

Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2023 – 04:05 pm GMT

PDB ID	:	5FVN
Title	:	X-ray crystal structure of Enterobacter cloacae OmpE36 porin.
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		van den Berg, B.; Lakey, J.H.
Deposited on	:	2016-02-09
Resolution	:	1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp 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:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Motric	Whole archive	Similar resolution			
Wiethic	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$			
R _{free}	130704	1156 (1.46-1.46)			
Clashscore	141614	1202 (1.46-1.46)			
Ramachandran outliers	138981	1178(1.46-1.46)			
Sidechain outliers	138945	1178 (1.46-1.46)			
RSRZ outliers	127900	1139 (1.46-1.46)			

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	А	342	4% 97%	•
1	В	342	4% 95%	5%
1	С	342	2% 9 6%	•
1	D	342	<u>6%</u> 96%	•
1	Е	342	4% 97%	•



Mol	Chain	Length	Quality of ch	ain
1	F	342	% 	•
2	G	3	67%	33%
2	K	3	100%	
2	L	3	67%	33%
2	М	3	67%	33%
3	Н	5	60%	40%
3	Ι	5	40%	60%
3	Ν	5	60%	40%
4	J	4	50%	50%
4	0	4	50%	50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	DAO	В	412	-	-	-	Х
11	DAO	D	418	-	-	-	Х
11	DAO	D	424	-	-	-	Х



 $\mathbf{2}$

Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 19668 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	349	Total	С	Ν	0	S	4	8	0
1	Л	042	2722	1704	455	560	3	4	8	0
1	В	349	Total	С	Ν	0	S	0	4	0
1	D	042	2700	1685	451	561	3	0	4	0
1	С	249	Total	С	Ν	0	S	0	5	0
1		042	2704	1691	451	559	3	0	0	0
1	Л	349	Total	С	Ν	0	S	0	6	0
1	D	042	2710	1693	452	562	3	0	0	0
1	F	349	Total	С	Ν	0	S	0	6	0
1	Ľ	042	2708	1694	451	560	3	0	0	0
1	F	349	Total	С	Ν	Ο	S	0	1	0
	Г	042	2701	1689	452	557	3		4	U

• Molecule 1 is a protein called OMPC PORIN.

• Molecule 2 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-pho sphono-alpha-D-glucopyranose.

$$4P$$

$$\alpha \ 6 \qquad \beta \ 6 \qquad \alpha \ 4P$$

$$1P$$

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2 C	3	Total	С	Ν	Ο	Р	0	0	0
2	9		46	20	2	22	2		0	
2	K	3	2 Total C N O P	0	0	0				
	2 K	5	45	20	2	21	2	0	0	0
0	т	3	Total	С	Ν	Ο	Р	0	0	0
			46	20	2	22	2	0	0	
0	2 M	3	Total	С	Ν	Ο	Р	0	0	0
			46	20	2	22	2	0		0

• Molecule 3 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyran



osonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-de oxy-1-O-phosphono-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3 H	Б	Total	С	Ν	Ο	Р	0	0	0
0		5	74	35	2	35	2		0	
2	т	5	Total	С	Ν	Ο	Р	0	0	0
0	3 1	5	74	35	2	35	2	0		
2	3 N	5	Total	С	Ν	Ο	Р	0	0	0
3			74	35	2	35	2			0

• Molecule 4 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phospho no-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	т	4	Total	С	Ν	0	Р	0	0	0
4	J	4	61	28	2	29	2	0		
4	Ο	1	Total	С	Ν	0	Р	0	0	0
4		4	61	28	2	29	2			

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 6 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 2 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 4 & 4 \end{array}$	0	0
6	А	1	Total C 6 6	0	0
6	А	1	Total C 4 4	0	0
6	А	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 5 & 5 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 4 1 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 5 & 3 \end{array}$	0	0
6	А	1	Total C 8 8	0	0
6	А	1	Total C 7 7	0	0
6	В	1	Total C O 9 8 1	0	0
6	В	1	Total C 3 3	0	0
6	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 5 & 3 & 2 \end{array}$	0	0
6	В	1	Total C 8 8	0	0
6	В	1	Total C 8 8	0	0
6	С	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 3 & 3 \end{array}$	0	0
6	С	1	Total C 7 7	0	0
6	С	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 3 & 3 \end{array}$	0	0
6	С	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ 6 & 6 \end{array}$	0	0
6	С	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 3 & 3 \end{array}$	0	0
6	С	1	Total C 8 8	0	0
6	С	1	Total C O 11 10 1	0	0
6	С	1	Total C O 11 10 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	1	Total C O 10 9 1	0	0
6	С	1	Total C 7 7	0	0
6	D	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 4 & 4 \end{array}$	0	0
6	D	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 6 & 6 \end{array}$	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 8 8	0	0
6	D	1	Total C 8 8	0	0
6	D	1	Total C O 11 10 1	0	0
6	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 3 & 1 \end{array}$	0	0
6	D	1	Total C 6 6	0	0
6	Е	1	Total C 6 6	0	0
6	F	1	Total C 3 3	0	0
6	F	1	Total C 4 4	0	0
6	F	1	Total C 8 8	0	0

• Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
7	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 8 is 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid (three-letter code: KDO) (formula: $C_8H_{14}O_8$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 15 8 7 \end{array}$	0	0
8	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 15 8 7 \end{array}$	0	0
8	Е	1	Total C O 15 8 7	0	0

• Molecule 9 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: $C_{14}H_{28}O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total C O 15 13 2	0	0
9	А	1	Total C O 13 11 2	0	0
9	А	1	Total C O 16 14 2	0	0
9	А	1	Total C O 14 12 2	0	0
9	В	1	Total C O 14 12 2	0	0
9	В	1	Total C O 15 13 2	0	0
9	В	1	Total C O 13 11 2	0	0
9	В	1	Total C O 16 14 2	0	0
9	С	1	Total C O 14 12 2	0	0
9	С	1	Total C O 16 14 2	0	0
9	С	1	$\begin{array}{c cccc} \hline 10 & 11 & 2 \\ \hline Total & C & O \\ \hline 11 & 9 & 2 \\ \end{array}$	0	0
9	С	1	Total C O 16 14 2	0	0
9	С	1	Total C O 13 11 2	0	0
9	С	1	$\begin{array}{c cccc} 10 & 11 & 2 \\ \hline Total & C & O \\ 16 & 14 & 2 \\ \end{array}$	0	0
9	С	1	Total C O 13 11 2	0	0
9	С	1	Total C O 16 14 2	0	0
9	D	1	Total C O 14 12 2	0	0
9	D	1	Total C O 11 9 2	0	0
9	D	1	Total C O 13 11 2	0	0
9	D	1	Total C O 11 9 2	0	0
9	D	1	Total C O 16 14 2	0	0
9	D	1	Total C O 13 11 2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 16 14 2	0	0
9	D	1	Total C O 14 12 2	0	0
9	Е	1	Total C O 14 12 2	0	0
9	Е	1	Total C O 14 12 2	0	0
9	Е	1	Total C O 12 10 2	0	0
9	Е	1	Total C O 15 13 2	0	0
9	F	1	Total C O 14 12 2	0	0
9	F	1	Total C O 12 10 2	0	0
9	F	1	Total C O 13 11 2	0	0
9	F	1	Total C O 12 10 2	0	0
9	F	1	Total C O 16 14 2	0	0
9	F	1	Total C O 14 12 2	0	0
9	F	1	$\begin{array}{c cc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 11 & 9 & 2 \end{array}$	0	0
9	F	1	Total C O 16 14 2	0	0

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• Molecule 10 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 5 1 \end{array}$	0	0
10	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 5 1 \end{array}$	0	0
10	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 7 & 1 \end{array}$	0	0
10	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 9 8 1 \end{array}$	0	0
10	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 4 1 \end{array}$	0	0
10	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 5 1 \end{array}$	0	0
10	Ε	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 5 1 \end{array}$	0	0
10	F	1	Total C O 11 10 1	0	0
10	F	1	Total C O 12 11 1	0	0

• Molecule 11 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 4 1 \end{array}$	0	0
11	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 7 1 \end{array}$	0	0
11	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 4 1 \end{array}$	0	0
11	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 4 1 \end{array}$	0	0
11	С	1	Total C O 13 12 1	0	0
11	С	1	Total C O 10 9 1	0	0
11	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 7 & 1 \end{array}$	0	0
11	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 5 1 \end{array}$	0	0
11	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 2 & 1 \end{array}$	0	0
11	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 4 1 \end{array}$	0	0
11	Е	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 4 1 \end{array}$	0	0
11	Е	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 4 1 \end{array}$	0	0
11	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 4 1 \end{array}$	0	0
11	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	1	$\begin{array}{c cc} Total & C & O \\ 8 & 7 & 1 \end{array}$	0	0

• Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	С	1	Total Ca 1 1	0	0
12	F	1	Total Ca 1 1	0	0

• Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	А	321	Total O 321 321	0	0
13	В	316	Total O 316 316	0	0
13	С	324	Total O 324 324	0	0
13	D	296	Total O 296 296	0	0
13	Е	303	Total O 303 303	0	0
13	F	350	Total O 350 350	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: OMPC PORIN

• Molecule 1: OMPC PORIN



Cl	nai	n I	? :	%									98%	.
A1	M36	W56 BE7	Y58	D84	D89	F136	R166	R170	E186	<mark>0233</mark>	R242	F342		

• Molecule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phos phono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain G:	67%	33%

GP11 Z9M2 KD03

 $\bullet \ {\rm Molecule \ 2: \ 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic \ acid-(2-6)-2-amino-2-deoxy-4-O-phos phono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose}$

Chain K	: 100%	
GP11 Z9M2 KD03		
• Molecu phono-be	ule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-am eta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D	ino-2-deoxy-4-O-phos 9-glucopyranose

Chain L:

33%

GP11 Z9M2 KD03

 $\bullet \ {\rm Molecule \ 2: \ 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic \ acid-(2-6)-2-amino-2-deoxy-4-O-phos phono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose}$

Chain M:	67%	33%

67%

GP 11 Z9M2 KD 03

• Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranos e

Chain H:	60%	40%

GP11 Z9M2 KDD3 KDD4 GMH5

• Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose e



Chain I:	40%	60%						
GP11 29/2 K003 K004 GMH5								
• Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose								
Chain N:	60%	40%						
GP 11 29M2 KDD3 KDD3 KDD4 GMH5								
• Molecule 4: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-o ct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-ami no-2-deoxy-1-O-phosphono-alpha-D-glucopyranose								
Chain J:	50%	50%						

