

Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 06:19 PM EDT

PDB ID : 4JCF

Title : S268F Variant of JC Polyomavirus Major Capsid Protein VP1 in Complex

with LSTc

Authors : Stehle, T.; Stroh, L.J.

Deposited on : 2013-02-21

Resolution : 2.20 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:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35.1

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)

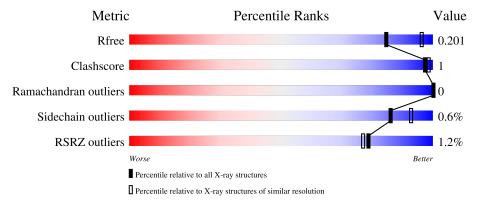
Validation Pipeline (wwPDB-VP) : 2.35.1

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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \ resolution} \\ (\#{\rm Entries, \ resolution \ range(\AA)}) \end{array}$
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	272	92%	• 5%
1	В	272	95%	5%
1	С	272	91%	• 6%
1	D	272	90%	• 6%
1	Е	272	92%	• 6%



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Mol	Chain	Length	Quality of chain	
2	F	3	67%	33%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10941 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 Major capsid protein VP1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	C	256	Total	С	N	Ο	S	0	4	0
1		250	2004	1268	341	384	11	U	4	
1	A	258	Total	С	N	О	S	0	2	0
1	Λ	250	2000	1265	340	384	11	U		
1	В	259	Total	С	N	О	S	0	5	0
1	Ъ	209	2022	1280	344	387	11	U	3	
1	D	257	Total	С	N	О	S	0	4	0
1		201	2000	1265	341	383	11	U	4	
1	Е	257	Total	С	N	О	S	0	2	0
1		257	1997	1266	340	380	11	U		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	18	GLY	-	expression tag	UNP P03089
С	19	SER	-	expression tag	UNP P03089
С	20	HIS	-	expression tag	UNP P03089
С	21	MET	-	expression tag	UNP P03089
С	268	PHE	SER	engineered mutation	UNP P03089
A	18	GLY	-	expression tag	UNP P03089
A	19	SER	-	expression tag	UNP P03089
A	20	HIS	-	expression tag	UNP P03089
A	21	MET	-	expression tag	UNP P03089
A	268	PHE	SER	engineered mutation	UNP P03089
В	18	GLY	-	expression tag	UNP P03089
В	19	SER	-	expression tag	UNP P03089
В	20	HIS	-	expression tag	UNP P03089
В	21	MET	-	expression tag	UNP P03089
В	268	PHE	SER	engineered mutation	UNP P03089
D	18	GLY	-	- expression tag	
D	19	SER	-	- expression tag	
D	20	HIS	-	- expression tag	
D	21	MET	-	expression tag	UNP P03089



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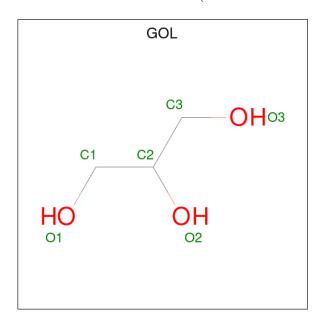
Chain	Residue	Modelled	Actual	Comment	Reference
D	268	PHE	SER	engineered mutation	UNP P03089
E	18	GLY	-	expression tag	UNP P03089
E	19	SER	-	expression tag	UNP P03089
E	20	HIS	_	expression tag	UNP P03089
E	21	MET	-	expression tag	UNP P03089
E	268	PHE	SER	engineered mutation	UNP P03089

• Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	F	3	Total 46	C N 25 2	O 19	0	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



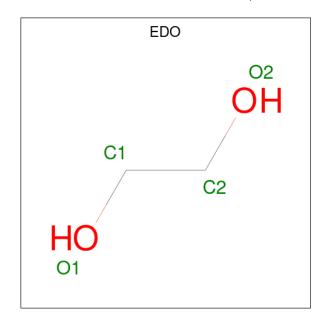
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	Е	1	Total C O 6 3 3	0	0

 \bullet Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



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

• Molecule 5 is water.

