

May 27, 2025 – 02:33 pm BST

PDB ID	:	$9HL6 / pdb_00009hl6$
EMDB ID	:	EMD-52245
Title	:	TRPML1 in complex with compound 4a
Authors	:	Reeks, J.; Mahajan, P.; Clark, M.; Cowan, S.R.; Di Daniel, E.; Earl, C.P.;
		Fisher, S.; Holvey, R.S.; Jackson, S.M.; Lloyd-Evans, E.; Morgillo, C.M.;
		Mortenson, P.N.; O'Reilly, M.; Richardson, C.J.; Schopf, P.; Tams, D.M.;
		Waller-Evans, H.; Ward, S.E.; Whibley, S.; Williams, P.A.; Johnson, C.N.
Deposited on	:	2024-12-04
Resolution	:	2.20 Å(reported)
Based on initial model	:	

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.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	FAILED
buster-report	:	1.1.7 (2018)
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)	:	2.43.1

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 2.20 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 15884 atoms, of which 124 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.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	Λ	457	Total	С	Ν	0	S	2	0
1	Л	407	3705	2432	614	634	25	2	0
1	С	457	Total	С	Ν	0	S	2	0
	407	3705	2432	614	634	25	2	U	
1	Р	457	Total	С	Ν	0	S	2	0
1	D	407	3705	2432	614	634	25	2	0
1 D	457	Total	С	Ν	0	S	2	0	
	D	407	3705	2432	614	634	25		0

• Molecule 1 is a protein called Mucolipin-1.

There are 196 discrepancies between the n	nodelled and reference sequences:
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Chain	Residue	Modelled	Actual	Comment	Reference
А	-47	MET	-	initiating methionine	UNP Q9GZU1
А	-46	HIS	-	expression tag	UNP Q9GZU1
А	-45	HIS	-	expression tag	UNP Q9GZU1
А	-44	HIS	-	expression tag	UNP Q9GZU1
А	-43	HIS	-	expression tag	UNP Q9GZU1
А	-42	HIS	-	expression tag	UNP Q9GZU1
А	-41	HIS	-	expression tag	UNP Q9GZU1
А	-40	HIS	-	expression tag	UNP Q9GZU1
А	-39	HIS	-	expression tag	UNP Q9GZU1
А	-38	GLY	-	expression tag	UNP Q9GZU1
А	-37	GLY	-	expression tag	UNP Q9GZU1
А	-36	SER	-	expression tag	UNP Q9GZU1
А	-35	ASP	-	expression tag	UNP Q9GZU1
А	-34	TYR	-	expression tag	UNP Q9GZU1
А	-33	LYS	-	expression tag	UNP Q9GZU1
А	-32	ASP	-	expression tag	UNP Q9GZU1
А	-31	HIS	-	expression tag	UNP Q9GZU1
А	-30	ASP	-	expression tag	UNP Q9GZU1
A	-29	GLY	-	expression tag	UNP Q9GZU1
A	-28	ASP	-	expression tag	UNP Q9GZU1
A	-27	TYR	-	expression tag	UNP Q9GZU1
A	-26	LYS	_	expression tag	UNP Q9GZU1



Chain	Residue	Modelled	Actual	Comment	Reference
А	-25	ASP	-	expression tag	UNP Q9GZU1
А	-24	HIS	-	expression tag	UNP Q9GZU1
А	-23	ASP	-	expression tag	UNP Q9GZU1
А	-22	ILE	-	expression tag	UNP Q9GZU1
А	-21	ASP	-	expression tag	UNP Q9GZU1
А	-20	TYR	-	expression tag	UNP Q9GZU1
А	-19	LYS	-	expression tag	UNP Q9GZU1
А	-18	ASP	-	expression tag	UNP Q9GZU1
А	-17	ASP	-	expression tag	UNP Q9GZU1
А	-16	ASP	-	expression tag	UNP Q9GZU1
А	-15	ASP	-	expression tag	UNP Q9GZU1
А	-14	LYS	-	expression tag	UNP Q9GZU1
А	-13	GLY	-	expression tag	UNP Q9GZU1
А	-12	GLY	-	expression tag	UNP Q9GZU1
А	-11	SER	-	expression tag	UNP Q9GZU1
А	-10	GLY	-	expression tag	UNP Q9GZU1
А	-9	GLY	-	expression tag	UNP Q9GZU1
А	-8	SER	-	expression tag	UNP Q9GZU1
А	-7	GLU	-	expression tag	UNP Q9GZU1
А	-6	ASN	-	expression tag	UNP Q9GZU1
А	-5	LEU	-	expression tag	UNP Q9GZU1
А	-4	TYR	-	expression tag	UNP Q9GZU1
А	-3	PHE	-	expression tag	UNP Q9GZU1
А	-2	GLN	-	expression tag	UNP Q9GZU1
А	-1	GLY	-	expression tag	UNP Q9GZU1
А	0	PRO	-	expression tag	UNP Q9GZU1
А	1	GLY	-	expression tag	UNP Q9GZU1
С	-47	MET	-	initiating methionine	UNP Q9GZU1
С	-46	HIS	-	expression tag	UNP Q9GZU1
С	-45	HIS	-	expression tag	UNP Q9GZU1
С	-44	HIS	-	expression tag	UNP Q9GZU1
C	-43	HIS	-	expression tag	UNP Q9GZU1
С	-42	HIS	-	expression tag	UNP Q9GZU1
С	-41	HIS	-	expression tag	UNP Q9GZU1
С	-40	HIS	-	expression tag	UNP Q9GZU1
С	-39	HIS	-	expression tag	UNP Q9GZU1
C	-38	GLY	-	expression tag	UNP Q9GZU1
С	-37	GLY	-	expression tag	UNP Q9GZU1
C	-36	SER	-	expression tag	UNP Q9GZU1
C	-35	ASP	-	expression tag	UNP Q9GZU1
C	-34	TYR	-	expression tag	UNP $Q9\overline{GZU1}$
С	-33	LYS	-	expression tag	UNP Q9GZU1



