

wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2024 – 09:27 pm GMT

PDB ID : 5CPW

Title: Crystal structure of murine polyomavirus PTA strain VP1 in complex with

the GT1a glycan

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Deposited on : 2015-07-21

Resolution : 1.75 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:

Mol Probity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

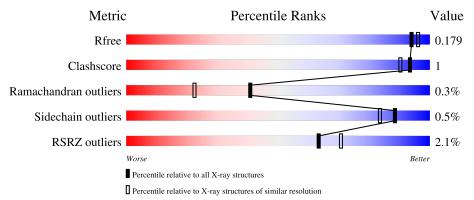
Validation Pipeline (wwPDB-VP) : 2.36

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	284	95%	
1	В	284	94%	
1	С	284	95%	
1	D	284	95%	•
1	Е	284	95%	



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Mol	Chain	Length	Quality of chain					
2	F	5	60%	40%				
2	G	5	20%	80%				
2	Н	5	40%	60%				
3	I	6	33%	67%				
3	J	6		100%				



2 Entry composition (i)

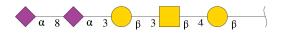
There are 5 unique types of molecules in this entry. The entry contains 13340 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 VP1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	278	Total	С	N	О	S	0	11	0
1	Λ	210	2225	1421	373	422	9	U	11	
1	В	278	Total	С	N	О	S	0	7	0
1	Ъ	210	2212	1408	374	422	8	0	'	
1	C	278	Total	С	N	О	S	0	5	0
1		210	2195	1400	369	418	8	0		
1	D	283	Total	С	N	О	S	0	7	0
1	ש	200	2249	1429	375	432	13	0	'	
1	Е	278	Total	С	N	О	S	0	8	0
1	E	218	2207	1408	372	419	8	0	0	

• Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	F	5	Total C N O 77 42 3 32	0	0	0
2	G	5	Total C N O 77 42 3 32	0	0	0
2	Н	5	Total C N O 77 42 3 32	0	0	0

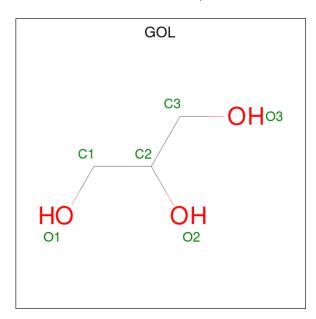
• Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose.





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	I	6	Total C N O 97 53 4 40	0	0	0
3	J	6	Total C N O 97 53 4 40	0	0	0

 \bullet Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	В	1	Total C O 4 2 2	0	0
4	В	1	Total C O 4 2 2	0	0
4	С	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0



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Mol	Chain	Residues	Ato	ms	ZeroOcc	AltConf
4	E	1	Total 4	C O 2 2	0	0

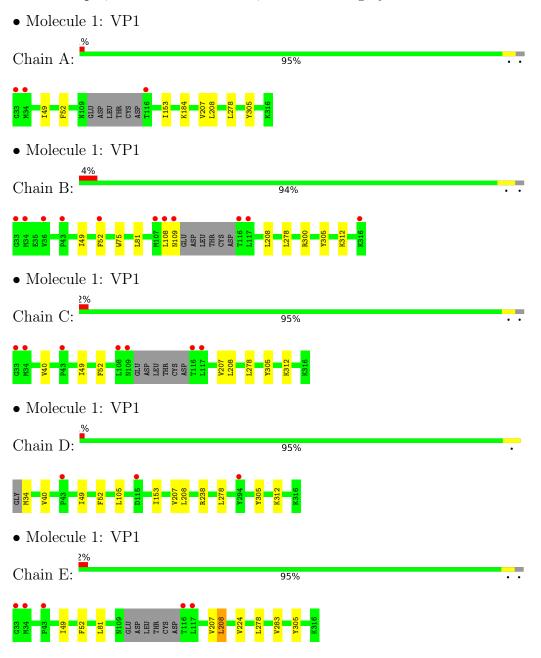
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	347	Total O 347 347	0	0
5	В	329	Total O 329 329	0	0
5	С	348	Total O 348 348	0	0
5	D	401	Total O 401 401	0	0
5	Е	370	Total O 370 370	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 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranos