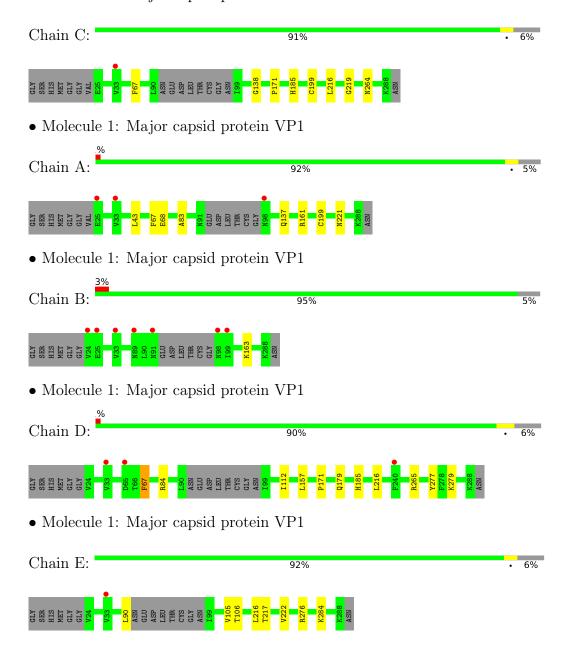
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	163	Total O 163 163	0	0
5	A	170	Total O 170 170	0	0
5	В	164	Total O 164 164	0	0
5	D	162	Total O 162 162	0	0
5	E	179	Total O 179 179	0	0



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: Major capsid protein VP1





 \bullet Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 67% 33%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	149.97Å 96.06Å 128.22Å	Depositor
a, b, c, α , β , γ	90.00° 110.36° 90.00°	Depositor
Resolution (Å)	44.64 - 2.20	Depositor
rtesolution (A)	44.60 - 2.20	EDS
% Data completeness	99.6 (44.64-2.20)	Depositor
(in resolution range)	99.6 (44.60-2.20)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.28 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
P. P.	0.164 , 0.201	Depositor
R, R_{free}	0.170 , 0.201	DCC
R_{free} test set	4321 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 42.2	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10941	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 3.74% 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: SIA, NAG, EDO, GAL, GOL

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	0.49	0/2052	0.67	1/2793~(0.0%)	
1	В	0.46	0/2083	0.67	0/2835	
1	С	0.50	0/2062	0.67	1/2804 (0.0%)	
1	D	0.49	0/2058	0.69	$1/2800 \ (0.0\%)$	
1	Е	0.49	0/2049	0.69	$1/2786 \ (0.0\%)$	
All	All	0.48	0/10304	0.68	$4/14018 \; (0.0\%)$	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	A	199	CYS	CB-CA-C	-5.75	98.89	110.40
1	Е	276	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	84	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	С	199	CYS	CB-CA-C	-5.05	100.29	110.40

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	2000	0	1920	4	0
1	В	2022	0	1952	1	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	2004	0	1945	3	0
1	D	2000	0	1927	5	0
1	Ε	1997	0	1932	3	0
2	F	46	0	40	1	0
3	A	6	0	8	0	0
3	В	6	0	8	0	0
3	С	6	0	8	0	0
3	D	6	0	8	0	0
3	Ε	6	0	8	0	0
4	A	4	0	6	0	0
5	A	170	0	0	0	0
5	В	164	0	0	1	0
5	С	163	0	0	0	0
5	D	162	0	0	0	0
5	Ε	179	0	0	0	0
All	All	10941	0	9762	16	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 (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:TYR:OH	1:D:279:LYS:HE2	2.06	0.55
1:A:43:LEU:HD21	1:A:83:ALA:HB2	1.89	0.55
1:C:171:PRO:HB3	1:C:185:HIS:CG	2.47	0.49
1:A:43:LEU:HD21	1:A:83:ALA:CB	2.45	0.47
1:B:163:LYS:HG2	5:B:555:HOH:O	2.13	0.47
1:D:171:PRO:HB3	1:D:185:HIS:CG	2.51	0.46
1:D:67:PHE:CE1	2:F:3:SIA:H113	2.53	0.43
1:A:68:GLU:HG3	1:A:161:ARG:NH1	2.34	0.43
1:C:138:GLY:HA2	1:C:219:GLY:O	2.19	0.42
1:E:90:LEU:HD21	1:E:284:LYS:HE2	2.01	0.42
1:D:157:LEU:O	1:D:179:GLN:HA	2.21	0.41
1:D:112:ILE:HD11	1:D:277:TYR:HB2	2.02	0.41
1:E:217:THR:HG22	1:E:222:VAL:HG11	2.02	0.41
1:A:137:GLN:HE21	1:A:221:ASN:HA	1.86	0.40
1:E:105:VAL:HG12	1:E:106:THR:HG23	2.04	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	A	$256/272\ (94\%)$	247 (96%)	9 (4%)	0	100	100	
1	В	260/272~(96%)	251 (96%)	9 (4%)	0	100	100	
1	С	$256/272\ (94\%)$	247 (96%)	9 (4%)	0	100	100	
1	D	257/272~(94%)	251 (98%)	6 (2%)	0	100	100	
1	E	255/272~(94%)	249 (98%)	6 (2%)	0	100	100	
All	All	1284/1360 (94%)	1245 (97%)	39 (3%)	0	100	100	

There are no Ramachandran outliers to report.

