

wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 01:36 pm GMT

PDB ID : 6GN6

Title : Alpha-L-fucosidase isoenzyme 1 from Paenibacillus thiaminolyticus

Authors: Kovalova, T.; Koval, T.; Lipovova, P.; Dohnalek, J.

Deposited on : 2018-05-30

Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure 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/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 as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

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)

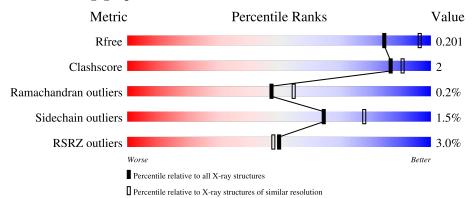
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	A	447	88%	6%	6%
1	В	447	89%		6%
1	С	447	89%	5%	6%
1	D	447	89%	6%	5%
1	Е	447	90%	•	• 6%



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Mol	Chain	Length	Quality of chain	
1	F	447	90%	5% •
2	G	2	100%	
2	Н	2	50% 50%	
2	I	2	50% 50%	
2	J	2	100%	
2	K	2	100%	
2	L	2	50% 50%	
2	M	2	100%	
2	N	2	100%	

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
2	GLC	J	2	-	-	-	X



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 22428 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.

• Molecule 1 is a protein called Alpha-L-fucosidase.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	421	Total	С	N	О	S	0	2	0
1	Λ	421	3416	2184	593	626	13	U		
1	В	421	Total	С	N	О	S	0	3	0
1	Ъ	421	3424	2190	595	626	13	U	3	
1	С	421	Total	С	N	О	S	0	1	0
1		421	3408	2179	590	626	13	U	1	
1	D	425	Total	С	N	О	S	0	1	0
1	D	420	3444	2202	599	629	14	U	1	
1	Е	421	Total	С	N	О	S	0	2	0
1	l L	421	3416	2184	593	626	13	U		
1	F	428	Total	С	N	О	S	0	2	0
1	I'	420	3473	2218	605	636	14	U		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP E3PQQ9
A	-19	GLY	-	expression tag	UNP E3PQQ9
A	-18	HIS	-	expression tag	UNP E3PQQ9
A	-17	HIS	-	expression tag	UNP E3PQQ9
A	-16	HIS	-	expression tag	UNP E3PQQ9
A	-15	HIS	-	expression tag	UNP E3PQQ9
A	-14	HIS	-	expression tag	UNP E3PQQ9
A	-13	HIS	-	expression tag	UNP E3PQQ9
A	-12	HIS	-	expression tag	UNP E3PQQ9
A	-11	HIS	-	expression tag	UNP E3PQQ9
A	-10	HIS	-	expression tag	UNP E3PQQ9
A	-9	HIS	-	expression tag	UNP E3PQQ9
A	-8	SER	-	expression tag	UNP E3PQQ9
A	-7	SER	=	expression tag	UNP E3PQQ9
A	-6	GLY	=	expression tag	UNP E3PQQ9
A	-5	HIS	-	expression tag	UNP E3PQQ9
A	-4	ILE	-	expression tag	UNP E3PQQ9



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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP E3PQQ9
A	-2	GLY	-	expression tag	UNP E3PQQ9
A	-1	ARG	-	expression tag	UNP E3PQQ9
A	0	HIS	-	expression tag	UNP E3PQQ9
В	-20	MET	-	initiating methionine	UNP E3PQQ9
В	-19	GLY	ı	expression tag	UNP E3PQQ9
В	-18	HIS	-	expression tag	UNP E3PQQ9
В	-17	HIS	-	expression tag	UNP E3PQQ9
В	-16	HIS	-	expression tag	UNP E3PQQ9
В	-15	HIS	-	expression tag	UNP E3PQQ9
В	-14	HIS	-	expression tag	UNP E3PQQ9
В	-13	HIS	-	expression tag	UNP E3PQQ9
В	-12	HIS	-	expression tag	UNP E3PQQ9
В	-11	HIS	-	expression tag	UNP E3PQQ9
В	-10	HIS	-	expression tag	UNP E3PQQ9
В	-9	HIS	-	expression tag	UNP E3PQQ9
В	-8	SER	-	expression tag	UNP E3PQQ9
В	-7	SER	-	expression tag	UNP E3PQQ9
В	-6	GLY	-	expression tag	UNP E3PQQ9
В	-5	HIS	-	expression tag	UNP E3PQQ9
В	-4	ILE	-	expression tag	UNP E3PQQ9
В	-3	GLU	-	expression tag	UNP E3PQQ9
В	-2	GLY	-	expression tag	UNP E3PQQ9
В	-1	ARG	-	expression tag	UNP E3PQQ9
В	0	HIS	-	expression tag	UNP E3PQQ9
С	-20	MET	-	initiating methionine	UNP E3PQQ9
С	-19	GLY	-	expression tag	UNP E3PQQ9
С	-18	HIS	-	expression tag	UNP E3PQQ9
С	-17	HIS	-	expression tag	UNP E3PQQ9
С	-16	HIS	ı	expression tag	UNP E3PQQ9
С	-15	HIS	ı	expression tag	UNP E3PQQ9
С	-14	HIS	-	expression tag	UNP E3PQQ9
С	-13	HIS	ı	expression tag	UNP E3PQQ9
С	-12	HIS	-	expression tag	UNP E3PQQ9
С	-11	HIS	-	expression tag	UNP E3PQQ9
С	-10	HIS	-	expression tag	UNP E3PQQ9
С	-9	HIS	-	expression tag	UNP E3PQQ9
С	-8	SER	-	expression tag	UNP E3PQQ9
С	-7	SER		expression tag	UNP E3PQQ9
С	-6	GLY	-	expression tag	UNP E3PQQ9
С	-5	HIS	-	expression tag	UNP E3PQQ9
С	-4	ILE	-	expression tag	UNP E3PQQ9



