



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:39 PM BST

PDB ID : 5W75  
Title : Crystal Structure of Reconstructed Bacterial Elongation Factor Node 168  
Authors : Ortlund, E.A.  
Deposited on : 2017-06-19  
Resolution : 2.30 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  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

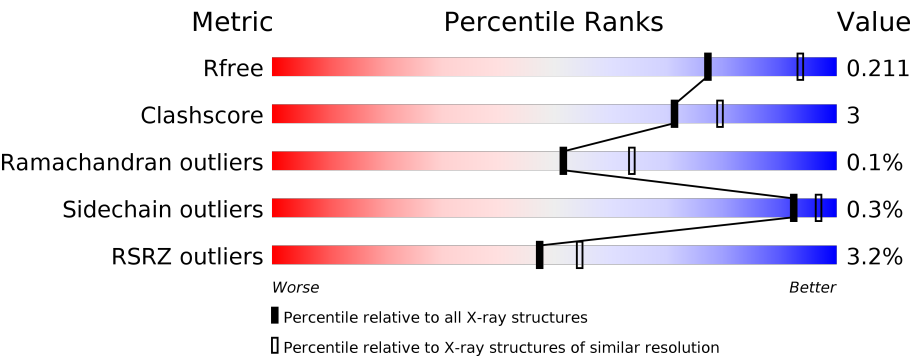
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.



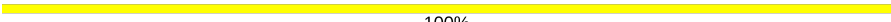
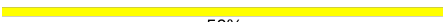

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	392	<div><div>3%</div><div><div></div><div>91%</div><div>7%</div><div></div></div><div></div></div>
1	B	392	<div><div>4%</div><div><div></div><div>91%</div><div>7%</div><div></div></div><div></div></div>
1	C	392	<div><div>3%</div><div><div></div><div>90%</div><div>8%</div><div></div></div><div></div></div>
1	D	392	<div><div>3%</div><div><div></div><div>91%</div><div>8%</div><div></div></div><div></div></div>
2	E	2	<div><div></div><div><div></div><div>100%</div><div></div></div><div></div></div>
2	F	2	<div><div></div><div><div></div><div>100%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 50%  50%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13025 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 Elongation factor Tu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3004	1906	512	572	14			
1	B	385	Total	C	N	O	S	0	0	0
			3010	1909	513	574	14			
1	C	387	Total	C	N	O	S	0	0	0
			3023	1916	516	577	14			
1	D	387	Total	C	N	O	S	0	0	0
			3023	1916	516	577	14			

There are 24 discrepancies between the modelled and reference sequences:

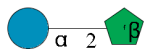
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	VAL	ILE	conflict	UNP B9K884
A	127	GLY	GLU	conflict	UNP B9K884
A	324	PHE	THR	conflict	UNP B9K884
A	336	THR	ALA	conflict	UNP B9K884
A	?	-	GLY	deletion	UNP B9K884
A	395	LEU	-	expression tag	UNP B9K884
B	21	VAL	ILE	conflict	UNP B9K884
B	127	GLY	GLU	conflict	UNP B9K884
B	324	PHE	THR	conflict	UNP B9K884
B	336	THR	ALA	conflict	UNP B9K884
B	?	-	GLY	deletion	UNP B9K884
B	395	LEU	-	expression tag	UNP B9K884
C	21	VAL	ILE	conflict	UNP B9K884
C	127	GLY	GLU	conflict	UNP B9K884
C	324	PHE	THR	conflict	UNP B9K884
C	336	THR	ALA	conflict	UNP B9K884
C	?	-	GLY	deletion	UNP B9K884
C	395	LEU	-	expression tag	UNP B9K884
D	21	VAL	ILE	conflict	UNP B9K884
D	127	GLY	GLU	conflict	UNP B9K884
D	324	PHE	THR	conflict	UNP B9K884

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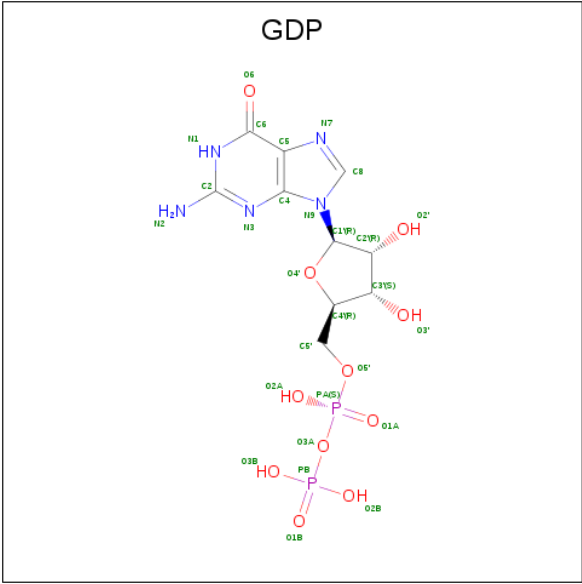
Chain	Residue	Modelled	Actual	Comment	Reference
D	336	THR	ALA	conflict	UNP B9K884
D	?	-	GLY	deletion	UNP B9K884
D	395	LEU	-	expression tag	UNP B9K884

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



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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O P	0	0
			28	10	5	11 2		

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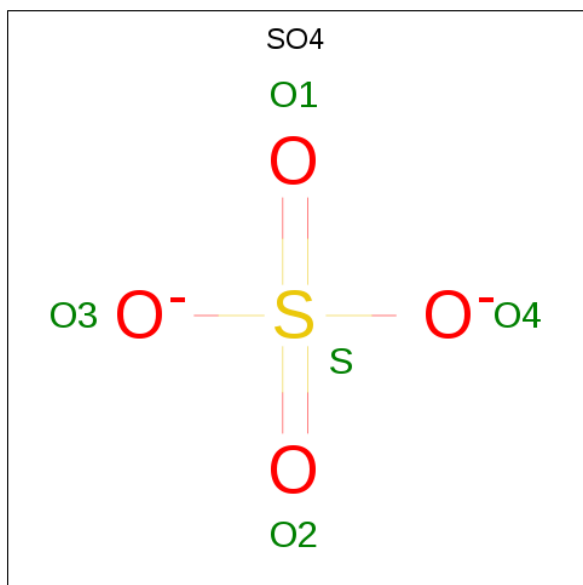
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

- Molecule 6 is water.

