

wwPDB EM Validation Summary Report (i)

Apr 3, 2024 – 01:04 PM EDT

PDB ID : 9B4H: EMD-43892 EMDB ID Title : Chlamydomonas reinhardtii mastigoneme filament Authors : Dai, J.; Ma, M.; Zhang, R.; Brown, A. Deposited on 2024-03-20 : 3.10 Å(reported) Resolution : Based on initial model :

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

Overall quality at a glance (i) 1

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

The reported resolution of this entry is 3.10 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.



Ramachandran outliers	154571	4023	
Sidechain outliers	154315	3826	
The table below summaris	ses the geometric issue	es observed across the	polymeric chains and their fit
to the map. The red. oran	ge, vellow and green	segments of the bar in	dicate the fraction of residues
that contain outliers for >	>=3, 2, 1 and 0 type	s of geometric quality	criteria respectively. A grey
segment represents the fr	action of residues th	at are not modelled.	The numeric value for each

lue 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	1987	90%	6% ·				
1	В	1987	90%	6% ·				
2	Х	8572	•	9%				
3	A1	2	50%	50%				
3	A2	2	50%	50%				
3	A3	2	50%	50%				
3	a1	2	50%	50%				
3	a2	2	50%	50%				
3	a3	2	10	00%				



Mol	Chain	Length	Quality of chain
4	A4	2	100%
4	A5	2	100%
4	A7	2	50% 50%
4	B0	2	50% 50%
4	B1	2	100%
4	B3	2	100%
4	B4	2	100%
4	B5	2	100%
4	B7	2	100%
4	B9	2	100%
4	C0	2	100%
4	C1	2	100%
4	C2	2	100%
4	C3	2	100%
4	C4	2	100%
4	C5	2	100%
4	C6	2	100%
4	C7	2	100%
4	C8	2	100%
4	C9	2	100%
4	D0	2	100%
4	D1	2	50% 50%
4	D2	2	100%
4	D3	2	100%
4	D4	2	100%

Continued from previous page...



Mol	Chain	Length	Quality of chain
4	D5	2	100%
4	D6	2	100%
4	D7	2	100%
4	D8	2	100%
4	D9	2	100%
4	E0	2	100%
4	E1	2	100%
4	E2	2	100%
4	E3	2	100%
4	E4	2	100%
4	E5	2	100%
4	E7	2	100%
4	E8	2	100%
4	F0	2	100%
4	F2	2	100%
4	F3	2	100%
4	F5	2	100%
4	F8	2	100%
4	a5	2	50% 50%
4	a7	2	50% 50%
4	b0	2	100%
4	b1	2	100%
4	b3	2	100%
4	b4	2	100%
4	b5	2	100%

Continued from previous page...



Mol	Chain	Length	Quality of chain
4	b7	2	100%
4	b9	2	100%
4	c0	2	100%
4	c1	2	100%
4	c2	2	100%
4	c3	2	100%
4	c4	2	100%
4	c5	2	100%
4	c6	2	100%
4	c7	2	100%
4	c8	2	100%
4	c9	2	100%
4	d0	2	100%
4	d1	2	50% 50%
4	d2	2	100%
4	d3	2	100%
4	d4	2	100%
4	d5	2	100%
4	d6	2	100%
4	d7	2	100%
4	d8	2	50% 50%
4	d9	2	100%
4	e0	2	100%
4	e1	2	100%
4	e2	2	100%

Continued from previous page...MolChainLength



Mol	Chain	Length	Quality of chain	
4	e3	2	50% 50%	•
4	e4	2	100%	•
4	e5	2	100%	
4	e6	2	50% 50%	
4	e7	2	50% 50%	•
4	e8	2	100%	•
4	fO	2	50% 50%	•
4	f2	2	50% 50%	•
4	f3	2	100%	•
4	f5	2	100%	•
4	f8	2	100%	•
5	A6	4	100%	
5	A9	4	100%	
5	B6	4	100%	
5	F6	4	100%	
5	F7	4	100%	
5	a6	4	100%	
5	a9	4	25% 75%	•
5	b6	4	100%	
5	f6	4	100%	
5	f7	4	100%	•
6	E6	8	100%	•
7	a4	2	100%	•
8	e9	6	100%	•

Continued from previous page...

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	34V	a4	1	Х	-	_	-
9	A1AIO	А	2004	Х	-	-	-
9	A1AIO	А	2006	Х	-	-	-
9	A1AIO	А	2009	Х	-	-	-
9	A1AIO	А	2011	Х	-	-	-
9	A1AIO	А	2012	Х	-	-	-
9	A1AIO	А	2014	Х	-	-	-
9	A1AIO	А	2016	Х	-	-	-
9	A1AIO	А	2018	Х	-	-	-
9	A1AIO	А	2025	Х	-	-	-
9	A1AIO	А	2035	Х	-	-	-
9	A1AIO	А	2037	Х	-	-	-
9	A1AIO	А	2038	X	-	-	-
9	A1AIO	А	2040	X	-	-	-
9	A1AIO	А	2052	X	-	-	-
9	A1AIO	В	2004	X	-	-	-
9	A1AIO	В	2006	Х	-	-	-
9	A1AIO	В	2009	Х	-	-	-
9	A1AIO	В	2011	X	-	-	-
9	A1AIO	В	2012	Х	-	-	-
9	A1AIO	В	2014	Х	-	-	-
9	A1AIO	В	2016	Х	-	-	-
9	A1AIO	В	2030	Х	-	-	-
9	A1AIO	В	2031	Х	-	-	-
9	A1AIO	В	2032	Х	-	-	-
9	A1AIO	В	2033	X	-	-	-
9	A1AIO	В	2034	X		-	-
9	A1AIO	В	2046	X	_	-	-
9	A1AIO	В	2047	X	-	-	-
9	A1AIO	В	2053	X	-	-	-



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 32328 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.

 $\bullet\,$ Molecule 1 is a protein called Tyrosine-protein kin ase ephrin type A/B receptor-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	1908	Total 13867	C 8726	N 2262	O 2798	S 81	0	0
1	В	1908	Total 13867	C 8726	N 2262	0 2798	S 81	0	0

• Molecule 2 is a protein called C-type lectin domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	Х	109	Total 834	C 509	N 116	O 208	S 1	0	0

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	A	Aton	ns	AltConf	Trace	
9	Δ.1	2	Total	С	Ν	0	0	0
່ງ	AI	2	28	16	2	10	0	0
2	1.9	2	Total	С	Ν	0	0	0
່ງ	A2	2	28	16	2	10	0	0
3	Λ 3	2	Total	С	Ν	0	0	0
5	AJ	2	28	16	2	10	0	0
3	.1	9	Total	С	Ν	0	0	0
5	aı		28	16	2	10	0	0
2		9	Total	С	Ν	0	0	0
5	5 az	2	28	16	2	10	0	0
3	.3	2	Total	С	Ν	0	0	0
J	aJ	2	28	16	2	10	U	0

• Molecule 4 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e.



Mol	Chain	Residues	At	oms		AltConf	Trace
4	Δ.4	9	Total	С	0	0	0
4	Λ4	2	18	10	8	0	0
	A 5	2	Total	С	Ο	0	0
	110	2	18	10	8	0	0
4	Α7	2	Total	С	Ο	0	0
		_	18	10	8	Ŭ	
4	B0	2	Total	C	O	0	0
			18	$\frac{10}{3}$	8		
4	B1	2	Total	C 10	0	0	0
			18	$\frac{10}{C}$	8		
4	B3	2		10	0	0	0
			18 Total	$\frac{10}{C}$	8		
4	B4	2	1000	10	8	0	0
			Total	$\frac{10}{C}$	0		
4	B5	2	18	10	8	0	0
			Total	$\frac{10}{C}$	0		
4	B7	2	18	10	8	0	0
			Total	$\frac{10}{C}$	0		
4	B9	2	18	10	8	0	0
	Co	2	Total	С	0	0	
4	CO	2	18	10	8	0	0
4	C1	0	Total	С	0	0	0
4	U1	2	18	10	8	0	0
4	C2	9	Total	С	0	0	0
4	02	2	18	10	8	0	0
4	C3	2	Total	С	Ο	0	0
	00	2	18	10	8	0	0
4	C4	2	Total	С	Ο	0	0
		-	18	10	8		
4	C5	2	Total	\mathbf{C}	U o	0	0
			18	$\frac{10}{C}$	8		
4	C6	2	10tal	U 10	0	0	0
			1ð Tetel	$\frac{10}{C}$	<u>ð</u>		
4	C7	2	10tal 19	10	Q Q	0	0
			Total	$\frac{10}{C}$	0		
4	C8	2	18	10	8	0	0
			Total	$\frac{10}{C}$	0		
4	C9	2	18	10	8	0	0
			Total	$\frac{10}{C}$	0		
4	D0	2	18	10	8	0	0
	54	2	Total	C	0		
4	DI	2	18	10	8	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf	Trace		
4	Da	0	Total	С	Ο	0	0	
4	D2	2	18	10	8	0	0	
4	Dэ	0	Total	С	Ο	0	0	
4	D3	2	18	10	8	0	0	
4	D 4	0	Total	С	0	0	0	
4	D4	2	18	10	8	0	0	
4	Dr	0	Total	С	0	0	0	
4	D3	2	18	10	8	0	0	
4	De	0	Total	С	Ο	0	0	
4	Do	2	18	10	8	0	0	
4	D7	0	Total	С	0	0	0	
4	Dí	2	18	10	8	0	0	
4	Do	0	Total	С	0	0	0	
4	D8	2	18	10	8	0	0	
4	DO	0	Total	С	0	0	0	
4	D9	2	18	10	8	0	0	
4	FO	0	Total	С	Ο	0	0	
4	EU	2	18	10	8	0	0	
4	D 1	0	Total	С	Ο	0	0	
4	EI	Z	18	10	8	0	0	
4	ΓΩ	0	Total	С	Ο	0	0	
4	EZ	2	18	10	8	0	0	
4	\mathbf{F}^{I}	0	Total	С	Ο	0	0	
4	Ľ4	2	18	10	8	0	0	
4	٣ĸ	n	Total	С	Ο	0	0	
4	EÐ	2	18	10	8	0	0	
4	F٥	ე	Total	С	0	0	0	
4	Eo	2	18	10	8	0	0	
4	FO	ე	Total	С	Ο	0	0	
4	ΓU	2	18	10	8	0	0	
4	F 3	2	Total	С	0	0	0	
4	гэ	2	18	10	8	0	0	
4	F8	9	Total	С	0	0	0	
4	10	2	18	10	8	0	0	
1	95	9	Total	С	0	0	0	
4	au		18	10	8	U	U	
4	a7	9	Total	С	0	0	0	
±			18	10	8		U	
4	b0	9	Total	С	0	0	0	
4		b0	bU	2	18	10	8	0
1	b1	9	Total	С	0	0	0	
- 1	4 b1	b1 2	18	10	8		U	



Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf	Trace	
4	1.0	0	Total	С	Ο	0	0
4	60	Z	18	10	8	0	0
4	L 4	0	Total	С	0	0	0
4	04	Z	18	10	8	0	0
4	15	0	Total	С	Ο	0	0
4	GG	Z	18	10	8	0	0
4	h7	0	Total	С	0	0	0
4	D7	2	18	10	8	0	0
4	b0	n	Total	С	0	0	0
4	60	2	18	10	8	0	0
4	-0	0	Total	С	Ο	0	0
4	co	2	18	10	8	0	0
4	1	0	Total	С	Ο	0	0
4	CI	2	18	10	8	0	0
4	റി	n	Total	С	Ο	0	0
4	CZ	2	18	10	8	0	0
4		2	Total	С	Ο	0	0
4	03	2	18	10	8	0	
4	4	0	Total	С	Ο	0	0
4	C4	2	18	10	8	0	0
4	o5	2	Total	С	0	0	0
4	0	2	18	10	8	0	0
4	ch	9	Total	С	0	0	0
4	0	2	18	10	8	0	
4	c7	9	Total	С	0	0	0
-1	CI	2	18	10	8	0	0
4	c8	9	Total	С	0	0	0
т	0		18	10	8	0	0
4	c0	9	Total	С	Ο	0	0
	0	2	18	10	8	0	0
4	d1	9	Total	С	Ο	0	0
	ui	2	18	10	8	0	0
	d2	2	Total	С	Ο	0	
, I	42	<u></u>	18	10	8		0
	d3	2	Total	\mathbf{C}	Ο	0	0
-	40		18	10	8		0
4	d4	2	Total	\mathbf{C}	Ο	0	0
		-	18	10	8		0
4	45	9	Total	С	0	Ο	0
	40	2	18	10	8	0	U
4	ല	2	Total	С	Ο	0	
4 e0	2	18	10	8		U	



Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf	Trace	
4	- 1	0	Total	С	Ο	0	0
4	er	2	18	10	8	0	0
4	- 0	0	Total	С	Ο	0	0
4	ez	2	18	10	8	0	0
4	. 4	0	Total	С	Ο	0	0
4	e4	2	18	10	8	0	0
4	- 5	0	Total	С	Ο	0	0
4	eə	2	18	10	8	0	0
4	- P	0	Total	С	Ο	0	0
4	eo	2	18	10	8	0	0
4	fO	0	Total	С	Ο	0	0
4	10	2	18	10	8	0	0
4	fð	0	Total	С	Ο	0	0
4	15	2	18	10	8	0	0
4	fE	ე	Total	С	Ο	0	0
4	10	2	18	10	8	0	0
4	fo	ე	Total	С	Ο	0	
4	10	2	18	10	8	0	0
4	ГЭ	ე	Total	С	0	0	0
4	ĿЭ	2	18	10	8	0	0
4	f2	n	Total	С	Ο	0	0
4		2	18	10	8	0	0
4		ე	Total	С	Ο	0	0
4	er	2	18	10	8	0	0
4	06	9	Total	С	Ο	0	0
4	eo	2	18	10	8	0	0
4	03	9	Total	С	Ο	0	0
-1	60	2	18	10	8	0	0
4	65	9	Total	С	Ο	0	0
т	u.	2	18	10	8	0	0
	d7	9	Total	С	Ο	0	0
	ui	2	18	10	8	0	0
	48	2	Total	\mathbf{C}	Ο	0	
	uu	-	18	10	8		0
4	46	2	Total	С	Ο	0	
	40		18	10	8		0
	d0	2	Total	\mathbf{C}	Ο	0	
		<u> </u>	18	10	8		
4	F5	2	Total	С	Ο	0	0
		2	18	10	8		0
	F2	2	Total	\mathbf{C}	0	0	
4 F ⁻ 2		18	10	8		U	



Continued from previous page...

Mol	Chain	Residues	At	\mathbf{oms}		AltConf	Trace
4	$\mathrm{E7}$	2	Total 18	C 10	0 8	0	0

• Molecule 5 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(5-5)-beta-L-arabinofuranose.

Mol	Chain	Residues	Ato	oms		AltConf	Trace
5	16	4	Total	С	0	0	0
0	AU	4	36	20	16	0	0
5	4.0	4	Total	С	0	0	0
0	ЛJ	1	36	20	16	0	0
5	B6	4	Total	С	Ο	0	0
0	D0	1	36	20	16	0	0
5	F6	4	Total	С	Ο	Ο	0
0	10	1	36	20	16	0	0
5	F7	1	Total	С	Ο	0	Ο
0	11	Ŧ	36	20	16	0	
5	аб	4	Total	\mathbf{C}	Ο	0	0
0	au	a0	36	20	16	0	
5	₂ 0	4	Total	С	Ο	0	0
		1	36	20	16		0
5	b6	4	Total	\mathbf{C}	Ο	0	0
		1	36	20	16	0	0
5	f6	4	Total	С	Ο	0	0
	10	4	36	20	16		0
5	f7	f7 4	Total	С	Ο	0	0
0 17	11		36	20	16		U

• Molecule 6 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	At	\mathbf{oms}		AltConf	Trace
6	E6	8	Total 72	C 40	O 32	0	0

• Molecule 7 is an oligosaccharide called beta-L-arabinofuranose-(1-4)-beta-L-ribulofuranose.

Mol	Chain	Residues	Atoms		AltConf	Trace	
7	a4	2	Total 18	C 10	0 8	0	0



• Molecule 8 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms		AltConf	Trace	
0	-0	6	Total	С	0	0	0
0	8 e9	0	54	30	24	0	U

• Molecule 9 is beta-L-glucofuranose (three-letter code: A1AIO) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 11 6 5 \end{array}$	0
9	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 11 6 5 \end{array}$	0
9	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 11 6 5 \end{array}$	0
9	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 11 6 5 \end{array}$	0
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \overline{\text{O}} \\ 11 & 6 & 5 \end{array}$	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	А	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 11 & 6 & 5 \end{array}$	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 11 & 6 & 5 \end{array}$	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	В	1	Total C O	0
9	В	1	Total C O	0
		-	11 6 5	Ŭ
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 11 6 5 \end{array}$	0
9	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 11 6 5 \end{array}$	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 11 & 6 & 5 \end{array}$	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 11 6 5 \end{array}$	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 11 & 6 & 5 \end{array}$	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	Total C O 11 6 5	0
9	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 11 6 5 \end{array}$	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 11 & 6 & 5 \end{array}$	0
9	В	1	Total C O 11 6 5	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	В	1	Total C O 11 6 5	0

• Molecule 10 is alpha-D-galactopyranose (three-letter code: GLA) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
10	Δ	1	Total C O	0
10	Л	1	11 6 5	0
10	Δ	1	Total C O	0
10	11	I	11 6 5	0
10	Δ	1	Total C O	0
10	11	Ĩ	11 6 5	0
10	А	1	Total C O	0
10	11	Ĩ	11 6 5	0
10	Δ	1	Total C O	0
10	11	I	11 6 5	0
10	Δ	1	Total C O	0
10	11	1	11 6 5	0
10	Δ	1	Total C O	0
10	11	I	11 6 5	0
10	Δ	1	Total C O	0
10	11	I	11 6 5	0
10	Δ	1	Total C O	0
10	1	I	11 6 5	0
10	Δ	1	Total C O	0
10	11	1	11 6 5	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
10	٨	1	Total C O	0
10	A	L	11 6 5	0
10	٨	1	Total C O	0
10	A	L	11 6 5	0
10	Λ	1	Total C O	0
10	Л	T	11 6 5	0
10	В	1	Total C O	0
10	D	I	11 6 5	0
10	В	1	Total C O	0
10	D	T	11 6 5	0
10	В	1	Total C O	0
10	D	T	11 6 5	0
10	В	1	Total C O	0
10	Б	1	11 6 5	0
10	В	1	Total C O	0
10	D	1	11 6 5	0
10	В	1	Total C O	0
10		-	11 6 5	
10	В	1	Total C O	0
		-	11 6 5	Ŭ
10	В	1	Total C O	0
		-	11 6 5	Ŭ
10	В	1	Total C O	0
		-	11 6 5	Ŭ
10	В	1	Total C O	0
	_	_	11 6 5	
10	В	1	Total C O	0
			11 6 5	_
10	В	1	Total C O	0
	_	_	11 6 5	~
10	В	1	Total C O	0
		÷	11 6 5	



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: Tyrosine-protein kinase ephrin type A/B receptor-like domain-containing protein

Chain A:	90%	6% •	
MET MET MET MET MET PRO ALA ARG ARG ARG ARG ARG ARG ARG ARG ARG AR	VALC VALC LEU VAL VAL VAL ALA ALA ALA ALA ALA ALA ALA	R206 R239 Y262 7415 8430	
A443 ◆ A470 E502 ◆ E502 ◆ E502 ◆ E565 E565 S67 S662 F662	D7 26 F7 33 F7 39 C7 90 F8 33 F907 F907 F907 F907 F907 F133 C1110 D1145 D1145 D1145 D1145 D1145 D1145 D1145 D1145 D1145	K1286 C1317 N1379 D1394 K1399	
S1443 S1488 S1488 B1534 F1537 F1537 F1537 F1537 F1537 F1537 F1571 F1677	1/1688 1/1688 1/1688 1/178 1/1723 1/1746 <th 1746<<="" th=""><th>P1860 S1966 S1966 P1865 P1865 P1865 P1865 P1865 P1865</th></th>	<th>P1860 S1966 S1966 P1865 P1865 P1865 P1865 P1865 P1865</th>	P1860 S1966 S1966 P1865 P1865 P1865 P1865 P1865 P1865
S1869 P1870 P1872 P1872 P1875 P1875 P1875 P1876 P1876 P1876 P1880 P1880 P1882 P1882 P1882 P1882 P1886 P1886 P1886 P1886 P1886 P1886 P1886 P1886 P1889 P1887 P1887	P1893 P1894 P1894 P1894 P1896 P1890 P1900 P1900 P1900 P1910 P1910 P1911 P1911 P1911 P1911 P19115 P19112 P19112 P19113 P19115 P19113 P19115 P19113 P19115 P19115 P19113 P19115 P19	P1920 P1921 P1923 P1923 P1929 P1929 P1931	
P1982 V1943 V1943 P1946 P1946 P1946 P1946 CLV ALA ALA ALA ALA ALA ALA ALA ALA ALA A	ALA ALA GLU GLU GLU GLU ALA ASP CLU PRO GLU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP		
• Molecule 1: Tyrosine-protein tein	n kinase ephrin type A/B receptor-	like domain-containing pro-	
Chain B:	90%	6% ·	





A FIG71 7 T1677 88 T1677 99 11677 99 11677 99 11677 99 11677 98 11677 99 11677 99 11677 99 11688 99 1188 98 11686 111 11666 112 11866 113 11866 114 11866 115 11866 116 11866 118 11866 118 11866 118 11866 118 11866 118 11866 118 11866 118 11866 118 11866 118 11866 118 11866 118 11866 118 11866 118 11886 118 1

ALA GLU GLU GLU GLU GLU GLU AASP CLU MET GLU MET GLU GLU ASP GLU GLU GLU

• Molecule 2: C-type lectin domain-containing protein

Chain X: 99% NEW PRODUCTION OF THE PRODUCTI PRODUCT OF CONTRACT OF CONTRAC PROPERTIGATION OF THE CONTRACT PROCONCIPACIÓN DE LA CONCINENCIA DE LA CONCINENC REAL OF A CONTRACT OF A CONTRA ALLEAU AL SERVICE AND ADDRESS AND ADDRESS AND ADDRESS AD PRODUCT STATEMENT STATEMEN