Chain	Residue	Modelled	Actual	Comment	Reference
С	-32	ASP	-	expression tag	UNP Q9GZU1
С	-31	HIS	-	expression tag	UNP Q9GZU1
С	-30	ASP	-	expression tag	UNP Q9GZU1
С	-29	GLY	-	expression tag	UNP Q9GZU1
С	-28	ASP	-	expression tag	UNP Q9GZU1
С	-27	TYR	-	expression tag	UNP Q9GZU1
С	-26	LYS	-	expression tag	UNP Q9GZU1
С	-25	ASP	-	expression tag	UNP Q9GZU1
С	-24	HIS	-	expression tag	UNP Q9GZU1
С	-23	ASP	-	expression tag	UNP Q9GZU1
С	-22	ILE	-	expression tag	UNP Q9GZU1
С	-21	ASP	-	expression tag	UNP Q9GZU1
С	-20	TYR	-	expression tag	UNP Q9GZU1
С	-19	LYS	-	expression tag	UNP Q9GZU1
С	-18	ASP	-	expression tag	UNP Q9GZU1
С	-17	ASP	-	expression tag	UNP Q9GZU1
С	-16	ASP	-	expression tag	UNP Q9GZU1
С	-15	ASP	-	expression tag	UNP Q9GZU1
С	-14	LYS	-	expression tag	UNP Q9GZU1
С	-13	GLY	-	expression tag	UNP Q9GZU1
С	-12	GLY	-	expression tag	UNP Q9GZU1
С	-11	SER	-	expression tag	UNP Q9GZU1
С	-10	GLY	-	expression tag	UNP Q9GZU1
С	-9	GLY	-	expression tag	UNP Q9GZU1
С	-8	SER	-	expression tag	UNP Q9GZU1
С	-7	GLU	-	expression tag	UNP Q9GZU1
С	-6	ASN	-	expression tag	UNP Q9GZU1
С	-5	LEU	-	expression tag	UNP Q9GZU1
С	-4	TYR	-	expression tag	UNP Q9GZU1
С	-3	PHE	-	expression tag	UNP Q9GZU1
С	-2	GLN	-	expression tag	UNP Q9GZU1
С	-1	GLY	-	expression tag	UNP Q9GZU1
С	0	PRO	-	expression tag	UNP Q9GZU1
С	1	GLY	-	expression tag	UNP Q9GZU1
В	-47	MET	-	initiating methionine	UNP Q9GZU1
В	-46	HIS	-	expression tag	UNP Q9GZU1
В	-45	HIS	-	expression tag	UNP Q9GZU1
В	-44	HIS	-	expression tag	UNP Q9GZU1
В	-43	HIS	-	expression tag	UNP Q9GZU1
В	-42	HIS	-	expression tag	UNP Q9GZU1
В	-41	HIS	-	expression tag	UNP Q9GZU1
В	-40	HIS	-	expression tag	UNP Q9GZU1