GP11 Z9M2 KD03 KD04

GP1 Z9M KD0 KD0

 \bullet Molecule 4: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain O:	50%	50%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	109.75Å 123.26 Å 116.01 Å	Deperitor
a, b, c, α , β , γ	90.00° 91.01° 90.00°	Depositor
$\mathbf{Posolution} \left(\overset{\circ}{\mathbf{A}} \right)$	115.99 - 1.45	Depositor
Resolution (A)	48.60 - 1.45	EDS
% Data completeness	100.0 (115.99-1.45)	Depositor
(in resolution range)	99.9(48.60-1.45)	EDS
R _{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.73 (at 1.45 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
B B.	0.155 , 0.183	Depositor
II, II, <i>free</i>	0.167 , 0.192	DCC
R_{free} test set	13912 reflections (2.56%)	wwPDB-VP
Wilson B-factor $(Å^2)$	14.5	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , 60.8	EDS
L-test for $twinning^2$	$< L > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19668	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 13.10% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, DAO, GP1, GMH, C8E, Z9M, KDO, SO4, FTT, MYR, PO4

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.54	0/2799	0.83	4/3785~(0.1%)	
1	В	0.52	0/2768	0.82	8/3743~(0.2%)	
1	С	0.51	0/2775	0.81	4/3753~(0.1%)	
1	D	0.52	0/2784	0.86	5/3765~(0.1%)	
1	Е	0.53	0/2782	0.82	4/3763~(0.1%)	
1	F	0.49	0/2769	0.77	4/3745~(0.1%)	
All	All	0.52	0/16677	0.82	29/22554~(0.1%)	

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	D	1	1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	242	ARG	NE-CZ-NH1	-14.26	113.17	120.30
1	D	242	ARG	NE-CZ-NH2	10.48	125.54	120.30
1	А	242	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	F	242	ARG	NE-CZ-NH2	9.71	125.15	120.30
1	С	242	ARG	NE-CZ-NH2	9.45	125.03	120.30
1	А	242	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	Ε	242	ARG	NE-CZ-NH2	8.72	124.66	120.30
1	В	242	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	С	170	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	F	242	ARG	NE-CZ-NH1	-7.45	116.58	120.30



Mol	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	Е	242	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	С	242	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	В	132	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	А	74	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	F	170	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	Ε	132	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	В	268	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	С	170	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	213	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	В	242	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	В	74	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	В	170	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	В	170	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	92	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	F	170	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	А	170	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	37	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	Е	213	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	В	166	ARG	NE-CZ-NH2	-5.07	117.77	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	84	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	83	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2722	0	2520	2	0
1	В	2700	0	2475	8	0
1	С	2704	0	2491	6	0



	Choin	Non H	page	U(addad)	Clashes	Summ Clashes
	D	NOII-II				Symm-Clasnes
	D	2710	0	2492	4	0
	E	2708	0	2498	<u>3</u>	0
	F	2701	0	2488	2	0
2	G	40	0	17	2	0
2	K	45	0	15	0	0
2	L	46	0	17	2	0
2	M	46	0	17	3	0
3	H	74	0	40	1	0
3		74	0	38	4	0
3	N	74	0	37	1	0
4	J	61	0	28	2	0
4	0	61	0	29	2	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
6	A	50	0	76	3	0
6	В	33	0	56	2	0
6	С	69	0	122	4	0
6	D	59	0	102	1	0
6	E	6	0	11	0	0
6	F	15	0	27	2	0
7	A	5	0	0	0	0
7	В	5	0	0	0	0
7	С	5	0	0	0	0
7	D	5	0	0	0	0
7	E	5	0	0	0	0
7	F	5	0	0	0	0
8	A	15	0	12	2	0
8	D	15	0	12	2	0
8	E	15	0	12	3	0
9	A	58	0	84	0	0
9	В	58	0	85	0	0
9	С	115	0	172	0	0
9	D	108	0	154	0	0
9	Ε	55	0	75	0	0
9	F	108	0	153	2	0
10	A	6	0	6	0	0
10	В	6	0	6	0	0
10	C	17	0	22	0	0
10	D	11	0	10	0	0
10	Е	6	0	6	0	0
10	F	23	0	34	0	0
11	А	13	0	14	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	В	5	0	4	0	0
11	С	36	0	51	0	0
11	D	14	0	10	0	0
11	Е	10	0	8	0	0
11	F	18	0	18	0	0
12	С	1	0	0	0	0
12	F	1	0	0	0	0
13	А	321	0	0	1	0
13	В	316	0	0	5	0
13	С	324	0	0	1	0
13	D	296	0	0	4	0
13	Е	303	0	0	0	0
13	F	350	0	0	0	0
All	All	19668	0	16544	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
8:E:403:KDO:C2	2:M:3:KDO:O4	1.81	1.29
8:D:413:KDO:C2	2:L:3:KDO:O4	1.84	1.24
8:A:412:KDO:C2	2:G:3:KDO:O4	1.85	1.24
6:A:408:C8E:H112	13:A:755:HOH:O	1.73	0.88
1:D:251:LYS:HG3	13:D:719:HOH:O	1.73	0.86
3:I:3:KDO:HO4	3:I:4:KDO:C2	1.90	0.81
6:F:401:C8E:H11	9:F:407:FTT:C10	2.11	0.80
1:D:236:GLN:HG3	13:D:719:HOH:O	1.87	0.74
1:C:69:ASN:H	6:C:405:C8E:H13	1.55	0.72
4:0:3:KDO:HO4	4:O:4:KDO:C2	2.09	0.65
3:N:3:KDO:C4	3:N:4:KDO:C2	2.75	0.62
1:D:236:GLN:CG	13:D:719:HOH:O	2.45	0.60
4:J:3:KDO:C4	4:J:4:KDO:C2	2.76	0.59
8:E:403:KDO:C2	2:M:3:KDO:C4	2.79	0.58
6:D:409:C8E:H81	13:D:587:HOH:O	2.04	0.58
3:I:3:KDO:C4	3:I:4:KDO:C2	2.79	0.57
1:B:236:GLN:HG3	13:B:727:HOH:O	2.06	0.56
1:B:236:GLN:CG	13:B:727:HOH:O	2.53	0.56
1:C:68:GLU:HB2	6:C:405:C8E:C1	2.37	0.55
1:C:68:GLU:HA	6:C:405:C8E:H22	1.87	0.55



	A + 0	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:H:3:KDO:C4	3:H:4:KDO:C2	2.83	0.54	
8:D:413:KDO:C2	2:L:3:KDO:C4	2.86	0.52	
1:A:59:GLN:HE22	6:A:408:C8E:H132	1.76	0.51	
4:0:3:KDO:C4	4:0:4:KDO:C2	2.82	0.51	
6:B:403:C8E:H101	13:B:737:HOH:O	2.11	0.51	
3:I:3:KDO:O4	3:I:4:KDO:C1	2.55	0.49	
1:C:68:GLU:HB2	6:C:405:C8E:H11	1.94	0.48	
1:B:103:TRP:CE2	1:B:222:LYS:HE2	2.48	0.48	
1:E:137:PHE:HB2	1:E:139:LEU:HD13	1.97	0.47	
3:I:3:KDO:H5	3:I:5:GMH:O2	2.16	0.45	
1:B:35:TYR:CD1	6:B:403:C8E:H102	2.53	0.44	
1:B:236:GLN:HG2	13:B:727:HOH:O	2.17	0.43	
1:B:9:ASN:HB3	13:C:610:HOH:O	2.18	0.43	
8:A:412:KDO:C2	2:G:3:KDO:C4	2.89	0.43	
6:F:403:C8E:H13	9:F:406:FTT:H22	2.01	0.43	
1:E:103:TRP:CE2	1:E:222:LYS:HE2	2.54	0.43	
1:B:295:ASP:OD1	1:B:311:ASP:OD1	2.37	0.42	
4:J:3:KDO:O4	4:J:4:KDO:C1	2.55	0.42	
8:E:403:KDO:C3	2:M:3:KDO:O4	2.63	0.42	
1:D:56:TRP:CZ2	1:D:58:TYR:HB2	2.55	0.42	
1:F:56:TRP:CZ2	1:F:58:TYR:HB2	2.56	0.41	
1:B:6:LYS:HE2	13:B:660:HOH:O	2.20	0.41	
1:C:56:TRP:CZ2	1:C:58:TYR:HB2	2.55	0.41	
1:A:113:ASP:OD2	6:A:407:C8E:H102	2.21	0.41	
1:C:295:ASP:OD1	1:C:311:ASP:OD1	2.40	0.40	
1:E:56:TRP:CD1	1:F:36:MET:HG2	2.57	0.40	

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	348/342~(102%)	332~(95%)	16 (5%)	0	100 100
1	В	344/342~(101%)	329~(96%)	14 (4%)	1 (0%)	41 18
1	С	345/342~(101%)	330~(96%)	14 (4%)	1 (0%)	41 18
1	D	346/342~(101%)	329~(95%)	16 (5%)	1 (0%)	41 18
1	Е	346/342~(101%)	330~(95%)	16 (5%)	0	100 100
1	F	344/342~(101%)	332~(96%)	12 (4%)	0	100 100
All	All	2073/2052~(101%)	1982~(96%)	88 (4%)	3~(0%)	51 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	136	PHE
1	С	136	PHE
1	D	83	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	283/275~(103%)	279~(99%)	4 (1%)	67 37
1	В	279/275~(102%)	276~(99%)	3(1%)	73 48
1	С	280/275~(102%)	277~(99%)	3 (1%)	73 48
1	D	281/275~(102%)	278~(99%)	3 (1%)	73 48
1	Е	281/275~(102%)	278~(99%)	3 (1%)	73 48
1	F	279/275~(102%)	276~(99%)	3 (1%)	73 48
All	All	1683/1650~(102%)	1664 (99%)	19 (1%)	71 48

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	89	ASP
1	А	166	ARG



Mol	Chain	Res	Type
1	А	233	GLN
1	А	320	LYS
1	В	89	ASP
1	В	166	ARG
1	В	233	GLN
1	С	89	ASP
1	С	166	ARG
1	С	233	GLN
1	D	89	ASP
1	D	166	ARG
1	D	233	GLN
1	Е	89	ASP
1	Е	166	ARG
1	Е	233	GLN
1	F	89	ASP
1	F	166	ARG
1	F	233	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

35 monosaccharides are modelled in this entry.

