

Feb 7, 2022 – 03:27 pm GMT

PDB ID : 70CI	
EMDB ID : EMD-12808	
Title : Cryo-EM structure of yeast Ost6p containing oligosaccharyltransfe	erase
$\operatorname{complex}$	
Authors : Wild, R.; Neuhaus, J.D.; Eyring, J.; Irobalieva, R.N.; Kowal, J.; Lin, G	C.W.;
Locher, K.P.; Aebi, M.	
Deposited on : $2021-04-27$	
Resolution : $3.46 \text{ Å}(\text{reported})$	
Based on initial model : 6EZN	

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 following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.0.dev 97
Mogul	:	1.8.4, 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)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 3.46 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.



Motric	Whole archive	EM structures
IVIEUTIC	$(\# {\rm Entries})$	$(\# { m Entries})$
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 $\geq=3, 2, 1$ and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq=5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	476	7% 75%	16%	9%
2	В	130	68%	15%	17%
3	С	332	• 33% • 64%		
4	D	36	• 86%		11% •
5	Е	86	86%		13% •
6	F	718	75%	14%	11%
7	G	430	5%	14%	9%
8	Н	286	24%	12%	10%



Mol	Chain	Length	Qualit	ty of chain
			88%	
9	Ι	24		100%
1.0				
10	K	2		100%
11	J	7	43%	57%

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
14	AJP	В	202	X	-	-	-
14	AJP	D	102	Х	-	-	-



2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 17077 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 Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	434	Total 3503	C 2275	N 558	0 664	S 6	0	0

• Molecule 2 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2.

Mol	Chain	Residues		At	oms		AltConf	Trace	
2	В	108	Total 869	C 588	N 139	0 136	S 6	0	0

• Molecule 3 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST6.

Mol	Chain	Residues		At	oms		AltConf	Trace	
3	С	119	Total 933	C 638	N 138	0 148	S 9	0	0

• Molecule 4 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST4.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
4	D	35	Total 267	C 172	N 40	O 51	S 4	0	0

• Molecule 5 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5.

Mol	Chain	Residues		Ate	\mathbf{oms}	AltConf	Trace		
5	Е	85	Total 666	C 448	N 99	0 118	S 1	0	0

• Molecule 6 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3.



Mol	Chain	Residues		At	AltConf	Trace			
6	F	639	Total 5130	C 3394	N 817	O 896	S 23	0	0

• Molecule 7 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	393	Total 3177	C 2041	N 524	O 609	${f S}\ 3$	0	0

• Molecule 8 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Н	258	Total 1873	C 1228	N 311	0 331	${ m S} { m 3}$	0	0

• Molecule 9 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST6 - TM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Ι	24	Total 120	C 72	N 24	O 24	0	0

• Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
10	Κ	2	Total 28	C 16	N 2	0 10	0	0

• Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyra nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





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

• Molecule 12 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf
10	Λ	1	Total	С	Ν	0	Р	0
12	A	1	35	25	1	8	1	0
19	В	1	Total	С	Ν	0	Р	0
12	D	1	33	23	1	8	1	0
19	С	1	Total	С	Ν	Ο	Р	0
12	U	1	36	26	1	8	1	0
19	р	1	Total	С	Ν	Ο	Р	0
14	D	1	38	28	1	8	1	0
12	F	1	Total	\mathbf{C}	Ν	Ο	Р	0
14	Ľ	1	42	32	1	8	1	0
12	н	1	Total	Ċ	N	Ō	Р	0
14	11		44	34	1	8	1	0

• Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atom	s	AltConf
12	Λ	1	Total C	N O	0
15	Π	T	14 8	1 5	0
12	С	1	Total C	N O	0
10	G	I	28 16	2 10	0
12	С	1	Total C	N O	0
10	G	L	28 16	2 10	U

- Molecule 14 is Digitonin (three-letter code: AJP) (formula: $\mathrm{C}_{56}\mathrm{H}_{92}\mathrm{O}_{29}).$



Mol	Chain	Residues	Atoms	AltConf
14	В	1	Total C O 54 39 15	0



Mol	Chain	Residues	Atoms	AltConf
14	D	1	Total C O 43 33 10	0

• Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	F	1	Total 1 1	Mg 1	0

• Molecule 16 is Dolichylphosphate (three-letter code: V8K) (formula: $C_{55}H_{91}O_4P$).

	V8K		
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Mol	Chain	Residues	Atoms				AltConf
16	F	1	Total 60	$\begin{array}{c} \mathrm{C} \\ 55 \end{array}$	0 4	Р 1	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1



K297

• Molecule 4: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST4



 \bullet Molecule 5: Dolichyl-diphosphooligos accharide--protein glycosyltransferase subunit OST5



• Molecule 6: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



77%

Chain G:



14%

9%



• Molecule 8: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1



 \bullet Molecule 9: Dolichyl-diphosphooligos
accharide--protein glycosyltransferase subunit OST6 - TM1

																				8	889	6	
С	h	ai	n	I:																			10
•	•	•	•	•	•	•	•	•	•	••	•	•	•	•		•	•	•	•	•	•		
	2	e.	4	LC.		7	œ	6	10	Ħ	12	13	14	15	16	17	18	19	20	21	22	23	24
×	×	×	×	×	: ×	×	~	×	×	×	×	×	×	~	~	~	×	×	×	×	×	~ :	×

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

100%

NAG1 NAG2

 $\label{eq:mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose - (1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose - (1-4)-2-acetamido$

Chain J: 43% 57%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN5 MAN6 MAN7



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	220536	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
		D :/
Microscope	FEI ITIAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT $(4k \ge 4k)$	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	322.56, 322.56, 322.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: V8K, MG, AJP, MAN, BMA, PEE, 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 angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/3605	0.49	0/4908	
2	В	0.27	0/891	0.45	0/1203	
3	С	0.27	0/961	0.43	0/1301	
4	D	0.25	0/270	0.39	0/365	
5	Ε	0.27	0/684	0.41	0/926	
6	F	0.28	0/5281	0.49	0/7186	
7	G	0.26	0/3259	0.48	0/4431	
8	Н	0.26	0/1912	0.49	0/2606	
All	All	0.27	0/16863	0.48	0/22926	