Chain	Residue	Modelled	Actual	Comment	Reference
В	-39	HIS	-	expression tag	UNP Q9GZU1
В	-38	GLY	_	expression tag	UNP Q9GZU1
В	-37	GLY	-	expression tag	UNP Q9GZU1
В	-36	SER	-	expression tag	UNP Q9GZU1
В	-35	ASP	-	expression tag	UNP Q9GZU1
В	-34	TYR	-	expression tag	UNP Q9GZU1
В	-33	LYS	_	expression tag	UNP Q9GZU1
В	-32	ASP	-	expression tag	UNP Q9GZU1
В	-31	HIS	-	expression tag	UNP Q9GZU1
В	-30	ASP	-	expression tag	UNP Q9GZU1
В	-29	GLY	-	expression tag	UNP Q9GZU1
В	-28	ASP	-	expression tag	UNP Q9GZU1
В	-27	TYR	-	expression tag	UNP Q9GZU1
В	-26	LYS	-	expression tag	UNP Q9GZU1
В	-25	ASP	-	expression tag	UNP Q9GZU1
В	-24	HIS	-	expression tag	UNP Q9GZU1
В	-23	ASP	-	expression tag	UNP Q9GZU1
В	-22	ILE	-	expression tag	UNP Q9GZU1
В	-21	ASP	-	expression tag	UNP Q9GZU1
В	-20	TYR	-	expression tag	UNP Q9GZU1
В	-19	LYS	-	expression tag	UNP Q9GZU1
В	-18	ASP	-	expression tag	UNP Q9GZU1
В	-17	ASP	-	expression tag	UNP Q9GZU1
В	-16	ASP	-	expression tag	UNP Q9GZU1
В	-15	ASP	-	expression tag	UNP Q9GZU1
В	-14	LYS	-	expression tag	UNP Q9GZU1
В	-13	GLY	-	expression tag	UNP Q9GZU1
В	-12	GLY	-	expression tag	UNP Q9GZU1
В	-11	SER	-	expression tag	UNP Q9GZU1
В	-10	GLY	-	expression tag	UNP Q9GZU1
В	-9	GLY	-	expression tag	UNP Q9GZU1
В	-8	SER	-	expression tag	UNP Q9GZU1
В	-7	GLU	-	expression tag	UNP Q9GZU1
В	-6	ASN	-	expression tag	UNP Q9GZU1
В	-5	LEU	-	expression tag	UNP Q9GZU1
В	-4	TYR	-	expression tag	UNP Q9GZU1
В	-3	PHE	-	expression tag	UNP Q9GZU1
В	-2	GLN	-	expression tag	UNP Q9GZU1
В	-1	GLY	-	expression tag	UNP Q9GZU1
В	0	PRO	-	expression tag	UNP Q9GZU1
В	1	GLY	-	expression tag	UNP Q9GZU1
D	-47	MET	-	initiating methionine	UNP Q9GZU1



Chain	Residue	Modelled	Actual	Comment	Reference
D	-46	HIS	-	expression tag	UNP Q9GZU1
D	-45	HIS	-	expression tag	UNP Q9GZU1
D	-44	HIS	_	expression tag	UNP Q9GZU1
D	-43	HIS	-	expression tag	UNP Q9GZU1
D	-42	HIS	-	expression tag	UNP Q9GZU1
D	-41	HIS	-	expression tag	UNP Q9GZU1
D	-40	HIS	-	expression tag	UNP Q9GZU1
D	-39	HIS	-	expression tag	UNP Q9GZU1
D	-38	GLY	-	expression tag	UNP Q9GZU1
D	-37	GLY	-	expression tag	UNP Q9GZU1
D	-36	SER	-	expression tag	UNP Q9GZU1
D	-35	ASP	-	expression tag	UNP Q9GZU1
D	-34	TYR	-	expression tag	UNP Q9GZU1
D	-33	LYS	-	expression tag	UNP Q9GZU1
D	-32	ASP	-	expression tag	UNP Q9GZU1
D	-31	HIS	-	expression tag	UNP Q9GZU1
D	-30	ASP	-	expression tag	UNP Q9GZU1
D	-29	GLY	-	expression tag	UNP Q9GZU1
D	-28	ASP	_	expression tag	UNP Q9GZU1
D	-27	TYR	_	expression tag	UNP Q9GZU1
D	-26	LYS	-	expression tag	UNP Q9GZU1
D	-25	ASP	_	expression tag	UNP Q9GZU1
D	-24	HIS	-	expression tag	UNP Q9GZU1
D	-23	ASP	-	expression tag	UNP Q9GZU1
D	-22	ILE	-	expression tag	UNP Q9GZU1
D	-21	ASP	-	expression tag	UNP Q9GZU1
D	-20	TYR	-	expression tag	UNP Q9GZU1
D	-19	LYS	-	expression tag	UNP Q9GZU1
D	-18	ASP	-	expression tag	UNP Q9GZU1
D	-17	ASP	-	expression tag	UNP Q9GZU1
D	-16	ASP	-	expression tag	UNP Q9GZU1
D	-15	ASP	-	expression tag	UNP Q9GZU1
D	-14	LYS	-	expression tag	UNP Q9GZU1
D	-13	GLY	-	expression tag	UNP Q9GZU1
D	-12	GLY	-	expression tag	UNP Q9GZU1
D	-11	SER	-	expression tag	UNP Q9GZU1
D	-10	GLY	-	expression tag	UNP Q9GZU1
D	-9	GLY	-	expression tag	UNP Q9GZU1
D	-8	SER	-	expression tag	UNP Q9GZU1
D	-7	GLU	-	expression tag	UNP Q9GZU1
D	-6	ASN	-	expression tag	UNP Q9GZU1
D	-5	LEU	-	expression tag	UNP Q9GZU1



Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	TYR	-	expression tag	UNP Q9GZU1
D	-3	PHE	-	expression tag	UNP Q9GZU1
D	-2	GLN	-	expression tag	UNP Q9GZU1
D	-1	GLY	-	expression tag	UNP Q9GZU1
D	0	PRO	-	expression tag	UNP Q9GZU1
D	1	GLY	-	expression tag	UNP Q9GZU1

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



Mol	Chain	Residues	Atoms	AltConf	Trace
2	E	2	Total C N O	0	0
2	Ľ	2	28 16 2 10	0	0
2	F	9	Total C N O	0	0
2	Ľ	2	28 16 2 10	0	0
2	С	9	Total C N O	0	0
	G	2	28 16 2 10	0	0
9	Ц	9	Total C N O	0	0
	11	2	28 16 2 10	0	0

• Molecule 3 is PENTANE (CCD ID: LNK) (formula: C_5H_{12}).





Mol	Chain	Residues	Atoms	AltConf
3	А	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 5 & 5 \end{array}$	0
3	С	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 5 & 5 \end{array}$	0
3	В	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 5 & 5 \end{array}$	0
3	D	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 5 & 5 \end{array}$	0

• Molecule 4 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms	AltConf
4	А	1	Total C 8 8	0
4	А	1	Total C 8 8	0
4	С	1	Total C 8 8	0
4	С	1	Total C 8 8	0
4	В	1	Total C 8 8	0
4	В	1	Total C 8 8	0
4	D	1	Total C 8 8	0
4	D	1	Total C 8 8	0





Mol	Chain	Residues	Atoms	AltConf
5	А	1	Total C 16 16	0
5	А	1	Total C 16 16	0
5	С	1	Total C 16 16	0
5	В	1	Total C 16 16	0

• Molecule 6 is HEXANE (CCD ID: HEX) (formula: $\mathrm{C}_{6}\mathrm{H}_{14}).$





Mol	Chain	Residues	Atoms	AltConf
6	А	1	Total C 6 6	0
6	С	1	Total C 6 6	0
6	В	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 6 & 6 \end{array}$	0
6	D	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 6 & 6 \end{array}$	0

• Molecule 7 is (2R)-3-{[(S)-hydroxy{[(1S,2R,3R,4S,5S,6R)-2,4,6-trihydroxy-3,5-bis(phosphonooxy)cyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl dioctanoate (CCD ID: EUJ) (formula: $C_{25}H_{49}O_{19}P_3$).



Mol	Chain	Residues	Atoms				AltConf	
7	Λ	1	Total	С	Ο	Р	0	
· ·	Л	L	47	25	19	3	0	
7	С	1	Total	С	Ο	Р	0	
1		1	47	25	19	3	0	
7	D	1	Total	С	Ο	Р	0	
(D	L	47	25	19	3	0	
7	р	D 1		С	Ο	Р	0	
(D		47	25	19	3	0	

• Molecule 8 is 4-[[(3R)-3-[1-(4-chloranyl-2-fluoranyl-phenyl)piperidin-4-yl]-3-methyl-2H-indol-1-yl]sulfonyl]-N,N-dimethyl-benzenesulfonamide (CCD ID: A1IV1) (formula: $C_{28}H_{31}ClFN_3O_4S_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Atoms							AltConf	
0	8 A	Λ 1	1	Total	С	Cl	F	Η	Ν	Ο	S	0
0		1	70	28	1	1	31	3	4	2	0	
0	С	C 1	Total	С	Cl	F	Η	Ν	0	S	0	
0			70	28	1	1	31	3	4	2	0	
0	D	1	Total	С	Cl	F	Η	Ν	Ο	S	0	
0	8 B	1	70	28	1	1	31	3	4	2	0	
8 D	1	Total	С	Cl	F	Η	Ν	Ο	S	0		
		70	28	1	1	31	3	4	2	0		

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	AltConf
9	А	78	Total O 78 78	0
9	С	77	Total O 77 77	0
9	В	79	Total O 79 79	0
9	D	78	Total O 78 78	0

MolProbity failed to run properly - this section is therefore empty.