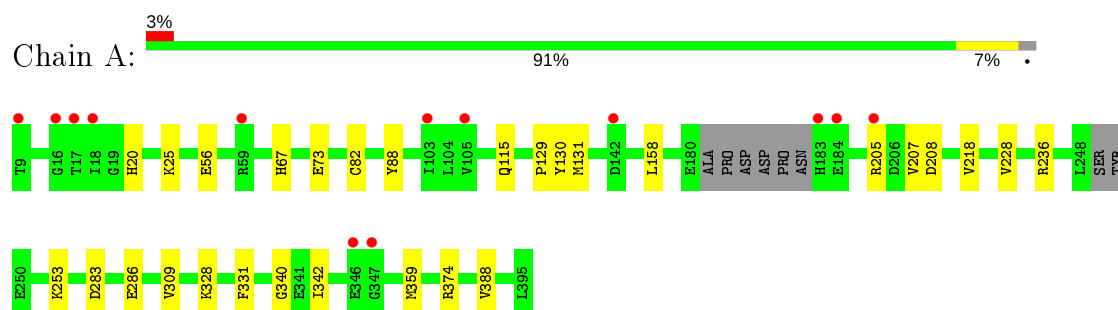
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	165	Total 165	O 165	0	0
6	B	164	Total 164	O 164	0	0
6	C	134	Total 134	O 134	0	0
6	D	189	Total 189	O 189	0	0



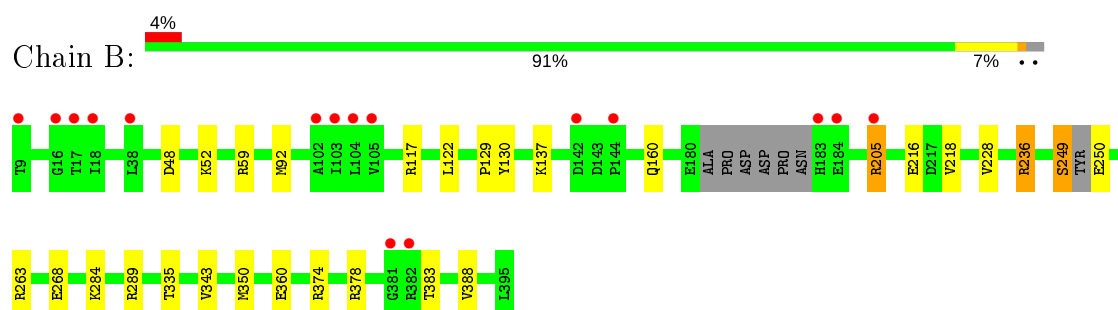
### 3 Residue-property plots [i](#)

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.

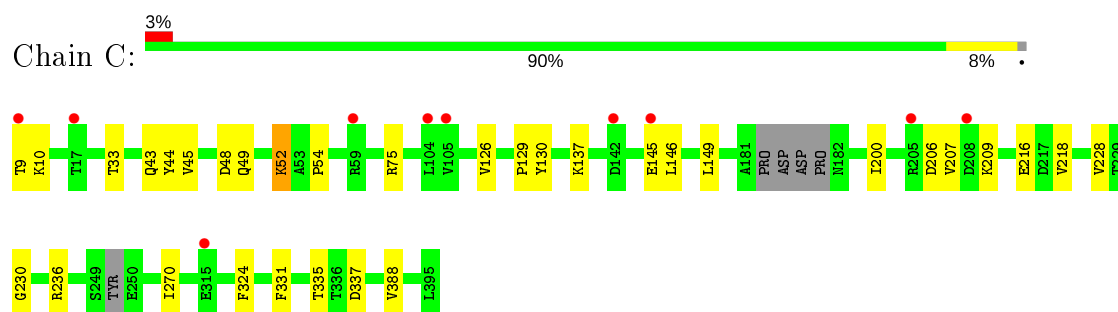
#### • Molecule 1: Elongation factor Tu



#### • Molecule 1: Elongation factor Tu

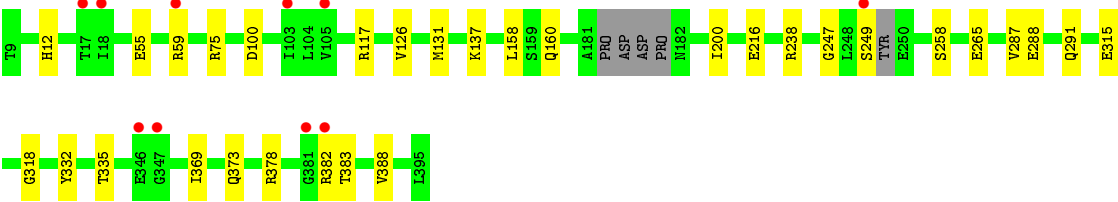


#### • Molecule 1: Elongation factor Tu



#### • Molecule 1: Elongation factor Tu





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

Chain E: 100%



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

Chain F: 100%



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

Chain G: 100%



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

Chain H: 50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.42Å 173.42Å 208.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 2.30 29.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.70-2.30) 90.5 (29.71-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.29 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.194 , 0.220 0.193 , 0.211	Depositor DCC
$R_{free}$ test set	2000 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: GDP, 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	0/3060	0.47	0/4141
1	B	0.26	0/3067	0.46	0/4152
1	C	0.28	0/3081	0.48	0/4173
1	D	0.26	0/3081	0.47	0/4173
All	All	0.27	0/12289	0.47	0/16639

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	3004	0	3022	16	0
1	B	3010	0	3028	20	0
1	C	3023	0	3040	32	0
1	D	3023	0	3040	20	0
2	E	23	0	21	0	0
2	F	23	0	20	0	0
2	G	23	0	21	0	0
2	H	23	0	19	1	0
3	A	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	12	1	0
3	C	28	0	12	1	0
3	D	28	0	11	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	10	0	0	0	0
5	B	30	0	0	0	0
5	C	30	0	0	0	0
5	D	35	0	0	0	0
6	A	165	0	0	0	2
6	B	164	0	0	1	0
6	C	134	0	0	3	2
6	D	189	0	0	4	0
All	All	13025	0	12258	86	2

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 3.

