

# wwPDB EM Validation Summary Report (i)

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PDB ID	:	8FQC
EMDB ID	:	EMD-29383
Title	:	Structure of baseplate with receptor binding complex of Agrobacterium phage
		Milano
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Deposited on	:	2023-01-05
Resolution	:	3.20  Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev $70$
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 3.20 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.



(# Entries)	(#Entries)
154571	4023
154315	3826
	(#Entries) 154571 154315

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 of 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  $\leq=5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	C1	457	68% ••	29%
2	E1	136	96%	•
2	a1	136	96%	•
2	f1	136	96%	•
2	g1	136	96%	
3	F1	396	97%	••
3	G1	396	95%	
3	h1	396	97%	•••
3	i1	396	97%	•••



Mol	Chain	Length	Quality of chain						
4	H1	178		98%					
4	j1	178		98%					
5	I1	503		98%	••				
5	K1	503		95%	• •				
5	k1	503		96%	••				
5	m1	503		96%	• •				
6	J1	286		93%	6%				
6	l1	286		97%	•				
7	P1	587	27%	72%					
7	Q1	587	28% •	71%					
7	R1	587	29% •	71%					
7	r1	587	27% •	72%					
7	s1	587	29% •	71%					
7	t1	587	29%	71%					
8	S1	300	39%	60%					
8	T1	300	39%	60%					
8	V1	300	39%	• 60%					
8	W1	300	40%	60%					
8	X1	300	40%	60%					
8	Y1	300	40%	60%					
8	u1	300	39%	60%					
8	v1	300	39%	• 60%					
8	w1	300	40%	60%					
8	x1	300	39%	60%					
8	y1	300	40%	60%					

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Conti	nuea jron	i previous	page								
Mol	Chain	Length	Quality of chain								
8	z1	300									
9	U1	398	97%								
9	e1	398	97%								
10	А	188	78%	10% • 11%							

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# 2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 66089 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 Baseplate hub protein, gp26.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	326	Total 2551	C 1610	N 434	O 500	S 7	0	0

• Molecule 2 is a protein called Tail-tube, gp21.

Mol	Chain	Residues		At	oms		AltConf	Trace	
2 E1	<b>F</b> 1	121	Total	С	Ν	0	S	0	0
	101	995	617	165	206	7	0	0	
9	9 91	131	Total	С	Ν	0	S	0	0
	aı		995	617	165	206	7	0	0
0	f1	131	Total	С	Ν	0	S	0	0
	11		995	617	165	206	7	0	0
2	g1	121	Total	С	Ν	0	S	0	0
		151	995	617	165	206	7	0	0

• Molecule 3 is a protein called Baseplate Wedge 2 protein, gp29.

Mol	Chain	Residues		At		AltConf	Trace		
3 F1	<b>F</b> 1	303	Total	С	Ν	0	$\mathbf{S}$	0	0
	090	3016	1900	515	580	21	0	0	
2	G1	202	Total	С	Ν	0	S	0	0
3 GI	595	3016	1900	515	580	21	0	0	
2	h1	202	Total	С	Ν	0	S	0	0
0	111		3016	1900	515	580	21	0	0
3	i1	303	Total	С	Ν	0	S	0	0
		11 393	3016	1900	515	580	21	0	0

• Molecule 4 is a protein called Baseplate wedge 1, gp28.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H1	176	Total 1334	C 817	N 244	0 264	S 9	0	0



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Mol	Chain	Residues	Atoms					AltConf	Trace
4	j1	176	Total 1334	C 817	N 244	0 264	S 9	0	0

• Molecule 5 is a protein called Tail sheath protein, gp20.

Mol	Chain	Residues		At		AltConf	Trace			
5 I1	T1	408	Total	С	Ν	0	S	0	0	
	490	3739	2342	633	742	22	0	0		
5	K1	IZ 1	404	Total	С	Ν	0	S	0	0
0 KI	494	3706	2322	628	735	21	0	0		
5	l-1	498	Total	С	Ν	0	S	0	0	
D KI	KI		3739	2342	633	742	22		0	
5	m1	1	404	Total	С	Ν	0	S	0	0
		494	3706	2322	628	735	21	0	U	

• Molecule 6 is a protein called Baseplate Wedge 3 protein, gp30.

Mol	Chain	Residues		At	oms			AltConf	Trace
6	T1	285	Total	С	Ν	0	$\mathbf{S}$	0	0
0	91	285	2185	1390	355	420	20	0	0
6	11	285	Total	С	Ν	0	S	0	0
0	11	200	2185	1390	355	420	20	U	U

• Molecule 7 is a protein called Tail Spike protein, gp124.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	P1	162	Total	С	Ν	0	$\mathbf{S}$	0	0
1	11	102	1227	782	194	248	3	0	0
7	01	173	Total	С	Ν	0	$\mathbf{S}$	0	0
1	Q1	175	1308	835	210	260	3	0	0
7	R1	173	Total	С	Ν	0	$\mathbf{S}$	0	0
1	101	175	1308	835	210	260	3	0	0
7	r1	162	Total	С	Ν	0	$\mathbf{S}$	0	0
1	11	102	1227	782	194	248	3	0	0
7	e1	173	Total	С	Ν	Ο	$\mathbf{S}$	0	0
1	51	175	1308	835	210	260	3	0	0
7	+1	173	Total	С	N	0	S	0	0
	υL	175	1308	835	210	260	3	0	0

• Molecule 8 is a protein called Short Tail Fibers, gp31.