3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	327826	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 $(e^-/\text{\AA}^2)$	42.95	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.576	Depositor
Minimum map value	-1.311	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.437	Depositor
Map size (Å)	379.42902, 379.42902, 379.42902	wwPDB
Map dimensions	590, 590, 590	wwPDB
Map angles ($^{\circ}$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6431, 0.6431, 0.6431	Depositor



4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

8 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	Turne	Chain	Dec	Tiple	Bo	ond leng	ths	Bond angles			
INIOI	туре	Unam	nes	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	Е	1	1,2	14,14,15	0.75	0	17,19,21	1.80	3 (17%)	
2	NAG	Е	2	2	14,14,15	0.83	0	17,19,21	0.95	0	
2	NAG	F	1	1,2	14,14,15	0.74	0	17,19,21	1.82	3 (17%)	
2	NAG	F	2	2	14,14,15	0.82	0	17,19,21	0.95	0	
2	NAG	G	1	1,2	14,14,15	0.75	0	17,19,21	1.79	3 (17%)	
2	NAG	G	2	2	14,14,15	0.83	0	17,19,21	0.95	0	
2	NAG	Н	1	1,2	14,14,15	0.75	0	17,19,21	1.80	3 (17%)	
2	NAG	Н	2	2	14,14,15	0.83	0	17,19,21	0.95	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
2	NAG	Е	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Е	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Н	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Н	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	1	NAG	C1-O5-C5	5.29	119.36	112.19
2	Н	1	NAG	C1-O5-C5	5.21	119.25	112.19
2	Е	1	NAG	C1-O5-C5	5.20	119.24	112.19
2	G	1	NAG	C1-O5-C5	5.13	119.15	112.19
2	Н	1	NAG	C4-C3-C2	-2.97	106.67	111.02
2	Е	1	NAG	C4-C3-C2	-2.96	106.68	111.02
2	F	1	NAG	C4-C3-C2	-2.94	106.72	111.02
2	G	1	NAG	C4-C3-C2	-2.93	106.72	111.02
2	G	1	NAG	O4-C4-C5	2.23	114.83	109.30
2	F	1	NAG	O4-C4-C5	2.23	114.83	109.30
2	Н	1	NAG	O4-C4-C5	2.22	114.82	109.30
2	Е	1	NAG	O4-C4-C5	2.21	114.79	109.30



There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Е	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	Н	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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















4.6 Ligand geometry (i)

28 ligands 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).

Mol Type	Turne	Chain	Dec	Tink	Bo	ond leng	ths	Bond angles		
1VIOI	туре	Unain	nes	LIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OCT	D	602	-	7,7,7	0.24	0	$6,\!6,\!6$	0.18	0
5	R16	С	607	-	15,15,15	0.24	0	14,14,14	0.12	0