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Chain	Residue	Modelled Modelled	Actual	Comment	Reference
С	-3	GLU	_	expression tag	UNP E3PQQ9
С	-2	GLY	_	expression tag	UNP E3PQQ9
С	-1	ARG	-	expression tag	UNP E3PQQ9
С	0	HIS	_	expression tag	UNP E3PQQ9
D	-20	MET	_	initiating methionine	UNP E3PQQ9
D	-19	GLY	-	expression tag	UNP E3PQQ9
D	-18	HIS	_	expression tag	UNP E3PQQ9
D	-17	HIS	-	expression tag	UNP E3PQQ9
D	-16	HIS	-	expression tag	UNP E3PQQ9
D	-15	HIS	-	expression tag	UNP E3PQQ9
D	-14	HIS	_	expression tag	UNP E3PQQ9
D	-13	HIS	_	expression tag	UNP E3PQQ9
D	-12	HIS	-	expression tag	UNP E3PQQ9
D	-11	HIS	_	expression tag	UNP E3PQQ9
D	-10	HIS	_	expression tag	UNP E3PQQ9
D	-9	HIS	_	expression tag	UNP E3PQQ9
D	-8	SER	-	expression tag	UNP E3PQQ9
D	-7	SER	_	expression tag	UNP E3PQQ9
D	-6	GLY	-	expression tag	UNP E3PQQ9
D	-5	HIS	-	expression tag	UNP E3PQQ9
D	-4	ILE	_	expression tag	UNP E3PQQ9
D	-3	GLU	_	expression tag	UNP E3PQQ9
D	-2	GLY	_	expression tag	UNP E3PQQ9
D	-1	ARG	-	expression tag	UNP E3PQQ9
D	0	HIS	-	expression tag	UNP E3PQQ9
Е	-20	MET	-	initiating methionine	UNP E3PQQ9
Е	-19	GLY	-	expression tag	UNP E3PQQ9
Е	-18	HIS	-	expression tag	UNP E3PQQ9
Е	-17	HIS	-	expression tag	UNP E3PQQ9
Е	-16	HIS	-	expression tag	UNP E3PQQ9
Е	-15	HIS	-	expression tag	UNP E3PQQ9
Е	-14	HIS	-	expression tag	UNP E3PQQ9
Е	-13	HIS	-	expression tag	UNP E3PQQ9
Е	-12	HIS	-	expression tag	UNP E3PQQ9
Е	-11	HIS	-	expression tag	UNP E3PQQ9
Е	-10	HIS	-	expression tag	UNP E3PQQ9
Е	-9	HIS	-	expression tag	UNP E3PQQ9
Е	-8	SER	-	expression tag	UNP E3PQQ9
Е	-7	SER	-	expression tag	UNP E3PQQ9
Е	-6	GLY	-	expression tag	UNP E3PQQ9
Е	-5	HIS	-	expression tag	UNP E3PQQ9
Е	-4	ILE	-	expression tag	UNP E3PQQ9



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Chain	Residue	Modelled	Actual	Comment	Reference
Е	-3	GLU	-	expression tag	UNP E3PQQ9
Е	-2	GLY	-	expression tag	UNP E3PQQ9
Е	-1	ARG	-	expression tag	UNP E3PQQ9
Е	0	HIS	-	expression tag	UNP E3PQQ9
F	-20	MET	-	initiating methionine	UNP E3PQQ9
F	-19	GLY	-	expression tag	UNP E3PQQ9
F	-18	HIS	-	expression tag	UNP E3PQQ9
F	-17	HIS	-	expression tag	UNP E3PQQ9
F	-16	HIS	-	expression tag	UNP E3PQQ9
F	-15	HIS	-	expression tag	UNP E3PQQ9
F	-14	HIS	-	expression tag	UNP E3PQQ9
F	-13	HIS	-	expression tag	UNP E3PQQ9
F	-12	HIS	-	expression tag	UNP E3PQQ9
F	-11	HIS	-	expression tag	UNP E3PQQ9
F	-10	HIS	-	expression tag	UNP E3PQQ9
F	-9	HIS	-	expression tag	UNP E3PQQ9
F	-8	SER	-	expression tag	UNP E3PQQ9
F	-7	SER	-	expression tag	UNP E3PQQ9
F	-6	GLY	-	expression tag	UNP E3PQQ9
F	-5	HIS	-	expression tag	UNP E3PQQ9
F	-4	ILE	=	expression tag	UNP E3PQQ9
F	-3	GLU	-	expression tag	UNP E3PQQ9
F	-2	GLY	=	expression tag	UNP E3PQQ9
F	-1	ARG	-	expression tag	UNP E3PQQ9
F	0	HIS	-	expression tag	UNP E3PQQ9

• Molecule 2 is an oligosaccharide called alpha-D-glucopyranose. (1-4)-alpha-D-glucopyranose.



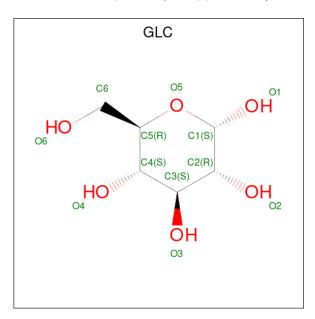
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace	
2	G	2	Total C O	0	0	0	
			23 12 11			ŭ .	
2	Н	2	Total C O	0	0	0	
	11	2	23 12 11			J	
2	Ţ	2	Total C O	0	0	0	
2	1	2	23 12 11	0	0	0	
2	Ţ	J 2	Total C O	0	0	0	
	J		23 12 11	U	U		



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace		
2	K	2	Total C O	0	0	0		
	11	2	23 12 11	0	U			
2	Т	2	Total C O	0	0	0		
2	ш	2	23 12 11	0				
2	M	2	Total C O	0	0	0		
	111	1V1	101	2	23 12 11	0	0	0
2	N	2	Total C O	0	0	0		
	2 N	2	23 12 11	U	0			

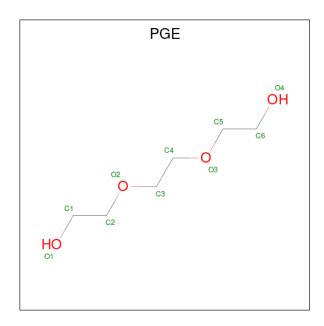
• Molecule 3 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	В	1	Total C O 12 6 6	0	0
3	С	1	Total C O 12 6 6	0	0
3	D	1	Total C O 12 6 6	0	0
3	E	1	Total C O 12 6 6	0	0
3	F	1	Total C O 12 6 6	0	0

 \bullet Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $\mathrm{C_6H_{14}O_4}).$

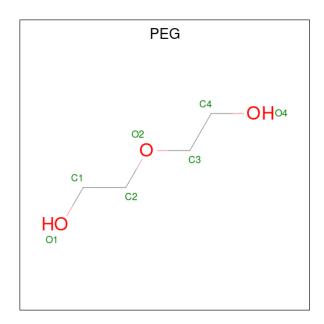




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O	0	0
4	Λ	1	10 6 4	U	U
4	A	1	Total C O	0	0
4	11	1	10 6 4	O	0
4	В	1	Total C O	0	0
	Ъ	1	10 6 4	0	0
4	$^{\rm C}$	1	Total C O	0	0
	C	1	10 6 4	0	0
4	$^{\rm C}$	1	Total C O	0	0
	C	1	10 6 4	U	0
4	D	1	Total C O	0	0
	D	1	10 6 4	O	
4	D	1	Total C O	0	0
T	D	1	10 6 4	O	Ü
4	E	1	Total C O	0	0
T	L	1	10 6 4	O	U
4	E	1	Total C O	0	0
-	L	1	10 6 4	J	0
4	F	1	Total C O	0	0
4	I.	I I	10 6 4	U	

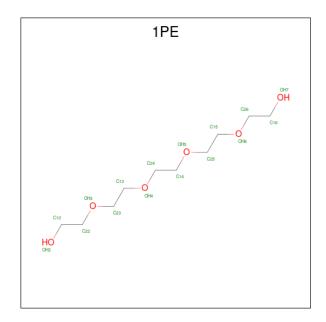
 $\bullet \ \ Molecule \ 5 \ is \ DI(HYDROXYETHYL)ETHER \ (three-letter \ code: \ PEG) \ (formula: \ C_4H_{10}O_3).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total C O 7 4 3	0	0
5	В	1	Total C O 7 4 3	0	0