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



Mal	Turne	Chain	Dec	Timle	Bo	ond leng	ths	Bond angles		
NIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	GP1	G	1	2,9	15,16,16	1.51	1 (6%)	$23,\!24,\!24$	1.03	1 (4%)
2	Z9M	G	2	2,9	15,15,16	1.34	1 (6%)	$18,\!22,\!24$	1.09	0
2	KDO	G	3	2	15,15,16	0.82	0	$19,\!21,\!24$	1.37	3 (15%)
3	GP1	Н	1	3,9	15,16,16	1.52	1 (6%)	23,24,24	1.50	3 (13%)
3	Z9M	Н	2	3,9	15,15,16	1.14	1 (6%)	18,22,24	0.91	0
3	KDO	Н	3	3	15,15,16	1.19	1 (6%)	19,21,24	1.30	3 (15%)
3	KDO	Н	4	3	15,15,16	0.76	0	19,21,24	1.52	3 (15%)
3	GMH	Н	5	3	13,13,14	0.63	0	17,18,20	1.23	2 (11%)
3	GP1	Ι	1	3,9	15,16,16	1.66	1 (6%)	23,24,24	1.07	2 (8%)
3	Z9M	Ι	2	3,9	15,15,16	1.53	1 (6%)	18,22,24	1.15	1 (5%)
3	KDO	Ι	3	3	15,15,16	1.23	1 (6%)	19,21,24	1.56	4 (21%)
3	KDO	Ι	4	3,12	15,15,16	0.68	0	19,21,24	1.52	2 (10%)
3	GMH	Ι	5	3	13,13,14	0.99	1 (7%)	17,18,20	1.52	4 (23%)
4	GP1	J	1	4,9	15,16,16	1.40	1 (6%)	23,24,24	1.30	3 (13%)
4	Z9M	J	2	4,9	15,15,16	1.24	1 (6%)	18,22,24	0.70	0
4	KDO	J	3	4	15,15,16	1.13	1 (6%)	19,21,24	1.34	2 (10%)
4	KDO	J	4	4	15,15,16	0.81	0	19,21,24	1.64	5 (26%)
2	GP1	K	1	2,9	15,16,16	1.47	1 (6%)	23,24,24	1.67	5 (21%)
2	Z9M	K	2	2,9	15,15,16	1.36	1 (6%)	18,22,24	1.00	1 (5%)
2	KDO	K	3	2	14,14,16	0.76	0	16,19,24	2.19	2 (12%)
2	GP1	L	1	2,9	15,16,16	1.41	1 (6%)	23,24,24	0.94	1 (4%)
2	Z9M	L	2	2,9	15,15,16	1.29	1 (6%)	18,22,24	0.90	0
2	KDO	L	3	2	15,15,16	0.76	0	19,21,24	1.53	6 (31%)
2	GP1	М	1	2,9	15,16,16	1.53	1 (6%)	23,24,24	0.94	1 (4%)
2	Z9M	М	2	2,9	15,15,16	1.46	1 (6%)	18,22,24	0.81	0
2	KDO	М	3	2	15,15,16	0.74	0	19,21,24	1.39	3 (15%)
3	GP1	Ν	1	3,9	15,16,16	1.78	1 (6%)	23,24,24	0.93	1 (4%)
3	Z9M	Ν	2	3,9	15,15,16	1.52	1 (6%)	18,22,24	1.05	1 (5%)
3	KDO	N	3	3	15,15,16	1.18	1 (6%)	19,21,24	1.59	5 (26%)
3	KDO	N	4	3,12	15,15,16	0.63	0	19,21,24	1.54	3 (15%)
3	GMH	Ν	5	3	13,13,14	0.73	0	17,18,20	1.64	3 (17%)
4	GP1	О	1	4,9	15,16,16	1.45	1 (6%)	23,24,24	1.39	2 (8%)
4	Z9M	Ο	2	4,9	15,15,16	1.31	1 (6%)	18,22,24	0.68	0
4	KDO	Ο	3	4	15,15,16	1.05	2 (13%)	19,21,24	1.44	4 (21%)
4	KDO	Ο	4	4	15,15,16	0.74	0	19,21,24	1.53	3 (15%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GP1	G	1	2,9	-	2/6/27/27	0/1/1/1
2	Z9M	G	2	2,9	-	0/7/24/27	0/1/1/1
2	KDO	G	3	2	-	0/10/26/30	0/1/1/1
3	GP1	Н	1	3,9	-	1/6/27/27	0/1/1/1
3	Z9M	Н	2	3,9	-	0/7/24/27	0/1/1/1
3	KDO	Н	3	3	-	0/10/26/30	0/1/1/1
3	KDO	Н	4	3	-	1/10/26/30	0/1/1/1
3	GMH	Н	5	3	-	0/6/23/26	0/1/1/1
3	GP1	I	1	3,9	-	0/6/27/27	0/1/1/1
3	Z9M	Ι	2	$3,\!9$	-	2/7/24/27	0/1/1/1
3	KDO	Ι	3	3	-	1/10/26/30	0/1/1/1
3	KDO	Ι	4	3,12	-	1/10/26/30	0/1/1/1
3	GMH	Ι	5	3	-	4/6/23/26	0/1/1/1
4	GP1	J	1	4,9	-	1/6/27/27	0/1/1/1
4	Z9M	J	2	4,9	-	0/7/24/27	0/1/1/1
4	KDO	J	3	4	-	0/10/26/30	0/1/1/1
4	KDO	J	4	4	-	0/10/26/30	0/1/1/1
2	GP1	Κ	1	2,9	-	0/6/27/27	0/1/1/1
2	Z9M	K	2	2,9	-	0/7/24/27	0/1/1/1
2	KDO	Κ	3	2	-	2/10/22/30	0/1/1/1
2	GP1	L	1	2,9	-	1/6/27/27	0/1/1/1
2	Z9M	L	2	2,9	_	0/7/24/27	0/1/1/1
2	KDO	L	3	2	-	1/10/26/30	0/1/1/1
2	GP1	М	1	2,9	-	1/6/27/27	0/1/1/1
2	Z9M	М	2	2,9	-	0/7/24/27	0/1/1/1
2	KDO	М	3	2	-	2/10/26/30	0/1/1/1
3	GP1	Ν	1	3,9	_	0/6/27/27	0/1/1/1
3	Z9M	Ν	2	$3,\!9$	-	0/7/24/27	0/1/1/1
3	KDO	Ν	3	3	-	0/10/26/30	0/1/1/1
3	KDO	Ν	4	3,12	-	4/10/26/30	0/1/1/1
3	GMH	Ν	5	3	-	3/6/23/26	0/1/1/1
4	GP1	Ο	1	4,9	-	1/6/27/27	0/1/1/1
4	Z9M	0	2	4,9	-	0/7/24/27	0/1/1/1
4	KDO	0	3	4	-	0/10/26/30	0/1/1/1
4	KDO	0	4	4	-	2/10/26/30	0/1/1/1

All (25) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Ν	1	GP1	P4B-O1	6.46	1.71	1.59
3	Ι	1	GP1	P4B-O1	-5.77	1.48	1.59
3	Н	1	GP1	P4B-O1	-5.54	1.48	1.59
3	Ν	2	Z9M	P1-O4	-5.48	1.49	1.59
2	G	1	GP1	P4B-O1	-5.42	1.49	1.59
2	М	1	GP1	P4B-O1	-5.39	1.49	1.59
3	Ι	2	Z9M	P1-O4	-5.38	1.49	1.59
2	М	2	Z9M	P1-O4	-5.30	1.49	1.59
2	Κ	1	GP1	P4B-O1	-5.26	1.49	1.59
4	0	1	GP1	P4B-O1	-5.23	1.49	1.59
4	J	1	GP1	P4B-O1	-5.08	1.49	1.59
2	Κ	2	Z9M	P1-O4	-5.07	1.49	1.59
2	L	1	GP1	P4B-O1	-5.03	1.49	1.59
2	G	2	Z9M	P1-O4	-4.81	1.50	1.59
4	0	2	Z9M	P1-O4	-4.68	1.50	1.59
2	L	2	Z9M	P1-O4	-4.44	1.50	1.59
4	J	2	Z9M	P1-O4	-4.29	1.51	1.59
3	Н	2	Z9M	P1-O4	-3.89	1.52	1.59
3	Ι	3	KDO	O5-C5	-3.84	1.33	1.43
3	Н	3	KDO	O5-C5	-3.53	1.34	1.43
3	Ν	3	KDO	O5-C5	-3.13	1.35	1.43
4	J	3	KDO	C2-C1	-3.11	1.49	1.52
4	0	3	KDO	O1B-C1	-2.55	1.22	1.30
4	0	3	KDO	C2-C1	-2.46	1.50	1.52
3	Ι	5	GMH	O5-C5	2.22	1.45	1.43

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	K	3	KDO	O6-C6-C5	7.59	117.80	109.94
2	K	1	GP1	01-P4B-08B	-5.39	88.58	109.39
3	Н	1	GP1	01-P4B-08B	4.91	128.34	109.39
3	N	5	GMH	C1-O5-C5	4.77	119.30	111.48
4	0	1	GP1	O1-C1-C2	4.54	116.62	108.40
3	Н	4	KDO	O6-C2-C3	4.45	116.58	110.46
3	Ι	4	KDO	O6-C2-C3	4.44	116.57	110.46
4	0	4	KDO	O6-C2-C3	4.43	116.56	110.46
3	Ι	5	GMH	O5-C1-C2	-3.58	105.25	110.77
4	J	4	KDO	O6-C2-C3	3.54	115.32	110.46
3	Н	4	KDO	C6-O6-C2	3.50	118.83	111.34
3	Н	5	GMH	C1-O5-C5	3.47	117.17	111.48
3	N	2	Z9M	C1-O5-C5	3.45	116.87	112.19
4	J	1	GP1	01-C1-C2	3.37	114.50	108.40