PHE	THR	GLN	ASP	GLY	SER	PRO PPO	THR	PHE	GI.N	TRP	ALA	ALA	VAL	TYR	THR	PRD	ARG	PRO	VAL	ALA	CYS	ALA	SER VAT	ASP	PRO	THR	GLY	PHE	GLN TYR	VAL	PRO ALA	GLY	CYS	VAL	GLN	LEU PRO	ALA	CYS	ARG	ALA ALA	THR	ALA	ASN
ALA	ILE	ALA	PRO	PRO	PRO	PRO	PRO	ALA	PRO PRO	PRO	PRO	ALA	THR	ALA	VAL	THR	ARG	VAL	CLY GLY	TYR	LEU	TYR	SER 1 FII	TYR	ASN	GLU	ALA ALA	LEU	TYR	PRO	GLU AL.A	ALA	ALA TVB	CYS	ARG	ALA GLY	GLY	GLY TYR	LEU	ALA SER	PHE	HIS	0ELU LEU
ALA	GLU	PHE	ALA	VAL	SER	TYR Met	THR	THR	THR AI.A	THR	ALA	LEU	ALA ALA	GLY	ASP	SER	VAL	TRP	ILE	TYR	ASP	GLU	ILE CI V	ARG	ASN	GLU	TEU	LEU	ARG	TEU	ASP GLY	GLY	PRO AT A	ALA	TRP	STH STH	PHE	GLY	PRO	THR	ASP	THR	ATD OTA
ASN	ASP	CYS AT A	ALA	VAL	GLN	LEU	GLY	GLY	GLN TRP	VAL	MET	ASP	CYS	LEU	GLU	ARG	PRO	PHE	ILE	LYS	ARG	LEU	LEU LEU	ILE	SER	ALA	PRO	ALA	PR.O	PRO	ALA ALA	VAL	ALA AT A	SER	PRO	PR.0 PR.0	LEU	ALA SER	LEU	PRU ALA	TEU	ARG	VICH
THR	VAL	ALA	VAL	LEU	GLN	TYR VAI	ALA	SER	PRO ALA	LEU	SER	TYR	ALA	ALA	ASP	ALA ALA	CYS	THR	GLN	TYR TYR	GLY	VAL	LEU	TRP	PHE	ALA	ALA	SER	GLU PHE	ASN	ALA VAL	MET	LEU	LEU	GLN	ALA ASP	VAL	GLY	LEU	ASP ASP	PRO	SER	TRP
PHE	GLY	LEU	ARG	SER	ALA	ASN	ALA	ASP	TRP PHE	TRP	TYR	GLY	THR	THR	LEU	GI.Y	THR	ALA	MET	ALA ASP	PRO	ALA	GLN	LEU	PHE	ASN	THR	SER	ALA	CYS	ALA	TEU	GLY	SER	LEU	TYR	GLN	ASP	ASN	GLY GLY	GLY	ASP	ARG
CYS	VAL	ALA	SER	VAL	ASP	ALA	GLY	GLY	SER TYR	CYS	TYR	ARG	ASP	ASP	ARG	ALA CYS	ASP	GLN	ARG	0TY	PHE	ILE	CYS	VAL	ASP	ASP	MET	PRO	LEU AL.A	PRO	SER	PRO	GLN GLN	PRO	PRO	PRO	PR0	GLY	PRO	LEU	PRO	PRO	PR0
ALA	PRO	PRO CT V	PRO	ASP	ASP	PRO PPO	SER	PRO	PRO AI.A	PRO	SER	ASP	HIS	ALA	PRO	PHE	PRO	PRO	ALA	PHE	VAL	PRO	CI II CI II	PRO	ALA	ALA	PRO	GLN	LYS	PRO	THR	PRO	PRO AT A	PRO	PRO	GLY SER	ASP	TRP	SER	ALA PRO	TRP	GLU	PR0
SER	ARG	PRO ATA	THR	PRO	PRO	PHE	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO	PRO	ALA	PRO	PRO	PRO	GLY	PRO	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO	PRO	PRO PRO	PRO	PRO GLN	SIH	PRO	LEU	PRO	PHE ALA	PRO	GLU	PRO	TYR	PRO	ASP	PR0
GLU	ALA	PRO DBO	PRO	PRO	PHE	GLU	GLY	VAL	P1453 P1454	P1455	P1456	P1457	P1459	P1460	P1461	P1462 P1463	P1464	P1465	1460	P1468 P1469	LEU	PRO	PRO SFR	GLN	PRO	GLY	VAL	SER	P1480 P1481	P1482	P1483 P1484	P1485	P1486 D1487	P1488	P1489	P1490 G1491	T1492	P1493	P1496	P1499	LEU	ALA	ALA
ALA	PRO	GLY	PRO	THR	PRO	ALA	ALA	GLU	SER	ALA	VAL	P1520	P1522	P1523	P1524	P1526	P1527	P1528	P1529	P1531	P1532	R1533	T1534 DB0	PRO	LEU	PRO	LYS	ALA	GLII	SIH	ALA P1546	P1547	P1548 D1540	P1550	P1551	P1552 P1553	P1554	P1556		P1559 S1560	T1561	P1562	A1564
HYP	SER	GLN	ALA	ALA	VAL	THR	SER	ALA	SER	PRO	PRO	ALA	PRO	GLY	A1585	P1587	P1588	P1589	P1590	P1592	P1593	P1594	P1595 D1596	F1030 P1597	P1598		P1601 P1602	T1603	ALA GLY	ALA	PRO GLY	ALA	P1610 D1611	P1612	P1613	P1614 P1615	P1616	P1617 P1618	P1619	P1620	P1623	D1624	41020 P1626
S1627	A1628	HYP AT A	ALA	PRO	VAL	PRO AT A	ALA	PRO	GLN	SER	PRO	PRO AT A	GLU	ASP	SER	GL.Y	ALA	VAL	PRO	PRO	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO	PRO	GLN THR	PRO	PRO ALA	CLN	PRO SED	GLY	THR	ALA	SER	PRO PRO	PRO	PRU PRO	PRO	PRO	PRO PRO
PRO	PRO	GLY	PRO	ASP	PRO	SER AT A	PRO	ALA	VAL	ALA	ALA	PR0	VAL	PRO	PRO	PRO	VAL	PRO	ALA	ASP	THR	TYR	THR AT A	PRO	PRO	PRO	PRO	PRO	PRO PRO	PRO	PR.O	PRO	PR0 CI V	THR	PRO	PRU	GLY	PRO	THR	GLU PRO	GLN	ALA	PRO
PRO	PRO	PRO	PRO	PRO	PRO	PRO	THR	PRO	SER ALA	PRO	ALA	ALA	SER	GLN	PRO	UAL.	PRO	SER	VAL	PRO	ASP	ALA	PRO PRO	PRO	GLY	LEU	GLY	ALA	PRO PRO	PRO	PRO PRO	PRO	PRO PPO	PRO	PRO	PRO	PRO	GLY VAL	PRO	THR	ALA	SER	PRO
GLY	ALA	PRO	PRO	PRO	PRO	PRO PPO	PRO	PRO	PRO GLY	ALA	PRO	ASP	PRO	ALA	ALA	L'EU	ALA	PRO	ARG	ASP	THR	GLN	SER	GLY	ALA	PRO	PRO	ALA	LEU PRO	GLY	ALA PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLY	VAL	PRO	THR
ALA	GLY	ALA	GLY	ALA	PRO	PRO PPO	PRO	PRO	PR.O PR.O	PRO	PRO	PRO CT V	SER	PRO	ASP	PRO	SER	ALA	PRO AT A	ALA ALA	PRO	SER	VAL	ALA	ALA	PRO	PRO	SER	PR.O PR.O	ALA	GLU	SER	THR	ALA	VAL	PRO PRO	PRO	PRO	PRO	DRO PRO	PRO	PRO	PRO PRO
PRO	GLN	THR	PRO	ALA	PR0 PR0	ALA	THR	ALA	ALA SFR	PRO	PRO	PRO Dar	PRO	PRO	PRO	PRO	PRO	PRO	GLY	PRO	ASP	GLN	PR0 SFB	ALA	PRO	ALA	PRO	ALA	ALA	ALA	VAL	SER	PRO DBO	VAL	PRO	ALA PRO	ASP	TYR	THR	ALA PRO	PRO	PRO	PRO PRO
PRO	PRO	PRO	PRO	PRO	PRO	GLY	PRO	PRO	SER GLY	GLN	PRO	THR	PRO	GLN	ALA	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO PRO	GLY	THR	PRO	ALA	PRO	ALA	PRO	SER	PRO	SER	PRO	ALA	ALA LYS	VAL	ASP SER	PRO	PRO PRO	GLY	LEU	ASP



Page 25	
---------	--

ALA	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO	PRO PRO	PRO	GLY	VAL	PRO	ALA	ALA	SER ATA	PRO	GLY	PRO	PRO	PRO	PRO PRO	PRO	PRO PRO	PRO	PRO PPO	GLY	ALA	PRO ASP	GLN	PRO AT A	THR	PRO	LEU AT A	PRO	ARG	PRO	THR	GLN	THR PRO	GLY	ALA	PRO	PRO
ALA	PRO	GLY	ALA	PRO	PRO	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO PRO	GLY	MET	PRO PRO	THR	ALA	AL.A	PRO	GLY	ALA PRO	PRO	PR.O PR.O	PRO	PRO PPO	PRO	PRO	PRO PRO	GLY	SER	ASP	CLLN	PRO SFR	ALA	PRO	ALA	PRO	SER	VAL PRO	ALA	ALA	GLN	PRO
SER	PRO	ALA	GLU	SER	THR	ALA	VAL	PR.O	PRO	PRO	PRO	PRO	PRO	PRO	PR.O	PRO	PRO	THR	PRO	PRO	ALA GLN	PRO	ALA GLY	THR	ALA ATA	SER	PRO	PRO PRO	PRO	PRO	PRO	PRO	PR.O	PRO	GLY	SER	ASP	GLN	PR0 SER	ALA	PRO	THR	PRO
ALA	PRO	ALA	VAL	SER	PRO	VAL	PRO	ALA	ASP	THR	TYR	ALA	PRO	PRO	PR.O	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLY THR	PRO	PR0 sep	GLY	GLN	PR0 THR	GLU	PR0	ALA	PRO	PRO PRO	PRO	PRO	PRO Dad	PRO	PRO	PRO PRO	GLY	THR	SER	ALA
PRO AT A	ALA	PRO	SER	PRO	SER	PRO	ALA	ALA I VS	VAL	ASP	SER	PRO	PRO	GLY	LEU	ASP	ALA	PRO	PRO	PRO	PRO	PRO	PRO PRO	PRO	PRO PPO	PRO	GLY	VAL PRO	PRO	THR	THR	ALA	PRO GI V	ALA	PRO	PRO Dad	PRO	PRO	PRO PRO	PRO	PRO	PRO	GLY
ALA	ASP	GLN	PRO ATA	ALA	PRO	ALA ARG	PRO	GLY	ASP	ALA	PRO	ALA	PRO	PRO	PRO AT A	GLN	PRO	AL.A	PRO	PRO	PRO	PRO	PRO PRO	PRO	PRO PPO	PRO	PRO	PRO	VAL	PRO	PRO	THR	PRO ASP	ALA	ALA	ALA	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO
PR0	GLY	SER	PRO ASP	GLN	PRO	ALA HIS	PRO	ALA THR	PRO	SER	VAL	PRO ALA	ALA	PRO	GLN	PRO	PRO	ASP	LYS	GLU	ASP ALA	ALA	PR.0 PR.0	PRO	PR.0	PRO	PRO	PR0 PR0	PRO	PR0	PRO	GLY	VAL	ASP	ALA	PRO	THR	THR	GLN AI.A	PRO	ALA	ALA PRO	PRO
PRO	PRO	PRO	PR.O PR.O	PRO	PRO	GLY	THR	PRO THR	MET	PRO	GLY	ALA PRO	THR	LYS	PRO CI V	ALA	PRO I EU	AL.A	PRO	GLU	GLN PRD	ALA	GLU	ALA	PR.O	GLY	ALA	PRO PRO	PRO	PRO	PRO	PRO	PR.O	PRO	PRO	PRO PBO	ASP	ALA	PRO LEU	PRO	PRO	ALA	ARG
ALA	ASP	ALA	PRO PRO	PRO	PRO	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO PRO	PRO	GLY	ALA PRO	ASP	ALA	AT.A	ALA	PRO	ALA GLN	PRO	THR ALA	SER	THR	PRO	ASP	ALA PRO	PRO	PRO	ALA LEU	PRO	ASP AT A	PRO	PRO	PRO Dao	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO
TY	RO R	RO	LA I	AL .	TA	SP	TA	RO RO	N. O.	RO	RO	RU RU		RO	RO P	TY	LA	D dS	ILN	RO	T.A	RO	RG	RO	T.Y	SP	LA	R0 LA	TA	RO DO	RO RO	TA	EN .	TY	TA	RO PO	RO	RO	RO	RO	RO	L L L	RO
0,00	E E E	AL P			HR A	SP A	AA	A P	A P	SO P	SO P		- L L L L	20 P		, 0 , 0	20 A		ER G	20 E	N A	SO P	A A	SO P	A D		SR A		A	A P	N P	30 A		TI C	SP A	S P	P P	A P	A P	EO P	P C	0, 0, 7 4	20 P
		۰۸ ۵			E .	A D	P AI	A D	E A	R	R PI			A PI	A D		0 0 0			I I I I I I I I I I I I I I I I I I I		I d	о Н. Н.	R PI		T H	IS I	A VI	. U	R Al		Y PI	A D	. ~ 	A AS		N AS	O AI	A AI U PI	PI	A Pi		Y Pi
PR	PR DR	PR DR	R PR	PR DR	: CI	PR DR	AS AS	AL DR	VA (E	日日	19 10	T H	AL AL	AL DR	E BR	PR	AT AT	PR	PR 1	HH I	PR	EL PR	E	PR DR	E E	PR	AL GL	PR	EL	DR DR	GL	AL AL	: E	I AL	H E	3 5	PR	L AL CL	IH	AL	A HA	CL
AL/	PRC	PRC	PRC	PRC	PRC	PRC	PRC	PRC	PRC	ASF	AL/		PRC	PRC	PRC AT /	ARC	AL/	ASF	AL/	PRC	PRC	PRC	PRC	PRC	PRC	PRC	PRC	GLY ALA	PRC	ASF	PRC	AL/	AL/ PRC	AL/	GLN	PRC	AL/	SEF	HL.	PRC	ASF	PRC	PRC
PRO AT A	LEU	PRO	ASP	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLY	VAL	PRO	LYS	AT.A	ALA	VAL	ASP ALA	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	ATD GTY	PRO	ASP	GLN	ALA	ALA	PRO	SER	PRO	GLY ALA	PRO	GLY	THR	ALA
PRO	PRO	ALA	HIS	ASP	ALA	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO CI V	VAL	PRO	PRO	ALA	PRO	GLY THR	THR	PRO	PRO	PR0 PP0	PRO	PRO	PRO PRO	PRO	PRO	PRO	GLN	THR	ALA	MET	PRO	VAL	PRO	SER	GLY	GLN	ALA	ALA
PRO TI E	ALA	PRO	SER	PRO	VAL	GLU GLU	ASP	ALA	ALA	PRO	PRO	PRO	PRO	PRO	PRO DRO	PRO	PRO	PRO	PRO	GLY	THR PRO	ALA	ALA PRO	PRO	GLN	SER	ALA	PR0 GLN	ALA	PRO	PRO	PRO	PR.0 PR.0	PRO	PRO	PR0	PRO	GLY	THR PRO	ASP	ALA	ALA	MET
PRO	LEU	PRO	ASP	PRO	LEU	PRO	GLY	ALA VAT	GLN	GLN	PRO	PRU ALA	ALA	PRO	CLY GLY	PRO	PRO	PRO	PRO	PRO	PRO PRO	PRO	PRO PRO	PRO	PRO	ALA	PRO	PRO VAL	PRO	4TD	PRO	ASN	ALA ATA	PRO	PRO	PRO	PRO	PRO	PRO PRO	PRO	PRO	GLY	ALA
PRO A CD	GLN	PRO	ALA	PRO	ALA	PRO	GLY	PRO	ALA	PRO	SER	ALA PRO	PRO	PRO	HIS I FII	PRO	ASP	PRO	PRO	PRO	PRO	PRO	PRO PRO	PRO	PRO PPO	PRO	PRO	GLY VAL	PRO	PRO	ILE	PRO	ASP	ALA	ALA	ALA	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO
PRO AT V	SER	PRO	ASP	PRO	ALA	PRO	ALA	SER	ASP	ALA	PRO	GLY PRO	THR	ALA	PR.O	PRO	ALA	DRO	ASP	THR	PRO	PRO	PR0 PR0	PRO	PRO DBO	PRO	PR0	PRO PRO	PRO	ASP	ALA PRO	PRO	SER	ARG	THR	HIS	GLY	LYS	GLY	ASP	ASP	ASP	PHE
ALA	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO	PRO GI V	MET	PRO	ASP	PRO	ALA	VAL	PRO SFR	GLN	PRO	AL.A	PRO	MET	PRO	ALA	ALA GLU	GLN	VAL	ALA	SER	PR0 PR0	ARG	LEU	PRO	PRO	PR.O	PRO	PRO	PR0	PRO	PRO	PRO PRO	THR	THR	PRO	PRO



GLU	ASP	HIS	THR AI A	PRO	ALA	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO GLY	THR	PRO	MET	PRO	SER VAL	PRO	ALA	THR PRO	GLU	ASP VAL	SER	VAL	ARG	ASP	ALA PRO	PRO PRO	SER	PRO	GLY ALA	PRO	PRO	PRO PRO	PRO	PRO	PRO PRO
PRO	PRO	GLY	ALA	PRO	ALA	PRO	PRO	GLN	ALA	SER	PRO	PRO	PRO	PR.O	PRO	PRO	PRO	PRO	GLY THR	PRO	ASP	ALA PRO	ALA	ASP TLE	LYS	ASP TRP	SER	PRO	ASP ALA	PRO ALA	ALA	PRO	PRO ALA	LEU	ASP	ALA PRO	PRO	PRO	PRO PRO
PRO	PRO	PRO	PR.O	PRO	GLY	PRO	PRO	PRO TUD	PRO	VAL	ASP ALA	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO	PR.O PR.O	PRO	PRO	SER VAL	PRO	PR0 PR0	PRO	LEU	ASP	GLY	VAL PRO	ASP LEU	PRO	SER	PRO PRO	PRO	ASP	GLN	GLY	PRO	PRO PRO
PRO	PRO	PRO	PR.O	PRO	PRO	PRO	GLY	VAL	PRO	PRO	LEU	SER	PRO	PR.O PR.O	ASP	ALA	PRO	PRO	PR.O PR.O	PRO	PRO	PRO PRO	PRO	PRO GLY	ALA	PRU ALA	MET	THR	VAL PRO	THR GLN	PRO CT V	ALA	PRO GLN	PRO	ASP	ALA AI.A	ASP	PRO	ALA VAL
PRO	ASP	LEU	PRO PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO PRO	ALA	ILE	PRO PRO	PRO	THR	ASP	ALA	ALA L'EII	SER	PRO	LEU PRO	PRO	PRO PRO	PRO	PRO PRO	PRO PRO	PRO	PRO PRO	GLY THR	PRO PHF	THR	PRO ASP	THR	ALA	ASP TRP	SER	PRO	ASP ALA
PRO	ALA ALA	PRO	PRO PRO	GLY	GLU	ASN	ALA	PRO	PRO	PRO	PRO PRO	PRO	PRO	PRO PRO	PRO	PRO	GLY	ALA	PRO PRO	ALA	GLN	PRO PRO	GLN	ASP ALA	SER	PRO PRO	PRO PRO	PRO	PRO PRO	PRO PRO	PRO	GLY	THR PRO	ASP	PRO	ALA ASP	ILE	ASP	TRP SER
GLN	ASP	ALA	PRO AT A	THR	PRO	PRO	ALA	LEU	ASP	ALA	PRO PRO	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO	PRO PRO	GLY	VAL	PRO PRO	PRO	THR PRO	VAL	ASP ALA	PRO PRO	PRO	PRO PRO	PRO PRO	PRO	PRO	PRO PRO	PRO CT V	ALA	PR.O PR.O	PRO	VAL.	LEU ASP
VAL	GLY VAL	PRO	ASP	PRO	PRO	PRU	PRO	PRO	ASP	GLN	PRO CI V	ALA	PRO	PRO PRO	PRO	PRO	PRO	PRO	PRO PRO	PRO	PRO	PR0 GLY	ALA	PRO PRO	PRO	ASN	THR	PRO	ALA PRO	PRO PRO	PRO	PRO	PRO PRO	PRO	PRO	PRO GLY	THR	ASP	MET PRO
MET	VAL PRO	ARG	ALA	ASN	ALA	ASN	VAL	PRO	PRO	PRO	ALA I FII	PRO	ALA	SER	PRO	ASP	PRO	PRO	PRO PRO	PRO	PRO	PRO PRO	PRO	PRO PRO	PRO	GLY	SER	ALA	SER PRO	TLE PRO	LEU	VAL	SER PRO	PRO	PRO	PRO PRO	PRO	PRO	PRO PRO
PRO	SER	THR	PRO ASP	THR	PRO	LEU	PRO	ASN 1 ETI	PRO	PRO	SER	PRO	MET	PRO PRO	GLU	ILE	PRO	PRO	ASP ALA	PRO	PRO	PRO PRO	PRO	PRO PRO	PRO	PRO PRO	PRO	PRO	ASP VAL	PRO PRO	PRO CI V	SER	PRO PRO	LEU	SER	PRO	PRO	PRO	PRO PRO
PRO	PRO	PRO	PRO AT A	THR	PRO	ACF AI.A	PRO	ALA	ILE	LYS	ASP	SER	CLN	PRO ASP	ALA	PRO	ALA ALA	PRO	PRO PRO	ALA	PHE	PRO ASP	ALA	PRO PRO	PRO	PRO PRO	PRO PRO	PRO	PRO PRO	PRO PRO	PRO GI V	ALA	PRO PRO	PRO	PRO	LYS ASP	SER	PRO	PR0 PR0
PRO	PRO	PRO	PR.O	PRO	PRO	PRO	GLY	VAL	PRO	THR	PRO CI II	PHE	ASP	PRO GLY	VAL	PRO	LEU	PRO	PRO SER	PRO	PRO	PRO PRO	ASP	GLN	SER	ALA PRO	PRO	PRO	PRO PRO	PRO PRO	PRO	PRO	PRO PRO	GLY	PRO	PRO GLY	VAL	GL.Y	LEU PRO
ASP	PRO	PRO	PRO PRO	PRO	PRO	PRO	PRO	PRO	GLY	THR	PRO	MET	PRO	THR	PRO	GLY	PRO	GLY	PRO PRO	PRO	PRO	PRO PRO	PRO	PRO PRO	PRO	GLY	ALA	ALA	ARG ASP	PRO PRO	PRO	PRO	PRO PRO	PRO	PRO	PRO PRO	PRO	MET	PRO PRO
GLY	PRO	SER	SER	LEU	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLY ALA	PRO	PRO	PRO	ASN	PRO	GLN	GLN	PRO PRO	PRO	LEU GLU	PRO	ASP MET	PRO	PRO	ASP PHE	PRO SER	THR	PRO	PRO PRO	PRO	PRO	PRO PRO	PRO	PRO	PRO PRO
GLY	PRO	PRO	PR.O	SER	PRO	PRO	ASP	ALA	PRO	PRO	PRO PRO	PRO	PRO	PR.O PR.O	PRO	PRO	GLU	PRO	PR.O PR.O	PRO	SER	GLY	VAL	PRO LEU	ALA	PRU LEU	ALA	GLY	LEU PRO	PR0 PR0	PRO	ARG	PRO ARG	PRO	PRO	PRO LYS	PRO	PRO	PRO PRO
PRO	PRO PRO	PRO	ASP	PRO	PRO	AT.A AI.A	PRO	ASP	PRO	ILE	PRO CI N	SER	PRO	PR.O PR.O	PRO	PRO	PRO	PRO	PR.O PR.O	PRO	ILE	PRO PRO	PRO	PR.O PR.O	PRO	PRO PRO	PRO PRO	PRO	PRO PRO	PR0 LEU	ALA	SER	PRO PRO	PRO	PRO	PR.0 PR.0	PRO	UTU GLU	PR.O THR
ALA	VAL	ASP	GLN	LEU	GLY	GL.N	PRO	PRO	PRO	PRO	PRO I FII	ASN	LEU	THR ASP	VAL	SER	ALA	ASN	THR	GLY	GLY	ARG THR	THR	GLY	ASP	ALA VAL	PRO	ALA	VAL THR	SER	PRO CI V	ASN	THR PHE	ASP	ASP	ALA TYR	ARG	VAL.	PRO VAL
VAL	ALA	ASN	VAL THR	VAL	VAL	ASP	ALA	TRP MET	GLN	PRO	GLN I FII	TYR	GLU	LYS	ARG	ARG	GLU	PHE	ALA	VAL	MET	GLN	VAL	LEU PRO	PHE	GLN	TYR I FII	ILE	ARG VAL	ARG VAL	ASN 1 VS	TEU	THR TRP	ARG	GLY	ASP TYR	LEU	GLU	GLN ARG
ASN	THR	LEU	THR AT A	ARG	GLY	PRO	PRO	PR0 SED	PRO	PRO	ALA	PRO	ARG	ALA PRO	GLY	SER	ALA	LEU	SER	PRO	PRO	PRO PRO	PRO	PR.O PR.O	PRO	PRU SER	ASN	THR	SER TYR	PR0 ARG	MET THR	TEU	PHE	GLN	TYR	AL.A GI.U	MET	THR	GLU ALA
ASP	ARG	ALA	GLY	GLY	SER	ALA ALA	LEU	VAL	SER	PHE	GLN	SER	ARG	PRO	VAL	TYR	ALA LEU	SER	LEU GL.Y	ALA	THR	SER	THR	SER TYR	THR	VAL TYR	THR	ARG	LEU	VAL THR	ASP	GLN	PR0 PR0	GLN	THR	LEU	GLY	PRO	GLU VAL



