



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 12:47 PM BST

PDB ID : 6BHJ  
Title : Structure of HIV-1 Reverse Transcriptase Bound to a 38-mer Hairpin Template-Primer RNA-DNA Aptamer  
Authors : Ruiz, F.X.; Miller, M.T.; Tuske, S.; Das, K.; Arnold, E.  
Deposited on : 2017-10-30  
Resolution : 2.81 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

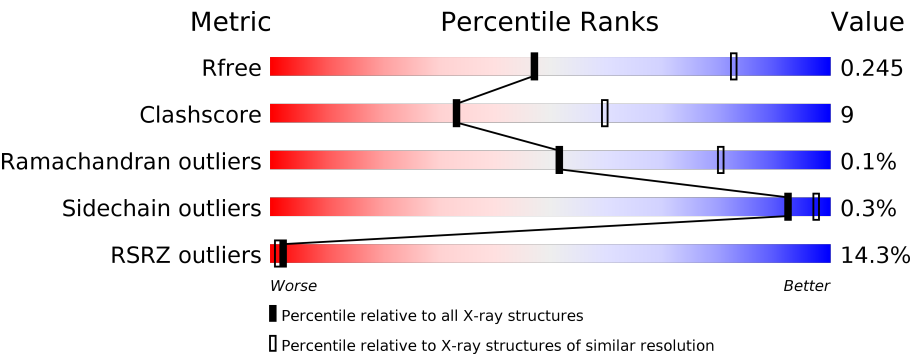
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

# 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 2.81 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	557	<div><div>13%</div><div>92%</div><div>7% ..</div></div>
1	C	557	<div><div>25%</div><div>90%</div><div>9% .</div></div>
2	B	444	<div><div>5%</div><div>90%</div><div>. 6%</div></div>
2	D	444	<div><div>8%</div><div>88%</div><div>. 8%</div></div>
3	E	38	<div><div>18%</div><div>47%</div><div>26%</div><div>8%</div></div>
3	F	38	<div><div>45%</div><div>16%</div><div>45%</div><div>32%</div><div>8%</div></div>

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Mol	Chain	Length	Quality of chain
4	G	2	
4	H	2	

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
6	GOL	B	2003	-	-	X	-
6	GOL	C	602	-	-	-	X
6	GOL	D	502	-	-	X	X
7	SO4	C	601	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17498 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 HIV-1 REVERSE TRANSCRIPTASE P66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4509	2919	751	832	7			
1	C	553	Total	C	N	O	S	0	0	0
			4504	2916	750	831	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	LYS	ARG	variant	UNP A0A076Q3N8
A	280	SER	CYS	engineered mutation	UNP A0A076Q3N8
A	498	ASN	ASP	engineered mutation	UNP A0A076Q3N8
C	172	LYS	ARG	variant	UNP A0A076Q3N8
C	280	SER	CYS	engineered mutation	UNP A0A076Q3N8
C	498	ASN	ASP	engineered mutation	UNP A0A076Q3N8

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3439	2242	568	622	7			
2	D	410	Total	C	N	O	S	0	0	0
			3394	2213	561	613	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP A0A076Q3N8
B	-14	ALA	-	expression tag	UNP A0A076Q3N8
B	-13	HIS	-	expression tag	UNP A0A076Q3N8
B	-12	HIS	-	expression tag	UNP A0A076Q3N8
B	-11	HIS	-	expression tag	UNP A0A076Q3N8
B	-10	HIS	-	expression tag	UNP A0A076Q3N8

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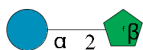
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP A0A076Q3N8
B	-8	HIS	-	expression tag	UNP A0A076Q3N8
B	-7	ALA	-	expression tag	UNP A0A076Q3N8
B	-6	LEU	-	expression tag	UNP A0A076Q3N8
B	-5	GLU	-	expression tag	UNP A0A076Q3N8
B	-4	VAL	-	expression tag	UNP A0A076Q3N8
B	-3	LEU	-	expression tag	UNP A0A076Q3N8
B	-2	PHE	-	expression tag	UNP A0A076Q3N8
B	-1	GLN	-	expression tag	UNP A0A076Q3N8
B	0	GLY	-	expression tag	UNP A0A076Q3N8
B	172	LYS	ARG	variant	UNP A0A076Q3N8
B	280	SER	CYS	engineered mutation	UNP A0A076Q3N8
D	-15	MET	-	initiating methionine	UNP A0A076Q3N8
D	-14	ALA	-	expression tag	UNP A0A076Q3N8
D	-13	HIS	-	expression tag	UNP A0A076Q3N8
D	-12	HIS	-	expression tag	UNP A0A076Q3N8
D	-11	HIS	-	expression tag	UNP A0A076Q3N8
D	-10	HIS	-	expression tag	UNP A0A076Q3N8
D	-9	HIS	-	expression tag	UNP A0A076Q3N8
D	-8	HIS	-	expression tag	UNP A0A076Q3N8
D	-7	ALA	-	expression tag	UNP A0A076Q3N8
D	-6	LEU	-	expression tag	UNP A0A076Q3N8
D	-5	GLU	-	expression tag	UNP A0A076Q3N8
D	-4	VAL	-	expression tag	UNP A0A076Q3N8
D	-3	LEU	-	expression tag	UNP A0A076Q3N8
D	-2	PHE	-	expression tag	UNP A0A076Q3N8
D	-1	GLN	-	expression tag	UNP A0A076Q3N8
D	0	GLY	-	expression tag	UNP A0A076Q3N8
D	172	LYS	ARG	variant	UNP A0A076Q3N8
D	280	SER	CYS	engineered mutation	UNP A0A076Q3N8

- Molecule 3 is DNA/RNA hybrid called 38-MER RNA-DNA Aptamer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			726	331	130	230	35			
3	F	35	Total	C	N	O	P	0	0	0
			726	331	130	230	35			

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

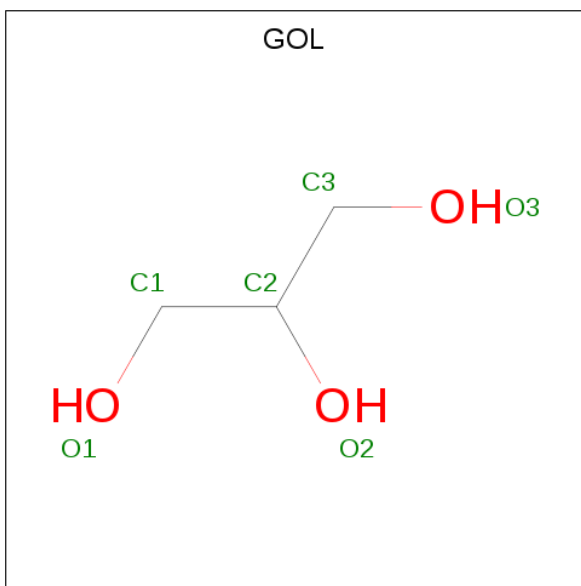


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total	C	O	0	0	0
			23	12	11			
4	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



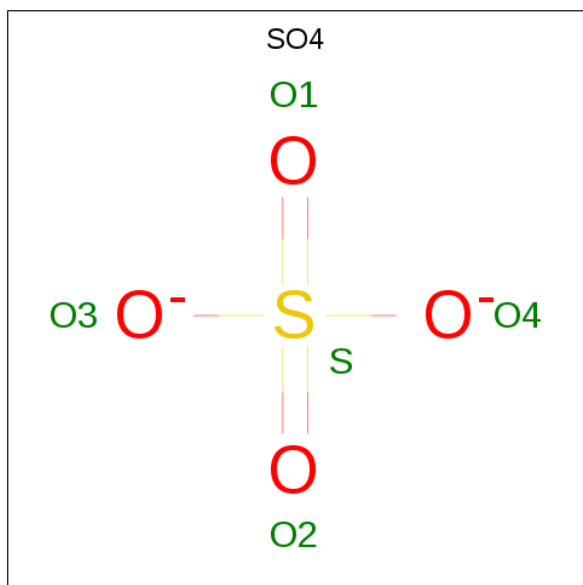
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

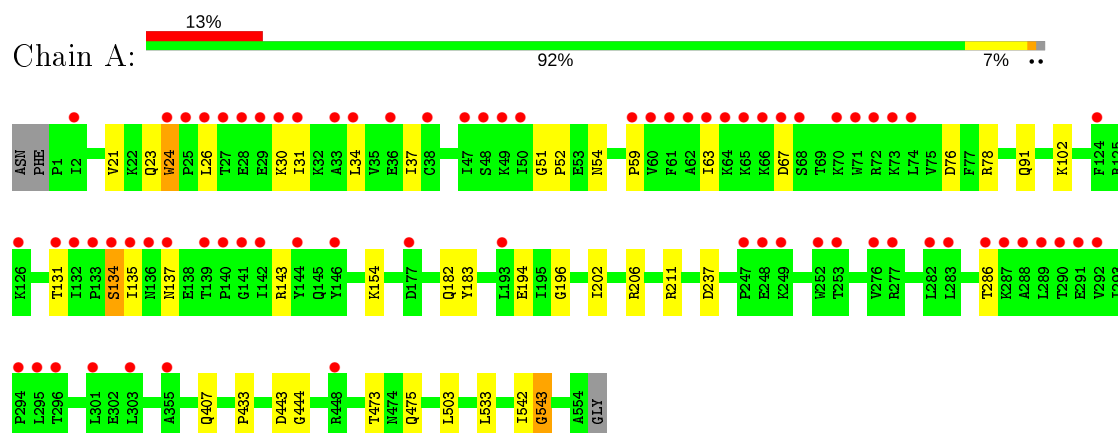
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	22	Total	O	0	0
			22	22		
8	B	43	Total	O	0	0
			43	43		
8	C	25	Total	O	0	0
			25	25		
8	D	20	Total	O	0	0
			20	20		
8	E	1	Total	O	0	0
			1	1		