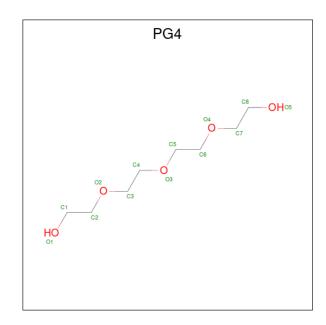
 \bullet Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $\mathrm{C_{10}H_{22}O_6}).$



M	[ol	Chain	Residues	Atoms	ZeroOcc	AltConf
(6	В	1	Total C O 16 10 6	0	0
(6	F	1	Total C O 16 10 6	0	0

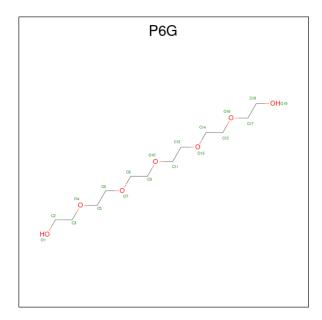


 \bullet Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $\mathrm{C_8H_{18}O_5}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	Total C O 13 8 5	0	0

 \bullet Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $\mathrm{C_{12}H_{26}O_{7}}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	С	1	Total C O 19 12 7	0	0
8	Е	1	Total C O 19 12 7	0	0



• Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	С	1	Total Na 1 1	0	0
9	F	1	Total Na 1 1	0	0

• Molecule 10 is water.

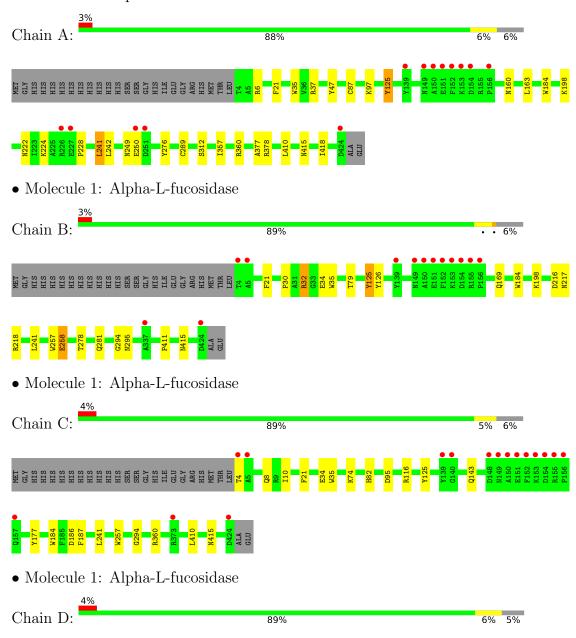
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	255	Total O 255 255	0	0
10	В	247	Total O 247 247	0	0
10	С	218	Total O 218 218	0	0
10	D	226	Total O 226 226	0	0
10	E	226	Total O 226 226	0	0
10	F	220	Total O 220 220	0	0



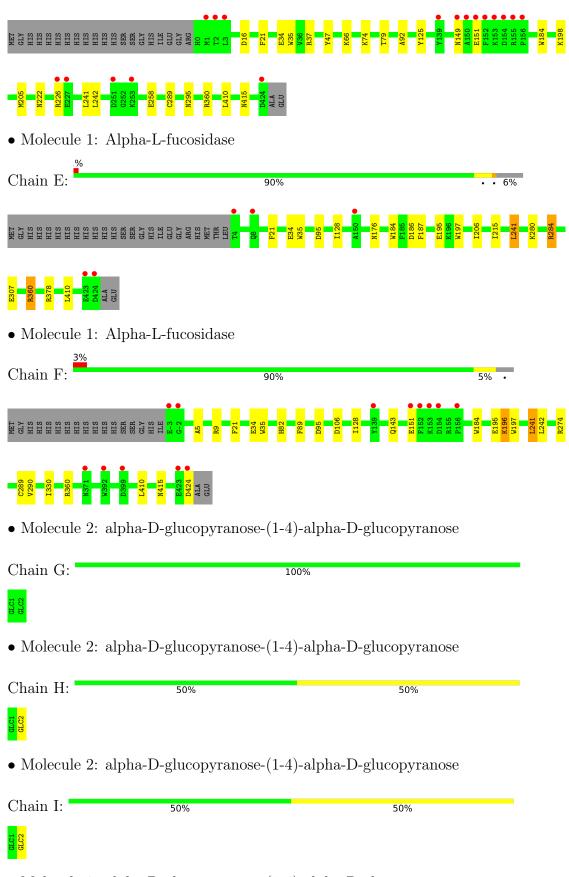
3 Residue-property plots (i)

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: Alpha-L-fucosidase







• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



Chain J:	100	0%
GLC2 GLC2		
• Molecule 2:	alpha-D-glucopyranose-(1-4))-alpha-D-glucopyranose
Chain K:	10	00%
GLC2 GLC2		
• Molecule 2:	alpha-D-glucopyranose-(1-4))-alpha-D-glucopyranose
Chain L:	50%	50%
GLC2 GLC2		
• Molecule 2:	alpha-D-glucopyranose-(1-4))-alpha-D-glucopyranose
Chain M:	10	00%
GLC1 GLC2		
• Molecule 2:	alpha-D-glucopyranose-(1-4))-alpha-D-glucopyranose
Chain N:	10	00%
GE01 GE02		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	107.77Å 148.76Å 194.90Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 - 2.20	Depositor
rtesolution (A)	48.93 - 2.20	EDS
% Data completeness	99.2 (48.93-2.20)	Depositor
(in resolution range)	99.2 (48.93-2.20)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.23 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
D.D.	0.167 , 0.217	Depositor
R, R_{free}	0.176 , 0.201	DCC
R_{free} test set	7763 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 52.7	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22428	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.50% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ 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: PEG, 1PE, NA, P6G, GLC, PG4, PGE

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).

Mol	Chain	Bond lengths		Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.80	0/3524	0.87	1/4790 (0.0%)	
1	В	0.85	$1/3536 \ (0.0\%)$	0.89	0/4806	
1	С	0.82	0/3513	0.83	0/4776	
1	D	0.83	$1/3550 \ (0.0\%)$	0.84	0/4825	
1	Е	0.84	0/3524	0.89	2/4790 (0.0%)	
1	F	0.80	0/3582	0.86	0/4867	
All	All	0.82	$2/21229 \ (0.0\%)$	0.86	3/28854 (0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
1	В	258	GLU	CD-OE2	5.64	1.31	1.25
1	D	92	ALA	C-O	-5.42	1.13	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	241	LEU	CA-CB-CG	6.28	129.75	115.30
1	Е	284	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	Ε	241	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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



the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3270	22	0
1	В	3424	0	3279	12	0
1	С	3408	0	3257	10	0
1	D	3444	0	3303	14	0
1	Ε	3416	0	3270	14	0
1	F	3473	0	3329	17	0
2	G	23	0	21	0	0
2	Н	23	0	21	0	0
2	I	23	0	21	0	0
2	J	23	0	21	0	0
2	K	23	0	21	0	0
2	L	23	0	21	1	0
2	M	23	0	21	0	0
2	N	23	0	21	0	0
3	A	12	0	12	1	0
3	В	12	0	12	2	0
3	С	12	0	12	3	0
3	D	12	0	12	2	0
3	${ m E}$	12	0	12	2	0
3	F	12	0	12	3	0
4	A	20	0	28	1	0
4	В	10	0	14	0	0
4	С	20	0	28	1	0
4	D	20	0	28	2	0
4	Ε	20	0	28	0	0
4	F	10	0	14	0	0
5	В	14	0	20	1	0
6	В	16	0	22	0	0
6	F	16	0	22	0	0
7	В	13	0	18	1	0
8	С	19	0	26	0	0
8	Ε	19	0	26	0	0
9	С	1	0	0	0	0
9	F	1	0	0	0	0
10	A	255	0	0	1	0
10	В	247	0	0	0	0
10	С	218	0	0	1	0
10	D	226	0	0	0	0
10	E	226	0	0	2	0
10	F	220	0	0	1	0
All	All	22428	0	20222	88	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 2.

