

#### Sep 16, 2024 - 09:47 pm BST

PDB ID	:	80LB			
EMDB ID	:	EMD-16954			
Title	:	SA11 Rotavirus Non-tripsinized Triple Layered Particle			
Authors	:	Asensio-Cob, D.; Perez-Mata, C.; Gomez-Blanco, J.; Vargas, J.; Rodriguez,			
		J.M.; Luque, D.			
Deposited on	:	2023-03-30			
Resolution	:	3.40  Å(reported)			
This is a Full wwPDB EM Validation 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.dev112
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

# 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 3.40 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)	${f EM} {f structures} \ (\#{f Entries})$
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	882	88%	11%
1	В	882	90%	• 9%
2	с	326	84%	16%
2	d	326	79%	21%
2	е	326	83%	17%
2	f	326	84%	16%
2	g	326	6% 85%	15%
2	h	326		15%
2	i	326	6% 84%	16%



Mol	Chain	Length	Quality of chain	
2	j	326	83%	17%
2	k	326	5% 84%	• 16%
2	1	326	<mark>6%</mark> 84%	• 15%
2	m	326	80%	20%
2	n	326	85%	15%
2	0	326	5%	20%
3	С	397	13%	
3	D	397	11%	
3	Е	397	12%	
3	F	397	13%	
3	G	397	14%	
3	Н	397	99%	·
3	Ι	397	15%	
3	J	397	13%	
3	Κ	397	12%	
3	L	397	14%	
3	М	397	12%	
3	Ν	397	14%	
3	О	397	12%	



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 82097 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 Inner capsid protein VP2.

Mol	Chain	Residues		Α	toms			AltConf	Trace
1	А	781	Total 6377	C 4051	N 1100	O 1189	${ m S}\ 37$	0	0
1	В	800	Total 6540	C 4155	N 1126	O 1222	S 37	0	0

• Molecule 2 is a protein called Outer capsid glycoprotein VP7.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	С	274	Total         C         N         O         S           2167         1377         342         432         16	0	0
2	d	258	Total         C         N         O         S           2039         1295         320         408         16	0	0
2	е	270	Total         C         N         O         S           2141         1361         339         425         16	0	0
2	f	275	Total         C         N         O         S           2181         1386         346         433         16	0	0
2	g	276	Total         C         N         O         S           2185         1388         347         434         16	0	0
2	h	277	Total         C         N         O         S           2190         1391         348         435         16	0	0
2	i	273	Total         C         N         O         S           2163         1375         341         431         16	0	0
2	j	270	Total         C         N         O         S           2141         1361         339         425         16	0	0
2	k	275	Total         C         N         O         S           2181         1386         346         433         16	0	0
2	1	276	Total         C         N         O         S           2190         1391         348         435         16	0	0
2	m	260	Total         C         N         O         S           2053         1304         323         410         16	0	0
2	n	277	Total         C         N         O         S           2190         1391         348         435         16	0	0
2	О	261	Total         C         N         O         S           2059         1307         324         412         16	0	0



Mol	Chain	Residues		At	oms			AltConf	Trace
9	C	207	Total	С	Ν	0	S	0	0
3	U	- 397	3163	2007	550	592	14	0	0
9	П	207	Total	С	Ν	0	S	0	0
3	D	- 397	3163	2007	550	592	14	0	0
3	F	307	Total	С	Ν	0	S	0	0
5	Ľ	591	3163	2007	550	592	14	0	0
3	F	307	Total	С	Ν	0	S	0	0
5	Ľ	091	3163	2007	550	592	14	0	0
3	C	307	Total	С	Ν	Ο	$\mathbf{S}$	0	0
5	G	091	3163	2007	550	592	14	0	0
3	н	307	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0
5	11	091	3163	2007	550	592	14	0	0
3	Т	307	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0
0	1	001	3163	2007	550	592	14	0	0
3	т	307	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0
0	5	591	3163	2007	550	592	14	0	0
3	K	397	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0
0	11	001	3163	2007	550	592	14	0	0
3	T.	397	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0
		001	3163	2007	550	592	14	0	0
3	М	397	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0
0	111	001	3163	2007	550	592	14	0	0
3	Ν	397	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0
	11		3163	2007	550	592	14	0	
3	0	397	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0
		001	3163	2007	550	592	14		

• Molecule 3 is a protein called Intermediate capsid protein VP6.

