

# wwPDB EM Validation Summary Report (i)

Nov 22, 2022 – 11:49 AM JST

PDB ID	:	7EEB
EMDB ID	:	EMD-31076
Title	:	Structure of the CatSpermasome
Authors	:	Wu, J.P.; Ke, M.
Deposited on	:	2021-03-18
Resolution	:	2.90  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 43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
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)	:	2.31.3

# 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 2.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 >=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 <=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	А	955	5% 15% 11	% •		73%				
2	В	588	20% 29%	189	<b>%</b> ••		52%			
3	С	395	18%	51%		19%		30%		
4	D	442	39%	6	16%		45%			
5	Е	1109	<b></b>	60%			31%		• 5%	
6	F	1145	<b>_</b>	67%			21%	•	9%	
7	G	805	6%	60%			26%	•	11%	
8	Н	985	6%	65%			27%		• 7%	

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Mol	Chain	Length	(	Quality of cha	ain	
0	Т	706	F 00/	83%	220/	150/
9		700	50%	88%	33%	• 15%
10	J	171		82%		12% 6%
11	М	116	39% 61%		36%	•
12	Ν	28	61%	93%		7%
13	Ι	216	7	81%		19%
14	K	194	60%	%	5%	26%
15	0	7	14%	570/	٥ <i>٢</i> د	20%
10	0	1	50%	57%		29%
16	Р	2	50%		50%	
16	S	2	50%		50%	
16	Т	2	50%		50%	
16	V	2	50% 		50%	
16	X	2	50%		50%	
16	a	2	50%		50%	
				100%		
16	d	2	50%		50%	
17	Q	3	33%	33%	3	3%
17	R	3	33%		67%	
17	U	3		100%		
17	W	3	67%			33%
17	b	3	67%			33%
18	Y	5	40%	40%	40%	6
	-			-		
18	С	5	40%		60%	
19	Z	7	14%	57%		29%

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The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	NAG	Х	1	-	-	Х	-
17	NAG	U	1	-	-	Х	-
19	NAG	Ζ	1	-	-	Х	-



# 2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 47874 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 Enhanced green fluorescent protein, Cation channel sperm-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	258	Total 2112	C 1422	N 322	O 357	S 11	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-268	ASP	-	expression tag	UNP C5MKY7
А	-267	TYR	-	expression tag	UNP C5MKY7
А	-266	LYS	-	expression tag	UNP C5MKY7
А	-265	ASP	-	expression tag	UNP C5MKY7
А	-264	HIS	-	expression tag	UNP C5MKY7
А	-263	ASP	-	expression tag	UNP C5MKY7
А	-262	GLY	-	expression tag	UNP C5MKY7
А	-261	ASP	-	expression tag	UNP C5MKY7
А	-260	TYR	-	expression tag	UNP C5MKY7
А	-259	LYS	-	expression tag	UNP C5MKY7
А	-258	ASP	-	expression tag	UNP C5MKY7
А	-257	HIS	-	expression tag	UNP C5MKY7
А	-256	ASP	-	expression tag	UNP C5MKY7
А	-255	ILE	-	expression tag	UNP C5MKY7
А	-254	ASP	-	expression tag	UNP C5MKY7
А	-253	TYR	-	expression tag	UNP C5MKY7
А	-252	LYS	-	expression tag	UNP C5MKY7
А	-251	ASP	-	expression tag	UNP C5MKY7
А	-250	ASP	-	expression tag	UNP C5MKY7
А	-249	ASP	-	expression tag	UNP C5MKY7
А	-248	ASP	-	expression tag	UNP C5MKY7
А	-247	LYS	-	expression tag	UNP C5MKY7
А	-7	GLU	-	linker	UNP C5MKY7
А	-6	ASN	-	linker	UNP C5MKY7
А	-5	LEU	-	linker	UNP C5MKY7
А	-4	TYR	-	linker	UNP C5MKY7
А	-3	PHE	-	linker	UNP C5MKY7

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Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	GLN	-	linker	UNP C5MKY7
А	-1	GLY	-	linker	UNP C5MKY7
А	0	SER	-	linker	UNP C5MKY7

• Molecule 2 is a protein called Cation channel sperm-associated protein 2.

Mol	Chain	Residues		At	AltConf	Trace			
2	В	281	Total 2343	C 1585	N 363	0 384	S 11	0	0

• Molecule 3 is a protein called Cation channel sperm-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	278	Total 2277	C 1506	N 359	0 400	S 12	0	0

• Molecule 4 is a protein called Cation channel sperm-associated protein 4.

Mol	Chain	Residues		At	AltConf	Trace			
4	D	242	Total 1965	C 1325	N 300	0 325	S 15	0	0

• Molecule 5 is a protein called Cation channel sperm-associated protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Е	1053	Total 8470	$\begin{array}{c} \mathrm{C} \\ 5502 \end{array}$	N 1387	O 1537	S 44	0	0

• Molecule 6 is a protein called Cation channel sperm-associated protein subunit gamma 2.

Mol	Chain	Residues		Α	AltConf	Trace			
6	F	1042	Total 8454	C 5515	N 1354	O 1538	S 47	0	0

• Molecule 7 is a protein called Cation channel sperm-associated protein subunit delta.

Mol	Chain	Residues		A	AltConf	Trace			
7	G	714	Total 5680	C 3669	N 923	O 1056	S 32	0	0

• Molecule 8 is a protein called Cation channel sperm-associated protein subunit epsilon.