e	
Chain F: 60%	40%
GAL1 NGA2 GAL3 SIA5 SIA5	
	c acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-Deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose
Chain G: 20%	80%
GAL1 NGA2 GAE3 SIA5 SIA5	
	c acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-Deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose
Chain H: 40%	60%
ACALA CALA SIA5 SIA5	
	c acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-Doxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuram
Chain I: 33%	67%
MGA2 MGA2 GAL3 SIA6 SIA6	
	c acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-Doxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuram
Chain J:	100%
CAL1 NGA2 CAL3 SIA4 SIA6	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	219.60Å 219.60Å 99.74Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.59 - 1.75	Depositor
Resolution (A)	47.54 - 1.75	EDS
% Data completeness	97.5 (47.59-1.75)	Depositor
(in resolution range)	97.6 (47.54-1.75)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) > 1$	1.32 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
D D	0.160 , 0.181	Depositor
R, R_{free}	0.159 , 0.179	DCC
R_{free} test set	8140 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 47.5	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13340	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.35% 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: NGA, GOL, SIA, GAL

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		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.39	0/2306	0.56	0/3141	
1	В	0.38	0/2277	0.55	0/3100	
1	С	0.38	0/2266	0.56	0/3089	
1	D	0.39	0/2324	0.58	0/3165	
1	Е	0.41	0/2279	0.58	0/3106	
All	All	0.39	0/11452	0.57	0/15601	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2225	0	2219	5	0
1	В	2212	0	2188	9	0
1	С	2195	0	2179	5	0
1	D	2249	0	2230	11	0
1	Е	2207	0	2188	7	0
2	F	77	0	65	0	0
2	G	77	0	65	0	0
2	Н	77	0	65	0	0



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	97	0	81	0	0
3	J	97	0	81	0	0
4	A	8	0	8	1	0
4	В	8	0	8	0	0
4	С	4	0	4	0	0
4	D	8	0	8	1	0
4	Ε	4	0	4	0	0
5	A	347	0	0	0	0
5	В	329	0	0	0	0
5	С	348	0	0	1	0
5	D	401	0	0	0	0
5	Е	370	0	0	0	0
All	All	13340	0	11393	33	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.

The worst 5 of 33 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:E:49:ILE:HD11	1:E:278:LEU:HD23	1.71	0.71
1:D:52[A]:PHE:CD1	1:E:208:LEU:HD13	2.27	0.69
1:A:49:ILE:HD11	1:A:278:LEU:HD23	1.78	0.66
1:B:49:ILE:HD11	1:B:278:LEU:HD23	1.78	0.66
1:C:49:ILE:HD11	1:C:278:LEU:CD2	2.32	0.59

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	284/284 (100%)	276 (97%)	7 (2%)	1 (0%)	34	17
1	В	280/284~(99%)	273 (98%)	7 (2%)	0	100	100
1	С	280/284~(99%)	271 (97%)	8 (3%)	1 (0%)	34	17
1	D	288/284 (101%)	278 (96%)	9 (3%)	1 (0%)	41	22
1	E	281/284 (99%)	273 (97%)	7 (2%)	1 (0%)	34	17
All	All	1413/1420 (100%)	1371 (97%)	38 (3%)	4 (0%)	41	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	VAL
1	D	207	VAL
1	С	207	VAL
1	Ε	207	VAL

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	250/250 (100%)	249 (100%)	1 (0%)	91 87
1	В	246/250 (98%)	245 (100%)	1 (0%)	91 87
1	C	245/250 (98%)	244 (100%)	1 (0%)	91 87
1	D	254/250 (102%)	252 (99%)	2 (1%)	81 72
1	E	246/250 (98%)	245 (100%)	1 (0%)	91 87
All	All	1241/1250 (99%)	1235 (100%)	6 (0%)	88 83

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	34	MET
1	D	208	LEU
1	Е	208	LEU
1	В	208	LEU



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Mol	Chain	Res	Type
1	A	208	LEU

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

Mol	Chain	Res	Type
1	D	293	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

27 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	Mol Type Cha		Chain Res Link		Во	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	GAL	F	1	2	12,12,12	0.52	0	17,17,17	0.65	0	
2	NGA	F	2	2	14,14,15	0.39	0	17,19,21	0.69	0	
2	GAL	F	3	2	11,11,12	0.45	0	15,15,17	0.59	0	
2	SIA	F	4	2	20,20,21	0.59	0	24,28,31	1.03	2 (8%)	
2	SIA	F	5	2	20,20,21	0.57	0	24,28,31	1.02	2 (8%)	
2	GAL	G	1	2	12,12,12	0.54	0	17,17,17	0.81	1 (5%)	
2	NGA	G	2	2	14,14,15	0.39	0	17,19,21	0.81	1 (5%)	
2	GAL	G	3	2	11,11,12	0.55	0	15,15,17	0.63	0	
2	SIA	G	4	2	20,20,21	0.59	0	24,28,31	0.99	1 (4%)	
2	SIA	G	5	2	20,20,21	0.59	0	24,28,31	0.98	2 (8%)	