Mol	Chain	Residues		At	oms			AltConf	Trace
0	C1	110	Total	С	Ν	0	S	0	0
0	51	119	878	545	150	174	9	0	0
0	TT1	110	Total	С	Ν	0	S	0	0
0	11	119	878	545	150	174	9	0	0
8	V1	110	Total	С	Ν	0	S	0	0
0	V I	119	878	545	150	174	9	0	0
8	W1	110	Total	С	Ν	0	S	0	0
0	VV 1	115	878	545	150	174	9	0	0
8	X1	110	Total	С	Ν	Ο	$\mathbf{S}$	0	0
0	$\Lambda_1$	115	878	545	150	174	9	0	0
8	V1	110	Total	С	Ν	Ο	$\mathbf{S}$	0	0
0	11	115	878	545	150	174	9	0	0
8	v1	110	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0
	V I	115	878	545	150	174	9	0	0
8	w1	110	Total	С	Ν	Ο	$\mathbf{S}$	0	0
	** 1	115	878	545	150	174	9	0	0
8	v1	119	Total	С	Ν	Ο	$\mathbf{S}$	0	0
		110	878	545	150	174	9	0	0
8	v1	119	Total	С	Ν	Ο	$\mathbf{S}$	0	0
	у <b>т</b>	110	878	545	150	174	9	0	0
8	111	119	Total	С	Ν	Ο	$\mathbf{S}$	0	0
	ui	110	878	545	150	174	9		
8	z1	119	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0
	21	110	878	545	150	174	9		

• Molecule 9 is a protein called Baseplate Centerpiece, gp25.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	U1	394	Total 3027	C 1910	N 522	O 590	${ m S}{ m 5}$	0	0
9	e1	394	Total 3027	C 1910	N 522	O 590	${ m S}{ m 5}$	0	0

• Molecule 10 is a protein called Baseplate Central Spike, gp27.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	А	168	Total 1289	C 799	N 223	0 264	${ m S} { m 3}$	0	0

• Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Ator	ns	AltConf
11	А	1	Total 1	Fe 1	0



# 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Baseplate hub protein, gp26





• Molecule 3: Baseplate Wedge 2 protein, gp29

Chain F1: 97% ME7 SEF • Molecule 3: Baseplate Wedge 2 protein, gp29 Chain G1: 95% . .. MET SER C3 T4 T5 T5 • Molecule 3: Baseplate Wedge 2 protein, gp29 Chain h1: 97% • Molecule 3: Baseplate Wedge 2 protein, gp29 Chain i1: 97% . . MET • Molecule 4: Baseplate wedge 1, gp28 Chain H1: 98% • Molecule 4: Baseplate wedge 1, gp28 Chain j1: 98% MET THR • Molecule 5: Tail sheath protein, gp20 Chain I1: 98%





• Molecule 5: Tail sheath protein, gp20

Chain K1:	95% •••
MET MET ALA GLN GLN GLA GLA GLA GLA GLA GLA GLA GLA GLA GLA	P378 N379 T415 ASP ASP ASP ASP ASP ASP ASP ASP
• Molecule 5: Tail sheath prote	in, gp20
Chain k1:	96%
MET ALA GLN GLN GLN GLN CJL F21 F21 F22 F22 F22 F22 F22 F22 F22 F22	D499 N500 ASP ARG
• Molecule 5: Tail sheath prote	in, gp20
Chain m1:	96% ••
MET ALA ALA GLN GLN GLA GLA GLA C12 T17 T17 T17 T17 C182 C182 C182 C182 C182 C182 C182 C182	R481 L497 ASN ASN ASN ASN ASG
• Molecule 6: Baseplate Wedge	3 protein, gp30
Chain J1:	93% 6%
M1 N2 V3 L4 L5 L5 E3 E3 E3 E3 C125 C125 C126 C126 C206 E203 E203 E207 E211 C211 C212 C212 C212 C212 C212 C212	V213 F276 ASP ASP
• Molecule 6: Baseplate Wedge	3 protein, gp30
Chain l1:	97% •
M1 N2 V3 V3 V15 V15 V151 A151 A285 ASP	
• Molecule 7: Tail Spike protein	n, gp124
Chain P1: 27%	72%
MET ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLA CLA CLA CLA CLA CLA CLA CLA CLA CLA	TLE SIER GLU CLU CLU CLU CLU CLU THR THR THR THR THR THR ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
THR CLY ASP ASP ASC VAL ASC VAL CLU CLY CLY THR TTR TTR TTR ASN ASN ASN ASN ASP ASP ASP ASP ASP ASP ASP ASP ASP ASC ASP ASC ASP ASC ASC ASC ASC ASC ASC ASC ASC ASC ASC	THR VAL VAL CLY CLY CLY CLY CLY VAL CLY VAL CLY CLY CLY CLY CLY CLY CLY CLY CLY CL
GLY ASIN CLY CLY CLY CLY CLY CLY CLY CLY ASIN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	THR THR THR TYR TYR TYR THR GLV GLV GLV CYS GLV CYS GLV CYS ASN ALA ALA ALA ALA ALA ALA ALA ALA ALA AL