PHE	VAL	PRO LEU	TYR	GLY	TYR	CLII	LEU	GLY	ALA	ALA	TYR	ASP LEU	LEU	ASP	GLY	ILE	ASN	ASP	ASP	VAL.	ILE	ILE	ASN	LEU	ARG	TRP	ASN	SER	GLU	CYS	CYS	THR	THR	PHE	ILE	ASP	THR	GLN	VAL	GLU	PRO	ASP	PRO	PHE
TLE	VAL	THR TYR	ASP	VAL	ASP	PHE VAL.	TRP	ASN	ALA	PRO	THR	CAL GLN	ARG	LYS	VAL	VAL	TYR	ASP	PRO	CYS ALA	GLN	ALA	SER	GI.Y	VAL	GLU	ARG THR	CYS	PRO	THR	ARG	CYS	SER	VAL I ETI	GLY	GLY	VAL	GLY	SER	ALA THR	LEU	PHE SER	ASP	ILE
ARG	ASP	LEU ALA	THR	PRO	THR	GLU PRO	ASP	PRO	ASN	PRO	GLY GLY	THR	TEU	GLY	ILE	THR	LEU	SER	SER	PRO	VAL	TYR	ASP	THR	ILE	PRO	ASN I FII	GLN	LEU	PR0	LEU	GLY	LEU	PHE	VAL	ILE	PRO	ASN	LEU	ASP GLY	THR	PRO GLV	LEU	GLN
GL Y	THR	LEU THR	TYR	LEU	VAL	GLY	PRO	TRP	GLU	PRO	GLY	TYR TLE	ALA	ASN	ASP	ARG	ASP	ASP	SER	GLN	CLN	HIS	VAL	VAL	ARG	TYR	ALA GI II	TEU	VAL	THR	THR	PRO	THR	PRO PRO	ASN	THR	PRO	ALA	ILE	THR	ASP	VAL	ASP	VAL
SER	GLY	ASN	ALA	ILE	GLN	VAL	LEU	VAL	VAL	LEU	CYS	PRO ALA	THR	LEU	PRO VAT	LEU	CYS	PRO	PRO	GLU	ARG	VAL	LEU	ALA ARG	PRO	VAL	TRP	CYS	ALA	GLU	VAL	GLY	VAL	PRO	PHE	PHE	THR	ALA	LEU	GLY GLY	ALA	ALA ALA	VAL	PRO
AT.A	VAL	THR	ASN	THR	PRO	VAL	ARG	LEU	ASP	ASN	LYS	T YR LEU	VAL	THR	TLE	ASP	ASN	ALA	THR	ALA ALA	ARG	CYS	PRO	ASP	GLY	ASP	PRO THR	GLY	PRO	ASP	SER	VAL	THR	ALA THR	ASP	ALA	GLU	GLY	ASP	ILE SER	TYR	LYS VAL	HIS	ALA
PHE	CYS	ALA ASP	VAL	SER	ALA	GLY VAL.	ASP	THR	TRP	GLU	ALA	VAL GL.Y	TEU	ALA	ALA	GLN	PHE	GL Y	ASN	VAL LEU	LYS	ALA	GLY	ARG	VAL	ILE	TVB	THR	VAL	ASP	THR	GLY	ALA	THR	GLN	ILE	SER	THR	LEU	LEU VAL	MET	GLN	CYS	GLU
ASP	GLY	GLU VAL	GLN	CYS	ASP	GLY THR	CYS	THR	PHE	ASN	CYS	ASP	PRO	SER	THR	ILE	THR	LEU	THR	DHE	GLY	ASN	GLY	ASP	ASP	THR	THR CI V	SER	GLY	ASN	VAL	ASP	GLY	SER	PHE	VAL	ASP	SER	ASN	THR	THR	SER THR	VAL	ASN
ASP	ILE	THR GLY	GLY	GLY	SER	ILE	THR	ALA	ALA	SER	GLY	ALA PRO	VAL	VAL	SER	ASN	GLU	PRO	PRO	V AL TLE	ALA	LEU	ARG	ASN	THR	LEU	LEU	GLN	THR	GLN	VAL	GLN	ASN	PHE	TRP	ARG	ASN	CYS ARG	ALA	SER GLU	GLY	PRO	PRO	ALA
THR	LEU	GLU	LEU	GLY	GLN	ALA PHE	ASP	PRO	GLU	GLY	ASN	THR	ASN	THR	TVB	VAL	CYS	PRO	PRO	VAL ALA	CYS	LEU	ALA	THR	SER	SIH	LEU	CYS	ALA	SIH	GLU	THR	SER	LYS	VAL	ARG	GLY	CYS	ASP	THR GLY	ALA	ASP PRO	GLY	ASN
TLE	PHE	ASN VAL	ILE	PHE	VAL	CYS	ASN	GLY	VAL PRO	ARG	GLN	SER ALA	GLN	VAL	THR	THR	VAL	LEU	ILE AT A	ALA ARG	TAS	CYS	ALA	ALA GL.Y	TEU	TYR	GLU	ASP	GLY	CYS	GLU	VAL	PRO	CYS AT A	ALA	LYS	ALA	VAL	ALA	ASP	GLN	VAL VAL	ASN	ASN
THR	TEU	PRO ALA	LEU	ARG	LEU	PRO PRO	GLY	SER	ALA	GLU	ASN	ALA PRO	VAL	SER	ALA AT A	GLY	VAL	PRO	LEU	LEU	THR	GLN	ILE	THR	TYR	GLY	VAL	ALA	PRO	SER	PHE	PRO	CYS	ALA SFR	TYR	ASP	ALA	ALA	ALA	CYS AI.A	ALA	ILE ALA	MET	ASP
VAL.	GLU	ASP GLY	ASP	LEU	SER	PHE	ASN	VAL	ASP	ALA	THR	ASP CYS	SER	GLY	LYS	PRO	ASN	THR	CYS	ARG	CYS	ARG	PRO	GLU	TEU	SER	CI V	LYS	CYS	PRO PRO	GLY	TYR	ARG	LEU ABG	TYR	PHE	VAL	ASP	ASN	SER GLY	GLY	ILE SER	GLU	ALA
PHE	TRP	ASN PHE	ILE	VAL	SER	VAL	VAL	ASN	VAL	TRP	PHE	LEU MET	PRO	PRO	SER	ASN	ILE	SER	ALA	ALA	SER	ASN	SER	ASN	ALA	THR	ARG	PHE	MET	GLN	ILE	VAL	ASN	ALA THR	ARG	SER	ARG	PHE PHE	LEU	VAL GLY	GLN	LEU	ARG	PHE
GL Y	VAL	ASP LEU	LYS	ASP	ARG	SER. AL.A	ASN	VAL	SER	LEU	ALA	LEU VAL	ASN	THR	ASN	ASP	GLU	GLY	GLN	AT.A	ILE	ASN	ALA	ASP	CYS	ILE	CYS	ILE	ASN	VAL THR	LEU	DHE	THR	THR CI V	LEU	GLN	VAL	TYR	THR	VAL PRO	GLU	VAL	CLU	ILE
PHE	CLU	PR0 ASP	ASN	PHE	PRO	PR.O	GLY	ARG	ARG	PRO	PRO	PRO VAL	PRO	PRO	SER	PRO	PRO	SER	PRO AT A	PRD	ARG	PRO	PRO	PRO	PRO	ALA	PRO PRO	PRO	PRO	PRO	GLY	SER	PRO	PR.O	ALA	PRO	PRO	PRO	PRO	SER	PRO	PR.O THR	PRO	PRO
SER	PRO	PR0 GLN	PRO	PR0 GED	PRO	PRO PRO	PRO	PRO	PRO	ALA	PRO	PRO	PRO	SER	PRO PRO	ALA	PRO	PRO	PRO	V AL PRD	PRO	SER	PRO	ALA PRO	PRO	ARG	PRO PRO	ALA	PRO	THR	PRO	SER	PRO	PRO AT A	PRO	PRO	SER	PRO	LEU	PRO PRO	PRO	SER	GLY	PRO
PRU	PRO	GLY ASN	GLY	ASN	GLY	ARG	LEU	ILE	GLY	THR	PRO	ALA VAI.	ALA	PRO	ALA	ALA	PRO	ALA	ASN	ARG VAL	TRP	SER	TRP	GLY	ASP	TYR	GLU MFT	GLY	ALA	VAL TRP	SER	PRO	PRO	PRO I FII	GLN	ARG	LEU	ASN	GLN	LEU ARG	ARG	SER	SER	GLU
PRO	GLY	ALA ALA	ALA	GLY AT A	GLY	ALA	VAL	SER	TYR	ASP	ASP	ASP GLY	ASP	GLY	GLU AT A	ASP	TRP	ALA	PRO	PRO	PRO	ALA	ASP	TYR GLII	GLU	GLU	ASP	GLU	GLN	VAL	MET	VAL VAL	SER	ALA AT A	GLY	THR	HIS	GL Y PRO	GLY	ASP SER	ASP	ASP	PRO	LEU
PRO	TRP	GLY	SER	ALA	ALA	TRP	GLY	PRO	ALA	ALA	GLY	VAL AL.A	ARG	LYS	ALA	GLY	ALA	ALA	GL Y	GL.Y	SER	GLY	GLY	ALA GLN	SER	ALA	PRO AT A	PRO	ALA	SER	VAL	VAL	PRO	SER	LEU	HIS	THR	ALA LEU	MET	AI.A	SER	ALA	SER	GLU



_	_	_	_	_	_	_	_	_	_	_	_	_			_	_	_	_	_	_	_	_	_	_	_	_	_		_	_		_	_	_	_	_		_		_	_
ALA	GLY	PRO	ASP	PRO LEU	TEU	SER GLY	ALA	GLY	PRO	GLY	SER	GLY	ALA	GLY ALA	SER	ALA	GLY	ALA	PRO	ALA	ASN	THR	ALA	ALA	VAL LEU	GLY	ALA GLY	GLU	TUE	ALA	ALA	SER.	LEU	SER	GLY	ALA	ILE	GI.N	LEU	SIH	LYS
PRO AT A	LEU	GLN GLN	GLN	GLN ALA	ALA	ALA ALA	TEU	ALA	GLN	ALA	GLY PRO	SIH	GLN	GLY	TEU	PRO	ALA	THR	ALA	TYR	GLU	PRO PHE	GLY	GLY	HE SHE	GLY	GLY ALA	ASP	THR	ALA	SER	TEU	TEU	GLY ALA	ALA	ALA AT A	SIH	PRO ALA	ALA	GLY	ASN
GLY AL A	GLY	GLY GLY	LEU	VAL GLY	GLN	VAL VAL	ARG	GLY	ALA	ALA	LYS	ARG	ALA	SER VAL	GLY	VAL	GLY	LYS	VAL	THR	ARG	GLU GLV	GLU	GLN	ASP ASP	LEU	PR0 GLY	SER	GLY AT A	LEU	ARG	ALA	ALA	LEU GLU	GLU	ALA	ARG	ALA	THR	ALA AT A	ALA
LA	SP	RO T A	LA	ER LA	LA	LA ER	AL	LA	LA LA	LA	LE	RO	RG	YS T.Y	TN	LY VS	LY	ER	AL AL	LY	LA	LA HR	AL	LU LU	LA T.A	AL	LA ET	HE	ER	LA	LA	ER	EU	AL HR	LA	SP	IIS	EU SD	RO	RG	LE
40	. A	- Ц			A	4 0	>	- P	4 4	A	H C	, <u>с</u>	A ,			0 -	10	0		5 E	A	⊲ ⊢		С	A A		α 2		0.6	4 4	Α.	- 0			A	4 U	2 =			4 -	
LYS	GLY	PRO	GLY	GLY	ALA	ASP ASP	PHE	ASN	HIS	GLU	LEU MET	GLY	SER	ALA L'VS	PRO	GLN	ALA	ALA	TAS	ASP	ASP	ALA	ALA	GLY	ALA ASP	GLU	PRO	ARG	ARG	VAL	VAL	THR	LEU	LEU SER	GLU	GLN	VAL	PRO ALA	LEU	ALA	ILE
SER	ARG	LEU	GLN	SER GLN	ARG	GLU LEU	ASP	ALA	ARG	LEU	PRO	THR	ALA	GL.Y	VAL	VAL	GLN	VAL	GLY GLY	ARG	GLY	ARG	ARG	ARG	ARG LEU	LEU	GLN THR	THR	SER	SER	VAL	ALA ASN	GLN	THR ALA	SER	CYS	PRO	ALA TLF	ASN	ALA	ASN
LEU	THR	ASN	THR	ALA PRO	PRO	PR0 THR	THR	THR	MET	TYR	LEU ALA	VAL	THR	SER	LEU	ILE	ASP	ILE	ASP	VAL	ASN	ARG ALA	LEU	SER	ALA	MET	ASN	SER	THR	THR	ILE	VAL	LEU	ASP GLU	LYS	THP	ALA	THR	VAL	LYS	GLU
SER	TYR	VAL	TYR	LYS ASN	LEU	ALA THR	THR	TYR	SER	ALA	CLU CLU	ASN	ARG	ASN	THR	VAL	TEU	ASN	LEU	ALA	LEU	ALA AL.A	ALA	ASP	ALA THR	ASN	SER	LEU	LEU	ALA	LEU	GLY	LEU	LEU	GLY	ALA	THR	SER ALA	ALA	CT II CT II	ALA
ASP	LEU	GLY	THR	THR AI.A	MET	LEU VAL	ASP	GLY T ETI	GLY	LEU	SER	GLU	ASN	T.R.P PHE	PHE	GLU	TYR	GLN	GLN	CYS LEU	ILE	GLN	SER	GLY	GLY GLY	THR	THR	ASN	PHE	ILE	ASN	GLU	GLN	GLN ALA	ALA	LEU	TYR	ASP 1 FU	GLU	THR	ARG
- <u></u>	ч Ч	9.9	3 9	9 9		A D	A.	7. 8	9 63	B	D N		щ.	a F	, X	ڻ د	; 2	H	D. II	n X	e. 1	Х, д	I D.	R	3 6	A.	A.	A.	Y	W X	D: A	, e	P.	X. DI	X		4 64		ξ. <u>Δ</u> .	<u>е</u> , р	ų.
NA TA	AL	PF	РН	P.F. P.F.	PH	ALAR	AL	15 CI	TH	E	E LE	AL	Ξ	GI MF	GI	AF	AF	SE	Ë :		TH	10 HS.	15	Ë ;	H K	AL	AL	AL	19 GI	GI	E E	75 EL	AL	CI CI CI	GI	PF	ASA	PH	AS	AS	AL
ALA	ALA	ALA	GLY	SER GLY	TYR	ALA	VAL	ARG	ABF	ARG	CLN	THR	GLY	THR VAL	PRO	SER	VAL	SER	ALA	GLU LEU	PRO	GL.Y	TEU	THR	ARG	LEU	GLN TYR	GLY	GLY	GLU	LEU	VAL	ALA	ALA GLY	ARG	PRO	ALA	GLY	THR	VAL	TYR
ASP	ARG	CLY GLY	PRO	GLU ARG	ARG	ARG THR	ALA	GLY	ALA ARG	GLY	ASN	VAL	VAL	GLY GLY	TEU	MET	HIS	GLN	VAL	ARG	ARG	LEU	CLN	VAL	VAL LEU	GLY	ARG	SER	GLU	CYS	GLN	LYS	PHE	GLY PRO	LEU	ARG AT A	GLU	CYS VAL	ARG	SER	TYR
SER	TYS	ASN	GLN	ASP LEU	GLY	GLY ILE	GLY	GLU	PRO	VAL	PHE	ARG	SER	SER	ILE	TYR	PRO	ASP	VAL	GLY	ARG	ALA TRP	ALA	TYR	ASN	PHE	SER	GLY	ASN	GLU	ILE	THR	LEU	LYS LEU	PRO	PHE	PHE	THR HTS	TYR	PRO	PRO
GLY	PRO	ASP	TYR	PRO VAL	PHE	PHE ASP	THR	ARG I ETI	GLY	ALA	ASP	ALA	ARG	LYS L.F.II	LEU	THR	LEU	GLU	ASP	GLY ARG	TYR	LEU SER	PRO	ILE	SER	SER	GLU L.F.U	ARG	LEU	LEU	LEU	V AL TYR	ASN	PR0 ASP	ALA	VAT	PHE	GLY TYR	LEU	ARG	ALA
TRP	TRP	3LY	ASP	GLY VAL	VAL	ARG LEU	ARG	GLN	ILE	ALA	ALA TLF	PRO	ALA	THR	TYR	3LY Tvs	PHE	ILE	SER	HIS	3LN	TYR TYR	MET	PHE	PRO	ASP	TRP TLE	MET	VAL	PHE	ILE	LEU	HIS	LEU ALA	SER	THR	LEU	ASP	VAL	ARG AT A	LEU
N	0 Z	0 1		NU	A	R D	¥	D		A	۲ ۲		A	- - -		ы c	, 0	ß	5	ר ג	ß	ග ප	2 64	2	م. تع م		24 C	ы	<u>с</u> , _г	3 4	<u>с,</u> :	о ц	A	at 03	D	ы 2	4 EL	A	A D	ц н	1 5
13 CL	35	AR		GL	AL	E IS	GL	19	5 3	AL	19	E	AL:	AS GL	E	Hd	AR	LY	AR	AR VA	Γλ	LY	ΥT	E	AR	WE	HT R	Hd	AT N	AL	EL E	UA VA	AL	SE	LE	H U		AL	3	VA	LE
TYR	PHE	VAL	VAL	ALA SER	PRO	GLY	PRO	THR	THR	THR	TYR	VAL	TYR	ASP ALA	ASP	VAL	ALA	PRO	ALA	PHE	PHE	MET	ASN	TYS.	GLII	ARG	GLY TRP	ASN	PRO	TEU	ALA	VAL	LEU	GLN	PHE	GLN	ARG	SER	TEU	LYS	THR
ASN	THR	ILE	LEU	ALA ALA	THR	ALA ALA	ALA	MET	PRO	PRO	SER	PRO	PRO	GLY	GLY	ASP	ARG	TRP	LEU	LEU PRO	ASP	ASP VAL	SER	GLY	LEU	ALA	LEU GLY	ASP	MET	SER	TYR	ASP	ASN	GLU	TYR	LEU	ASN	LEU TYR	PHE	VAL	GLN
SER	VAL	LEU	MET	LEU MET	VAL	ARG LEU	MET	HIS	VAL	SER	PHE GLN	PRO	SIH	LEU AL.A	VAL	ILE	GLY	ALA	ILE	ALA ARG	AL.A	TLE	MET	LEU	TYR	TRP	ALA VAL	ILE	ALA	MET	VAL	VAL VAL	MET	LEU	MET	LEU	ILE	ILE ALA	PHE	GLY	ARG
LEU	GLN	LEU	THR	ILE SER	GLY	SER	TYR	ALA	ALA	ARG	TRP	TEU	ILE	LYS HTS	SER	ASP	GLY	ASN	ARG	ALA THR	ILE	GLU	MET	LEU	ASP	ASN	THR VAL	ILE	LEU	GLY	GLY GLY	SER	LEU	VAL	ALA	LEU	ARG	GLY	GLY	ALA	PHE