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	с	2	Total Ca 2 2	0
4	d	2	Total Ca 2 2	0
4	е	2	Total Ca 2 2	0
4	f	2	Total Ca 2 2	0
4	g	2	Total Ca 2 2	0
4	h	2	Total Ca 2 2	0



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Mol	Chain	Residues	Atoms	AltConf
4	i	2	Total Ca 2 2	0
4	j	2	Total Ca 2 2	0
4	k	2	Total Ca 2 2	0
4	1	2	Total Ca 2 2	0
4	m	2	Total Ca 2 2	0
4	n	2	Total Ca 2 2	0
4	0	2	Total Ca 2 2	0

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms	AltConf
5	d	1	Total C N O	0
0	u	1	15  8  1  6	0
5	0	1	Total C N O	0
0	е	1	15  8  1  6	0
5	f	1	Total C N O	0
0	1	1	15  8  1  6	0
5	h	1	Total C N O	0
0	11	1	15  8  1  6	U



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
5	÷	1	Total C N O	0
5	J	1	15  8  1  6	0
5	l,	1	Total C N O	0
5	K	1	15  8  1  6	0
5	1	1	Total C N O	0
5	1	1	15  8  1  6	0
5	m	1	Total C N O	0
0	111	1	15  8  1  6	0
5	n	1	Total C N O	0
5 II	1	15  8  1  6	0	
F	0	1	Total C N O	0
5	0		15  8  1  6	

• Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
6	С	1	Total Zn 1 1	0
6	Н	1	Total Zn 1 1	0
6	Ι	1	Total Zn 1 1	0
6	L	1	Total Zn 1 1	0
6	Ο	1	Total Zn 1 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.

 $\bullet$  Molecule 1: Inner capsid protein VP2



# Q215 Q215 R225 R225 R236 A236 R268 A236 R269 A236 R263 A236 R263 A236 R264 A236 R264 A236 R264 A236 R264 A236 R264 A236 R264 A266 R264 A266 R265 A266 R266 A266 R267 A R267 A R266 A R267 A R266 A R267 A R268 A R268 A R275 A



A428 L431 A432 A432 T436 P440 6443 A461 A461	148/ 148/ 1493 1502 1512 1512	D5 26 S5 30 G5 34 G5 34 G5 34 D5 44 L5 48 L5 48 L5 48 L5 42 L5 48	M5 65 E5 76 K577 S598 S598 A622 A623 A623
A630 G637 S642 S642 S642 S645 K649 K649 A657 C669 L674 P675	VG76 R679 R679 R680 1683 E895 K700 K700	0704 1725 1725 1729 1737 1737 1737 1736 1737 1748 1748 1748 1748 1748	L763
• Moloculo 2: Outor consid	d glycoprotoin VP7		
Chain c:	84%	16%	
MET TYR GLY GLY GLU TLE GLU THR THR THR THR THR THR THR THR THR THR	ASN TILE TILE LUEU LUEU LUEU LUEU TLEU ASP ASP ASP TLE TLE TLE TLE TLE TLE TLE	PHE TILE TILE TILE TILE TILE TILE PRE PRE PRE PRE PRE PRE CS4 CS4 CS4	862 D64 T65 A66 Y67
•     • <td>d glycoprotein VP7</td> <td>D304 V324 ARC VAL</td> <td></td>	d glycoprotein VP7	D304 V324 ARC VAL	
Chain d:	79%	21%	
MET TYR GLY GLY GLY CLU TYR THR THR THR THR THR THR THR THR THR TH	TYR TYR TLE LLE LLEU LFU LFU TLE TLE MRC TLE TLE TLE TLE TLE TLE TLE TYR TYR	PHE TLE TLE TLE VAL TLE VAL FLC FLC ALA ALA ALA ALA ALA ALA ALA ALA ALA	ASN L57 862 M63
D64 d110 1124 S128 T178 D179 C232 C232	D267 R312 R313 R313 R313 R313 R313 R313 R313		
• Molecule 2: Outer capsio	d glycoprotein VP7		
Chain e:	83%	17%	•
MET TYR GLIY GLIU CLU CLU CLU CLU THR THR THR THR THR THR THR THR THR THR	TYR THE LECU LECU LECU LECU LECU LECU LECU THE MET MET MET THE THE THE THE THE THE	PHEU TILE TILE VAL TILE VAL LIEU PHE PHE PHE PHE CLAV ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	ASN 157 160 160
S62 M63 D64 T65 A66 E74 E74 C110 €110 S115 S115	D136 D136 C232 C232 C232 L252 L252 K312 K312 K312 K313 R313	► ► ► ► ► ► ► ► ► ► ► ► ► ► ► ► ► ► ►	
• Molecule 2: Outer capsio	d glycoprotein VP7		
Chain f:	84%	16%	