Mol	Chain	Residues		Atoms					Trace
0	п	016	Total	С	Ν	Ο	$\mathbf{S}$	0	0
0	11	910	7502	4865	1208	1389	40	0	0

• Molecule 9 is a protein called Kazal-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	597	Total 4694	C 3079	N 747	O 829	S 39	0	0

• Molecule 10 is a protein called Transmembrane protein 249.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace	
10	J	161	Total 794	С 472	N 161	O 161	0	0

• Molecule 11 is a protein called Transmembrane protein 262.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	М	116	Total 946	C 625	N 159	0 151	S 11	0	0

• Molecule 12 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Ν	28	Total 140	C 84	N 28	O 28	0	0

• Molecule 13 is a protein called EF-hand calcium-binding domain-containing protein 9.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
13	Ι	174	Total 863	C 515	N 174	0 174	0	0

• Molecule 14 is a protein called Cation channel sperm-associated protein subunit zeta.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
14	K	143	Total 710	C 424	N 143	0 143	0	0

• Molecule 15 is an oligosaccharide called beta-D-mannopyranose-(1-2)-beta-D-mannopyranos e-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopy



ranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
15	О	7	Total 83	C 46	N 2	O 35	0	0

• Molecule 16 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Aton	ns		AltConf	Trace
16	P	9	Total C	Ν	0	0	0
10	1	2	28 16	2	10	0	0
16	S	9	Total C	Ν	Ο	0	0
10	0	2	28 16	2	10	0	0
16	т	9	Total C	Ν	0	0	0
10	T	2	28 16	2	10	0	0
16	V	9	Total C	Ν	0	0	0
10	v	2	28   16	2	10	0	0
16	x	9	Total C	Ν	0	0	0
10	Λ	2	28   16	2	10	0	0
16	0	9	Total C	Ν	0	0	0
10	a	2	28 16	2	10	0	0
16	d	9	Total C	Ν	0	0	0
10	u	2	28 16	2	10	0	0

• Molecule 17 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns	AltConf	Trace	
17	Q	3	Total 39	C 22	N 2	0 15	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace	
17	В	3	Total C N O	0	0	
11	п	5	39  22  2  15	0	0	
17	ΤT	2	Total C N O	0	0	
11	U	5	39  22  2  15	0	0	
17	W	2	Total C N O	0	0	
11	vv	5	39  22  2  15	0	0	
17	h	3	Total C N O	0	0	
17	D	5	39 $22$ $2$ $15$	U	0	

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• Molecule 18 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns	AltConf	Trace	
18	Y	5	Total 61	С 34	N 2	O 25	0	0
18	с	5	Total 61	С 34	N 2	O 25	0	0

• Molecule 19 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyrano se-(1-6)]beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopy ranose.



Mol	Chain	Residues	AltConf	Trace				
19	Z	7	Total 83	C 46	N 2	O 35	0	0

• Molecule 20 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
20	А	1	Total Na 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
20	D	1	Total Na 1 1	0

• Molecule 21 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5 -en (three-letter code: 9Z9) (formula:  $C_{34}H_{56}O_5$ ).



Mol	Chain	Residues	Atoms	AltConf
21	А	1	Total C O 117 102 15	0
21	А	1	Total         C         O           117         102         15	0
21	А	1	Total         C         O           117         102         15	0

• Molecule 22 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	A	Aton	ns		AltConf
20	F	1	Total	С	Ν	0	0
	Ľ	L	56	32	4	20	0
22	F	1	Total	С	Ν	0	0
	Ľ	T	56	32	4	20	0
22	F	1	Total	С	Ν	0	0
	Ľ	I	56	32	4	20	0
22	F	1	Total	С	Ν	0	0
	Ľ	I	56	32	4	20	0
22	F	1	Total	С	Ν	0	0
	Г	T	14	8	1	5	0
22	C	1	Total	С	Ν	0	0
	G	T	42	24	3	15	0
22	C	1	Total	$\mathbf{C}$	Ν	Ο	0
	G	T	42	24	3	15	0
22	С	1	Total	С	Ν	0	0
	G	I I	42	24	3	15	0
22	Ц	1	Total	С	Ν	0	0
	11		14	8	1	5	U



# 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: Enhanced green fluorescent protein, Cation channel sperm-associated protein 1



















 T603

 T615

 T615

 T615

 T615

 T615

 T615

 A619

 A614

 A625

 A626

 A627

 A628

 A628

 A629

 A626

 A621

 A626

 A629

 A626

 A629

 A641

 A642

 A643

 A644

 A644

 A645



# Y687 Y687 F689 F707 F711 F707 F707 F719 F715 F715 F716 F717 F718 F719 F712 F712 F713 F723 F724 F725 F726 F723 F724 F723 F724 F725 F724 F725 F724 F735 F735 F736 F737 F738 F739 F744 F745

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• Molecule 9: Kazal-like domain-containing protein