The worst 5 of 88 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:C:95[A]:ASP:OD1	10:C:601:HOH:O	1.69	1.10
1:E:95[B]:ASP:OD1	10:E:601:HOH:O	1.85	0.93
1:F:95[B]:ASP:OD1	10:F:601:HOH:O	1.89	0.91
1:D:149:ASN:OD1	1:D:151:GLU:HG2	1.78	0.83
1:E:360:ARG:HH21	1:E:360:ARG:HG3	1.57	0.69

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	Perce	ntiles
1	A	421/447 (94%)	410 (97%)	10 (2%)	1 (0%)	47	55
1	В	422/447 (94%)	403 (96%)	18 (4%)	1 (0%)	47	55
1	С	420/447 (94%)	404 (96%)	15 (4%)	1 (0%)	47	55
1	D	424/447 (95%)	410 (97%)	13 (3%)	1 (0%)	47	55
1	Е	421/447 (94%)	408 (97%)	13 (3%)	0	100	100
1	F	428/447 (96%)	413 (96%)	14 (3%)	1 (0%)	47	55
All	All	$2536/2682\ (95\%)$	2448 (96%)	83 (3%)	5 (0%)	47	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	ASN
1	D	415	ASN
1	В	415	ASN



Continued from previous page...

Mol	Chain	Res	Type
1	С	415	ASN
1	F	415	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain 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	A	352/372~(95%)	348 (99%)	4 (1%)	73 85
1	В	353/372 (95%)	348 (99%)	5 (1%)	67 80
1	\mathbf{C}	351/372 (94%)	345 (98%)	6 (2%)	60 74
1	D	355/372 (95%)	350 (99%)	5 (1%)	67 80
1	${ m E}$	352/372~(95%)	347 (99%)	5 (1%)	67 80
1	F	358/372 (96%)	351 (98%)	7 (2%)	55 69
All	All	2121/2232 (95%)	2089 (98%)	32 (2%)	65 78

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	184	TRP
1	F	196	LYS
1	С	143	GLN
1	С	125	TYR
1	F	241	LEU

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)

16 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).

N T - 1	(T)	Cl :-	D	T : 1-	Вс	ond leng	ths	В	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	G	1	2	12,12,12	0.72	0	17,17,17	0.58	0
2	GLC	G	2	2	11,11,12	0.93	0	15,15,17	0.68	0
2	GLC	Н	1	2	12,12,12	0.67	0	17,17,17	0.60	0
2	GLC	Н	2	2	11,11,12	0.67	0	15,15,17	1.01	1 (6%)
2	GLC	I	1	2	12,12,12	0.70	0	17,17,17	0.64	0
2	GLC	I	2	2	11,11,12	0.90	0	15,15,17	1.14	1 (6%)
2	GLC	J	1	2	12,12,12	0.52	0	17,17,17	0.75	0
2	GLC	J	2	2	11,11,12	0.52	0	15,15,17	0.86	0
2	GLC	K	1	2	12,12,12	0.74	0	17,17,17	0.86	0
2	GLC	K	2	2	11,11,12	0.71	0	15,15,17	1.15	0
2	GLC	L	1	2	12,12,12	0.71	0	17,17,17	1.18	1 (5%)
2	GLC	L	2	2	11,11,12	0.72	0	15,15,17	1.05	2 (13%)
2	GLC	M	1	2	12,12,12	0.79	0	17,17,17	0.70	0
2	GLC	M	2	2	11,11,12	1.17	0	15,15,17	1.07	0
2	GLC	N	1	2	12,12,12	0.59	0	17,17,17	0.60	0
2	GLC	N	2	2	11,11,12	0.66	0	15,15,17	0.84	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.

N	/Iol	\mathbf{Type}	Chain	Res	Link	Chirals	Torsions	Rings
	2	GLC	G	1	2	-	0/2/22/22	0/1/1/1
	2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
	2	GLC	Н	1	2	-	0/2/22/22	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	Н	2	2	-	2/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/22/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	GLC	L	1	2	-	2/2/22/22	0/1/1/1
2	GLC	L	2	2	-	0/2/19/22	0/1/1/1
2	GLC	M	1	2	-	0/2/22/22	0/1/1/1
2	GLC	M	2	2	-	0/2/19/22	0/1/1/1
2	GLC	N	1	2	-	2/2/22/22	0/1/1/1
2	GLC	N	2	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	L	2	GLC	C3-C4-C5	2.32	114.39	110.24
2	L	2	GLC	O4-C4-C3	-2.22	105.22	110.35
2	Н	2	GLC	O5-C5-C6	2.12	110.52	107.20
2	I	2	GLC	C1-C2-C3	2.05	112.19	109.67
2	L	1	GLC	O2-C2-C3	-2.05	105.61	110.35

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Н	2	GLC	C4-C5-C6-O6
2	L	1	GLC	C4-C5-C6-O6
2	L	1	GLC	O5-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6
2	Н	2	GLC	O5-C5-C6-O6

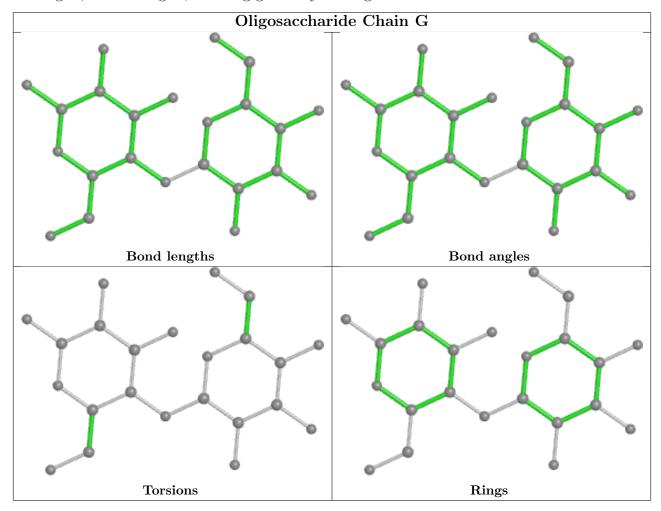
There are no ring outliers.