MET TYR GLY LLZ LLZ CLU CLU THR THR THR THR THR THR THR THR THR TLE TLE TLE	ASN TYR LLE LLE LLE LLE LLE LLE LLE MET ARG ARG ARG PHE PHE PHE	LLE LLE VAL LTE LEU PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO
165 A66 A89 C110 C110 L133 L133 D109	L100 A181 C232 C253 C253 E256 E256 E256 E256 E256 E256 E256 E256	K312 N326
• Molecule 2: Outer caps	id glycoprotein VP7	
Chain g:	85%	15%
MET TYR GLY CLZ CLZ TYR THR THR THR THR THR THR THR THR THR TH	ASN TYR TYR LLELE LLELE LLELE LLELE THR ASP ASP ASP ASP ASP TILE TLLE TLLE TLLE TLLE TLLE LLU	ILLE ILLE VAL ILLE ILEU SER PRO PRO PRO ARG AIA ARG AIA ARG AIA ARG AI3 ARG AI3 ARG AI3 ARG AI3 AI3 AI3 AI3 AI3 AI3 AI3 AI3 AI3 AI3
L133 A156 A156 C191 V218 V218 V218 C292 C232 C	L271 4 T276 4 E282 4 B304 4 S319 4 V326	
• Molecule 2: Outer caps	id glycoprotein VP7	
Chain h:	85%	15%
MET TYR GLY CLY CLU CLU THR THR THR THR THR THR THR THR THR THR	ASN TYR TILE LLEU LLEU LLEU LLEU LLEU MET ARG ARC TLE TLE TLE TLE TLE TLE TLE TLE TLE TLE	LILE ILLE VAL LEU VAL LEU SER PHE PHE LEU ASO ASO ASO ASO ASO ASO ASO ASO ASO ASO
I124 + S128 + D136 + C232 + C232 + C232 + K312 + K312 + K313 +	N326	
• Molecule 2: Outer caps	id glycoprotein VP7	
Chain i:	84%	16%
MET MET GIV CILZ CILZ CILZ CILZ VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL	ASN TYR ASN LUE LUE LUE LVS SER SER ARG ARG TTR ARG TTR TTR TTR TTR TTR TTR TTR TTR TTR	LLE TLE VAL LEU SER PHE PHE PHE CLEU VSS CS4 M63 M63 M63 M63 M63 M63 M63
E74 L77 L77 A89 A90 A90 A90 C110 C110 C114 C1124 S123	L133 ← D136 ← C232 ← T241 ← T241 ← R324 AR5 ← VAL	
• Molecule 2: Outer caps	id glycoprotein VP7	
Chain j:	83%	17%
MET 1112 1112 1112 1112 1112 1114 1114 111	ASN TYR LLE LLE LLE LLE LLE LLE MET ARG ARG TYR ARG TYR TYR PHE	LLE VAL VAL LEU VAL LEU PRO PRO PRO ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG



T65           A66           E74           E74           C110           C110           D136           T200	2231 1269 1304 ♦ 8313 8314 ♦	
• Molecule 2: Outer cap	sid glycoprotein VP7	
Chain k:	84%	• 16%
MET TYR GLY GLY TLE GLU THR THR THR THR THR THR THR THR THR THR	LEU ASN TYR TLEU LEU LEU LEU LEU ARF PHE TTR ARF THR ARF TTR ARF TTR ARF THR ARF THR ARF	ILE ILE VAL LEU LEU SER SER SER ARG GIA MSC GIA D64 GII0 O64 CIA CIA CIA CIA CIA CIA CIA CIA CIA CIA
L133 D136 L147 L148 A156 A156 C191 E216	1226 ♦ D267 ♦ D267 ♦ D267 ♦ D304 ♦	
• Molecule 2: Outer cap	sid glycoprotein VP7	
Chain l:	84%	• 15%
MET TYR GLY GLY GLU TYR THR THR THR THR THR THR THR THR THR TH	LEU ASN TYR TUE LEU LEU LEU LEU MET ARR ARP PHE LEU TYR TYR TYR TYR TYR TYR TYR TYR TYR TYR	TLE TLE VALE FRO FRO FRO FRO FRO FRO FRO FRO FRO FRO
E74	C232 C232 C232 C232 C232 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3	
• Molecule 2: Outer cap	sid glycoprotein VP7	
Chain m:	80%	20%
MET TYR GLY GLY TLE GLU THR THR THR THR THR THR THR THR THR THR	LEU ASN TYR TILE LEU LEU LEU LEU ARG ARG TILE TILE TILE TILE TYR ARG FHE TUE TUE TUE TYR	ILE ILE VAL LEU VAL LEU SER ASN ASN CIN GSA CSA CSA CSA CSA CSA CSA CSA CSA CSA C
A90 G110 S115 S128 S128 L133 A156	E216 E216 D231 C232 SER SER A23 A23 A23 A23 A23 A23 A23 A24 A12 A12 A12 A12 A12 A12 A12 A12 A12 A12	
• Molecule 2: Outer cap	sid glycoprotein VP7	
Chain n:	85%	15%
MET 1778 1778 11.16 11.16 11.16 11.16 11.16 11.16 11.16 11.16 11.16 11.16 11.16 11.16 11.16 11.16	LLEU ASN TYFR TYFR LLEU LLYS SEER TYFR MET MET MET MET MET MET TLE TLE TTE TTE TTE PHE	ILE ILE VAL ILEU VAL ILEU SER PHE PHE IEU ASO ASO ASO ASO ASO ASO ASO ASO ASO ASO



• Molecule 2: Outer capsid glycoprotein VP7



Chain o:	80%	20%	
MET TYR GLY ILE GLU TYR THR THR VAL	LEU LEU LEU LEU LEU LEU LEU LEU LEU ASN ASN LEU LEU LEU NET TYR ASN ASN ASN LEU LEU TYR ASN ASN TYR ASN TYR ASN TYR ASN TILE LEU LEU LEU LEU LEU LEU LEU LEU LEU L	PRO PHE LEU ALA GLN ASN TYR CS4	T60 1664 A66
E74 A90 A10 G110	1124 1133 1133 1133 1133 1133 1133 1133 1133 1234		
• Molecule	3: Intermediate capsid protein VP6		
Chain C:	13%		I
M1 D2 V3 S6 L7 L7	LIU K17 L18 C21 C21 C21 C21 C21 C21 C21 C21 C22 C21 C22 C33 C43 C43 C43 C43 C43 C43 C43 C43 C43	S115 K118 K123 K123	E137 E137 N140 N143 L157 C197 A198 A198 V217
1224 1238 1238 A241 D242	1253 ← 1253 ← 1253 ← 1255 1253 ← 1255 1255 1255 1252 12307 ← 12307 ← 12307 ← 12307 ← 12307 ← 12307 ← 11391 ← 1391		
• Molecule	3: Intermediate capsid protein VP6		
Chain D:	11%		
M1 D2 V3 S8 S8 K9	110 113 118 118 118 118 118 118 118	N143	A198 1205 V217 V217 E230 E230 P256 P256
L1265	N346 1371 1387 K397 K397		
• Molecule	3: Intermediate capsid protein VP6		
Chain E:	12%		1
MI L7 D13	D29 N35 N35 A2 A2 C43 C43 C43 C43 C43 C43 C43 C43 C43 C43	1157 11	A241 A241 C243 F249 F266 F263 F263 R266
D286 N299 V304	N310 N310 N345 N345 V349 V349 V349 V388 V388 V388 V388 V388 V388 V388 V395 K397		
• Molecule	3: Intermediate capsid protein VP6		
Chain F:	13%		
M1 L7 D13 A14	N14 228 130 131 131 135 138 138 138 138 138 138 138 138 138 138	K118 1122 K123 K123 E137	N1440 N1440 N1443 N1443 N1443 N1443 N1443 N1448 N1448 N1498 N1498 N2417 N2417 N241 N241 N241 N241 N241 N241 N241 N241
	PROTEIN DATA BANK		



