



wwPDB EM Model Validation Summary Report ⓘ

Apr 30, 2020 – 12:44 PM EDT

PDB ID : 6V0F
EMDB ID : EMD-20996
Title : Lipophilic Envelope-spanning Tunnel B (LetB), Model 4
Authors : Isom, G.L.; Coudray, N.; MacRae, M.R.; McManus, C.T.; Ekiert, D.C.; Bhabha, G.
Deposited on : 2019-11-18
Resolution : 2.96 Å(reported)
Based on initial model : 5UW2

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

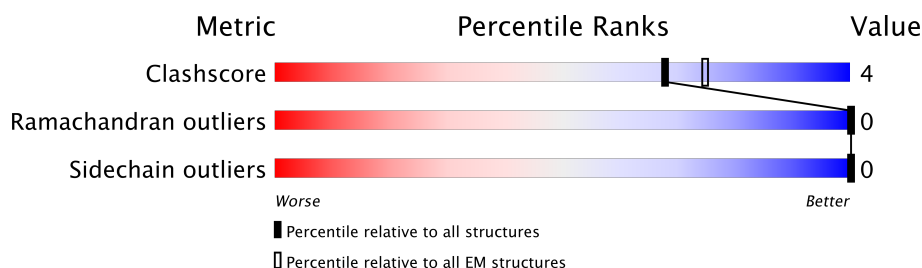
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY







The reported resolution of this entry is 2.96 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. 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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	832	 36% 6% 58%
1	B	832	 36% 6% 58%
1	C	832	 37% 5% 58%
1	D	832	 37% 6% 58%
1	E	832	 37% 6% 58%
1	F	832	 36% 6% 58%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15942 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 Intermembrane transport protein YebT.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		
1	B	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		
1	C	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		
1	D	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		
1	E	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		
1	F	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		

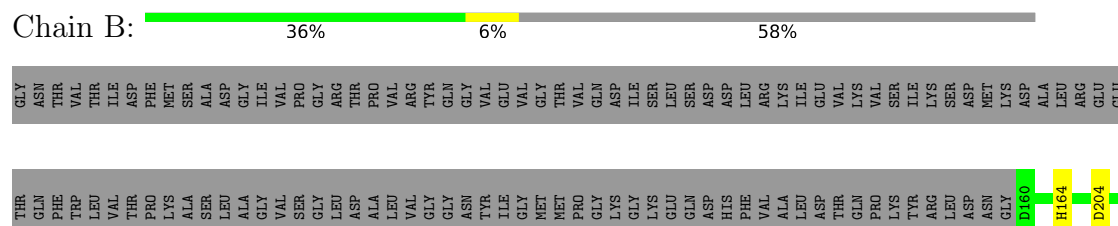
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Intermembrane transport protein YebT