ILE	LEU	VAL	LEU	AT.A	PHE	PHE	ALA TLF	LEU	LEU ARG	GLN	GLN	MET	LEU ARG	ARG	TRP	SIH	ALA	ALA PRO	THR	VAL	GLU	ASP	LEU ARG	SIH	PHE	ARG	TRP	VAL GLN	ARG	TRP	ASP	ALA PRO	SER	LYS	ARG LEU	ASP	LEU THR	ILE ASP
TRP	VAL	ARG	PRO	UAL.	ARG	THR	TRP ALA	TYR	SER VAL	TEU	TYR SFR	ALA	VAL. VAL.	ARG	GLY	ALA	ALA	VAL ALA	GLY	GLY	ALA	LEU	ALA LYS	ARG	HIS PRO	THR	SIH	GLN	VAL THR	GLU	ALA	VAL LEU	LEU	GLY	GLY PRO	PRO	GLY	ASN SER
PRO	ASP	GLU PRO	ASP	ARG	TYR	PRO	ARG TYR	ASN	ARG	ALA	MET	MET	VAL	GLU	GLU	LEU	LEU	VAL ASN	LYS	GLU	ARG	ARG	GLU LEU	PHE	PHE	MET	THR	ASN	GLU	GLY	THR	LYS ARG	MET	ALA	MET GLY	ALA	PRO ARG	ARG ALA
ALA	AL.A	ALA	ALA	VAL	ASP	SER	ALA ARG	ALA	MET ALA	ASP	SER I FII	ALA	SER	LEU	LEU	ARG	PHE	GLY	ARG	VAL	ARG	ARG	ALA ALA	ARG	SER PHE	ASP	GLU	MET HIS	GLN	ARG	ARG	GLY	THR	ALA	GLY GLY	SER	GLY SER	ALA ASP
GLY	SER	DHE	SER	GLY SFR	LEU	GLY	GLY SER	ALA	GLY	GLY	ASP SFR	GLU	ASN SER	ASP	ASP	MET	LEU	PRO THR	GLY	VAL	VAL	GLY	SER LEU	LYS	ARG	GLY	LYR GLY	VAL HIS	ASN	GLN	VAL	HIS	LEU	LEU	GLN	ALA	GLN	THR ALA
MET	ARG	ASN	SIH	THE	ARG	ASN	MET GLY	ARG	GLU	GLY	ASP	PRO	GLN	LEU	ALA	LEU	PHE	VAL ALA	GLN	PHE	GLY	GLN	TLE PRO	GLU	PR0 GLU	ARG	PRO	PRO GLY	VAL	PRO	LEU	TYR ARG	GLN	VAL	GLN	ALA	GLY SER	GLY ASN
SER	LEU	ASN	VAL	GL Y AT A	GLY	ALA	PRO ALA	PRO	ALA ALA	PRO	GLY GLY	PRO	PRO ARG	PRO	GLY	SER	ARG	GLY	GLY	ALA	MET	MET	GLY GLN	SER	GLN	ALA	ALA PRO	ALA PRO	THR	GLY	VAL	ALA ALA	VAL	ASP	THR ASN	THR	PRO GLU	GL Y MET
LEU	THR	ALA	LEU	GLN	MET	ALA	PR0 PR0	SER	THR	ALA	ASN AI A	ALA	VAL SER	ALA	ASP	THR	VAL	PRO ALA	GLU	ALA	GLU ALA	SER	SER AL.A	SER	VAL THR	ASP	GLY ALA	PR0 ARG	ALA	PRO	PRO	GLY GLY	ALA	SER	ARG ALA	ARG	PHE ALA	ALA ASP
LEU	GLU	PRO	GLY	ASN THR	THR	THR	ALA GLY	GLU	GLU ALA	PRO	ALA SFR	PRO	GLY VAL	ALA	SER	GLY	ALA	VAL GLY	SER	PRO	GLY	ARG	ASN	SER	VAL SER	GLY	GLN	GLY GLY	SER	THR	ARG	SER MET	LEU	ARG	HIS LEU	GLN	PRO GLU	PRO ARG
ALA	ALA	PHE	ALA	PRO	ALA	ALA	THR LEU	GLY	LEU	GLY	GLN I FII	GLY	SER	SER	SER	ARG	SER	SER	SER	MET	VAL MET	PRO	ALA GLY	SER	GLY SER	ALA	T YR PHE	THR PRO	SER	SER	GLY	GLY ALA	ALA	ALA	ALA THR	ALA	PRO GLY	GLY PRO
THR	ALA	THR	GLY	GLY THR	ASP	GLY	ALA AI.A	PRO	GLN PRO	GLU	PRO I FII	THR	ILE ARG	ARG	PR0	ILE	HIS	LYS MET	ARG	SER	GLY	ALA	ALA AI.A	ALA	VAL ALA	GLY	MET	ARG SER	PHE	SER	ALA	PR0 GLY	GLU	THR	PRO ALA	SER	PRO THR	GL Y AL A
THR	SER	SER	ALA	ALA	ALA	ALA	SER LEU	ILE	THR SER	PRO	GLY	TYR	GLY ARG	SER	GL Y	SER	THR	SER	ALA	ARG	GLY	VAL	ALA THR	PRO	ARG GLY	ASP	VAL	SER	GLN	SER	TEU	PRO LEU	ASP	THR	ILE ILE	PHE	ALA THR	SER ALA
ALA	VAL	GLN	ARG	THR	SER	VAL	LEU GLN	LEU	LEU ARG	GLU	LEU	GLY	VAL GLN	ALA	ASP	ASP	ALA	MET LEU	ARG	SER	THK	VAL	LEU TLE	GLU	ARG LEU	SER	ALA GLY	SER VAL	PRO PHE	PRO	ARG	ALA ALA	ARG	VAL	PROGLY	VAL	MET GLY	SER PRO
ALA	SER	PRO	PRO	VAL	PRO	ASN	GLU L'YS	PRO	GLY	TRP	GLU	ALA	ALA VAL	ALA	ARG	ALA	ALA	ALA ASN	ALA	ALA	ALA	ALA	GLN	ALA	ALA VAL	GLY	ALA	SER PRO	ARG	GLY	SER	LEU ARG	VAL	VAL	GLU ASP	GLY	ALA GLY	GLY ALA
ALA	SIH	HIS GLY	GLY	ALA	GLY AT A	ALN	VAL	ASP	GL V GL V	ASP	MET	PRO	LEU PRO	PRO	PRO	ALA	LEU	ARG GLY	VAL	ASP	TYR	THR	ALA SFR	PRO	ARG SER	LEU	ALA ALA	LEU GLN	AL.A	ARG	ALA	ALA GLY	PRO	SER	GLY LEU	LEU	THR PRO	PRO THR
PRO	THR	GLU	ALA	PRU	GLU	ALA	LEU PRO	PRO	ALA ALA	ALA	LYS SFB	ALA	GLU PRO	ALA	GLN	GLU	GLU	ALA PRO	ALA	GLY GLY	GLU SER	ARG	VAL VAL	SER	ARG ALA	ALA	GLN	ALA GLY	MET	PRO VAL	ASP	GLU MET	ARG	VAL	GLU PRO	GLU	PR0 GLU	LEU VAL
THR	PHE	VAL	GLN	CI V	MET	SER	ARG ALA	ALA	GLY ASP	ALA	ALA ATA	LEU	ALA ALA	ALA	ALA	ALA	ALA	GLU	ASP	GLU	ARG	GLU	ARG GLU	ALA	LEU ALA	ALA	GLU	GLY LEU	ASP SFR	LEU	PRO	PRO PRO	GLY	LER	SER SER	SER	GLY GLN	VAL HIS
VAL	PRO	ALA PRO	TYR	GLY PRO	VAL	TYR	GLY ALA	ALA	PRO HIS	ILE	ALA	LEU	GLU MET	ALA	GLY	ARG	PRO	SER	GLY	ALA	GLN	SER	SER ASP	PRO	ALA ILE	LYS	VAL LEU	SER PRO	ALA	GLU AT.A	SIH	ARG ARG	ALA	THR	PRO LYS	SER	SER HIS	GLY SER
ARG	VAL	GLY SER	PRO	11H.	PRO PRO	JLU	ALA TLE	ARG	ARG LEU	SER	PRO 21 II	THR	SER	LEU	SER	PRO	3L Y	SER	ALA	VAL	VAL	ALA	ALA	ALA	ARG	ALA	JLU 3LU	GLU MLA	SER	ARG	ASN	LEU PRO	LEU	SER	PRO	3LY	SER SER	ARG PRO
ALA	SER	GLN	ARG	ASP GLIT	dLN GLN	VAL	GLU VAL	LEU	ALA LEU	PRO	ASP THR	VAL	PR0 GLU	GLY	CL II	ALA	GLU	ALA GLY	GLY	PRO	ASP	GLU .	PRO VAL	GLN	GLU	GLY	GLU	GLY	HIS	ALA	GLU	ALA SER	ARG	LEU	GLY ARG	GLN	PRU SER	ARG ILE



ALA	PHE SER	GLU	SER	MET	ARG	ARG	ALA	ASP	GLN	GLU	ASP	ASP	GLU	ASP	GLU	PRO	PRU	ALA	THR	ALA	ALA	GLY	ALA	GLY	ALA	GLN	ALA	GLU	PRO	AL.A	PRO	PRO	ALA	GLY	TYR	PRO	PRO	PRO	NEK	GLU	PRO	ALA	GLN	SER
GLU	PRO LEU	GLU	GLY	ARG	PRO	ARG	PRO	ARG	SER	VAL	LEU	VAL	GLY	PRU	PRO	PRO	PRO	PRO	GLY	GLY	PRO	ALA	PRO	VAL	ARG	ARG	ALA	ALA	SER	AT.A	SER	LEU	GLY	THR	THR	GLN	ALA	SER	LEU DEL	ALA	GLU	ALA	THR	GLY
GLU	GLY	VAL	ALA PRO	PRO	GLN	TEU	THR	GLU	GLU	ALA	SER	VAL	ILE	GI.N	ALA	LEU	GLY THR	SER	ALA	PRO	PRO	ILE	GLY	LYS	ALA	THR	ARG	VAL	GLN	PRO	PRO	ASP	GLU	ARG	ARG	GLN SER	GLN	LEU	ALA	GLN	GLN	GLU	TEU	ALA
ALA	ALA GLN	ALA	ALA VAT	ALA	MET	ARG	MET	SER	ASN	ALA	SER	ARG	VAL	SER	ARG	ALA	THR	PHE	SER	ALA	ALA ALA	ALA	PRO	GLY	ALA	GLY	LEU	LEU	GLN	MET	ASP	SER	GLY	SER	GLY	ALA ALA	THR	ASP	ALA	GLY	GLY	GLY AT A	GLY	PRO
SER	SER	SER	ALA	PRO	PRO	PRO	GLY	ALA	ALA	ALA	PRO	LEU	ARG	GL.Y	ARG	ARG	ALA L'EII	LEU	ALA	SER	GLN	SER	GLY	ALA	PHE	GLY	LEU	ALA	ALA	GL.Y	GLU	GLU	SER	ASN	ALA	GLN	MET	ALA	ALA	ALA	LEU	GLU	TYS	GLN
ALA	GLU	ALA	ALA	LYS	ALA TVD	VAL	ASP	LEU	MET	ASN	MET	ARG	SER	MET	SER	ALA	THR GLY	GLU	ARG	LEU	LEU	SER	GLY	ARG	GLY	SER	ALA	GLY	PRO	ALLS ALLS	ALA	ALA	PRO	ALA	LEU	GLY ALA	ALA	GLY	GLY	SER	ARG	GLN	SER	LEU
ALA	GLU	VAL	SER	CLY CLY	SER AT A	GLY	LEU	GLN	GLN	ASP	LEU	SER	GLY	MET	GLN	LEU	PRO	SER	GLY	SER	VAL	ALA	PRO	ARG	ALA	PRO	PRO WET	ALA	ALA	CI.Y	SER	LEU	LYS	PRO	GLY	THR GLY	ARG	SER	SER	ASN	LEU	PR0 PP0	MET	SER
PRO	GLY	ALA	THR	ALA	ALA	GLY	SER	GLU	GLY	ALA	SER	GLY	LEU	чь т РR П	ILE	VAL	PRO PRO	PRO	PRO	LEU	THR	ASN	ALA	PR0	ALI	PRO	GLN	VAL	SER	GLN LEU	MET	GL Y GL Y	GLY	SER	GLN	GLY SER	PHE	GLY	ALA	SER	PRO	SER AI A	ALA	ARG
SER	ALA	ALA	GLN	GLN	LEU	ALA	PHE THR	GLY	ASP	LEU	VAL	GLU	ASP	ASP	TEU	ASP	SER	GLY	SER	MET	ARG	ALA	PRO	ALA	PRO	THR	PRO r vc	ARG	ARG	GLN AT.A	GLY	ASP	GLU											

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A1:	50%	50%	
NAG1 NAG2			
• Molecule a opyranose	3: 2-acetamido-2-deoxy-bet	ta-D-glucopyranose-(1-4)-2-acetamido-	2-deoxy-beta-D-gluc
Chain A2:	50%	50%	
NAG1 NAG2			
• Molecule a opyranose	3: 2-acetamido-2-deoxy-bet	ta-D-glucopyranose-(1-4)-2-acetamido-	2-deoxy-beta-D-gluc
Chain A3:	50%	50%	
NAG1 NAG2			
• Molecule a opyranose	3: 2-acetamido-2-deoxy-bet	ta-D-glucopyranose-(1-4)-2-acetamido-	2-deoxy-beta-D-gluc
Chain a1:	50%	50%	



NAG1 NAG2

• Molecule 3: 2-a	acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-acetamido-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-a	do-2-deoxy-beta-D-gluc
opyranose		

Chain a2:	50%	50%	
NAG1 NAG2			
• Molecule 3 opyranose	2-acetamido-2-deoxy-beta-D	0-glucopyranose-(1-4)-2-acetamido	-2-deoxy-beta-D-gluc
Chain a3:	1	00%	
NAG1 NAG2			
• Molecule 4	beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain A4:		100%	
FUB 1 FUB 2			
• Molecule 4	beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain A5:		100%	·
FUB2 FUB2			
• Molecule 4	beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain A7:	50%	50%	
FUB2 FUB2			
• Molecule 4	beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain B0:	50%	50%	1
FUB1 FUB2			
• Molecule 4	beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain B1:	:	100%	i -



FUB1 FUB2

• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain B3:	100%
FUB1 FUB2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain B4:	100%
FUB1 FUB2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain B5:	100%
FUB1 FUB2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain B7:	100%
FUB2 FUB2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain B9:	100%
FUB1 FUB2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain C0:	100%
FUB 1 FUB 2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain C1:	100%
E UB 1 E UB 2	

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



Chain C2:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain C3:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain C4:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain C5:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain C6:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain C7:	100%
FUB2 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain C8:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain C9:	100%



FUB1 FUB2

• Molecule 4	: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain D0:	100%
FUB1 FUB2	
• Molecule 4:	: beta-L-arabinofuranose- $(1-2)$ -beta-L-arabinofuranose
Chain D1:	50%
FUB2	
• Molecule 4	: beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain D2:	100%
FUB1 FUB2	
• Molecule 4:	: beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain D3:	100%
FUB1 FUB2	
• Molecule 4	: beta-L-arabinofuranose- $(1-2)$ -beta-L-arabinofuranose
Chain D4:	100%
FUB1 FUB2	
• Molecule 4:	: beta-L-arabinofuranose- $(1-2)$ -beta-L-arabinofuranose
Chain D5:	100%
FUB2 FUB2	
• Molecule 4:	: beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain D6:	100%
FUB1 FUB2	



• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain D7:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain D8:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain D9:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain E0:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain E1:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain E2:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain E4:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain E5:	100%

WORLDWIDE PROTEIN DATA BANK

FUB1 FUB2

• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain E8:	100%
FUB1 FUB2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain F0:	100%
FUB1 FUB2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain F3:	100%
FUB1 FUB2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain F8:	100%
FUB1 FUB2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain a5:	50% 50%
FUB1 FUB2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain a7:	50% 50%
FUB 2 FUB 2	
• Molecule	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose
Chain b0:	100%
FUB1 FUB2	

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose


Chain b1:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain b3:	100%
FUB2 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain b4:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain b5:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain b7:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain b9:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain c0:	100%
FUB1 FUB2	
• Molecule 4:	beta-L-arabino furanose-(1-2)-beta-L-arabino furanose
Chain c1:	100%



FUB1 FUB2

• Molecule 4: beta-L-arabinofuranose-(1-	-2)-beta-L-arabinofuranose
Chain c2:	100%
FUB2 FUB2	
• Molecule 4: beta-L-arabinofuranose-(1-	2)-beta-L-arabinofuranose
Chain c3:	100%
FUB1 FUB2	
• Molecule 4: beta-L-arabinofuranose-(1-	2)-beta-L-arabinofuranose
Chain c4:	100%
F UB1 F UB2	
• Molecule 4: beta-L-arabinofuranose-(1-	2)-beta-L-arabinofuranose
Chain c5:	100%
FUB1 FUB2	
• Molecule 4: beta-L-arabinofuranose-(1-	2)-beta-L-arabinofuranose
Chain c6:	100%
FUB 2 FUB 2	
• Molecule 4: beta-L-arabinofuranose-(1-	2)-beta-L-arabinofuranose
Chain c7:	100%
FUB2	
• Molecule 4: beta-L-arabinofuranose-(1-	2)-beta-L-arabinofuranose
Chain c8:	100%
FUB2 FUB2	

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



Chain c9:	100%	
FUB1 FUB2		
• Molecule 4	: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain d1:	50% 50%	
FUB2		
• Molecule 4	: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain d2:	100%	
FUB1 FUB2		
• Molecule 4	: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain d3:	100%	
FUB1 FUB2		
• Molecule 4	1: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain d4:	100%	
FUB1 FUB2		
• Molecule 4	: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain d5:	100%	
FUB2 FUB2		
• Molecule 4	: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain e0:	100%	
FUB1 FUB2		
• Molecule 4	1: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain e1:	100%	



FUB1 FUB2

• Molecule 4: beta-L-	-arabinofuranose-(1-2)-beta-L-arabinofuranos	se
Chain e2:	100%	
FUB2 FUB2		
• Molecule 4: beta-L-	-arabinofuranose-(1-2)-beta-L-arabinofuranos	se
Chain e4:	100%	
FUB1 FUB2		
• Molecule 4: beta-L-	-arabinofuranose-(1-2)-beta-L-arabinofuranos	se
Chain e5:	100%	
FUB1 FUB2		
• Molecule 4: beta-L-	-arabinofuranose-(1-2)-beta-L-arabinofuranos	se
Chain e8:	100%	
FUB1 FUB2		
• Molecule 4: beta-L-	-arabinofuranose-(1-2)-beta-L-arabinofuranos	se
Chain f0:	50% 50%	
FUB1 FUB2		
• Molecule 4: beta-L-	-arabinofuranose-(1-2)-beta-L-arabinofuranos	se
Chain f3:	100%	
FUB1 FUB2		
• Molecule 4: beta-L-	-arabinofuranose-(1-2)-beta-L-arabinofuranos	se
Chain f5:	100%	
FUB1 FUB2		

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



Chain f8:	100%	
FUB1 FUB2		
• Molecule 4	l: beta-L-arabinofuranose-(1-2)-beta-L-a	arabinofuranose
Chain E3:	100%	
FUB1 FUB2		
• Molecule 4	l: beta-L-arabinofuranose-(1-2)-beta-L-a	arabinofuranose
Chain f2:	50%	50%
F UB1 F UB2		
• Molecule 4	l: beta-L-arabinofuranose-(1-2)-beta-L-a	arabinofuranose
Chain e7:	50%	50%
FUB2		
• Molecule 4	e: beta-L-arabinofuranose-(1-2)-beta-L-a	arabinofuranose
Chain e6:	50%	50%
FUB1 FUB2		
• Molecule 4	l: beta-L-arabinofuranose-(1-2)-beta-L-a	arabinofuranose
Chain e3:	50%	50%
FUB1 FUB2		
• Molecule 4	l: beta-L-arabinofuranose-(1-2)-beta-L-a	arabinofuranose
Chain d9:	100%	
FUB1 FUB2		
• Molecule 4	e: beta-L-arabinofuranose-(1-2)-beta-L-a	arabinofuranose
Chain d7:	100%	



FUB1 FUB2

• Molecule 4	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain d8:	50% 50%	
• Molecule 4	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain d6:	100%	
FUB1 FUB2		
• Molecule 4 Chain d0:	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
FUB2 FUB2		
• Molecule 4	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain F5:	100%	
• Molecule 4	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain F2: -	100%	
• Molecule 4	4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose	
Chain E7:	100%	
• Molecule !	5. beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-bet	a-L-arabinofuranose
(1-2)-beta-L	-arabinofuranose	
Chain A6:	100%	

FUB1 FUB2 FUB3 FUB4



 \bullet Molecule 5: beta-L-arabino furanose-(1-2)-beta-L-arabino furanose-(5-5)-beta-L-arabino furanose-(1-2)-beta-L-arabino fura

Chain A9:

100%

FUB1 FUB2 FUB3 FUB4

 \bullet Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain B6:

100%



 \bullet Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F6:

100%

FUB1 FUB2 FUB3 FUB4

 \bullet Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F7:

100%

FUB1 FUB2 FUB3 FUB3

 \bullet Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain a6:

100%

FUB1 FUB2 FUB3 FUB4

 \bullet Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

C1 · 0		
Chain a9:	25%	75%

FUB1 FUB2 FUB3 FUB4

 \bullet Molecule 5: beta-L-arabino furanose-(1-2)-beta-L-arabino furanose-(5-5)-beta-L-arabino furanose-(1-2)-beta-L-arabino fura



Chain b6:	100%
FUB1 FUB2 FUB3 FUB4	
• Molecule (1-2)-beta-	5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose- L-arabinofuranose
Chain f6:	100%
FUB1 FUB2 FUB3 FUB4	
• Molecule (1-2)-beta-	5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose- L-arabinofuranose
Chain f7:	100%
FUB1 FUB2 FUB3 FUB4	
• Molecule (1-2)-beta- a-L-arabine	6: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose- L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose
Chain E6:	100%
FUB1 FUB2 FUB4 FUB5 FUB5 FUB5 FUB7 FUB8	
• Molecule	7: beta-L-arabinofuranose-(1-4)-beta-L-ribulofuranose
Chain a4:	100%
34V1 FUB2	

 $\bullet \ Molecule \ 8: \ beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-$

Chain e9:

100%

FUB1 FUB2 FUB3 FUB4 FUB5 FUB5



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	687452	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	39	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.771	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	711.68, 711.68, 711.68	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	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: HYP, GLA, FUB, 34V, A1AIO, 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		
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/13729	0.49	0/18855	
1	В	0.27	0/13729	0.50	1/18855~(0.0%)	
2	Х	0.21	0/157	0.51	0/190	
All	All	0.27	0/27615	0.49	1/37900~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	1643	ASN	CB-CA-C	-5.12	100.17	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	1850	ARG	Sidechain

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	1849/1987~(93%)	1792 (97%)	57 (3%)	0	100	100
1	В	1849/1987~(93%)	1783 (96%)	65 (4%)	1 (0%)	51	83
2	Х	21/8572~(0%)	18 (86%)	1 (5%)	2 (10%)	0	3
All	All	3719/12546~(30%)	3593~(97%)	123 (3%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	1854	SER
2	Х	1627	SER
2	Х	1560	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	Percentiles
1	А	1451/1514~(96%)	1392~(96%)	59~(4%)	30 64
1	В	1451/1514~(96%)	1395 (96%)	56 (4%)	32 65
2	Х	17/6717~(0%)	15 (88%)	2(12%)	5 21
All	All	2919/9745~(30%)	2802 (96%)	117 (4%)	35 65

5 of 117 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	1943	VAL
1	В	1861	SER
1	В	660	CYS
1	В	1859	SER
1	В	1677	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
1	В	1853	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