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$
4	J	4	KDO	O4-C4-C3	-3.22	101.96	109.94
3	Ν	4	KDO	O1A-C1-C2	-3.20	115.01	122.57
2	Κ	1	GP1	O9B-P4B-O1	3.13	120.00	105.99
4	J	4	KDO	C6-O6-C2	3.09	117.94	111.34
3	Ν	3	KDO	C6-O6-C2	3.09	117.94	111.34
4	J	3	KDO	C4-C5-C6	-3.08	104.22	110.41
4	0	4	KDO	C6-O6-C2	3.05	117.87	111.34
3	Ν	4	KDO	O6-C2-C3	3.05	114.65	110.46
2	G	3	KDO	C4-C5-C6	-3.02	104.35	110.41
3	Ι	3	KDO	O5-C5-C4	-3.00	104.25	109.99
4	J	1	GP1	O9B-P4B-O1	2.92	119.06	105.99
3	Ι	3	KDO	C3-C4-C5	2.89	114.88	110.69
3	Н	1	GP1	O9B-P4B-O1	-2.88	93.07	105.99
2	Κ	1	GP1	O1-C1-C2	2.87	113.60	108.40
3	Ι	2	Z9M	C1-O5-C5	2.83	116.03	112.19
4	0	3	KDO	C6-O6-C2	2.81	117.36	111.34
4	0	3	KDO	C4-C5-C6	-2.79	104.81	110.41
2	L	3	KDO	C4-C5-C6	-2.74	104.91	110.41
3	Ι	3	KDO	C4-C5-C6	-2.73	104.91	110.41
2	Κ	3	KDO	O1B-C1-C2	2.71	120.77	113.03
3	Ν	1	GP1	O3-C3-C2	-2.71	105.34	110.22
2	М	3	KDO	C6-O6-C2	2.70	117.12	111.34
3	Н	3	KDO	C4-C5-C6	-2.69	104.99	110.41
2	Κ	2	Z9M	C1-O5-C5	2.67	115.81	112.19
3	Н	5	GMH	C1-C2-C3	2.66	112.94	109.67
3	Ν	3	KDO	C4-C5-C6	-2.65	105.09	110.41
2	L	1	GP1	O1-C1-C2	2.55	113.02	108.40
4	0	4	KDO	O1A-C1-C2	-2.54	116.56	122.57
2	М	1	GP1	O1-C1-C2	2.49	112.91	108.40
2	М	3	KDO	C4-C5-C6	-2.49	105.41	110.41
3	N	4	KDO	01B-C1-C2	2.47	120.07	113.03
4	0	3	KDO	01A-C1-C2	-2.46	116.75	122.57
4	J	3	KDO	C6-O6-C2	2.44	116.56	111.34
3	Ι	5	GMH	O2-C2-C1	2.42	114.10	109.15
3	Ι	1	GP1	O1-C1-C2	2.42	112.78	108.40
3	Ι	5	GMH	C1-O5-C5	2.38	115.37	111.48
2	Κ	1	GP1	07B-P4B-O1	2.36	116.57	105.99
4	J	1	GP1	O3-C3-C4	-2.36	104.89	110.35
3	Н	3	KDO	C6-O6-C2	2.34	116.34	111.34
2	М	3	KDO	C3-C4-C5	2.33	114.07	110.69
3	N	3	KDO	O5-C5-C4	-2.32	105.56	109.99
3	Ν	3	KDO	C3-C4-C5	2.26	113.97	110.69



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Ι	1	GP1	O7B-P4B-O1	2.25	116.09	105.99
3	Н	4	KDO	O1A-C1-C2	-2.23	117.30	122.57
3	Ι	5	GMH	C1-C2-C3	-2.22	106.93	109.67
4	J	4	KDO	O4-C4-C5	2.21	114.56	110.14
3	Ν	5	GMH	O5-C1-C2	2.18	114.13	110.77
2	L	3	KDO	O4-C4-C5	-2.18	105.78	110.14
3	Ν	3	KDO	O1A-C1-C2	-2.16	117.46	122.57
2	Κ	1	GP1	O5-C1-O1	-2.16	108.55	111.36
2	L	3	KDO	O1B-C1-C2	2.15	119.16	113.03
3	Ν	5	GMH	O2-C2-C3	2.14	114.43	110.14
2	L	3	KDO	C6-O6-C2	2.14	115.92	111.34
2	L	3	KDO	C3-C4-C5	2.12	113.76	110.69
2	G	3	KDO	C6-O6-C2	2.09	115.81	111.34
4	0	1	GP1	O3-C3-C4	-2.08	105.53	110.35
4	J	4	KDO	O1A-C1-C2	-2.08	117.66	122.57
3	Ι	4	KDO	O8-C8-C7	-2.07	106.57	111.07
2	L	3	KDO	O1A-C1-C2	-2.07	117.69	122.57
4	0	3	KDO	O1B-C1-C2	2.04	118.87	113.03
3	Н	1	GP1	O1-C1-C2	2.04	112.10	108.40
3	Н	3	KDO	C3-C4-C5	2.03	113.64	110.69
2	G	1	GP1	O1-C1-C2	2.02	112.06	108.40
2	G	3	KDO	O5-C5-C6	2.01	115.26	109.94
3	Ι	3	KDO	C6-O6-C2	2.00	115.63	111.34

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
3	Ι	5	GMH	C5-C6-C7-O7
3	Ι	5	GMH	O6-C6-C7-O7
3	N	4	KDO	C5-C6-C7-C8
3	Ν	4	KDO	O6-C6-C7-O7
3	Ν	5	GMH	O5-C5-C6-O6
2	G	1	GP1	C1-O1-P4B-O8B
2	Κ	3	KDO	C6-C7-C8-O8
3	Ι	5	GMH	O5-C5-C6-C7
3	Ι	2	Z9M	C4-O4-P1-O9
3	Ι	4	KDO	C5-C6-C7-C8
3	Ι	5	GMH	O5-C5-C6-O6
3	Ν	4	KDO	O1A-C1-C2-O6
4	0	4	KDO	O1A-C1-C2-O6
2	G	1	GP1	C1-O1-P4B-O9B



Mol	Chain	Res	Type	Atoms
2	L	1	GP1	C1-O1-P4B-O7B
2	М	1	GP1	C1-O1-P4B-O7B
3	Н	1	GP1	C1-O1-P4B-O9B
3	Ι	2	Z9M	C4-O4-P1-O7
3	N	5	GMH	C4-C5-C6-O6
4	J	1	GP1	C1-O1-P4B-O9B
4	0	1	GP1	C1-O1-P4B-O7B
3	Н	4	KDO	O1A-C1-C2-O6
2	K	3	KDO	O7-C7-C8-O8
2	L	3	KDO	O1B-C1-C2-C3
2	М	3	KDO	O1A-C1-C2-C3
2	М	3	KDO	O1B-C1-C2-C3
3	Ι	3	KDO	O1A-C1-C2-C3
3	N	4	KDO	O1A-C1-C2-C3
3	N	5	GMH	C4-C5-C6-C7
4	0	4	KDO	O1A-C1-C2-C3

There are no ring outliers.

14 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	KDO	2	0
2	L	3	KDO	2	0
3	Ι	3	KDO	4	0
3	Ι	5	GMH	1	0
4	J	3	KDO	2	0
3	Н	3	KDO	1	0
4	J	4	KDO	2	0
3	Ι	4	KDO	3	0
4	0	3	KDO	2	0
4	0	4	KDO	2	0
3	Ν	4	KDO	1	0
2	М	3	KDO	3	0
3	H	4	KDO	1	0
3	N	3	KDO	1	0

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
































5.6 Ligand geometry (i)

Of 110 ligands modelled in this entry, 2 are monoatomic - leaving 108 for Mogul analysis.

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

Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	ths	Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	DAO	D	418	9	1,2,13	1.37	0	1,1,13	0.76	0
5	SO4	D	401	-	4,4,4	0.21	0	$6,\!6,\!6$	0.46	0
9	FTT	А	418	4,11	13,13,16	0.55	0	$13,\!13,\!17$	1.47	1 (7%)
9	FTT	D	425	4	13,13,16	0.54	0	$13,\!13,\!17$	1.55	2 (15%)
6	C8E	D	409	-	3,3,20	0.55	0	2,2,19	0.34	0
9	FTT	В	407	2	13,13,16	0.51	0	$13,\!13,\!17$	1.08	1 (7%)
9	FTT	D	414	2	13,13,16	0.57	0	13,13,17	0.69	1 (7%)
9	FTT	В	409	11,3	12,12,16	0.59	0	12,12,17	1.11	2 (16%)
11	DAO	В	412	9	4,4,13	0.62	0	3,3,13	0.71	0



N.T. 1	T		D	T ! 1.	Bo	ond leng	\mathbf{ths}	Bond angles		
NIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	KDO	Е	403	-	$15,\!15,\!16$	0.68	0	$19,\!21,\!24$	1.70	3 (15%)
10	MYR	С	419	9	7,7,15	0.60	0	6,6,15	0.56	0
9	FTT	А	415	2,10	15,15,16	0.43	0	15, 15, 17	0.92	1 (6%)
10	MYR	F	411	9	10,10,15	0.43	0	9,9,15	0.63	0
6	C8E	В	401	-	8,8,20	0.38	0	7,7,19	0.58	0
6	C8E	А	404	-	5,5,20	0.30	0	4,4,19	0.26	0
6	C8E	D	406	-	7,7,20	0.33	0	$6,\!6,\!19$	0.46	0
7	PO4	Ε	402	-	4,4,4	0.63	0	$6,\!6,\!6$	0.81	0
6	C8E	С	403	-	2,2,20	0.25	0	0,1,19	-	_
6	C8E	A	408	-	7,7,20	0.48	0	6,6,19	0.44	0
9	FTT	С	422	4	$15,\!15,\!16$	0.28	0	$15,\!15,\!17$	1.40	3 (20%)
9	FTT	В	410	10,3	$15,\!15,\!16$	0.44	0	$15,\!15,\!17$	0.85	0
6	C8E	С	409	-	9,9,20	0.35	0	8,8,19	0.43	0
11	DAO	F	413	9	4,4,13	0.65	0	3,3,13	0.54	0
6	C8E	С	402	-	6,6,20	0.53	0	$5,\!5,\!19$	0.82	0
9	FTT	F	416	4,10	15,15,16	0.29	0	15,15,17	0.81	0
7	PO4	F	404	-	4,4,4	0.54	0	6,6,6	0.80	0
8	KDO	А	412	-	$15,\!15,\!16$	0.87	1 (6%)	19,21,24	1.44	3 (15%)
6	C8E	А	407	-	4,4,20	0.50	0	$3,\!3,\!19$	0.25	0
9	FTT	С	416	10,3	10,10,16	0.69	0	10, 10, 17	1.20	1 (10%)
6	C8E	F	402	-	3,3,20	0.35	0	2,2,19	0.62	0
9	FTT	А	413	2	$14,\!14,\!16$	0.38	0	$14,\!14,\!17$	0.76	0
9	FTT	В	408	3	14,14,16	0.40	0	14, 14, 17	0.72	0
11	DAO	С	420	9	12,12,13	0.44	0	11,11,13	0.58	0
6	C8E	A	405	-	3,3,20	0.38	0	2,2,19	0.64	0
9	FTT	С	423	4,11	12,12,16	0.63	0	$12,\!12,\!17$	1.19	1 (8%)
6	C8E	А	402	-	2,2,20	0.45	0	$1,\!1,\!19$	0.11	0
6	C8E	С	408	-	10,10,20	0.35	0	9,9,19	0.39	0
9	FTT	E	406	2	13,13,16	0.35	0	13,13,17	0.89	0
10	MYR	A	416	9	5,5,15	0.64	0	4,4,15	0.72	0
6	C8E	D	403	-	5,5,20	0.32	0	4,4,19	0.32	0
9	FTT	F	410	3	15,15,16	0.38	0	$15,\!15,\!17$	1.29	3 (20%)
9	FTT	D	422	2,10	15,15,16	0.37	0	$15,\!15,\!17$	0.80	0
9	FTT	Ε	404	11,2	13, 13, 16	0.61	0	$13,\!13,\!17$	1.31	1 (7%)
6	C8E	D	402	-	3,3,20	0.35	0	2,2,19	0.67	0
6	C8E	В	404	-	7,7,20	0.29	0	$6,\!6,\!19$	0.34	0
11	DAO	F	418	9	7,7,13	0.57	0	6,6,13	0.58	0
10	MYR	В	411	9	$5,\!5,\!15$	0.61	0	4,4,15	0.78	0
5	SO4	A	401	-	4,4,4	0.19	0	$6,\!6,\!6$	0.57	0
9	FTT	D	421	11,2	12,12,16	0.57	0	$12,\!12,\!17$	1.11	1 (8%)
11	DAO	F	412	9	4,4,13	0.63	0	$3,\!3,\!13$	0.64	0