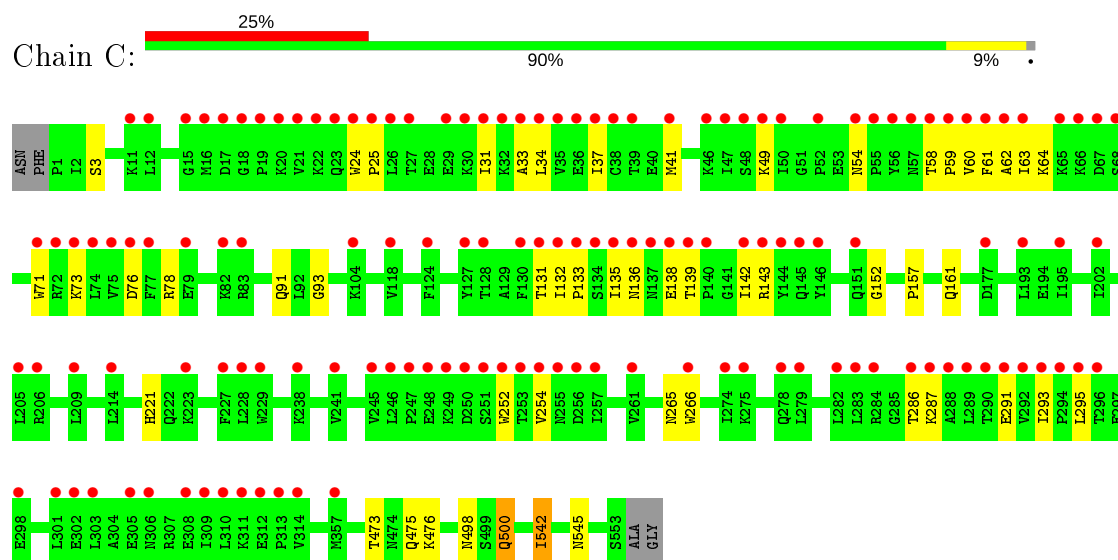
### 3 Residue-property plots [i](#)

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.

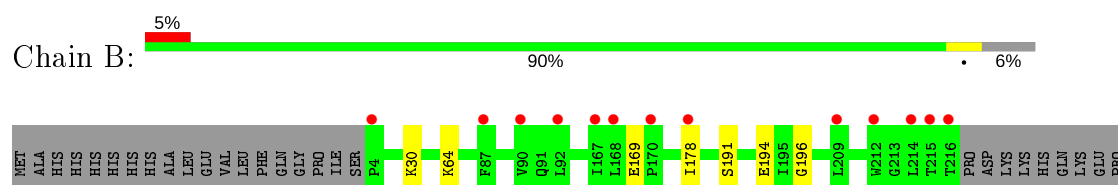
#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 subunit



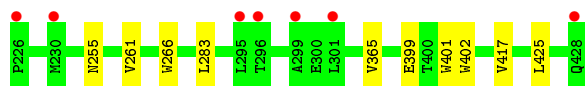
#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 subunit



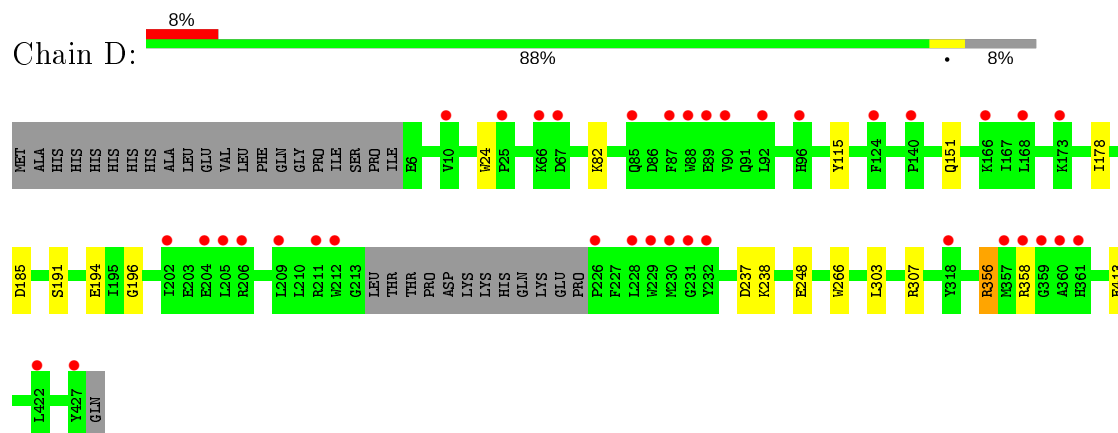
#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 subunit



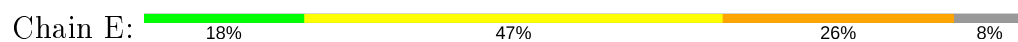




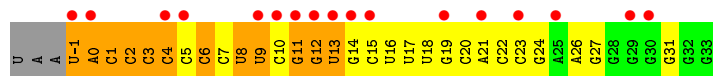
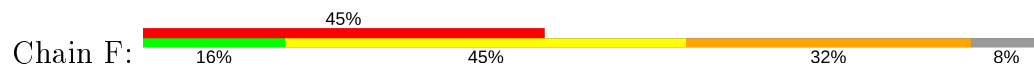
- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 subunit



- Molecule 3: 38-MER RNA-DNA Aptamer



- Molecule 3: 38-MER RNA-DNA Aptamer



- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.06Å 127.46Å 132.12Å 90.00° 101.81° 90.00°	Depositor
Resolution (Å)	47.69 – 2.81 47.69 – 2.81	Depositor EDS
% Data completeness (in resolution range)	92.4 (47.69-2.81) 92.4 (47.69-2.81)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.203 , 0.244 0.203 , 0.245	Depositor DCC
$R_{free}$ test set	2679 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.9	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 79.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 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: GOL, MG, GLC, SO4, FRU

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	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.26	0/4627	0.44	1/6286 (0.0%)
1	C	0.26	0/4622	0.45	1/6279 (0.0%)
2	B	0.27	0/3539	0.43	0/4807
2	D	0.25	0/3493	0.42	0/4745
3	E	1.41	10/811 (1.2%)	1.69	27/1254 (2.2%)
3	F	1.42	10/811 (1.2%)	1.67	26/1254 (2.1%)
All	All	0.49	20/17903 (0.1%)	0.68	55/24625 (0.2%)

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
2	D	0	1
3	E	0	1
3	F	0	1
All	All	0	3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	13	U	O5'-C5'	-15.95	1.17	1.42
3	F	13	U	O5'-C5'	-15.93	1.17	1.42
3	F	12	G	O3'-P	-11.38	1.47	1.61
3	E	12	G	O3'-P	-11.22	1.47	1.61
3	F	13	U	C3'-O3'	10.44	1.56	1.42
3	E	13	U	C3'-O3'	10.26	1.56	1.42
3	F	3	C	O3'-P	-9.29	1.50	1.61
3	E	3	C	O3'-P	-9.22	1.50	1.61
3	F	4	C	C4'-C3'	7.72	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	C	C4'-C3'	7.65	1.61	1.53
3	F	4	C	C5'-C4'	-7.26	1.42	1.51
3	E	4	C	C5'-C4'	-7.15	1.42	1.51
3	E	13	U	C4'-C3'	-6.19	1.46	1.53
3	F	13	U	C4'-C3'	-6.19	1.46	1.53
3	E	11	G	O5'-C5'	-5.54	1.33	1.42
3	F	11	G	O5'-C5'	-5.45	1.34	1.42
3	F	0	A	C3'-O3'	-5.14	1.34	1.42
3	E	0	A	C3'-O3'	-5.09	1.35	1.42
3	E	12	G	C3'-O3'	-5.08	1.35	1.42
3	F	12	G	C3'-O3'	-5.07	1.35	1.42