All (86) 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:B:236:ARG:NH1	1:B:268:GLU:OE2	2.03	0.91
1:C:33:THR:HG21	1:C:45:VAL:H	1.37	0.90
1:C:207:VAL:O	1:C:236:ARG:NH1	2.05	0.89
1:D:59:ARG:NH2	6:D:501:HOH:O	2.04	0.87
1:D:318:GLY:O	1:D:382:ARG:NH1	2.15	0.80
1:C:33:THR:CG2	1:C:45:VAL:H	1.98	0.75
1:C:49:GLN:O	6:C:501:HOH:O	2.04	0.75
1:D:131:MET:HE2	1:D:158:LEU:HD21	1.72	0.71
1:C:9:THR:HG22	1:C:10:LYS:H	1.55	0.70
1:C:207:VAL:HB	1:C:236:ARG:NH1	2.07	0.70
1:D:287:VAL:HA	1:D:291:GLN:HE22	1.60	0.65
1:D:126:VAL:HG12	1:D:388:VAL:HG11	1.79	0.64
1:C:145:GLU:O	1:C:149:LEU:CD2	2.45	0.64
1:C:216:GLU:HG3	1:C:230:GLY:HA2	1.80	0.63
1:B:48:ASP:O	1:B:52:LYS:HG2	2.01	0.60
1:D:315:GLU:OE1	6:D:502:HOH:O	2.17	0.60
1:A:331:PHE:HZ	1:A:342:ILE:HD11	1.67	0.60
1:D:238:ARG:NH1	6:D:503:HOH:O	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:LYS:HE3	1:D:55:GLU:O	2.03	0.57
1:C:48:ASP:O	1:C:52:LYS:HG3	2.05	0.57
1:A:374:ARG:HG2	1:A:388:VAL:HG22	1.87	0.56
1:C:145:GLU:O	1:C:149:LEU:HD22	2.06	0.55
1:C:126:VAL:HG12	1:C:388:VAL:HG11	1.89	0.54
1:C:145:GLU:O	1:C:149:LEU:HD23	2.07	0.54
1:C:206:ASP:HA	1:C:209:LYS:HD2	1.89	0.54
1:B:216:GLU:HG3	1:B:335:THR:HG21	1.91	0.53
1:C:33:THR:CG2	1:C:44:TYR:HA	2.39	0.52
1:D:288:GLU:H	1:D:291:GLN:NE2	2.07	0.52
1:A:131:MET:HE2	1:A:158:LEU:HD21	1.92	0.52
1:A:207:VAL:HG23	1:A:236:ARG:HG2	1.92	0.52
1:D:137:LYS:HG2	3:D:401:GDP:C6	2.45	0.51
1:C:218:VAL:HG22	1:C:228:VAL:HG12	1.92	0.50
1:D:216:GLU:HG3	1:D:335:THR:HG21	1.93	0.50
1:A:73:GLU:N	1:A:73:GLU:OE2	2.42	0.49
1:C:129:PRO:HB2	1:C:130:TYR:CD2	2.47	0.49
1:D:378:ARG:HG2	1:D:383:THR:HA	1.92	0.49
1:C:75:ARG:NH2	1:C:200:ILE:O	2.39	0.49
1:C:52:LYS:O	1:C:52:LYS:HD3	2.12	0.48
1:C:207:VAL:HB	1:C:236:ARG:HH12	1.78	0.48
1:D:117:ARG:NH1	1:D:160:GLN:OE1	2.48	0.47
1:C:137:LYS:HG2	3:C:401:GDP:C6	2.50	0.47
1:A:218:VAL:HG22	1:A:228:VAL:HG12	1.95	0.47
1:C:33:THR:HG23	1:C:43:GLN:O	2.15	0.46
1:D:369:ILE:HA	1:D:373:GLN:HE22	1.81	0.46
1:C:49:GLN:O	1:C:52:LYS:HD2	2.16	0.46
1:C:146:LEU:HA	1:C:149:LEU:HD23	1.98	0.45
1:B:350:MET:HE1	1:C:324:PHE:HB2	1.98	0.45
1:C:52:LYS:NZ	6:C:506:HOH:O	2.49	0.45
1:A:129:PRO:HB2	1:A:130:TYR:CD2	2.51	0.45
1:A:20:HIS:HA	1:A:115:GLN:HB2	1.98	0.45
1:C:216:GLU:HG2	1:C:335:THR:HG21	1.99	0.45
1:B:378:ARG:HE	1:B:383:THR:HG1	1.61	0.45
1:A:56:GLU:OE1	1:A:67:HIS:HE1	1.99	0.44
1:B:218:VAL:HG22	1:B:228:VAL:HG12	1.98	0.44
1:C:54:PRO:HD3	6:C:506:HOH:O	2.17	0.44
1:A:205:ARG:HG3	1:A:207:VAL:HG12	1.99	0.44
1:A:25:LYS:HE2	1:A:25:LYS:HB2	1.70	0.44
1:B:205:ARG:HG2	1:B:205:ARG:H	1.61	0.44
1:B:263:ARG:NH1	1:D:100:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLU:O	1:B:289:ARG:HG3	2.17	0.44
1:B:59:ARG:NH2	6:B:502:HOH:O	2.35	0.43
1:B:129:PRO:HB2	1:B:130:TYR:CD2	2.52	0.43
1:B:137:LYS:HG2	3:B:401:GDP:C6	2.53	0.43
1:B:117:ARG:HH12	1:B:160:GLN:HE22	1.66	0.43
1:B:249:SER:HB2	1:B:250:GLU:H	1.65	0.43
1:C:145:GLU:C	1:C:149:LEU:HD23	2.38	0.43
1:A:82:CYS:HB2	1:A:88:TYR:CE1	2.54	0.43
1:B:263:ARG:HB3	1:D:12:HIS:HB2	2.01	0.42
1:D:258:SER:OG	1:D:265:GLU:OE2	2.31	0.42
1:A:309:VAL:HG11	1:A:359:MET:HE1	2.00	0.42
1:D:247:GLY:O	1:D:249:SER:N	2.53	0.42
1:C:236:ARG:HG2	1:C:270:ILE:HG22	2.02	0.42
3:D:401:GDP:C2'	3:D:401:GDP:O5'	2.65	0.42
1:B:343:VAL:HB	1:B:360:GLU:HB2	2.01	0.42
6:D:611:HOH:O	2:H:2:FRU:H3	2.20	0.41
1:B:92:MET:HE1	1:B:122:LEU:HB3	2.01	0.41
1:A:283:ASP:HB3	1:A:286:GLU:HG3	2.01	0.41
1:C:331:PHE:O	1:C:337:ASP:HA	2.20	0.41
1:A:253:LYS:HB3	1:A:253:LYS:HE2	1.97	0.41
1:A:328:LYS:HA	1:A:340:GLY:O	2.20	0.41
1:B:374:ARG:HG2	1:B:388:VAL:HG22	2.03	0.40
1:B:117:ARG:HH12	1:B:160:GLN:NE2	2.18	0.40
1:D:75:ARG:NH2	1:D:200:ILE:O	2.38	0.40
1:C:149:LEU:HD22	1:C:149:LEU:H	1.86	0.40
1:D:332:TYR:CE1	1:D:378:ARG:HB2	2.57	0.40
1:C:33:THR:HG22	1:C:44:TYR:HA	2.03	0.40