- Molecule 1: Intermembrane transport protein YebT

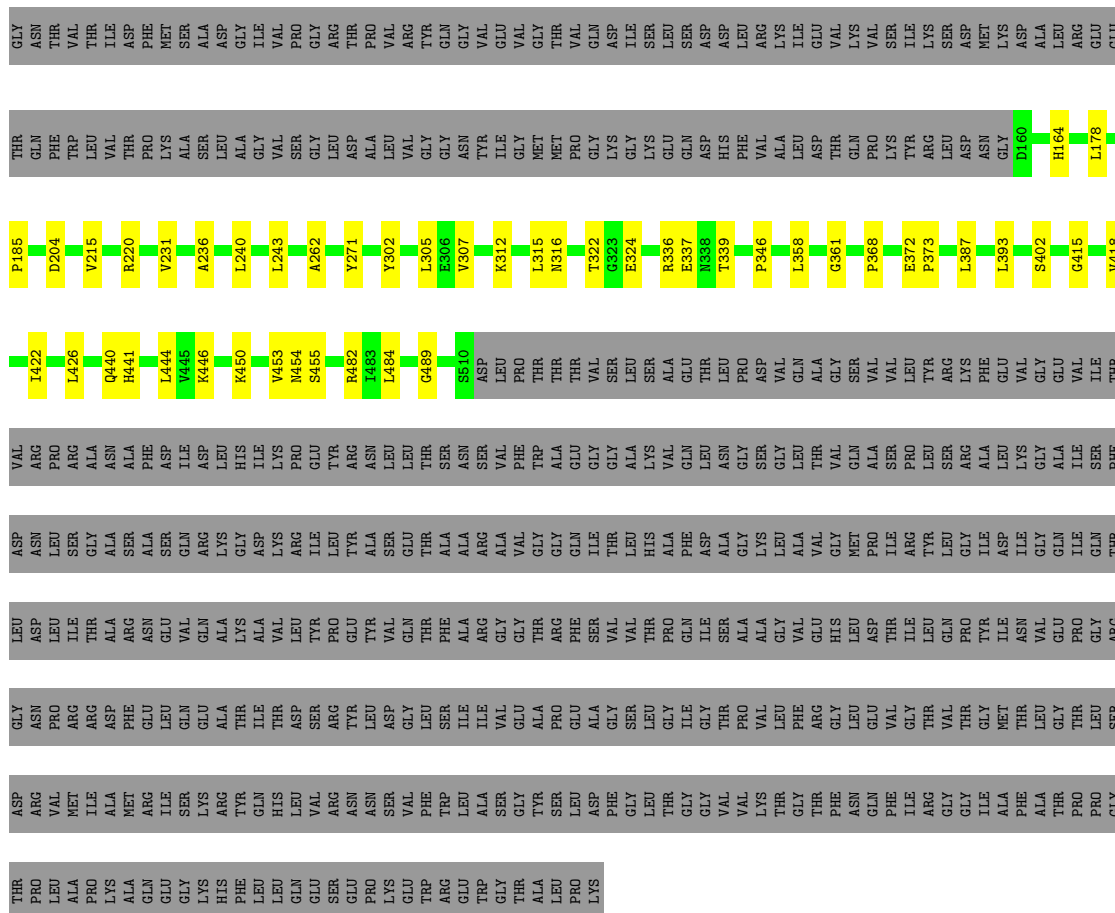


V215	R220	V231	A236	L240	L243	A262	Y271	Y302	L305	E306	V307	K312	L315	N316	T322	G323	E324	R336	E337	T339	P346	L358	G361	V367	P368	E372	P373	L387	L393	S402	L411	G415	V418		
I422	L426	H441	ASP	L444	K446	K450	V453	N454	R456	S472	E475	I483	L484	G489	A499	S510	ASP	LEU	PRO	THR	THR	VAL	SER	LEU	ASP	VAL	GLN	ALA	THR	SER	VAL	THR	PHE	GLY	
GLY	GLY	VAL	VAL	ARG	ALA	ASN	ASP	LEU	GLY	LYS	PRO	TYR	ASN	LEU	THR	ASN	ASN	PHE	THR	ALA	GLY	LYS	VAL	GLY	SER	GLY	GLN	VAL	GLY	ALA	VAL	LEU	ASP	LYS	
ALA	ILE	SER	PHE	LEU	ASN	SER	GLN	ARG	LYS	ASP	ILE	LEU	TYR	ALA	GLY	ALA	ARG	ALA	VAL	GLY	GLY	THR	HIS	ALA	VAL	GLN	THR	VAL	GLY	PRO	ILE	ARG	TYR	ILE	ASP
GLN	ILE	GLN	THR	LEU	ASP	GLU	VAL	GLN	ALA	VAL	THR	PRO	GLU	TYR	THR	THR	ARG	GLY	THR	GLY	THR	VAL	THR	PRO	GLN	GLY	GLY	GLU	HIS	LEU	ASP	THR	ILE	ASN	
VAL	GLY	PRO	GLY	PRO	ARG	ASP	GLN	GLY	ALA	THR	SER	ARG	TYR	LEU	ASP	LEU	ILE	VAL	GLY	ARG	ALA	SER	LEU	GLY	VAL	ALA	VAL	PHE	GLY	GLY	VAL	VAL	GLY	THR	THR
LEU	THR	SER	ASP	VAL	MET	ARG	LYS	THR	GLN	THR	VAL	VAL	ASN	PHE	GLY	TRP	ILE	VAL	SER	PRO	ALA	SER	LEU	GLY	VAL	VAL	THR	GLY	GLY	PRO	VAL	PHE	GLY	THR	ALA
ALA	THR	PRO	THR	LEU	ALA	ALA	GLY	LEU	HIS	LEU	GLU	SER	GLY	VAL	THR	THR	ALA	GLY	GLY	LEU	THR	GLY	THR	THR	VAL	VAL	GLY	GLY	THR	ASN	GLN	PHE	ILE	ARG	PHE
LYS																																			