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEX	D	604	-	$5,\!5,\!5$	0.24	0	4,4,4	0.14	0
6	HEX	С	604	-	$5,\!5,\!5$	0.25	0	4,4,4	0.14	0
3	LNK	A	601	-	$4,\!4,\!4$	0.26	0	3, 3, 3	0.24	0
6	HEX	В	605	-	$5,\!5,\!5$	0.25	0	$4,\!4,\!4$	0.15	0
8	A1IV1	А	607	-	42,43,43	0.37	0	57,67,67	1.07	4 (7%)
3	LNK	С	601	-	4,4,4	0.26	0	3,3,3	0.24	0
4	OCT	В	603	-	7,7,7	0.24	0	6,6,6	0.18	0
8	A1IV1	С	606	-	42,43,43	0.37	0	57,67,67	1.07	4 (7%)
5	R16	А	608	-	$15,\!15,\!15$	0.24	0	14,14,14	0.12	0
3	LNK	D	601	-	4,4,4	0.27	0	3,3,3	0.25	0
4	OCT	А	602	-	7,7,7	0.24	0	$6,\!6,\!6$	0.18	0
5	R16	А	604	-	$15,\!15,\!15$	0.23	0	14,14,14	0.12	0
7	EUJ	В	606	-	47,47,47	0.47	0	61,65,65	0.46	0
4	OCT	В	604	-	7,7,7	0.23	0	$6,\!6,\!6$	0.17	0
4	OCT	А	603	-	7,7,7	0.24	0	$6,\!6,\!6$	0.17	0
4	OCT	С	603	-	7,7,7	0.24	0	$6,\!6,\!6$	0.17	0
7	EUJ	D	605	-	$47,\!47,\!47$	0.47	0	$61,\!65,\!65$	0.46	0
8	A1IV1	D	606	-	42,43,43	0.38	0	57,67,67	1.08	4 (7%)
7	EUJ	С	605	-	47,47,47	0.46	0	$61,\!65,\!65$	0.46	0
7	EUJ	А	606	-	47,47,47	0.47	0	$61,\!65,\!65$	0.46	0
8	A1IV1	В	607	-	42,43,43	0.38	0	57,67,67	1.08	4 (7%)
5	R16	В	601	-	$15,\!15,\!15$	0.24	0	14,14,14	0.12	0
3	LNK	В	602	-	4,4,4	0.27	0	$3,\!3,\!3$	0.24	0
4	OCT	D	603	-	7,7,7	0.24	0	6,6,6	0.16	0
6	HEX	А	605	-	5, 5, 5	0.24	0	4,4,4	0.14	0
4	OCT	C	602	-	7,7,7	0.24	0	$6,\!6,\!6$	0.18	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
4	OCT	D	602	-	-	1/5/5/5	-
5	R16	С	607	-	-	5/13/13/13	-
6	HEX	D	604	-	-	1/3/3/3	-
6	HEX	С	604	-	-	1/3/3/3	-
3	LNK	А	601	-	-	0/2/2/2	-
6	HEX	В	605	-	-	1/3/3/3	-
8	A1IV1	А	607	-	-	10/34/59/59	0/5/5/5
3	LNK	С	601	-	-	0/2/2/2	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OCT	В	603	-	-	2/5/5/5	-
8	A1IV1	С	606	-	-	10/34/59/59	0/5/5/5
5	R16	А	608	-	-	5/13/13/13	-
3	LNK	D	601	-	-	0/2/2/2	-
4	OCT	А	602	-	-	2/5/5/5	-
5	R16	А	604	-	-	5/13/13/13	-
7	EUJ	В	606	-	-	10/44/68/68	0/1/1/1
4	OCT	В	604	-	-	2/5/5/5	-
4	OCT	А	603	-	-	2/5/5/5	-
4	OCT	С	603	-	-	2/5/5/5	-
7	EUJ	D	605	-	-	10/44/68/68	0/1/1/1
8	A1IV1	D	606	-	-	10/34/59/59	0/5/5/5
7	EUJ	С	605	-	-	10/44/68/68	0/1/1/1
7	EUJ	А	606	-	-	10/44/68/68	0/1/1/1
8	A1IV1	В	607	-	-	10/34/59/59	0/5/5/5
5	R16	В	601	-	-	6/13/13/13	-
3	LNK	В	602	-	-	0/2/2/2	-
4	OCT	D	603	-	-	2/5/5/5	-
6	HEX	А	605	-	-	1/3/3/3	-
4	OCT	С	602	_	_	2/5/5/5	-

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	В	607	A1IV1	C10-S11-N14	-3.46	102.20	106.92
8	А	607	A1IV1	C10-S11-N14	-3.44	102.23	106.92
8	D	606	A1IV1	C10-S11-N14	-3.44	102.23	106.92
8	С	606	A1IV1	C10-S11-N14	-3.41	102.27	106.92
8	С	606	A1IV1	C28-C22-N21	2.94	123.96	120.47
8	А	607	A1IV1	C28-C22-N21	2.93	123.96	120.47
8	D	606	A1IV1	C28-C22-N21	2.90	123.92	120.47
8	В	607	A1IV1	C28-C22-N21	2.88	123.89	120.47
8	D	606	A1IV1	F29-C28-C22	2.56	120.75	118.42
8	С	606	A1IV1	F29-C28-C22	2.48	120.68	118.42
8	В	607	A1IV1	F29-C28-C22	2.48	120.68	118.42
8	А	607	A1IV1	F29-C28-C22	2.44	120.64	118.42
8	D	606	A1IV1	C25-C27-C28	2.16	119.07	117.48



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$				
8	А	607	A1IV1	C25-C27-C28	2.14	119.06	117.48				
8	В	607	A1IV1	C25-C27-C28	2.12	119.05	117.48				
8	С	606	A1IV1	C25-C27-C28	2.06	119.00	117.48				