	T a	Chain	Dag	T : 1-	Bo	ond leng	ths	В	Bond angles		
NIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
9	FTT	F	406	2	13,13,16	0.53	0	$13,\!13,\!17$	1.03	1 (7%)	
6	C8E	В	402	-	2,2,20	0.45	0	0,1,19	-	-	
6	C8E	С	405	-	2,2,20	0.18	0	0,1,19	-	-	
11	DAO	С	414	9	4,4,13	0.63	0	3,3,13	0.58	0	
6	C8E	С	410	-	6,6,20	0.32	0	$5,\!5,\!19$	0.47	0	
8	KDO	D	413	-	15,15,16	0.90	1 (6%)	$19,\!21,\!24$	1.68	<mark>3 (15%)</mark>	
11	DAO	А	417	9	4,4,13	0.64	0	3,3,13	1.00	0	
6	C8E	Е	401	-	5,5,20	0.29	0	4,4,19	0.35	0	
10	MYR	Е	409	9	5,5,15	0.62	0	4,4,15	0.65	0	
11	DAO	Е	405	9	4,4,13	0.67	0	3,3,13	1.03	0	
9	FTT	D	417	2	10,10,16	0.62	0	$10,\!10,\!17$	1.12	1 (10%)	
9	FTT	С	424	4,10	15,15,16	0.32	0	$15,\!15,\!17$	0.87	0	
9	FTT	F	408	11,3	12,12,16	0.70	0	$12,\!12,\!17$	1.00	1 (8%)	
11	DAO	С	421	9	9,9,13	0.58	0	8,8,13	0.44	0	
6	C8E	F	403	-	7,7,20	0.35	0	$6,\!6,\!19$	0.47	0	
9	FTT	D	415	11,2	10,10,16	0.56	0	10, 10, 17	1.47	1 (10%)	
9	FTT	F	407	11,3	11,11,16	0.74	0	$11,\!11,\!17$	1.24	1 (9%)	
9	FTT	F	409	10,3	11,11,16	0.64	0	11,11,17	0.97	1 (9%)	
9	FTT	С	413	11,3	13,13,16	0.72	0	13,13,17	1.36	1 (7%)	
7	PO4	С	411	-	4,4,4	0.84	0	$6,\!6,\!6$	0.97	0	
9	FTT	С	417	11,3	$15,\!15,\!16$	0.44	0	$15,\!15,\!17$	0.81	0	
11	DAO	D	424	9	4,4,13	0.63	0	$3,\!3,\!13$	0.67	0	
6	C8E	С	406	-	7,7,20	0.30	0	$6,\!6,\!19$	0.41	0	
6	C8E	F	401	-	2,2,20	0.24	0	$0,\!1,\!19$	-	-	
6	C8E	D	410	-	5,5,20	0.26	0	$4,\!4,\!19$	0.35	0	
6	C8E	A	406	-	4,4,20	0.34	0	$3,\!3,\!19$	0.32	0	
6	C8E	В	403	-	4,4,20	0.29	0	$3,\!3,\!19$	0.31	0	
11	DAO	A	419	9	7,7,13	0.50	0	$6,\!6,\!13$	0.83	0	
9	FTT	F	415	4,11	10,10,16	0.57	0	$10,\!10,\!17$	1.46	1 (10%)	
6	C8E	С	407	-	10,10,20	0.34	0	9,9,19	0.44	0	
6	C8E	А	409	-	7,7,20	0.28	0	$6,\!6,\!19$	0.50	0	
9	FTT	А	414	11,2	12,12,16	0.53	0	$12,\!12,\!17$	1.45	2 (16%)	
9	FTT	D	420	2	15,15,16	0.34	0	$15,\!15,\!17$	0.83	0	
11	DAO	С	426	9	7,7,13	0.55	0	$6,\!6,\!13$	0.69	0	
6	C8E	D	408	-	10,10,20	0.39	0	$9,\!9,\!19$	0.26	0	
10	MYR	D	419	9	4,4,15	0.69	0	3,3,15	0.90	0	
9	FTT	F	414	4	13,13,16	0.41	0	$13,\!13,\!17$	0.60	0	
11	DAO	E	410	9	4,4,13	0.63	0	$3,\!3,\!13$	0.78	0	
9	FTT	E	407	11,2	11,11,16	0.53	0	$11,\!11,\!17$	1.33	2 (18%)	
7	PO4	В	406	-	4,4,4	1.10	0	$6,\!6,\!6$	0.66	0	



Mal	Tuno	Chain	Dog	Link	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
6	C8E	D	407	-	7,7,20	0.30	0	$6,\!6,\!19$	0.29	0
11	DAO	D	412	-	$5,\!5,\!13$	0.54	0	4,4,13	0.84	0
9	FTT	Е	408	2,10	14,14,16	0.55	0	$14,\!14,\!17$	0.97	1 (7%)
7	PO4	D	411	-	4,4,4	0.60	0	6,6,6	1.15	0
6	C8E	В	405	-	7,7,20	0.30	0	6,6,19	0.67	0
9	FTT	С	415	3	15,15,16	0.56	0	$15,\!15,\!17$	1.06	1 (6%)
9	FTT	С	418	11,3	12,12,16	0.61	0	$12,\!12,\!17$	1.01	1 (8%)
6	C8E	С	404	-	5,5,20	0.24	0	4,4,19	0.33	0
9	FTT	D	416	2,10	12,12,16	0.57	0	12,12,17	0.86	0
6	C8E	А	410	-	6,6,20	0.25	0	$5,\!5,\!19$	0.48	0
10	MYR	D	423	9	$5,\!5,\!15$	0.60	0	$4,\!4,\!15$	0.74	0
6	C8E	А	403	-	3,3,20	0.40	0	2,2,19	0.62	0
10	MYR	F	417	9	$11,\!11,\!15$	0.44	0	$10,\!10,\!15$	0.63	0
6	C8E	С	401	-	2,2,20	0.28	0	0,1,19	-	-
7	PO4	А	411	-	4,4,4	0.97	0	6,6,6	0.78	0
6	C8E	D	405	-	5,5,20	0.28	0	4,4,19	0.34	0
10	MYR	С	425	9	8,8,15	0.46	0	7,7,15	0.64	0
6	C8E	D	404	-	5,5,20	0.28	0	4,4,19	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FTT	А	418	4,11	-	5/12/12/15	-
9	FTT	D	425	4	-	4/12/12/15	-
6	C8E	D	409	-	-	0/0/1/18	-
9	FTT	В	407	2	-	1/12/12/15	-
9	FTT	D	414	2	-	7/12/12/15	-
9	FTT	В	409	11,3	-	3/11/11/15	-
11	DAO	В	412	9	-	1/1/2/11	-
8	KDO	Е	403	-	-	1/10/26/30	0/1/1/1
10	MYR	С	419	9	-	0/4/5/13	-
9	FTT	А	415	2,10	-	7/14/14/15	-
10	MYR	F	411	9	-	0/7/8/13	-
6	C8E	В	401	-	-	3/6/6/18	-
6	C8E	А	404	-	-	1/3/3/18	-
6	C8E	D	406	-	_	4/5/5/18	-
6	C8E	А	408	-	-	3/5/5/18	-