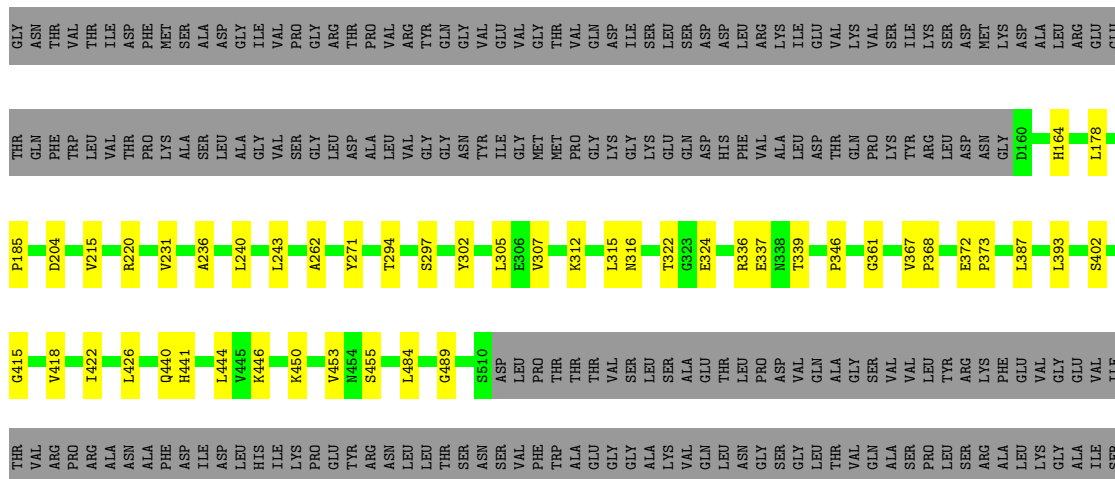
● Molecule 1: Intermembrane transport protein YebT

Chain C:		37%										5%										58%																								
GLY	ASN	THR	VAL	THR	ILE	ASP	PHE	MET	SER	ALA	GLY	ILE	VAL	PRO	GLY	ARG	THR	PRO	VAL	ARG	THR	GLN	GLY	THR	VAL	GLN	ASP	ILE	SER	LEU	ARG	LYS	VAL	SER	ILE	LYS	SER	ASP	MET	LYS	ASP	ALA	LEU	ARG	GLU	
L444	R220	V231	A236	L240	L243	Y271	Y302	L305	E306	V307	K312	L315	N316	T322	G323	E324	R336	E337	N338	T339	P346	L358	G361	P368	E372	P373	L387	L393	S402	G415	V418	L422	L426	Q440	H441											
ALA	ASN	ALA	PHE	ILE	ASP	LEU	HIS	ILE	LYS	PRO	GLY	TYR	ARG	ASN	LEU	GLY	THR	THR	VAL	GLY	THR	ASN	LEU	GLY	THR	ALA	GLY	VAL	ARG	GLY	VAL	THR	TYR	GLN	PRO	LYS	TYR	ILE	ARG	LEU	ASP	ASN	GLY	D160	H164	D204
GLY	ALA	SER	ALA	GLN	ARG	LYS	GLY	ASP	LYS	ARG	THR	ALA	ALA	VAL	GLY	GLY	ILE	THR	LEU	ALA	ASP	GLY	THR	VAL	GLY	VAL	THR	PRO	ILE	ARG	VAL	GLY	GLN	GLY	THR	ILE	ALA	THR	LEU	ASP	ASN	LEU	SER			
THR	ALA	ARG	ASN	VAL	GLN	ALA	LYS	THR	ALA	TYR	GLY	ALA	ALA	GLY	THR	PHE	ALA	ALA	THR	GLY	ILE	SER	THR	VAL	GLY	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
ARG	ASP	PHE	GLU	GLN	SER	THR	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
ILE	ALA	MET	ARG	ILE	LYS	THR	GLN	ASN	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	