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	13	U	C5'-C4'-C3'	-20.02	83.97	116.00
3	E	13	U	C5'-C4'-C3'	-19.99	84.02	116.00
3	E	9	U	C4'-C3'-O3'	16.47	145.94	113.00
3	F	9	U	C4'-C3'-O3'	16.45	145.91	113.00
3	F	13	U	C4'-C3'-O3'	11.15	135.31	113.00
3	E	13	U	C4'-C3'-O3'	11.13	135.26	113.00
3	E	2	C	P-O5'-C5'	11.12	138.69	120.90
3	F	2	C	P-O5'-C5'	11.06	138.59	120.90
3	F	1	C	P-O5'-C5'	-9.85	105.15	120.90
3	E	1	C	P-O5'-C5'	-9.81	105.20	120.90
3	F	11	G	C5'-C4'-C3'	-8.59	102.26	116.00
3	E	11	G	C5'-C4'-C3'	-8.48	102.42	116.00
3	F	0	A	C4'-C3'-O3'	8.06	129.12	113.00
3	E	0	A	C4'-C3'-O3'	8.03	129.06	113.00
3	F	10	C	C5'-C4'-C3'	-7.67	103.73	116.00
3	E	10	C	C5'-C4'-C3'	-7.62	103.81	116.00
3	E	4	C	C5'-C4'-O4'	7.16	117.69	109.10
3	F	-1	U	O5'-P-OP2	-7.12	99.29	105.70
3	F	-1	U	O5'-P-OP1	-7.12	99.29	105.70
3	E	-1	U	O5'-P-OP2	-7.08	99.32	105.70
3	F	4	C	C5'-C4'-O4'	7.08	117.59	109.10
3	E	-1	U	O5'-P-OP1	-7.03	99.37	105.70
3	F	11	G	C4'-C3'-O3'	6.55	126.10	113.00
3	E	11	G	C4'-C3'-O3'	6.47	125.95	113.00
3	F	10	C	C5'-C4'-O4'	6.36	116.73	109.10
3	E	10	C	C5'-C4'-O4'	6.33	116.70	109.10
3	E	12	G	C2'-C3'-O3'	6.33	123.83	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	13	U	O4'-C4'-C3'	6.30	111.14	106.10
3	F	12	G	C2'-C3'-O3'	6.30	123.78	113.70
3	F	13	U	O4'-C4'-C3'	6.30	111.14	106.10
3	F	4	C	P-O3'-C3'	6.17	127.11	119.70
3	E	4	C	P-O3'-C3'	6.16	127.09	119.70
1	C	542	ILE	CB-CA-C	-5.99	99.61	111.60
3	E	8	U	C5'-C4'-O4'	5.87	116.14	109.10
3	F	13	U	C3'-C2'-O2'	-5.87	96.29	113.30
3	E	13	U	C3'-C2'-O2'	-5.86	96.30	113.30
3	F	8	U	C5'-C4'-O4'	5.83	116.09	109.10
3	E	6	C	P-O3'-C3'	-5.72	112.83	119.70
3	F	6	C	P-O3'-C3'	-5.70	112.86	119.70
3	E	1	C	O5'-C5'-C4'	5.59	122.33	111.70
3	F	1	C	O5'-C5'-C4'	5.59	122.32	111.70
3	E	8	U	C3'-C2'-C1'	5.50	105.90	101.50
3	F	8	U	C3'-C2'-C1'	5.49	105.89	101.50
1	A	24	TRP	C-N-CD	5.46	139.87	128.40
3	F	9	U	C2'-C3'-O3'	-5.34	97.76	109.50
3	F	11	G	P-O3'-C3'	5.33	126.09	119.70
3	E	11	G	P-O5'-C5'	5.30	129.38	120.90
3	E	11	G	P-O3'-C3'	5.29	126.05	119.70
3	E	9	U	C2'-C3'-O3'	-5.29	97.87	109.50
3	F	11	G	P-O5'-C5'	5.26	129.31	120.90
3	E	13	U	C5'-C4'-O4'	5.14	115.27	109.10
3	F	13	U	C5'-C4'-O4'	5.13	115.25	109.10
3	E	5	C	C5'-C4'-O4'	5.08	115.19	109.10
3	E	10	C	O4'-C4'-C3'	-5.03	98.97	104.00
3	F	5	C	C5'-C4'-O4'	5.02	115.12	109.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	356	ARG	Peptide
3	E	13	U	Sidechain
3	F	13	U	Sidechain

## 5.2 Too-close contacts ⓘ

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	4509	0	4572	63	1
1	C	4504	0	4565	89	1
2	B	3439	0	3468	25	0
2	D	3394	0	3421	29	0
3	E	726	0	379	43	0
3	F	726	0	379	71	0
4	G	23	0	21	0	0
4	H	23	0	21	6	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	24	0	32	11	0
6	C	6	0	8	0	0
6	D	6	0	8	6	0
7	C	5	0	0	0	0
8	A	22	0	0	0	0
8	B	43	0	0	0	0
8	C	25	0	0	0	0
8	D	20	0	0	0	0
8	E	1	0	0	0	0
All	All	17498	0	16874	283	1

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 9.