Mol	Mol Type Chain		Res	Link	Во	Bond lengths			Bond angles		
WIOI	Туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	GAL	Н	1	2	12,12,12	0.51	0	17,17,17	0.81	1 (5%)	
2	NGA	Н	2	2	14,14,15	0.48	0	17,19,21	0.63	0	
2	GAL	Н	3	2	11,11,12	0.71	0	15,15,17	0.70	0	
2	SIA	Н	4	2	20,20,21	0.67	0	24,28,31	1.10	2 (8%)	
2	SIA	Н	5	2	20,20,21	0.60	0	24,28,31	0.97	2 (8%)	
3	GAL	I	1	3	12,12,12	0.50	0	17,17,17	0.97	2 (11%)	
3	NGA	I	2	3	14,14,15	0.48	0	17,19,21	0.79	1 (5%)	
3	GAL	I	3	3	11,11,12	0.52	0	15,15,17	0.70	0	
3	SIA	I	4	3	20,20,21	0.58	0	24,28,31	0.87	0	
3	SIA	I	5	3	20,20,21	0.66	0	24,28,31	1.05	2 (8%)	
3	SIA	I	6	3	20,20,21	0.63	0	24,28,31	1.15	1 (4%)	
3	GAL	J	1	3	12,12,12	0.51	0	17,17,17	0.98	1 (5%)	
3	NGA	J	2	3	14,14,15	0.42	0	17,19,21	0.84	1 (5%)	
3	GAL	J	3	3	11,11,12	0.59	0	15,15,17	0.83	1 (6%)	
3	SIA	J	4	3	20,20,21	0.59	0	24,28,31	0.97	1 (4%)	
3	SIA	J	5	3	20,20,21	0.60	0	24,28,31	0.96	1 (4%)	
3	SIA	J	6	3	20,20,21	0.62	0	24,28,31	1.03	2 (8%)	

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	GAL	F	1	2	-	2/2/22/22	0/1/1/1
2	NGA	F	2	2	-	0/6/23/26	0/1/1/1
2	GAL	F	3	2	-	0/2/19/22	0/1/1/1
2	SIA	F	4	2	-	4/18/34/38	0/1/1/1
2	SIA	F	5	2	-	0/18/34/38	0/1/1/1
2	GAL	G	1	2	-	2/2/22/22	0/1/1/1
2	NGA	G	2	2	-	0/6/23/26	0/1/1/1
2	GAL	G	3	2	-	0/2/19/22	0/1/1/1
2	SIA	G	4	2	-	6/18/34/38	0/1/1/1
2	SIA	G	5	2	-	0/18/34/38	0/1/1/1
2	GAL	Н	1	2	-	1/2/22/22	0/1/1/1
2	NGA	Н	2	2	-	0/6/23/26	0/1/1/1
2	GAL	Н	3	2	-	0/2/19/22	0/1/1/1
2	SIA	Н	4	2	-	5/18/34/38	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	Н	5	2	-	0/18/34/38	0/1/1/1
3	GAL	I	1	3	-	2/2/22/22	0/1/1/1
3	NGA	I	2	3	-	0/6/23/26	0/1/1/1
3	GAL	I	3	3	-	0/2/19/22	0/1/1/1
3	SIA	I	4	3	-	2/18/34/38	0/1/1/1
3	SIA	I	5	3	-	0/18/34/38	0/1/1/1
3	SIA	I	6	3	-	4/18/34/38	0/1/1/1
3	GAL	J	1	3	-	1/2/22/22	0/1/1/1
3	NGA	J	2	3	-	0/6/23/26	0/1/1/1
3	GAL	J	3	3	-	0/2/19/22	0/1/1/1
3	SIA	J	4	3	_	4/18/34/38	0/1/1/1
3	SIA	J	5	3	-	0/18/34/38	0/1/1/1
3	SIA	J	6	3	-	5/18/34/38	0/1/1/1