197 non-standard protein/DNA/RNA residues 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	Trune	Chain	Dec	Timle	B	ond leng	gths	B	ond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	HYP	А	1918	1	6,8,9	0.49	0	5,10,12	2.08	1 (20%)
1	HYP	В	1911	1	6,8,9	0.45	0	5,10,12	1.94	1 (20%)
1	HYP	В	1923	1	6,8,9	0.48	0	$5,\!10,\!12$	1.81	1 (20%)
1	HYP	А	1920	1	6,8,9	0.46	0	5,10,12	2.13	2 (40%)
2	HYP	Х	1592	2	6,8,9	0.43	0	5,10,12	1.94	1 (20%)
1	HYP	А	1927	1	6,8,9	0.48	0	5,10,12	1.98	1 (20%)
2	HYP	Х	1457	2	6,8,9	0.43	0	5,10,12	1.95	1 (20%)
2	HYP	Х	1626	2	6,8,9	0.53	0	5,10,12	1.68	1 (20%)
2	HYP	Х	1602	2	6,8,9	0.46	0	5,10,12	1.73	1 (20%)
2	HYP	Х	1587	2	6,8,9	0.45	0	5,10,12	1.91	2 (40%)
2	HYP	Х	1591	2	6,8,9	0.42	0	5,10,12	1.82	1 (20%)



Mol	Type	Chain	Dog	Link	В	ond leng	gths	B	Bond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	HYP	Х	1610	2	$6,\!8,\!9$	0.45	0	$5,\!10,\!12$	1.91	1 (20%)
2	HYP	Х	1590	2	6,8,9	0.44	0	$5,\!10,\!12$	2.01	1 (20%)
1	HYP	А	1897	1	6,8,9	0.46	0	5,10,12	2.00	3 (60%)
2	HYP	Х	1620	2	6,8,9	0.46	0	5,10,12	1.87	1 (20%)
2	HYP	Х	1523	2	6,8,9	0.43	0	5,10,12	1.85	1 (20%)
2	HYP	Х	1595	2	6,8,9	0.46	0	5,10,12	1.56	1 (20%)
1	HYP	В	1880	1	6,8,9	0.47	0	5,10,12	1.64	1 (20%)
1	HYP	А	1878	1	6,8,9	0.46	0	5,10,12	1.98	1 (20%)
1	HYP	В	1920	1	6,8,9	0.45	0	5,10,12	1.89	2 (40%)
1	HYP	В	1921	1	6,8,9	0.53	0	5,10,12	1.62	2 (40%)
2	HYP	Х	1532	2	6,8,9	0.50	0	5,10,12	1.87	2 (40%)
1	HYP	А	1930	1	6,8,9	0.45	0	5,10,12	1.65	1 (20%)
2	HYP	Х	1485	2	6,8,9	0.45	0	5,10,12	1.85	2 (40%)
1	HYP	В	1893	1	6,8,9	0.45	0	5,10,12	1.81	2 (40%)
2	HYP	Х	1462	2	6,8,9	0.44	0	5,10,12	1.71	1 (20%)
1	HYP	А	1928	1	6,8,9	0.48	0	5,10,12	1.96	2 (40%)
1	HYP	А	1922	1	6,8,9	0.48	0	5,10,12	2.04	1 (20%)
1	HYP	В	1890	1	$6,\!8,\!9$	0.49	0	$5,\!10,\!12$	1.27	0
1	HYP	В	1915	1	$6,\!8,\!9$	0.44	0	$5,\!10,\!12$	1.74	1 (20%)
2	HYP	Х	1520	2	$6,\!8,\!9$	0.45	0	$5,\!10,\!12$	1.84	1 (20%)
1	HYP	А	1911	1	6, 8, 9	0.45	0	$5,\!10,\!12$	1.83	3 (60%)
1	HYP	А	1857	1	6,8,9	0.45	0	$5,\!10,\!12$	1.65	2 (40%)
2	HYP	Х	1522	2	$6,\!8,\!9$	0.44	0	$5,\!10,\!12$	1.75	1 (20%)
1	HYP	В	1901	1	$6,\!8,\!9$	0.45	0	$5,\!10,\!12$	1.64	2 (40%)
2	HYP	Х	1459	2	6,8,9	0.43	0	5,10,12	1.90	2 (40%)
2	HYP	Х	1521	2	6,8,9	0.44	0	5,10,12	1.95	2 (40%)
2	HYP	Х	1551	2	6,8,9	0.45	0	5,10,12	2.00	1 (20%)
2	HYP	Х	1589	2	6,8,9	0.43	0	5,10,12	1.89	1 (20%)
1	HYP	А	1917	1	6,8,9	0.46	0	5,10,12	1.86	3 (60%)
1	HYP	В	1875	1	6,8,9	0.47	0	5,10,12	1.73	1 (20%)
1	HYP	В	1899	1	6,8,9	0.45	0	5,10,12	1.76	1 (20%)
2	HYP	Х	1469	2	6,8,9	0.49	0	5,10,12	1.70	1 (20%)
1	HYP	В	1865	1	6,8,9	0.57	0	5,10,12	1.49	0
1	HYP	В	1858	1	6,8,9	0.58	0	5,10,12	1.41	1 (20%)
1	HYP	В	1887	1	6,8,9	0.46	0	$5,\!10,\!12$	1.89	2 (40%)



Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	В	ond ang	gles
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	HYP	А	1872	1	6, 8, 9	0.48	0	$5,\!10,\!12$	1.48	1 (20%)
2	HYP	Х	1488	2	6, 8, 9	0.45	0	$5,\!10,\!12$	1.93	1 (20%)
2	HYP	Х	1612	2	6, 8, 9	0.45	0	$5,\!10,\!12$	1.94	1 (20%)
1	HYP	А	1875	1	6,8,9	0.45	0	$5,\!10,\!12$	1.86	1 (20%)
2	HYP	Х	1617	2	6,8,9	0.44	0	5,10,12	1.88	2 (40%)
1	HYP	В	1862	1	6,8,9	0.45	0	5,10,12	1.81	1 (20%)
1	HYP	А	1907	1	6,8,9	0.46	0	5,10,12	1.82	2 (40%)
1	HYP	В	1916	1	6,8,9	0.46	0	5,10,12	1.85	2 (40%)
2	HYP	Х	1586	2	6,8,9	0.44	0	5,10,12	1.88	1 (20%)
2	HYP	Х	1614	2	6,8,9	0.44	0	5,10,12	1.89	2 (40%)
1	HYP	А	1932	1	6,8,9	0.50	0	5,10,12	1.84	2 (40%)
1	HYP	В	1888	1	6,8,9	0.45	0	5,10,12	1.94	1 (20%)
1	HYP	А	1883	1	6,8,9	0.50	0	5,10,12	1.74	1 (20%)
2	HYP	Х	1615	2	6,8,9	0.45	0	5,10,12	1.96	1 (20%)
1	HYP	В	1927	1	6,8,9	0.46	0	5,10,12	1.90	1 (20%)
2	HYP	Х	1468	2	6,8,9	0.44	0	5,10,12	1.95	1 (20%)
2	HYP	Х	1496	2	6,8,9	0.49	0	5,10,12	1.74	1 (20%)
2	HYP	Х	1546	2	6,8,9	0.46	0	5,10,12	1.93	1 (20%)
1	HYP	А	1890	1	6,8,9	0.47	0	5,10,12	1.79	1 (20%)
1	HYP	А	1902	1	6,8,9	0.45	0	5,10,12	1.84	2 (40%)
1	HYP	А	1860	1	6,8,9	0.47	0	5,10,12	1.85	1 (20%)
1	HYP	А	1898	1	6,8,9	0.45	0	5,10,12	1.89	2 (40%)
2	HYP	Х	1550	2	6,8,9	0.44	0	5,10,12	1.96	1 (20%)
1	HYP	В	1897	1	6,8,9	0.46	0	5,10,12	1.79	2 (40%)
2	HYP	Х	1465	2	6,8,9	0.46	0	5,10,12	1.75	1 (20%)
1	HYP	В	1878	1	6,8,9	0.47	0	5,10,12	1.70	1 (20%)
1	HYP	В	1872	1	6,8,9	0.45	0	5,10,12	1.94	2 (40%)
2	HYP	Х	1529	2	6,8,9	0.44	0	5,10,12	1.95	2 (40%)
2	HYP	Х	1601	2	6,8,9	0.44	0	5,10,12	1.98	1 (20%)
1	HYP	А	1863	1	6,8,9	0.50	0	5,10,12	2.32	2 (40%)
1	HYP	В	1906	1	6,8,9	0.45	0	5,10,12	1.91	2 (40%)
1	HYP	А	1931	1	6,8,9	0.44	0	5,10,12	1.84	2 (40%)
2	HYP	Х	1524	2	6,8,9	0.43	0	5,10,12	1.95	3 (60%)
1	HYP	А	1894	1	6,8,9	0.54	0	5,10,12	2.25	2 (40%)
1	HYP	А	1892	1	6,8,9	0.50	0	5,10,12	1.54	1 (20%)



Mal	Tuno	Chain	Dec	Tiple	B	ond leng	gths	В	Bond ang	gles
NIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	HYP	А	1865	1	6, 8, 9	0.48	0	$5,\!10,\!12$	1.89	2 (40%)
1	HYP	А	1908	1	6, 8, 9	0.46	0	$5,\!10,\!12$	1.86	1 (20%)
2	HYP	Х	1453	2	6,8,9	0.47	0	$5,\!10,\!12$	1.77	2 (40%)
1	HYP	А	1913	1	6,8,9	0.45	0	$5,\!10,\!12$	1.85	1 (20%)
2	HYP	Х	1526	2	6,8,9	0.43	0	$5,\!10,\!12$	2.03	1 (20%)
2	HYP	Х	1531	2	6,8,9	0.43	0	5,10,12	1.99	1 (20%)
1	HYP	А	1916	1	6,8,9	0.46	0	5,10,12	1.68	2 (40%)
1	HYP	А	1888	1	6,8,9	0.45	0	5,10,12	1.86	1 (20%)
1	HYP	В	1929	1	6,8,9	0.46	0	$5,\!10,\!12$	1.83	2 (40%)
1	HYP	А	1864	1	6,8,9	0.52	0	5,10,12	2.35	2 (40%)
2	HYP	Х	1464	2	6,8,9	0.44	0	5,10,12	1.82	1 (20%)
1	HYP	А	1877	1	6,8,9	0.51	0	5,10,12	2.12	2 (40%)
1	HYP	В	1913	1	6,8,9	0.48	0	5,10,12	1.80	1 (20%)
2	HYP	Х	1554	2	6,8,9	0.44	0	5,10,12	1.89	2 (40%)
1	HYP	В	1932	1	6,8,9	0.47	0	$5,\!10,\!12$	2.07	2 (40%)
1	HYP	А	1910	1	6,8,9	0.46	0	5,10,12	1.90	1 (20%)
2	HYP	Х	1553	2	6,8,9	0.44	0	$5,\!10,\!12$	1.89	2 (40%)
1	HYP	А	1866	1	6,8,9	0.49	0	5,10,12	1.63	1 (20%)
1	HYP	В	1902	1	6,8,9	0.45	0	5,10,12	1.99	2 (40%)
2	HYP	Х	1588	2	6,8,9	0.45	0	5,10,12	1.87	1 (20%)
1	HYP	В	1922	1	6,8,9	0.47	0	5,10,12	1.97	2 (40%)
2	HYP	Х	1613	2	6,8,9	0.45	0	5,10,12	1.94	1 (20%)
2	HYP	Х	1461	2	6,8,9	0.44	0	$5,\!10,\!12$	1.88	1 (20%)
1	HYP	В	1864	1	6,8,9	0.50	0	$5,\!10,\!12$	2.21	3 (60%)
1	HYP	А	1885	1	6,8,9	0.51	0	$5,\!10,\!12$	2.45	2 (40%)
2	HYP	Х	1455	2	6,8,9	0.44	0	$5,\!10,\!12$	1.86	1 (20%)
2	HYP	Х	1456	2	6,8,9	0.43	0	5,10,12	1.89	2 (40%)
2	HYP	Х	1484	2	6,8,9	0.43	0	5,10,12	1.93	2 (40%)
1	HYP	А	1873	1	6,8,9	0.47	0	$5,\!10,\!12$	1.79	1 (20%)
2	HYP	Х	1458	2	6,8,9	0.43	0	5,10,12	1.87	1 (20%)
1	HYP	В	1868	1	6,8,9	0.49	0	5,10,12	2.10	1 (20%)
2	HYP	Х	1483	2	6,8,9	0.46	0	5,10,12	1.93	1 (20%)
2	HYP	Х	1454	2	6,8,9	0.47	0	$5,\!10,\!12$	1.36	0
1	HYP	А	1868	1	6,8,9	0.50	0	$5,\!10,\!12$	1.92	1 (20%)
2	HYP	X	1460	2	6,8,9	0.45	0	$5,\!10,\!\overline{12}$	1.85	1 (20%)



Mal	Turne	Chain	Dec	Tiple	B	ond leng	gths	B	Bond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	HYP	А	1929	1	6,8,9	0.47	0	$5,\!10,\!12$	1.90	3 (60%)
1	HYP	В	1894	1	6,8,9	0.47	0	$5,\!10,\!12$	1.91	1 (20%)
2	HYP	Х	1555	2	6,8,9	0.43	0	$5,\!10,\!12$	1.98	3 (60%)
1	HYP	В	1910	1	6,8,9	0.45	0	5,10,12	2.15	1 (20%)
2	HYP	Х	1596	2	6,8,9	0.46	0	5,10,12	1.92	1 (20%)
1	HYP	А	1867	1	6,8,9	0.45	0	5,10,12	1.91	2 (40%)
1	HYP	А	1893	1	6,8,9	0.45	0	5,10,12	1.82	2 (40%)
2	HYP	Х	1619	2	6,8,9	0.43	0	5,10,12	1.94	1 (20%)
1	HYP	А	1882	1	6,8,9	0.45	0	5,10,12	1.92	2 (40%)
1	HYP	В	1856	1	6,8,9	0.51	0	5,10,12	2.06	2 (40%)
1	HYP	В	1873	1	6,8,9	0.48	0	5,10,12	1.46	0
2	HYP	Х	1559	2	6,8,9	0.47	0	5,10,12	1.86	1 (20%)
1	HYP	А	1905	1	6,8,9	0.44	0	$5,\!10,\!12$	1.63	2 (40%)
1	HYP	В	1857	1	6,8,9	0.47	0	$5,\!10,\!12$	1.61	1 (20%)
2	HYP	Х	1481	2	6,8,9	0.44	0	5,10,12	1.90	1 (20%)
2	HYP	Х	1556	2	6,8,9	0.45	0	5,10,12	1.90	1 (20%)
2	HYP	Х	1548	2	6,8,9	0.45	0	5,10,12	2.02	1 (20%)
1	HYP	В	1877	1	6,8,9	0.55	0	5,10,12	2.24	2 (40%)
1	HYP	В	1931	1	6,8,9	0.44	0	5,10,12	1.84	2 (40%)
1	HYP	А	1914	1	6,8,9	0.52	0	5,10,12	2.35	2 (40%)
1	HYP	В	1917	1	6,8,9	0.48	0	5,10,12	1.69	2 (40%)
2	HYP	Х	1528	2	6,8,9	0.44	0	5,10,12	1.84	1 (20%)
2	HYP	Х	1552	2	6,8,9	0.44	0	5,10,12	1.92	2 (40%)
2	HYP	Х	1480	2	6,8,9	0.46	0	5,10,12	1.89	1 (20%)
1	HYP	В	1855	1	6,8,9	0.52	0	5,10,12	2.18	3 (60%)
1	HYP	А	1912	1	6,8,9	0.50	0	5,10,12	2.37	1 (20%)
2	HYP	Х	1499	2	6,8,9	0.45	0	5,10,12	1.85	2 (40%)
1	HYP	А	1899	1	6,8,9	0.50	0	5,10,12	1.64	1 (20%)
1	HYP	А	1870	1	6,8,9	0.48	0	5,10,12	1.83	1 (20%)
2	HYP	X	1562	2	6,8,9	0.47	0	5,10,12	1.84	1 (20%)
2	HYP	X	1623	2	6,8,9	0.46	0	5,10,12	1.87	1 (20%)
2	HYP	X	1527	2	6,8,9	0.43	0	5,10,12	1.87	1 (20%)
2	HYP	X	1525	2	6,8,9	0.43	0	5,10,12	1.93	2 (40%)
1	HYP	В	1866	1	6,8,9	0.48	0	5,10,12	2.02	2 (40%)
2	HYP	Х	1598	2	6,8,9	0.49	0	5,10,12	2.02	2 (40%)



Mal	Tune	Chain	Dec	Tiple	B	ond leng	gths	В	Bond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	HYP	А	1901	1	6, 8, 9	0.45	0	$5,\!10,\!12$	1.86	2 (40%)
2	HYP	Х	1489	2	6, 8, 9	0.46	0	$5,\!10,\!12$	1.87	2 (40%)
1	HYP	А	1923	1	6,8,9	0.50	0	5,10,12	2.01	1 (20%)
1	HYP	В	1885	1	6,8,9	0.53	0	$5,\!10,\!12$	2.35	2 (40%)
2	HYP	Х	1549	2	6,8,9	0.45	0	5,10,12	1.94	1 (20%)
1	HYP	В	1930	1	6,8,9	0.46	0	5,10,12	1.87	2 (40%)
2	HYP	Х	1530	2	6,8,9	0.43	0	5,10,12	1.97	1 (20%)
2	HYP	Х	1493	2	6,8,9	0.45	0	5,10,12	1.91	1 (20%)
1	HYP	В	1883	1	6,8,9	0.48	0	$5,\!10,\!12$	1.78	1 (20%)
1	HYP	В	1860	1	6,8,9	0.51	0	5,10,12	2.26	1 (20%)
1	HYP	А	1921	1	6,8,9	0.55	0	$5,\!10,\!12$	1.44	0
1	HYP	В	1898	1	6,8,9	0.43	0	$5,\!10,\!12$	1.91	3 (60%)
1	HYP	В	1870	1	6, 8, 9	0.47	0	$5,\!10,\!12$	1.86	1 (20%)
1	HYP	В	1928	1	6,8,9	0.52	0	$5,\!10,\!12$	1.57	1 (20%)
2	HYP	Х	1547	2	6,8,9	0.44	0	$5,\!10,\!12$	1.92	1 (20%)
1	HYP	А	1858	1	6,8,9	0.52	0	$5,\!10,\!12$	1.63	1 (20%)
1	HYP	А	1903	1	6,8,9	0.47	0	$5,\!10,\!12$	1.89	1 (20%)
1	HYP	А	1862	1	6,8,9	0.46	0	5,10,12	1.84	1 (20%)
1	HYP	А	1855	1	6,8,9	0.44	0	5,10,12	1.84	1 (20%)
1	HYP	В	1882	1	6,8,9	0.46	0	5,10,12	1.81	2 (40%)
2	HYP	Х	1593	2	6,8,9	0.44	0	5,10,12	1.93	1 (20%)
1	HYP	В	1908	1	6,8,9	0.48	0	$5,\!10,\!12$	1.93	1 (20%)
2	HYP	Х	1618	2	6,8,9	0.43	0	$5,\!10,\!12$	1.94	2 (40%)
1	HYP	А	1915	1	6,8,9	0.45	0	5,10,12	1.81	2 (40%)
1	HYP	А	1906	1	6,8,9	0.44	0	5,10,12	1.77	2 (40%)
1	HYP	В	1905	1	6,8,9	0.49	0	5,10,12	1.62	2 (40%)
2	HYP	Х	1463	2	6,8,9	0.43	0	5,10,12	1.89	2 (40%)
1	HYP	В	1892	1	6,8,9	0.50	0	5,10,12	1.41	1 (20%)
1	HYP	В	1914	1	6,8,9	0.54	0	5,10,12	2.36	2 (40%)
2	HYP	Х	1487	2	6,8,9	0.44	0	5,10,12	1.86	1 (20%)
1	HYP	А	1856	1	6,8,9	0.49	0	5,10,12	2.01	3 (60%)
2	HYP	X	1597	2	6,8,9	0.45	0	5,10,12	2.07	2 (40%)
2	HYP	X	1594	2	6,8,9	0.49	0	5,10,12	1.41	0
2	HYP	X	1616	2	6,8,9	0.44	0	$5,\!10,\!12$	1.87	2(40%)
2	HYP	Х	1486	2	6,8,9	0.44	0	$5,\!10,\!12$	1.65	1 (20%)



Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	B	ond ang	gles
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	HYP	В	1907	1	6,8,9	0.45	0	$5,\!10,\!12$	1.89	2 (40%)
2	HYP	Х	1482	2	6,8,9	0.45	0	5,10,12	1.93	2 (40%)
1	HYP	А	1880	1	6,8,9	0.48	0	5,10,12	1.81	1 (20%)
1	HYP	А	1887	1	6,8,9	0.46	0	$5,\!10,\!12$	2.01	3 (60%)
1	HYP	В	1903	1	6,8,9	0.45	0	5,10,12	1.85	1 (20%)
1	HYP	В	1912	1	6,8,9	0.51	0	5,10,12	2.06	2 (40%)
1	HYP	В	1863	1	6,8,9	0.49	0	$5,\!10,\!12$	2.06	1 (20%)
1	HYP	В	1918	1	6,8,9	0.51	0	$5,\!10,\!12$	1.69	1 (20%)
2	HYP	Х	1611	2	6,8,9	0.45	0	$5,\!10,\!12$	1.92	1 (20%)
2	HYP	Х	1490	2	6,8,9	0.48	0	5,10,12	1.92	1 (20%)
1	HYP	В	1867	1	6,8,9	0.46	0	5,10,12	1.98	2 (40%)

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
1	HYP	А	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1920	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1592	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1927	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1457	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1626	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1602	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1587	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1591	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1610	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1590	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1620	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1523	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1595	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1921	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1532	2	-	0/0/11/13	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	А	1930	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1485	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1893	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1462	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1915	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1520	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1522	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1901	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1459	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1521	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1551	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1589	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1899	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1469	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1872	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1488	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1612	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1875	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1617	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1916	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1586	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1614	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1883	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1615	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1927	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1468	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1496	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1546	2	-	0/0/11/13	0/1/1/1

Continued from previous page...



001000	nucu jio		is page.	••			
Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	А	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1898	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1550	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1465	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1872	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1529	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1601	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1524	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1453	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1526	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1531	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1864	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1464	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1554	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1910	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1553	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1902	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1588	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1922	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1613	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1461	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1885	1	-	0/0/11/13	0/1/1/1

Continued from previous page...