5FVN

Conti	nueu jro	m previoi	is page	•••			
Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FTT	С	422	4	-	4/14/14/15	-
9	FTT	В	410	10,3	-	5/14/14/15	-
6	C8E	С	409	-	-	2/7/7/18	-
11	DAO	F	413	9	-	0/1/2/11	-
6	C8E	С	402	-	-	2/4/4/18	-
9	FTT	F	416	4,10	-	6/14/14/15	-
8	KDO	А	412	-	-	1/10/26/30	0/1/1/1
6	C8E	А	407	-	-	2/2/2/18	-
9	FTT	С	416	10,3	-	1/9/9/15	-
6	C8E	F	402	-	-	0/1/1/18	-
9	FTT	А	413	2	-	3/13/13/15	-
9	FTT	В	408	3	-	1/13/13/15	-
11	DAO	С	420	9	-	0/9/10/11	-
6	C8E	А	405	-	-	0/1/1/18	-
9	FTT	С	423	4,11	-	1/11/11/15	-
6	C8E	С	408	-	-	3/8/8/18	-
9	FTT	Ε	406	2	-	2/12/12/15	-
10	MYR	А	416	9	-	0/2/3/13	-
6	C8E	D	403	-	-	0/3/3/18	-
9	FTT	F	410	3	-	5/14/14/15	-
9	FTT	D	422	2,10	-	5/14/14/15	-
9	FTT	Е	404	11,2	-	6/12/12/15	-
6	C8E	D	402	-	-	1/1/1/18	-
6	C8E	В	404	-	-	2/5/5/18	-
11	DAO	F	418	9	-	2/4/5/11	-
10	MYR	В	411	9	-	1/2/3/13	-
9	FTT	D	421	11,2	-	0/11/11/15	-
11	DAO	F	412	9	-	0/1/2/11	-
9	FTT	F	406	2	-	1/12/12/15	-
11	DAO	С	414	9	-	1/1/2/11	-
6	C8E	С	410	-	-	2/4/4/18	-
8	KDO	D	413	-	-	2/10/26/30	0/1/1/1
11	DAO	А	417	9	-	1/1/2/11	-
6	C8E	E	401	-	-	3/3/3/18	-
10	MYR	E	409	9	-	1/2/3/13	-
11	DAO	E	405	9	-	0/1/2/11	-
9	FTT	D	417	2	-	3/9/9/15	-
9	FTT	С	424	4,10	-	3/14/14/15	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FTT	F	408	11,3	-	5/11/11/15	-
11	DAO	С	421	9	-	1/6/7/11	-
6	C8E	F	403	-	-	2/5/5/18	-
9	FTT	D	415	11,2	-	1/9/9/15	-
9	FTT	F	407	11,3	-	3/10/10/15	-
9	FTT	F	409	10,3	-	2/10/10/15	-
9	FTT	С	413	11,3	-	2/12/12/15	-
9	FTT	С	417	11,3	-	2/14/14/15	-
11	DAO	D	424	9	-	1/1/2/11	-
6	C8E	С	406	-	-	0/5/5/18	-
6	C8E	D	410	-	-	0/3/3/18	-
6	C8E	А	406	-	-	0/2/2/18	-
6	C8E	В	403	-	-	1/2/2/18	-
11	DAO	А	419	9	-	0/4/5/11	-
9	FTT	F	415	4,11	-	1/9/9/15	-
6	C8E	С	407	-	-	1/8/8/18	-
6	C8E	А	409	-	-	0/5/5/18	-
9	FTT	А	414	11,2	-	0/11/11/15	-
9	FTT	D	420	2	-	3/14/14/15	-
11	DAO	С	426	9	-	3/4/5/11	-
6	C8E	D	408	-	-	1/8/8/18	-
10	MYR	D	419	9	-	1/1/2/13	-
9	FTT	F	414	4	-	2/12/12/15	-
11	DAO	Е	410	9	-	1/1/2/11	-
9	FTT	Е	407	11,2	-	1/10/10/15	-
6	C8E	D	407	-	-	2/5/5/18	-
11	DAO	D	412	-	-	2/2/3/11	-
9	FTT	Е	408	2,10	-	7/13/13/15	-
6	C8E	В	405	-	-	1/5/5/18	-
9	FTT	С	415	3	-	2/14/14/15	-
9	FTT	С	418	11,3	-	4/11/11/15	-
6	C8E	С	404	-	-	1/3/3/18	-
9	FTT	D	416	2,10	-	6/11/11/15	-
6	C8E	А	410	-	-	0/4/4/18	-
10	MYR	D	423	9	-	1/2/3/13	-
6	C8E	А	403	-	-	0/1/1/18	_
10	MYR	F	417	9		3/8/9/13	-
6	C8E	D	405	_	-	0/3/3/18	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MYR	С	425	9	-	2/5/6/13	-
6	C8E	D	404	-	-	0/3/3/18	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
8	D	413	KDO	C2-C1	-2.78	1.50	1.52
8	А	412	KDO	C2-C1	-2.54	1.50	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
8	Е	403	KDO	O6-C2-C3	5.14	117.53	110.46
8	D	413	KDO	O6-C2-C3	4.84	117.12	110.46
9	А	418	FTT	O2-C1-C2	-4.80	111.43	125.43
9	D	425	FTT	O2-C1-C2	-4.38	112.67	125.43
9	С	413	FTT	O2-C1-C2	-4.38	112.68	125.43
9	F	415	FTT	O2-C1-C2	-4.20	113.19	125.43
8	А	412	KDO	O6-C2-C3	4.02	115.99	110.46
9	D	415	FTT	O2-C1-C2	-3.91	114.03	125.43
9	С	423	FTT	O2-C1-C2	-3.63	114.84	125.43
9	А	414	FTT	O2-C1-C2	-3.59	114.97	125.43
8	А	412	KDO	C6-O6-C2	3.51	118.85	111.34
8	D	413	KDO	C6-O6-C2	3.48	118.78	111.34
8	Е	403	KDO	C6-O6-C2	3.48	118.77	111.34
9	В	407	FTT	O2-C1-C2	-3.44	115.39	125.43
9	Е	404	FTT	O2-C1-C2	-3.32	115.76	125.43
9	F	406	FTT	O2-C1-C2	-3.29	115.83	125.43
8	D	413	KDO	O1A-C1-C2	-3.05	115.36	122.57
9	С	418	FTT	O2-C1-C2	-3.02	116.64	125.43
9	D	417	FTT	O2-C1-C2	-2.96	116.79	125.43
9	С	416	FTT	O2-C1-C2	-2.88	117.02	125.43
9	F	407	FTT	O2-C1-C2	-2.87	117.07	125.43
9	Е	407	FTT	O2-C1-C2	-2.77	117.34	125.43
9	D	421	FTT	O2-C1-C2	-2.73	117.47	125.43
9	F	408	FTT	O2-C1-C2	-2.71	117.54	125.43
8	Е	403	KDO	01A-C1-C2	-2.59	116.46	122.57
9	В	409	FTT	02-C1-C2	-2.38	118.50	125.43
9	F	410	FTT	C5-C4-C3	-2.31	108.20	114.85
9	Е	407	FTT	C3-C2-C1	2.27	116.74	112.75
9	F	410	FTT	02-C1-C2	-2.27	118.81	125.43
9	А	415	FTT	C5-C4-C3	-2.23	108.44	114.85



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
9	А	414	FTT	C4-C3-C2	-2.22	105.33	112.91
9	F	409	FTT	O2-C1-C2	-2.19	119.04	125.43
9	С	422	FTT	C11-C10-C9	-2.19	103.31	114.42
9	D	425	FTT	C3-C2-C1	-2.19	108.90	112.75
8	А	412	KDO	O1A-C1-C2	-2.17	117.43	122.57
9	Ε	408	FTT	C10-C9-C8	-2.14	103.57	114.42
9	D	414	FTT	O2-C1-C2	-2.10	119.30	125.43
9	F	410	FTT	C4-C3-C2	-2.10	105.73	112.91
9	С	422	FTT	C7-C6-C5	-2.09	103.80	114.42
9	С	415	FTT	C4-C3-C2	-2.08	105.80	112.91
9	С	422	FTT	C5-C4-C3	-2.03	109.00	114.85
9	В	409	FTT	C3-C2-C1	2.01	116.28	112.75

There are no chirality outliers.

All (177) torsion outliers are listed below:
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Mol	Chain	Res	Type	Atoms
9	А	418	FTT	O2-C1-C2-C3
9	А	418	FTT	C2-C3-C4-C5
9	А	418	FTT	O3-C3-C4-C5
9	С	417	FTT	C1-C2-C3-C4
9	С	417	FTT	C1-C2-C3-O3
9	D	414	FTT	C1-C2-C3-O3
9	Е	404	FTT	C1-C2-C3-C4
9	Е	404	FTT	C1-C2-C3-O3
9	F	407	FTT	O2-C1-C2-C3
9	F	410	FTT	C1-C2-C3-O3
10	В	411	MYR	C1-C2-C3-C4
10	D	423	MYR	C1-C2-C3-C4
6	А	408	C8E	O12-C13-C14-O15
6	С	409	C8E	C6-C7-C8-O9
6	А	408	C8E	O9-C10-C11-O12
6	D	407	C8E	C2-C3-C4-C5
9	А	418	FTT	C4-C5-C6-C7
9	D	425	FTT	C11-C10-C9-C8
6	С	407	C8E	С11-С10-О9-С8
9	А	415	FTT	C10-C11-C12-C13
9	D	422	FTT	C9-C10-C11-C12
6	С	408	C8E	C2-C3-C4-C5
6	D	408	C8E	C2-C3-C4-C5
9	А	415	FTT	С11-С10-С9-С8
9	D	417	FTT	C5-C6-C7-C8



Mol	Chain	Res	Type	Atoms
9	В	408	FTT	C9-C10-C11-C12
11	С	414	DAO	C1-C2-C3-C4
9	F	410	FTT	C6-C7-C8-C9
9	А	413	FTT	C9-C10-C11-C12
9	D	422	FTT	C6-C7-C8-C9
6	В	403	C8E	O9-C10-C11-O12
9	В	410	FTT	C9-C10-C11-C12
9	Е	408	FTT	C7-C8-C9-C10
9	В	410	FTT	C11-C10-C9-C8
9	F	410	FTT	C7-C8-C9-C10
11	F	418	DAO	C3-C4-C5-C6
9	Е	408	FTT	C4-C5-C6-C7
9	С	422	FTT	C6-C7-C8-C9
9	D	422	FTT	C10-C11-C12-C13
9	D	416	FTT	O3-C3-C4-C5
9	Е	404	FTT	O3-C3-C4-C5
9	F	408	FTT	O3-C3-C4-C5
9	Е	408	FTT	C6-C7-C8-C9
9	F	416	FTT	C7-C8-C9-C10
6	С	409	C8E	C7-C8-O9-C10
6	В	401	C8E	C2-C3-C4-C5
6	С	408	C8E	C4-C5-C6-C7
9	С	413	FTT	C4-C5-C6-C7
9	F	416	FTT	C10-C11-C12-C13
9	В	410	FTT	C10-C11-C12-C13
9	А	418	FTT	C6-C7-C8-C9
6	Е	401	C8E	C2-C3-C4-C5
9	D	420	FTT	C10-C11-C12-C13
9	А	413	FTT	C10-C11-C12-C13
9	F	407	FTT	C6-C7-C8-C9
9	С	415	FTT	C10-C11-C12-C13
6	F	403	C8E	C2-C3-C4-C5
9	С	418	FTT	C6-C7-C8-C9
9	D	422	FTT	C1-C2-C3-O3
9	E	408	FTT	C1-C2-C3-O3
9	F	409	FTT	C1-C2-C3-O3
9	F	416	FTT	C1-C2-C3-O3
6	В	404	C8E	C5-C6-C7-C8
6	С	402	C8E	C4-C5-C6-C7
9	F	407	FTT	C7-C8-C9-C10
9	D	414	FTT	C5-C6-C7-C8
9	С	422	FTT	C10-C11-C12-C13