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	3503	0	3378	48	0
2	В	869	0	899	16	0
3	С	933	0	956	7	0
4	D	267	0	280	4	0
5	Е	666	0	677	8	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	5130	0	5053	71	0
7	G	3177	0	3058	38	0
8	Н	1873	0	1787	21	0
9	Ι	120	0	26	0	0
10	K	28	0	25	0	0
11	J	83	0	70	0	0
12	А	35	0	44	2	0
12	В	33	0	40	0	0
12	С	36	0	46	0	0
12	D	38	0	50	0	0
12	F	42	0	58	1	0
12	Н	44	0	62	2	0
13	А	14	0	13	0	0
13	G	28	0	26	1	0
14	В	54	0	0	1	0
14	D	43	0	0	1	0
15	F	1	0	0	0	0
16	F	60	0	0	0	0
All	All	17077	0	16548	199	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:411:ASP:HB3	1:A:415:GLY:HA2	1.70	0.72
6:F:42:ILE:HG13	6:F:43:ILE:H	1.57	0.69
6:F:77:PRO:O	7:G:318:GLN:NE2	2.27	0.67
6:F:588:LEU:O	6:F:592:ARG:HG2	1.96	0.65
6:F:580:GLY:O	6:F:585:ASN:ND2	2.23	0.65
7:G:354:THR:HG22	7:G:372:VAL:HG22	1.77	0.65
6:F:168:GLU:HA	6:F:171:ALA:HB3	1.80	0.64
6:F:40:GLU:OE2	6:F:497:ARG:NH1	2.29	0.64
7:G:163:VAL:HG11	7:G:191:ILE:HD13	1.79	0.64
4:D:29:ASP:OD2	6:F:141:SER:OG	2.16	0.64
1:A:232:GLN:NE2	1:A:375:ASP:OD2	2.28	0.64
6:F:364:HIS:HB3	6:F:462:PHE:HD1	1.64	0.62
1:A:31:TRP:HB3	1:A:55:ILE:HD11	1.81	0.62
6:F:391:TYR:CE2	6:F:412:VAL:HB	2.35	0.61
7:G:60:ASN:OD1	7:G:61:SER:N	2.33	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:F:617:ASP:OD1	6:F:618:ALA:N	2.31	0.61
7:G:57:LEU:HD11	7:G:62:THR:HG21	1.83	0.60
1:A:378:GLU:OE2	1:A:420:THR:OG1	2.19	0.60
6:F:554:GLU:OE2	6:F:693:ARG:NH2	2.35	0.60
8:H:276:THR:O	8:H:280:ARG:HG2	2.03	0.59
1:A:33:ASN:HD22	1:A:170:THR:HG22	1.69	0.58
7:G:27:LEU:HB3	7:G:79:ILE:HD13	1.84	0.58
1:A:124:SER:HB3	1:A:127:GLU:HB2	1.84	0.58
3:C:284:LEU:O	3:C:288:VAL:HG23	2.04	0.58
1:A:377:VAL:HG21	1:A:426:LEU:HD12	1.86	0.57
1:A:64:THR:HG23	1:A:119:PHE:HB2	1.87	0.57
6:F:159:ARG:NH1	6:F:168:GLU:OE2	2.38	0.56
1:A:36:TYR:O	1:A:173:ALA:HA	2.05	0.56
1:A:199:ASN:OD1	1:A:200:GLY:N	2.38	0.56
1:A:144:TYR:HB3	1:A:145:PRO:HD3	1.87	0.56
7:G:193:ASN:OD1	7:G:194:ALA:N	2.39	0.55
6:F:222:VAL:O	6:F:226:ILE:HG12	2.07	0.55
7:G:264:ILE:HG13	7:G:364:LEU:HD21	1.88	0.55
6:F:479:VAL:HG13	6:F:480:VAL:HG23	1.88	0.55
14:B:202:AJP:C83	14:B:202:AJP:C81	2.85	0.54
6:F:603:LYS:HZ2	6:F:605:ARG:HE	1.55	0.54
2:B:113:GLU:HG2	6:F:192:MET:HB2	1.90	0.54
8:H:154:ILE:HG12	8:H:155:LEU:HD12	1.89	0.54
7:G:115:PRO:HD3	7:G:178:SER:HB3	1.88	0.53
6:F:213:PHE:HE2	6:F:391:TYR:HE1	1.55	0.53
8:H:50:ASP:O	8:H:152:ARG:NH1	2.42	0.53
2:B:79:ALA:HB2	2:B:128:PHE:HD2	1.73	0.53
6:F:425:PHE:HB3	6:F:429:LEU:HD12	1.90	0.53
4:D:7:LEU:HD22	6:F:37:ILE:HG13	1.91	0.53
1:A:408:SER:OG	1:A:409:TYR:N	2.41	0.53
6:F:62:SER:OG	6:F:63:PHE:N	2.42	0.53
2:B:62:CYS:O	2:B:65:ILE:HG22	2.10	0.52
1:A:40:ILE:HB	1:A:177:LEU:HD23	1.91	0.51
1:A:156:LEU:HD21	1:A:230:LEU:HD11	1.92	0.51
6:F:45:GLU:O	6:F:48:PRO:HD2	2.10	0.51
8:H:94:MET:HE1	8:H:119:ASP:H	1.74	0.51
6:F:425:PHE:O	6:F:429:LEU:N	2.42	0.51
1:A:97:LEU:HG	1:A:98:ALA:H	1.75	0.51
1:A:298:GLY:O	1:A:343:ASN:ND2	2.43	0.51
6:F:356:TRP:CD1	6:F:357:PRO:HD3	2.46	0.51
1:A:306:ASP:OD1	1:A:307:LEU:N	2.42	0.50