All (2) 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)
6:A:651:HOH:O	6:C:578:HOH:O[1_455]	2.05	0.15
6:A:502:HOH:O	6:C:501:HOH:O[1_455]	2.07	0.13

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	378/392 (96%)	369 (98%)	9 (2%)	0	100	100
1	B	381/392 (97%)	372 (98%)	8 (2%)	1 (0%)	41	50
1	C	385/392 (98%)	375 (97%)	10 (3%)	0	100	100
1	D	385/392 (98%)	380 (99%)	5 (1%)	0	100	100
All	All	1529/1568 (98%)	1496 (98%)	32 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	249	SER

### 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	325/332 (98%)	324 (100%)	1 (0%)	92	97
1	B	326/332 (98%)	324 (99%)	2 (1%)	86	94
1	C	327/332 (98%)	326 (100%)	1 (0%)	92	97
1	D	327/332 (98%)	327 (100%)	0	100	100
All	All	1305/1328 (98%)	1301 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	208	ASP
1	B	205	ARG
1	B	236	ARG
1	C	52	LYS

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	67	HIS
1	B	160	GLN
1	D	291	GLN
1	D	373	GLN

### 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 ⓘ

8 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	$\# Z  > 2$
2	GLC	E	1	2	11,11,12	1.10	2 (18%)	15,15,17	1.76	1 (6%)
2	FRU	E	2	2	11,12,12	2.40	3 (27%)	10,18,18	4.80	3 (30%)
2	GLC	F	1	2	11,11,12	1.31	2 (18%)	15,15,17	0.90	0
2	FRU	F	2	2	11,12,12	1.14	1 (9%)	10,18,18	1.56	2 (20%)
2	GLC	G	1	2	11,11,12	0.53	0	15,15,17	1.31	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FRU	G	2	2	11,12,12	2.28	3 (27%)	10,18,18	5.74	2 (20%)
2	GLC	H	1	2	11,11,12	2.64	4 (36%)	15,15,17	2.27	6 (40%)
2	FRU	H	2	2	11,12,12	1.55	3 (27%)	10,18,18	1.24	1 (10%)

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	GLC	E	1	2	-	0/2/19/22	0/1/1/1
2	FRU	E	2	2	-	2/5/24/24	0/1/1/1
2	GLC	F	1	2	-	0/2/19/22	0/1/1/1
2	FRU	F	2	2	-	2/5/24/24	0/1/1/1
2	GLC	G	1	2	-	0/2/19/22	0/1/1/1
2	FRU	G	2	2	-	2/5/24/24	0/1/1/1
2	GLC	H	1	2	-	2/2/19/22	0/1/1/1
2	FRU	H	2	2	-	0/5/24/24	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	FRU	O5-C2	5.84	1.52	1.43
2	G	2	FRU	O5-C2	5.75	1.52	1.43
2	H	1	GLC	C2-C3	-5.28	1.44	1.52
2	H	1	GLC	O2-C2	-4.42	1.34	1.43
2	H	1	GLC	O3-C3	-3.88	1.33	1.43
2	G	2	FRU	O2-C2	3.75	1.47	1.40
2	E	2	FRU	O2-C2	3.50	1.46	1.40
2	H	2	FRU	O3-C3	-2.87	1.37	1.42
2	F	1	GLC	O4-C4	-2.65	1.36	1.43
2	F	2	FRU	O3-C3	-2.64	1.37	1.42
2	F	1	GLC	O2-C2	-2.51	1.38	1.43
2	E	1	GLC	O5-C1	2.39	1.47	1.43
2	E	1	GLC	O5-C5	2.35	1.48	1.43
2	H	2	FRU	O5-C5	-2.31	1.38	1.43
2	H	1	GLC	O4-C4	-2.29	1.37	1.43
2	G	2	FRU	O3-C3	2.24	1.47	1.42
2	E	2	FRU	C4-C5	2.24	1.58	1.53
2	H	2	FRU	C4-C3	-2.12	1.44	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	FRU	O2-C2-O5	-16.28	78.07	109.50
2	E	2	FRU	O2-C2-O5	-13.08	84.26	109.50
2	G	2	FRU	O5-C5-C4	-7.58	86.65	105.49
2	E	2	FRU	O5-C5-C4	-6.56	89.18	105.49
2	E	1	GLC	O5-C5-C6	5.49	115.81	107.20
2	H	1	GLC	C1-O5-C5	5.48	119.62	112.19
2	E	2	FRU	O3-C3-C4	3.53	125.53	113.32
2	F	2	FRU	C6-C5-C4	-3.25	107.25	115.09
2	H	1	GLC	C6-C5-C4	-3.16	105.59	113.00
2	H	1	GLC	O3-C3-C2	-3.05	104.15	109.99
2	H	1	GLC	O5-C5-C6	-3.05	102.42	107.20
2	G	1	GLC	O5-C5-C6	2.98	111.88	107.20
2	F	2	FRU	O2-C2-O5	2.75	114.81	109.50
2	G	1	GLC	O2-C2-C1	2.55	114.37	109.15
2	H	1	GLC	O6-C6-C5	-2.37	103.17	111.29
2	H	1	GLC	C1-C2-C3	-2.37	106.76	109.67
2	G	1	GLC	C1-C2-C3	-2.18	106.99	109.67
2	H	2	FRU	C6-C5-C4	-2.03	110.18	115.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	FRU	O1-C1-C2-O2
2	G	2	FRU	O1-C1-C2-O2
2	F	2	FRU	C4-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6
2	F	2	FRU	O5-C5-C6-O6
2	G	2	FRU	O5-C5-C6-O6
2	E	2	FRU	O5-C5-C6-O6