DB

Y121	<mark>q122</mark>	V123	Q124 F125	S126	L127 T128	R129	T130 E131	W132	Y133 1124	L134 M135	D136	F137	D139	Y140	1141	A142	5143 F144	V145	V146	A147 1148	I149	<b>I150</b>	A151 H152	F153	G154 S155	K156	G157	R159	T160	R161	162 1163	A164	A165 8166	C167	I168	L169 M170	G171	L172	E173	S174	M175 1 176	E177	A178	F1/9 P180
F181	F182	T183	Y184 🕈 E185	I186	1187	P189	G190 🕈 R191	Q192	S193	E195	L196	C197	E199	E200	N201	E202	R204	N205	1206	1207 C208	G209	N210	S211	P213	N214	S216	K217	1219	Y220	F221	1223	G224	<mark>(225</mark>		1228	H229 G230	1231	A232	G233	M234	P235	1230 Y237	1238	G240
41	42	43	44 45	46	47 48	49	50	52		55	66	57		•	61	<mark>62</mark>	64	65	66	67	69	<b>4</b>	71	73	75	29 2		2 6	•••	81 • • •	83 2	84	يو يو	87	88		91	92	63 63	94	95	6	8	
• 12	T2	F2	12 F2	D2		P2	T2 S2	S2	€ G	F2	Y2			G2	₩2	S2	Y2		12				G2 M2	V2	G2 G2			F2	<b>q</b> 2	P2	P2	K2	E2 KO	T2	V2	E2 12	E2	●	<b>A</b> 2	K2		q2 q2		
S301	G302	W303	W304 K305	T306	F307 L308	I309	I310 A311	A312	I313 5214	5314 F315	C316	V317	5319 F319	M320	M321	V322	5223 F324	P325	T326	5327 L328	P329	<b>G</b> 330	A331 H332	K333	L334 R335	L336	A337	R339	K340	E341 PRO	PRO THD	ILE	ASP	ARG	LYS	MET	LYS ILE	<b>q355</b>	P356	H357	L358	G360		
F361	L362	H363	N364	W366	H367	L369	K370	P372	L373	L375	T376	Q377	01CA	C380	K381	V382	5303 E384	Y385	L386	T387 F388	N389	T390	S391 L392	Y393	F394	P396	H397 H398	L399	1400 1401	Q402	F403	L404 I405	T406	P407	1409	A410	S411	L412	L413 T414	G415	A416	F417	V418 L419	P420
421	•																																											
9	G422	1423	I424 G425	H426	F427 L428	G429	G430	1432	V433	D4.34 R435	L436	E437	r4.30	N440	K441	N442	L444	K445	F446	T447 L448	V449	T450	T451	V453	S454 V455	G456	L457	L459	L460	1461 E460	F463	V464	E465	0467	T468	T469	F471	A472	G473	1474	N475 F476	D477	Y478	04/9 G480
/481 <b>•</b> G	1482 <b>•</b> 6422	1483 🔶 1423	484 • 1424 • 1485 • G425 •	1486 🔶 H426	.487 ♥ F427 ♥ F428 ● L428 ●	1489 🔶 G429 🔶	0490 ♥ G430 ♥ 3491 ● L431 ●	1492 🔶 1432	V433	1495 • R435	1496 🔶 L436	2497 E437	1430 M430	S500 ♦ N440 ♦	501 🔶 K441 🔶	(502 • N442	504 ♦ L444 ♦	1505 🔶 K445	506 F446	3507 T447	509 ♦ V449	5510 <b>•</b> T450	(511 (1451) (512 (1452)	(513 • V453 •	514         S454           5515         V455	516 ♦ G456 ♦	2517 • L457 • 1518 • 16		521 L460	(522 • 1461 • • • • • • • • • • • • • • • • • • •	$F_{1524} \bullet F_{463} \bullet F_{46} \bullet F_{46} \bullet F_{46} \bullet F_{46} \bullet F_{46} \bullet F_{46} \bullet$	(525 🔶 V464	1526 E465		[529 🔶 T468 🔶	1469 T469		(533 • A472 •	(534 G473	1474 • 1474 • 1536			[539 Y478 Y478	G480
	G482 G422	• [1483 • I423	• L484 • I424 • G485 • G425 •	♦ N486 ♦ H426		A489 G429	● D490 ● G430 ● G431 ● C491 ● I431 ●	N492 • I432	E493	C495	♦ D496 ♦ L436	C497 E437	1430 M430		► L501 ► K441	Y502 N442		• I505 • K445	C506 F446	G507 ♥ T447 B508 ♦ L448	D509	♦ E510 ♦ T450 ♦	♦ K511 ♥ T451 ♥ E512 ♦ V452 ●	Y513	F514 S515 V455	P516	F518	A519	C521	K522 1461	$\begin{array}{c c} \bullet \\ \bullet \\ \bullet \\ T524 \\ \bullet \\ F463 \\ \bullet \\ F$	K525	V526 E465		T529	E530 T469	♦ T532 ♦ F471	♦ Y533 ♦ A472 ♦	Y534 6473	♦ N535 ♥ I474 ♦ C536			1539 Y478 K540	
	<b>G542</b> ♦ G482 ♦ G422	L543 • Q483 • I423	A544 C L484 L424 C L425 C C425 C	S546 ♦ N486 ♦ H426 ♦	D547    L487    F427	E549 A A489 G429	G550         D490         G430           0551         C491         1431	F552 • N492 • 1432		A555 C495 R435	I556 ♦ D496 ♦ L436 ♦	A557 C497 E437	T559 T499 T439	C560 S500 N440	D561 • L501 • K441 •	S562 V502 N442	C564 S504 L144	L565 + I505 + K445 +	K566 C506 🔶 F446	P568 G507 T447 T447	L569 D509 V449	F571 $\blacklozenge$ E510 $\blacklozenge$ T450 $\blacklozenge$	A572	F573 Y513 Y513 Y453	F575 F514 S454 S515 V455	B576 P516 C456 C456	T578 C517 L457	F580 A519 L459		N582 K522 I461	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	S585 • K525 • V464	I586 V526 E465		1589 • T529 • T468	S590         E530         1469           T591         K531         T470	$1331 \qquad \qquad 1532 \qquad \qquad 1532 \qquad \qquad 1471 \qquad \qquad$	L593	Q594 + Y534 G473	SE95 A N535 A 1474 C536 C536 C536			N599 T539 Y478	F600 • G480 • G480 •
Y481	G482 🔶 G422	Q483 🔶 I423	L484 • I424 • G425 • G425 •	N486 H426	L487 • F427 • T488 • L428 •	A489 🔶 G429	D490 C430 C430 C431 C431 C491 C491 C491 C491 C491 C491 C491 C49	N492	E493 (V433 (V433) Vлол (Vлол	C495 R435	D496 🔶 L436 🔶	C497 E437	T499 T439 T439		L501 🔶 K441 🔶	Y502 • N442	1503 0444 0 1444	1505 🔶 K445 🔶	C506 F446	G507 T447 L448	D509	E510 🕈 T450 🌵	K511 T451 E512 V452	Y513	F514 <b>S454</b>	P516 6456	C517 L457		C521 L460	K522 • 1461	T524 F463	K525	V526 E465		T529	E530 Ф T469 Ф V T470 Ф		Y533   A472	Y534 G473	N535 1474 C536			I539 Y478 K	