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
6:F:201:TYR:HH	6:F:215:THR:HG1	1.59	0.50
1:A:453:ILE:HG21	5:E:75:THR:HG21	1.94	0.50
7:G:84:THR:HG22	7:G:85:LYS:H	1.77	0.50
12:A:1301:PEE:H8	12:F:902:PEE:H1	1.94	0.50
7:G:55:GLU:N	7:G:55:GLU:OE1	2.45	0.50
8:H:76:ASN:ND2	8:H:149:ASN:OD1	2.45	0.50
8:H:77:LYS:O	8:H:141:SER:OG	2.19	0.50
6:F:359:PHE:O	6:F:363:THR:OG1	2.28	0.49
6:F:80:ARG:NH1	6:F:536:ASN:HD21	2.10	0.49
8:H:76:ASN:HD22	8:H:149:ASN:HA	1.77	0.49
5:E:15:SER:OG	5:E:16:PHE:N	2.45	0.49
6:F:80:ARG:CZ	6:F:536:ASN:HD21	2.25	0.49
7:G:327:LEU:HB3	7:G:339:TYR:HB3	1.93	0.49
6:F:50:PHE:HE2	6:F:86:LEU:HD13	1.78	0.49
1:A:42:VAL:HG12	1:A:47:ILE:HD12	1.95	0.49
1:A:449:LYS:HB3	1:A:450:PRO:HD3	1.94	0.49
14:D:102:AJP:C81	14:D:102:AJP:C83	2.91	0.49
1:A:184:GLU:O	1:A:222:ILE:HG13	2.13	0.49
1:A:249:ILE:HB	1:A:345:LEU:HD13	1.94	0.48
1:A:156:LEU:O	1:A:223:VAL:HA	2.13	0.48
7:G:333:ASP:OD1	7:G:334:SER:N	2.38	0.48
2:B:50:PHE:HB2	8:H:214:TRP:HZ2	1.78	0.48
3:C:289:PRO:HG2	6:F:427:ILE:HG21	1.95	0.48
6:F:221:HIS:CE1	6:F:387:PHE:HB2	2.48	0.48
7:G:379:ALA:HB3	7:G:382:GLU:OE1	2.13	0.48
3:C:273:LEU:O	3:C:277:VAL:HG23	2.13	0.48
6:F:44:HIS:ND1	6:F:163:GLY:HA3	2.29	0.48
7:G:271:HIS:HB3	7:G:292:TYR:HD1	1.79	0.48
8:H:84:LEU:HB3	8:H:93:GLU:OE1	2.13	0.47
6:F:566:VAL:O	6:F:682:LEU:HD12	2.15	0.47
5:E:44:LEU:HA	5:E:47:VAL:HG12	1.96	0.47
6:F:382:LYS:HB2	6:F:385:HIS:ND1	2.29	0.47
12:H:1101:PEE:H27	12:H:1101:PEE:H33	1.68	0.47
1:A:38:ARG:HB2	1:A:51:ILE:HG22	1.96	0.47
6:F:648:ASP:OD2	6:F:651:ARG:NH2	2.48	0.47
7:G:32:GLN:HB2	13:G:502:NAG:H62	1.95	0.47
6:F:82:THR:HG22	6:F:86:LEU:HD22	1.96	0.47
2:B:65:ILE:HD11	2:B:71:ASN:HB3	1.97	0.46
1:A:97:LEU:HD13	1:A:116:ILE:HD11	1.96	0.46
7:G:182:LEU:HD22	7:G:188:ILE:HG21	1.97	0.46
8:H:179:GLU:OE2	8:H:181:HIS:NE2	2.48	0.46



Atom-1	Atom-2	Interatomic	Clash overlap (Å)
$1 \cdot \Lambda \cdot 1 / A \cdot TVB \cdot CF2$	7.C.71.IVS.HC3	$\frac{115tallee(A)}{2.50}$	$\frac{0.46}{0.46}$
1.A.144.1110.002	1·Δ·88·GLU·HG2	1.97	0.40
1.A.00.1 ΠΕ.ΠΕ2	1.A.00.010.1102	<u> </u>	0.40
6·F·152·II F·O	6.F.159.ILF.HC13	2.14	0.40
7·C·331·CLV·HA3	7.C.338.TVB.HB2	1.08	0.40
7.C.34.THR.HC22	7:G:35:GLU:HG2	1.90	0.40
$1 \cdot \Delta \cdot 2/5 \cdot \text{TRP} \cdot \text{HR2}$	5.E.86.VAL.HC12	1.97	0.40
6.F.138.LVS.HC2	6·F·130·ΔSP·H	1.50	0.45
2·B·86·GLV·HA2	2.B.80.VAL.HC22	1.01	0.45
12.H.1101.PEE.H14	12.H.1101.PEE.H20	1.30	0.45
6·F·118·PHF·HZ	6·F·170·ILF·HD12	1.12	0.45
6·F·213·PHE·CE2	6.F.301.TVB.HE1	2 3/	0.45
8·H·236·CLV·HA3	8·H·274·THB·HC21	1.08	0.45
7.C.201.CLU.HC3	7.G.201.GLU.O	2.16	0.45
7.C.355.PHF.HB2	7.G.201.GE0.0	2.10	0.45
$1 \cdot \Delta \cdot 351 \cdot V \Delta I \cdot O$	5.F.13.SFB.HB2	2.17	0.45
6.F.356.TRP.CC	6.F.357.PRO.HD3	2.17	0.45
2.B.38.II F.HD11	2.B.45.IVS.HC3	1.08	0.45
7·C·//00·PHE·HB2	2.D.40.D15.HG5 8.H.914.TBP.CH2	2.50	0.44
7.G.84.THB.HG22	7.C.85.LVS.N	2.02	0.44
8·H·35·SEB·HA	8.H.115.LEU.HB2	1 99	0.44
3·C·237·VAL·HG23	3·C·242·ILE·HB	1.00	0.44
6·F·471·ABC·HH11	6·F·471·ABC·HC3	1.55	0.44
1·A·372·THB·H	1.A.428.SEB.HB3	1.82	0.11
6·F·625·ABG·HH11	6·F·625·ABG·HG3	1.82	0.11
3·C·284·LEU·HD12	3:C:284:LEU:HA	1.83	0.44
5:E:57:LEU:O	5:E:61:THR:HG23	2.18	0.44
2·B·72·PHE·HE2	7·G·389·ILE·HD13	1.83	0.44
4:D:27:ALA:HB2	6:F:429:LEU:HD13	2.00	0.44
1:A:270:ARG:HG3	1:A:274:MET:HE3	1.99	0.43
2:B:34:TYR:OH	2:B:48:ASP:OD2	2.35	0.43
7:G:66:VAL:HG12	7:G:93:GLN:OE1	2.18	0.43
7:G:152:VAL:HG13	7:G:171:ASP:HB3	2.00	0.43
7:G:195:PRO:HG2	7:G:198:SER:HB3	1.99	0.43
1:A:196:GLY:HA3	1:A:203:PHE:CZ	2.54	0.43
2:B:109:ARG:NH2	2:B:113:GLU:OE2	2.40	0.43
6:F:48:PRO:HB3	6:F:165:TYR:HB3	2.00	0.43
6:F:262:ARG:HG2	6:F:262:ARG:HH11	1.82	0.43
1:A:208:TRP:HB2	1:A:211:ILE:HD11	1.99	0.43
6:F:273:PHE:O	6:F:276:ILE:HG22	2.18	0.43
1:A:36:TYR:CE2	1:A:164:PRO:HB3	2.53	0.43