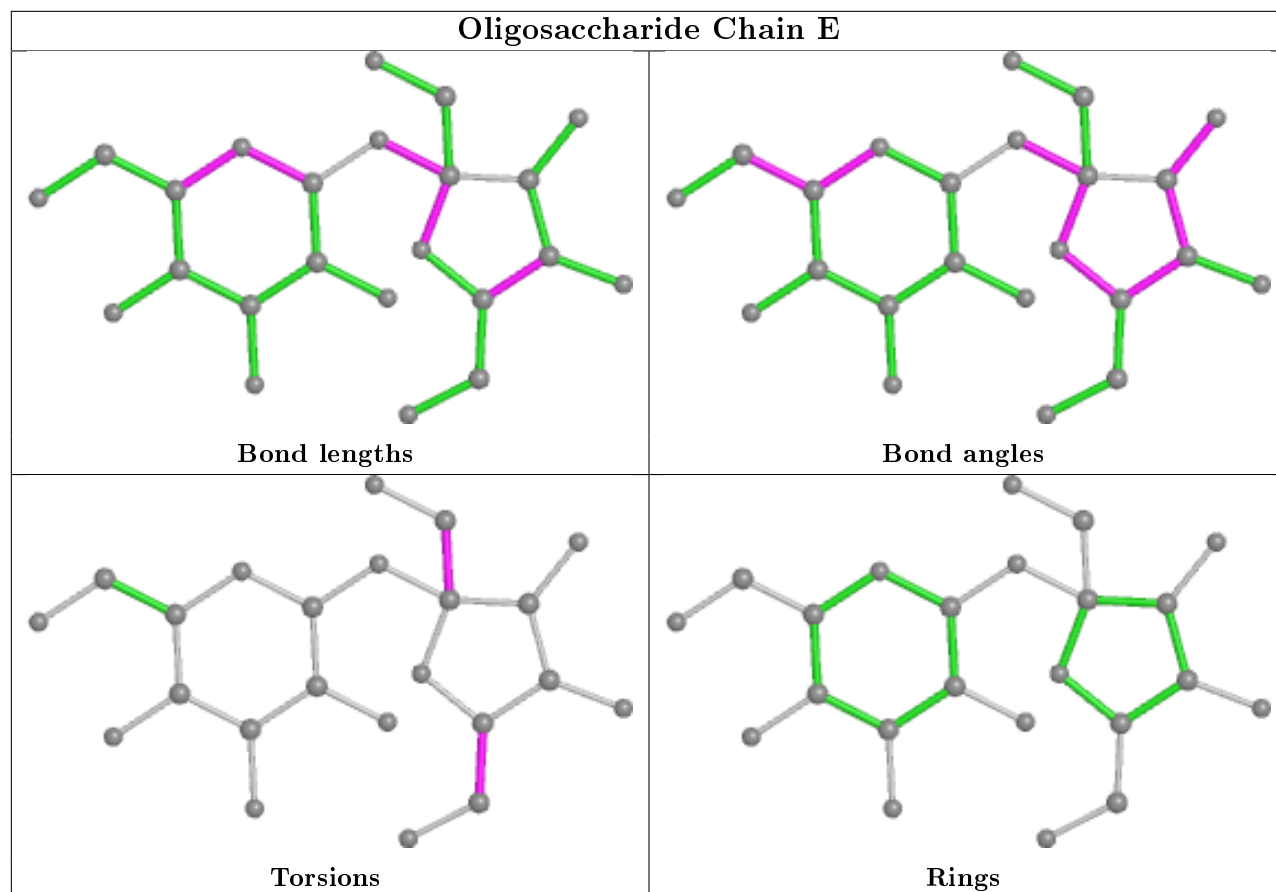
There are no ring outliers.