LEU ASN SER PRO GLY THR MET ILE VAL	ASN ASN ARG SER ARG	VAL LYS ALA VAL LEU HIS	ALA ALA ASN MET ILE VAT	ALL GLN ILE GLY VAL	ILE GLU SER LEU ALA	SER THR PRO ASP ASN GLY	PHE LEU ALA VAL MET SER	SER SER LEU ASP PRO	LEU THR SER THR TYR
GLY THR ILE SER CYS CYS	PRO PHE VAL PHE PHE GLN	ASP PHE GLY ARG ASP ASN	ASP ASP THR ASP ALA LEU ASM	GLY GLY PRO LYS PHE ILE	VAL SER ASN GLY ARG	ASP VAL HIS GLY ASN TYR	ASP PRO ALA PHE TYR ALA	LEU PRO ASN GLY GLN THR	LEU ASN SER HIS PHE
ALA GLY ILE ASP ALA ALA CLU GLU THR	LEU GLN GLU TYR SER	PRO LEU ASP ARG LEU VAL	PRU VAL ASP LEU GLY PHE SFB	DER PHE GLY GLY TRP	THR ASP GLY GLU THR	ILE GLY ALA HIS VAL VAL	SER ARG SER THR ILE VAL	PRU GLU ASN MET ALA GLY	SER VAL PHE SER THR
ASP SER SER THR LEU ASP GLY VAL VAL	ASN ILE VAL VAL CLY	PRO SER VAL VAL VAL GLY GLY	VAL THR ILE VAL ASP GLY TI F	ALA ALA PHE ALA SER	SER SER PHE ASN LEU	ASP PRO GLY GLN THR VAL	ARG VAL VAL THR THR SER	ASP GLY THR PHE ASP TYR	ALA ALA LEU THR LEU
VAL GLY HIS ARG GLU VAL VAL TYR VAL	ASN								
• Molecule	7: Tail	Spike pro	otein, gp	124					
Chain Q1:		28%	·			71%			-
MET ALA K3 K3 G0 G116 C1117 S118 S118	V119 D175 PRO SER	GLN ILE LEU SER GLU	UAL THR LEU ARG VAL	TYR VAL THR GLY ASP	ASP ALA THR ALA ASP	GLY THR LEU ALA LYS PRO	PHE ALA TTHR VAL SER ALA	ALA ILE GLY VAL ALA ALA THR	THR GLY ASP ARG VAL
GLU TTR PRO GLY GLY TTR TTR GLY GLY	ASN PHE ALA PRO LYS	SER ASP VAL VAL VAL VAL	GLY GLV GLY VAL VAL	ASP GLY ASP VAL THR	ILE ALA ALA GLY VAL	SER GLY ALA LEU VAL ASP	GLY LEU PHE VAL ASP GLY	SER VAL LEU VAL ASN GLY	ALA ASN GLY SER VAL
HR HE SSN SSN EER AL AL	SN SN EU LA HR	LY SN SN HR LY AL	HHE RG SNN SNN SNN SNN SNN SNN SNN SNN SNN SNN	LE LA LA LA	LE AL SN LY HR	LY LA LLU LE LE	HE ER LLY AL AL	LU SSN EU EU EU	ER RO HR
					A A V I			09 H H H H H H H H H H H H H H H H H H H	H H H S H
	HEVALS				AS A				
GL LE PR PH PH GLL ASS	PH GL AR AS AS	AT THAT AND	PR GL	ASI ASI ABI ASI ASI ASI ASI ASI ASI ASI ASI ASI AS	VAI HII GL GL ASI ASI TYT	ASI PRU PHT TYT AL	PRE 6 CLS	ASI SES PHT AL	GL ASI AL
LEU GLU LEU GLU TYR SER PRO	LEU ASP ARG LEU VAL	PRO VAL ASP LEU GLY	PHE THR GLY TRP	ASP ASP GLY GLU THR THR	GLY ALA HIS VAL VAL	SER ARG SER THR TLE VAL	PRO GLU MET ALA GLY	SEK VAL PHE SER THR ASP	SER SER THR LEU ASP
GLY VAL LEU ASN ASN TLE VAL VAL CLY GLY	SER VAL VAL VAL GLY THR	VAL THR ILE VAL ASP GLY	ALA ALA THR PHE ALA SER SER SER	SER SER PHE ASN LEU ASP	PRO GLY GLN THR VAL	ARG VAL VAL THR THR SER	ASP GLY GLY THR PHE ASP TYR	ALA ALA LEU LEU LEU VAL	GLY HIS ARG GLU VAL
VAL TYR VAL ASN									
• Molecule	7: Tail S	Spike pro	otein, gp	124					
Chain R1:		29%	·			71%			
MET ALA K3 G21 E22 C24 C24 C24	D175 D175 PRO SER GLN	ILE LEU SER GLU GLU	VAL THR LEU ARG ASP ASP TYB	LIR VAL THR GLY ASP ASP	ALA THR ALA ASP GLY	THR LEU ALA LYS PRO PHE	ALA THR VAL SER ALA ALA	LLE GLY VAL ALA THR THR	GLY ASP ARG VAL GLU
ILE TYR PRO GLY THR TYR ILE GLY ASN	PHE ALA PRO LYS SER	ASP VAL THR VAL VAL GLY	GLU GLV GLY VAL VAL TLE	GLY GLY ASP VAL THR ILE	ALA ALA GLY VAL SER	GLY ALA LEU VAL ASP GLY	LEU PHE VAL ASP GLY SER	VAL LEU VAL ASN GLY ALA	ASN GLY SER VAL THR
PHE ARG ASN SER ASN GLU ASN	VAL VAL LEU ALA THR GLY	ASN ASN THR GLY VAL TYR	PHE PHE GLU ASN ASP ASP	GLU GLU ALA ALA ILE	VAL ASN GLY THR GLY	ASN ALA GLU PHE TLE PHE	SER GLY GLY VAL SER GLU	ASN ASP PHE PHE LEU ASN	SER PRO GLY THR MET
ILE VAL GLU ASN ARG SER ARG VAL VAL	ALA VAL LEU HIS GLU	ALA GLY ASN MET ILE VAL	ALN ASN GLY VAL ILE	SER LEU SER SER	PRO ASP ASN GLY PHE	LEU ALA VAL MET SER SER	SER LEU PHE ASP PRO LEU	THR SER THR TYR GLY	ILE SER LYS THR GLY