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	А	606	EUJ	C2B-C1B-O3C-C3C
7	А	606	EUJ	O1B-C1B-O3C-C3C
7	С	605	EUJ	C2B-C1B-O3C-C3C
7	С	605	EUJ	O1B-C1B-O3C-C3C
7	В	606	EUJ	C2B-C1B-O3C-C3C
7	В	606	EUJ	O1B-C1B-O3C-C3C
7	D	605	EUJ	C2B-C1B-O3C-C3C
7	D	605	EUJ	O1B-C1B-O3C-C3C
8	А	607	A1IV1	C15-C16-C18-C31
8	А	607	A1IV1	C17-C16-C18-C19
8	А	607	A1IV1	C17-C16-C18-C31
8	А	607	A1IV1	C32-C16-C18-C19
8	А	607	A1IV1	C32-C16-C18-C31
8	А	607	A1IV1	C28-C22-N21-C30
8	С	606	A1IV1	C15-C16-C18-C31
8	С	606	A1IV1	C17-C16-C18-C19
8	С	606	A1IV1	C17-C16-C18-C31
8	С	606	A1IV1	C32-C16-C18-C19
8	С	606	A1IV1	C32-C16-C18-C31
8	С	606	A1IV1	C28-C22-N21-C30
8	В	607	A1IV1	C15-C16-C18-C31
8	В	607	A1IV1	C17-C16-C18-C19
8	В	607	A1IV1	C17-C16-C18-C31
8	В	607	A1IV1	C32-C16-C18-C19
8	В	607	A1IV1	C32-C16-C18-C31
8	В	607	A1IV1	C28-C22-N21-C30
8	D	606	A1IV1	C15-C16-C18-C31
8	D	606	A1IV1	C17-C16-C18-C19
8	D	606	A1IV1	C17-C16-C18-C31
8	D	606	A1IV1	C32-C16-C18-C19
8	D	606	A1IV1	C32-C16-C18-C31
8	D	606	A1IV1	C28-C22-N21-C30
7	А	606	EUJ	C1-O1-P1-O13
7	С	605	EUJ	C1-O1-P1-O13



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Mol	Chain	Res		Atoms
7	B	606	EU.I	C1-01-P1-013
7	D	605	EUI	C1-O1-P1-O13
4	A	603	OCT	C3-C4-C5-C6
4	C	603	OCT	C3-C4-C5-C6
4	B	604	OCT	C3 C4 C5 C6
4	D	603	OCT	C3-C4-C5-C6
7		606	EUI	C2-C1-O1-P1
7	A	606	EUI	C6-C1-O1-P1
7	C	605	EUI	C2-C1-O1-P1
7	C	605	EUI	C6-C1-O1-P1
7	B	606	EUI	C2 C1 O1 P1
7	B	606	EUJ EUI	C6 C1 O1 P1
7	D	605	EUI	C2 C1 O1 P1
7	D	605	FUI	C2-C1-O1-I I C6 C1 O1 P1
1 5	D B	601	D16	$\begin{array}{c} 0 - 0 - 0 - 1 - 1 \\ 0 - 0 - 0 - 1 \\ 0 - 0 - 1 \\$
5		604	D16	$\begin{array}{c} 0.01 \\ 0.02 \\ 0.03 \\ 0.02 \\ 0.02 \\ 0.02 \\ 0.02 \\ 0.04 \\ 0.$
5	A C	607	D16	C_{21} C_{22} C_{23} C_{24}
5		608	D16	$\begin{array}{c} \text{C31-C32-C33-C34} \\ \text{C31-C32-C32-C34} \\ \end{array}$
	A	600	$\frac{R10}{D16}$	C_{21} C_{22} C_{23} C_{24} C_{25}
	A	608	R10 D16	0.32 - 0.33 - 0.34 - 0.35
0 F		007 C04	R10	0.32 - 0.33 - 0.34 - 0.35
5	A	604 C01	RI0 D1C	C32-C33-C34-C35
5	В	601	RI0 D10	C32-C33-C34-C35
5	A	608	RI0	C37-C38-C39-C40
5	A	604	RI0	C37-C38-C39-C40
8	A	607	AIIVI	C23-C22-N21-C30
8	C	606	AIIVI	C23-C22-N21-C30
8	B	607	AIIVI	C23-C22-N21-C30
8	D	606	AllV1	C23-C22-N21-C30
5	В	601	R16	C37-C38-C39-C40
4	A	603	OCT	C1-C2-C3-C4
4		603	OCT	C1-C2-C3-C4
4	D	603	OCT D12	C1-C2-C3-C4
5	C	607	R16	C37-C38-C39-C40
4	В	604	OCT	C1-C2-C3-C4
5	A	604	R16	C28-C29-C30-C31
5	C	607	R16	C28-C29-C30-C31
5	A	608	R16	C28-C29-C30-C31
7	А	606	EUJ	C1-O1-P1-O11
7	С	605	EUJ	C1-O1-P1-O11
7	В	606	EUJ	C1-O1-P1-O11
7	D	605	EUJ	C1-O1-P1-O11
5	В	601	R16	C28-C29-C30-C31