1 monomer is involved in 1 short contact:

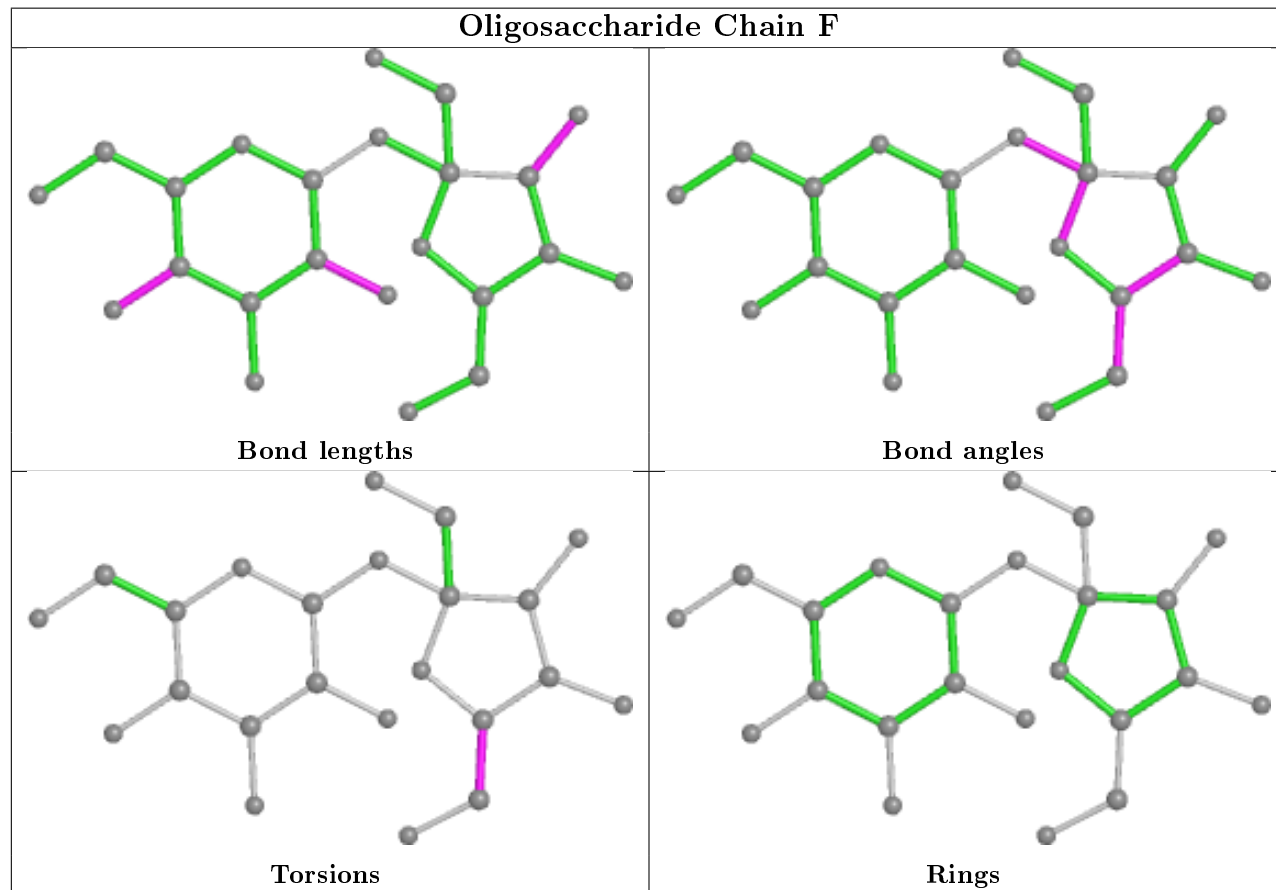
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	FRU	1	0