# NALLILLE LEUVALLILLE VALLILLE TYR VAL ASN • Molecule 7: Tail Spike protein, gp124 Chain r1: 27% 72% MET ALAS ALYS LYS ALGU ARG PRO PRO GLN VAL CLY VAL CLY VAL PRO ASN ACLART ALLART ALLAR TYR THR THR THR THR THR THR THR THR THR ASSN THR THR ASSN THR ASSN THR ASSN PHERE ALLARY ALL LEU VAL GLY ARG GLU VAL VAL VAL TYR VAL VAL • Molecule 7: Tail Spike protein, gp124 Chain s1: 29% 71% PHERE PHERE ARGORD THE MET VALUAL SERRAS SERRAS SERRAS SERRAS SERRAS SERRAS SERRAS SERRAS SERVAL SERVAL SERVAL SERVAL SERVAL SERVAL SERRAS SERAS SERRAS GGLY PHEC CYS CYS PHE CYS PHE CYS PHE ASS PHE ASS PHE ASS PHE CYS PHE CYS PHE CYS PHE CYS PHE CYS PHE CYS PHE ASS PHE



#### LLEU THR CHILU CHILU CHILU CHILU CHILEU CHIL

#### 

#### VAL TYR VAL ASN

• Molecule 7: Tail Spike protein, gp124

Chain t1:	29%	71%
MET ALA KIA B175 PR0 PR0 SER CLM ILE ILE SER SER CLM CLU GLU	GLU VAL LEU VAL LEU ARG ARG ARG ARP ARR ARP ARA ARP ARA ARP ARA ARP ARA ARP ARA ARP ARA ARP ARA ARP ARA ARP ARA ARC ARA ARC ARA ARC ARA ARC ARA ARC ARC	ALA ALA VAL SER ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
11LE GLY ASN ASN PHE ASN PRO LYS SER ASP VAL THR VAL VAL	GLY CELU OLIZU OLIZU VALL ALSE ALSE ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	PHE VAL ASP ASP ASP SER SER VAL ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN
THR GLU ASN VAL VAL LEU ALA ALA ASN ASN ASN THR ASN THR CLY	TYR ARG ASU ASU ASU ASU ASN CYS ASN ALA ALA ALA ASN ALA ASN ALA ASN ALA ASN ALA ASN ALA ASN ALA ASN ALA ASN ASN ASL ASD ASD ASD ASD ASD ASD ASD ASD ASD ASD	CLY CLY CLY CLY CLY CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
ARG VAL LYS ALA ALA VAL LEU HTS GLU ALA GLV ASN MET ILE	VAL VAL ASN ASN ASN ASN VAL TLE CLU CLU CLU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	SER LEU PHE ASP ASP ASP ASP ASP THR THR THR THR THR THR THR THR CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS
GLN ASP GLY GLY ASP ASP ASP THR THR THR THR THR THR TLBU	ASN PRO PRO PHE TLYS PHE TLYS ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	PRO ASN GLY GLN CLN CLN CLN CLN ASN ASN ASN ASN ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU
SER PRO LEU ASP ASP VAL VAL VAL ASP LEU CEU GLY GLY	SER PHE THR GLY GLY THR GLY THR THR THR THR THR ALA ANA ANA SER SER SER SER SER SER SER SER SER SER	ASN ASN MET ALA ALA ASN SER SER SER SER SER SER SER SER SER SER
GLY PRO SER VAL VAL VAL CLY THR THR THR THR THR THR THR THR THR GLY	11.E 11.E 11.E 11.E 21.E 21.E 21.E 21.F 21.E 21.F 21.F 21.F 21.F 21.F 21.F 21.F 21.F	GLY THR PHE PHE ASP ASP ASP ASP CLU CLEU VAL CLEU VAL CLU VAL CLU VAL CLU VAL CLU VAL ASN ASS
• Molecule 8: Sho	rt Tail Fibers, gp31	
Chain S1:	39%	60%
MET ALA G3 C12 C12 C12 G121 G121 GLY THR THR THR THR CYS	GLN LLE GLN GLN GLN GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY	VAL PHC PHC ALA ALA ALA ALA ALA ALA CLY GLY GLY GLY GLY GLN GLN GLN GLN
ASN GLN LEU PHE ASP ASP SER ARG ALA GLY CLY PHE TRP	ASP VAL SER CIN SER CIN SER ALA ALA ALA ALA ALA ALA ALA ALA CIV CIV CIV CIV CIV CIV CIV CIV	VAL SUR SUR CIUU CIUU PHE TIE TIE TIE CIU CIU CIU CIU CIU CIU CIU CIU CIU CIU
PHE ALA ALA ALA VAL PRO PRO THR GLV GLV THR THR THR THR THR ASP	GLY GLY GLY GLA ARG CLA ALA ALA ALA ALA ALA ALA ALA ALA ALA	LLEU LLEU PLEO LLEU LLEU LLEU LLEU ASP ASP ASP ASP ASP ASP CLY VAL TLE ARG CLY TRA CLY TRA CLY TRA CLY TRA CLY TRA CLI TLE ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP
TRP ASP GLY VAL GLN VAL		
• Molecule 8: Sho	rt Tail Fibers, gp31	
Chain T1:	39%	60%