1 monomer is involved in 1 short contact:

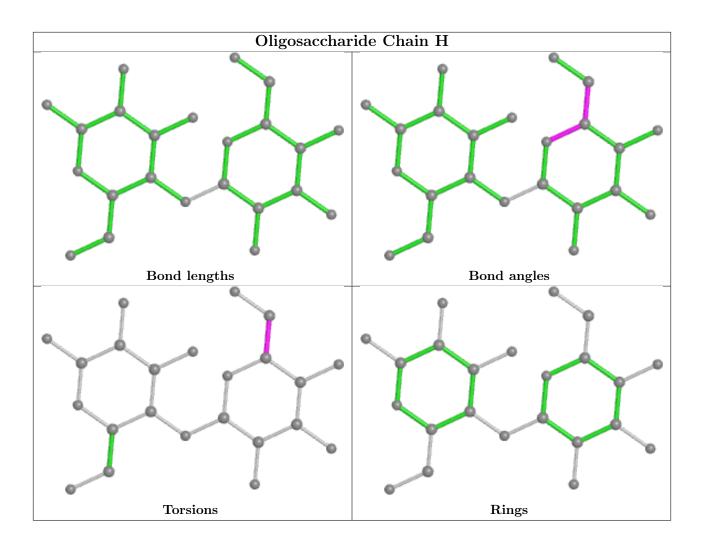
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	GLC	1	0



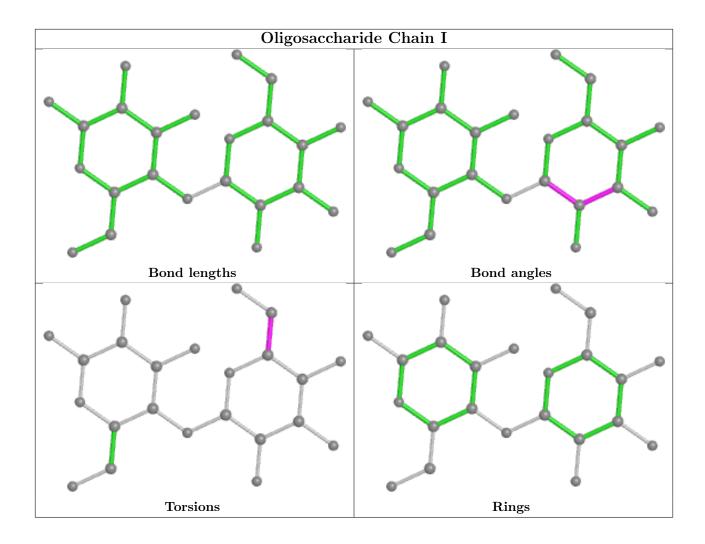
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