All (283) 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)
3:F:19:DG:C2'	3:F:20:DC:H5'	1.06	1.51
1:A:63:ILE:HD11	3:E:-1:U:P	1.51	1.49
1:A:30:LYS:O	1:A:34:LEU:HD13	1.26	1.33
3:F:19:DG:H2''	3:F:20:DC:C5'	0.84	1.32
1:A:30:LYS:O	1:A:34:LEU:CD1	1.85	1.25
1:C:473:THR:HG21	3:F:19:DG:H4'	1.21	1.18
2:D:303:LEU:HD22	2:D:307:ARG:NH1	1.59	1.17
1:C:59:PRO:HG2	1:C:76:ASP:HB3	1.28	1.13
3:E:19:DG:H2''	3:E:20:DC:O5'	1.35	1.13
3:F:19:DG:H2'	3:F:20:DC:H5'	1.26	1.09
1:C:76:ASP:HA	3:F:0:A:H4'	1.28	1.08
2:B:402:TRP:HE1	6:B:2003:GOL:H32	1.11	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:THR:CG2	1:C:59:PRO:HD2	1.84	1.08
3:F:18:DU:H4'	3:F:19:DG:O5'	1.50	1.05
3:E:18:DU:H4'	3:E:19:DG:O5'	1.50	1.05
1:C:54:ASN:HB3	1:C:143:ARG:NH2	1.71	1.04
3:F:19:DG:C2'	3:F:20:DC:C5'	1.80	1.04
1:A:76:ASP:HA	3:E:0:A:H4'	1.40	1.02
1:A:542:ILE:HD11	2:B:261:VAL:HG11	1.38	1.02
2:B:402:TRP:NE1	6:B:2003:GOL:H32	1.74	1.02
1:C:265:ASN:ND2	3:F:6:C:O2'	1.92	1.02
1:C:54:ASN:HB3	1:C:143:ARG:HH22	1.23	1.02
1:A:26:LEU:HD23	1:A:31:ILE:HG12	1.41	1.02
3:F:19:DG:H2''	3:F:20:DC:H5''	1.06	1.02
1:A:63:ILE:CD1	3:E:-1:U:P	2.47	1.01
1:C:54:ASN:CB	1:C:143:ARG:HH22	1.74	1.01
1:A:26:LEU:HG	1:A:31:ILE:HG13	1.41	0.99
1:C:287:LYS:HD3	1:C:291:GLU:OE2	1.60	0.99
3:F:16:DU:H2'	3:F:17:DU:OP1	1.61	0.98
3:E:16:DU:H2'	3:E:17:DU:OP1	1.61	0.97
1:A:54:ASN:O	1:A:143:ARG:NH2	1.98	0.96
1:C:131:THR:HG22	1:C:143:ARG:HG2	1.43	0.96
1:A:78:ARG:NH2	3:E:-1:U:O2'	1.99	0.96
1:C:58:THR:HG22	1:C:59:PRO:HD2	1.46	0.94
3:E:22:DC:H5''	3:E:22:DC:H6	1.28	0.94
2:B:402:TRP:HE1	6:B:2003:GOL:C3	1.80	0.94
1:A:102:LYS:HE3	1:A:237:ASP:OD1	1.66	0.94
3:F:22:DC:H5''	3:F:22:DC:H6	1.28	0.94
2:D:303:LEU:HD22	2:D:307:ARG:CZ	1.98	0.92
1:C:252:TRP:HD1	1:C:295:LEU:HD13	1.37	0.89
1:C:31:ILE:HG23	1:C:132:ILE:HD11	1.56	0.88
1:C:252:TRP:CD1	1:C:295:LEU:HD13	2.09	0.87
2:D:303:LEU:HD22	2:D:307:ARG:HH12	1.36	0.87
1:C:91:GLN:HB2	1:C:161:GLN:HE22	1.42	0.85
1:A:26:LEU:HD11	1:A:30:LYS:CB	2.06	0.85
3:F:19:DG:C5	3:F:20:DC:C4	2.64	0.85
1:C:49:LYS:HE2	1:C:142:ILE:CD1	2.07	0.85
1:C:473:THR:CG2	3:F:19:DG:H4'	2.07	0.84
1:C:58:THR:HG23	1:C:59:PRO:HD2	1.58	0.84
3:E:19:DG:H2''	3:E:20:DC:C5'	2.09	0.83
1:C:252:TRP:CD1	1:C:295:LEU:CD1	2.61	0.82
1:A:26:LEU:HD11	1:A:30:LYS:HB3	1.62	0.81
2:D:24:TRP:CD2	6:D:502:GOL:H31	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASN:O	1:C:143:ARG:NH2	2.14	0.79
1:C:473:THR:HG21	3:F:19:DG:C4'	2.09	0.78
3:F:19:DG:C6	3:F:20:DC:C4	2.72	0.78
1:C:475:GLN:NE2	3:F:16:DU:O2	2.15	0.78
2:D:303:LEU:HB3	2:D:307:ARG:NH1	1.98	0.78
2:D:303:LEU:CD2	2:D:307:ARG:NH1	2.43	0.78
2:D:303:LEU:HB3	2:D:307:ARG:HH12	1.48	0.78
1:A:26:LEU:O	1:A:31:ILE:HD11	1.82	0.77
3:F:19:DG:C6	3:F:20:DC:N3	2.53	0.77
1:A:21:VAL:CG1	1:A:59:PRO:HG3	2.14	0.77
1:C:49:LYS:HE2	1:C:142:ILE:HD12	1.64	0.77
1:C:287:LYS:HD3	1:C:291:GLU:CD	2.05	0.77
3:E:19:DG:C2'	3:E:20:DC:O5'	2.23	0.77
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.68	0.76
1:A:30:LYS:O	1:A:34:LEU:HD12	1.86	0.76
3:F:22:DC:H5''	3:F:22:DC:C6	2.19	0.75
1:C:33:ALA:CB	1:C:71:TRP:CD1	2.69	0.75
1:C:131:THR:CG2	1:C:143:ARG:HG2	2.16	0.75
2:B:402:TRP:HE1	6:B:2003:GOL:H11	1.50	0.74
3:E:19:DG:H5''	3:E:19:DG:H8	1.53	0.74
1:A:76:ASP:HA	3:E:0:A:C4'	2.18	0.73
1:C:135:ILE:HG22	1:C:136:ASN:N	2.03	0.72
1:C:59:PRO:CG	1:C:76:ASP:HB3	2.15	0.72
3:F:19:DG:H5''	3:F:19:DG:H8	1.54	0.72
1:A:443:ASP:OD1	1:A:444:GLY:N	2.23	0.71
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.72	0.71
1:A:26:LEU:CD2	1:A:31:ILE:HG12	2.20	0.71
1:C:135:ILE:CG2	1:C:136:ASN:N	2.53	0.71
2:D:303:LEU:CD2	2:D:307:ARG:HH12	2.00	0.71
1:C:265:ASN:ND2	3:F:6:C:HO2'	1.89	0.70
1:C:54:ASN:CA	1:C:143:ARG:HH22	2.04	0.70
3:E:22:DC:H5''	3:E:22:DC:C6	2.19	0.70
1:A:433:PRO:HG3	2:B:255:ASN:HD22	1.56	0.70
6:D:502:GOL:O1	4:H:2:FRU:H5	1.92	0.70
1:C:54:ASN:C	1:C:143:ARG:HH22	1.95	0.69
1:C:500:GLN:CD	1:C:500:GLN:H	1.94	0.69
1:A:26:LEU:HD11	1:A:30:LYS:HB2	1.74	0.69
1:A:26:LEU:HD23	1:A:31:ILE:CG1	2.21	0.69
1:C:33:ALA:HB1	1:C:71:TRP:CD1	2.28	0.68
1:C:286:THR:O	1:C:287:LYS:HG3	1.92	0.68
1:A:26:LEU:CG	1:A:31:ILE:HG13	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:CE	1:A:237:ASP:OD1	2.40	0.68
2:D:413:GLU:OE2	4:H:1:GLC:O4	2.12	0.68
1:A:34:LEU:HD12	1:A:34:LEU:N	2.08	0.67
1:C:58:THR:HG22	1:C:59:PRO:CD	2.23	0.67
3:F:19:DG:C3'	3:F:20:DC:C5'	2.71	0.67
2:D:24:TRP:CE3	6:D:502:GOL:H12	2.29	0.67
3:E:16:DU:C2'	3:E:17:DU:OP1	2.40	0.66
1:C:132:ILE:HG13	1:C:133:PRO:HD2	1.78	0.66
1:C:476:LYS:HE3	3:F:20:DC:OP1	1.95	0.66
1:C:59:PRO:HG2	1:C:76:ASP:CB	2.16	0.66
1:A:26:LEU:O	1:A:31:ILE:CD1	2.43	0.66
1:C:476:LYS:CE	3:F:20:DC:OP1	2.43	0.66
1:C:63:ILE:HD11	3:F:-1:U:P	2.36	0.66
1:A:21:VAL:HG12	1:A:59:PRO:HG3	1.77	0.65
1:C:152:GLY:HA2	3:F:1:C:O4'	1.97	0.65
1:C:135:ILE:HG21	1:C:138:GLU:HB2	1.78	0.65
1:C:54:ASN:HB3	1:C:143:ARG:CZ	2.26	0.65
1:C:91:GLN:OE1	1:C:161:GLN:NE2	2.29	0.65
1:C:91:GLN:NE2	1:C:93:GLY:O	2.29	0.65
2:D:303:LEU:CB	2:D:307:ARG:HH12	2.10	0.65
1:A:24:TRP:CD1	1:A:59:PRO:HB3	2.31	0.64
1:C:476:LYS:HE3	3:F:20:DC:P	2.36	0.64
2:D:115:TYR:CE2	2:D:185:ASP:OD1	2.51	0.64
3:F:16:DU:C2'	3:F:17:DU:OP1	2.40	0.64
1:A:473:THR:HG21	3:E:19:DG:H4'	1.80	0.64
2:B:402:TRP:NE1	6:B:2003:GOL:H11	2.13	0.63
1:C:476:LYS:HG3	3:F:20:DC:OP1	1.98	0.63
1:C:135:ILE:CG2	1:C:136:ASN:H	2.12	0.62
1:A:26:LEU:CD1	1:A:30:LYS:HB2	2.28	0.62
3:F:21:DA:H8	3:F:21:DA:O5'	1.83	0.62
2:D:115:TYR:HE2	2:D:185:ASP:OD1	1.80	0.62
2:D:303:LEU:CG	2:D:307:ARG:HH12	2.13	0.62
2:D:413:GLU:OE2	4:H:1:GLC:C4	2.48	0.62
1:C:476:LYS:CG	3:F:20:DC:OP1	2.48	0.62
1:A:286:THR:O	1:A:286:THR:HG22	2.00	0.62
2:B:402:TRP:NE1	6:B:2003:GOL:C3	2.50	0.62
2:D:82:LYS:NZ	4:H:1:GLC:O4	2.33	0.61
1:C:58:THR:CG2	1:C:59:PRO:CD	2.72	0.61
1:C:76:ASP:HA	3:F:0:A:C4'	2.17	0.61
1:A:26:LEU:HG	1:A:31:ILE:CG1	2.23	0.61
3:E:22:DC:C5'	3:E:22:DC:H6	2.10	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:CD2	1:A:31:ILE:CG1	2.79	0.60
1:C:91:GLN:HB2	1:C:161:GLN:NE2	2.13	0.60
1:C:252:TRP:CD1	1:C:295:LEU:CD2	2.85	0.60
1:C:33:ALA:HB2	1:C:71:TRP:CD1	2.36	0.60
1:C:157:PRO:HG2	3:F:2:C:O4'	2.01	0.60