ASN PHE CLUN CLUN CLUN CLUN CLUN CLUN CLUN CLUN
PHE TYR TYR TYR TYR THR THR THR THR THR THR THR THR THR TH
TRP GLSP VAL GLN VAL
• Molecule 8: Short Tail Fibers, gp31
Chain V1: 39% • 60%
MET MET ALA ALA ALA CC CC CC CC CC CC CC CC CC CC CC CC CC
PRO PRO ASN ASP PHE ASP PHE ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP
SER PHE THR THR THR THR THR THR THR THR THR THR
CLN TRP ASP VAL VAL VAL
• Molecule 8: Short Tail Fibers, gp31
Chain W1: 40% 60%
MET MET ALA ALA ALA CALA CALA CALA CALA CALA ALA
LEU PHE ASP SER ASP ALA ALA ALA GLY GLY CLY CLN GLY CLN GLY CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN
TYR     LEU     MET       WUL     PHE     MET       WUL     PHE     MET       WUL     SER     GLY       THR     GLY     TRP       GLY     TRP     GLY       MAP     TRP     GLY       MAP     TRP     GLY       MAP     TRP     GLY       MAP     GLY     GLY       MAP     GLY     GLY       MAP     GLY     GLY       MAP     GLY     GLY       MAD     GLY     GLY       MAD     GLY     GLY       MAL     GLY
GLY     TYR     LEU     MET       VAL     PARE     LEU     MET       CUN     THR     LEU     MET       CUN     THR     CLN     THR     CLN       CUN     THR     CLN     CLN     CLN       CUN     THR     CLN     CLN     CLN       CUN     CLN     CLN     CLN     CLN
Image: Second
Image: State of the state
Image:
Image:
Image:



• Molecule 8:	Short Tail Fibers, g	gp31
Chain Y1:	40%	60%
MET ALA G3 G121 G121 GLN VAL GLN THR LEU	CYS CYS GLM LBU FRO FRO GLM ALA ALA ALA ALA ASP ASP ASP ASP TRP	LEBU ALA CYS CYS CYS CYS CYS CYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
LEU PHE ASP SER TRP ARG ALA GLY GLY PHE	TRP ASP VAL SER SER CLN SER THR ALA ALA ALA ALA ALA ALA PHE VAL	ARE ARE ARE ARE ARE ARE ARE ALV ALL ALL ALL ALA ALA ALA ALA ALA ALA
TYR VAL PRO FRO GLY GLV THR THR ALA ALA ILE	ASP GLY GLY GLY GLN ARG GLN ALA ALA ALA ALA TLE TLE TLE CYS CIYS	GLN GLN TYRP TYRP TYRP TYRP TYRP CLN GLN ALA ALA ALA ALA ALA ALA CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY
GLY VAL GLN VAL		
• Molecule 8:	Short Tail Fibers, g	gp31
Chain v1:	39%	• 60%
MET ALA G3 K37 C38 G121 G121 VAL	GLY THR LEU CYS CYS CYS GLN FLEU GLN GLN ASP ASP	ASP ASP ASP ALA ALA ALA ASP CYS CYS CYS CYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
GLN ASN GLN LEU PHE ASP SER TRP ALA ALA	GLY GLY PHE TRP ASP ASP VAL SER GLN GLN GLN ALA ALA ALA ALA ALA ALA	ALA ALA PHE VAL VAL ARG SER ARG CLY CLU CLU CLU CLU CLU CLU CLV CLU CLV CLU CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV
THR PHE ALA TYR VAL PRO THR GLY GLY THR	THR ALA ALA ASP ASP GLY GLY GLY ALA ALA ALA ALA ALA ALA ALE	PHE LYS CVS GLY GLY GLN ALA ALA ALA ALA ALA ALA ALA ALA ALA A
ILE TRP ASP GLY VAL GLN VAL VAL		
• Molecule 8:	Short Tail Fibers, g	gp31
Chain w1:	40%	60%
MET ALA G3 G121 GLN VAL GLY THR LEU	CYS CYS GLN LEU FRO CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	LEU ALA O'S CYS CYS CYS CYS CYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
LEU PHE ASP SER TRP ARG ALA GLY GLY PHE	TRP ASP VAL SER SER GLN SER THR ALA ALA ALA ALA ALA VAL	ARE ARE ARE ARE ARE CLY CLY CLY CLY CLY CLY CLY CLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A
TYR VAL PRO PRO GLY GLV THR THR THR THR TLA	ASP GLY GLY GLY GLY GLN GLN ALA ALA ALA ALA ALA ALA LYS CLY SY CLY	ASIN ASIN TYRP TYRP TYRP ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
GLY VAL GLN VAL		
• Molecule 8:	Short Tail Fibers, g	gp31
Chain x1:	39%	60%
MET ALA G3 G3 G121 GLN VAL GLY GLY	THR LEU CYS CYS CYS CYS CIN FRO FRO FRO FRO FRO CIN ASP ASP	TASP TASP ALA ALA ALA CYS CYS CYS CYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL



ASN ASN FIE FIE FIE FIE FIE FIE FIE FIE FIE FIE	TYR GLN SER SER SER GLU TRP GLU SER SER THR
PHE PHE TYR VAL ALA TYR PRO CLY CLU THR THR THR ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	ARAS VAL ARG ARG CLY GLY GLN ARG LEU CLN TLEU CLN
TRP GLY VAL GLN VAL	
• Molecule 8: Short Tail Fibers, gp31	
Chain y1: 40% 60%	
MET MET ALA ALA GIZI GIZI GIZI CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	dur VAL TLE GLY GLY VAL TLE PRO GLN GLN GLN GLN
LEU PHE ASP ASP ASP ASP ALA ALA ALA ALA THR THR THR ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	SER TLE SER SER GLU GLU PRO PRO SER THR PHE ALA
TYR YAL PRO FIHR FIHR FIHR THR THR THR THR THR ASP CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	AND THR PRO GLY GLN GLN LEU GLN ILE TRP ASP
GLY CUML VAL	
• Molecule 8: Short Tail Fibers, gp31	
Chain ul: 39% 60%	
Chain ul: 39% 60%	GLY GLY GLY GLY GLY GLY GLY GLY TLE PRO
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	ALA ALA TYR GLY GLN GLY GLN GLY SER GLY ULE CLY CLY GLY GLY CLY CLY SER PRO
HIH     39%     60%       THR     111     39%     60%       THR     111     111     111       TRR     111     111     111	ARG ALA GLA ARG ALA GLA ARG GLN GLY THR SER GLY PRO TLE CLY CLY CLY CLY CLY CLY CLY CLY ARG GLU CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY
$M_{11}$ $39\%$ $60\%$ $M_{11}$ $M_{11}$ $39\%$ $60\%$ $M_{11}$	ARG ALA GLA ARG ALA GLA ARG GLN GLY THR SER GLY CLY FIN SER GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C
Chain ul:       39%       60%         Image: Provide state stat	ARG ALA GLY VAL TYR GLY ARG ALA GLY ARG GLN GLY THR SER GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C
Chain ul:       39%       60%         Image: State of the st	ARG ALA GLY VAL TYR GLY ARG ALA GLY ARG GLN GLY THR SER GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C
Chain ul:       39%       60%         Image: Source of the state of the s	ALM ALC ALL ALC ALL ALC ALL ALL ALL ALL ALL
Chain ul:       39%       60%         # # #       60%         # # #       60%         #       60%         #       60%         #       60%         #       60%         #       60%         #       60%         #       60%         #       60%         #	IN         SAM         ALG         U.L         OLI         OLI           GLY         LEU         V.AL         TYR         OLI         OLI           OLY         ELU         V.AL         TYR         GLY         OLI           OLY         GLY         MAG         GLN         GLY         GLY           ALA         CLY         YR         GLN         GLN         GLY           TYR         GLY         PRO         TLE         VAL         GLY           GLN         GLY         THR         SER         GLY         GLY           GLN         GLY         PRO         TLE         VAL         GLY           SER         GLY         THR         GLU         GLY         GLY           SER         TLE         VAL         TR         GLU         GLY           GLU         GLY         GLU         TR         GLY         GLY           GLU         GLY         GLN         GLU         GLY         GLY           GLU         GLY         GLN         GLU         GLY         GLY           GLU         GLY         GLN         GLN         GLY         GLY
Chain ul:       39%       60%         III III       39%       60%         III III IIII       39%       60%         III IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	ST         LIA         LIA         LIA         OLI         OLI           VAL         GLY         LEU         ALA         OLI         OLI           VAL         GLY         LEU         VAL         TYR         GLY           ARG         GLY         TYR         GLY         CLY           ARG         GLY         TYR         GLY         CLY           VAL         TYR         GLY         NAG         GLY           ARG         GLY         THR         SER         GLY           VAL         TYR         GLY         PRO         TLE           THR         SER         GLY         GLY         GLY           THR         SER         GLY         GLY         GLY           FIRE         VAL         TYR         GLY         GLY           FIRE         VAL         TYR         GLY         GLY           GLY         SER         GLY         GLY         GLY           FIRE         VAL         TRP         GLY         GLY           GLY         SER         GLY         GLY         GLY           FIRE         GLY         GLY         GLY         GLY



• • •

• Molecule 9: Baseplate Centerpiece, gp25

Chain U1: 97%



• Molecule 9: Baseplate Centerpiece, gp25

Chain e1: 97% ···



• Molecule 10: Baseplate Central Spike, gp27

Chain A:	78%	10% •	11%
MET THR THR THR THR THR TRR ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	836 836 836 836 836 840 840 841 948 742 841 742 150 150 150 150 873 873 873 873 876	D114 S115 I116	D181 P185 LYS ARG ASP



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14856	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \times 4k)$	Depositor
Maximum map value	1.478	Depositor
Minimum map value	-0.780	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	624.24005,  624.24005,  624.24005	wwPDB
Map dimensions	578, 578, 578	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor



# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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).

Mal	Chain	Bond	lengths	Bo	ond angles
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	C1	0.38	0/2598	0.57	0/3525
2	E1	0.46	0/1011	0.52	0/1382
2	a1	0.40	0/1011	0.52	0/1382
2	f1	0.38	0/1011	0.51	0/1382
2	g1	0.41	0/1011	0.52	0/1382
3	F1	0.42	0/3085	0.49	0/4207
3	G1	0.47	0/3085	0.55	0/4207
3	h1	0.42	0/3085	0.48	0/4207
3	i1	0.46	0/3085	0.54	0/4207
4	H1	0.37	0/1353	0.51	0/1831
4	j1	0.37	0/1353	0.51	0/1831
5	I1	0.41	0/3815	0.53	0/5211
5	K1	0.38	0/3781	0.51	0/5165
5	k1	0.42	0/3815	0.52	0/5211
5	m1	0.37	0/3781	0.50	0/5165
6	J1	0.44	0/2237	0.53	0/3063
6	l1	0.41	0/2237	0.50	0/3063
7	P1	0.33	0/1269	0.45	0/1755
7	Q1	0.35	0/1352	0.50	0/1868
7	R1	0.30	0/1352	0.47	0/1868
7	r1	0.33	0/1269	0.45	0/1755
7	s1	0.36	0/1352	0.46	0/1868
7	t1	0.32	0/1352	0.47	0/1868
8	S1	0.29	0/892	0.46	0/1217
8	T1	0.28	0/892	0.46	0/1217
8	V1	0.28	0/892	0.49	0/1217
8	W1	0.32	0/892	0.44	0/1217
8	X1	0.30	0/892	0.46	0/1217
8	Y1	0.29	0/892	0.45	0/1217
8	u1	0.31	0/892	0.48	0/1217
8	v1	0.30	0/892	0.47	0/1217
8	w1	0.28	0/892	0.45	0/1217