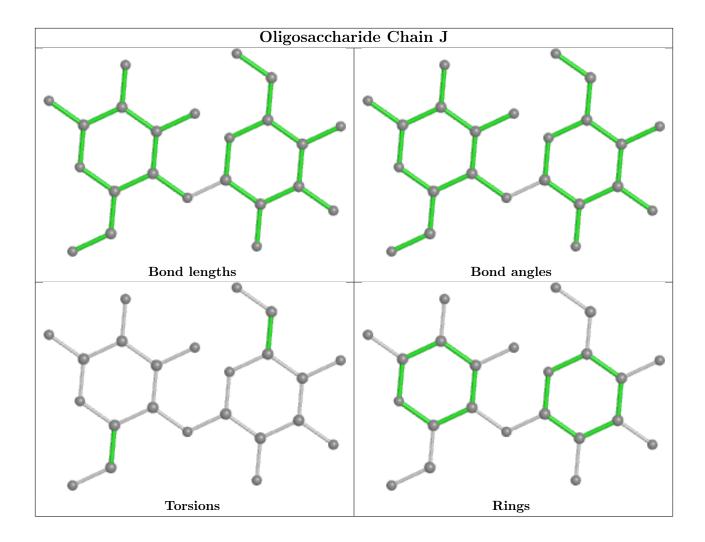




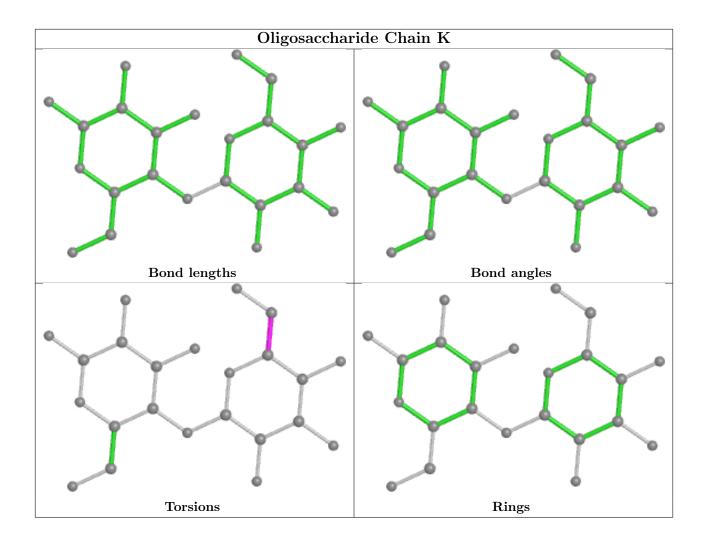




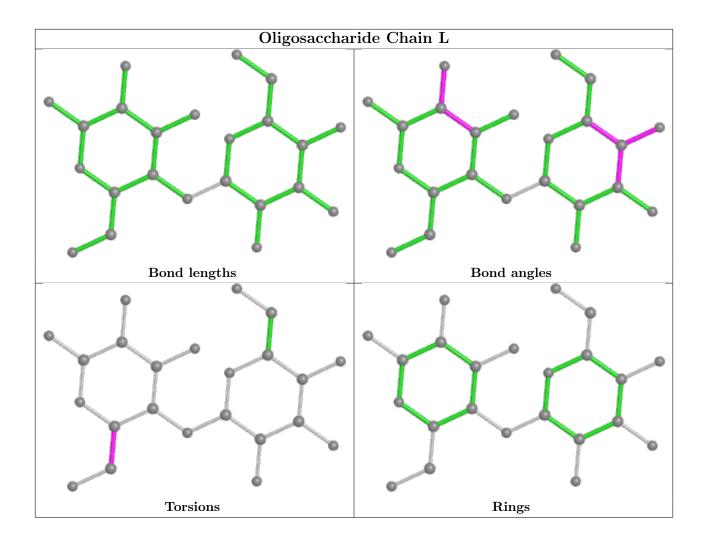




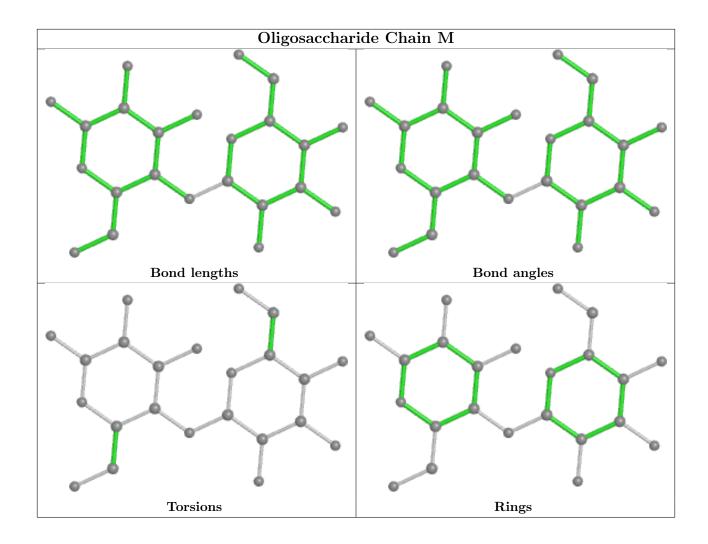




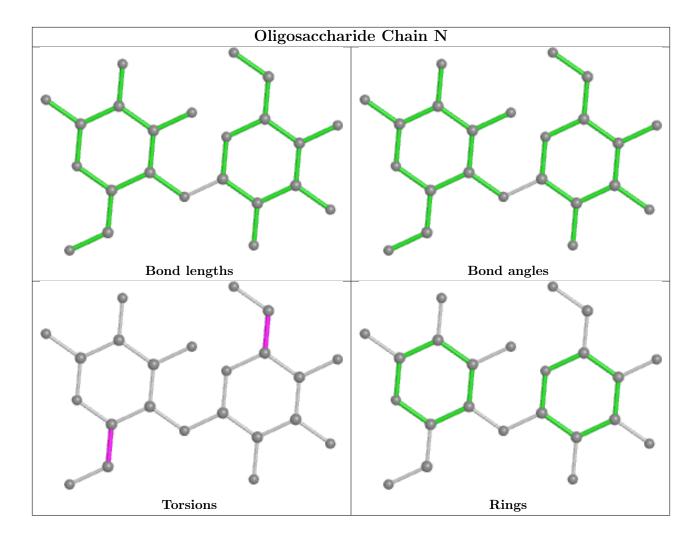












5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
MIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	D	501	-	12,12,12	0.93	1 (8%)	17,17,17	2.18	7 (41%)
4	PGE	A	504	-	9,9,9	0.71	0	8,8,8	0.82	0
3	GLC	Е	501	-	12,12,12	0.74	0	17,17,17	2.11	6 (35%)
4	PGE	Е	506	-	9,9,9	0.86	0	8,8,8	0.77	0
4	PGE	С	504	-	9,9,9	0.56	0	8,8,8	0.46	0



Mol	Trino	Chain	Dag	Link	Во	ond leng	ths	В	ond ang	gles
IVIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	В	505	-	15,15,15	0.60	0	14,14,14	0.32	0
6	1PE	F	505	9	15,15,15	0.77	0	14,14,14	0.53	0
5	PEG	В	503	_	6,6,6	0.66	0	5,5,5	0.24	0
3	GLC	В	501	-	12,12,12	0.78	0	17,17,17	2.34	10 (58%)
8	P6G	С	502	9	18,18,18	0.77	0	17,17,17	0.93	0
7	PG4	В	506	-	12,12,12	0.68	0	11,11,11	0.37	0
3	GLC	A	501	-	12,12,12	0.75	0	17,17,17	2.39	9 (52%)
4	PGE	F	504	-	9,9,9	0.74	0	8,8,8	0.78	0
5	PEG	В	502	-	6,6,6	0.53	0	5,5,5	0.31	0
4	PGE	В	504	-	9,9,9	0.85	0	8,8,8	0.88	0
3	GLC	С	501	-	12,12,12	0.76	0	17,17,17	2.01	5 (29%)
4	PGE	D	503	-	9,9,9	0.57	0	8,8,8	0.56	0
4	PGE	A	505	_	9,9,9	0.78	0	8,8,8	0.89	0
3	GLC	F	501	_	12,12,12	0.72	0	17,17,17	2.22	6 (35%)
4	PGE	D	502	-	9,9,9	0.76	0	8,8,8	0.78	0
4	PGE	Е	507	-	9,9,9	0.90	0	8,8,8	0.77	0
4	PGE	С	503	-	9,9,9	1.08	0	8,8,8	1.47	2 (25%)
8	P6G	Е	508	-	18,18,18	0.81	0	17,17,17	0.98	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
3	GLC	D	501	-	-	1/2/22/22	0/1/1/1
4	PGE	A	504	_	-	4/7/7/7	-
3	GLC	Ε	501	-	-	0/2/22/22	0/1/1/1
4	PGE	Ε	506	-	-	2/7/7/7	-
4	PGE	С	504	-	-	2/7/7/7	-
6	1PE	В	505	-	-	6/13/13/13	-
6	1PE	F	505	9	-	7/13/13/13	-
5	PEG	В	503	-	-	2/4/4/4	-
3	GLC	В	501	-	-	0/2/22/22	0/1/1/1
8	P6G	С	502	9	-	7/16/16/16	-
7	PG4	В	506	-	-	2/10/10/10	-
3	GLC	A	501	-	-	2/2/22/22	0/1/1/1
4	PGE	F	504	-	-	7/7/7/7	-
5	PEG	В	502	-	-	2/4/4/4	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	В	504	-	-	2/7/7/7	-
3	GLC	С	501	-	-	2/2/22/22	0/1/1/1
4	PGE	D	503	-	-	5/7/7/7	-
4	PGE	A	505	-	-	1/7/7/7	-
3	GLC	F	501	_	-	0/2/22/22	0/1/1/1
4	PGE	D	502	-	-	5/7/7/7	-
4	PGE	E	507	-	-	4/7/7/7	-
4	PGE	С	503	-	-	5/7/7/7	-
8	P6G	Е	508	-	-	8/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$oxed{Ideal(\AA)}$
3	D	501	GLC	O5-C5	-2.18	1.39	1.44

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
3	F	501	GLC	O5-C1-C2	-5.24	100.93	110.28
3	Ε	501	GLC	O5-C1-C2	-4.82	101.69	110.28
3	A	501	GLC	C4-C3-C2	4.36	118.44	110.82
3	D	501	GLC	O2-C2-C1	4.32	119.19	109.16
3	С	501	GLC	O5-C1-C2	-3.96	103.22	110.28

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	С	503	PGE	C3-C4-O3-C5
6	F	505	1PE	OH5-C14-C24-OH4
6	В	505	1PE	ОН4-С13-С23-ОН3
6	В	505	1PE	OH6-C15-C25-OH5
4	Е	507	PGE	O2-C3-C4-O3

There are no ring outliers.

