



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 04:51 AM EDT

PDB ID : 5FZ2  
EMDB ID: : EMD-3362  
Title : Natively membrane-anchored full-length Herpes simplex virus 1 glycoprotein B  
Authors : Zeev-Ben-Mordehai, T.; Vasishtan, D.; Duran, A.H.; Vollmer, B.; White, P.; Pandurangan, A.P.; Siebert, C.A.; Topf, M.; Grunewald, K.  
Deposited on : unknown  
Resolution : 23.00 Å(reported)  
Based on PDB ID : 2GUM

This is a wwPDB/EMDataBank EM Map/Model Validation Summary 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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

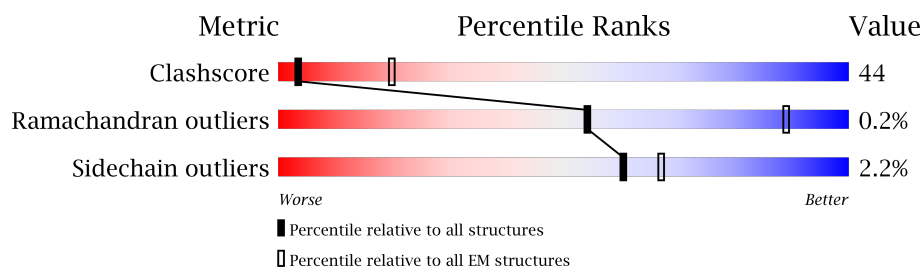
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 23.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	1-A	904	
1	1-B	904	
1	1-C	904	
1	2-A	904	
1	2-B	904	
1	2-C	904	
1	3-A	904	
1	3-B	904	
1	3-C	904	

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Mol	Chain	Length	Quality of chain
1	4-A	904	<div><div></div><div></div><div></div><div></div></div>
1	4-B	904	<div><div></div><div></div><div></div><div></div></div>
1	4-C	904	<div><div></div><div></div><div></div><div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 32768 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.

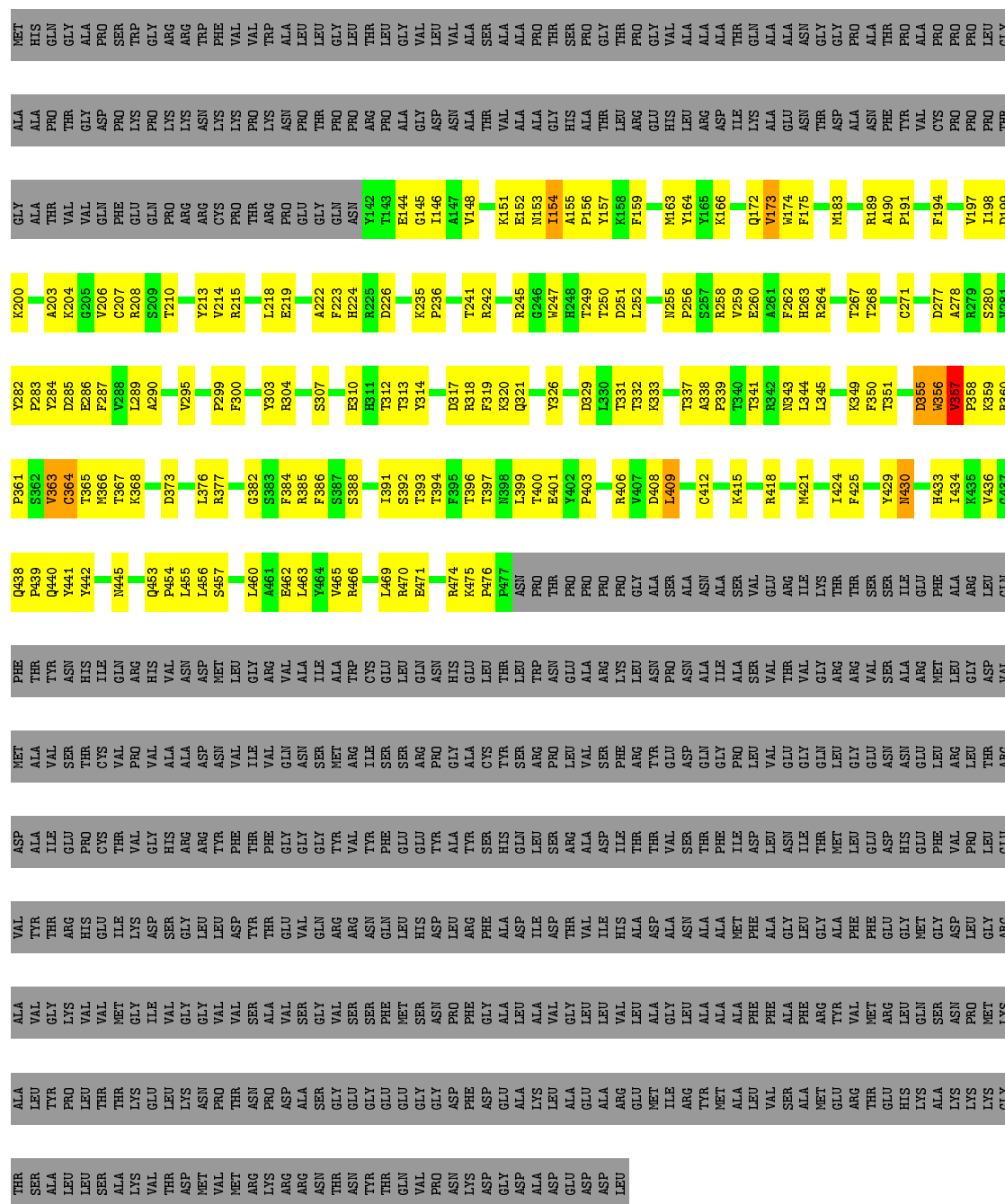
- Molecule 1 is a protein called ENVELOPE GLYCOPROTEIN B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	336	Total	C	N	O	S	0	1
			2728	1729	475	513	11		
1	2-A	336	Total	C	N	O	S	0	1
			2728	1729	475	513	11		
1	3-A	336	Total	C	N	O	S	0	1
			2728	1729	475	513	11		
1	4-A	336	Total	C	N	O	S	0	1
			2728	1729	475	513	11		
1	1-B	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	2-B	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	3-B	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	4-B	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	1-C	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	2-C	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	3-C	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	4-C	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		




- Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain 1-B:  18% 18% . 63%



- Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain 1-C:  18% 18% . 63%

- Molecule 1: ENVELOPE GLYCOPROTEIN B

WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

 **EMDataBank**  
Unified Data Resource for 3DEM






[illegible]

- Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain 3-A:  18% 19% . 63%

GLY	ARG	ARG	GLU	LEU	THR	ASP	LEU	VAL36	R360	R2719	I198	ALA	MET
ARG	ASP	VAL	GLN	GLN	ARG	VAL	GLN	Q437	R361	R2719	I198	ALA	HIS
ALA	MET	ASP	PHE	PHE	THR	ALA	PHE	Q362	R362	R281	D199	THR	GLY
VAL	ALA	THR	THR	THR	ILE	ALA	THR	P439	R363	R282	D200	VAL	GLY
GLY	VAL	ARG	THR	THR	THR	VAL	THR	T384	R364	R283	A203	VAL	ALA
LYS	SER	GLU	ASN	ASN	THR	GLY	ASN	Q440	R365	R284	K204	GLN	PRO
VAL	THR	VAL	HIS	HIS	PRO	VAL	THR	Y441	R366	R285	G205	PHE	SER
VAL	VAL	VAL	CYS	ILE	CYS	THR	ILE	Y442	R367	D286	V206	GLU	TRP
MET	MET	THR	ILE	ILE	THR	VAL	ILE	M445	R368	F287	C207	GLN	GLY
GLY	PRO	GLY	ARG	ARG	VAL	VAL	ARG	Q453	D373	V288	R208	LYS	ARG
ILE	VAL	VAL	HIS	HIS	VAL	VAL	VAL	P454	D373	L289	G209	LYS	TRP
VAL	ALA	ALA	ASN	ASN	ASN	ALA	ASN	L455	L376	A290	T210	ASN	ARG
GLY	ASP	ASP	ASP	ASP	ARG	ALA	ASP	L456	R377	V295	V213	LYS	PHE
VAL	VAL	VAL	MET	MET	THR	VAL	MET	S457	R377	V295	V214	VAL	VAL
ASP	VAL	VAL	ASP	ASP	THR	VAL	ASP	G382	G382	P299	R215	LYS	TRP
THR	THR	THR	THR	THR	THR	THR	THR	S383	G382	P299	R215	LYS	TRP
ALA	ALA	PHE	PHE	ARG	PHE	VAL	ARG	L460	F384	F300	L218	PRO	ALA
VAL	VAL	GLY	GLY	VAL	GLY	VAL	VAL	L461	R385	F300	E219	PRO	LEU
GLY	ASN	GLN	GLN	GLN	GLY	GLN	GLN	L462	F386	Y303	R222	THR	GLY
VAL	GLY	GLY	GLY	ILE	GLY	SER	ILE	Y464	S387	R304	A222	PRO	LEU
VAL	VAL	VAL	ARG	ARG	VAL	MET	ALA	R465	S388	E310	F223	ARG	THR
SER	SER	VAL	THR	THR	VAL	ARG	THR	R466	S388	H311	D224	PRO	LEU
SER	SER	THR	CYS	CYS	CYS	ILE	GLY	L469	T391	T312	E225	ALA	GLY
PHE	PHE	THR	GLN	GLN	THR	SER	THR	R470	S392	T313	D226	GLY	VAL
MET	MET	GLU	LEU	LEU	GLU	SER	LEU	E471	T393	Y314	R235	ASP	LEU