Mal	Chain	Bond	lengths	Bo	ond angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
8	x1	0.28	0/892	0.49	0/1217
8	y1	0.31	0/892	0.45	0/1217
8	z1	0.31	0/892	0.44	0/1217
9	U1	0.44	0/3093	0.49	0/4214
9	e1	0.44	0/3093	0.50	1/4214~(0.0%)
10	А	0.62	0/1320	0.91	3/1791~(0.2%)
All	All	0.40	0/67510	0.51	4/92226~(0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
9	e1	138	LEU	CA-CB-CG	5.73	128.49	115.30
10	А	116	ILE	N-CA-C	-5.73	95.53	111.00
10	А	181	ASP	CB-CG-OD2	5.18	122.96	118.30
10	А	72	GLY	N-CA-C	-5.14	100.25	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	Perce	entiles
1	C1	320/457~(70%)	247 (77%)	65 (20%)	8 (2%)	5	32
2	E1	129/136~(95%)	117 (91%)	12 (9%)	0	100	100
2	a1	129/136~(95%)	117 (91%)	12 (9%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	f1	129/136~(95%)	118 (92%)	11 (8%)	0	100	100
2	g1	129/136~(95%)	118 (92%)	10 (8%)	1 (1%)	19	58
3	F1	391/396~(99%)	371~(95%)	19~(5%)	1 (0%)	41	74
3	G1	391/396~(99%)	366 (94%)	21 (5%)	4 (1%)	15	54
3	h1	391/396~(99%)	378~(97%)	10 (3%)	3 (1%)	19	58
3	i1	391/396~(99%)	363 (93%)	26 (7%)	2(0%)	29	67
4	H1	174/178~(98%)	149 (86%)	24 (14%)	1 (1%)	25	64
4	j1	174/178~(98%)	145 (83%)	27 (16%)	2 (1%)	14	51
5	I1	496/503~(99%)	439 (88%)	56 (11%)	1 (0%)	47	79
5	K1	492/503~(98%)	421 (86%)	64 (13%)	7 (1%)	11	46
5	k1	496/503~(99%)	441 (89%)	53 (11%)	2(0%)	34	69
5	m1	492/503~(98%)	404 (82%)	80 (16%)	8 (2%)	9	43
6	J1	283/286~(99%)	258 (91%)	20 (7%)	5 (2%)	8	41
6	l1	283/286~(99%)	253 (89%)	27 (10%)	3 (1%)	14	51
7	P1	160/587~(27%)	146 (91%)	13 (8%)	1 (1%)	25	64
7	Q1	171/587~(29%)	155 (91%)	12 (7%)	4 (2%)	6	34
7	R1	171/587~(29%)	158 (92%)	12 (7%)	1 (1%)	25	64
7	r1	160/587~(27%)	147 (92%)	12 (8%)	1 (1%)	25	64
7	s1	171/587~(29%)	158 (92%)	10 (6%)	3 (2%)	8	41
7	t1	171/587~(29%)	156 (91%)	15 (9%)	0	100	100
8	S1	117/300~(39%)	109 (93%)	8 (7%)	0	100	100
8	T1	117/300~(39%)	112 (96%)	4 (3%)	1 (1%)	17	56
8	V1	117/300~(39%)	109~(93%)	8 (7%)	0	100	100
8	W1	117/300~(39%)	109 (93%)	8 (7%)	0	100	100
8	X1	117/300~(39%)	107~(92%)	10 (8%)	0	100	100
8	Y1	117/300~(39%)	111 (95%)	6 (5%)	0	100	100
8	u1	117/300 (39%)	110 (94%)	6 (5%)	1 (1%)	17	56
8	v1	117/300~(39%)	107 (92%)	10 (8%)	0	100	100
8	w1	$\overline{117/300}~(39\%)$	114 (97%)	3 (3%)	0	100	100
8	x1	$117/\overline{300}\ (\overline{39\%})$	105 (90%)	12 (10%)	0	100	100
8	y1	117/300 (39%)	110 (94%)	7 (6%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
8	z1	117/300~(39%)	108~(92%)	7~(6%)	2(2%)	9	42
9	U1	392/398~(98%)	368~(94%)	21 (5%)	3(1%)	19	58
9	e1	392/398~(98%)	361~(92%)	30~(8%)	1 (0%)	41	74
10	А	166/188~(88%)	142 (86%)	13 (8%)	11 (7%)	1	9
All	All	8648/13631~(63%)	7807~(90%)	764 (9%)	77 (1%)	21	56

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5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F1	375	ASP
6	J1	2	ASN
5	K1	378	PRO
7	Q1	117	ILE
7	Q1	119	VAL

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	C1	281/383~(73%)	271~(96%)	10 (4%)	35	69
2	E1	115/116~(99%)	115 (100%)	0	100	100
2	a1	115/116~(99%)	115 (100%)	0	100	100
2	f1	115/116~(99%)	115 (100%)	0	100	100
2	g1	115/116~(99%)	115 (100%)	0	100	100
3	F1	330/333~(99%)	324 (98%)	6(2%)	59	82
3	G1	330/333~(99%)	317~(96%)	13~(4%)	32	67
3	h1	330/333~(99%)	324~(98%)	6(2%)	59	82
3	i1	330/333~(99%)	321 (97%)	9~(3%)	44	75
4	H1	145/147~(99%)	145 (100%)	0	100	100
4	j1	145/147~(99%)	145 (100%)	0	100	100
5	I1	404/408~(99%)	399~(99%)	5 (1%)	71	88



