



# Full wwPDB EM Model Validation Report ⓘ

Apr 30, 2020 – 12:48 PM EDT

PDB ID : 6V0I  
EMDB ID : EMD-20999  
Title : Lipophilic Envelope-spanning Tunnel B (LetB), Model 7  
Authors : Isom, G.L.; Coudray, N.; MacRae, M.R.; McManus, C.T.; Ekiert, D.C.; Bhabha, G.  
Deposited on : 2019-11-18  
Resolution : 3.43 Å(reported)  
Based on initial model : 5UW2

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

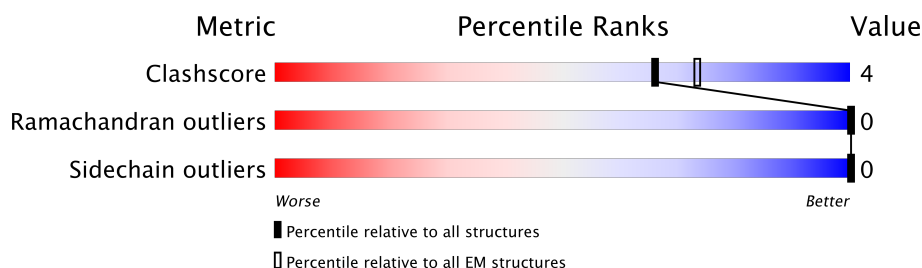
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*







The reported resolution of this entry is 3.43 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  $\geq 3$ , 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	 37% 5% 58%
1	B	832	 37% 5% 58%
1	C	832	 37% 5% 58%
1	D	832	 37% 5% 58%
1	E	832	 37% 5% 58%
1	F	832	 37% 5% 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		



V206	L206	L207	E208	F211	R220	V227	V231	A236	L246	Y271	Y302	V307	K312	E324	S330	V331	V332	T333	L334	L335	R336	E337	N338	T339	R340	P368	E372	P373	P390	D391	V392	L393	I437	E438	P439	K450	V453	N454	S455	D458								
L469	L469	L469	S472	E475	W476	R482	I483	L484	S510	ASP	LEU	PRO	THR	THR	LEU	PRO	ASP	VAL	GLN	ALA	GLY	SER	VAL	LEU	TYR	ARG	LYS	PHE	GLY	VAL	GLY	GLU	VAL	ILE	THR	VAL	PRO	ARG	ALA	PHE	ASP	ILE	ASP	LEU				
LYS	HIS	LYS	PRO	GLY	TYR	LEU	ASN	ASN	SER	VAL	GLY	ALA	LYS	ALA	GLY	SER	GLY	VAL	GLN	VAL	GLY	SER	VAL	TYR	TYR	ARG	LYS	PHE	GLY	VAL	GLY	GLU	VAL	ILE	THR	ASN	ASN	LEU	SER	GLY	ALA	ASN	ALA	PHE	ASP	GLN	LYS	
GLY	ASP	LYS	ARG	ILE	TYR	GLU	ASN	ALA	ARG	VAL	THR	LEU	HIS	ALA	GLY	LYS	LEU	ALA	GLN	THR	GLY	VAL	GLN	TYR	TYR	ARG	LYS	PHE	GLY	VAL	GLY	GLU	VAL	ILE	THR	ASN	ASN	LEU	SER	GLY	ALA	ASN	ALA	PHE	ASP	GLN	LYS	
LYS	ALA	VAL	LEU	THR	TYR	PRO	TYR	VAL	ARG	GLY	ILE	LEU	THR	ALA	ALA	LYS	GLY	VAL	GLN	THR	GLY	HIS	VAL	ILE	GLN	GLY	VAL	ILE	ALA	ASP	ILE	LYS	VAL	GLY	GLU	ALA	THR	GLY	ALA	ASN	ALA	PHE	ASP	GLN	ALA			
THR	ILE	THR	ASP	SER	ASN	ARG	TYR	GLU	ARG	THR	SER	VAL	THR	GLN	GLY	ILE	GLY	PHE	GLN	THR	GLY	VAL	GLN	TYR	TYR	ARG	LYS	PHE	GLY	VAL	GLY	GLU	PRO	ILE	THR	ASN	ASN	LEU	SER	GLY	ALA	ASN	ALA	PHE	ASP	GLN	ALA	
TYR	GLN	HIS	LEU	VAL	ARG	ASN	ASN	ALA	ILE	VAL	GLY	GLY	LEU	GLY	PRO	VAL	VAL	PHE	GLY	THR	GLY	ASN	GLY	VAL	VAL	TYR	ARG	LYS	PHE	GLY	VAL	GLY	GLU	PRO	ARG	THR	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
PHE	LEU	LEU	GLN	GLU	SER	GLU	TRP	ARG	THR	ALA	THR	GLY	LEU	THR	VAL	VAL	GLY	THR	THR	THR	ASN	PHE	GLY	GLY	GLY	GLY	GLY	GLY	ILE	ALA	PHE	ALA	THR	THR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	