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	Perce	ntiles
1	A	219/237~(92%)	218 (100%)	1 (0%)	88	94
1	В	223/237 (94%)	223 (100%)	0	100	100
1	С	223/237 (94%)	221 (99%)	2 (1%)	78	88
1	D	220/237 (93%)	217 (99%)	3 (1%)	67	80
1	E	219/237 (92%)	218 (100%)	1 (0%)	88	94
All	All	1104/1185 (93%)	1097 (99%)	7 (1%)	86	93

All (7) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	С	67	PHE
1	С	216	LEU
1	A	67	PHE
1	D	67	PHE
1	D	216	LEU
1	D	265	ARG
1	Е	216	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	123	ASN
1	С	137	GLN
1	A	130	ASN
1	A	137	GLN
1	В	137	GLN
1	D	137	GLN
1	Е	137	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

3 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).

Ţ.	Mol	Type	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Pog	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	les
'	IVIOI	туре		n nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2										
	2	NAG	F	1	2	15,15,15	0.55	0	21,21,21	1.10	2 (9%)										



Mol	Trus	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	in Res	Timle	Bond lengths			Bond angles		
MIOI	Mol Type Chain Res	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2									
2	GAL	F	2	2	11,11,12	0.62	0	15,15,17	1.06	1 (6%)								
2	SIA	F	3	2	20,20,21	0.58	0	24,28,31	1.18	3 (12%)								

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	NAG	F	1	2	-	0/6/26/26	0/1/1/1
2	GAL	F	2	2	-	1/2/19/22	0/1/1/1
2	SIA	F	3	2	-	1/18/34/38	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	F	1	NAG	C1-C2-N2	-3.26	106.95	110.73
2	F	3	SIA	C6-O6-C2	2.44	116.56	111.34
2	F	3	SIA	O1B-C1-C2	2.26	119.48	113.03
2	F	3	SIA	O6-C2-C1	2.21	112.04	107.70
2	F	2	GAL	C1-C2-C3	2.17	112.34	109.67
2	F	1	NAG	O7-C7-N2	2.10	125.82	121.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	SIA	O8-C8-C9-O9
2	F	2	GAL	O5-C5-C6-O6

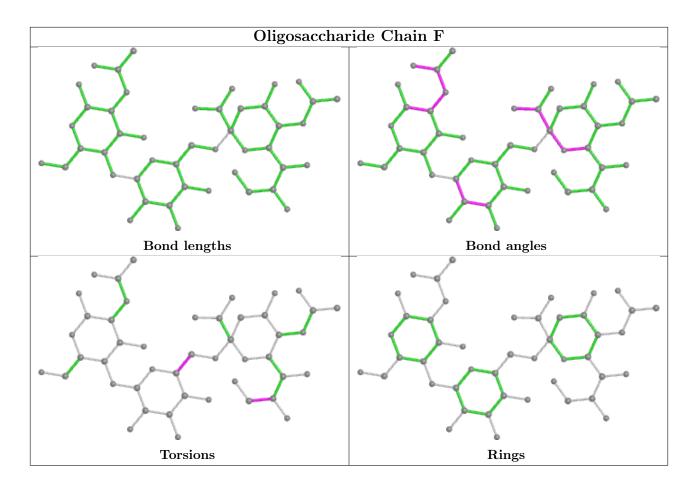
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	SIA	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)

6 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).