	A t and D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:395:PRO:HG3	1:A:434:GLN:H	1.84	0.43
6:F:47:ASP:HB3	6:F:48:PRO:HD3	2.01	0.43
2:B:124:VAL:HG11	6:F:248:VAL:HG13	1.99	0.43
6:F:134:THR:HB	6:F:143:GLY:HA2	2.01	0.43
2:B:35:PHE:HA	2:B:38:ILE:HG22	2.00	0.43
6:F:171:ALA:HB1	6:F:208:TRP:CE3	2.54	0.42
6:F:638:PRO:HG3	6:F:655:ILE:HG22	2.01	0.42
7:G:268:HIS:O	7:G:294:VAL:HA	2.19	0.42
7:G:296:PHE:CE2	7:G:312:ILE:HD13	2.54	0.42
8:H:114:ASP:OD1	8:H:117:LYS:N	2.52	0.42
6:F:168:GLU:OE1	6:F:168:GLU:N	2.49	0.42
8:H:269:ALA:HB3	8:H:270:PRO:HD3	2.01	0.42
1:A:75:PHE:HE1	1:A:96:LEU:HD22	1.84	0.42
2:B:73:PRO:HG3	7:G:392:SER:HB3	2.00	0.42
6:F:61:ASN:HB3	6:F:65:LYS:HE2	2.00	0.42
1:A:80:PHE:HB3	1:A:136:PHE:HB2	2.01	0.42
6:F:76:TYR:CE1	6:F:512:LYS:HE2	2.54	0.42
6:F:508:ASP:OD1	6:F:511:SER:HB3	2.20	0.42
6:F:156:TYR:HD1	6:F:407:LEU:HD11	1.84	0.42
6:F:394:LEU:HD23	6:F:394:LEU:HA	1.85	0.42
8:H:234:PHE:CZ	8:H:238:ILE:HD11	2.53	0.42
5:E:51:SER:OG	5:E:52:SER:N	2.53	0.42
6:F:53:ARG:NH2	6:F:71:ASP:OD1	2.46	0.42
1:A:409:TYR:CE1	12:A:1301:PEE:H14	2.54	0.42
6:F:373:GLY:O	6:F:377:LEU:HG	2.20	0.42
4:D:18:MET:SD	6:F:24:ILE:HG12	2.60	0.42
8:H:124:GLN:NE2	8:H:164:ASP:O	2.50	0.42
6:F:161:VAL:HG12	6:F:162:ALA:H	1.85	0.42
1:A:351:VAL:HG12	1:A:359:PHE:CE2	2.55	0.41
6:F:186:GLN:HE22	6:F:383:ASP:HB3	1.85	0.41
7:G:273:HIS:HB2	7:G:277:THR:O	2.20	0.41
8:H:98:PRO:HB3	8:H:111:TYR:CZ	2.55	0.41
1:A:264:LEU:HD23	1:A:264:LEU:H	1.85	0.41
2:B:45:LYS:O	2:B:49:THR:HG22	2.20	0.41
6:F:75:TRP:NE1	6:F:534:ASP:OD1	2.53	0.41
6:F:355:SER:OG	6:F:357:PRO:HD2	2.19	0.41
6:F:370:PHE:HB3	6:F:371:PRO:HD3	2.02	0.41
1:A:32:GLU:O	1:A:55:ILE:HD12	2.20	0.41
6:F:380:ASP:N	6:F:380:ASP:OD1	2.52	0.41
6:F:667:ASP:N	6:F:667:ASP:OD1	2.54	0.41
7:G:141:ARG:NH1	7:G:201:GLU:OE2	2.54	0.41



	page	T , , •	
Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:398:PHE:HB3	1:A:423:TYR:CE2	2.56	0.41
1:A:72:SER:HB2	1:A:111:GLU:O	2.20	0.41
6:F:603:LYS:HG2	6:F:605:ARG:HH21	1.85	0.41
7:G:163:VAL:O	7:G:261:LYS:HE2	2.21	0.41
3:C:318:ILE:HD12	3:C:332:PHE:CE1	2.56	0.41
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.95	0.41
6:F:497:ARG:HG2	6:F:526:MET:SD	2.61	0.41
7:G:135:PRO:HG2	7:G:138:HIS:ND1	2.36	0.41
1:A:449:LYS:NZ	5:E:86:VAL:HB	2.36	0.41
2:B:48:ASP:OD1	2:B:49:THR:N	2.54	0.41
2:B:49:THR:HG23	8:H:214:TRP:HE1	1.85	0.41
6:F:377:LEU:HD22	6:F:385:HIS:CD2	2.55	0.41
7:G:318:GLN:HB2	7:G:353:PHE:CE1	2.56	0.41
7:G:346:LEU:HD13	7:G:375:ILE:HD13	2.03	0.41
3:C:232:THR:HG22	3:C:232:THR:O	2.20	0.40
8:H:83:LEU:HD12	8:H:136:THR:O	2.21	0.40
1:A:144:TYR:HH	1:A:186:TYR:HE1	1.69	0.40
1:A:307:LEU:HB2	6:F:501:TYR:CE1	2.57	0.40
8:H:144:ALA:HB1	8:H:148:GLU:OE2	2.22	0.40
7:G:385:ARG:HA	7:G:385:ARG:HD2	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	А	430/476~(90%)	414 (96%)	16 (4%)	0	100	100	
2	В	106/130~(82%)	103 (97%)	3 (3%)	0	100	100	
3	С	117/332~(35%)	116 (99%)	1 (1%)	0	100	100	
4	D	33/36~(92%)	32 (97%)	1 (3%)	0	100	100	