● Molecule 1: Intermembrane transport protein YebT

Chain C:		37%										5%										58%																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
GLY	ASN	THR	VAL	THR	THR	ASP	PHE	MET	SER	ALA	SER	ALA	ASP	GLY	ILE	VAL	VAL	PRO	GLY	ARG	THR	THR	VAL	ARG	TYR	GLN	GLY	VAL	GLY	GLN	GLY	GLN	GLY	ASP	ASP	LEU	LEU	LYS	ILE	VAL	GLY	VAL	LYS	SER	LYS	THR	ASP	GLN	PHE	THR	GLN	E208	S472	PRO	ARG	LEU	TYR	GLY	THR	VAL	ASP	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	59687	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

### 5.1 Standard geometry

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	0.37	0/2702	0.68	0/3666
1	B	0.37	0/2702	0.68	0/3666
1	C	0.37	0/2702	0.68	0/3666
1	D	0.37	0/2702	0.68	0/3666
1	E	0.37	0/2702	0.68	0/3666
1	F	0.37	0/2702	0.68	0/3666
All	All	0.37	0/16212	0.68	0/21996

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	2657	0	2711	23	0
1	B	2657	0	2711	25	0
1	C	2657	0	2711	24	0
1	D	2657	0	2711	26	0
1	E	2657	0	2711	24	0
1	F	2657	0	2711	24	0
All	All	15942	0	16266	140	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 (140) 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:393:LEU:HB3	1:B:437:ILE:HB	1.74	0.70
1:C:393:LEU:HB3	1:C:437:ILE:HB	1.74	0.70
1:E:393:LEU:HB3	1:E:437:ILE:HB	1.74	0.70
1:D:393:LEU:HB3	1:D:437:ILE:HB	1.74	0.69
1:F:393:LEU:HB3	1:F:437:ILE:HB	1.74	0.69
1:A:393:LEU:HB3	1:A:437:ILE:HB	1.74	0.69
1:A:336:ARG:HA	1:A:373:PRO:HA	1.79	0.65
1:E:336:ARG:HA	1:E:373:PRO:HA	1.79	0.65
1:B:336:ARG:HA	1:B:373:PRO:HA	1.79	0.64
1:D:336:ARG:HA	1:D:373:PRO:HA	1.79	0.64
1:F:336:ARG:HA	1:F:373:PRO:HA	1.79	0.63
1:C:336:ARG:HA	1:C:373:PRO:HA	1.79	0.63
1:D:312:LYS:HB3	1:D:324:GLU:HG2	1.85	0.59
1:C:312:LYS:HB3	1:C:324:GLU:HG2	1.85	0.59
1:E:312:LYS:HB3	1:E:324:GLU:HG2	1.85	0.58
1:F:312:LYS:HB3	1:F:324:GLU:HG2	1.85	0.58
1:B:312:LYS:HB3	1:B:324:GLU:HG2	1.85	0.57
1:A:332:VAL:HA	1:A:335:LEU:HD12	1.87	0.57
1:B:332:VAL:HA	1:B:335:LEU:HD12	1.87	0.57
1:A:312:LYS:HB3	1:A:324:GLU:HG2	1.85	0.57
1:C:332:VAL:HA	1:C:335:LEU:HD12	1.87	0.57
1:F:332:VAL:HA	1:F:335:LEU:HD12	1.87	0.57
1:D:332:VAL:HA	1:D:335:LEU:HD12	1.87	0.56
1:C:220:ARG:NH2	1:C:271:TYR:OH	2.39	0.56
1:E:332:VAL:HA	1:E:335:LEU:HD12	1.87	0.56
1:F:220:ARG:NH2	1:F:271:TYR:OH	2.39	0.56
1:A:220:ARG:NH2	1:A:271:TYR:OH	2.39	0.56
1:D:220:ARG:NH2	1:D:271:TYR:OH	2.39	0.55
1:E:220:ARG:NH2	1:E:271:TYR:OH	2.39	0.55
1:B:220:ARG:NH2	1:B:271:TYR:OH	2.39	0.55