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	I	5	SIA	C6-O6-C2	2.86	117.47	111.34
2	F	5	SIA	C6-O6-C2	2.67	117.05	111.34
3	I	2	NGA	C1-O5-C5	2.50	115.58	112.19
3	J	2	NGA	C1-O5-C5	2.49	115.57	112.19
2	G	2	NGA	C1-O5-C5	2.48	115.56	112.19

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

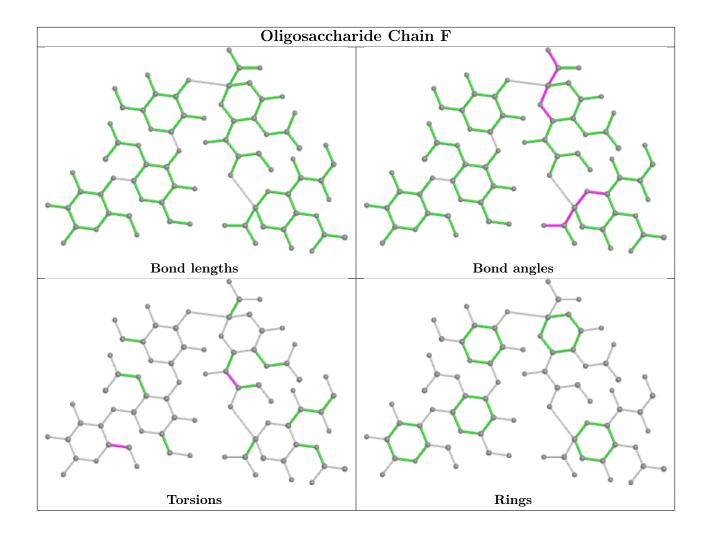
Mol	Chain	Res	Type	Atoms
3	I	6	SIA	O7-C7-C8-O8
3	I	6	SIA	C6-C7-C8-O8
3	I	6	SIA	C6-C7-C8-C9
3	J	6	SIA	O8-C8-C9-O9
2	F	1	GAL	O5-C5-C6-O6

There are no ring outliers.

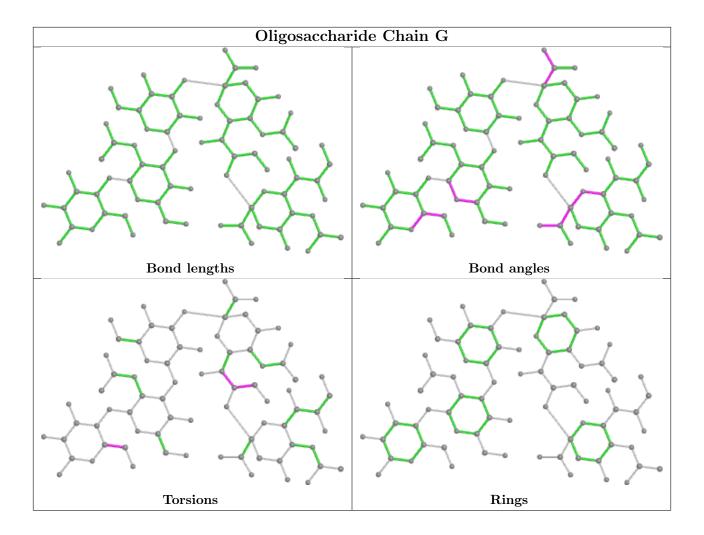
No monomer is involved in short contacts.