12 monomers are involved in 19 short contacts:

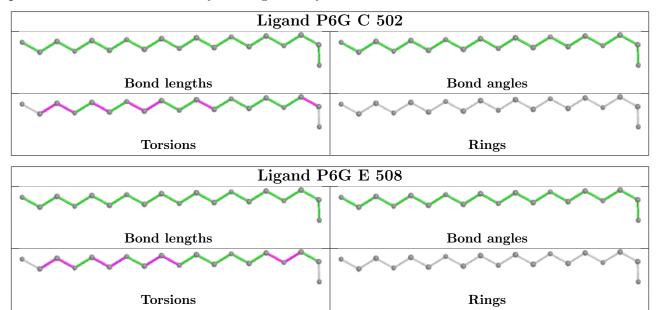
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	GLC	2	0



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	PGE	1	0
3	Ε	501	GLC	2	0
3	В	501	GLC	2	0
7	В	506	PG4	1	0
3	A	501	GLC	1	0
5	В	502	PEG	1	0
3	С	501	GLC	3	0
4	D	503	PGE	1	0
3	F	501	GLC	3	0
4	D	502	PGE	1	0
4	С	503	PGE	1	0

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





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 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	<rsrz></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q < 0.9
1	A	421/447 (94%)	-0.20	13 (3%) 49 47	19, 31, 57, 86	0
1	В	421/447 (94%)	-0.20	13 (3%) 49 47	19, 28, 55, 90	0
1	С	421/447 (94%)	-0.10	16 (3%) 40 38	20, 33, 59, 94	1 (0%)
1	D	425/447 (95%)	-0.05	17 (4%) 38 36	19, 31, 63, 110	0
1	Е	421/447 (94%)	-0.22	5 (1%) 79 77	17, 30, 57, 79	0
1	F	428/447 (95%)	-0.12	13 (3%) 50 48	20, 32, 60, 87	0
All	All	2537/2682 (94%)	-0.15	77 (3%) 50 48	17, 31, 59, 110	1 (0%)

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	156	PRO	7.1
1	С	154	ASP	6.3
1	В	150	ALA	5.8
1	В	5	ALA	5.4
1	С	424	ASP	5.3

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

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

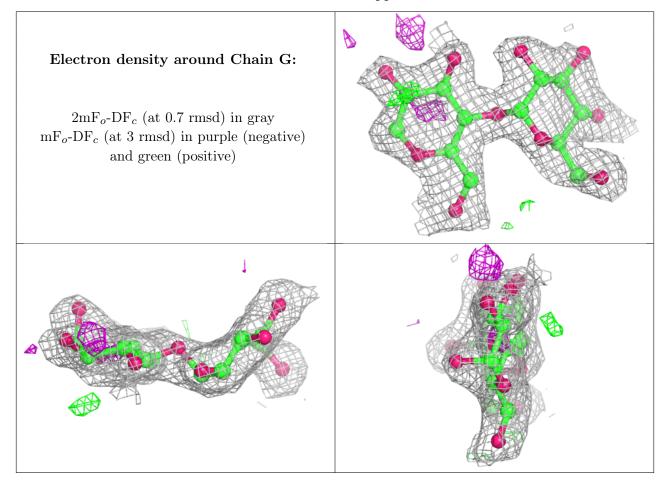
6.3 Carbohydrates (i)

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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
2	GLC	J	1	12/12	0.68	0.38	75,91,99,110	0
2	GLC	J	2	11/12	0.74	0.52	89,97,104,106	0
2	GLC	L	2	11/12	0.78	0.26	33,39,42,44	11
2	GLC	I	1	12/12	0.79	0.28	58,67,73,73	0
2	GLC	G	1	12/12	0.79	0.23	55,58,64,66	0
2	GLC	I	2	11/12	0.80	0.37	63,73,80,81	0
2	GLC	K	2	11/12	0.81	0.28	59,67,76,84	0
2	GLC	G	2	11/12	0.82	0.22	49,57,63,66	0
2	GLC	Н	2	11/12	0.84	0.45	64,76,82,85	0
2	GLC	Н	1	12/12	0.86	0.33	52,72,84,103	0
2	GLC	M	2	11/12	0.86	0.22	49,56,58,59	0
2	GLC	N	2	11/12	0.86	0.34	61,68,72,73	0
2	GLC	N	1	12/12	0.87	0.42	58,66,73,78	0
2	GLC	L	1	12/12	0.87	0.22	28,41,44,46	12
2	GLC	M	1	12/12	0.89	0.19	47,53,58,59	0
2	GLC	K	1	12/12	0.89	0.28	44,54,59,66	0

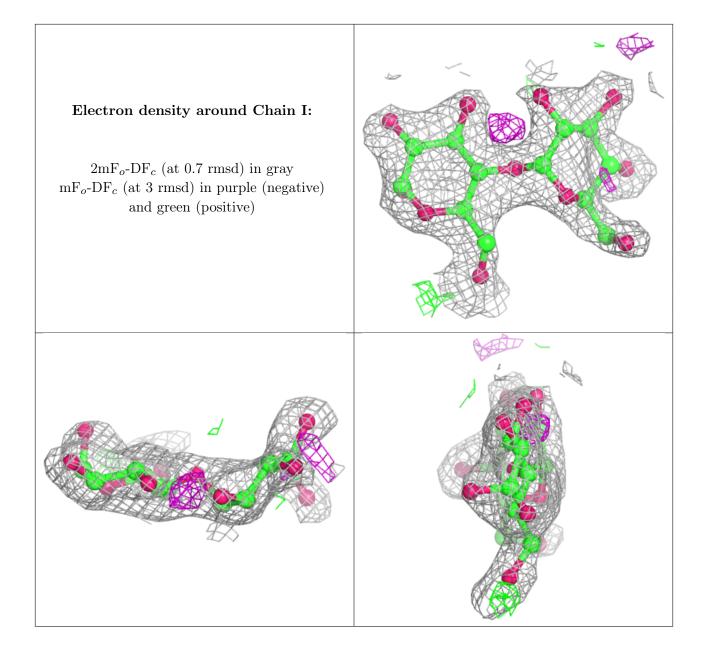
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





Electron density around Chain H: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



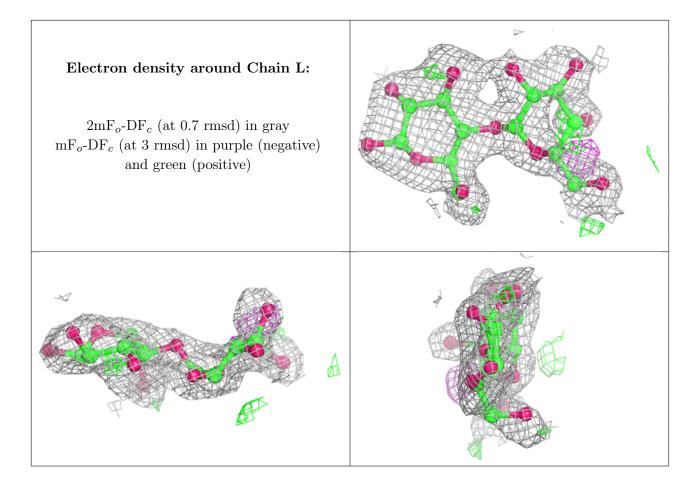




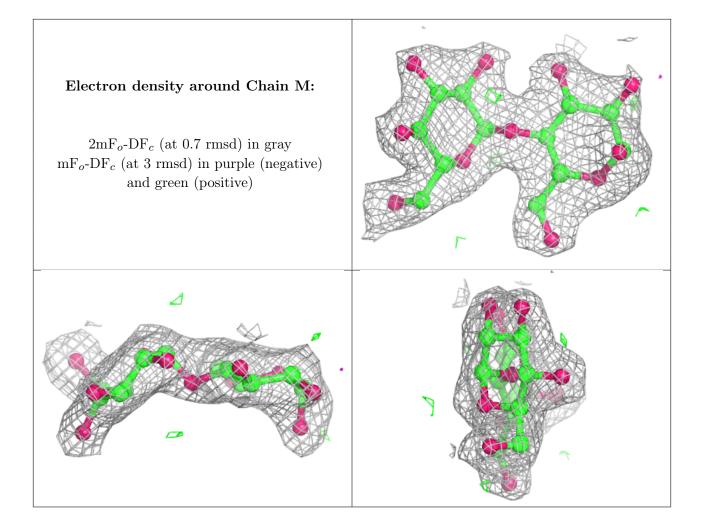


Electron density around Chain K: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