1:C:54:ASN:CB	1:C:143:ARG:NH2	2.44	0.60
1:C:287:LYS:CD	1:C:291:GLU:OE2	2.45	0.59
1:C:60:VAL:HG12	1:C:61:PHE:H	1.67	0.59
1:C:60:VAL:HG12	1:C:61:PHE:N	2.17	0.59
3:E:15:C:O2	3:E:19:DG:N1	2.34	0.59
1:C:34:LEU:CD2	1:C:73:LYS:HG3	2.33	0.59
1:C:91:GLN:CB	1:C:161:GLN:HE22	2.13	0.59
1:C:34:LEU:HD11	1:C:62:ALA:HB2	1.83	0.59
2:D:24:TRP:CG	6:D:502:GOL:H31	2.38	0.58
1:C:78:ARG:NH2	3:F:-1:U:O2'	2.36	0.58
2:D:24:TRP:CD2	6:D:502:GOL:C3	2.86	0.58
1:A:433:PRO:CG	2:B:255:ASN:HD22	2.15	0.57
1:A:23:GLN:NE2	1:A:137:ASN:OD1	2.36	0.57
3:E:26:DA:H2'	3:E:27:DG:C8	2.39	0.57
3:F:26:DA:H2'	3:F:27:DG:C8	2.40	0.57
1:C:252:TRP:CD1	1:C:295:LEU:HD22	2.39	0.57
3:F:22:DC:C5'	3:F:22:DC:H6	2.10	0.56
3:E:19:DG:H5''	3:E:19:DG:C8	2.38	0.56
1:A:134:SER:OG	1:A:135:ILE:N	2.39	0.55
3:F:15:C:O2	3:F:19:DG:N1	2.34	0.55
3:F:12:G:O5'	3:F:12:G:H8	1.89	0.55
1:A:26:LEU:CG	1:A:31:ILE:CG1	2.84	0.55
2:B:402:TRP:HE1	6:B:2003:GOL:C1	2.16	0.55
3:F:18:DU:C4'	3:F:19:DG:O5'	2.37	0.55
1:A:21:VAL:HG11	1:A:59:PRO:CG	2.37	0.55
3:F:19:DG:C2'	3:F:20:DC:H5''	1.86	0.55
2:D:303:LEU:HD22	2:D:307:ARG:NH2	2.22	0.55
3:F:23:DC:H2''	3:F:24:DG:H5'	1.89	0.55
2:B:402:TRP:CD1	6:B:2003:GOL:H32	2.42	0.54
3:E:12:G:O5'	3:E:12:G:H8	1.90	0.54
1:C:132:ILE:HG23	1:C:132:ILE:O	2.07	0.54
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.41	0.54
3:E:11:G:C2	3:E:24:DG:C2	2.96	0.54
3:E:18:DU:H1'	3:E:19:DG:C5	2.43	0.54
3:F:11:G:C2	3:F:24:DG:C2	2.96	0.54
3:E:23:DC:H2''	3:E:24:DG:H5'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:CG2	2:B:283:LEU:HD13	2.35	0.53
3:F:19:DG:C3'	3:F:20:DC:H5'	2.19	0.53
1:A:34:LEU:HD12	1:A:34:LEU:H	1.73	0.53
2:B:399:GLU:HG2	6:B:2003:GOL:H12	1.90	0.53
2:D:413:GLU:OE2	4:H:1:GLC:H4	2.08	0.53
1:A:542:ILE:HD11	2:B:261:VAL:CG1	2.26	0.53
3:F:18:DU:H1'	3:F:19:DG:C5	2.43	0.53
3:F:19:DG:O6	3:F:20:DC:N4	2.41	0.53
1:A:21:VAL:HG11	1:A:59:PRO:HG3	1.91	0.53
3:E:3:C:O2'	3:E:4:C:H5'	2.09	0.53
2:B:64:LYS:H	6:B:2005:GOL:H12	1.75	0.52
3:F:19:DG:C8	3:F:19:DG:H5''	2.38	0.52
1:A:21:VAL:CG1	1:A:59:PRO:CG	2.86	0.51
2:D:151:GLN:HB3	2:D:185:ASP:OD2	2.10	0.51
1:C:138:GLU:O	1:C:139:THR:HG23	2.11	0.51
3:F:3:C:O2'	3:F:4:C:H5'	2.09	0.51
1:C:252:TRP:CD1	1:C:295:LEU:HD11	2.43	0.51
3:E:18:DU:C4'	3:E:19:DG:O5'	2.37	0.51
3:F:19:DG:C6	3:F:20:DC:N4	2.79	0.51
1:C:286:THR:O	1:C:287:LYS:CG	2.59	0.51
1:A:26:LEU:HD21	1:A:31:ILE:HA	1.93	0.51
1:A:202:ILE:O	1:A:206:ARG:HB2	2.11	0.51
1:C:252:TRP:NE1	1:C:295:LEU:CD2	2.73	0.50
1:C:252:TRP:NE1	1:C:295:LEU:HD22	2.26	0.50
1:C:254:VAL:HG22	1:C:293:ILE:HD13	1.94	0.50
1:A:26:LEU:CD1	1:A:30:LYS:CB	2.84	0.50
2:D:24:TRP:CE3	6:D:502:GOL:H31	2.47	0.50
3:E:0:A:OP1	3:E:1:C:OP2	2.30	0.49
3:F:8:U:H2'	3:F:9:U:C6	2.47	0.49
3:F:0:A:OP1	3:F:1:C:OP2	2.30	0.49
3:F:19:DG:N7	3:F:20:DC:C5	2.80	0.49
1:A:51:GLY:H	1:A:52:PRO:CD	2.25	0.49
1:A:154:LYS:HA	3:E:1:C:O2'	2.13	0.49
3:E:8:U:H2'	3:E:9:U:C6	2.47	0.49
3:F:7:C:N4	3:F:26:DA:N6	2.61	0.49
3:E:21:DA:H2'	3:E:22:DC:C6	2.48	0.49
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.28	0.48
1:C:54:ASN:C	1:C:143:ARG:NH2	2.61	0.48
3:E:23:DC:H2'	3:E:24:DG:C8	2.48	0.48
1:C:132:ILE:CG1	1:C:133:PRO:HD2	2.43	0.48
3:E:7:C:N4	3:E:26:DA:N6	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:HG22	1:C:64:LYS:N	2.29	0.47
1:C:266:TRP:CE2	3:F:31:DG:H4'	2.49	0.47
3:F:23:DC:H2'	3:F:24:DG:C8	2.49	0.47
2:D:303:LEU:CB	2:D:307:ARG:NH1	2.72	0.47
1:C:49:LYS:CE	1:C:142:ILE:HD12	2.40	0.47
3:E:17:DU:H1'	3:E:18:DU:H5	1.96	0.47
3:E:7:C:H2'	3:E:8:U:C6	2.49	0.47
3:F:17:DU:H1'	3:F:18:DU:H5	1.96	0.47
3:F:7:C:H2'	3:F:8:U:C6	2.49	0.47
1:A:503:LEU:HD11	1:A:533:LEU:HB3	1.97	0.47
3:F:19:DG:C5'	3:F:19:DG:C8	2.99	0.46
1:C:135:ILE:HG23	1:C:136:ASN:H	1.79	0.46
1:C:33:ALA:CB	1:C:71:TRP:CG	2.98	0.46
2:B:30:LYS:HZ1	6:B:2005:GOL:H31	1.80	0.46
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.97	0.46
3:F:19:DG:N7	3:F:20:DC:C4	2.83	0.46
3:E:19:DG:C5'	3:E:19:DG:C8	2.98	0.46
3:F:11:G:H2'	3:F:12:G:C8	2.50	0.46
1:A:34:LEU:CD1	1:A:34:LEU:N	2.79	0.45
3:E:11:G:H2'	3:E:12:G:C8	2.51	0.45
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.29	0.45
3:F:18:DU:H2''	3:F:18:DU:O2	2.16	0.45
1:C:500:GLN:H	1:C:500:GLN:NE2	2.14	0.45
1:C:542:ILE:O	1:C:542:ILE:HG22	2.16	0.45
2:D:194:GLU:OE1	2:D:196:GLY:N	2.48	0.45
3:F:18:DU:H1'	3:F:19:DG:N7	2.31	0.45
1:A:34:LEU:O	1:A:37:ILE:N	2.49	0.45
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.99	0.44
1:A:407:GLN:NE2	2:B:417:VAL:O	2.50	0.44
3:E:18:DU:H1'	3:E:19:DG:N7	2.31	0.44
3:F:19:DG:C5'	3:F:19:DG:H8	2.27	0.44
1:C:24:TRP:HE3	1:C:25:PRO:HD2	1.82	0.44
3:F:19:DG:C5	3:F:20:DC:N3	2.82	0.44
3:F:19:DG:C1'	3:F:20:DC:H5''	2.45	0.44
1:C:37:ILE:HG22	1:C:41:MET:HG3	1.99	0.44
1:A:543:GLY:N	2:B:283:LEU:O	2.51	0.44
3:E:18:DU:H2''	3:E:18:DU:O2	2.16	0.44
2:D:237:ASP:OD1	2:D:238:LYS:HG2	2.18	0.43
3:E:7:C:H42	3:E:26:DA:N6	2.17	0.43
2:D:413:GLU:HG3	4:H:1:GLC:O6	2.19	0.43
1:C:254:VAL:HG23	1:C:291:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:CG2	1:C:64:LYS:N	2.82	0.42
1:A:78:ARG:HG3	3:E:0:A:O3'	2.19	0.42
2:D:356:ARG:O	2:D:358:ARG:N	2.53	0.42
3:F:12:G:O5'	3:F:12:G:C8	2.72	0.42
2:B:266:TRP:CZ3	2:B:425:LEU:HD21	2.54	0.42
2:B:194:GLU:OE1	2:B:196:GLY:N	2.52	0.42
3:F:7:C:H42	3:F:26:DA:N6	2.17	0.42
2:D:178:ILE:HG12	2:D:191:SER:HB3	2.02	0.42
1:A:475:GLN:NE2	3:E:16:DU:O2	2.52	0.42
1:A:194:GLU:OE1	1:A:196:GLY:N	2.52	0.41
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.01	0.41
3:E:22:DC:C5'	3:E:22:DC:C6	2.94	0.41
1:C:252:TRP:HE1	1:C:295:LEU:HD22	1.85	0.41
3:E:14:G:O5'	3:E:14:G:H8	2.03	0.41
1:A:91:GLN:NE2	1:A:183:TYR:CE1	2.89	0.41
1:C:286:THR:OG1	3:F:9:U:H4'	2.20	0.41
3:F:14:G:H8	3:F:14:G:O5'	2.03	0.41
1:A:51:GLY:N	1:A:52:PRO:CD	2.84	0.41
1:C:132:ILE:O	1:C:132:ILE:CG2	2.68	0.40
3:E:16:DU:C2'	3:E:16:DU:O2	2.70	0.40
3:F:16:DU:O2	3:F:16:DU:C2'	2.70	0.40
3:F:18:DU:C2'	3:F:18:DU:O2	2.69	0.40
3:F:19:DG:C1'	3:F:20:DC:C5'	2.84	0.40
1:C:498:ASN:ND2	1:C:545:ASN:OD1	2.34	0.40
3:F:19:DG:C5	3:F:20:DC:C5	3.07	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:NH1	1:C:3:SER:OG[2_455]	1.25	0.95