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

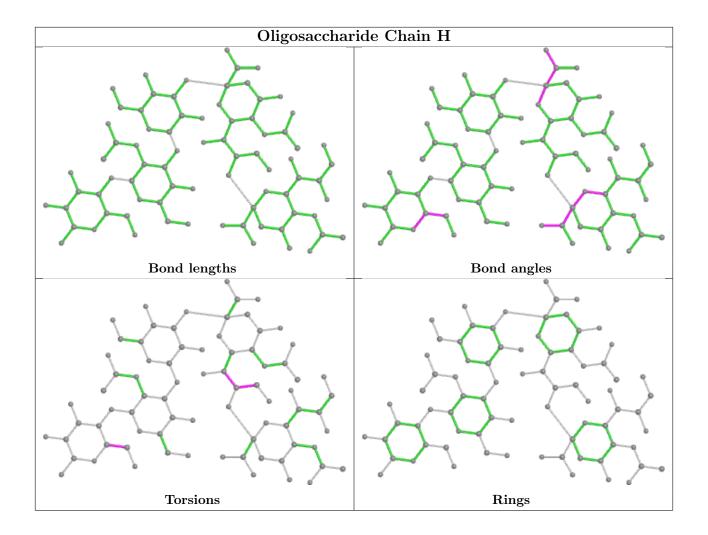




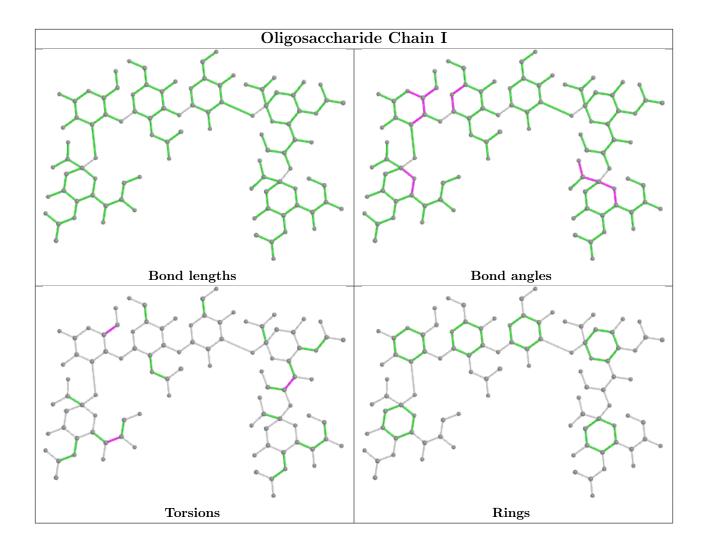




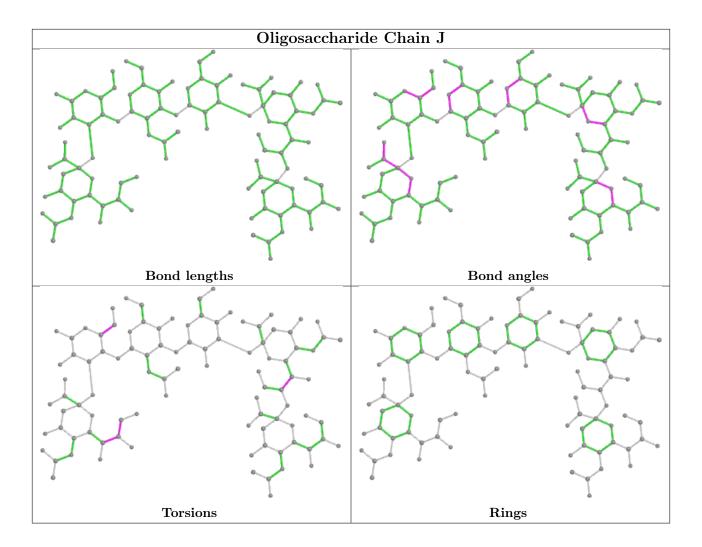












5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mal	Trino	Chain	Res	Link	В	Bond lengths			Bond angles		
Mol	Type	Chain		Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
4	GOL	A	401	-	3,3,5	0.48	0	2,2,5	0.36	0	
4	GOL	Е	401	-	3,3,5	0.43	0	2,2,5	0.44	0	
4	GOL	В	402	-	3,3,5	0.47	0	2,2,5	0.29	0	
4	GOL	A	402	-	3,3,5	0.44	0	2,2,5	0.44	0	
4	GOL	С	401	-	3,3,5	0.45	0	2,2,5	0.34	0	
4	GOL	D	401	-	3,3,5	0.46	0	2,2,5	0.35	0	



Mol	Type	Chain	Res	Link	В	Bond lengths			ond ang	gles
IVIOI	туре				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	402	-	3,3,5	0.50	0	2,2,5	0.32	0
4	GOL	В	401	-	3,3,5	0.44	0	2,2,5	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	401	-	-	0/1/1/4	-
4	GOL	E	401	-	-	0/1/1/4	-
4	GOL	В	402	-	-	1/1/1/4	-
4	GOL	A	402	-	-	0/1/1/4	-
4	GOL	С	401	-	-	1/1/1/4	-
4	GOL	D	401	-	-	1/1/1/4	-
4	GOL	D	402	-	-	1/1/1/4	-
4	GOL	В	401	-	-	1/1/1/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	С	401	GOL	O1-C1-C2-O2
4	D	402	GOL	O1-C1-C2-O2
4	В	402	GOL	O1-C1-C2-O2
4	В	401	GOL	O1-C1-C2-O2
4	D	401	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