Mol	Chain	Res	Type	Atoms
9	Е	406	FTT	C9-C10-C11-C12
6	D	406	C8E	C1-C2-C3-C4
9	В	410	FTT	C11-C12-C13-C14
6	D	407	C8E	C4-C5-C6-C7
10	С	425	MYR	C3-C4-C5-C6
10	F	417	MYR	C7-C8-C9-C10
9	С	413	FTT	O2-C1-C2-C3
9	D	415	FTT	O2-C1-C2-C3
9	D	422	FTT	C5-C6-C7-C8
11	А	417	DAO	C1-C2-C3-C4
11	D	424	DAO	C1-C2-C3-C4
9	D	416	FTT	C2-C3-C4-C5
9	Е	404	FTT	C2-C3-C4-C5
9	F	408	FTT	C2-C3-C4-C5
6	Е	401	C8E	C1-C2-C3-C4
6	В	401	C8E	C3-C4-C5-C6
9	D	414	FTT	C9-C10-C11-C12
6	В	405	C8E	C2-C3-C4-C5
9	С	418	FTT	C4-C5-C6-C7
9	D	416	FTT	C6-C7-C8-C9
9	D	414	FTT	C11-C10-C9-C8
9	D	425	FTT	C9-C10-C11-C12
6	В	401	C8E	C6-C7-C8-O9
9	С	424	FTT	C5-C6-C7-C8
9	D	420	FTT	C9-C10-C11-C12
9	F	414	FTT	C9-C10-C11-C12
6	Е	401	C8E	C3-C4-C5-C6
9	Е	408	FTT	C9-C10-C11-C12
6	С	404	C8E	C3-C4-C5-C6
9	С	422	FTT	C4-C5-C6-C7
11	F	418	DAO	C4-C5-C6-C7
6	D	406	C8E	C5-C6-C7-C8
9	С	424	FTT	C11-C10-C9-C8
9	В	409	FTT	C5-C6-C7-C8
6	C	410	C8E	C1-C2-C3-C4
10	F	417	MYR	C11-C10-C9-C8
9	F	414	FTT	C4-C5-C6-C7
9	D	414	FTT	C1-C2-C3-C4
9	F	409	FTT	C1-C2-C3-C4
9	F	410	FTT	C1-C2-C3-C4
9	F	416	FTT	C1-C2-C3-C4
9	D	414	FTT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
6	С	408	C8E	C11-C10-O9-C8
9	В	410	FTT	C1-C2-C3-O3
6	D	402	C8E	C1-C2-C3-C4
10	Е	409	MYR	C1-C2-C3-C4
11	С	421	DAO	C1-C2-C3-C4
11	С	426	DAO	C1-C2-C3-C4
11	D	412	DAO	C1-C2-C3-C4
9	D	417	FTT	C6-C7-C8-C9
6	В	404	C8E	C3-C4-C5-C6
11	С	426	DAO	C4-C5-C6-C7
9	D	420	FTT	C4-C5-C6-C7
9	D	425	FTT	C7-C8-C9-C10
11	D	412	DAO	C2-C3-C4-C5
6	С	402	C8E	C3-C4-C5-C6
9	С	416	FTT	O2-C1-C2-C3
9	С	418	FTT	O2-C1-C2-C3
9	С	423	FTT	O2-C1-C2-C3
9	D	416	FTT	O2-C1-C2-C3
9	D	425	FTT	O2-C1-C2-C3
9	Е	404	FTT	O2-C1-C2-C3
9	F	408	FTT	O2-C1-C2-C3
9	F	415	FTT	O2-C1-C2-C3
9	С	422	FTT	C5-C6-C7-C8
11	С	426	DAO	C2-C3-C4-C5
8	D	413	KDO	O1A-C1-C2-O6
8	Е	403	KDO	O1A-C1-C2-O6
10	D	419	MYR	C1-C2-C3-C4
11	В	412	DAO	C1-C2-C3-C4
11	Е	410	DAO	C1-C2-C3-C4
9	D	414	FTT	C4-C5-C6-C7
9	D	416	FTT	C3-C4-C5-C6
9	Е	406	FTT	C4-C5-C6-C7
9	А	413	FTT	C4-C5-C6-C7
9	А	415	FTT	C5-C6-C7-C8
9	С	415	FTT	C7-C8-C9-C10
6	А	404	C8E	C1-C2-C3-C4
9	F	410	FTT	C11-C12-C13-C14
9	А	415	FTT	C11-C12-C13-C14
9	F	416	FTT	C11-C10-C9-C8
6	А	408	C8E	C14-C13-O12-C11
6	D	406	C8E	C3-C4-C5-C6
9	A	415	FTT	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
9	А	415	FTT	C7-C8-C9-C10
9	В	409	FTT	C11-C10-C9-C8
9	F	416	FTT	C4-C5-C6-C7
9	Е	407	FTT	C2-C3-C4-C5
9	F	408	FTT	C6-C7-C8-C9
10	С	425	MYR	C2-C3-C4-C5
6	А	407	C8E	С11-С10-О9-С8
10	F	417	MYR	C6-C7-C8-C9
9	В	407	FTT	C5-C6-C7-C8
6	D	406	C8E	C4-C5-C6-C7
6	F	403	C8E	C3-C4-C5-C6
9	F	406	FTT	O2-C1-C2-C3
9	D	416	FTT	C5-C6-C7-C8
8	А	412	KDO	O1A-C1-C2-O6
9	С	424	FTT	C11-C12-C13-C14
9	F	408	FTT	C3-C4-C5-C6
6	А	407	C8E	C7-C8-O9-C10
9	Ε	408	FTT	C1-C2-C3-C4
9	С	418	FTT	C3-C4-C5-C6
9	Ε	408	FTT	C3-C4-C5-C6
8	D	413	KDO	O1B-C1-C2-C3
6	C	410	C8E	C4-C5-C6-C7
9	В	409	FTT	C6-C7-C8-C9
9	Е	404	FTT	C4-C5-C6-C7
9	D	417	FTT	O3-C3-C4-C5
9	A	415	FTT	C9-C10-C11-C12

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There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	409	C8E	1	0
8	Е	403	KDO	3	0
6	А	408	C8E	2	0
8	А	412	KDO	2	0
6	А	407	C8E	1	0
9	F	406	FTT	1	0
6	С	405	C8E	4	0
8	D	413	KDO	2	0
6	F	403	C8E	1	0
9	F	407	FTT	1	0
6	F	401	C8E	1	0



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	В	403	C8E	2	0

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



























5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ	2>2	$OWAB(Å^2)$	$Q{<}0.9$
1	А	342/342~(100%)	0.17	14 (4%) 37	40	9, 15, 28, 59	1 (0%)
1	В	342/342~(100%)	0.17	14 (4%) 37	40	9, 15, 31, 77	0
1	С	342/342~(100%)	0.09	7 (2%) 65	67	9, 14, 30, 54	0
1	D	342/342~(100%)	0.25	21 (6%) 21	23	10, 16, 31, 96	0
1	Ε	342/342~(100%)	0.16	14 (4%) 37	40	10, 15, 32, 58	0
1	F	342/342~(100%)	0.00	3 (0%) 84	86	9, 14, 25, 40	0
All	All	2052/2052~(100%)	0.14	73 (3%) 42	46	9, 15, 30, 96	1 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	139	LEU	8.7
1	D	83	GLY	8.0
1	А	139	LEU	7.1
1	Е	139	LEU	6.9
1	D	137	PHE	6.5
1	D	84	ASP	6.1
1	В	137	PHE	6.1
1	D	138	GLY	5.6
1	А	138	GLY	5.6
1	А	82	PHE	5.6
1	В	136	PHE	5.2
1	С	138	GLY	5.1
1	D	136	PHE	5.1
1	D	139	LEU	5.1
1	А	137	PHE	5.0
1	D	265	PHE	5.0
1	В	84	ASP	4.9
1	В	138	GLY	4.9
1	D	134	SER	4.7



Mol	Chain	Res	Type	RSRZ
1	В	82	PHE	4.7
1	Е	82	PHE	4.4
1	В	83	GLY	4.3
1	Е	137	PHE	4.3
1	Е	138	GLY	4.2
1	Е	265	PHE	4.1
1	В	140	VAL	3.8
1	D	82	PHE	3.6
1	D	49	GLN	3.6
1	D	159	GLU	3.6
1	D	85	ALA	3.6
1	А	159	GLU	3.5
1	Е	84	ASP	3.2
1	A	83	GLY	3.2
1	Е	85	ALA	3.2
1	Е	141	ASP	3.1
1	Е	264	ASP	3.1
1	А	84	ASP	2.9
1	В	265	PHE	2.9
1	С	226	ASN	2.8
1	В	85	ALA	2.8
1	С	137	PHE	2.8
1	D	135	ASP	2.8
1	С	139	LEU	2.7
1	F	186	GLU	2.7
1	С	84	ASP	2.7
1	А	136	PHE	2.7
1	F	84	ASP	2.6
1	В	264[A]	ASP	2.6
1	С	82	PHE	2.6
1	A	264	ASP	2.6
1	D	86	GLY	2.5
1	D	261	TYR	2.5
1	E	140	VAL	2.5
1	В	49	GLN	2.5
1	A	265	PHE	2.5
1	Е	83	GLY	2.4
1	Е	136	PHE	2.4
1	D	140	VAL	2.4
1	В	86	GLY	2.4
1	A	141	ASP	2.3
1	С	141	ASP	2.3



Mol	Chain	Res	Type	RSRZ	
1	D	264[A]	ASP	2.3	
1	А	49	GLN	2.3	
1	F	136	PHE	2.3	
1	D	186	GLU	2.3	
1	D	45	GLN	2.3	
1	D	188	PHE	2.2	
1	Е	159	GLU	2.2	
1	Е	263	PHE	2.1	
1	А	261	TYR	2.1	
1	В	141	ASP	2.1	
1	А	45	GLN	2.0	
1	D	226	ASN	2.0	

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	KDO	Κ	3	14/16	0.62	0.29	42,49,65,65	0
3	GMH	Ι	5	13/14	0.77	0.21	$36,\!45,\!58,\!69$	0
3	GMH	Н	5	13/14	0.80	0.28	32,36,40,48	0
2	GP1	K	1	16/16	0.85	0.31	34,37,66,67	0
3	GMH	Ν	5	13/14	0.86	0.21	31,36,54,59	0
2	KDO	М	3	15/16	0.88	0.21	23,27,35,38	0
2	KDO	G	3	15/16	0.89	0.28	24,29,40,48	0
2	KDO	L	3	15/16	0.89	0.25	25,28,40,44	0
3	KDO	Н	3	15/16	0.90	0.21	22,26,33,41	0
3	KDO	Н	4	15/16	0.92	0.14	18,20,25,27	0
2	Z9M	Κ	2	15/16	0.92	0.21	25,29,34,40	0
4	KDO	J	4	15/16	0.92	0.12	12,19,22,23	0
4	KDO	0	3	15/16	0.92	0.14	13,21,31,35	0
2	GP1	L	1	16/16	0.93	0.19	24,26,44,49	0
2	GP1	G	1	16/16	0.93	0.21	22,27,48,52	0
4	KDO	Ō	4	15/16	0.93	0.12	17,18,21,24	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors(A^2)	$\mathbf{Q}{<}0.9$	
3	KDO	N	3	15/16	0.94	0.14	$18,\!25,\!33,\!37$	0	
3	KDO	N	4	15/16	0.94	0.12	15,16,20,29	0	
2	Z9M	G	2	15/16	0.94	0.22	22,24,31,34	0	
4	KDO	J	3	15/16	0.94	0.12	16,21,30,34	0	
3	GP1	Н	1	16/16	0.94	0.13	22,24,50,51	0	
3	KDO	Ι	3	15/16	0.94	0.10	18,23,31,31	0	
2	GP1	М	1	16/16	0.94	0.15	$23,\!26,\!47,\!49$	0	
3	Z9M	Н	2	15/16	0.95	0.16	20,21,26,26	0	
3	KDO	Ι	4	15/16	0.95	0.09	14,15,19,24	0	
4	GP1	0	1	16/16	0.95	0.09	18,20,41,43	0	
2	Z9M	L	2	15/16	0.95	0.17	23,24,30,30	0	
4	GP1	J	1	16/16	0.95	0.08	$17,\!19,\!44,\!44$	0	
2	Z9M	М	2	15/16	0.96	0.20	$21,\!21,\!26,\!27$	0	
3	GP1	N	1	16/16	0.97	0.07	16,19,34,34	0	
3	Z9M	Ι	2	15/16	0.97	0.06	18,21,41,41	0	
4	Z9M	0	2	15/16	0.97	0.06	17,18,24,27	0	
4	Z9M	J	2	15/16	0.97	0.07	16,17,26,26	0	
3	GP1	Ι	1	16/16	0.97	0.07	17,19,33,35	0	
3	Z9M	N	2	15/16	0.98	0.07	18,21,29,32	0	