## 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	552/557 (99%)	527 (96%)	23 (4%)	2 (0%)	34	64
1	C	551/557 (99%)	533 (97%)	18 (3%)	0	100	100
2	B	412/444 (93%)	403 (98%)	9 (2%)	0	100	100
2	D	406/444 (91%)	397 (98%)	9 (2%)	0	100	100
All	All	1921/2002 (96%)	1860 (97%)	59 (3%)	2 (0%)	51	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	SER
1	A	543	GLY

### 5.3.2 Protein sidechains ⓘ

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	495/497 (100%)	493 (100%)	2 (0%)	91	97
1	C	495/497 (100%)	493 (100%)	2 (0%)	91	97
2	B	377/403 (94%)	376 (100%)	1 (0%)	92	97
2	D	372/403 (92%)	371 (100%)	1 (0%)	92	97
All	All	1739/1800 (97%)	1733 (100%)	6 (0%)	92	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	182	GLN
2	B	169	GLU
1	C	221	HIS
1	C	500	GLN
2	D	266	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
2	B	255	ASN
1	C	161	GLN
1	C	265	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

4 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	GLC	G	1	4	11,11,12	1.08	1 (9%)	15,15,17	2.16	5 (33%)
4	FRU	G	2	4	11,12,12	0.58	0	10,18,18	0.94	0
4	GLC	H	1	4	11,11,12	0.70	0	15,15,17	1.25	2 (13%)
4	FRU	H	2	4	11,12,12	0.64	0	10,18,18	1.83	3 (30%)

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	GLC	G	1	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FRU	G	2	4	-	1/5/24/24	0/1/1/1
4	GLC	H	1	4	-	0/2/19/22	0/1/1/1
4	FRU	H	2	4	-	2/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	GLC	C2-C3	-2.19	1.49	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	C2-C3-C4	-5.04	102.17	110.89
4	G	1	GLC	C1-O5-C5	4.18	117.86	112.19
4	H	2	FRU	O1-C1-C2	-3.35	104.73	111.86
4	G	1	GLC	C3-C4-C5	-3.18	104.57	110.24
4	H	2	FRU	O4-C4-C3	-2.80	103.78	112.15
4	H	1	GLC	C1-C2-C3	-2.55	106.53	109.67
4	H	2	FRU	O3-C3-C4	-2.49	104.71	113.32
4	H	1	GLC	O6-C6-C5	-2.33	103.28	111.29
4	G	1	GLC	C1-C2-C3	-2.30	106.84	109.67
4	G	1	GLC	C6-C5-C4	-2.18	107.90	113.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	FRU	C4-C5-C6-O6
4	H	2	FRU	O5-C5-C6-O6
4	G	2	FRU	O1-C1-C2-C3

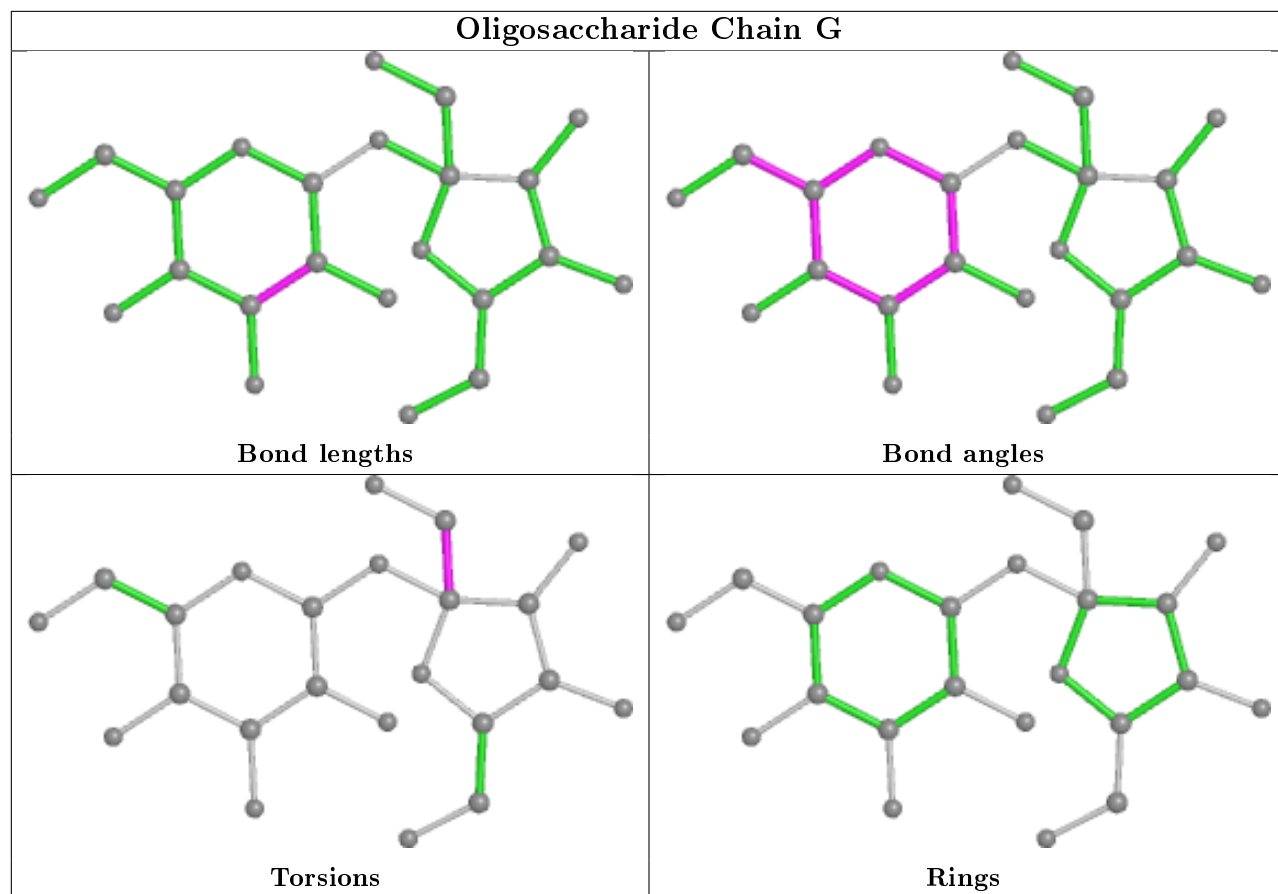
There are no ring outliers.

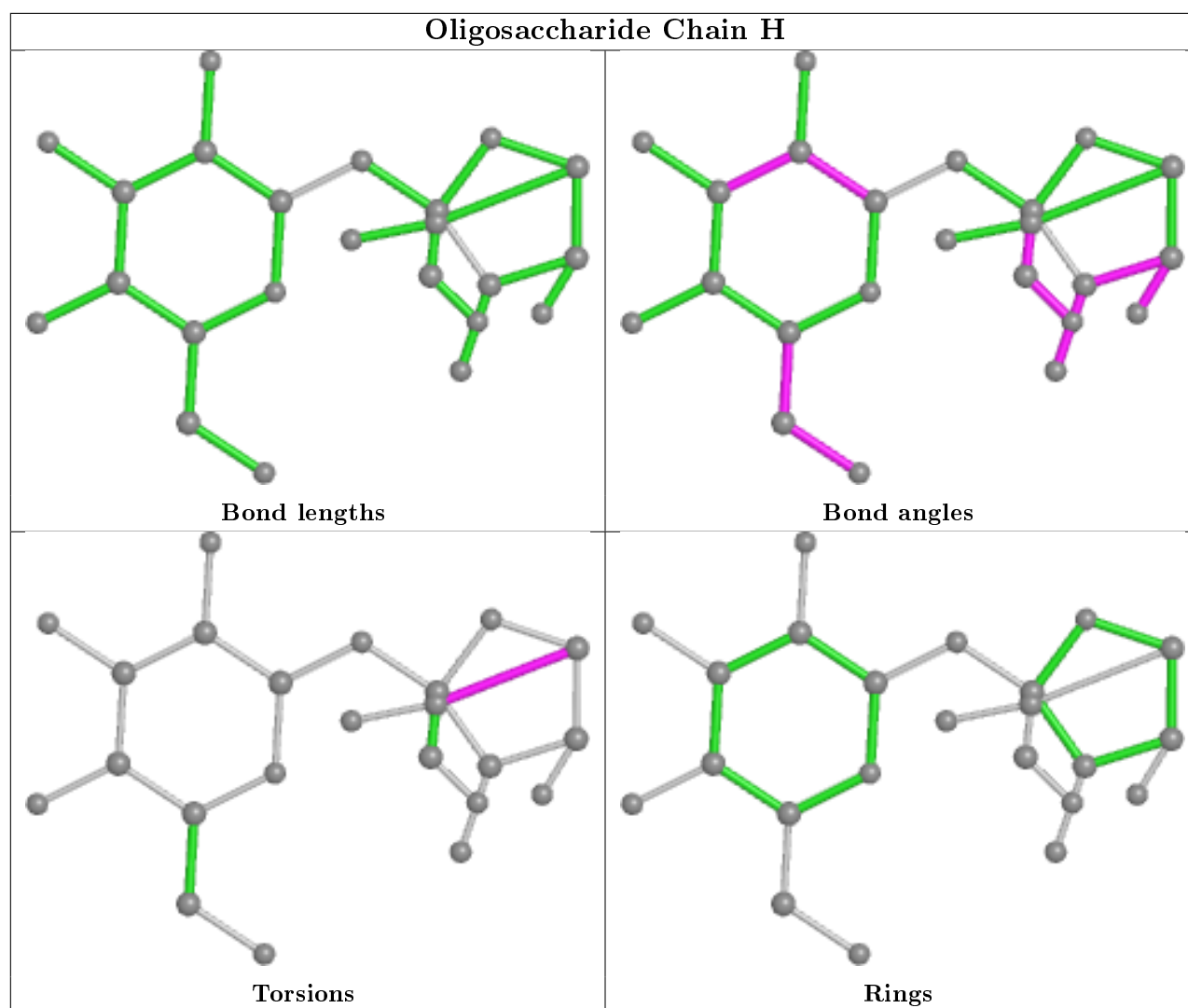
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	GLC	5	0
4	H	2	FRU	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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	GOL	B	2003	-	5,5,5	0.27	0	5,5,5	0.65	0
6	GOL	B	2004	-	5,5,5	0.38	0	5,5,5	0.24	0
6	GOL	C	602	-	5,5,5	0.17	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	B	2005	-	5,5,5	0.11	0	5,5,5	0.68	0
6	GOL	D	502	-	5,5,5	0.23	0	5,5,5	0.26	0
6	GOL	B	2002	-	5,5,5	0.30	0	5,5,5	0.72	0
7	SO4	C	601	-	4,4,4	0.26	0	6,6,6	0.18	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
6	GOL	B	2003	-	-	2/4/4/4	-
6	GOL	B	2004	-	-	0/4/4/4	-
6	GOL	C	602	-	-	0/4/4/4	-
6	GOL	B	2005	-	-	0/4/4/4	-
6	GOL	D	502	-	-	2/4/4/4	-
6	GOL	B	2002	-	-	1/4/4/4	-