001000	nucu jio		is page.	••			
Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	Х	1455	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1456	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1484	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1873	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1458	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1868	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1483	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1454	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1868	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1460	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1894	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1555	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1910	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1596	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1893	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1619	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1873	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1559	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1481	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1556	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1548	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1917	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1528	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1552	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1480	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1912	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1499	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1870	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1562	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1623	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1527	2	-	0/0/11/13	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	Х	1525	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1866	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1598	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1901	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1489	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1885	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1549	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1930	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1530	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1493	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1928	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1547	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1882	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1593	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1618	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1905	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1463	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1914	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1487	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1856	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1597	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1594	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1616	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1486	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1907	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1482	2	-	0/0/11/13	0/1/1/1
1	HYP	А	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	А	1887	1	-	0/0/11/13	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	В	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	В	1918	1	-	0/0/11/13	0/1/1/1
2	HYP	Х	1611	2	-	0/0/11/13	0/1/1/1
2	HYP	Х	1490	2	-	0/0/11/13	0/1/1/1
1	HYP	В	1867	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 285 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	А	1912	HYP	CB-CG-CD	-4.36	97.92	103.27
1	В	1914	HYP	CB-CG-CD	-4.24	98.07	103.27
1	В	1860	HYP	CB-CG-CD	-4.18	98.14	103.27
1	А	1914	HYP	CB-CG-CD	-4.08	98.27	103.27
1	А	1885	HYP	CB-CG-CD	-3.92	98.46	103.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

240 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	Res	Tink	Bo	ond leng	$_{\rm sths}$	Bond angles			
Moi Type Chain	Unain	1105		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
3	NAG	A1	1	1,3	14,14,15	0.77	0	17,19,21	1.02	1 (5%)	
3	NAG	A1	2	3	14,14,15	0.72	0	17,19,21	0.87	0	
3	NAG	A2	1	1,3	14,14,15	0.72	0	17,19,21	1.23	2 (11%)	



N T 1	т	<u> </u>	Ъ	т. 1	Bo	ond leng	\mathbf{ths}	В	ond ang	les
NIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	NAG	A2	2	3	14,14,15	0.73	0	17,19,21	0.83	0
3	NAG	A3	1	1,3	14,14,15	0.81	0	17,19,21	0.98	1 (5%)
3	NAG	A3	2	3	14,14,15	0.76	0	17,19,21	0.93	0
4	FUB	A4	1	4	9,9,10	1.08	0	10,12,14	0.79	0
4	FUB	A4	2	9,4	9,9,10	1.03	0	10,12,14	0.82	0
4	FUB	A5	1	4	9,9,10	1.03	0	10,12,14	0.86	0
4	FUB	A5	2	9,4	9,9,10	1.03	0	10,12,14	0.81	0
5	FUB	A6	1	5	9,9,10	1.06	0	10,12,14	0.85	0
5	FUB	A6	2	5,9	9,9,10	1.08	0	10,12,14	0.81	0
5	FUB	A6	3	5	9,9,10	1.04	0	10,12,14	0.88	0
5	FUB	A6	4	5,9	9,9,10	1.05	0	$10,\!12,\!14$	0.84	0
4	FUB	A7	1	4	9,9,10	1.06	0	$10,\!12,\!14$	0.90	0
4	FUB	A7	2	9,4	9,9,10	1.11	0	10,12,14	0.93	1 (10%)
5	FUB	A9	1	5	9,9,10	1.05	0	10,12,14	0.80	0
5	FUB	A9	2	5,9	9,9,10	1.07	0	10,12,14	0.79	0
5	FUB	A9	3	5	9,9,10	1.04	0	10,12,14	0.90	0
5	FUB	A9	4	5,9	9,9,10	1.05	0	10,12,14	0.80	0
4	FUB	B0	1	4	9,9,10	1.10	0	10,12,14	0.99	1 (10%)
4	FUB	B0	2	9,4	9,9,10	1.02	0	10,12,14	0.83	0
4	FUB	B1	1	4	9,9,10	1.05	0	10,12,14	0.85	0
4	FUB	B1	2	9,4	9,9,10	1.05	0	10,12,14	0.78	0
4	FUB	B3	1	4	9,9,10	1.01	0	10,12,14	0.94	0
4	FUB	B3	2	9,4	9,9,10	1.08	0	10,12,14	0.91	0
4	FUB	B4	1	4	9,9,10	1.02	0	10,12,14	0.79	0
4	FUB	B4	2	9,4	9,9,10	1.03	0	10,12,14	0.90	0
4	FUB	B5	1	4	9,9,10	1.04	0	10,12,14	0.79	0
4	FUB	B5	2	9,4	9,9,10	1.05	0	10,12,14	0.79	0
5	FUB	B6	1	5	9,9,10	1.05	0	10,12,14	0.78	0
5	FUB	B6	2	5,9	9,9,10	1.04	0	$10,\!12,\!14$	0.79	0
5	FUB	B6	3	5	9,9,10	1.02	0	$10,\!12,\!14$	0.86	0
5	FUB	B6	4	5,9	$9,\!9,\!10$	1.05	0	$10,\!12,\!14$	0.88	0
4	FUB	B7	1	4	$9,\!9,\!10$	1.05	0	$10,\!12,\!14$	0.77	0
4	FUB	B7	2	9,4	$9,\!9,\!10$	1.05	0	$10,\!12,\!14$	0.88	0
4	FUB	B9	1	4	9,9,10	1.04	0	10,12,14	0.82	0
4	FUB	B9	2	9,4	9,9,10	1.04	0	10,12,14	0.86	0
4	FUB	CO	1	4	9,9,10	$1.0\overline{2}$	0	10,12,14	0.99	0
4	FUB	CO	2	9,4	9,9,10	1.04	0	10,12,14	0.80	0
4	FUB	C1	1	4	9,9,10	1.03	0	10,12,14	0.83	0
4	FUB	C1	2	9,4	9,9,10	1.02	0	10,12,14	0.88	0
4	FUB	C2	1	4	9,9,10	1.03	0	10,12,14	0.81	0
4	FUB	C2	2	9,4	9,9,10	1.03	0	10,12,14	0.86	0
4	FUB	C3	1	4	$9,\!9,\!10$	1.03	0	10,12,14	0.88	0



N T 1	т		Ъ	T • 1	Bond lengths		Bond angles			
NIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	FUB	C3	2	9,4	9,9,10	1.04	0	$10,\!12,\!14$	0.91	0
4	FUB	C4	1	4	9,9,10	1.04	0	10,12,14	0.81	0
4	FUB	C4	2	9,4	9,9,10	1.02	0	10,12,14	0.89	0
4	FUB	C5	1	4	9,9,10	1.04	0	10,12,14	0.87	0
4	FUB	C5	2	9,4	9,9,10	1.04	0	10,12,14	0.91	0
4	FUB	C6	1	4	9,9,10	1.04	0	10,12,14	0.81	0
4	FUB	C6	2	9,4	9,9,10	1.02	0	$10,\!12,\!14$	0.88	0
4	FUB	C7	1	4	9,9,10	1.03	0	$10,\!12,\!14$	0.80	0
4	FUB	C7	2	9,4	9,9,10	1.03	0	10,12,14	0.92	0
4	FUB	C8	1	4	9,9,10	1.03	0	10,12,14	0.86	0
4	FUB	C8	2	9,4	9,9,10	1.02	0	10,12,14	0.88	0
4	FUB	C9	1	4	9,9,10	1.03	0	10,12,14	0.88	0
4	FUB	C9	2	9,4	9,9,10	1.03	0	10,12,14	0.87	0
4	FUB	D0	1	4	9,9,10	1.04	0	10,12,14	0.92	0
4	FUB	D0	2	9,4	9,9,10	1.03	0	10,12,14	0.90	0
4	FUB	D1	1	4	9,9,10	1.04	0	10,12,14	1.14	1 (10%)
4	FUB	D1	2	9,4	9,9,10	1.04	0	10,12,14	0.85	0
4	FUB	D2	1	4	9,9,10	1.07	0	10,12,14	0.93	0
4	FUB	D2	2	9,4	9,9,10	1.05	0	10,12,14	0.80	0
4	FUB	D3	1	4	9,9,10	1.04	0	10,12,14	0.77	0
4	FUB	D3	2	9,4	9,9,10	1.04	0	10,12,14	0.92	0
4	FUB	D4	1	4	9,9,10	1.05	0	$10,\!12,\!14$	0.74	0
4	FUB	D4	2	9,4	9,9,10	1.05	0	10,12,14	0.89	0
4	FUB	D5	1	4	$9,\!9,\!10$	1.06	0	$10,\!12,\!14$	0.89	0
4	FUB	D5	2	9,4	9,9,10	1.06	0	$10,\!12,\!14$	0.88	0
4	FUB	D6	1	4	$9,\!9,\!10$	1.04	0	$10,\!12,\!14$	0.80	0
4	FUB	D6	2	9,4	9,9,10	1.08	0	$10,\!12,\!14$	1.03	0
4	FUB	D7	1	4	$9,\!9,\!10$	1.06	0	$10,\!12,\!14$	0.97	0
4	FUB	D7	2	9,4	$9,\!9,\!10$	1.07	0	$10,\!12,\!14$	0.88	0
4	FUB	D8	1	4	9,9,10	1.05	0	10,12,14	0.79	0
4	FUB	D8	2	9,4	$9,\!9,\!10$	1.04	0	$10,\!12,\!14$	0.86	0
4	FUB	D9	1	4	$9,\!9,\!10$	1.06	0	$10,\!12,\!14$	0.90	0
4	FUB	D9	2	9,4	9,9,10	1.07	0	$10,\!12,\!14$	0.83	0
4	FUB	EO	1	4	9,9,10	1.05	0	$10,\!12,\!14$	0.80	0
4	FUB	EO	2	9,4	9,9,10	1.05	0	10,12,14	0.76	0
4	FUB	E1	1	4	$9,\!9,\!10$	1.05	0	$10,\!12,\!14$	0.83	0
4	FUB	E1	2	9,4	9,9,10	1.05	0	$10,\!12,\!14$	0.95	0
4	FUB	E2	1	4	9,9,10	1.03	0	$10,\!12,\!14$	0.85	0
4	FUB	E2	2	9,4	9,9,10	1.07	0	$10,\!12,\!14$	0.85	0
4	FUB	E3	1	4	9,9,10	1.06	0	$10,\!12,\!14$	0.86	0
4	FUB	E3	2	9,4	9,9,10	1.04	0	10,12,14	0.89	0
4	FUB	E4	1	4	$9,\!9,\!10$	1.02	0	$10,\!12,\!14$	1.07	1 (10%)



Ъ / . 1	—		D	T	Bond lengths		Bond angles			
IVIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	FUB	E4	2	9,4	9,9,10	1.07	0	10,12,14	1.13	1 (10%)
4	FUB	E5	1	4	9,9,10	1.04	0	10,12,14	0.79	0
4	FUB	E5	2	9,4	9,9,10	1.04	0	10,12,14	0.84	0
6	FUB	E6	1	6	9,9,10	1.06	0	10,12,14	0.85	0
6	FUB	E6	2	9,6	9,9,10	1.04	0	10,12,14	0.74	0
6	FUB	E6	3	6	9,9,10	1.03	0	$10,\!12,\!14$	0.84	0
6	FUB	E6	4	9,6	9,9,10	1.06	0	10,12,14	0.75	0
6	FUB	E6	5	6	$9,\!9,\!10$	1.02	0	$10,\!12,\!14$	0.85	0
6	FUB	E6	6	9,6	$9,\!9,\!10$	1.06	0	$10,\!12,\!14$	0.75	0
6	FUB	E6	7	6	$9,\!9,\!10$	1.04	0	$10,\!12,\!14$	0.73	0
6	FUB	E6	8	9,6	$9,\!9,\!10$	1.05	0	$10,\!12,\!14$	0.83	0
4	FUB	E7	1	4	$9,\!9,\!10$	1.07	0	$10,\!12,\!14$	0.78	0
4	FUB	E7	2	9,4	$9,\!9,\!10$	1.07	0	10,12,14	0.90	0
4	FUB	E8	1	4	$9,\!9,\!10$	1.03	0	$10,\!12,\!14$	0.80	0
4	FUB	E8	2	9,4	$9,\!9,\!10$	1.03	0	$10,\!12,\!14$	0.85	0
4	FUB	F0	1	4	$9,\!9,\!10$	1.03	0	$10,\!12,\!14$	0.87	0
4	FUB	F0	2	9,4	$9,\!9,\!10$	1.05	0	$10,\!12,\!14$	0.84	0
4	FUB	F2	1	4	$9,\!9,\!10$	1.04	0	$10,\!12,\!14$	0.78	0
4	FUB	F2	2	9,4	$9,\!9,\!10$	1.08	0	$10,\!12,\!14$	0.90	0
4	FUB	F3	1	4	$9,\!9,\!10$	1.07	0	$10,\!12,\!14$	0.86	0
4	FUB	F3	2	9,4	$9,\!9,\!10$	1.06	0	$10,\!12,\!14$	0.90	0
4	FUB	F5	1	4	$9,\!9,\!10$	1.06	0	$10,\!12,\!14$	0.78	0
4	FUB	F5	2	9,4	$9,\!9,\!10$	1.07	0	$10,\!12,\!14$	0.89	0
5	FUB	F6	1	5	$9,\!9,\!10$	1.06	0	$10,\!12,\!14$	0.78	0
5	FUB	F6	2	5,9	9,9,10	1.07	0	10,12,14	0.84	0
5	FUB	F6	3	5	9,9,10	1.05	0	10,12,14	0.82	0
5	FUB	F6	4	5,9	9,9,10	1.07	0	10,12,14	0.86	0
5	FUB	F7	1	5	9,9,10	1.04	0	10,12,14	0.77	0
5	FUB	F7	2	5,9	9,9,10	1.07	0	10,12,14	0.77	0
5	FUB	F7	3	5	9,9,10	1.02	0	10,12,14	0.80	0
5	FUB	F7	4	5,9	9,9,10	1.04	0	10,12,14	0.81	0
4	FUB	F8	1	4	9,9,10	1.06	0	10,12,14	0.78	0
4	FUB	F8	2	9,4	9,9,10	1.07	0	10,12,14	0.90	0
3	NAG	al	1	1,3	14,14,15	0.74	0	17,19,21	0.86	1 (5%)
3	NAG	a1	2	3	14,14,15	0.72	0	17,19,21	0.82	0
3	NAG	a2	1	1,3	$14,\!14,\!15$	0.73	0	$17,\!19,\!21$	1.17	1(5%)
3	NAG	a2	2	3	14,14,15	0.74	0	17,19,21	0.83	0
3	NAG	a3	1	1,3	14,14,15	0.78	0	17,19,21	1.53	2 (11%)
3	NAG	a3	2	3	14,14,15	0.73	0	17,19,21	1.24	2 (11%)
7	34V	a4	1	7	9,9,10	1.27	0	10,12,15	0.91	1 (10%)
7	FUB	a4	2	7,9	9,9,10	1.33	2 (22%)	10,12,14	1.24	2 (20%)



Mal	Turne	Chain	Dec	Tinle	Bo	ond leng	ths	B	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	FUB	a5	1	4	9,9,10	1.08	0	10,12,14	0.93	0
4	FUB	a5	2	9,4	9,9,10	1.36	2 (22%)	10,12,14	1.09	1 (10%)
5	FUB	a6	1	5	9,9,10	1.10	1 (11%)	10,12,14	1.08	0
5	FUB	a6	2	$5,\!9$	$9,\!9,\!10$	1.33	0	10,12,14	1.26	1 (10%)
5	FUB	a6	3	5	$9,\!9,\!10$	1.17	1 (11%)	10,12,14	1.24	1 (10%)
5	FUB	a6	4	5,9	9,9,10	1.25	1 (11%)	10,12,14	1.12	1 (10%)
4	FUB	a7	1	4	9,9,10	1.13	0	10,12,14	0.98	0
4	FUB	a7	2	9,4	$9,\!9,\!10$	1.37	2 (22%)	10,12,14	0.99	1 (10%)
5	FUB	a9	1	5	$9,\!9,\!10$	1.32	1 (11%)	10,12,14	1.02	1 (10%)
5	FUB	a9	2	5,9	$9,\!9,\!10$	1.33	1 (11%)	10,12,14	0.91	0
5	FUB	a9	3	5	9,9,10	1.10	0	10,12,14	0.96	0
5	FUB	a9	4	5,9	$9,\!9,\!10$	1.33	1 (11%)	10,12,14	1.06	1 (10%)
4	FUB	b0	1	4	$9,\!9,\!10$	1.45	2 (22%)	10,12,14	1.29	2 (20%)
4	FUB	b0	2	9,4	$9,\!9,\!10$	1.36	1 (11%)	10,12,14	1.00	1 (10%)
4	FUB	b1	1	4	9,9,10	1.41	2 (22%)	10,12,14	1.28	2 (20%)
4	FUB	b1	2	9,4	9,9,10	1.30	0	10,12,14	1.02	1 (10%)
4	FUB	b3	1	4	9,9,10	1.07	0	10,12,14	1.01	1 (10%)
4	FUB	b3	2	9,4	9,9,10	1.36	1 (11%)	10,12,14	1.38	2 (20%)
4	FUB	b4	1	4	9,9,10	1.37	1 (11%)	10,12,14	0.97	1 (10%)
4	FUB	b4	2	9,4	9,9,10	1.43	2 (22%)	10,12,14	1.12	1 (10%)
4	FUB	b5	1	4	9,9,10	1.14	0	10,12,14	1.39	1 (10%)
4	FUB	b5	2	9,4	9,9,10	1.24	0	10,12,14	1.12	1 (10%)
5	FUB	b6	1	5	9,9,10	1.35	2 (22%)	10,12,14	1.08	1 (10%)
5	FUB	b6	2	5,9	9,9,10	1.39	2 (22%)	10,12,14	1.11	1 (10%)
5	FUB	b6	3	5	9,9,10	1.31	1 (11%)	10,12,14	1.04	1 (10%)
5	FUB	b6	4	5,9	9,9,10	1.34	1 (11%)	10,12,14	1.09	1 (10%)
4	FUB	b7	1	4	9,9,10	1.24	0	10,12,14	1.00	1 (10%)
4	FUB	b7	2	9,4	9,9,10	1.39	2 (22%)	10,12,14	1.06	1 (10%)
4	FUB	b9	1	4	9,9,10	1.27	0	10,12,14	0.95	1 (10%)
4	FUB	b9	2	9,4	9,9,10	1.28	0	10,12,14	0.97	1 (10%)
4	FUB	c0	1	4	9,9,10	1.32	1 (11%)	10,12,14	1.23	2 (20%)
4	FUB	c0	2	9,4	9,9,10	1.27	1 (11%)	10,12,14	1.20	2 (20%)
4	FUB	c1	1	4	9,9,10	1.38	2 (22%)	10,12,14	1.04	1 (10%)
4	FUB	c1	2	9,4	9,9,10	1.24	1 (11%)	10,12,14	1.05	1 (10%)
4	FUB	c2	1	4	9,9,10	1.35	1 (11%)	10,12,14	1.01	1 (10%)



Mal	Trune	Chain	Dec	Timle	Bond lengths			В	Bond angles			
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
4	FUB	c2	2	9,4	$9,\!9,\!10$	1.26	0	10,12,14	1.02	1 (10%)		
4	FUB	c3	1	4	$9,\!9,\!10$	1.30	1 (11%)	10,12,14	1.23	2 (20%)		
4	FUB	c3	2	9,4	9,9,10	1.43	2 (22%)	10,12,14	1.01	1 (10%)		
4	FUB	c4	1	4	9,9,10	1.31	0	10,12,14	1.01	1 (10%)		
4	FUB	c4	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	1.14	1 (10%)		
4	FUB	c5	1	4	9,9,10	1.18	0	10,12,14	1.02	1 (10%)		
4	FUB	c5	2	9,4	9,9,10	1.27	0	10,12,14	0.93	1 (10%)		
4	FUB	c6	1	4	9,9,10	1.40	2 (22%)	10,12,14	1.11	1 (10%)		
4	FUB	c6	2	9,4	9,9,10	1.29	1 (11%)	10,12,14	0.98	1 (10%)		
4	FUB	c7	1	4	9,9,10	1.42	2 (22%)	10,12,14	1.31	2 (20%)		
4	FUB	c7	2	9,4	9,9,10	1.28	0	10,12,14	1.15	1 (10%)		
4	FUB	c8	1	4	9,9,10	1.15	0	10,12,14	0.97	1 (10%)		
4	FUB	c8	2	9,4	9,9,10	1.44	2 (22%)	10,12,14	1.08	1 (10%)		
4	FUB	c9	1	4	9,9,10	1.16	0	10,12,14	1.36	2 (20%)		
4	FUB	c9	2	9,4	9,9,10	1.36	2 (22%)	10,12,14	1.35	2 (20%)		
4	FUB	d0	1	4	9,9,10	1.16	0	10,12,14	0.97	1 (10%)		
4	FUB	d0	2	9,4	9,9,10	1.44	2 (22%)	10,12,14	1.08	1 (10%)		
4	FUB	d1	1	4	9,9,10	1.08	0	10,12,14	0.86	0		
4	FUB	d1	2	9,4	$9,\!9,\!10$	1.10	0	10,12,14	1.57	4 (40%)		
4	FUB	d2	1	4	$9,\!9,\!10$	1.09	0	10,12,14	1.15	1 (10%)		
4	FUB	d2	2	9,4	$9,\!9,\!10$	1.29	0	10,12,14	1.00	1 (10%)		
4	FUB	d3	1	4	9,9,10	1.27	0	10,12,14	0.96	1 (10%)		
4	FUB	d3	2	9,4	9,9,10	1.33	1 (11%)	10,12,14	1.05	1 (10%)		
4	FUB	d4	1	4	9,9,10	1.16	0	10,12,14	0.94	1 (10%)		
4	FUB	d4	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	0.96	1 (10%)		
4	FUB	d5	1	4	9,9,10	1.23	0	10,12,14	1.03	1 (10%)		
4	FUB	d5	2	9,4	9,9,10	1.41	2 (22%)	10,12,14	1.18	1 (10%)		
4	FUB	d6	1	4	9,9,10	1.17	0	10,12,14	0.94	1 (10%)		
4	FUB	d6	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	0.96	1 (10%)		
4	FUB	d7	1	4	9,9,10	1.46	2 (22%)	10,12,14	1.19	1 (10%)		
4	FUB	d7	2	9,4	9,9,10	1.33	1 (11%)	10,12,14	0.99	1 (10%)		
4	FUB	d8	1	4	9,9,10	1.09	0	10,12,14	1.00	0		
4	FUB	d8	2	9,4	9,9,10	1.38	2 (22%)	10,12,14	1.00	1 (10%)		
4	FUB	d9	1	4	9,9,10	1.27	0	10,12,14	0.90	1 (10%)		
4	FUB	d9	2	9,4	9,9,10	1.44	2 (22%)	10,12,14	1.03	1 (10%)		