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

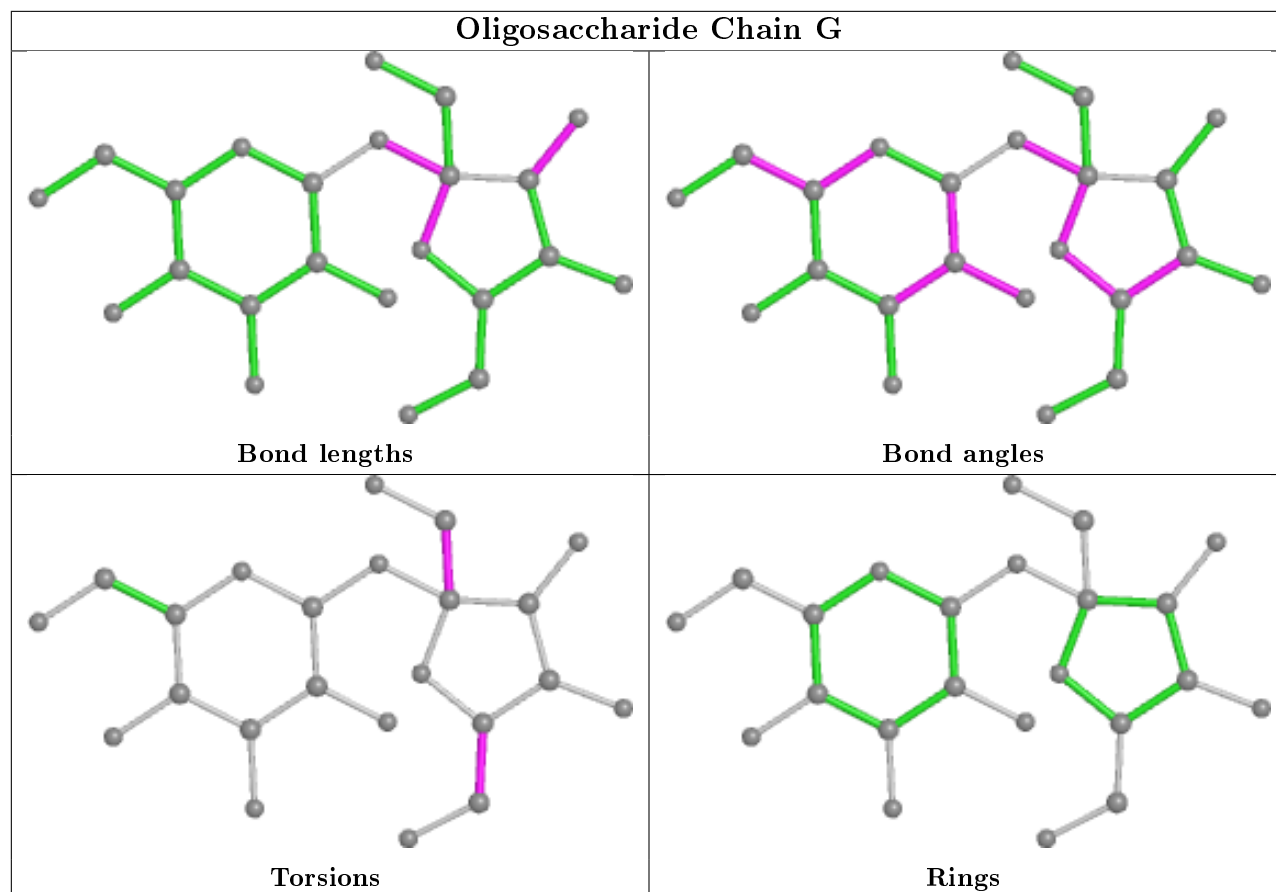
## Oligosaccharide Chain E



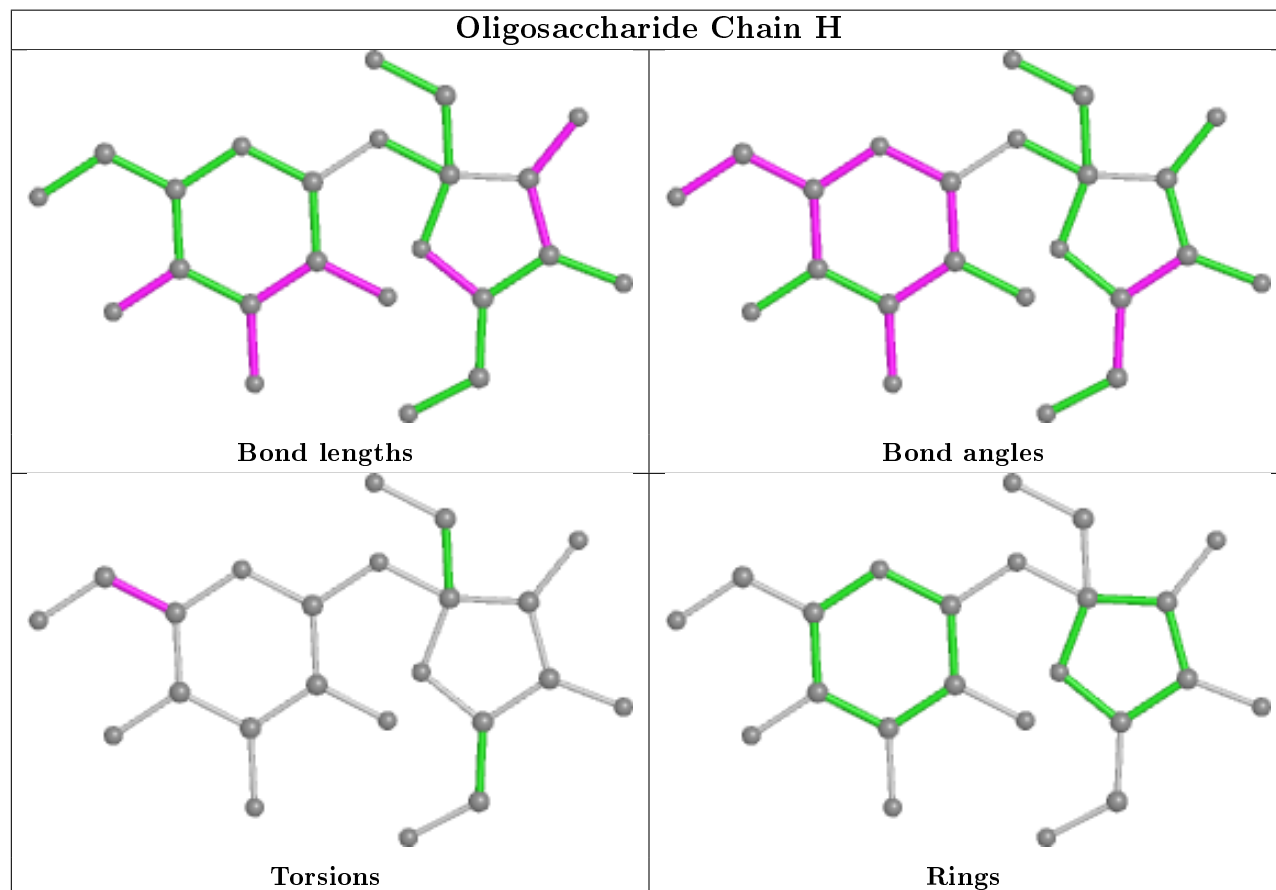
## Oligosaccharide Chain F



## Oligosaccharide Chain G



## Oligosaccharide Chain H



## 5.6 Ligand geometry

Of 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 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
5	SO4	A	404	-	4,4,4	0.13	0	6,6,6	0.09	0
5	SO4	C	407	-	4,4,4	0.13	0	6,6,6	0.06	0
3	GDP	D	401	4	24,30,30	2.67	8 (33%)	31,47,47	4.22	10 (32%)
5	SO4	C	408	-	4,4,4	0.14	0	6,6,6	0.11	0
5	SO4	B	406	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	D	405	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GDP	C	401	4	24,30,30	1.87	8 (33%)	31,47,47	4.87	13 (41%)
5	SO4	C	403	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	B	403	-	4,4,4	0.16	0	6,6,6	0.11	0
5	SO4	C	404	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	D	406	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	D	409	-	4,4,4	0.14	0	6,6,6	0.11	0
5	SO4	C	405	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	404	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	C	406	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	B	405	-	4,4,4	0.14	0	6,6,6	0.06	0
3	GDP	A	401	4	24,30,30	1.81	6 (25%)	31,47,47	4.94	13 (41%)
5	SO4	B	407	-	4,4,4	0.13	0	6,6,6	0.08	0
3	GDP	B	401	4	24,30,30	1.64	4 (16%)	31,47,47	4.87	10 (32%)
5	SO4	B	408	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	B	404	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	408	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	D	403	-	4,4,4	0.14	0	6,6,6	0.13	0
5	SO4	D	407	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	A	403	-	4,4,4	0.15	0	6,6,6	0.07	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	GDP	C	401	4	-	2/12/32/32	0/3/3/3
3	GDP	A	401	4	-	2/12/32/32	0/3/3/3
3	GDP	D	401	4	-	5/12/32/32	0/3/3/3
3	GDP	B	401	4	-	2/12/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	GDP	O4'-C1'	8.26	1.52	1.41
3	D	401	GDP	C2'-C1'	-4.58	1.46	1.53
3	D	401	GDP	C6-C5	-4.43	1.33	1.41
3	C	401	GDP	C6-C5	-4.11	1.34	1.41
3	B	401	GDP	C6-C5	-4.07	1.34	1.41
3	A	401	GDP	C6-C5	-3.93	1.34	1.41
3	D	401	GDP	C6-N1	3.91	1.39	1.33
3	B	401	GDP	C6-N1	3.86	1.39	1.33
3	A	401	GDP	C6-N1	3.78	1.39	1.33
3	C	401	GDP	C6-N1	3.68	1.39	1.33
3	D	401	GDP	PB-O1B	3.46	1.61	1.50
3	A	401	GDP	PB-O1B	3.26	1.61	1.50
3	C	401	GDP	PB-O1B	3.25	1.61	1.50