1:C:231:VAL:HB	1:D:236:ALA:H	1.73	0.54
1:B:472:SER:O	1:B:476:TRP:N	2.34	0.53
1:D:231:VAL:HB	1:E:236:ALA:H	1.73	0.53
1:B:231:VAL:HB	1:C:236:ALA:H	1.74	0.53
1:E:453:VAL:HG12	1:E:455:SER:H	1.74	0.53
1:A:231:VAL:HB	1:B:236:ALA:H	1.73	0.53
1:C:453:VAL:HG12	1:C:455:SER:H	1.74	0.53
1:F:453:VAL:HG12	1:F:455:SER:H	1.74	0.53
1:B:227:VAL:HB	1:B:246:LEU:HD21	1.91	0.53
1:C:227:VAL:HB	1:C:246:LEU:HD21	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:SER:O	1:D:476:TRP:N	2.34	0.52
1:A:453:VAL:HG12	1:A:455:SER:H	1.74	0.52
1:A:227:VAL:HB	1:A:246:LEU:HD21	1.91	0.52
1:D:302:TYR:HB3	1:D:307:VAL:HG21	1.92	0.52
1:D:453:VAL:HG12	1:D:455:SER:H	1.74	0.52
1:E:231:VAL:HB	1:F:236:ALA:H	1.73	0.52
1:F:302:TYR:HB3	1:F:307:VAL:HG21	1.92	0.51
1:B:453:VAL:HG12	1:B:455:SER:H	1.74	0.51
1:C:302:TYR:HB3	1:C:307:VAL:HG21	1.92	0.51
1:D:227:VAL:HB	1:D:246:LEU:HD21	1.91	0.51
1:F:227:VAL:HB	1:F:246:LEU:HD21	1.91	0.51
1:A:302:TYR:HB3	1:A:307:VAL:HG21	1.92	0.51
1:A:458:ASP:HB3	1:A:469:LEU:HB2	1.92	0.51
1:B:458:ASP:HB3	1:B:469:LEU:HB2	1.92	0.51
1:E:227:VAL:HB	1:E:246:LEU:HD21	1.91	0.51
1:E:302:TYR:HB3	1:E:307:VAL:HG21	1.92	0.51
1:A:472:SER:O	1:A:476:TRP:N	2.34	0.50
1:F:458:ASP:HB3	1:F:469:LEU:HB2	1.92	0.50
1:E:458:ASP:HB3	1:E:469:LEU:HB2	1.92	0.50
1:D:458:ASP:HB3	1:D:469:LEU:HB2	1.92	0.50
1:C:458:ASP:HB3	1:C:469:LEU:HB2	1.92	0.50
1:B:302:TYR:HB3	1:B:307:VAL:HG21	1.92	0.50
1:D:450:LYS:HB2	1:D:484:LEU:HB2	1.94	0.50
1:A:330:SER:O	1:A:333:THR:OG1	2.27	0.50
1:E:450:LYS:HB2	1:E:484:LEU:HB2	1.94	0.50
1:F:472:SER:O	1:F:476:TRP:N	2.34	0.50
1:D:330:SER:O	1:D:333:THR:OG1	2.27	0.49
1:E:472:SER:O	1:E:476:TRP:N	2.34	0.49
1:A:450:LYS:HB2	1:A:484:LEU:HB2	1.94	0.49
1:B:330:SER:O	1:B:333:THR:OG1	2.27	0.49
1:F:450:LYS:HB2	1:F:484:LEU:HB2	1.94	0.49
1:B:450:LYS:HB2	1:B:484:LEU:HB2	1.94	0.48
1:C:450:LYS:HB2	1:C:484:LEU:HB2	1.94	0.48
1:E:330:SER:O	1:E:333:THR:OG1	2.27	0.48
1:A:236:ALA:H	1:F:231:VAL:HB	1.77	0.47
1:F:391:ASP:HB3	1:F:439:PRO:HG3	1.96	0.47
1:A:391:ASP:HB3	1:A:439:PRO:HG3	1.97	0.47
1:E:391:ASP:HB3	1:E:439:PRO:HG3	1.96	0.47
1:B:391:ASP:HB3	1:B:439:PRO:HG3	1.96	0.47
1:F:454:ASN:HD21	1:F:482:ARG:HB2	1.81	0.47
1:A:454:ASN:HD21	1:A:482:ARG:HB2	1.81	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:SER:O	1:C:333:THR:OG1	2.27	0.46
1:D:391:ASP:HB3	1:D:439:PRO:HG3	1.96	0.46
1:F:330:SER:O	1:F:333:THR:OG1	2.27	0.46
1:C:391:ASP:HB3	1:C:439:PRO:HG3	1.96	0.46