• Molecule 3: Intermediate capsid protein VP6









# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	10815	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	42	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II $(4k \ge 4k)$	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	1072.0, 1072.0, 1072.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: CA, ZN, NAG

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 Bond ang		ond angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.36	0/6494	0.62	1/8806~(0.0%)
1	В	0.37	0/6661	0.63	1/9033~(0.0%)
2	с	0.34	0/2213	0.60	0/3023
2	d	0.35	0/2081	0.63	0/2844
2	е	0.35	0/2186	0.60	0/2986
2	f	0.33	0/2227	0.60	0/3042
2	g	0.32	0/2231	0.58	0/3047
2	h	0.33	0/2236	0.59	0/3054
2	i	0.35	0/2209	0.61	0/3018
2	j	0.37	0/2186	0.64	0/2986
2	k	0.36	0/2227	0.60	0/3042
2	1	0.35	0/2236	0.64	0/3054
2	m	0.33	0/2095	0.61	0/2863
2	n	0.34	0/2236	0.60	1/3054~(0.0%)
2	0	0.32	0/2101	0.60	0/2871
3	С	0.32	0/3234	0.53	0/4402
3	D	0.32	0/3234	0.54	0/4402
3	Е	0.32	0/3234	0.54	0/4402
3	F	0.32	0/3234	0.54	0/4402
3	G	0.32	0/3234	0.54	0/4402
3	Н	0.33	0/3234	0.55	0/4402
3	Ι	0.32	0/3234	0.54	0/4402
3	J	0.32	0/3234	0.54	0/4402
3	Κ	0.32	0/3234	0.54	0/4402
3	L	0.32	0/3234	0.54	0/4402
3	М	0.32	0/3234	0.54	0/4402
3	N	0.32	0/3234	0.54	0/4402
3	0	0.32	0/3234	0.54	0/4402
All	All	0.34	0/83661	0.58	3/113949~(0.0%)

There are no bond length outliers.



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	В	669	ASP	CB-CG-OD1	5.80	123.52	118.30
1	А	810	ASP	CB-CG-OD1	5.18	122.97	118.30
2	n	165	CYS	C-N-CA	5.03	134.28	121.70

All (3) bond angle outliers are listed below:

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	ntiles
1	А	779/882~(88%)	728 (94%)	50~(6%)	1 (0%)	48	78
1	В	798/882~(90%)	753 (94%)	42~(5%)	3~(0%)	30	60
2	с	272/326~(83%)	251 (92%)	21 (8%)	0	100	100
2	d	256/326~(78%)	243~(95%)	13~(5%)	0	100	100
2	е	268/326~(82%)	251 (94%)	17~(6%)	0	100	100
2	f	273/326~(84%)	252~(92%)	21 (8%)	0	100	100
2	g	274/326~(84%)	264 (96%)	10 (4%)	0	100	100
2	h	275/326~(84%)	255~(93%)	20~(7%)	0	100	100
2	i	271/326~(83%)	253~(93%)	18 (7%)	0	100	100
2	j	268/326~(82%)	246 (92%)	22 (8%)	0	100	100
2	k	273/326~(84%)	251 (92%)	22 (8%)	0	100	100
2	1	$\overline{274/326}\ (84\%)$	252 (92%)	20 (7%)	2 (1%)	19	47



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	m	258/326~(79%)	242 (94%)	16~(6%)	0	100	100
2	n	275/326~(84%)	253~(92%)	22 (8%)	0	100	100
2	0	259/326~(79%)	238~(92%)	21 (8%)	0	100	100
3	С	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	D	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	Ε	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	F	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	G	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	Η	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	Ι	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	J	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	Κ	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	L	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	М	395/397~(100%)	380~(96%)	15~(4%)	0	100	100
3	Ν	395/397~(100%)	380 (96%)	15~(4%)	0	100	100
3	Ο	395/397~(100%)	380 (96%)	15 (4%)	0	100	100
All	All	10208/11163~(91%)	9672 (95%)	530 (5%)	6 (0%)	50	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	В	746	TYR
1	А	220	GLU
2	1	71	THR
1	В	747	ALA
1	В	809	ASN
2	1	314	SER