wwPDB EM Validation Summary Report

EMD-31076, 7EEB

• Molecule 10: Transmembrane protein 249

I 1661 W662 M663 S664 S665 Q666 Q666 L667 I 1668 I 1669 V670

Page 18



PROTEIN DATA BANK

• Molecule 11: Transmembrane protein 262 39% Chain M: 61% 36% ¥ T78 G79 D80 K81 F82 L83 L83 C85 C85 C85 F86 F86 A75 • Molecule 12: Unknown 61% Chain N: 93% 7% X25 X26 X27 X28 X28 X28 X28 X30 X31 5 • Molecule 13: EF-hand calcium-binding domain-containing protein 9 81% Chain I: 78% 19% L12 Y13 M14 D15 7 P5 G6 C7 F8 W1 ( V1) ARG YS YS ARG ARG • Molecule 14: Cation channel sperm-associated protein subunit zeta 74% Chain K: 69% 5% 26% T38 A39 N40 V41 S42 170 871 072 873 L74 N75 L76 G94 R95 S96 197 E98 r11 811 E11 S11 C11 Y64 S65 Q66 T67 I68 E77 E79 E79 E80 E80 U81 Q83 Q83 **q**84 A85 E90 51 H93 ARG LEU PRO THR ILE GLY



 $\label{eq:constraint} \bullet \mbox{Molecule 15: beta-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gl ucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-2-acetamido$ 



• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 50% 50%

• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:	50%	50%

#### NAG 1 NAG 2

• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:	50%	50%	
NAG2 NAG2			
• Molecule 16: copyranose	2-acetamido-2-deoxy-beta	a-D-glucopyranose-(1-4)-2-acetamic	lo-2-deoxy-beta-D-glu
	50%	_	
Chain V:	50%	50%	
NAG2			

• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



#### NAG1 NAG2

• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

	50%	
Chain a:	50%	50%
•		
NAG1		

• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu copyranose

_	100%				
Chain d:	50%	50%			
••					
NAG1 NAG2					

• Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose

Chain Q:	33%	33%	33%
NAG1 NAG2 BNA3 BNA3			

• Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose

Chain R:	33%	67%
NAG1 NAG2 BYA3		

• Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:	100%
NAG1 BMA3	

67%

• Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

33%

Chain W:

VAG1 VAG2 VAG2



• Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



 $\label{eq:constraint} \bullet \mbox{Molecule 18: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos$ 



 $\bullet$  Molecule 18: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose ose

Chain c:	40%	60%
<mark>NAG1</mark> NAG2 BMA3 BMA4 BMA5		

 $\label{eq:constraint} \bullet \mbox{Molecule 19: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc$ 





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	560730	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	4.093	Depositor
Minimum map value	-2.371	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	430.91998, 430.91998, 430.91998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^{\circ}$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	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: BMA, NA, NAG, 9Z9

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	Bond lengths		angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.40	0/2159	0.59	0/2933
2	В	0.42	0/2406	0.54	0/3270
3	С	0.40	0/2324	0.52	0/3141
4	D	0.43	0/2015	0.54	0/2739
5	Ε	0.48	0/8706	0.70	0/11819
6	F	0.49	0/8695	0.64	0/11809
7	G	0.39	0/5823	0.60	0/7921
8	Н	0.36	0/7706	0.56	0/10491
9	L	0.31	0/4817	0.46	0/6543
10	J	0.31	0/791	0.45	0/1096
11	М	0.43	0/972	0.55	0/1314
13	Ι	0.79	0/862	0.75	0/1201
14	K	0.46	0/707	0.71	0/982
All	All	0.43	0/47983	0.60	0/65259

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 (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	А	2112	0	2211	155	0

Continued on next page...