1:D:339:THR:HG23	1:D:368:PRO:HA	1.98	0.46
1:C:472:SER:O	1:C:476:TRP:N	2.34	0.46
1:F:339:THR:HG23	1:F:368:PRO:HA	1.98	0.46
1:A:339:THR:HG23	1:A:368:PRO:HA	1.98	0.45
1:C:454:ASN:HD21	1:C:482:ARG:HB2	1.81	0.45
1:D:454:ASN:HD21	1:D:482:ARG:HB2	1.80	0.45
1:E:454:ASN:HD21	1:E:482:ARG:HB2	1.81	0.45
1:A:454:ASN:ND2	1:A:482:ARG:HB2	2.32	0.45
1:C:339:THR:HG23	1:C:368:PRO:HA	1.98	0.45
1:C:454:ASN:ND2	1:C:482:ARG:HB2	2.32	0.45
1:D:454:ASN:ND2	1:D:482:ARG:HB2	2.32	0.45
1:B:454:ASN:ND2	1:B:482:ARG:HB2	2.32	0.45
1:E:339:THR:HG23	1:E:368:PRO:HA	1.98	0.45
1:E:454:ASN:ND2	1:E:482:ARG:HB2	2.32	0.45
1:B:454:ASN:HD21	1:B:482:ARG:HB2	1.80	0.45
1:F:454:ASN:ND2	1:F:482:ARG:HB2	2.32	0.45
1:F:337:GLU:N	1:F:372:GLU:O	2.46	0.45
1:B:208:GLU:HB2	1:B:211:PHE:HD2	1.83	0.44
1:B:339:THR:HG23	1:B:368:PRO:HA	1.98	0.44
1:D:337:GLU:N	1:D:372:GLU:O	2.46	0.44
1:A:337:GLU:N	1:A:372:GLU:O	2.46	0.44
1:A:208:GLU:HB2	1:A:211:PHE:HD2	1.83	0.44
1:E:208:GLU:HB2	1:E:211:PHE:HD2	1.82	0.44
1:E:337:GLU:N	1:E:372:GLU:O	2.46	0.44
1:C:208:GLU:HB2	1:C:211:PHE:HD2	1.83	0.43
1:D:208:GLU:HB2	1:D:211:PHE:HD2	1.83	0.43
1:F:208:GLU:HB2	1:F:211:PHE:HD2	1.83	0.43
1:E:472:SER:HB3	1:E:475:GLU:HG3	2.02	0.42
1:B:472:SER:HB3	1:B:475:GLU:HG3	2.02	0.42
1:B:337:GLU:N	1:B:372:GLU:O	2.46	0.42
1:A:472:SER:HB3	1:A:475:GLU:HG3	2.02	0.42
1:F:472:SER:HB3	1:F:475:GLU:HG3	2.02	0.42
1:D:338:ASN:HA	1:D:340:ARG:HH12	1.84	0.41
1:D:367:VAL:HA	1:D:368:PRO:HD3	1.86	0.41
1:D:472:SER:HB3	1:D:475:GLU:HG3	2.02	0.41
1:E:338:ASN:HA	1:E:340:ARG:HH12	1.84	0.41
1:A:338:ASN:HB2	1:A:390:PRO:HG3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:ASN:HB2	1:F:390:PRO:HG3	2.03	0.41
1:C:472:SER:HB3	1:C:475:GLU:HG3	2.02	0.41
1:E:338:ASN:HB2	1:E:390:PRO:HG3	2.03	0.41
1:A:338:ASN:HA	1:A:340:ARG:HH12	1.84	0.41
1:B:338:ASN:HB2	1:B:390:PRO:HG3	2.03	0.41
1:F:338:ASN:HA	1:F:340:ARG:HH12	1.85	0.41
1:B:338:ASN:HA	1:B:340:ARG:HH12	1.84	0.41
1:D:338:ASN:HB2	1:D:390:PRO:HG3	2.02	0.41
1:C:338:ASN:HA	1:C:340:ARG:HH12	1.84	0.40
1:C:337:GLU:N	1:C:372:GLU:O	2.46	0.40
1:C:178:LEU:HD21	1:C:185:PRO:HB3	2.04	0.40
1:D:164:HIS:CD2	1:D:204:ASP:HB3	2.57	0.40
1:B:164:HIS:CD2	1:B:204:ASP:HB3	2.57	0.40
1:D:178:LEU:HD21	1:D:185:PRO:HB3	2.04	0.40
1:E:178:LEU:HD21	1:E:185:PRO:HB3	2.04	0.40
1:F:178:LEU:HD21	1:F:185:PRO:HB3	2.04	0.40
1:B:161:LEU:O	1:B:206:LEU:HA	2.22	0.40
1:C:338:ASN:HB2	1:C:390:PRO:HG3	2.02	0.40