#### 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	Percentil	$\mathbf{es}$
1	А	714/812~(88%)	712 (100%)	2~(0%)	91 95	
1	В	732/812~(90%)	731 (100%)	1 (0%)	92 97	·
2	с	245/296~(83%)	245 (100%)	0	100 10	0
2	d	233/296~(79%)	233 (100%)	0	100 10	0
2	е	243/296~(82%)	243 (100%)	0	100 10	0
2	f	247/296~(83%)	247~(100%)	0	100 10	0
2	g	247/296~(83%)	247 (100%)	0	100 10	0
2	h	247/296~(83%)	247~(100%)	0	100 10	0
2	i	245/296~(83%)	245 (100%)	0	100 10	0
2	j	243/296~(82%)	242 (100%)	1 (0%)	89 93	
2	k	247/296~(83%)	245~(99%)	2(1%)	79 87	ſ
2	1	248/296~(84%)	248 (100%)	0	100 10	0
2	m	234/296~(79%)	234 (100%)	0	100 10	0
2	n	247/296~(83%)	247 (100%)	0	100 10	0
2	О	235/296~(79%)	235~(100%)	0	100 10	0
3	С	351/351~(100%)	351~(100%)	0	100 10	0
3	D	351/351~(100%)	351~(100%)	0	100 10	0
3	Ε	351/351~(100%)	351~(100%)	0	100 10	0
3	F	351/351~(100%)	351~(100%)	0	100 10	0
3	G	351/351~(100%)	351~(100%)	0	100 10	0
3	Η	351/351~(100%)	348~(99%)	3~(1%)	75 86	
3	Ι	351/351~(100%)	351 (100%)	0	100 10	0
3	J	351/351~(100%)	351 (100%)	0	100 10	0
3	Κ	351/351~(100%)	351 (100%)	0	100 10	0
3	L	351/351~(100%)	351 (100%)	0	100 10	0
3	М	351/351~(100%)	351 (100%)	0	100 10	0
3	Ν	351/351~(100%)	351 (100%)	0	100 10	0
3	Ο	351/351~(100%)	351 (100%)	0	100 10	0
All	All	$91\overline{70/10035}\ (91\%)$	9161 (100%)	9 (0%)	92 97	

All (9) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	218	GLU
1	А	220	GLU
1	В	225	ARG
2	j	75	THR
2	k	147	THR
2	k	148	LEU
3	Н	65	LEU
3	Н	68	THR
3	Н	69	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	248	HIS
1	А	269	ASN
1	А	307	GLN
1	А	391	GLN
1	А	478	ASN
1	А	484	GLN
1	А	492	ASN
1	А	493	GLN
1	А	540	ASN
1	А	569	HIS
1	А	869	ASN
1	В	89	GLN
1	В	235	GLN
1	В	242	ASN
1	В	248	HIS
1	В	252	HIS
1	В	285	ASN
1	В	307	GLN
1	В	467	ASN
1	В	475	HIS
1	В	506	ASN
1	В	555	ASN
1	В	637	GLN
1	В	748	GLN
1	В	755	ASN
1	В	869	ASN
2	с	199	ASN
2	с	294	GLN
2	с	308	GLN
2	d	166	ASN



Mol	Chain	Res	Type
2	d	294	GLN
2	е	182	ASN
2	е	294	GLN
2	f	199	ASN
2	g	138	ASN
2	g	149	GLN
2	g	294	GLN
2	i	182	ASN
2	i	294	GLN
2	k	138	ASN
2	k	182	ASN
2	k	235	HIS
2	1	161	ASN
2	1	182	ASN
2	1	280	GLN
2	1	294	GLN
2	m	182	ASN
2	m	305	GLN
2	m	308	GLN
2	n	52	ASN
2	n	182	ASN
2	n	235	HIS
2	n	294	GLN
2	n	305	GLN
2	0	161	ASN
2	0	177	GLN
3	С	42	ASN
3	С	94	ASN
3	С	207	GLN
3	С	210	HIS
3	С	312	GLN
3	С	381	ASN
3	D	42	ASN
3	D	94	ASN
3	D	207	GLN
3	D	210	HIS
3	D	312	GLN
3	D	381	ASN
3	E	42	ASN
3	E	94	ASN
3	Ε	207	GLN
3	E	210	HIS