Chain D: 37% 6% 58%

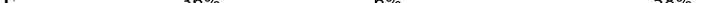


Chain E: 37% 6% 58%



[illegible]

- Molecule 1: Intermembrane transport protein YebT

Chain F:  36% 6% 58%

PRO	GLY	LEU	GLY	GLN	SER	ILE	V418	V215	THR	GLY
GLY	THR	SER	ARG	THR	PHE	THR	V418	V215	GLN	ASN
THR	ASP	ASP	GLY	THR	ASP	VAL	I422	R220	PHE	THR
PRO	PRO	ARG	ASN	ASP	ASN	ARG	L426	V231	TRP	VAL
ALA	ALA	MET	ARG	ILE	SER	ARG	L426	V231	VAL	ILE
PRO	THR	ILE	ARG	THR	GLY	ALA	Q440	A236	THR	ASP
LYS	LYS	ALA	ASP	ALA	ALA	ASN	H441	A236	PRO	PHE
HIS	MET	MET	PHE	ARG	SER	ALA	L444	L240	LYS	SER
GLN	GLN	ARG	GLU	ASN	ALA	PHE	L444	L240	ALA	SER
GLY	GLY	ILE	LEU	GLY	SER	ASP	V445	L243	SER	ALA
LYS	LYS	SER	GLN	VAL	GLN	ILE	K446	L243	LEU	ASP
ARG	ARG	LYS	GLU	GLN	ARG	ASP	K450	A262	ALA	GLY
PHE	PHE	TYR	THR	LYS	GLY	HIS	Y271	Y271	GLY	ILE
LEU	LEU	GLN	ILE	ALA	ASP	ILE	V453	T294	PRO	GLY
GLN	GLN	LEU	HIS	VAL	LYS	LYS	V454	T294	ARG	THR
LEU	LEU	LEU	ASP	ARG	ARG	PRO	S455	S297	ASP	THR
VAL	VAL	VAL	ASP	TYR	ILE	GLU	R456	S297	ALA	PRO
GLU	GLU	ARG	ARG	PRO	LEU	TYR	L484	Y302	VAL	ARG
ASN	ASN	TYR	TYR	GLY	ALA	ASN	G489	Y302	VAL	VAL
SER	SER	SER	VAL	VAL	SER	LEU	G489	L305	GLY	TYR
VAL	VAL	VAL	VAL	GLN	GLU	LEU	A499	F306	GLY	GLN
TRP	TRP	PHE	LEU	THR	THR	THR	A499	V307	ASN	GLY
ARG	ARG	TRP	SER	PHE	ALA	SER	S510	K312	TYR	VAL
GLU	GLU	LEU	ILE	ALA	ALA	ASN	ASP	K312	ILE	GLY
TRP	TRP	ALA	ILE	ARG	ARG	SER	ASP	L315	GLY	VAL
GLY	GLY	SER	VAL	GLY	ALA	VAL	LEU	N316	MET	GLY
THR	THR	GLY	GLY	GLY	VAL	PHE	PRO	N316	MET	THR
ALA	ALA	TYR	ALA	THR	GLY	TRP	THR	T322	PRO	VAL
SER	SER	SER	PRO	ARG	GLY	ALA	THR	T322	GLY	GLN
PRO	PRO	LEU	GLU	PHE	GLN	GLU	THR	G323	LYS	ASN
LYS	LYS	ASP	ALA	SER	ILE	GLY	VAL	E324	GLY	ILE
		PHE	GLY	VAL	THR	GLY	SER	R336	LYS	SER
		GLY	SER	VAL	LEU	ALA	LEU	R336	GLU	LEU
		LEU	LEU	THR	HIS	LYS	SER	E337	GLN	SER
		THR	GLY	PRO	ALA	VAL	ALA	N338	ASP	ASP
		GLY	ILE	GLN	PHE	GLN	GLU	T339	HIS	ASP
		GLY	GLY	ILE	ASP	LEU	THR	T339	PHE	LEU
		VAL	THR	SER	ALA	ASN	LEU	P346	VAL	ARG
		VAL	PRO	ALA	GLY	GLY	PRO	P346	ALA	LYS
		LYS	VAL	ALA	LYS	SER	ASP	L358	LEU	ILE
		THR	LEU	GLY	LEU	GLY	VAL	L358	GLU	ASP
		GLY	PHE	VAL	ALA	THR	GLN	G361	THR	THR
		THR	THR	GLU	VAL	LEU	ALA	G361	GLN	LYS
		PHE	GLY	HIS	GLY	VAL	GLY	V367	PRO	VAL
		ASN	LEU	LEU	MET	GLN	SER	P368	LYS	SER
		GLN	GLU	ASP	PRO	ALA	VAL	P368	TYR	ILE
		PHE	VAL	ILE	ILE	SER	VAL	E372	ARG	LYS
		ARG	GLY	ILE	ARG	PRO	LEU	P372	LEU	SER
		GLY	THR	LEU	TYR	TYR	THR	P372	ASP	ASP
		GLY	VAL	GLN	LEU	SER	ARG	L387	ASN	MET
		GLY	THR	PRO	GLY	ARG	LYS	L387	GLY	LYS
		ILE	GLY	TYR	ILE	ALA	PHE	L393	ASP	ASP
		ALA	MET	ILE	ASP	LEU	GLU	L393	ALA	ALA
		PHE	THR	ASN	ILE	LYS	VAL	S402	LEU	ARG
		ALA	LEU	VAL	GLY	GLY	GLY	S402	ARG	ARG
		THR	GLY	VAL	GLN	ALA	VAL	G415	GLU	GLU
		PRO	THR	PRO	THR	ILE	THR	D204	THR	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	144219	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.46	0/2702	0.74	4/3666 (0.1%)
1	B	0.46	0/2702	0.74	4/3666 (0.1%)
1	C	0.46	0/2702	0.74	4/3666 (0.1%)
1	D	0.46	0/2702	0.74	4/3666 (0.1%)
1	E	0.46	0/2702	0.74	4/3666 (0.1%)
1	F	0.46	0/2702	0.74	4/3666 (0.1%)
All	All	0.46	0/16212	0.74	24/21996 (0.1%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	240	LEU	CA-CB-CG	9.09	136.21	115.30
1	C	240	LEU	CA-CB-CG	9.08	136.19	115.30
1	F	240	LEU	CA-CB-CG	9.08	136.19	115.30
1	D	240	LEU	CA-CB-CG	9.07	136.17	115.30
1	B	240	LEU	CA-CB-CG	9.07	136.17	115.30