	Mol	Chain	Res	Type	Clashes	Symm-Clashes
	4	A	401	GOL	1	0
ſ	4	D	402	GOL	1	0

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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	278/284 (97%)	-0.41	3 (1%) 80 86	11, 16, 37, 70	0
1	В	278/284 (97%)	-0.23	11 (3%) 38 45	14, 20, 40, 70	0
1	С	278/284 (97%)	-0.21	7 (2%) 57 63	13, 20, 43, 70	0
1	D	283/284 (99%)	-0.43	3 (1%) 80 86	11, 17, 33, 63	0
1	E	278/284 (97%)	-0.39	5 (1%) 68 76	11, 16, 39, 69	0
All	All	1395/1420 (98%)	-0.33	29 (2%) 63 71	11, 18, 39, 70	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	33	GLY	5.3
1	В	34	MET	5.1
1	Е	34	MET	4.7
1	С	34	MET	4.6
1	С	116	THR	4.5

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.

\mathbf{Mol}	\mathbf{Type}	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{ ilde{A}}^2)$	Q<0.9
2	GAL	G	1	12/12	0.80	0.22	35,48,58,62	0



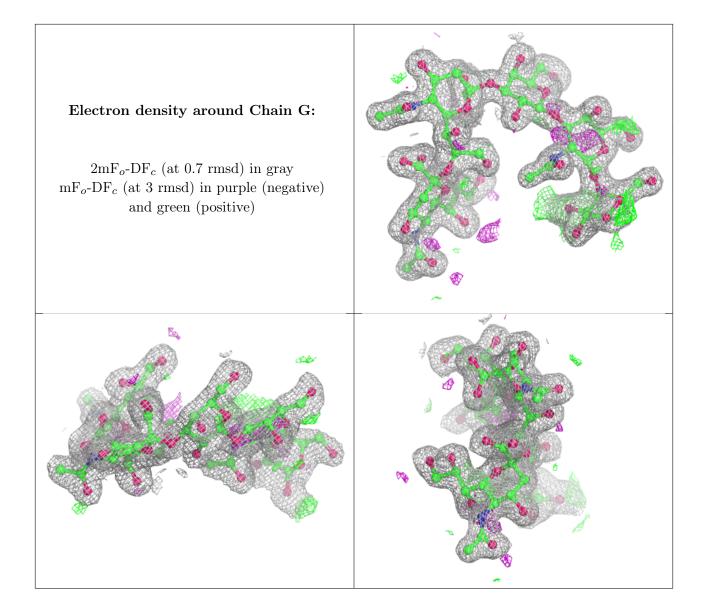
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
2	GAL	Н	1	12/12	0.86	0.23	42,48,52,58	0
3	GAL	I	1	12/12	0.87	0.20	36,45,48,55	0
3	GAL	J	1	12/12	0.88	0.17	31,42,47,62	0
3	SIA	J	6	20/21	0.89	0.28	42,52,77,80	0
2	GAL	F	1	12/12	0.90	0.19	32,47,58,75	0
3	SIA	I	6	20/21	0.90	0.23	44,55,79,88	0
2	NGA	G	2	14/15	0.92	0.22	24,31,42,43	0
2	NGA	Н	2	14/15	0.92	0.20	24,35,44,45	0
3	NGA	I	2	14/15	0.95	0.12	18,27,33,37	0
2	NGA	F	2	14/15	0.95	0.12	19,30,40,62	0
2	SIA	F	5	20/21	0.95	0.09	20,23,30,31	0
2	SIA	G	5	20/21	0.95	0.14	22,28,32,35	0
2	SIA	G	4	20/21	0.96	0.08	18,21,31,39	0
2	GAL	G	3	11/12	0.96	0.10	18,20,26,28	0
3	SIA	I	5	20/21	0.96	0.08	18,23,30,33	0
2	GAL	Н	3	11/12	0.96	0.09	18,20,22,23	0
2	SIA	Н	4	20/21	0.96	0.09	15,20,28,32	0
3	NGA	J	2	14/15	0.96	0.12	19,31,35,36	0
2	SIA	Н	5	20/21	0.96	0.14	21,27,33,37	0
3	SIA	I	4	20/21	0.97	0.06	13,16,22,28	0
3	GAL	J	3	11/12	0.97	0.06	14,16,20,21	0
3	SIA	J	4	20/21	0.97	0.06	13,16,23,27	0
3	SIA	J	5	20/21	0.97	0.06	17,21,25,30	0
2	SIA	F	4	20/21	0.97	0.06	12,16,24,32	0
3	GAL	I	3	11/12	0.98	0.05	14,16,18,19	0
2	GAL	F	3	11/12	0.98	0.05	15,17,21,22	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.