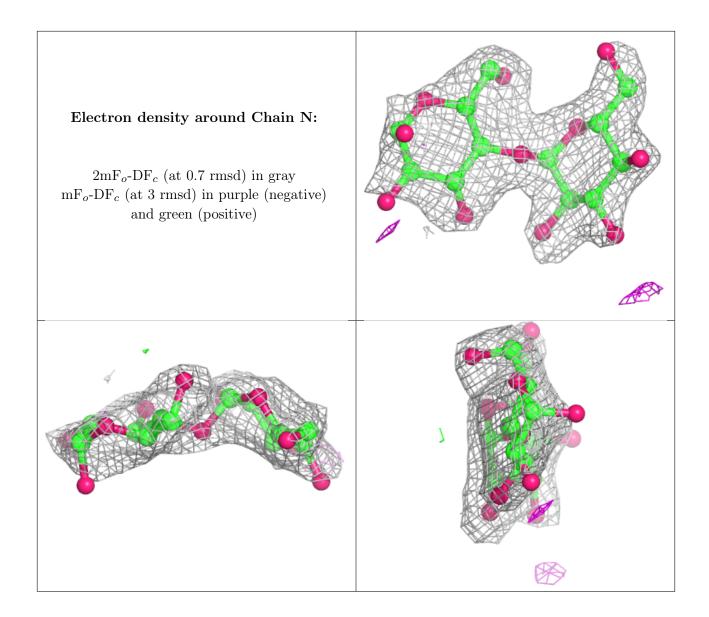












6.4 Ligands (i)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
6	1PE	F	505	16/16	0.71	0.25	56,73,82,83	0
4	PGE	Е	506	10/10	0.72	0.18	62,67,77,78	0
4	PGE	A	505	10/10	0.73	0.34	60,74,83,84	0
4	PGE	D	502	10/10	0.73	0.21	65,72,75,81	0
4	PGE	В	504	10/10	0.75	0.29	65,69,81,83	0
6	1PE	В	505	16/16	0.75	0.18	60,70,76,77	0
3	GLC	С	501	12/12	0.75	0.22	37,57,66,74	0

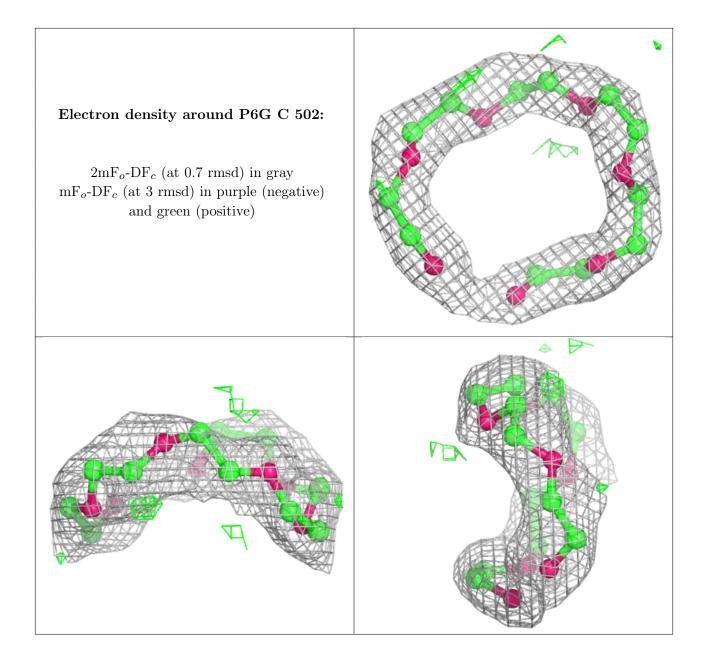


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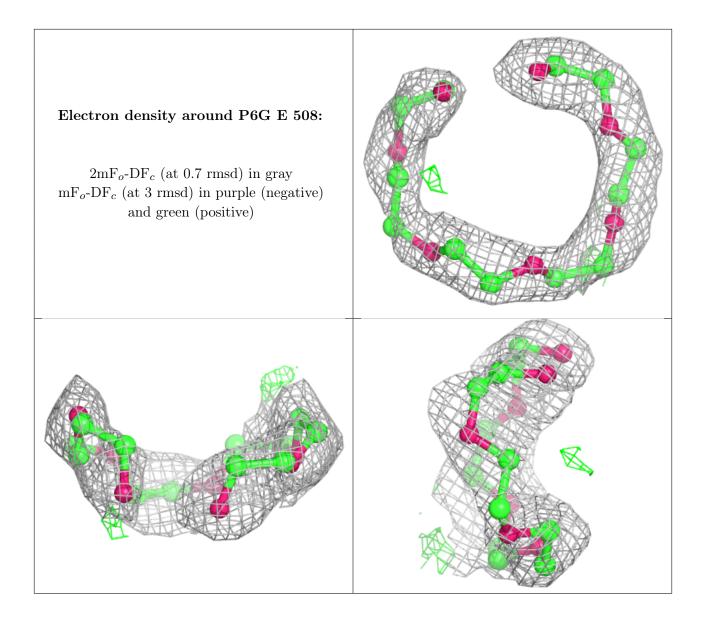
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
9	NA	С	505	1/1	0.75	0.23	69,69,69,69	0
9	NA	F	506	1/1	0.76	0.24	63,63,63,63	0
4	PGE	A	504	10/10	0.77	0.17	63,80,84,85	0
4	PGE	С	503	10/10	0.81	0.21	55,69,78,80	0
7	PG4	В	506	13/13	0.82	0.18	56,64,81,94	0
8	P6G	С	502	19/19	0.82	0.18	52,65,81,81	0
3	GLC	F	501	12/12	0.83	0.20	37,55,61,69	0
4	PGE	F	504	10/10	0.83	0.17	49,74,86,90	0
4	PGE	Е	507	10/10	0.84	0.23	62,64,69,72	0
3	GLC	A	501	12/12	0.85	0.23	36,52,64,73	0
8	P6G	Е	508	19/19	0.85	0.19	52,70,77,80	0
3	GLC	D	501	12/12	0.85	0.21	33,51,59,59	0
4	PGE	D	503	10/10	0.85	0.16	61,67,71,72	0
3	GLC	В	501	12/12	0.87	0.18	40,53,57,65	0
3	GLC	Е	501	12/12	0.88	0.16	34,52,57,68	0
5	PEG	В	503	7/7	0.88	0.29	60,63,67,68	0
4	PGE	С	504	10/10	0.88	0.26	58,65,74,77	0
5	PEG	В	502	7/7	0.89	0.27	54,60,62,63	0

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.