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
5	Ε	83/86~(96%)	81 (98%)	2(2%)	0	100	100	
6	F	631/718~(88%)	618~(98%)	12 (2%)	1 (0%)	47	80	
7	G	391/430~(91%)	381~(97%)	10 (3%)	0	100	100	
8	Н	256/286~(90%)	244~(95%)	12~(5%)	0	100	100	
All	All	2047/2494~(82%)	1989~(97%)	57 (3%)	1 (0%)	100	100	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	45	GLU

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	389/426~(91%)	389 (100%)	0	100 100		
2	В	94/115~(82%)	94 (100%)	0	100 100		
3	С	100/301~(33%)	100 (100%)	0	100 100		
4	D	32/33~(97%)	32 (100%)	0	100 100		
5	Ε	74/75~(99%)	74 (100%)	0	100 100		
6	F	538/613~(88%)	538 (100%)	0	100 100		
7	G	351/392~(90%)	351 (100%)	0	100 100		
8	Н	174/249~(70%)	174 (100%)	0	100 100		
All	All	1752/2204~(80%)	1752 (100%)	0	100 100		

There are no protein residues with a non-rotameric sidechain to report.

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
6	F	186	GLN
	<i>a</i>	1	



Continued from previous page...

Mol	Chain	Res	Type
6	F	536	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)

9 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	$\operatorname{ain} \operatorname{Res} L^{\frac{1}{2}}$	Tink	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
	Type	Unain			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	J	1	11,6	14,14,15	0.33	0	17,19,21	0.48	0
11	NAG	J	2	11	14,14,15	0.20	0	17,19,21	0.50	0
11	BMA	J	3	11	11,11,12	0.47	0	$15,\!15,\!17$	0.84	0
11	MAN	J	4	11	11,11,12	0.65	0	15,15,17	1.22	1 (6%)
11	MAN	J	5	11	11,11,12	0.72	0	15,15,17	1.02	1 (6%)
11	MAN	J	6	11	11,11,12	0.64	0	15,15,17	0.94	1 (6%)
11	MAN	J	7	11	11,11,12	0.68	0	15,15,17	0.96	1 (6%)
10	NAG	K	1	1,10	14,14,15	0.35	0	17,19,21	0.65	0
10	NAG	K	2	10	14,14,15	0.22	0	17,19,21	0.52	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
11	NAG	J	1	11,6	-	2/6/23/26	0/1/1/1
11	NAG	J	2	11	-	2/6/23/26	0/1/1/1
11	BMA	J	3	11	-	1/2/19/22	0/1/1/1
11	MAN	J	4	11	-	0/2/19/22	0/1/1/1
11	MAN	J	5	11	-	1/2/19/22	0/1/1/1
11	MAN	J	6	11	-	0/2/19/22	0/1/1/1
11	MAN	J	7	11	-	0/2/19/22	0/1/1/1
10	NAG	K	1	1,10	-	3/6/23/26	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
11	J	4	MAN	O2-C2-C3	-3.21	103.72	110.14
11	J	5	MAN	O2-C2-C3	-2.74	104.64	110.14
11	J	7	MAN	O2-C2-C3	-2.23	105.66	110.14
11	J	6	MAN	O2-C2-C3	-2.20	105.74	110.14

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
10	Κ	2	NAG	O5-C5-C6-O6
11	J	3	BMA	O5-C5-C6-O6
10	Κ	2	NAG	C4-C5-C6-O6
11	J	5	MAN	O5-C5-C6-O6
11	J	2	NAG	C4-C5-C6-O6
11	J	2	NAG	O5-C5-C6-O6
11	J	1	NAG	C4-C5-C6-O6
10	Κ	1	NAG	C3-C2-N2-C7
11	J	1	NAG	O5-C5-C6-O6
10	К	1	NAG	C4-C5-C6-O6
10	К	1	NAG	O5-C5-C6-O6

All (11) torsion outliers are listed below:

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.









5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is 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).

Mol T	Turne	Chain	Res	Link	Bond lengths			Bond angles		
	туре				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
13	NAG	G	502	7	14,14,15	0.51	0	17,19,21	0.44	0



Mal	T a	Chain	Dar	T : 1-	Bo	ond leng	ths	В	ond ang	les
IVIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
12	PEE	С	1801	-	$35,\!35,\!50$	1.64	5 (14%)	$38,\!40,\!55$	1.29	5 (13%)
12	PEE	F	902	-	41,41,50	1.58	5 (12%)	43,46,55	1.22	3 (6%)
12	PEE	А	1301	-	34,34,50	1.68	5 (14%)	$37,\!39,\!55$	1.31	4 (10%)
13	NAG	G	501	7	14,14,15	0.23	0	17,19,21	0.36	0
12	PEE	Н	1101	-	43,43,50	1.53	5 (11%)	$46,\!48,\!55$	1.22	4 (8%)
12	PEE	В	201	-	32,32,50	1.56	4 (12%)	$35,\!37,\!55$	1.14	4 (11%)
14	AJP	D	102	-	49,49,95	0.54	1 (2%)	74,80,149	1.35	9 (12%)
14	AJP	В	202	-	61,61,95	0.45	0	92,98,149	1.30	10 (10%)
16	V8K	F	903	15	59,59,59	1.85	8 (13%)	68,72,72	1.69	21 (30%)
12	PEE	D	101	-	37,37,50	1.46	4 (10%)	40,42,55	1.16	3 (7%)
13	NAG	А	1302	1	14,14,15	0.24	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
13	NAG	G	502	7	-	3/6/23/26	0/1/1/1
12	PEE	С	1801	-	-	16/39/39/54	-
12	PEE	А	1301	-	-	20/38/38/54	-
12	PEE	F	902	-	-	25/45/45/54	-
13	NAG	G	501	7	-	0/6/23/26	0/1/1/1
12	PEE	Н	1101	-	-	24/47/47/54	-
14	AJP	D	102	-	16/16/19/38	3/6/121/220	0/7/7/11
12	PEE	В	201	-	-	14/36/36/54	-
14	AJP	В	202	-	21/21/24/38	3/12/147/220	0/8/8/11
16	V8K	F	903	15	-	27/67/67/67	-
12	PEE	D	101	-	-	20/41/41/54	-
13	NAG	А	1302	1	-	2/6/23/26	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
16	F	903	V8K	P57-O56	7.87	1.85	1.60
16	F	903	V8K	C45-C46	7.80	1.54	1.34
12	F	902	PEE	C39-C38	4.35	1.57	1.31
12	Н	1101	PEE	C39-C38	4.34	1.56	1.31