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
6	B	2003	GOL	C1-C2-C3-O3
6	D	502	GOL	O1-C1-C2-C3
6	D	502	GOL	O1-C1-C2-O2
6	B	2002	GOL	O1-C1-C2-C3
6	B	2003	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2003	GOL	9	0
6	B	2005	GOL	2	0
6	D	502	GOL	6	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	554/557 (99%)	0.65	72 (12%) <span>3</span> <span>2</span>	46, 96, 199, 268	0
1	C	553/557 (99%)	1.26	140 (25%) <span>0</span> <span>0</span>	41, 133, 228, 281	0
2	B	416/444 (93%)	0.21	20 (4%) <span>30</span> <span>21</span>	41, 78, 149, 224	0
2	D	410/444 (92%)	0.39	37 (9%) <span>9</span> <span>5</span>	43, 101, 184, 262	0
3	E	32/38 (84%)	0.28	0 <span>100</span> <span>100</span>	110, 159, 204, 220	0
3	F	32/38 (84%)	2.07	17 (53%) <span>0</span> <span>0</span>	205, 240, 283, 298	0
All	All	1997/2078 (96%)	0.69	286 (14%) <span>2</span> <span>1</span>	41, 99, 217, 298	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	ALA	15.8
1	A	67	ASP	14.0
1	C	26	LEU	11.9
1	C	290	THR	10.3
1	C	61	PHE	10.3
1	C	34	LEU	9.6
1	A	63	ILE	9.4
1	C	252	TRP	9.1
1	C	254	VAL	8.9
1	C	37	ILE	8.8
1	A	26	LEU	8.6
1	A	61	PHE	8.5
1	C	62	ALA	8.5
1	C	133	PRO	8.0
1	C	142	ILE	7.9
1	A	133	PRO	7.9
1	A	24	TRP	7.7
1	C	136	ASN	7.7
1	C	59	PRO	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	132	ILE	7.4
1	A	64	LYS	7.3
1	C	21	VAL	7.2
1	C	288	ALA	7.1
1	A	33	ALA	7.1
1	C	282	LEU	7.0
1	C	48	SER	6.9
1	C	60	VAL	6.8
1	A	72	ARG	6.7
1	A	27	THR	6.7
1	C	25	PRO	6.5
1	C	205	LEU	6.5
1	A	73	LYS	6.4
2	D	360	ALA	6.4
1	C	23	GLN	6.4
1	C	38	CYS	6.4
1	C	66	LYS	6.3
1	C	138	GLU	6.2
1	A	134	SER	6.1
1	C	63	ILE	6.1
1	C	245	VAL	6.0
1	C	144	TYR	5.9
1	C	49	LYS	5.9
1	A	66	LYS	5.8
2	B	216	THR	5.7
2	D	90	VAL	5.7
1	C	146	TYR	5.6
1	C	71	TRP	5.5
1	C	74	LEU	5.5
1	C	247	PRO	5.5
2	D	228	LEU	5.4
1	C	132	ILE	5.3
1	A	289	LEU	5.3
1	C	292	VAL	5.3
1	C	30	LYS	5.3
1	C	73	LYS	5.2
1	A	295	LEU	5.2
1	C	12	LEU	5.2
2	B	214	LEU	5.2
1	C	313	PRO	5.2
1	C	50	ILE	5.2
1	C	302	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	24	TRP	5.1
1	A	28	GLU	5.0
1	C	67	ASP	5.0
1	C	76	ASP	4.9
2	D	202	ILE	4.9
1	A	287	LYS	4.9
1	C	255	ASN	4.9
2	D	87	PHE	4.9
1	C	75	VAL	4.8
1	C	131	THR	4.8
1	C	250	ASP	4.8
1	C	19	PRO	4.7
1	C	124	PHE	4.7
1	C	22	LYS	4.7
1	C	137	ASN	4.6
1	A	290	THR	4.5
1	C	135	ILE	4.5
1	C	253	THR	4.5
1	A	30	LYS	4.5
1	A	252	TRP	4.5
1	C	246	LEU	4.5
1	C	283	LEU	4.5
2	D	232	TYR	4.5
1	C	140	PRO	4.4
1	C	229	TRP	4.4
1	C	295	LEU	4.4
1	C	31	ILE	4.4
1	A	288	ALA	4.4
1	C	77	PHE	4.3
1	A	25	PRO	4.3
2	B	226	PRO	4.3
1	A	283	LEU	4.3
1	C	284	ARG	4.3
1	C	311	LYS	4.3
1	A	34	LEU	4.2
1	A	29	GLU	4.2
1	C	312	GLU	4.2
1	A	49	LYS	4.2
2	D	209	LEU	4.2
1	A	286	THR	4.2
1	A	135	ILE	4.2
1	C	257	ILE	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	17	ASP	4.2
1	C	228	LEU	4.1
1	C	56	TYR	4.1
2	D	89	GLU	4.1
1	A	249	LYS	4.1
1	C	294	PRO	4.1
1	C	39	THR	4.1
1	A	136	ASN	4.0
1	A	71	TRP	4.0
2	D	85	GLN	4.0
1	C	293	ILE	3.9
1	C	54	ASN	3.9
1	C	72	ARG	3.9
2	D	168	LEU	3.8
1	C	301	LEU	3.8
2	B	215	THR	3.8
1	C	58	THR	3.7
1	C	309	ILE	3.7
1	C	193	LEU	3.7
2	B	428	GLN	3.7
1	A	247	PRO	3.7
3	F	0	A	3.7
1	C	134	SER	3.7
2	D	358	ARG	3.6
3	F	15	C	3.6
1	A	68	SER	3.6
1	C	177	ASP	3.6
1	A	282	LEU	3.6
1	A	140	PRO	3.6
3	F	10	C	3.6
1	C	29	GLU	3.6
2	D	226	PRO	3.6
1	A	142	ILE	3.5
1	C	143	ARG	3.5
2	D	211	ARG	3.5
1	C	151	GLN	3.5
2	D	212	TRP	3.5
1	A	277	ARG	3.5
2	D	361	HIS	3.5
1	C	52	PRO	3.5
1	C	303	LEU	3.4
2	D	427	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	310	LEU	3.4
1	C	83	ARG	3.4
1	C	145	GLN	3.4
1	C	82	LYS	3.4
3	F	5	C	3.3
1	C	41	MET	3.3
1	C	248	GLU	3.3
3	F	19	DG	3.3
1	C	15	GLY	3.3
1	A	60	VAL	3.3
1	C	298	GLU	3.3
2	B	230	MET	3.3
2	D	205	LEU	3.3
1	C	306	ASN	3.2
1	A	294	PRO	3.2
1	C	274	ILE	3.2
1	C	36	GLU	3.2
1	A	131	THR	3.1
3	F	29	DG	3.1
1	A	31	ILE	3.1
1	A	124	PHE	3.1
1	C	251	SER	3.0
2	D	230	MET	3.0
1	C	32	LYS	3.0
1	C	209	LEU	3.0
1	A	144	TYR	3.0
1	C	314	VAL	3.0
1	C	27	THR	3.0
1	A	38	CYS	3.0
2	D	92	LEU	3.0
1	C	261	VAL	3.0
2	D	67	ASP	2.9
1	C	286	THR	2.9
1	A	70	LYS	2.9
1	A	137	ASN	2.9
1	A	177	ASP	2.9
1	A	303	LEU	2.9
2	B	4	PRO	2.9
1	A	141	GLY	2.9
2	B	295	LEU	2.9
3	F	25	DA	2.9
3	F	23	DC	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	276	VAL	2.8
3	F	21	DA	2.8
1	C	33	ALA	2.8
1	A	139	THR	2.8
2	D	357	MET	2.8
1	A	253	THR	2.8
1	C	256	ASP	2.8
1	C	227	PHE	2.8
1	C	275	LYS	2.8
1	C	279	LEU	2.8
2	D	88	TRP	2.8
1	A	248	GLU	2.8
1	C	68	SER	2.8
1	A	126	LYS	2.7
1	C	291	GLU	2.7
3	F	4	C	2.7
1	A	74	LEU	2.7
2	B	301	LEU	2.7
1	C	16	MET	2.7
1	C	357	MET	2.7
2	D	124	PHE	2.6
1	C	65	LYS	2.6
1	A	146	TYR	2.6
1	C	18	GLY	2.6
1	C	202	ILE	2.6
1	C	55	PRO	2.6
1	A	59	PRO	2.6
1	C	289	LEU	2.6
2	D	25	PRO	2.6
2	D	231	GLY	2.5
1	C	287	LYS	2.5
2	D	206	ARG	2.5
1	A	193	LEU	2.5
1	C	139	THR	2.5
1	A	291	GLU	2.5
1	A	292	VAL	2.5
1	C	249	LYS	2.5
2	B	90	VAL	2.5
1	C	20	LYS	2.5
2	D	359	GLY	2.5
1	C	127	TYR	2.5
2	D	422	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	278	GLN	2.5
2	B	167	ILE	2.5
2	B	178	ILE	2.5
1	A	48	SER	2.4
1	C	35	VAL	2.4
2	D	318	TYR	2.4
1	C	241	VAL	2.4
1	C	79	GLU	2.4
1	C	47	ILE	2.4
1	C	206	ARG	2.4
2	B	296	THR	2.3
1	C	223	LYS	2.3
3	F	9	U	2.3
1	A	355	ALA	2.3
2	B	299	ALA	2.3
1	A	296	THR	2.3
3	F	12	G	2.3
1	C	11	LYS	2.3
3	F	14	G	2.3
3	F	30	DG	2.3
2	B	87	PHE	2.3
1	C	238	LYS	2.3
2	D	140	PRO	2.3
2	B	170	PRO	2.3
2	B	92	LEU	2.3
3	F	11	G	2.3
1	C	296	THR	2.2
1	A	2	ILE	2.2
1	C	214	LEU	2.2
1	A	448	ARG	2.2
1	C	57	ASN	2.2
1	C	266	TRP	2.2
1	C	130	PHE	2.2
2	D	204	GLU	2.2
2	B	168	LEU	2.2
1	A	36	GLU	2.1
2	B	209	LEU	2.1
1	A	65	LYS	2.1
1	C	195	ILE	2.1
1	C	118	VAL	2.1
1	A	50	ILE	2.1
2	D	66	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	166	LYS	2.1
2	D	173	LYS	2.1
1	A	301	LEU	2.1
1	C	104	LYS	2.1
1	C	305	GLU	2.1
1	C	46	LYS	2.1
3	F	13	U	2.1
1	C	308	GLU	2.0
2	D	10	VAL	2.0
2	D	96	HIS	2.0
2	B	212	TRP	2.0
2	D	229	TRP	2.0
1	A	47	ILE	2.0
3	F	-1	U	2.0
1	C	128	THR	2.0