Mol	Chain	Res	Type
3	Е	239	ASN
3	Е	312	GLN
3	Е	381	ASN
3	F	42	ASN
3	F	94	ASN
3	F	207	GLN
3	F	210	HIS
3	F	239	ASN
3	F	312	GLN
3	F	381	ASN
3	G	42	ASN
3	G	94	ASN
3	G	207	GLN
3	G	210	HIS
3	G	239	ASN
3	G	312	GLN
3	G	381	ASN
3	Н	42	ASN
3	Н	83	ASN
3	Н	94	ASN
3	Н	207	GLN
3	Н	210	HIS
3	Н	312	GLN
3	Н	381	ASN
3	Ι	32	GLN
3	Ι	36	GLN
3	Ι	42	ASN
3	Ι	94	ASN
3	Ι	207	GLN
3	Ι	210	HIS
3	Ι	239	ASN
3	Ι	312	GLN
3	Ι	381	ASN
3	J	42	ASN
3	J	94	ASN
3	J	207	GLN
3	J	210	HIS
3	J	312	GLN
3	J	381	ASN
3	K	42	ASN
3	K	94	ASN
3	K	207	GLN



Mol	Chain	Res	Type
3	K	210	HIS
3	K	312	GLN
3	K	381	ASN
3	L	42	ASN
3	L	83	ASN
3	L	94	ASN
3	L	207	GLN
3	L	210	HIS
3	L	310	ASN
3	L	312	GLN
3	L	381	ASN
3	М	42	ASN
3	М	83	ASN
3	М	94	ASN
3	М	207	GLN
3	М	310	ASN
3	М	312	GLN
3	М	381	ASN
3	Ν	42	ASN
3	Ν	94	ASN
3	Ν	207	GLN
3	Ν	210	HIS
3	Ν	299	ASN
3	N	312	GLN
3	N	381	ASN
3	0	36	GLN
3	0	42	ASN
3	0	94	ASN
3	0	207	GLN
3	0	210	HIS
3	0	239	ASN
3	0	312	GLN
3	0	381	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 oligosaccharides in this entry.

# 5.6 Ligand geometry (i)

Of 41 ligands modelled in this entry, 31 are monoatomic - leaving 10 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	Tuno	Chain	Dog	Link	Bond lengths			Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	h	401	-	15,15,15	0.45	0	21,21,21	0.85	0
5	NAG	n	401	-	15,15,15	0.42	0	21,21,21	0.57	0
5	NAG	d	401	-	15,15,15	0.55	0	21,21,21	1.31	3 (14%)
5	NAG	е	401	-	15,15,15	0.37	0	21,21,21	1.04	3 (14%)
5	NAG	f	401	2	15,15,15	0.48	0	21,21,21	0.77	0
5	NAG	1	401	-	15,15,15	0.49	0	21,21,21	1.29	4 (19%)
5	NAG	k	401	-	15,15,15	0.50	0	21,21,21	0.99	1 (4%)
5	NAG	j	401	-	15,15,15	0.51	0	21,21,21	1.23	3 (14%)
5	NAG	0	401	-	15,15,15	0.41	0	21,21,21	0.64	0
5	NAG	m	401	2	15,15,15	0.51	0	21,21,21	0.76	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
5	NAG	h	401	-	-	4/6/26/26	0/1/1/1
5	NAG	n	401	-	-	2/6/26/26	0/1/1/1
5	NAG	d	401	-	-	3/6/26/26	0/1/1/1
5	NAG	е	401	-	-	2/6/26/26	0/1/1/1
5	NAG	f	401	2	-	5/6/26/26	0/1/1/1
5	NAG	1	401	-	-	4/6/26/26	0/1/1/1
5	NAG	k	401	-	-	2/6/26/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	j	401	-	-	6/6/26/26	0/1/1/1
5	NAG	0	401	-	-	4/6/26/26	0/1/1/1
5	NAG	m	401	2	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	d	401	NAG	O5-C1-C2	3.20	112.73	109.52
5	d	401	NAG	C1-C2-N2	-2.82	107.46	110.73
5	1	401	NAG	O5-C5-C6	2.66	113.05	106.44
5	j	401	NAG	C3-C4-C5	-2.50	105.79	110.24
5	j	401	NAG	C1-C2-C3	2.48	113.93	110.54
5	d	401	NAG	C1-C2-C3	2.42	113.84	110.54
5	l	401	NAG	C3-C4-C5	-2.39	105.98	110.24
5	k	401	NAG	O5-C5-C4	2.23	113.75	109.69
5	l	401	NAG	O5-C1-C2	2.21	111.73	109.52
5	е	401	NAG	O5-C5-C6	2.20	111.91	106.44
5	е	401	NAG	C3-C4-C5	-2.08	106.53	110.24
5	l	401	NAG	C1-C2-C3	2.05	113.34	110.54
5	е	401	NAG	C1-O5-C5	-2.04	109.81	113.66
5	j	401	NAG	O5-C5-C6	2.03	111.47	106.44