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	2657	0	2711	26	0
1	B	2657	0	2711	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2657	0	2711	24	0
1	D	2657	0	2711	25	0
1	E	2657	0	2711	25	0
1	F	2657	0	2711	26	0
All	All	15942	0	16266	135	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.

The worst 5 of 135 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:231:VAL:HB	1:F:236:ALA:H	1.63	0.63
1:E:336:ARG:HA	1:E:373:PRO:HA	1.82	0.62
1:A:336:ARG:HA	1:A:373:PRO:HA	1.82	0.62
1:B:336:ARG:HA	1:B:373:PRO:HA	1.82	0.62
1:D:231:VAL:HB	1:E:236:ALA:H	1.65	0.62

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
1	B	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
1	C	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
1	D	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
1	E	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
1	F	349/832 (42%)	345 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2094/4992 (42%)	2070 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	293/683 (43%)	293 (100%)	0	100	100
1	B	293/683 (43%)	293 (100%)	0	100	100
1	C	293/683 (43%)	293 (100%)	0	100	100
1	D	293/683 (43%)	293 (100%)	0	100	100
1	E	293/683 (43%)	293 (100%)	0	100	100
1	F	293/683 (43%)	293 (100%)	0	100	100
All	All	1758/4098 (43%)	1758 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	354	ASN
1	D	316	ASN
1	F	345	ASN
1	D	164	HIS
1	D	345	ASN

5.3.3 RNA ⓘ

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](#)

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.