ASN	ASN	THR	ASN	ASN	THR	PRO	ASN	F395	T394	D317	P236	ALA	ALA
PRO	PRO	ALA	GLY	GLY	ALA	GLY	GLY	R474	T396	R318	D317	THR	SER
PHE	PHE	THR	GLU	GLU	THR	ALA	GLU	K475	T397	F319	T241	VAL	ALA
GLY	GLY	CYS	LEU	LEU	SER	THR	LEU	P476	R398	K320	R242	ALA	ALA
LEU	ALA	ALA	THR	THR	THR	VAL	THR	P477	L399	Q321	R245	GLY	PRO
LEU	LEU	LEU	GLN	GLN	GLN	SER	LEU	ASN	T400	R246	G246	HIS	SER
VAL	VAL	VAL	ILE	ILE	ILE	ARG	THR	PRO	E401	Y326	D247	ALA	PRO
VAL	VAL	VAL	ASN	ASN	ASN	PRO	ASN	THR	Y402	D329	E248	THR	GLY
GLY	GLY	THR	GLU	GLU	ARG	LEU	GLU	P403	P403	D329	E248	THR	GLY
LEU	LEU	ALA	ALA	ALA	VAL	VAL	ALA	PRO	PRO	L330	T249	LEU	PRO
LEU	LEU	LEU	ASP	ASP	ASP	SER	SER	P406	R406	T331	D250	ARG	GLY
VAL	VAL	VAL	ILE	ILE	PHE	PHE	LYS	Q407	V407	T332	D251	GLY	GLY
LEU	LEU	LEU	THR	THR	THR	ARG	LEU	D408	D408	T332	D251	GLY	VAL
ALA	ALA	ASP	THR	THR	THR	THR	ASN	L409	L409	K333	L252	HIS	VAL
ALA	ALA	GLY	VAL	VAL	VAL	GLU	PRO	G410	G410	T337	R255	ARG	ALA
LEU	LEU	ASN	SER	ASN	SER	ASP	ASN	D411	A338	R256	G256	ASP	ALA
ALA	ALA	ALA	GLN	GLN	THR	ASN		C412	P339	R257	K366	ASP	ALA
ALA	ALA	PHE	ILE	ILE	PHE	GLY	ILE	ALA	T340	R258	Q172	LYS	GLN
ALA	ALA	MET	ALA	ALA	ALA	PRO	ALA	R415	T341	V259	Q173	ALA	ALA
PHE	PHE	PHE	SER	SER	ASP	LEU	SER	VAL	R342	E260	H174	GLU	ALA
PHE	PHE	ALA	VAL	VAL	VAL	VAL	VAL	GLU	R418	A261	F175	ASN	ASN
GLY	GLY	GLY	ASN	ASN	GLU	GLU	THR	ARG	M421	T362	THR	ASP	GLY
LEU	LEU	ILE	ILE	ILE	ILE	GLY	VAL	ILE		R263	Y179	ALA	GLY
GLY	GLY	THR	THR	THR	THR	GLN	GLY	LYS		R264		ALA	PRO
ALA	ALA	MET	MET	MET	MET	LEU	ARG	THR	1424	K349	M183	ASN	ALA
VAL	VAL	LEU	LEU	LEU	LEU	GLY	ARG	THR	F425	F350	T267	PHE	ALA
PHE	PHE	GLU	GLU	GLU	GLU	SER	VAL	SER		T268	R189	TYR	PRO
MET	MET	ASP	ASP	ASN	ASN	ASN	VAL	SER	Y429	V269	A190	VAL	PRO
GLY	GLY	HIS	HIS	ILE	ILE	ILE	ALA	ILE	M430	M270	P191	CYS	ALA
GLU	GLU	GLU	GLU	GLU	GLU	GLU	ARG	GLU	R356	R271		PRO	PRO
SER	SER	PHE	PHE	MET	MET	LEU	MET	PHE	H433	V357	F194	PRO	PRO
ASN	ASN	VAL	VAL	VAL	VAL	ARG	LEU	ALA	1434	D277		PRO	LEU