Mal	Turne	Chain	Dec	Tink	Bond lengths		Bond angles			
NIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	FUB	e0	1	4	$9,\!9,\!10$	1.27	0	$10,\!12,\!14$	0.99	1 (10%)
4	FUB	e0	2	9,4	$9,\!9,\!10$	1.31	1 (11%)	$10,\!12,\!14$	1.28	2 (20%)
4	FUB	e1	1	4	9,9,10	1.11	0	10,12,14	1.04	1 (10%)
4	FUB	e1	2	9,4	9,9,10	1.40	2 (22%)	10,12,14	1.08	1 (10%)
4	FUB	e2	1	4	9,9,10	1.24	0	10,12,14	1.04	1 (10%)
4	FUB	e2	2	9,4	9,9,10	1.34	1 (11%)	10,12,14	0.98	1 (10%)
4	FUB	e3	1	4	9,9,10	1.10	0	10,12,14	1.00	0
4	FUB	e3	2	9,4	$9,\!9,\!10$	1.39	2 (22%)	$10,\!12,\!14$	1.00	1 (10%)
4	FUB	e4	1	4	9,9,10	1.13	1 (11%)	10,12,14	1.26	1 (10%)
4	FUB	e4	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	1.22	2 (20%)
4	FUB	e5	1	4	9,9,10	1.46	2 (22%)	10,12,14	1.19	1 (10%)
4	FUB	e5	2	9,4	9,9,10	1.32	1 (11%)	10,12,14	0.99	1 (10%)
4	FUB	e6	1	4	9,9,10	1.10	0	10,12,14	1.00	0
4	FUB	e6	2	9,4	$9,\!9,\!10$	1.37	1 (11%)	$10,\!12,\!14$	0.99	1 (10%)
4	FUB	e7	1	4	9,9,10	1.10	0	10,12,14	0.99	0
4	FUB	e7	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	0.99	1 (10%)
4	FUB	e8	1	4	$9,\!9,\!10$	1.27	0	10,12,14	0.91	1 (10%)
4	FUB	e8	2	9,4	$9,\!9,\!10$	1.42	2 (22%)	$10,\!12,\!14$	1.03	1 (10%)
8	FUB	e9	1	8	$9,\!9,\!10$	1.21	0	$10,\!12,\!14$	1.03	1 (10%)
8	FUB	e9	2	8,9	9,9,10	1.26	0	10,12,14	1.51	1 (10%)
8	FUB	e9	3	8	9,9,10	1.14	0	10,12,14	1.06	1 (10%)
8	FUB	e9	4	8,9	9,9,10	1.23	0	10,12,14	1.42	1 (10%)
8	FUB	e9	5	8	9,9,10	1.25	0	10,12,14	1.02	1 (10%)
8	FUB	e9	6	8,9	9,9,10	1.32	0	10,12,14	1.20	2 (20%)
4	FUB	f0	1	4	9,9,10	1.10	0	10,12,14	0.99	0
4	FUB	fO	2	9,4	$9,\!9,\!10$	1.37	2 (22%)	$10,\!12,\!14$	0.99	1 (10%)
4	FUB	f2	1	4	9,9,10	1.09	0	10,12,14	1.00	0
4	FUB	f2	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	0.99	1 (10%)
4	FUB	f3	1	4	9,9,10	1.17	0	10,12,14	1.01	1 (10%)
4	FUB	f3	2	9,4	9,9,10	1.46	2 (22%)	$10,\!12,\!14$	1.04	1 (10%)
4	FUB	f5	1	4	9,9,10	1.30	0	10,12,14	1.01	1 (10%)
4	FUB	f5	2	9,4	9,9,10	1.25	1 (11%)	10,12,14	1.40	2 (20%)
5	FUB	f6	1	5	9,9,10	1.16	0	10,12,14	1.06	1 (10%)
5	FUB	f6	2	5,9	9,9,10	1.34	1 (11%)	10,12,14	1.08	1 (10%)
5	FUB	f6	3	5	9,9,10	1.23	0	10,12,14	1.02	1 (10%)
5	FUB	f6	4	5,9	9,9,10	1.30	1 (11%)	10,12,14	1.49	2 (20%)



Mol	Turne	Chain	Dec	Link Bond lengths				Bond angles			
WIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
5	FUB	f7	1	5	$9,\!9,\!10$	1.36	1 (11%)	10,12,14	1.03	1 (10%)	
5	FUB	f7	2	5,9	9,9,10	1.30	0	10,12,14	1.24	1 (10%)	
5	FUB	f7	3	5	9,9,10	1.34	2 (22%)	10,12,14	1.03	1 (10%)	
5	FUB	f7	4	5,9	9,9,10	1.27	0	10,12,14	1.23	1 (10%)	
4	FUB	f8	1	4	9,9,10	1.22	0	10,12,14	1.05	1 (10%)	
4	FUB	f8	2	9,4	9,9,10	1.39	2 (22%)	10,12,14	1.31	2 (20%)	

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
3	NAG	A1	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A1	2	3	-	1/6/23/26	0/1/1/1
3	NAG	A2	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	A2	2	3	-	0/6/23/26	0/1/1/1
3	NAG	A3	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A3	2	3	-	0/6/23/26	0/1/1/1
4	FUB	A4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	A4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	A5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	A5	2	9,4	-	0/2/15/18	0/1/1/1
5	FUB	A6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	A6	2	5,9	-	0/2/15/18	0/1/1/1
5	FUB	A6	3	5	-	0/2/15/18	0/1/1/1
5	FUB	A6	4	5,9	-	0/2/15/18	0/1/1/1
4	FUB	A7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	A7	2	9,4	-	0/2/15/18	0/1/1/1
5	FUB	A9	1	5	-	0/2/15/18	0/1/1/1
5	FUB	A9	2	5,9	-	0/2/15/18	0/1/1/1
5	FUB	A9	3	5	-	0/2/15/18	0/1/1/1
5	FUB	A9	4	5,9	-	0/2/15/18	0/1/1/1
4	FUB	B0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	B1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B1	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	B3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B3	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	B4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B4	2	9,4	-	0/2/15/18	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	B5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B5	2	9,4	-	0/2/15/18	0/1/1/1
5	FUB	B6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	B6	2	5,9	-	0/2/15/18	0/1/1/1
5	FUB	B6	3	5	-	0/2/15/18	0/1/1/1
5	FUB	B6	4	5,9	-	0/2/15/18	0/1/1/1
4	FUB	B7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B7	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	B9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B9	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	CO	1	4	-	0/2/15/18	0/1/1/1
4	FUB	CO	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C1	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C3	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C5	2	9,4	-	1/2/15/18	0/1/1/1
4	FUB	C6	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C6	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C7	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C8	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C9	1	4	-	2/2/15/18	0/1/1/1
4	FUB	C9	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D1	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D3	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D4	1	4	-	2/2/15/18	0/1/1/1
4	FUB	D4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D5	2	9,4	-	0/2/15/18	0/1/1/1

Continued from previous page...



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	D6	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D6	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	D7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D7	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D8	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	D9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D9	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	EO	1	4	-	2/2/15/18	0/1/1/1
4	FUB	E0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E1	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E2	1	4	_	0/2/15/18	0/1/1/1
4	FUB	E2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E3	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E4	1	4	-	2/2/15/18	0/1/1/1
4	FUB	E4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E5	2	9,4	-	0/2/15/18	0/1/1/1
6	FUB	E6	1	6	-	0/2/15/18	0/1/1/1
6	FUB	E6	2	9,6	-	0/2/15/18	0/1/1/1
6	FUB	E6	3	6	-	0/2/15/18	0/1/1/1
6	FUB	E6	4	9,6	-	2/2/15/18	0/1/1/1
6	FUB	E6	5	6	-	2/2/15/18	0/1/1/1
6	FUB	E6	6	9,6	-	0/2/15/18	0/1/1/1
6	FUB	E6	7	6	-	0/2/15/18	0/1/1/1
6	FUB	E6	8	9,6	-	2/2/15/18	0/1/1/1
4	FUB	E7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E7	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E8	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	F0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	F2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	F3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F3	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	F'5		4	-	$\frac{0/2}{15}$	0/1/1/1
4	FUB	F'5	2	9,4	-	$\frac{0/2}{15}$	0/1/1/1
5	FUB	FÓ		b	-	0/2/15/18	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5		F6	2	5.0	Cimais	$\frac{2}{2}$	0/1/1/1
				5,9	-	2/2/13/18	0/1/1/1
5 5	FUB		3	5 0	-	$\frac{0/2}{15/18}$	0/1/1/1
5	FUD FUB	F0 F7	4	5,9	-	$\frac{0/2}{15/18}$	0/1/1/1 0/1/1/1
5	FUD	F7	1 0	5	-	0/2/15/18	0/1/1/1
	FUD	<u>Г (</u>	2	5,9	-	$\frac{2/2}{15/18}$	0/1/1/1
5	FUB	F (3	5 50	-	$\frac{0/2}{15/18}$	0/1/1/1
$\frac{3}{4}$	FUD		4	5,9	-	$\frac{0/2}{15/18}$	0/1/1/1
4	FUB FUB	<u>го</u> F8	1	4 0.4	-	$\frac{0/2}{15/18}$	0/1/1/1 0/1/1/1
4	NAG	- 10 	1	$\frac{9,4}{1.3}$	_	$\frac{0/2}{13/18}$	0/1/1/1 0/1/1/1
3	NAG	a1 a1	2	3	_	$\frac{0/6}{23/26}$	0/1/1/1
3	NAG	a1 a2	1	13	_	$\frac{0/0/23/20}{1/6/23/26}$	0/1/1/1
3	NAG	a2	2	3	_	$\frac{1}{0}/\frac{6}{23}/\frac{26}{26}$	0/1/1/1
3	NAG	a <u>2</u> a3	1	1.3	_	$\frac{2}{6}/\frac{23}{26}$	0/1/1/1
3	NAG	a3	2	3	_	0/6/23/26	0/1/1/1
7	34V	a9 a4	1	7	1/1/3/3	$\frac{0/3/25/20}{0/2/15/19}$	0/1/1/1
7	FUB	a4	2	7.9	-	$\frac{0/2}{15/18}$	0/1/1/1
4	FUB	a5	1	4	_	$\frac{2}{2}/\frac{2}{15}/18$	0/1/1/1
4	FUB	a5	2	9.4	_	$\frac{1/2}{15/18}$	0/1/1/1
5	FUB	a6	1	5	-	$\frac{1/2}{1/2}$	0/1/1/1
5	FUB	a6	2	5.9	-	$\frac{2}{2}/\frac{15}{18}$	0/1/1/1
5	FUB	a6	3	5	_	0/2/15/18	0/1/1/1
5	FUB	a6	4	5.9	-	$\frac{0/2}{15/18}$	0/1/1/1
4	FUB	a7	1	4	_	0/2/15/18	0/1/1/1
4	FUB	a7	2	9,4	_	2/2/15/18	0/1/1/1
5	FUB	a9	1	5	_	0/2/15/18	0/1/1/1
5	FUB	a9	2	5,9	_	$\frac{2}{2}/\frac{15}{18}$	0/1/1/1
5	FUB	a9	3	5	-	$\frac{2}{2/15/18}$	0/1/1/1
5	FUB	a9	4	5.9	_	$\frac{2}{2}/\frac{15}{18}$	0/1/1/1
4	FUB	b0	1	4	_	0/2/15/18	0/1/1/1
4	FUB	b0	2	9.4	-	$\frac{0/2}{15/18}$	0/1/1/1
4	FUB	b1	1	4	_	$\frac{2}{2}/\frac{15}{18}$	0/1/1/1
4	FUB	b1	2	9.4	_	0/2/15/18	0/1/1/1
4	FUB	b3	1	4	-	1/2/15/18	0/1/1/1
4	FUB	b3	2	9,4	_	0/2/15/18	0/1/1/1
4	FUB	b4	1	4	-	$\frac{2}{2}/\frac{15}{18}$	0/1/1/1
4	FUB	b4	2	9,4	_	0/2/15/18	0/1/1/1
4	FUB	b5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	b5	2	9.4	_	0/2/15/18	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUB	b6	1	5	-	2/2/15/18	0/1/1/1
5	FUB	b6	2	5,9	-	2/2/15/18	0/1/1/1
5	FUB	b6	3	5	-	2/2/15/18	0/1/1/1
5	FUB	b6	4	5,9	_	2/2/15/18	0/1/1/1
4	FUB	b7	1	4	-	1/2/15/18	0/1/1/1
4	FUB	b7	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	b9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	b9	2	9,4	_	2/2/15/18	0/1/1/1
4	FUB	c0	1	4	_	0/2/15/18	0/1/1/1
4	FUB	c0	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c1	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c2	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	c3	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c3	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	c5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c5	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c6	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c6	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	c7	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c7	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c8	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c8	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	c9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c9	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d0	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	d1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d1	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	d2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	d3	1	4	-	1/2/15/18	0/1/1/1
4	FUB	d3	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d4	1	4	-	2/2/15/18	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	d4	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d5	1	4	-	1/2/15/18	0/1/1/1
4	FUB	d5	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d6	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d6	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d7	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d7	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d8	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d8	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d9	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d9	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	e0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	e0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	e1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e1	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	e2	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e3	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e3	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	e4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	e5	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e5	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e6	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e6	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e7	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e7	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e8	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e8	2	9,4	-	0/2/15/18	0/1/1/1
8	FUB	e9	1	8	-	1/2/15/18	0/1/1/1
8	FUB	e9	2	8,9	-	1/2/15/18	0/1/1/1
8	FUB	e9	3	8	-	2/2/15/18	0/1/1/1
8	FUB	e9	4	8,9	-	2/2/15/18	0/1/1/1
8	FUB	e9	5	8	-	2/2/15/18	0/1/1/1
8	FUB	e9	6	8,9	-	2/2/15/18	0/1/1/1
4	FUB	f0	1	4	-	2/2/15/18	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	fO	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	f2	1	4	-	2/2/15/18	0/1/1/1
4	FUB	f2	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	f3	1	4	-	1/2/15/18	0/1/1/1
4	FUB	f3	2	9,4	-	1/2/15/18	0/1/1/1
4	FUB	f5	1	4	-	2/2/15/18	0/1/1/1
4	FUB	f5	2	9,4	-	0/2/15/18	0/1/1/1
5	FUB	f6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	f6	2	5,9	-	1/2/15/18	0/1/1/1
5	FUB	f6	3	5	-	2/2/15/18	0/1/1/1
5	FUB	f6	4	5,9	-	2/2/15/18	0/1/1/1
5	FUB	f7	1	5	-	0/2/15/18	0/1/1/1
5	FUB	f7	2	5,9	-	2/2/15/18	0/1/1/1
5	FUB	f7	3	5	-	0/2/15/18	0/1/1/1
5	FUB	f7	4	5,9	-	2/2/15/18	0/1/1/1
4	FUB	f8	1	4	-	1/2/15/18	0/1/1/1
4	FUB	f8	2	9,4	-	0/2/15/18	0/1/1/1

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
4	f3	2	FUB	C2-C3	-2.49	1.49	1.53
4	c7	1	FUB	O4-C1	-2.48	1.38	1.43
4	d7	1	FUB	C2-C3	-2.46	1.49	1.53
4	e4	2	FUB	O4-C1	-2.45	1.38	1.43
4	e5	1	FUB	C2-C3	-2.44	1.49	1.53

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
3	a3	1	NAG	O5-C1-C2	-4.39	104.35	111.29
8	e9	2	FUB	O4-C4-C3	-4.21	100.98	104.70
8	e9	4	FUB	O4-C4-C3	-3.96	101.20	104.70
3	a3	2	NAG	C1-O5-C5	3.52	116.96	112.19
5	a6	2	FUB	O4-C4-C3	-3.27	101.81	104.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	a4	1	34V	C3


Mol	Chain	Res	Type	Atoms
4	b4	1	FUB	O4-C4-C5-O5
4	b4	1	FUB	C3-C4-C5-O5
4	c3	1	FUB	C3-C4-C5-O5
4	c7	1	FUB	O4-C4-C5-O5
4	c7	1	FUB	C3-C4-C5-O5

5 of 168 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)

140 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).



Mal	Type	Chain	Bos	Link	Bo	Bond lengths			Bond angles		
	туре	Chan	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
9	A1AIO	В	2030	4	11,11,12	5.66	6 (54%)	14,15,17	1.55	2 (14%)	
10	GLA	А	2063	1	11,11,12	1.74	3 (27%)	15,15,17	1.00	1 (6%)	
9	A1AIO	А	2028	4	11,11,12	5.71	6 (54%)	$14,\!15,\!17$	1.46	2 (14%)	
10	GLA	А	2058	1	11,11,12	1.71	3 (27%)	$15,\!15,\!17$	0.98	1 (6%)	
9	A1AIO	В	2051	5	11,11,12	5.69	<u>6 (54%)</u>	14,15,17	1.43	2 (14%)	
9	A1AIO	А	2039	6	11,11,12	5.70	<u>6 (54%)</u>	14,15,17	1.62	3 (21%)	
9	A1AIO	А	2040	4	11,11,12	5.66	6 (54%)	14,15,17	1.57	2 (14%)	
9	A1AIO	А	2027	4	11,11,12	5.69	6 (54%)	14,15,17	1.55	2 (14%)	
9	A1AIO	А	2046	4	11,11,12	5.70	6 (54%)	14,15,17	1.54	2 (14%)	
9	A1AIO	В	2003	5	11,11,12	5.70	6 (54%)	14,15,17	1.47	1 (7%)	
9	A1AIO	В	2049	4	11,11,12	5.70	6 (54%)	14,15,17	1.51	2 (14%)	
10	GLA	А	2069	1	11,11,12	1.73	3 (27%)	15,15,17	0.93	1 (6%)	
9	A1AIO	В	2028	4	11,11,12	5.71	6 (54%)	14,15,17	1.35	2 (14%)	
9	A1AIO	В	2056	5	11,11,12	5.72	6 (54%)	14,15,17	1.46	2 (14%)	
10	GLA	В	2060	-	11,11,12	1.73	3 (27%)	15,15,17	1.02	1 (6%)	
10	GLA	А	2059	1	11,11,12	0.40	0	15,15,17	0.77	1 (6%)	
9	A1AIO	А	2009	4	11,11,12	5.69	6 (54%)	14,15,17	1.62	2 (14%)	
9	A1AIO	В	2021	4	11,11,12	5.71	6 (54%)	14,15,17	1.34	2 (14%)	
10	GLA	В	2065	1	11,11,12	1.69	3 (27%)	15,15,17	1.01	1 (6%)	
9	A1AIO	В	2016	4	11,11,12	5.64	6 (54%)	14,15,17	1.51	3 (21%)	
9	A1AIO	А	2038	4	11,11,12	5.66	6 (54%)	14,15,17	1.56	2 (14%)	
9	A1AIO	А	2021	4	11,11,12	5.71	6 (54%)	14,15,17	1.40	2 (14%)	
9	A1AIO	В	2020	4	11,11,12	5.67	6 (54%)	14,15,17	1.33	2 (14%)	
9	A1AIO	А	2042	4	11,11,12	5.71	6 (54%)	14,15,17	1.52	2 (14%)	
9	A1AIO	В	2045	4	11,11,12	5.71	6 (54%)	14,15,17	1.45	2 (14%)	
9	A1AIO	В	2050	4	11,11,12	5.67	6 (54%)	14,15,17	1.50	2 (14%)	
9	A1AIO	А	2048	4	11,11,12	5.70	6 (54%)	14,15,17	1.55	2 (14%)	
9	A1AIO	А	2037	4	11,11,12	5.70	6 (54%)	14,15,17	1.48	2 (14%)	
10	GLA	А	2064	1	11,11,12	1.72	3 (27%)	15,15,17	1.02	1 (6%)	
9	A1AIO	В	2035	8	11,11,12	5.72	6 (54%)	14,15,17	1.54	2 (14%)	
9	A1AIO	А	2054	6	11,11,12	5.73	6 (54%)	14,15,17	1.44	2 (14%)	
9	A1AIO	В	2032	4	11,11,12	5.70	6 (54%)	14,15,17	1.62	2 (14%)	
9	A1AIO	В	2037	4	11,11,12	5.69	6 (54%)	14,15,17	1.58	2 (14%)	
9	A1AIO	В	2054	8	11,11,12	5.69	6 (54%)	14,15,17	1.26	2 (14%)	
9	A1AIO	А	2041	4	11,11,12	5.72	6 (54%)	14,15,17	1.35	2 (14%)	



Mal	Type	Chain	Bos	Link	Bond lengths			Bond angles		
	туре	Citain	nes		Counts	Counts RMSZ $\# Z > 2$		Counts	RMSZ	# Z > 2
9	A1AIO	А	2002	4	11,11,12	5.71	6 (54%)	14,15,17	1.49	2 (14%)
9	A1AIO	В	2052	5	11,11,12	<mark>5.66</mark>	6 (54%)	14,15,17	1.65	3 (21%)
9	A1AIO	А	2049	4	11,11,12	<mark>5.68</mark>	6 (54%)	14,15,17	1.55	2 (14%)
10	GLA	В	2068	1	11,11,12	1.74	3 (27%)	$15,\!15,\!17$	0.88	0
10	GLA	А	2070	1	11,11,12	1.73	3 (27%)	$15,\!15,\!17$	0.96	1 (6%)
9	A1AIO	В	2008	4	11,11,12	5.70	6 (54%)	$14,\!15,\!17$	1.67	3 (21%)
9	A1AIO	А	2018	4	11,11,12	5.68	<u>6 (54%)</u>	14,15,17	1.53	2 (14%)
9	A1AIO	В	2011	5	11,11,12	5.65	6 (54%)	14,15,17	1.64	2 (14%)
9	A1AIO	В	2048	4	11,11,12	5.70	6 (54%)	14,15,17	1.45	2 (14%)
9	A1AIO	В	2039	5	11,11,12	5.73	6 (54%)	14,15,17	1.48	1 (7%)
9	A1AIO	В	2055	8	11,11,12	5.67	6 (54%)	14,15,17	1.57	2 (14%)
9	A1AIO	В	2040	5	11,11,12	5.67	6 (54%)	14,15,17	1.60	2 (14%)
9	A1AIO	В	2027	4	11,11,12	5.71	6 (54%)	14,15,17	1.51	2 (14%)
10	GLA	В	2069	1	11,11,12	1.72	3 (27%)	15,15,17	0.91	0
9	A1AIO	А	2005	5	11,11,12	5.74	6 (54%)	14,15,17	1.45	2 (14%)
9	A1AIO	В	2023	4	11,11,12	5.66	6 (54%)	14,15,17	1.52	3 (21%)
9	A1AIO	В	2001	7	11,11,12	5.69	6 (54%)	14,15,17	1.65	2 (14%)
9	A1AIO	А	2051	5	11,11,12	5.72	6 (54%)	14,15,17	1.50	2 (14%)
10	GLA	В	2059	1	11,11,12	0.41	0	15,15,17	0.77	1 (6%)
9	A1AIO	В	2009	4	11,11,12	5.65	6 (54%)	14,15,17	1.79	2 (14%)
10	GLA	В	2066	-	11,11,12	1.74	3 (27%)	15,15,17	0.99	1 (6%)
9	A1AIO	В	2038	4	11,11,12	5.72	6 (54%)	14,15,17	1.51	2 (14%)
9	A1AIO	В	2010	4	11,11,12	5.70	6 (54%)	14,15,17	1.46	2 (14%)
9	A1AIO	А	2017	4	11,11,12	5.71	6 (54%)	14,15,17	1.40	1 (7%)
9	A1AIO	В	2053	5	11,11,12	5.68	6 (54%)	14,15,17	1.52	2 (14%)
9	A1AIO	А	2045	4	11,11,12	5.69	6 (54%)	14,15,17	1.55	2 (14%)
9	A1AIO	В	2004	4	11,11,12	5.70	6 (54%)	14,15,17	1.61	2 (14%)
9	A1AIO	В	2006	4	11,11,12	5.72	6 (54%)	14,15,17	1.61	2 (14%)
9	A1AIO	В	2024	4	11,11,12	5.70	6 (54%)	14,15,17	1.42	2 (14%)
9	A1AIO	В	2019	4	11,11,12	5.67	6 (54%)	14,15,17	1.59	2 (14%)
9	A1AIO	А	2053	6	11,11,12	5.70	6 (54%)	14,15,17	1.60	2 (14%)
9	A1AIO	В	2029	4	11,11,12	5.72	6 (54%)	14,15,17	1.47	2 (14%)
10	GLA	А	2068	1	11,11,12	1.74	3 (27%)	15,15,17	0.91	0
9	A1AIO	В	2017	4	11,11,12	5.68	6 (54%)	14,15,17	1.55	2 (14%)
9	A1AIO	А	2022	4	11,11,12	5.70	6 (54%)	14,15,17	1.48	2 (14%)