Contre	nucu jion	i precious	puge			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	2343	0	2435	125	0
3	С	2277	0	2339	87	0
4	D	1965	0	2022	57	0
5	Е	8470	0	8412	552	0
6	F	8454	0	8306	294	0
7	G	5680	0	5593	367	0
8	Н	7502	0	7359	281	0
9	L	4694	0	4699	203	0
10	J	794	0	346	11	0
11	М	946	0	950	69	0
12	N	140	0	30	1	0
13	Ι	863	0	370	1	0
14	K	710	0	297	5	0
15	0	83	0	70	1	0
16	Р	28	0	25	1	0
16	S	28	0	25	2	0
16	Т	28	0	25	2	0
16	V	28	0	25	2	0
16	Х	28	0	25	9	0
16	a	28	0	25	0	0
16	d	28	0	25	0	0
17	Q	39	0	34	1	0
17	R	39	0	34	3	0
17	U	39	0	34	11	0
17	W	39	0	34	3	0
17	b	39	0	34	0	0
18	Y	61	0	52	2	0
18	с	61	0	52	0	0
19	Ζ	83	0	70	18	0
20	А	1	0	0	0	0
20	D	1	0	0	0	0
21	А	117	0	0	20	0
22	Е	56	0	52	2	0
22	F	14	0	13	2	0
22	G	42	0	39	3	0
22	Н	14	0	13	1	0
All	All	47874	0	46075	2052	0

Continued from previous page...

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 22.

The worst 5 of 2052 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:A:535:LEU:HD11	1:A:565:TYR:CD2	1.32	1.62
8:H:91:ASN:HD21	16:V:1:NAG:C1	1.03	1.58
8:H:292:ASN:HD22	16:X:1:NAG:C1	1.04	1.58
8:H:565:ASN:HD22	19:Z:1:NAG:C1	0.93	1.52
5:E:759:THR:HG22	6:F:861:TYR:CZ	1.47	1.46

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	Perc	entiles
1	А	256/955~(27%)	240 (94%)	15~(6%)	1 (0%)	34	66
2	В	279/588~(47%)	256 (92%)	22 (8%)	1 (0%)	34	66
3	С	276/395~(70%)	249 (90%)	27 (10%)	0	100	100
4	D	240/442~(54%)	225 (94%)	15 (6%)	0	100	100
5	Е	1047/1109~(94%)	968 (92%)	67 (6%)	12 (1%)	14	42
6	F	1040/1145~(91%)	975 (94%)	59~(6%)	6 (1%)	25	58
7	G	708/805~(88%)	663 (94%)	39 (6%)	6 (1%)	19	51
8	Н	912/985~(93%)	861 (94%)	46 (5%)	5(0%)	29	61
9	L	593/706~(84%)	549~(93%)	38~(6%)	6 (1%)	15	45
10	J	155/171~(91%)	142 (92%)	13 (8%)	0	100	100
11	М	114/116~(98%)	101 (89%)	11 (10%)	2(2%)	8	29
13	Ι	172/216~(80%)	163 (95%)	6 (4%)	3(2%)	9	31
14	К	137/194 (71%)	135 (98%)	1 (1%)	1 (1%)	22	54
All	All	5929/7827~(76%)	5527 (93%)	359 (6%)	43 (1%)	26	54

5 of 43 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
5	Е	335	GLU
5	Е	689	ILE
5	Е	756	ALA
5	Е	833	TYR
5	Е	948	PHE

#### 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	Percentiles		
1	А	237/846~(28%)	230~(97%)	7 (3%)	41	75	
2	В	262/546~(48%)	259~(99%)	3(1%)	73	92	
3	С	253/363~(70%)	252 (100%)	1 (0%)	91	97	
4	D	213/399~(53%)	210 (99%)	3 (1%)	67	89	
5	Е	957/1009~(95%)	907~(95%)	50 (5%)	23	55	
6	F	946/1035~(91%)	903~(96%)	43 (4%)	27	61	
7	G	642/720~(89%)	618 (96%)	24 (4%)	34	68	
8	Н	842/897~(94%)	828 (98%)	14 (2%)	60	86	
9	L	516/613~(84%)	505~(98%)	11 (2%)	53	81	
11	М	100/100~(100%)	98~(98%)	2 (2%)	55	82	
All	All	4968/6528~(76%)	4810 (97%)	158 (3%)	42	73	

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	224	TYR
8	Н	933	ILE
7	G	443	ASN
7	G	746	GLN
9	L	474	ILE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such side chains are listed below:



Mol	Chain	Res	Type
6	F	498	ASN
7	G	169	ASN
8	Н	888	ASN
6	F	621	ASN
6	F	673	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)

53 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Tuno	Chain	Dog	Tink	Bo	ond leng	ths	B	ond ang	gles
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	NAG	Ο	1	5,15	14,14,15	0.64	1 (7%)	17,19,21	0.77	1 (5%)
15	NAG	0	2	15	14,14,15	0.54	0	17,19,21	0.61	0
15	BMA	Ο	3	15	11,11,12	1.76	3 (27%)	$15,\!15,\!17$	1.35	2 (13%)
15	BMA	0	4	15	11,11,12	1.34	1 (9%)	$15,\!15,\!17$	1.34	3 (20%)
15	BMA	0	5	15	11,11,12	1.23	2 (18%)	15,15,17	1.62	3 (20%)
15	BMA	Ο	6	15	11,11,12	1.11	0	15,15,17	1.17	1 (6%)
15	BMA	Ο	7	15	11,11,12	0.63	0	15,15,17	1.07	1 (6%)
16	NAG	Р	1	16,5	14,14,15	0.68	1 (7%)	17,19,21	0.40	0
16	NAG	Р	2	16	14,14,15	0.23	0	17,19,21	0.47	0
17	NAG	Q	1	17,6	14,14,15	0.70	1 (7%)	17,19,21	0.50	0
17	NAG	Q	2	17	14,14,15	0.44	0	17,19,21	0.58	0
17	BMA	Q	3	17	11,11,12	0.56	0	$15,\!15,\!17$	1.10	2 (13%)