## 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](#)

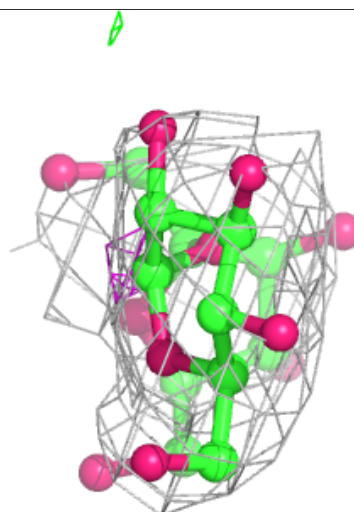
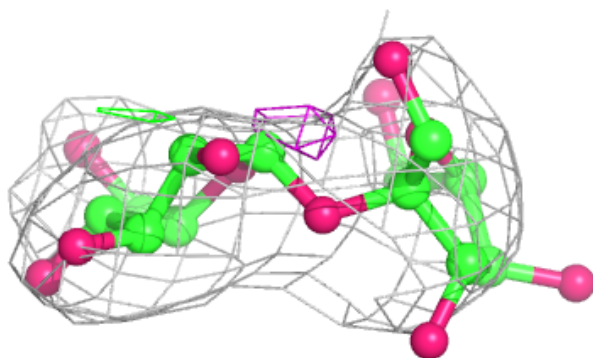
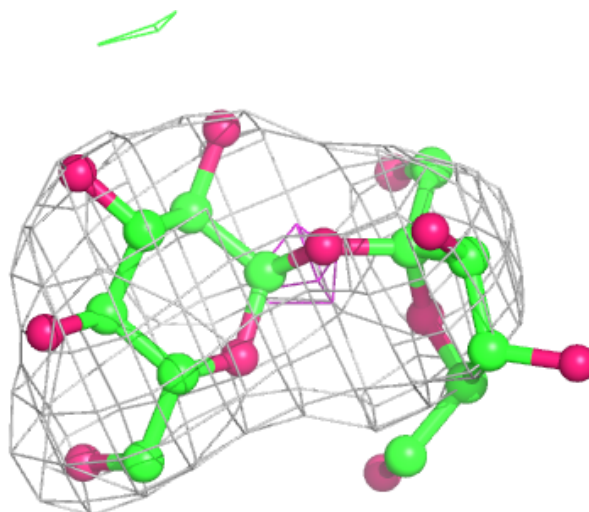
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

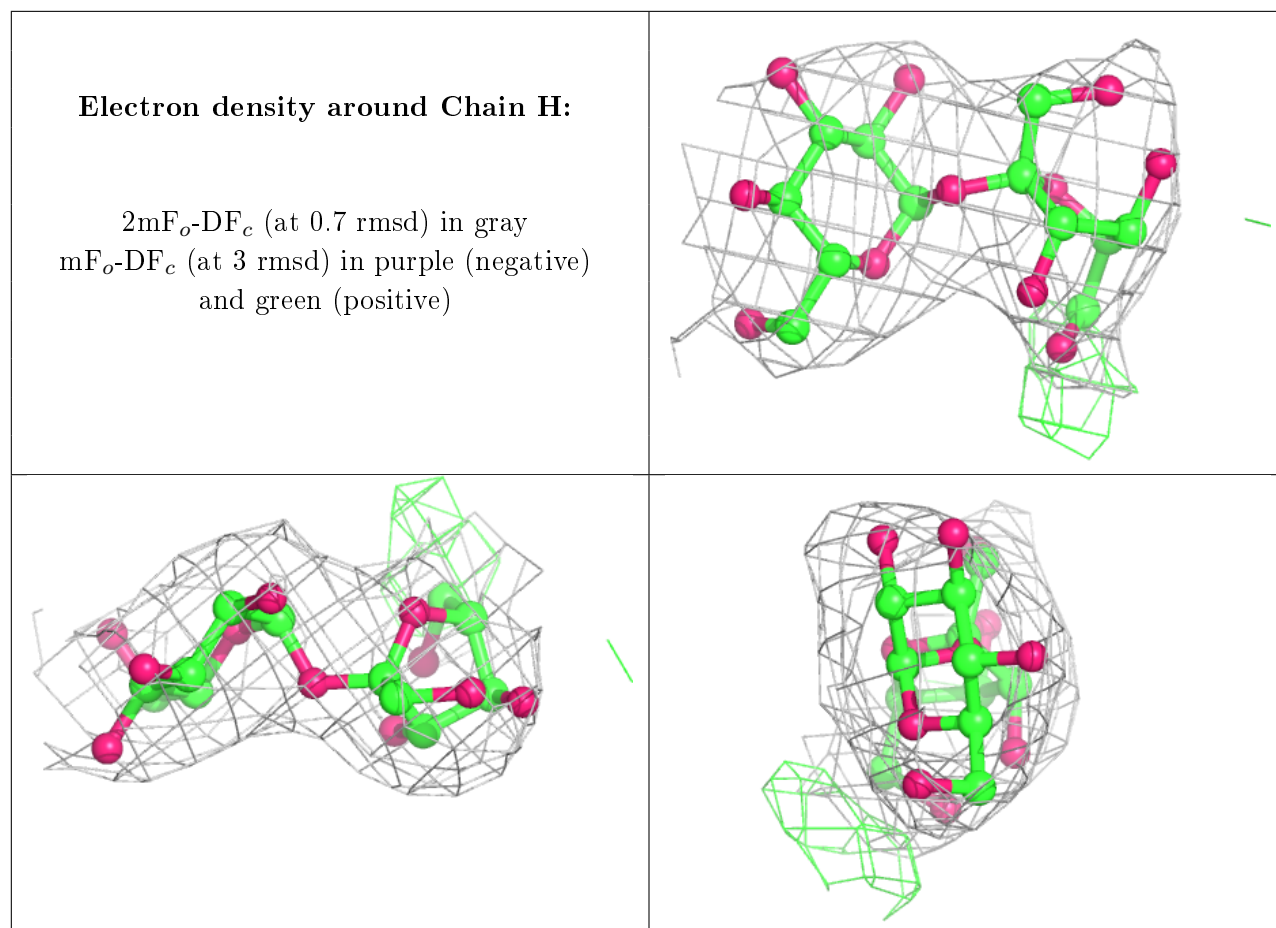
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FRU	G	2	12/12	0.84	0.26	151,163,168,169	0
4	GLC	H	1	11/12	0.88	0.19	113,116,124,125	0
4	FRU	H	2	12/12	0.89	0.22	136,147,152,152	0
4	GLC	G	1	11/12	0.94	0.25	87,116,134,142	0

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 G:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	SO4	C	601	5/5	0.10	0.43	207,208,210,212	0
6	GOL	D	502	6/6	0.66	0.47	92,102,107,109	0
6	GOL	C	602	6/6	0.77	0.57	98,108,110,113	0
6	GOL	B	2005	6/6	0.81	0.33	88,92,94,96	0
6	GOL	B	2004	6/6	0.83	0.31	77,81,86,87	0
6	GOL	B	2003	6/6	0.88	0.28	69,72,75,80	0
6	GOL	B	2002	6/6	0.89	0.20	68,73,79,80	0
5	MG	A	601	1/1	0.95	0.27	81,81,81,81	0
5	MG	C	603	1/1	0.95	0.38	77,77,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.