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	А	1301	PEE	C39-C38	4.23	1.57	1.28
12	С	1801	PEE	C39-C38	4.21	1.57	1.28
12	F	902	PEE	C18-C19	4.15	1.55	1.31
12	D	101	PEE	C18-C19	4.11	1.55	1.31
12	Н	1101	PEE	C18-C19	4.09	1.55	1.31
12	В	201	PEE	C19-C18	4.01	1.55	1.28
12	А	1301	PEE	C19-C18	4.00	1.55	1.28
12	D	101	PEE	O3-C30	3.66	1.44	1.33
12	С	1801	PEE	O3-C30	3.61	1.43	1.33
12	В	201	PEE	O3-C30	3.59	1.43	1.33
12	Н	1101	PEE	O3-C30	3.57	1.43	1.33
12	F	902	PEE	O3-C30	3.55	1.43	1.33
12	А	1301	PEE	O3-C30	3.55	1.43	1.33
12	С	1801	PEE	O2-C10	3.53	1.44	1.34
12	F	902	PEE	O2-C10	3.51	1.44	1.34
12	С	1801	PEE	C18-C19	3.47	1.55	1.29
12	В	201	PEE	O2-C10	3.39	1.43	1.34
12	Н	1101	PEE	O2-C10	3.39	1.43	1.34
12	D	101	PEE	O2-C10	3.38	1.43	1.34
12	А	1301	PEE	O2-C10	3.26	1.43	1.34
16	F	903	V8K	C46-C47	2.85	1.52	1.45
16	F	903	V8K	C54-C55	2.65	1.60	1.50
12	В	201	PEE	C11-C10	2.48	1.58	1.50
16	F	903	V8K	C45-C44	2.48	1.51	1.43
16	F	903	V8K	O56-C55	-2.40	1.34	1.44
12	F	902	PEE	C11-C10	2.38	1.57	1.50
12	А	1301	PEE	C11-C10	2.34	1.57	1.50
12	D	101	PEE	C11-C10	2.32	1.57	1.50
16	F	903	V8K	C11-C12	2.31	1.56	1.51
12	С	1801	PEE	C11-C10	2.27	1.57	1.50
12	Н	1101	PEE	C11-C10	2.25	1.57	1.50
14	D	102	AJP	C16-C11	-2.22	1.51	1.54
16	F	903	V8K	C16-C17	2.01	1.55	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
14	В	202	AJP	C12-C07-C08	-5.52	98.91	104.88
14	D	102	AJP	C12-C07-C08	-4.91	99.58	104.88
12	А	1301	PEE	O2-C10-C11	4.09	120.33	111.50
12	С	1801	PEE	O2-C10-C11	3.95	120.02	111.50
12	Н	1101	PEE	O2-C10-C11	3.95	120.01	111.50



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
12	D	101	PEE	O2-C10-C11	3.92	119.95	111.50
12	F	902	PEE	O2-C10-C11	3.89	119.88	111.50
14	В	202	AJP	C06-C07-C08	-3.84	97.34	104.34
12	В	201	PEE	O2-C10-C11	3.53	119.12	111.50
14	В	202	AJP	O09-C08-C10	3.36	117.08	110.17
14	В	202	AJP	O25-C23-C24	3.30	116.00	109.62
16	F	903	V8K	C16-C15-C14	3.30	122.72	111.88
14	D	102	AJP	C06-C07-C08	-3.06	98.77	104.34
16	F	903	V8K	C36-C35-C34	3.06	121.92	111.88
14	D	102	AJP	O09-C08-C10	3.05	116.45	110.17
12	F	902	PEE	O3-C30-C31	2.98	121.25	111.91
14	В	202	AJP	C11-C16-C15	-2.96	104.06	109.23
16	F	903	V8K	C16-C17-C19	2.95	127.09	121.12
14	D	102	AJP	C20-C21-C22	-2.90	109.33	114.09
16	F	903	V8K	C45-C46-C47	-2.84	118.44	126.42
16	F	903	V8K	C11-C10-C09	2.77	120.98	111.88
16	F	903	V8K	C26-C25-C24	2.76	120.96	111.88
12	Н	1101	PEE	O3-C30-C31	2.72	120.44	111.91
12	С	1801	PEE	C17-C18-C19	-2.70	109.64	131.07
16	F	903	V8K	C48-C47-C49	-2.69	118.31	123.59
14	В	202	AJP	C05-C06-C07	-2.69	98.99	103.37
14	D	102	AJP	C21-C20-C15	2.68	114.09	110.08
16	F	903	V8K	C31-C30-C29	2.68	120.68	111.88
16	F	903	V8K	C13-C12-C14	-2.67	116.84	123.68
16	F	903	V8K	C11-C12-C14	2.61	126.40	121.12
14	D	102	AJP	O09-C08-C07	-2.60	97.82	104.06
14	D	102	AJP	C20-C15-C16	-2.60	109.69	112.42
12	А	1301	PEE	O3-C30-C31	2.59	120.03	111.91
12	В	201	PEE	C17-C18-C19	-2.56	109.47	126.84
12	А	1301	PEE	C17-C18-C19	-2.55	109.48	126.84
12	С	1801	PEE	C37-C38-C39	-2.55	109.48	126.84
16	F	903	V8K	C40-C41-C42	2.55	121.36	112.98
12	D	101	PEE	O3-C30-C31	2.53	119.84	111.91
16	F	903	V8K	C40-C39-C37	2.52	133.72	127.66
14	D	102	AJP	C13-C12-C07	2.51	119.47	115.46
12	A	1301	PEE	C37-C38-C39	-2.47	110.07	126.84
12	С	1801	PEE	O3-C30-C31	2.45	119.60	111.91
14	В	202	AJP	C11-C12-C07	-2.41	96.07	100.19
16	F	903	V8K	O60-P57-O56	-2.39	100.37	106.73
16	F	903	V8K	C21-C20-C19	2.37	119.66	111.88
16	F	903	V8K	$C25-\overline{C26}-C27$	2.29	$1\overline{20.51}$	112.98
14	В	202	AJP	O09-C08-C07	-2.29	98.58	104.06