	<b>T</b>	Chain	Dec	T : 1-	Bo	ond leng	ths	Bond angles		les
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
17	NAG	R	1	17,6	14,14,15	0.50	0	17,19,21	0.50	0
17	NAG	R	2	17	14,14,15	0.32	0	17,19,21	0.62	0
17	BMA	R	3	17	11,11,12	0.97	1 (9%)	$15,\!15,\!17$	1.51	3 (20%)
16	NAG	S	1	16,6	14,14,15	0.80	1 (7%)	$17,\!19,\!21$	0.42	0
16	NAG	S	2	16	14,14,15	0.20	0	17,19,21	0.47	0
16	NAG	Т	1	16,6	14,14,15	0.29	0	17,19,21	0.57	0
16	NAG	Т	2	16	14,14,15	0.29	0	17,19,21	0.47	0
17	NAG	U	1	7,17	14,14,15	0.28	0	17,19,21	0.60	0
17	NAG	U	2	17	14,14,15	0.28	0	17,19,21	0.60	0
17	BMA	U	3	17	11,11,12	0.22	0	15,15,17	0.64	0
16	NAG	V	1	16	14,14,15	0.47	0	17,19,21	0.60	0
16	NAG	V	2	16	14,14,15	0.32	0	17,19,21	0.60	0
17	NAG	W	1	8,17	14,14,15	0.30	0	17,19,21	0.66	0
17	NAG	W	2	17	14,14,15	0.55	0	17,19,21	1.33	3 (17%)
17	BMA	W	3	17	11,11,12	0.63	0	$15,\!15,\!17$	1.04	2 (13%)
16	NAG	Х	1	16	14,14,15	0.79	1 (7%)	$17,\!19,\!21$	0.59	0
16	NAG	Х	2	16	14,14,15	0.17	0	17,19,21	0.45	0
18	NAG	Y	1	18,8	14,14,15	0.84	1 (7%)	17,19,21	0.62	0
18	NAG	Y	2	18	14,14,15	0.37	0	17,19,21	0.60	0
18	BMA	Y	3	18	11,11,12	0.96	1 (9%)	15,15,17	1.37	2 (13%)
18	BMA	Y	4	18	11,11,12	0.84	1 (9%)	15,15,17	0.94	1 (6%)
18	BMA	Y	5	18	11,11,12	0.76	0	15,15,17	0.89	0
19	NAG	Z	1	19	14,14,15	0.56	0	17,19,21	0.53	0
19	NAG	Z	2	19	14,14,15	0.69	1 (7%)	17,19,21	0.48	0
19	BMA	Z	3	19	11,11,12	0.87	0	$15,\!15,\!17$	0.93	1 (6%)
19	BMA	Z	4	19	11,11,12	1.10	1 (9%)	15, 15, 17	1.16	1 (6%)
19	BMA	Z	5	19	11,11,12	1.01	1 (9%)	$15,\!15,\!17$	1.21	2 (13%)
19	BMA	Z	6	19	11,11,12	0.64	0	15,15,17	0.93	1 (6%)
19	BMA	Ζ	7	19	11,11,12	0.56	0	15,15,17	0.80	0
16	NAG	a	1	16	14,14,15	0.40	0	17,19,21	0.61	0
16	NAG	a	2	16	14,14,15	0.45	0	17,19,21	0.62	1 (5%)
17	NAG	b	1	8,17	14,14,15	0.47	0	17,19,21	0.73	1 (5%)
17	NAG	b	2	17	14,14,15	0.39	0	17,19,21	0.52	0
17	BMA	b	3	17	11,11,12	0.77	0	15,15,17	0.70	0
18	NAG	с	1	18	14,14,15	0.29	0	17,19,21	0.46	0
18	NAG	с	2	18	14,14,15	0.41	0	17,19,21	0.43	0
18	BMA	с	3	18	11,11,12	0.54	0	$15,\!15,\!17$	1.18	1 (6%)
18	BMA	с	4	18	11,11,12	1.14	1 (9%)	$15,\!15,\!17$	1.30	3 (20%)
18	BMA	с	5	18	11,11,12	0.77	0	15,15,17	0.98	1 (6%)