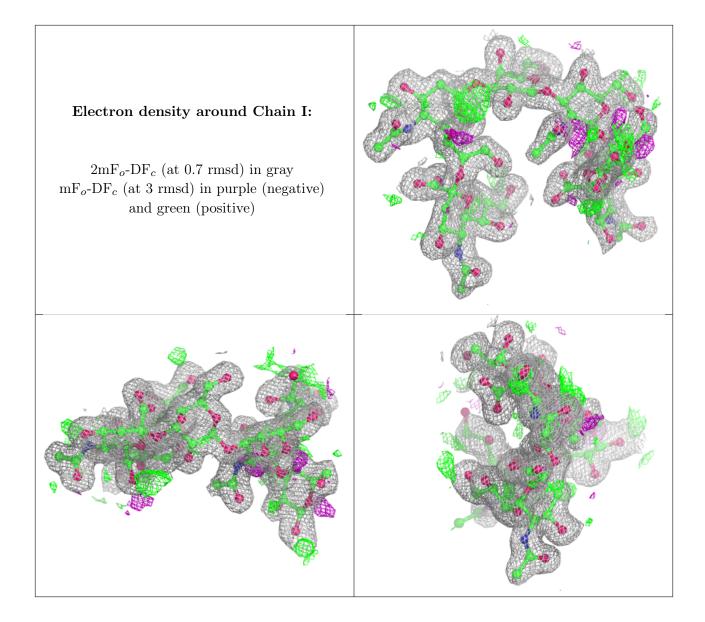




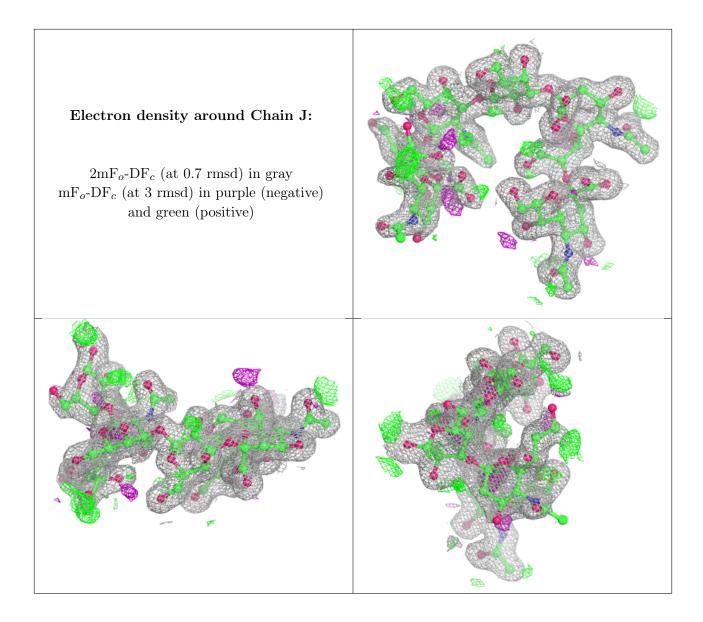












6.4 Ligands (i)

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	$\operatorname{B-factors}(\mathring{\mathrm{A}}^2)$	Q<0.9
4	GOL	D	402	4/6	0.74	0.14	39,40,47,48	0
4	GOL	С	401	4/6	0.80	0.14	45,48,55,61	0
4	GOL	В	402	4/6	0.82	0.17	37,44,46,55	0
4	GOL	A	402	4/6	0.84	0.12	39,41,49,51	0
4	GOL	A	401	4/6	0.85	0.13	39,40,43,43	0
4	GOL	Е	401	4/6	0.89	0.20	35,46,47,49	0
4	GOL	D	401	4/6	0.93	0.27	29,38,60,63	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	GOL	В	401	4/6	0.96	0.27	34,39,50,52	0

6.5 Other polymers (i)

There are no such residues in this entry.