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





































6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
11	DAO	Е	405	5/14	0.40	0.27	$52,\!54,\!57,\!63$	0
9	FTT	Е	404	14/17	0.52	0.25	38,46,48,57	0
9	FTT	С	413	14/17	0.53	0.26	33,47,58,61	0
10	MYR	А	416	6/16	0.56	0.32	47,52,55,57	0
11	DAO	А	417	5/14	0.60	0.39	$55,\!57,\!59,\!63$	0



Mol	Type	Chain	ls page	Atoms	BSCC	BSB	B -factors(\mathbf{A}^2)	0<0.9
11	DAO	С	<u>114</u>	5/1/	0.62	0.10	<u>10 50 63 63</u>	0
0	FTT	B	407	$\frac{14}{14}$	0.02	0.13	35 40 55 61	0
11	DAO	D	424	5/14	0.63	0.10	47.58.58.73	0
9	FTT	D	417	11/17	0.63	0.26	46.51.67.67	0
9	FTT	D	425	14/17	0.65	0.23	33.45.53.62	0
9	FTT	F	406	14/17	0.66	0.18	38.42.47.48	0
11	DAO	В	412	5/14	0.68	0.61	39.48.59.60	0
11	DAO	D	418	3/14	0.68	0.42	51,51,52,53	0
9	FTT	A	415	16/17	0.70	0.25	27,39,59,66	0
11	DAO	Е	410	5/14	0.70	0.36	49,54,55,56	0
10	MYR	Е	409	6/16	0.71	0.30	41,44,51,54	0
6	C8E	A	407	5/21	0.71	0.24	18,20,26,28	0
9	FTT	D	414	14/17	0.72	0.18	36,47,53,54	0
11	DAO	А	419	8/14	0.72	0.17	40,41,44,57	0
6	C8E	А	402	3/21	0.74	0.30	33,33,41,41	0
10	MYR	В	411	6/16	0.75	0.24	43,60,68,68	0
9	FTT	D	415	11/17	0.75	0.18	33,36,41,41	0
10	MYR	D	423	6/16	0.76	0.18	43,47,49,50	0
6	C8E	В	404	8/21	0.76	0.14	41,46,47,47	0
9	FTT	D	421	13/17	0.77	0.14	27,30,46,71	0
6	C8E	D	405	6/21	0.77	0.13	30,37,41,42	0
6	C8E	D	406	8/21	0.77	0.16	48,52,54,58	0
9	FTT	А	414	13/17	0.77	0.18	29,33,39,41	0
6	C8E	Е	401	6/21	0.78	0.19	44,52,63,65	0
10	MYR	D	419	5/16	0.79	0.27	16,25,37,38	0
6	C8E	А	409	8/21	0.80	0.18	29,34,38,38	0
6	C8E	С	406	8/21	0.80	0.17	30,33,33,35	0
6	C8E	D	404	6/21	0.80	0.13	32,41,41,43	0
6	C8E	В	405	8/21	0.81	0.11	38,39,41,41	0
6	C8E	С	403	3/21	0.81	0.12	45,45,46,50	0
6	C8E	А	410	7/21	0.81	0.19	38,39,40,41	0
10	MYR	F	411	11/16	0.81	0.12	$26,\!31,\!36,\!36$	0
9	FTT	А	418	14/17	0.81	0.18	39,44,66,68	0
6	C8E	D	407	8/21	0.81	0.17	$25,\!41,\!44,\!48$	0
6	C8E	С	409	10/21	0.82	0.13	35,38,50,54	0
6	C8E	С	410	7/21	0.82	0.25	$23,\!24,\!39,\!43$	0
6	C8E	В	402	3/21	0.82	0.10	46,46,50,55	0
6	C8E	D	408	11/21	0.82	0.23	27,41,43,43	0
9	FTT	E	407	12/17	0.82	0.14	26,29,36,39	0
6	C8E	С	408	11/21	0.83	0.21	36,39,45,49	0
6	C8E	A	404	6/21	0.83	0.13	39,46,50,51	0
6	C8E	В	403	5/21	0.83	0.20	30,32,33,41	0


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors $(Å^2)$	Q<0.9
6	-3 PC C8E	A	403	4/21	0.83	0.12	62 71 76 79	0
6	C8E	D	402	4/21	0.84	0.12	32 33 34 39	0
6	C8E	D	410	6/21	0.84	0.10	40 43 45 45	0
11	DAO	C	426	8/14	0.84	0.19	37 62 72 73	0
6	C8E	D	403	6/21	0.84	0.20	39 44 51 56	0
9	FTT	F	415	11/17	0.84	0.12	22.23.28.34	0
9	FTT	B	410	16/17	0.84	0.20	23,30,36,39	0
6	C8E	C	404	6/21	0.84	0.15	28.41.49.51	0
9	FTT	D	420	16/17	0.85	0.14	17.23.28.30	0
9	FTT	A	413	15/17	0.85	0.13	15.22.26.38	0
9	FTT	F	416	16/17	0.85	0.16	21.32.42.45	0
6	C8E	B	401	9/21	0.85	0.15	31.43.63.64	0
9	FTT	B	409	13/17	0.85	0.16	21.26.42.44	0
6	C8E	F	402	4/21	0.85	0.16	41.44.47.47	0
6	C8E	С	402	7/21	0.86	0.27	25,32,38,43	0
9	FTT	F	410	16/17	0.86	0.13	28,33,39,41	0
9	FTT	Е	408	15/17	0.86	0.23	25,31,40,41	0
11	DAO	D	412	6/14	0.86	0.10	44,48,51,57	0
6	C8E	A	406	5/21	0.87	0.11	57,64,67,74	0
10	MYR	F	417	12/16	0.87	0.12	29,32,44,50	0
9	FTT	D	422	16/17	0.87	0.18	28,36,41,43	0
6	C8E	А	405	4/21	0.87	0.12	77,80,84,87	0
11	DAO	F	418	8/14	0.87	0.18	34,49,64,66	0
8	KDO	D	413	15/16	0.88	0.20	14,22,27,27	0
9	FTT	D	416	13/17	0.88	0.16	29,43,53,54	0
6	C8E	D	409	4/21	0.88	0.29	21,23,30,39	0
6	C8E	А	408	8/21	0.88	0.22	19,29,52,66	0
10	MYR	С	425	9/16	0.88	0.15	33,55,63,71	0
7	PO4	D	411	5/5	0.88	0.24	32,37,40,47	0
7	PO4	Е	402	5/5	0.88	0.25	34,35,41,44	0
8	KDO	А	412	15/16	0.89	0.24	18,23,30,30	0
9	FTT	С	423	13/17	0.89	0.10	20,22,34,39	0
6	C8E	С	401	3/21	0.89	0.20	$45,\!45,\!50,\!51$	0
6	C8E	С	407	11/21	0.89	0.17	33,35,43,47	0
9	FTT	Е	406	14/17	0.90	0.10	$18,\!21,\!25,\!26$	0
11	DAO	С	421	10/14	0.90	0.12	$25,\!30,\!32,\!33$	0
9	FTT	C	415	16/17	0.90	0.13	23,32,37,38	0
9	FTT	F	409	12/17	0.91	0.11	21,26,34,38	0
8	KDO	E	403	15/16	0.91	0.16	19,21,26,27	0
7	PO4	A	411	5/5	0.91	0.20	36, 36, 41, 47	0
9	FTT	F	407	12/17	0.91	0.12	19,24,43,48	0
6	C8E	F	403	8/21	0.92	0.17	40,43,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
10	MYR	С	419	8/16	0.92	0.15	22,30,32,32	0
7	PO4	В	406	5/5	0.92	0.18	31,33,40,44	0
7	PO4	F	404	5/5	0.92	0.19	31,36,45,45	0
9	FTT	С	416	11/17	0.92	0.10	18,20,24,30	0
9	FTT	С	422	16/17	0.93	0.10	15,20,27,31	0
11	DAO	С	420	13/14	0.93	0.09	22,27,31,33	0
9	FTT	В	408	15/17	0.93	0.09	$19,\!21,\!36,\!37$	0
6	C8E	F	401	3/21	0.93	0.10	$21,\!21,\!30,\!37$	0
11	DAO	F	412	5/14	0.93	0.10	$26,\!27,\!35,\!40$	0
6	C8E	С	405	3/21	0.93	0.17	$26,\!26,\!28,\!35$	0
7	PO4	С	411	5/5	0.94	0.23	32,35,44,44	0
9	FTT	С	424	16/17	0.94	0.10	18,30,41,41	0
9	FTT	F	414	14/17	0.94	0.09	$16,\!18,\!24,\!27$	0
11	DAO	F	413	5/14	0.94	0.14	$33,\!34,\!49,\!62$	0
9	FTT	F	408	13/17	0.94	0.12	$19,\!31,\!46,\!46$	0
9	FTT	С	418	13/17	0.95	0.13	$19,\!26,\!52,\!55$	0
9	FTT	С	417	16/17	0.96	0.08	18,20,30,34	0
5	SO4	А	401	5/5	0.99	0.08	$17,\!19,\!22,\!27$	0
5	SO4	D	401	5/5	0.99	0.10	18,21,25,29	0
12	CA	C	412	1/1	1.00	0.08	$1\overline{2,12,12,12}$	0
12	CA	F	405	1/1	1.00	0.08	$13,\!13,\!13,\!13$	0

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The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











































6.5 Other polymers (i)

There are no such residues in this entry.