Mal	Type	Chain	Bos	Link	Bond lengths			Bond angles		
	туре	Ullalli	nes		Counts RMSZ $\# Z > 2$			Counts	RMSZ	# Z >2
9	A1AIO	А	2006	4	11,11,12	5.67	6 (54%)	14,15,17	1.71	2 (14%)
9	A1AIO	А	2026	4	11,11,12	5.70	6 (54%)	$14,\!15,\!17$	1.53	2 (14%)
9	A1AIO	А	2013	4	11,11,12	5.68	6 (54%)	$14,\!15,\!17$	1.46	2 (14%)
9	A1AIO	В	2033	4	11,11,12	5.66	6 (54%)	14,15,17	1.74	3 (21%)
9	A1AIO	А	2047	4	11,11,12	5.69	6 (54%)	14,15,17	1.55	2 (14%)
9	A1AIO	В	2036	4	11,11,12	5.71	6 (54%)	14,15,17	1.45	2 (14%)
10	GLA	А	2066	1	11,11,12	1.72	3 (27%)	15,15,17	0.92	0
9	A1AIO	А	2012	4	11,11,12	5.67	6 (54%)	14,15,17	1.58	2 (14%)
9	A1AIO	А	2033	4	11,11,12	5.72	6 (54%)	14,15,17	1.39	1 (7%)
9	A1AIO	А	2010	4	11,11,12	5.70	6 (54%)	14,15,17	1.43	2 (14%)
9	A1AIO	А	2031	4	11,11,12	5.70	6 (54%)	14,15,17	1.51	2 (14%)
10	GLA	А	2060	1	11,11,12	0.41	0	15,15,17	0.77	1 (6%)
10	GLA	В	2063	-	11,11,12	1.74	3 (27%)	15,15,17	1.22	1 (6%)
10	GLA	В	2067	1	11,11,12	1.73	3 (27%)	15,15,17	0.95	1 (6%)
9	A1AIO	А	2008	4	11,11,12	5.70	6 (54%)	14,15,17	1.49	2 (14%)
9	A1AIO	В	2046	4	11,11,12	5.64	6 (54%)	14,15,17	1.74	2 (14%)
9	A1AIO	В	2005	5	11,11,12	5.68	6 (54%)	14,15,17	1.46	3 (21%)
9	A1AIO	А	2025	4	11,11,12	5.70	6 (54%)	14,15,17	1.46	2 (14%)
9	A1AIO	А	2057	5	11,11,12	5.71	6 (54%)	14,15,17	1.41	2 (14%)
9	A1AIO	А	2055	6	11,11,12	5.71	6 (54%)	14,15,17	1.39	2 (14%)
9	A1AIO	В	2007	4	11,11,12	5.70	6(54%)	14,15,17	1.52	2 (14%)
9	A1AIO	А	2023	4	11,11,12	5.70	6(54%)	14,15,17	1.48	2 (14%)
9	A1AIO	А	2001	4	11,11,12	5.72	6 (54%)	14,15,17	1.49	2 (14%)
9	A1AIO	В	2013	4	11,11,12	5.69	6 (54%)	14,15,17	1.40	2 (14%)
9	A1AIO	В	2014	4	11,11,12	5.67	6 (54%)	14,15,17	1.46	2 (14%)
9	A1AIO	А	2003	5	11,11,12	5.70	6 (54%)	14,15,17	1.50	2 (14%)
9	A1AIO	В	2044	4	11,11,12	5.72	6 (54%)	14,15,17	1.45	2 (14%)
9	A1AIO	В	2026	4	11,11,12	5.69	6 (54%)	14,15,17	1.67	3 (21%)
9	A1AIO	А	2056	5	11,11,12	5.69	6(54%)	14,15,17	1.59	2 (14%)
9	A1AIO	В	2047	4	11,11,12	5.67	6 (54%)	14,15,17	1.74	3 (21%)
9	A1AIO	А	2011	5	11,11,12	5.68	6(54%)	14,15,17	1.56	2 (14%)
9	A1AIO	А	2044	5	11,11,12	5.71	6 (54%)	14,15,17	1.74	3 (21%)
10	GLA	А	2065	1	11,11,12	1.74	3 (27%)	15,15,17	0.93	1 (6%)
10	GLA	А	2067	1	11,11,12	1.75	3 (27%)	15,15,17	1.00	1 (6%)
9	A1AIO	А	2024	4	11,11,12	5.71	6 (54%)	14,15,17	1.52	2 (14%)



Mol	Type	Chain	Bos	Link	Bo	Bond lengths			Bond angles		
	Type	Ullalli	nes		Counts	Counts RMSZ $\# Z > 2$		Counts	RMSZ	# Z > 2	
9	A1AIO	В	2034	4	11,11,12	5.63	6 (54%)	14,15,17	1.74	2 (14%)	
9	A1AIO	А	2019	4	11,11,12	5.70	6 (54%)	14,15,17	1.41	2 (14%)	
9	A1AIO	В	2043	4	11,11,12	5.71	6 (54%)	$14,\!15,\!17$	1.45	2 (14%)	
9	A1AIO	А	2007	4	11,11,12	5.71	6 (54%)	$14,\!15,\!17$	1.53	2 (14%)	
10	GLA	В	2058	-	11,11,12	1.72	3 (27%)	15,15,17	1.02	1 (6%)	
9	A1AIO	В	2041	4	11,11,12	5.68	<u>6 (54%)</u>	14,15,17	1.65	3 (21%)	
9	A1AIO	А	2036	4	11,11,12	5.69	6 (54%)	14,15,17	1.47	2 (14%)	
10	GLA	А	2061	1	11,11,12	1.75	3 (27%)	15,15,17	0.98	1 (6%)	
10	GLA	А	2062	1	11,11,12	1.72	3 (27%)	15,15,17	0.98	1 (6%)	
9	A1AIO	А	2020	4	11,11,12	5.70	6 (54%)	14,15,17	1.42	2 (14%)	
9	A1AIO	А	2050	5	11,11,12	5.71	6 (54%)	14,15,17	1.31	2 (14%)	
9	A1AIO	В	2057	5	11,11,12	5.68	6 (54%)	14,15,17	1.54	2 (14%)	
9	A1AIO	А	2035	4	11,11,12	5.72	6 (54%)	14,15,17	1.36	2 (14%)	
10	GLA	В	2070	-	11,11,12	1.73	3 (27%)	15,15,17	0.98	1 (6%)	
9	A1AIO	В	2042	4	11,11,12	5.72	6 (54%)	14,15,17	1.44	2 (14%)	
9	A1AIO	А	2034	4	11,11,12	5.70	6 (54%)	14,15,17	1.59	2 (14%)	
9	A1AIO	В	2012	4	11,11,12	5.71	6 (54%)	14,15,17	1.47	2 (14%)	
9	A1AIO	В	2015	4	11,11,12	5.68	6 (54%)	14,15,17	1.64	3 (21%)	
9	A1AIO	А	2016	4	11,11,12	5.67	6 (54%)	14,15,17	1.59	2 (14%)	
9	A1AIO	В	2031	4	11,11,12	5.65	6 (54%)	14,15,17	1.67	3 (21%)	
9	A1AIO	А	2029	4	11,11,12	5.72	6 (54%)	14,15,17	1.36	2 (14%)	
9	A1AIO	А	2014	4	11,11,12	5.70	6 (54%)	14,15,17	1.49	2 (14%)	
10	GLA	В	2064	1	11,11,12	1.72	3 (27%)	15,15,17	0.97	1 (6%)	
9	A1AIO	А	2004	4	11,11,12	5.69	6 (54%)	14,15,17	1.52	2 (14%)	
9	A1AIO	В	2025	4	11,11,12	5.71	6 (54%)	14,15,17	1.53	2 (14%)	
9	A1AIO	В	2022	4	11,11,12	5.66	6 (54%)	14,15,17	1.49	2 (14%)	
9	A1AIO	В	2018	4	11,11,12	5.71	6 (54%)	14,15,17	1.37	2 (14%)	
9	A1AIO	В	2002	4	11,11,12	5.68	6 (54%)	14,15,17	1.57	2 (14%)	
9	A1AIO	А	2032	4	11,11,12	5.67	6 (54%)	14,15,17	1.53	2 (14%)	
9	A1AIO	А	2043	5	11,11,12	5.73	6 (54%)	14,15,17	1.52	2 (14%)	
9	A1AIO	А	2030	4	11,11,12	5.70	6 (54%)	14,15,17	1.38	2 (14%)	
9	A1AIO	А	2052	5	11,11,12	5.69	6 (54%)	14,15,17	1.50	2 (14%)	
9	A1AIO	А	2015	4	11,11,12	5.70	6 (54%)	14,15,17	1.39	2 (14%)	
10	GLA	В	2061	1	11,11,12	1.74	3 (27%)	15,15,17	0.91	0	
10	GLA	В	2062	1	11,11,12	1.73	3 (27%)	15,15,17	0.96	1 (6%)	



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
9	A1AIO	В	2030	4	1/1/4/5	4/6/19/22	0/1/1/1
10	GLA	А	2063	1	-	2/2/19/22	0/1/1/1
9	A1AIO	А	2028	4	-	0/6/19/22	0/1/1/1
10	GLA	А	2058	1	-	1/2/19/22	0/1/1/1
9	A1AIO	В	2051	5	-	1/6/19/22	0/1/1/1
9	A1AIO	А	2039	6	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2040	4	1/1/4/5	3/6/19/22	0/1/1/1
9	A1AIO	A	2027	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2046	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2003	5	-	3/6/19/22	0/1/1/1
9	A1AIO	В	2049	4	-	0/6/19/22	0/1/1/1
10	GLA	А	2069	1	-	1/2/19/22	0/1/1/1
9	A1AIO	В	2028	4	-	4/6/19/22	0/1/1/1
9	A1AIO	В	2056	5	-	0/6/19/22	0/1/1/1
10	GLA	В	2060	-	-	2/2/19/22	0/1/1/1
10	GLA	А	2059	1	-	0/2/19/22	0/1/1/1
9	A1AIO	А	2009	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	В	2021	4	-	3/6/19/22	0/1/1/1
10	GLA	В	2065	1	-	2/2/19/22	0/1/1/1
9	A1AIO	В	2016	4	1/1/4/5	6/6/19/22	0/1/1/1
9	A1AIO	А	2038	4	1/1/4/5	3/6/19/22	0/1/1/1
9	A1AIO	А	2021	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2020	4	-	4/6/19/22	0/1/1/1
9	A1AIO	А	2042	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2045	4	-	2/6/19/22	0/1/1/1
9	A1AIO	В	2050	4	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2048	4	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2037	4	1/1/4/5	0/6/19/22	0/1/1/1
10	GLA	А	2064	1	-	2/2/19/22	0/1/1/1
9	A1AIO	В	2035	8	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2054	6	-	1/6/19/22	0/1/1/1
9	A1AIO	В	2032	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	В	2037	4	-	2/6/19/22	0/1/1/1
9	A1AIO	В	2054	8	-	6/6/19/22	0/1/1/1

Continued on next page...



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1AIO	А	2041	4	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2002	4	-	2/6/19/22	0/1/1/1
9	A1AIO	В	2052	5	_	2/6/19/22	0/1/1/1
9	A1AIO	А	2049	4	-	2/6/19/22	0/1/1/1
10	GLA	В	2068	1	_	$\frac{2}{2}/\frac{2}{19}/22$	0/1/1/1
10	GLA	A	2070	1	-	0/2/19/22	0/1/1/1
9	A1AIO	В	2008	4	-	$\frac{2}{6}/19/22$	0/1/1/1
9	A1AIO	A	2018	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	В	2011	5	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	В	2048	4	-	$\frac{2}{6}/19/22$	0/1/1/1
9	A1AIO	В	2039	5	-	1/6/19/22	0/1/1/1
9	A1AIO	В	2055	8	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2040	5	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2027	4	-	0/6/19/22	0/1/1/1
10	GLA	В	2069	1	-	2/2/19/22	0/1/1/1
9	A1AIO	А	2005	5	-	2/6/19/22	0/1/1/1
9	A1AIO	В	2023	4	-	4/6/19/22	0/1/1/1
9	A1AIO	В	2001	7	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2051	5	-	0/6/19/22	0/1/1/1
10	GLA	В	2059	1	-	0/2/19/22	0/1/1/1
9	A1AIO	В	2009	4	1/1/4/5	0/6/19/22	0/1/1/1
10	GLA	В	2066	-	_	1/2/19/22	0/1/1/1
9	A1AIO	В	2038	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2010	4	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2017	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2053	5	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	А	2045	4	-	2/6/19/22	0/1/1/1
9	A1AIO	В	2004	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	В	2006	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	В	2024	4	-	1/6/19/22	0/1/1/1
9	A1AIO	В	2019	4	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2053	6	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2029	4	-	0/6/19/22	0/1/1/1
10	GLA	А	2068	1	-	0/2/19/22	0/1/1/1
9	A1AIO	В	2017	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2022	4	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2006	4	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	A	2026	4	-	0/6/19/22	0/1/1/1

Continued from previous page...

Continued on next page...



α \cdot \cdot \cdot	C	•	
Continued	trom	previous	page
		T · · · · · · · ·	1

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1AIO	А	2013	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2033	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	А	2047	4	-	2/6/19/22	0/1/1/1
9	A1AIO	В	2036	4	-	2/6/19/22	0/1/1/1
10	GLA	А	2066	1	-	0/2/19/22	0/1/1/1
9	A1AIO	А	2012	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	А	2033	4	-	1/6/19/22	0/1/1/1
9	A1AIO	A	2010	4	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2031	4	-	0/6/19/22	0/1/1/1
10	GLA	A	2060	1	-	0/2/19/22	0/1/1/1
10	GLA	В	2063	-	-	2/2/19/22	0/1/1/1
10	GLA	В	2067	1	-	2/2/19/22	0/1/1/1
9	A1AIO	А	2008	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2046	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	В	2005	5	-	6/6/19/22	0/1/1/1
9	A1AIO	А	2025	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	А	2057	5	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2055	6	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2007	4	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2023	4	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2001	4	-	1/6/19/22	0/1/1/1
9	A1AIO	В	2013	4	-	2/6/19/22	0/1/1/1
9	A1AIO	В	2014	4	1/1/4/5	3/6/19/22	0/1/1/1
9	A1AIO	А	2003	5	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2044	4	-	2/6/19/22	0/1/1/1
9	A1AIO	В	2026	4	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2056	5	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2047	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	A	2011	5	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	А	2044	5	-	2/6/19/22	0/1/1/1
10	GLA	А	2065	1	-	2/2/19/22	0/1/1/1
10	GLA	А	2067	1	-	0/2/19/22	0/1/1/1
9	A1AIO	А	2024	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2034	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	А	2019	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2043	4	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2007	4	-	0/6/19/22	0/1/1/1
10	GLA	В	2058	-	-	2/2/19/22	0/1/1/1

Continued on next page...



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1AIO	В	2041	4	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2036	4	-	0/6/19/22	0/1/1/1
10	GLA	А	2061	1	-	0/2/19/22	0/1/1/1
10	GLA	А	2062	1	-	0/2/19/22	0/1/1/1
9	A1AIO	А	2020	4	-	1/6/19/22	0/1/1/1
9	A1AIO	А	2050	5	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2057	5	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2035	4	1/1/4/5	5/6/19/22	0/1/1/1
10	GLA	В	2070	-	-	0/2/19/22	0/1/1/1
9	A1AIO	В	2042	4	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2034	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2012	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	В	2015	4	-	1/6/19/22	0/1/1/1
9	A1AIO	А	2016	4	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	В	2031	4	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	А	2029	4	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2014	4	1/1/4/5	0/6/19/22	0/1/1/1
10	GLA	В	2064	1	-	0/2/19/22	0/1/1/1
9	A1AIO	А	2004	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	В	2025	4	-	2/6/19/22	0/1/1/1
9	A1AIO	В	2022	4	-	0/6/19/22	0/1/1/1
9	A1AIO	В	2018	4	-	4/6/19/22	0/1/1/1
9	A1AIO	В	2002	4	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2032	4	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2043	5	-	0/6/19/22	0/1/1/1
9	A1AIO	А	2030	4	-	2/6/19/22	0/1/1/1
9	A1AIO	А	2052	5	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	А	2015	4	-	0/6/19/22	0/1/1/1
10	GLA	В	2061	1	-	2/2/19/22	0/1/1/1
10	GLA	В	2062	1	-	1/2/19/22	0/1/1/1

Continued from previous page...

The worst 5 of 753 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	А	2043	A1AIO	C05-C04	-15.64	1.28	1.53
9	В	2039	A1AIO	C05-C04	-15.61	1.28	1.53
9	А	2005	A1AIO	C05-C04	-15.61	1.28	1.53
9	А	2029	A1AIO	C05-C04	-15.59	1.28	1.53
9	А	2033	A1AIO	C05-C04	-15.58	1.28	1.53



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
9	В	2026	A1AIO	C02-C03-C04	-4.96	109.23	115.86
9	А	2044	A1AIO	C02-C03-C04	-4.83	109.40	115.86
9	В	2033	A1AIO	C02-C03-C04	-4.81	109.42	115.86
9	В	2047	A1AIO	C02-C03-C04	-4.80	109.44	115.86
9	В	2006	A1AIO	C02-C03-C04	-4.73	109.54	115.86

The worst 5 of 258 bond angle outliers are listed below:

5 of 29 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	А	2004	A1AIO	C06
9	А	2006	A1AIO	C06
9	А	2009	A1AIO	C06
9	А	2011	A1AIO	C06
9	А	2012	A1AIO	C06

5 of 166 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
9	А	2002	A1AIO	O12-C01-C02-O11
9	А	2005	A1AIO	O12-C01-C02-O11
9	А	2030	A1AIO	C01-C02-C03-O07
9	А	2033	A1AIO	C01-C02-C03-O07
9	А	2035	A1AIO	O12-C01-C02-C03

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 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-43892. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 256

Y Index: 256

Z Index: 256



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: 270

Y Index: 271

Z Index: 161

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



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

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 1110 nm^3 ; this corresponds to an approximate mass of 1002 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 0.323 ${\rm \AA}^{-1}$



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-43892 and PDB model 9B4H. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.5 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 (0.5).



9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.


9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

\mathbf{Chain}	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.8900	0.4880
А	0.8940	0.4900
A1	0.7140	0.4580
A2	0.8210	0.4630
A3	0.8930	0.5310
A4	0.8330	0.5290
A5	0.8330	0.4860
A6	0.8330	0.4760
A7	1.0000	0.5530
A9	0.8060	0.4870
В	0.8900	0.4890
B0	0.8890	0.4180
B1	0.7780	0.4140
B3	0.8330	0.4690
B4	0.7220	0.4660
B5	0.7220	0.5070
B6	0.8060	0.4670
B7	0.8890	0.4520
B9	0.6670	0.5150
C0	0.8330	0.4270
C1	0.7780	0.4790
C2	0.6670	0.4470
C3	0.9440	0.4330
C4	0.8330	0.4900
C5	0.7220	0.4670
C6	1.0000	0.4270
$\overline{C7}$	0.8890	0.4860
C8	0.7780	0.4280
C9	0.7780	0.4180
$\overline{\mathrm{D0}}$	0.8890	0.4360
D1	0.5560	0.3560
D2	0.6670	0.4780
D3	0.8330	0.5100
$\overline{\mathrm{D4}}$	0.8330	0.4810
D5	0.7780	0.4830

0.0 <.00

 $Continued \ on \ next \ page...$



Continued from previous page...

Chain	Atom inclusion	Q-score
D6	0.9440	0.5310
D7	0.8890	0.4730
D8	0.8330	0.4470
D9	0.8890	0.4850
E0	0.8330	0.4820
E1	0.7780	0.4790
E2	0.6670	0.4360
E3	0.8330	0.4660
E4	0.7220	0.3750
E5	0.7780	0.4620
E6	0.7780	0.4810
E7	0.7220	0.5030
E8	0.8330	0.4950
F0	0.7780	0.4980
F2	0.9440	0.5270
F3	0.9440	0.4910
F5	0.6670	0.4890
F6	0.8890	0.5040
F7	0.9170	0.5100
F8	0.9440	0.5430
X	0.9770	0.4900
a1	0.7500	0.4670
a2	0.7860	0.4180
a3	0.8570	0.5080
a4	0.8330	0.5080
a5	0.8330	0.4650
a6	0.8330	0.4790
a7	1.0000	0.5850
a9	0.8060	0.4960
b0	0.9440	0.4330
b1	0.6670	0.4610
b3	0.9440	0.5280
b4	0.8330	0.4610
b5	0.7780	0.4880
b6	0.8610	0.4400
b7	0.9440	0.4880
b9	0.8330	0.4850
c0	0.8330	0.4050
<u>c1</u>	0.8330	0.4300
<u>c2</u>	0.6670	0.4130
<u>c3</u>	0.9440	0.4320
c4	0.8330	0.4440

Continued on next page...



Chain	Atom inclusion	Q-score
c5	0.7780	0.4640
c6	1.0000	0.3930
c7	0.8890	0.4920
c8	0.8330	0.4650
c9	0.8330	0.4250
d0	0.7780	0.4100
d1	0.6670	0.3850
d2	0.7220	0.4600
d3	0.8890	0.5220
d4	0.8330	0.4840
d5	0.9440	0.5030
d6	0.9440	0.4680
d7	0.8890	0.4480
d8	0.7780	0.4470
d9	0.6670	0.4410
e0	0.8890	0.5090
e1	0.7780	0.5230
e2	0.7780	0.4800
e3	0.8330	0.4630
e4	0.7780	0.3930
e5	0.7780	0.4600
e6	0.8330	0.4700
e7	0.8330	0.4670
e8	0.8330	0.5300
e9	0.8330	0.4940
f0	0.8330	0.4820
f2	0.8890	0.4740
f3	0.9440	0.5090
f5	0.7220	0.5210
f6	0.9440	0.5080
f7	0.9170	0.5290
f8	1.0000	0.5210

Continued from previous page...