Mol	Type	Chain	Res	Link	В	Bond lengths			Bond angles		
MIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	GOL	В	301	-	5,5,5	0.43	0	5,5,5	0.46	0	
3	GOL	A	301	-	5,5,5	0.30	0	5,5,5	0.20	0	
4	EDO	A	302	_	3,3,3	0.40	0	2,2,2	0.50	0	
3	GOL	D	301	-	5,5,5	0.39	0	5,5,5	0.26	0	
3	GOL	С	304	_	5,5,5	0.30	0	5,5,5	0.14	0	
3	GOL	Е	301	-	5,5,5	0.38	0	5,5,5	0.38	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	GOL	В	301	-	-	2/4/4/4	-
3	GOL	A	301	-	-	2/4/4/4	-
4	EDO	A	302	-	-	1/1/1/1	-
3	GOL	D	301	-	-	4/4/4/4	-
3	GOL	С	304	-	-	2/4/4/4	-
3	GOL	E	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	304	GOL	C1-C2-C3-O3
3	A	301	GOL	C1-C2-C3-O3
3	A	301	GOL	O2-C2-C3-O3
3	В	301	GOL	O1-C1-C2-C3
3	D	301	GOL	C1-C2-C3-O3
3	D	301	GOL	O1-C1-C2-C3
3	Е	301	GOL	C1-C2-C3-O3
3	С	304	GOL	O2-C2-C3-O3
3	В	301	GOL	O1-C1-C2-O2
3	D	301	GOL	O2-C2-C3-O3
4	A	302	EDO	O1-C1-C2-O2
3	D	301	GOL	O1-C1-C2-O2
3	Е	301	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	258/272 (94%)	-0.47	3 (1%) 79 77	13, 19, 35, 49	0
1	В	259/272~(95%)	-0.34	7 (2%) 54 52	13, 20, 35, 55	0
1	С	256/272 (94%)	-0.48	1 (0%) 92 91	14, 20, 35, 48	0
1	D	257/272 (94%)	-0.47	3 (1%) 79 77	13, 20, 36, 54	0
1	E	257/272 (94%)	-0.52	1 (0%) 92 91	12, 19, 31, 48	0
All	All	1287/1360 (94%)	-0.45	15 (1%) 79 77	12, 20, 35, 55	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	33	VAL	5.6
1	D	33	VAL	5.0
1	В	33	VAL	4.3
1	В	24	VAL	3.7
1	A	98	ASN	3.4
1	Ε	33	VAL	3.4
1	В	91	ASN	2.8
1	В	98	ASN	2.8
1	D	240	PHE	2.5
1	В	99	ILE	2.5
1	A	33	VAL	2.4
1	В	25	GLU	2.4
1	В	89	ASN	2.2
1	A	25	GLU	2.1
1	D	65	ASP	2.1

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

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

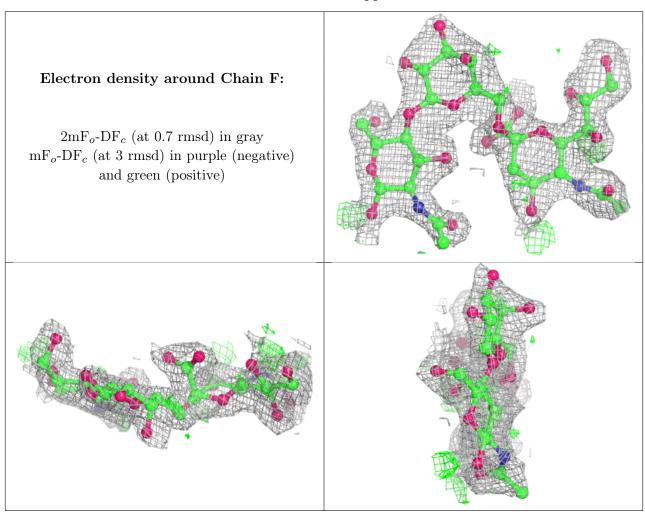


6.3 Carbohydrates (i)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	GAL	F	2	11/12	0.83	0.34	32,38,40,41	11
2	SIA	F	3	20/21	0.84	0.23	24,29,30,30	20
2	NAG	F	1	15/15	0.85	0.38	34,36,38,39	15

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{ ilde{A}}^2)$	Q<0.9
3	GOL	A	301	6/6	0.79	0.23	36,40,43,44	0
3	GOL	В	301	6/6	0.81	0.23	40,44,44,46	0
3	GOL	С	304	6/6	0.83	0.28	46,50,52,53	0
3	GOL	D	301	6/6	0.84	0.19	42,42,44,44	0
3	GOL	Е	301	6/6	0.92	0.20	33,36,38,38	0
4	EDO	A	302	4/4	0.92	0.20	39,39,40,41	0

6.5 Other polymers (i)

There are no such residues in this entry.