Mal Turna Ch	Chain	Dec	Tinle	Bo	ond leng	$_{\rm sths}$	Bond angles			
MOI	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	NAG	d	1	9,16	14,14,15	0.78	1 (7%)	17,19,21	0.75	0
16	NAG	d	2	16	14,14,15	0.35	0	17,19,21	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	0	1	5,15	-	1/6/23/26	0/1/1/1
15	NAG	Ο	2	15	-	2/6/23/26	0/1/1/1
15	BMA	Ο	3	15	-	2/2/19/22	0/1/1/1
15	BMA	0	4	15	-	2/2/19/22	0/1/1/1
15	BMA	0	5	15	-	2/2/19/22	0/1/1/1
15	BMA	0	6	15	-	2/2/19/22	0/1/1/1
15	BMA	0	7	15	-	2/2/19/22	0/1/1/1
16	NAG	Р	1	16,5	-	2/6/23/26	0/1/1/1
16	NAG	Р	2	16	-	2/6/23/26	0/1/1/1
17	NAG	Q	1	17,6	-	2/6/23/26	0/1/1/1
17	NAG	Q	2	17	-	2/6/23/26	0/1/1/1
17	BMA	Q	3	17	-	0/2/19/22	0/1/1/1
17	NAG	R	1	17,6	-	2/6/23/26	0/1/1/1
17	NAG	R	2	17	-	0/6/23/26	0/1/1/1
17	BMA	R	3	17	-	2/2/19/22	0/1/1/1
16	NAG	S	1	16,6	-	0/6/23/26	0/1/1/1
16	NAG	S	2	16	-	2/6/23/26	0/1/1/1
16	NAG	Т	1	16,6	-	4/6/23/26	0/1/1/1
16	NAG	Т	2	16	-	0/6/23/26	0/1/1/1
17	NAG	U	1	7,17	-	0/6/23/26	0/1/1/1
17	NAG	U	2	17	-	0/6/23/26	0/1/1/1
17	BMA	U	3	17	-	1/2/19/22	0/1/1/1
16	NAG	V	1	16	-	2/6/23/26	0/1/1/1
16	NAG	V	2	16	-	2/6/23/26	0/1/1/1
17	NAG	W	1	8,17	-	2/6/23/26	0/1/1/1
17	NAG	W	2	17	-	2/6/23/26	0/1/1/1
17	BMA	W	3	17	-	0/2/19/22	0/1/1/1
16	NAG	Х	1	16	-	2/6/23/26	0/1/1/1
16	NAG	Х	2	16	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	NAG	Y	1	18,8	-	2/6/23/26	0/1/1/1
18	NAG	Y	2	18	-	2/6/23/26	0/1/1/1
18	BMA	Y	3	18	-	1/2/19/22	0/1/1/1
18	BMA	Y	4	18	-	1/2/19/22	0/1/1/1
18	BMA	Y	5	18	-	2/2/19/22	0/1/1/1
19	NAG	Z	1	19	-	2/6/23/26	0/1/1/1
19	NAG	Z	2	19	-	2/6/23/26	0/1/1/1
19	BMA	Z	3	19	-	2/2/19/22	0/1/1/1
19	BMA	Ζ	4	19	-	1/2/19/22	0/1/1/1
19	BMA	Z	5	19	-	2/2/19/22	0/1/1/1
19	BMA	Ζ	6	19	-	0/2/19/22	0/1/1/1
19	BMA	Z	7	19	-	2/2/19/22	0/1/1/1
16	NAG	a	1	16	-	1/6/23/26	0/1/1/1
16	NAG	a	2	16	-	3/6/23/26	0/1/1/1
17	NAG	b	1	8,17	-	3/6/23/26	0/1/1/1
17	NAG	b	2	17	-	3/6/23/26	0/1/1/1
17	BMA	b	3	17	-	1/2/19/22	0/1/1/1
18	NAG	с	1	18	-	0/6/23/26	0/1/1/1
18	NAG	с	2	18	-	0/6/23/26	0/1/1/1
18	BMA	с	3	18	-	1/2/19/22	0/1/1/1
18	BMA	с	4	18	-	0/2/19/22	0/1/1/1
18	BMA	с	5	18	-	1/2/19/22	0/1/1/1
16	NAG	d	1	9,16	-	2/6/23/26	0/1/1/1
16	NAG	d	2	16	-	2/6/23/26	0/1/1/1

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The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
18	с	4	BMA	C1-C2	3.16	1.59	1.52
15	0	3	BMA	C2-C3	3.15	1.57	1.52
15	0	3	BMA	C4-C5	-2.92	1.46	1.53
18	Y	1	NAG	O5-C1	-2.91	1.39	1.43
16	S	1	NAG	O5-C1	-2.88	1.39	1.43

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
15	0	5	BMA	C1-C2-C3	-3.98	104.77	109.67
17	W	2	NAG	C1-O5-C5	3.71	117.22	112.19

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
15	0	4	BMA	O2-C2-C3	-3.50	103.13	110.14
15	0	5	BMA	O2-C2-C3	-3.49	103.14	110.14
18	с	4	BMA	O2-C2-C3	-3.23	103.66	110.14

Continued from previous page...

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Т	1	NAG	C3-C2-N2-C7
16	V	2	NAG	O5-C5-C6-O6
17	Q	1	NAG	O5-C5-C6-O6
15	0	4	BMA	O5-C5-C6-O6
16	V	1	NAG	O5-C5-C6-O6

There are no ring outliers.