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Mol	Chain	Res	Type	Atoms
8	A	607	A1IV1	C23-C22-N21-C20
8	С	606	A1IV1	C23-C22-N21-C20
8	В	607	A1IV1	C23-C22-N21-C20
8	D	606	A1IV1	C23-C22-N21-C20
6	С	604	HEX	C2-C3-C4-C5
8	А	607	A1IV1	C28-C22-N21-C20
8	С	606	A1IV1	C28-C22-N21-C20
8	В	607	A1IV1	C28-C22-N21-C20
8	D	606	A1IV1	C28-C22-N21-C20
8	А	607	A1IV1	C15-C16-C18-C19
8	С	606	A1IV1	C15-C16-C18-C19
8	В	607	A1IV1	C15-C16-C18-C19
8	D	606	A1IV1	C15-C16-C18-C19
5	А	608	R16	C30-C31-C32-C33
7	А	606	EUJ	C2-C3-O3-P3
7	С	605	EUJ	C2-C3-O3-P3
7	В	606	EUJ	C2-C3-O3-P3
7	D	605	EUJ	C2-C3-O3-P3
4	D	602	OCT	C5-C6-C7-C8
4	А	602	OCT	C5-C6-C7-C8
4	С	602	OCT	C5-C6-C7-C8
4	В	603	OCT	C5-C6-C7-C8
5	В	601	R16	C33-C34-C35-C36
6	В	605	HEX	C2-C3-C4-C5
7	А	606	EUJ	C1-O1-P1-O12
7	С	605	EUJ	C1-O1-P1-O12
7	В	606	EUJ	C1-O1-P1-O12
7	D	605	EUJ	C1-O1-P1-O12
6	А	605	HEX	C2-C3-C4-C5
6	D	604	HEX	C2-C3-C4-C5
5	A	604	R16	C33-C34-C35-C36
5	С	607	R16	C33-C34-C35-C36
7	A	606	EUJ	C4-C3-O3-P3
7	С	605	EUJ	C4-C3-O3-P3
7	B	606	EUJ	C4-C3-O3-P3
7	D	605	EUJ	C4-C3-O3-P3
5	B	601	R16	C30-C31-C32-C33
4	A	602	OCT	C2-C3-C4-C5
4	C	602	OCT	C2-C3-C4-C5
7	D	605	EUI	O2C-C1A-C2A-C3A
4	B	603	OCT	C2-C3-C4-C5
7	A	606	EUI	O2C-C1A-C2A-C3A
1 1	11	000	1 100	$+ \cup \Delta \cup = \cup I \Pi^{-} \cup \Delta \Pi^{-} \cup \partial \Pi^{-}$



	Jerre Frederic Frederic								
Mol	Chain	\mathbf{Res}	Type	Atoms					
7	С	605	EUJ	O2C-C1A-C2A-C3A					
7	В	606	EUJ	O2C-C1A-C2A-C3A					

There are no ring outliers.

No monomer is involved in short contacts.

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 must be highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

















4.7 Other polymers (i)

There are no such residues in this entry.



4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-52245. 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.

5.1 Orthogonal projections (i)

5.1.1 Primary map



5.1.2 Raw map



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



5.2 Central slices (i)

5.2.1 Primary map



X Index: 295



Y Index: 295



Z Index: 295

5.2.2 Raw map



X Index: 295

Y Index: 295



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



5.3 Largest variance slices (i)

5.3.1 Primary map



X Index: 274





Z Index: 232

5.3.2 Raw map



X Index: 274

Y Index: 274



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



5.4 Orthogonal standard-deviation projections (False-color) (i)

5.4.1 Primary map



5.4.2 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.



5.5 Orthogonal surface views (i)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.437. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.



Mask visualisation (i) 5.6

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

$emd_52245_msk_1.map$ (i) 5.6.1





6 Map analysis (i)

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

6.1 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.



6.2 Volume estimate (i)



The volume at the recommended contour level is 66 nm^3 ; this corresponds to an approximate mass of 60 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.



6.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.455 \AA^{-1}



7 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.

7.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.455 \AA^{-1}



7.2 Resolution estimates (i)

$\mathbf{B}_{\mathrm{assolution ostimato}}(\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)				
Resolution estimate (A)	0.143	0.5	Half-bit		
Reported by author	2.20	-	-		
Author-provided FSC curve	-	-	-		
Unmasked-calculated*	2.58	3.00	2.61		

*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 2.58 differs from the reported value 2.2 by more than 10 %



8 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-52245 and PDB model 9HL6. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.437 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.



8.2 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.

8.3 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 (0.437).



8.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.



8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.437) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.8750	0.7030	
А	0.8790	0.7030	
В	0.8770	0.7030	
С	0.8780	0.7030	
D	0.8790	0.7030	
Е	0.9290	0.6790	
F	0.9290	0.6800	
G	0.9290	0.6810	
Н	0.9290	0.6790	