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

- Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain 3-B:  18% 19% . 63%

[illegible]

- Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain 3-C:

[illegible]

• Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain 4-A:

[illegible]

GLY	ALA	THR	VAL	GLN	PHE	GLU	GLN	ASN	Y142	E144	G145	I146	A147	V148	K151	E152	I153	I154	A155	P156	Y157	K158	F159	M163	Y164	Y165	K166	Q172	V173	W174	F175	Y179	M183	R189	A190	P191	F194	V197												
I198	D199	K200	A203	K204	G205	V206	C207	R208	S209	T210	Y213	R214	R215	L218	E219	A222	F223	H224	R225	D226	K235	P236	T241	R242	R245	G246	W247	H248	T249	T250	D251	L252	N255	P256	S257	R258	V259	E260	A261	F262	H263	R264	T267	T268	V269	W270	C271	D277	A278	
R279	S280	Y281	Y282	Y283	Y284	D285	E286	T287	Y288	L289	A290	V295	P299	Y303	R304	T312	T313	Y314	D317	R318	F319	Q320	Q321	Y326	D329	L330	T331	T332	K333	T337	A338	P339	T340	T341	R342	N343	L344	L345	F425	K349	F350	T351	D355	W356	V357	P358	K359	R360	P361	S362
V363	C364	T365	M366	T367	K368	D373	L376	R377	L389	G392	S393	F394	R395	F396	S397	S398	I399	S392	T393	T394	F395	T396	N398	L399	T400	E401	P403	R406	V407	D408	L409	G410	D411	C412	R418	M421	I424	F425	Y429	M430	H433	I434	V435	V436	G437	Q438	P439	Q440		
Y441	Y442	M445	Q453	P454	L455	L456	S457	L460	L461	E462	L463	Y464	V465	R466	L469	R470	E471	R474	K475	P476	A477	ASN	PRO	PRO	PRO	PRO	PRO	PRO	GLY	ALA	ALA	ASN	ALA	SER	VAL	GLU	ARG	THR	ILE	GLU	PRO	PHE	ALA	ASP	THR	THR				
ASN	HIS	ILE	GLN	ARG	HIS	VAL	ASN	ASP	MET	LEU	GLY	ARG	VAL	GLN	VAL	ASN	ALA	ILE	ILE	GLY	THR	CYS	GLU	LEU	GLN	GLY	PRO	ASN	HIS	GLU	LEU	THR	TRP	ASN	GLY	ALA	THR	ILE	GLY	THR	VAL	GLU	THR	VAL	VAL					
SER	THR	CYS	VAL	PRO	GLY	VAL	ALA	ALA	ASP	ASN	ILE	VAL	GLN	ASN	GLY	THR	GLY	ALA	GLY	ALA	CYS	THR	SER	LEU	VAL	SER	PHE	LEU	THR	GLY	GLN	PRO	ALA	VAL	GLY	THR	VAL	GLY	GLN	THR	GLY	VAL	GLY	VAL	GLY	THR	ILE			
GLU	PRO	CYS	THR	VAL	LYS	GLY	HIS	ARG	GLY	PHE	THR	GLY	GLY	THR	THR	PHE	GLU	GLY	THR	SER	HIS	THR	THR	ALA	ALA	VAL	ILE	THR	THR	ASP	VAL	THR	THR	ASP	LEU	VAL	GLY	ASN	THR	VAL	ILE	THR	THR	THR	THR	THR				
ARG	HIS	GLU	ILE	MET	LYS	ASP	SER	GLY	LEU	THR	TYR	GLY	VAL	GLN	GLY	GLN	LEU	HIS	ASP	ARG	THR	ASN	GLY	VAL	VAL	ILE	HIS	ALA	ASP	GLY	ALA	MET	PHE	PHE	ALA	GLY	LEU	GLY	GLY	ASP	VAL	GLY	GLY	VAL	GLY					
LYS	VAL	VAL	GLY	ILE	ASP	VAL	GLY	VAL	VAL	THR	ALA	VAL	SER	GLY	PHE	GLY	THR	VAL	VAL	GLY	GLY	THR	GLY	LEU	VAL	VAL	VAL	ALA	ALA	ALA	ALA	PHE	PHE	ALA	PHE	ALA	THR	ARG	GLY	GLN	SER	ASP	VAL	PRO	LYS	ALA	THR			
PRO	LEU	THR	LYS	GLU	LEU	LYS	ASN	PRO	ASP	PRO	ARG	ASP	ALA	SER	GLY	GLY	GLY	GLY	GLY	PHE	ASP	GLY	GLY	LEU	ALA	VAL	GLY	LEU	ILE	ARG	THR	TYR	ALA	VAL	SER	THR	GLY	HIS	LEU	GLN	ALA	ALA	LYS	VAL	THR	ALA				
LEU	LEU	SER	ALA	VAL	VAL	ASP	MET	VAL	VAL	ARG	LYS	ARG	ARG	ASN	THR	THR	GLN	VAL	PRO	GLY	ASN	LYS	ASP	GLY	ASP	ALA	ASP	ALA	ASP	ALA	THR	GLY	ASP	GLY	THR	GLY	THR	GLY	THR	GLY	THR	THR	THR	THR	THR	THR	THR			

• Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain 4-B: 18% 18% 63%

MET	HIS	GLN	GLY	ALA	PRO	SER	THR	GLY	ARG	THR	PHE	VAL	VAL	THR	VAL	THR	LEU	LEU	GLY	GLY	LEU	VAL	ASN	THR	PRO	GLY	VAL	ALA	ALA	THR	PRO	GLY	VAL	ALA	ALA	ASP	ALA	THR	GLN	ALA	ALA	ASN	GLY	PRO	ALA	PRO	GLY			
S280	S280	Y281	Y282	Y283	Y284	D285	E286	T287	Y288	L289	A290	Y295	P299	Y303	R304	T312	T313	Y314	D317	R318	F319	K320	Q321	Y326	D329	L330	T331	T332	K333	T337	A338	P339	T340	T341	R342	N343	L344	L345	K349	F350	T351	D355	W356	V357	P358	K359	R360	P361	S362	V363
I198	D199	K200	A203	K204	G205	V206	C207	R208	S209	T210	Y213	Y214	R215	L218	E219	A222	F223	H224	R225	D226	K235	P236	T241	R242	R245	G246	W247	H248	T249	T250	D251	L252	N255	P256	S257	R258	V259	E260	A261	F262	H263	R264	T267	T268	V269	W270	C271	D277	A278	R279
GLY	ALA	THR	VAL	VAL	GLN	PHE	GLU	GLN	PRO	ARG	CYS	PRO	THR	THR	THR	ASN	Y142	T143	E144	G145	I146	A147	V148	K151	E152	N153	I154	A155	P156	Y157	K158	F159	M163	Y164	Y165	K166	Q172	V173	W174	F175	Y179	M183	R189	A190	P191	F194	V197			



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

## 4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of tilted images used	1909	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE-FLIPPED TILT SERIES PRIOR TO TOMOGRAPHIC RECONSTRUCTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	95000	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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	1-A	0.97	0/2800	1.07	1/3800 (0.0%)
1	1-B	0.97	0/2806	1.07	1/3810 (0.0%)
1	1-C	0.97	0/2806	1.07	1/3810 (0.0%)
1	2-A	0.98	0/2800	1.07	1/3800 (0.0%)
1	2-B	0.98	0/2806	1.07	1/3810 (0.0%)
1	2-C	0.98	0/2806	1.07	1/3810 (0.0%)
1	3-A	0.98	0/2800	1.07	1/3800 (0.0%)
1	3-B	0.98	0/2806	1.07	1/3810 (0.0%)
1	3-C	0.98	0/2806	1.07	1/3810 (0.0%)
1	4-A	0.98	0/2800	1.08	1/3800 (0.0%)
1	4-B	0.98	0/2806	1.07	1/3810 (0.0%)
1	4-C	0.98	0/2806	1.07	1/3810 (0.0%)
All	All	0.98	0/33648	1.07	12/45680 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	4
1	1-B	0	4
1	1-C	0	4
1	2-A	0	3
1	2-B	0	3
1	2-C	0	3
1	3-A	0	2
1	3-B	0	2
1	3-C	0	2
1	4-A	0	2
1	4-B	0	2
1	4-C	0	2
All	All	0	33