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	K1	400/408~(98%)	392~(98%)	8(2%)	55	80
5	k1	404/408~(99%)	393~(97%)	11 (3%)	44	75
5	m1	400/408~(98%)	394~(98%)	6~(2%)	65	85
6	J1	245/247~(99%)	231~(94%)	14~(6%)	20	56
6	l1	245/247~(99%)	239~(98%)	6~(2%)	49	77
7	P1	129/473~(27%)	129 (100%)	0	100	100
7	Q1	138/473~(29%)	135~(98%)	3~(2%)	52	79
7	R1	138/473~(29%)	135~(98%)	3~(2%)	52	79
7	r1	129/473~(27%)	127~(98%)	2(2%)	62	84
7	s1	138/473~(29%)	135~(98%)	3~(2%)	52	79
7	t1	138/473~(29%)	137~(99%)	1 (1%)	84	94
8	S1	97/229~(42%)	96~(99%)	1 (1%)	76	90
8	T1	97/229~(42%)	97~(100%)	0	100	100
8	V1	97/229~(42%)	95~(98%)	2(2%)	53	79
8	W1	97/229~(42%)	97~(100%)	0	100	100
8	X1	97/229~(42%)	97~(100%)	0	100	100
8	Y1	97/229~(42%)	97~(100%)	0	100	100
8	u1	97/229~(42%)	95~(98%)	2(2%)	53	79
8	v1	97/229~(42%)	95~(98%)	2(2%)	53	79
8	w1	97/229~(42%)	97~(100%)	0	100	100
8	x1	97/229~(42%)	96~(99%)	1 (1%)	76	90
8	y1	97/229~(42%)	97~(100%)	0	100	100
8	z1	97/229~(42%)	94~(97%)	3 (3%)	40	72
9	U1	$\overline{314/316}\ (99\%)$	308~(98%)	6 (2%)	57	81
9	e1	314/316~(99%)	309~(98%)	5 (2%)	62	84
10	А	143/162~(88%)	134 (94%)	9~(6%)	18	52
All	All	$71\overline{94/10979}~(66\%)$	7057~(98%)	137 (2%)	59	81

 $5~{\rm of}~137$  residues with a non-rotameric side chain are listed below:

			- <i>J</i> P S
7	r1	175	ASP
7	t1	175	ASP

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Mol	Chain	Res	Type
10	А	38	LYS
5	K1	12	ARG
6	J1	277	CYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such side chains are listed below:

Mol	Chain	Res	Type
2	a1	84	GLN
10	А	28	HIS
3	i1	355	ASN
8	z1	117	ASN
8	x1	17	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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-29383. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



6.1.2 Raw map



The images above show the map projected in three orthogonal directions.



# 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 289





Z Index: 289

#### 6.2.2 Raw map



X Index: 289

Y Index: 289

Z Index: 289

The images above show central slices of the map in three orthogonal directions.



## 6.3 Largest variance slices (i)

#### 6.3.1 Primary map









Z Index: 276

#### 6.3.2 Raw map



X Index: 0

Y Index: 289



The images above show the largest variance slices of the map in three orthogonal directions.



## 6.4 Orthogonal standard-deviation projections (False-color) (i)

#### 6.4.1 Primary map



#### 6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



#### 6.5 Orthogonal surface views (i)

#### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

#### 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



# 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



## 7.2 Volume estimate (i)



The volume at the recommended contour level is 7391  $\rm nm^3;$  this corresponds to an approximate mass of 6676 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



## 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.312  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

#### 8.1 FSC (i)



\*Reported resolution corresponds to spatial frequency of 0.312  ${\rm \AA^{-1}}$ 



## 8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.25	3.87	3.31
Unmasked-calculated*	4.42	8.07	4.58

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.2 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-29383 and PDB model 8FQC. Per-residue inclusion information can be found in section 3 on page 9.

## 9.1 Map-model overlays

#### 9.1.1 Map-model overlay (i)



#### 9.1.2 Map-model assembly overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



#### 9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

#### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).



## 9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

$\mathbf{Chain}$	Atom inclusion	Q-score
All	0.9810	0.4980
А	0.9070	0.3820
C1	0.9400	0.4770
E1	0.9870	0.5640
F1	0.9840	0.5370
G1	0.9880	0.5390
H1	0.9770	0.5290
I1	0.9860	0.5410
J1	0.9880	0.5400
K1	0.9790	0.4980
P1	0.9880	0.4520
$\overline{Q1}$	0.9890	0.4560
R1	0.9820	0.4260
S1	0.9780	0.3790
T1	0.9900	0.3780
U1	0.9780	0.5470
V1	0.9820	0.3670
W1	0.9910	0.4300
X1	0.9860	0.4260
Y1	0.9900	0.4110
al	0.9840	0.5560
e1	0.9790	0.5530
f1	0.9910	0.5590
g1	0.9820	0.5630
h1	0.9840	0.5390
i1	0.9860	0.5380
j1	0.9780	0.5300
k1	0.9890	0.5440
11	0.9840	0.5380
m1	0.9800	0.5010
r1	0.9860	0.4470
s1	0.9890	0.4560
t1	0.9870	0.4320
u1	0.9830	0.4140
v1	0.9760	0.3780



Continued from previous page...

Chain	Atom inclusion	Q-score
w1	0.9820	0.3860
x1	0.9680	0.3610
y1	0.9850	0.4160
z1	0.9780	0.4070