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	d	401	NAG	C1-C2-N2-C7
5	d	401	NAG	C8-C7-N2-C2
5	d	401	NAG	O7-C7-N2-C2
5	f	401	NAG	C3-C2-N2-C7
5	f	401	NAG	C8-C7-N2-C2
5	f	401	NAG	O7-C7-N2-C2
5	h	401	NAG	C1-C2-N2-C7
5	h	401	NAG	C8-C7-N2-C2
5	h	401	NAG	O7-C7-N2-C2
5	j	401	NAG	C1-C2-N2-C7
5	j	401	NAG	C8-C7-N2-C2
5	j	401	NAG	O7-C7-N2-C2
5	n	401	NAG	C8-C7-N2-C2
5	n	401	NAG	O7-C7-N2-C2



Mol	Chain	Res	Type	Atoms
5	0	401	NAG	C1-C2-N2-C7
5	0	401	NAG	C3-C2-N2-C7
5	0	401	NAG	C8-C7-N2-C2
5	0	401	NAG	O7-C7-N2-C2
5	1	401	NAG	C3-C2-N2-C7
5	е	401	NAG	C8-C7-N2-C2
5	е	401	NAG	O7-C7-N2-C2
5	j	401	NAG	O5-C5-C6-O6
5	1	401	NAG	C4-C5-C6-O6
5	k	401	NAG	C4-C5-C6-O6
5	1	401	NAG	O5-C5-C6-O6
5	f	401	NAG	O5-C5-C6-O6
5	j	401	NAG	C4-C5-C6-O6
5	j	401	NAG	C3-C2-N2-C7
5	1	401	NAG	C1-C2-N2-C7
5	k	401	NAG	O5-C5-C6-O6
5	f	401	NAG	C1-C2-N2-C7
5	h	401	NAG	O5-C5-C6-O6

Continued from previous page...

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-16954. 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: 400





Z Index: 400

#### 6.2.2 Raw map



X Index: 400

Y Index: 400

Z Index: 400

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: 380





Z Index: 380

#### 6.3.2 Raw map



X Index: 304

Y Index: 304



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 0.006. 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  $89021 \text{ nm}^3$ ; this corresponds to an approximate mass of 80415 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 0.294  $\rm \AA^{-1}$ 



# 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 0.294  $\mathrm{\AA^{-1}}$ 



# 8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estim	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit		
Reported by author	3.40	-	-		
Author-provided FSC curve	3.54	3.90	3.56		
Unmasked-calculated*	3.53	3.89	3.56		

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16954 and PDB model 80LB. Per-residue inclusion information can be found in section 3 on page 8.

## 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 0.006 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 (0.006).



## 9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 72% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.0590
А	0.6810	0.0430
В	0.6700	0.0470
С	0.6880	0.0470
D	0.7090	0.0570
Ε	0.6980	0.0580
F	0.6830	0.0610
G	0.6790	0.0440
Н	0.6880	0.0500
Ι	0.6850	0.0590
J	0.6910	0.0590
Κ	0.6980	0.0510
L	0.6920	0.0620
М	0.6970	0.0560
Ν	0.6980	0.0620
0	0.7030	0.0610
с	0.7800	0.0730
d	0.7930	0.0690
е	0.7780	0.0690
f	0.7770	0.0680
g	0.7770	0.0650
h	0.7750	0.0620
i	0.7790	0.0660
j	0.7940	0.0820
k	0.7790	0.0680
1	0.7670	0.0520
m	0.7900	0.0730
n	0.7880	0.0690
0	0.7930	0.0740