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
16	F	903	V8K	C18-C17-C19	-2.26	117.88	123.68
12	В	201	PEE	O3-C30-C31	2.26	119.00	111.91
16	F	903	V8K	C26-C27-C29	2.22	125.61	121.12
16	F	903	V8K	C44-C45-C46	-2.20	116.35	123.22
14	В	202	AJP	O34-C29-C30	2.20	115.47	109.45
16	F	903	V8K	C06-C07-C09	2.17	125.51	121.12
16	F	903	V8K	C10-C11-C12	2.15	120.03	112.98
16	F	903	V8K	O60-P57-O58	2.07	115.55	107.64
12	С	1801	PEE	C20-C19-C18	-2.06	109.39	126.37
12	F	902	PEE	C37-C38-C39	-2.06	108.95	124.73
12	Н	1101	PEE	C17-C18-C19	-2.05	108.98	124.73
14	D	102	AJP	C11-C12-C07	-2.03	96.72	100.19
12	В	201	PEE	O2-C10-O4	-2.02	118.82	123.70
14	В	202	AJP	C20-C21-C22	-2.01	110.78	114.09
12	D	101	PEE	C20-C19-C18	-2.01	109.33	124.73
12	Н	1101	PEE	C20-C19-C18	-2.00	109.35	124.73

All (37) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	В	202	AJP	C10
14	В	202	AJP	C28
14	В	202	AJP	C37
14	В	202	AJP	C26
14	В	202	AJP	C11
14	В	202	AJP	C02
14	В	202	AJP	C15
14	В	202	AJP	C27
14	В	202	AJP	C16
14	В	202	AJP	C12
14	В	202	AJP	C38
14	В	202	AJP	C23
14	В	202	AJP	C35
14	В	202	AJP	C30
14	В	202	AJP	C39
14	В	202	AJP	C07
14	В	202	AJP	C36
14	В	202	AJP	C22
14	В	202	AJP	C20
14	В	202	AJP	C19
14	В	202	AJP	C05
14	D	102	AJP	C07



Mol	Chain	Res	Type	Atom
14	D	102	AJP	C11
14	D	102	AJP	C10
14	D	102	AJP	C02
14	D	102	AJP	C15
14	D	102	AJP	C22
14	D	102	AJP	C23
14	D	102	AJP	C20
14	D	102	AJP	C27
14	D	102	AJP	C28
14	D	102	AJP	C16
14	D	102	AJP	C12
14	D	102	AJP	C19
14	D	102	AJP	C26
14	D	102	AJP	C30
14	D	102	AJP	C05

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All (157) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	А	1301	PEE	C1-O3P-P-O2P
12	А	1301	PEE	C1-O3P-P-O1P
12	А	1301	PEE	C1-O3P-P-O4P
12	А	1301	PEE	O4P-C4-C5-N
12	С	1801	PEE	C17-C18-C19-C20
12	С	1801	PEE	C4-O4P-P-O3P
12	С	1801	PEE	O4P-C4-C5-N
12	D	101	PEE	C17-C18-C19-C20
12	D	101	PEE	C11-C10-O2-C2
12	D	101	PEE	C4-O4P-P-O1P
12	D	101	PEE	O4P-C4-C5-N
12	F	902	PEE	C1-O3P-P-O1P
12	F	902	PEE	C4-O4P-P-O1P
12	Н	1101	PEE	O4-C10-O2-C2
12	Н	1101	PEE	C1-O3P-P-O4P
16	F	903	V8K	C19-C20-C21-C22
16	F	903	V8K	C20-C21-C22-C24
16	F	903	V8K	C20-C21-C22-C23
16	F	903	V8K	C24-C25-C26-C27
16	F	903	V8K	C32-C34-C35-C36
16	F	903	V8K	C37-C39-C40-C41
16	F	903	V8K	C40-C41-C42-C43
16	F	903	V8K	C40-C41-C42-C44



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Mol	Chain	Res	Type	Atoms
16	F	903	V8K	C55-O56-P57-O58
16	F	903	V8K	C55-O56-P57-O59
16	F	903	V8K	C55-O56-P57-O60
14	В	202	AJP	O40-C35-O34-C29
12	D	101	PEE	O4-C10-O2-C2
12	Н	1101	PEE	C11-C10-O2-C2
16	F	903	V8K	C10-C11-C12-C13
12	Н	1101	PEE	C31-C30-O3-C3
12	Н	1101	PEE	C11-C12-C13-C14
12	Н	1101	PEE	O5-C30-O3-C3
16	F	903	V8K	C15-C16-C17-C18
16	F	903	V8K	C30-C31-C32-C33
16	F	903	V8K	C35-C36-C37-C38
16	F	903	V8K	C15-C16-C17-C19
16	F	903	V8K	C30-C31-C32-C34
16	F	903	V8K	C35-C36-C37-C39
16	F	903	V8K	C14-C15-C16-C17
16	F	903	V8K	C39-C40-C41-C42
13	А	1302	NAG	C4-C5-C6-O6
12	А	1301	PEE	C31-C30-O3-C3
14	В	202	AJP	C36-C35-O34-C29
13	G	502	NAG	C8-C7-N2-C2
13	G	502	NAG	O7-C7-N2-C2
16	F	903	V8K	C10-C11-C12-C14
16	F	903	V8K	C45-C46-C47-C48
16	F	903	V8K	C45-C46-C47-C49
12	А	1301	PEE	C10-C11-C12-C13
12	А	1301	PEE	C16-C17-C18-C19
12	А	1301	PEE	C36-C37-C38-C39
12	А	1301	PEE	O5-C30-O3-C3
12	С	1801	PEE	C30-C31-C32-C33
12	F	902	PEE	C11-C10-O2-C2
12	F	902	PEE	C1-O3P-P-O4P
12	F	902	PEE	C4-O4P-P-O3P
12	F	902	PEE	O4-C10-O2-C2
14	D	102	AJP	O31-C30-C32-O33
12	С	1801	PEE	C11-C10-O2-C2
12	С	1801	PEE	C13-C14-C15-C16
12	C	1801	PEE	O4-C10-O2-C2
12	Н	1101	PEE	C14-C15-C16-C17
12	F	902	PEE	C10-C11-C12-C13
13	А	1302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms	
14	В	202	AJP	O31-C30-C32-O33	
12	В	201	PEE	C14-C15-C16-C17	
12	С	1801	PEE	C31-C32-C33-C34	
12	В	201	PEE	C32-C33-C34-C35	
12	D	101	PEE	C20-C21-C22-C23	
12	Н	1101	PEE	C31-C32-C33-C34	
12	А	1301	PEE	C12-C13-C14-C15	
12	С	1801	PEE	C12-C13-C14-C15	
12	D	101	PEE	C12-C13-C14-C15	
12	В	201	PEE	O4P-C4-C5-N	
12	D	101	PEE	C31-C32-C33-C34	
12	F	902	PEE	C12-C13-C14-C15	
12	А	1301	PEE	C32-C33-C34-C35	
12	D	101	PEE	C31-C30-O3-C3	
12	D	101	PEE	C10-C11-C12-C13	
12	А	1301	PEE	C11-C12-C13-C14	
12	Н	1101	PEE	C37-C38-C39-C40	
12	D	101	PEE	O5-C30-O3-C3	
12	Н	1101	PEE	C34-C35-C36-C37	
12	F	902	PEE	C15-C16-C17-C18	
12	Н	1101	PEE	C19-C20-C21-C22	
12	Н	1101	PEE	C35-C36-C37-C38	
12	Н	1101	PEE	C12-C13-C14-C15	
12	F	902	PEE	C34-C35-C36-C37	
12	С	1801	PEE	C32-C33-C34-C35	
12	В	201	PEE	C1-O3P-P-O4P	
12	F	902	PEE	C35-C36-C37-C38	
12	F	902	PEE	C1-C2-C3-O3	
12	Н	1101	PEE	C1-C2-C3-O3	
13	G	502	NAG	O5-C5-C6-O6	
12	А	1301	PEE	C30-C31-C32-C33	
12	D	101	PEE	C21-C22-C23-C24	
12	D	101	PEE	C19-C20-C21-C22	
12	Н	1101	PEE	C15-C16-C17-C18	
14	D	102	AJP	C27-C26-O25-C23	
16	F	903	V8K	C05-C06-C07-C08	
16	F	903	V8K	C05-C06-C07-C09	
12	F	902	PEE	C3-C2-O2-C10	
12	D	101	PEE	C13-C14-C15-C16	
12	Н	1101	PEE	C18-C19-C20-C21	
12	А	1301	PEE	O2-C2-C3-O3	
12	А	1301	PEE	C33-C34-C35-C36	