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%)	344 (99%)	5 (1%)	0	100	100
1	B	349/832 (42%)	344 (99%)	5 (1%)	0	100	100
1	C	349/832 (42%)	344 (99%)	5 (1%)	0	100	100
1	D	349/832 (42%)	344 (99%)	5 (1%)	0	100	100
1	E	349/832 (42%)	344 (99%)	5 (1%)	0	100	100
1	F	349/832 (42%)	344 (99%)	5 (1%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2094/4992 (42%)	2064 (99%)	30 (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. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	316	ASN
1	A	345	ASN
1	A	354	ASN
1	A	409	GLN
1	A	454	ASN
1	B	164	HIS
1	B	316	ASN
1	B	345	ASN
1	B	354	ASN
1	B	409	GLN
1	B	454	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	164	HIS
1	C	316	ASN
1	C	345	ASN
1	C	354	ASN
1	C	409	GLN
1	C	454	ASN
1	D	164	HIS
1	D	316	ASN
1	D	345	ASN
1	D	354	ASN
1	D	409	GLN
1	D	454	ASN
1	E	164	HIS
1	E	316	ASN
1	E	345	ASN
1	E	354	ASN
1	E	409	GLN
1	E	454	ASN
1	F	164	HIS
1	F	316	ASN
1	F	345	ASN
1	F	354	ASN
1	F	409	GLN
1	F	454	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 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.