21 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	0	4	BMA	1	0
15	0	5	BMA	1	0
16	S	1	NAG	2	0
17	Q	1	NAG	1	0
18	Y	1	NAG	1	0
19	Ζ	1	NAG	13	0
17	R	1	NAG	3	0
19	Ζ	5	BMA	1	0
17	U	2	NAG	6	0
18	Y	3	BMA	1	0
19	Ζ	2	NAG	4	0
16	Т	1	NAG	2	0
16	S	2	NAG	2	0
17	W	1	NAG	3	0
16	V	1	NAG	2	0
17	U	3	BMA	1	0
16	Х	1	NAG	9	0
18	Y	2	NAG	2	0
17	W	2	NAG	1	0
17	U	1	NAG	7	0
16	Р	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





















































# 5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mal	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
WIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
21	9Z9	А	703	-	44,44,44	0.70	1 (2%)	$66,\!68,\!68$	1.44	11 (16%)
22	NAG	Е	1204	5	14,14,15	0.32	0	17,19,21	0.42	0
22	NAG	G	903	7	14,14,15	0.48	0	$17,\!19,\!21$	0.81	1(5%)
22	NAG	Е	1202	5	14,14,15	0.31	0	17,19,21	0.39	0
22	NAG	Н	1001	-	14,14,15	0.41	0	17,19,21	0.49	0
22	NAG	F	1201	-	$14,\!14,\!15$	0.26	0	$17,\!19,\!21$	0.32	0
21	9Z9	А	704	-	44,44,44	0.70	1 (2%)	$66,\!68,\!68$	1.44	11 (16%)
22	NAG	G	901	7	14,14,15	0.42	0	17,19,21	0.49	0
22	NAG	G	902	7	$14,\!14,\!15$	0.19	0	$17,\!19,\!21$	0.40	0
21	9Z9	А	702	-	44,44,44	0.71	1 (2%)	$66,\!68,\!68$	1.44	12 (18%)
22	NAG	Е	1201	5	14,14,15	0.47	0	17,19,21	0.40	0
22	NAG	Е	1203	5	14,14,15	0.22	0	17,19,21	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	9Z9	А	703	-	-	0/12/100/100	0/6/6/6
22	NAG	Е	1204	5	-	0/6/23/26	0/1/1/1
22	NAG	G	903	7	-	2/6/23/26	0/1/1/1
22	NAG	Е	1202	5	-	0/6/23/26	0/1/1/1
22	NAG	Н	1001	-	-	2/6/23/26	0/1/1/1
22	NAG	F	1201	-	-	1/6/23/26	0/1/1/1
21	9Z9	А	704	-	-	0/12/100/100	0/6/6/6
22	NAG	G	901	7	-	2/6/23/26	0/1/1/1
22	NAG	G	902	7	-	2/6/23/26	0/1/1/1
21	9Z9	А	702	-	-	0/12/100/100	0/6/6/6
22	NAG	Е	1201	5	-	1/6/23/26	0/1/1/1
22	NAG	Е	1203	5	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
21	А	703	9Z9	C11-C08	-2.25	1.52	1.56
21	А	702	9Z9	C11-C08	-2.19	1.52	1.56
21	А	704	9Z9	C11-C08	-2.18	1.52	1.56

The worst 5 of 35 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
21	А	704	9Z9	C02-C06-C07	-4.41	107.85	114.38
21	А	702	9Z9	C02-C06-C07	-4.40	107.87	114.38
21	А	703	9Z9	C02-C06-C07	-4.36	107.93	114.38
21	А	703	9Z9	C21-C22-C23	-3.45	109.51	113.88
21	А	704	9Z9	C21-C22-C23	-3.43	109.55	113.88

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
22	G	903	NAG	C4-C5-C6-O6
22	G	901	NAG	O5-C5-C6-O6
22	G	903	NAG	O5-C5-C6-O6
22	G	902	NAG	O5-C5-C6-O6
22	G	901	NAG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	А	703	9Z9	9	0
22	Е	1204	NAG	1	0
22	G	903	NAG	1	0
22	Е	1202	NAG	1	0
22	Н	1001	NAG	1	0
22	F	1201	NAG	2	0
21	А	704	9Z9	6	0
22	G	901	NAG	1	0
22	G	902	NAG	1	0
21	А	702	9Z9	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









# 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-31076. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

# 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



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

## 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200  $\,$ 

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

## 6.3 Largest variance slices (i)

#### 6.3.1 Primary map



X Index: 235

Y Index: 218

Z Index: 260

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

## 6.4 Orthogonal surface views (i)

#### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



# 6.5 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 295  $\rm nm^3;$  this corresponds to an approximate mass of 266 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 0.345  $\rm \AA^{-1}$ 



# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31076 and PDB model 7EEB. Per-residue inclusion information can be found in section 3 on page 12.

# 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.4 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 (0.4).



## 9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 67% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6736	0.4260
А	0.6043	0.4150
В	0.4950	0.3700
С	0.5532	0.3920
D	0.6311	0.4380
Е	0.8544	0.5060
F	0.8964	0.5400
G	0.8252	0.4800
Н	0.8444	0.5020
Ι	0.0070	0.0540
J	0.1335	0.1840
K	0.0042	0.0140
L	0.0451	0.1190
М	0.5043	0.3680
N	0.3571	0.2590
0	0.7590	0.4420
Р	0.6429	0.4570
Q	0.9231	0.5490
R	0.8205	0.5000
S	0.8571	0.5240
Т	0.6429	0.4020
U	0.6154	0.3200
V	0.6429	0.4160
W	0.6667	0.4570
X	0.8571	0.4790
Y	0.6721	0.4120
Z	0.8675	0.4550
a	0.5000	0.3700
b	0.4615	0.2670
С	0.7705	0.4710
d	0.0000	0.0460