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-B	409	LEU	C-N-CA	5.22	133.26	122.30
1	4-A	409	LEU	C-N-CA	5.21	133.25	122.30
1	2-A	409	LEU	C-N-CA	5.20	133.23	122.30
1	2-B	409	LEU	C-N-CA	5.20	133.23	122.30
1	2-C	409	LEU	C-N-CA	5.20	133.23	122.30

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	154	ILE	Peptide
1	1-A	156	PRO	Peptide
1	1-A	355	ASP	Peptide
1	1-A	363	VAL	Peptide
1	1-B	154	ILE	Peptide

## 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	1-A	2728	0	2613	239	0
1	1-B	2732	0	2618	236	0
1	1-C	2732	0	2618	233	0
1	2-A	2728	0	2613	240	0
1	2-B	2732	0	2618	241	0
1	2-C	2732	0	2618	234	0
1	3-A	2728	0	2613	237	0
1	3-B	2732	0	2618	238	0
1	3-C	2732	0	2618	237	0
1	4-A	2728	0	2613	240	0
1	4-B	2732	0	2618	233	0
1	4-C	2732	0	2618	236	0
All	All	32768	0	31396	2844	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 44.

The worst 5 of 2844 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:304:ARG:HB2	1:B:356:TRP:HZ3	1.12	1.13
1:C:304:ARG:HB2	1:C:356:TRP:HZ3	1.12	1.11
1:B:363:VAL:HB	1:B:364:CYS:HA	1.35	1.07
1:A:304:ARG:HB2	1:A:356:TRP:HZ3	1.12	1.06
1:A:363:VAL:HB	1:A:364:CYS:HA	1.38	1.06

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 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	1-A	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	44	81
1	1-B	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	44	81
1	1-C	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	44	81
1	2-A	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	44	81
1	2-B	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	44	81
1	2-C	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	44	81
1	3-A	334/904 (37%)	327 (98%)	7 (2%)	0	100	100
1	3-B	334/904 (37%)	327 (98%)	7 (2%)	0	100	100
1	3-C	334/904 (37%)	327 (98%)	7 (2%)	0	100	100
1	4-A	334/904 (37%)	326 (98%)	7 (2%)	1 (0%)	44	81
1	4-B	334/904 (37%)	326 (98%)	7 (2%)	1 (0%)	44	81
1	4-C	334/904 (37%)	326 (98%)	7 (2%)	1 (0%)	44	81
All	All	4008/10848 (37%)	3921 (98%)	78 (2%)	9 (0%)	54	84

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	357	VAL
1	2-B	357	VAL
1	2-C	357	VAL
1	4-A	363	VAL
1	4-B	363	VAL

### 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	1-A	289/747 (39%)	282 (98%)	7 (2%)	54	78
1	1-B	290/747 (39%)	283 (98%)	7 (2%)	54	78
1	1-C	290/747 (39%)	283 (98%)	7 (2%)	54	78
1	2-A	289/747 (39%)	282 (98%)	7 (2%)	54	78
1	2-B	290/747 (39%)	283 (98%)	7 (2%)	54	78
1	2-C	290/747 (39%)	283 (98%)	7 (2%)	54	78
1	3-A	289/747 (39%)	283 (98%)	6 (2%)	59	80
1	3-B	290/747 (39%)	284 (98%)	6 (2%)	59	80
1	3-C	290/747 (39%)	284 (98%)	6 (2%)	59	80
1	4-A	289/747 (39%)	284 (98%)	5 (2%)	66	84
1	4-B	290/747 (39%)	285 (98%)	5 (2%)	66	84
1	4-C	290/747 (39%)	285 (98%)	5 (2%)	66	84
All	All	3476/8964 (39%)	3401 (98%)	75 (2%)	60	79

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2-B	364	CYS
1	2-C	430	ASN
1	4-B	430	ASN
1	2-B	430	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	2-C	356	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	2-C	443	GLN
1	3-A	443	GLN
1	4-C	430	ASN
1	3-A	153	ASN
1	3-A	430	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.