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EMD-12808, '	7OCI
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Mol	Chain	Res	Type	Atoms
12	С	1801	PEE	C31-C30-O3-C3
12	Н	1101	PEE	C32-C33-C34-C35
12	D	101	PEE	C4-O4P-P-O3P
12	А	1301	PEE	C13-C14-C15-C16
12	F	902	PEE	O2-C2-C3-O3
12	В	201	PEE	C34-C35-C36-C37
12	Н	1101	PEE	C16-C17-C18-C19
12	Н	1101	PEE	C20-C21-C22-C23
12	С	1801	PEE	C3-C2-O2-C10
12	В	201	PEE	O3P-C1-C2-O2
12	С	1801	PEE	O5-C30-O3-C3
12	Н	1101	PEE	O2-C2-C3-O3
12	В	201	PEE	C4-O4P-P-O3P
12	В	201	PEE	C1-O3P-P-O1P
12	D	101	PEE	C4-O4P-P-O2P
12	F	902	PEE	C1-O3P-P-O2P
12	F	902	PEE	C4-O4P-P-O2P
12	В	201	PEE	C16-C17-C18-C19
12	F	902	PEE	O3P-C1-C2-O2
14	D	102	AJP	O31-C26-O25-C23
12	А	1301	PEE	C1-C2-C3-O3
12	А	1301	PEE	C14-C15-C16-C17
12	D	101	PEE	C18-C19-C20-C21
12	F	902	PEE	C31-C30-O3-C3
12	А	1301	PEE	C4-O4P-P-O3P
12	D	101	PEE	C1-O3P-P-O4P
12	F	902	PEE	O5-C30-O3-C3
12	F	902	PEE	C40-C41-C42-C43
16	F	903	V8K	C42-C44-C45-C46
12	Н	1101	PEE	C22-C23-C24-C25
12	Н	1101	PEE	C39-C40-C41-C42
12	Н	1101	PEE	C13-C14-C15-C16
12	D	101	PEE	C34-C35-C36-C37
12	В	201	PEE	O2-C2-C3-O3
12	F	902	PEE	C38-C39-C40-C41
12	F	902	PEE	O3P-C1-C2-C3
12	С	1801	PEE	C15-C16-C17-C18
12	D	101	PEE	C16-C17-C18-C19
12	Н	1101	PEE	O3P-C1-C2-O2
12	F	902	PEE	C36-C37-C38-C39
12	В	201	PEE	O3P-C1-C2-C3
16	F	903	V8K	C34-C35-C36-C37



Mol	Chain	Res	Type	Atoms
12	С	1801	PEE	O3-C30-C31-C32
12	В	201	PEE	C1-O3P-P-O2P
12	В	201	PEE	C4-O4P-P-O1P
12	С	1801	PEE	C1-O3P-P-O2P
12	F	902	PEE	O4P-C4-C5-N
12	А	1301	PEE	O2-C10-C11-C12
12	F	902	PEE	C33-C34-C35-C36
12	В	201	PEE	C31-C32-C33-C34

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There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
13	G	502	NAG	1	0
12	F	902	PEE	1	0
12	А	1301	PEE	2	0
12	Н	1101	PEE	2	0
14	D	102	AJP	1	0
14	В	202	AJP	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 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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. 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-12808. 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.

Orthogonal projections (i) 6.1

6.1.1Primary map



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

6.2Central slices (i)

6.2.1Primary map



X Index: 192

Y Index: 192

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: 190

Y Index: 185

Z Index: 199

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 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



Mask visualisation (i) 6.5

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

$emd_{12808}msk_{1.map}$ (i) 6.5.1







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 93 nm^3 ; this corresponds to an approximate mass of 84 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 0.289 \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 0.289 \AA^{-1}



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)			
resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	3.46	-	-	
Author-provided FSC curve	3.88	4.30	3.94	
Unmasked-calculated*	-	-	-	

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.46 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12808 and PDB model 7OCI. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.022 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 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