3	C	401	GDP	PA-O1A	2.75	1.60	1.50
3	D	401	GDP	C2'-C3'	2.73	1.60	1.53
3	D	401	GDP	C2-N1	2.56	1.40	1.35
3	D	401	GDP	C5-C4	-2.47	1.34	1.40
3	A	401	GDP	PA-O1A	2.44	1.59	1.50
3	C	401	GDP	C5-C4	-2.43	1.34	1.40
3	B	401	GDP	C5-C4	-2.43	1.34	1.40
3	C	401	GDP	C2-N1	2.40	1.39	1.35
3	A	401	GDP	C5-C4	-2.37	1.34	1.40
3	B	401	GDP	C2-N1	2.33	1.39	1.35
3	A	401	GDP	C2-N1	2.20	1.39	1.35
3	C	401	GDP	C2'-C3'	-2.04	1.47	1.53
3	C	401	GDP	O4'-C4'	2.02	1.49	1.45

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	GDP	O4'-C1'-C2'	-20.85	76.46	106.93
3	B	401	GDP	O4'-C1'-C2'	-20.23	77.37	106.93
3	C	401	GDP	O4'-C1'-C2'	-20.17	77.45	106.93
3	D	401	GDP	C3'-C2'-C1'	-13.06	81.32	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	GDP	O4'-C4'-C3'	-11.28	82.79	105.11
3	A	401	GDP	O4'-C4'-C5'	-9.11	79.41	109.37
3	C	401	GDP	O4'-C4'-C5'	-8.95	79.92	109.37
3	B	401	GDP	O4'-C4'-C5'	-8.89	80.13	109.37
3	B	401	GDP	O4'-C4'-C3'	-8.09	89.10	105.11
3	C	401	GDP	O4'-C4'-C3'	-8.00	89.28	105.11
3	D	401	GDP	C2'-C3'-C4'	7.73	117.66	102.64
3	D	401	GDP	C5'-C4'-C3'	-7.68	86.39	115.18
3	A	401	GDP	O4'-C4'-C3'	-7.64	89.99	105.11
3	B	401	GDP	C3'-C2'-C1'	-6.47	91.23	100.98
3	C	401	GDP	C3'-C2'-C1'	-6.28	91.52	100.98
3	B	401	GDP	N3-C2-N1	-5.94	119.30	127.22
3	D	401	GDP	C1'-N9-C4	5.92	137.05	126.64
3	A	401	GDP	C3'-C2'-C1'	-5.91	92.08	100.98
3	D	401	GDP	N3-C2-N1	-5.69	119.63	127.22
3	A	401	GDP	N3-C2-N1	-5.60	119.76	127.22
3	C	401	GDP	C5'-C4'-C3'	5.52	135.88	115.18
3	B	401	GDP	C5'-C4'-C3'	5.41	135.46	115.18
3	C	401	GDP	N3-C2-N1	-5.40	120.02	127.22
3	A	401	GDP	C5'-C4'-C3'	5.23	134.78	115.18
3	A	401	GDP	C2-N3-C4	4.81	120.86	115.36
3	B	401	GDP	C2-N3-C4	4.75	120.78	115.36
3	D	401	GDP	C2-N3-C4	4.64	120.65	115.36
3	C	401	GDP	C2-N3-C4	4.62	120.63	115.36
3	B	401	GDP	O5'-C5'-C4'	3.08	119.58	108.99
3	A	401	GDP	C5-C6-N1	-3.03	119.29	123.43
3	C	401	GDP	O5'-C5'-C4'	3.02	119.40	108.99
3	A	401	GDP	O5'-C5'-C4'	3.00	119.32	108.99
3	B	401	GDP	C5-C6-N1	-2.99	119.34	123.43
3	D	401	GDP	C5-C6-N1	-2.91	119.46	123.43
3	C	401	GDP	C5-C6-N1	-2.87	119.51	123.43
3	D	401	GDP	PA-O3A-PB	-2.86	123.02	132.83
3	B	401	GDP	O2B-PB-O3A	2.84	114.16	104.64
3	C	401	GDP	O3B-PB-O3A	2.79	114.00	104.64
3	D	401	GDP	O5'-C5'-C4'	2.78	118.55	108.99
3	A	401	GDP	O3B-PB-O3A	2.61	113.39	104.64
3	C	401	GDP	O2B-PB-O3A	2.49	112.98	104.64
3	A	401	GDP	O2B-PB-O3A	2.34	112.49	104.64
3	C	401	GDP	O3A-PB-O1B	-2.29	98.49	111.19
3	A	401	GDP	C4-C5-N7	-2.16	107.14	109.40
3	A	401	GDP	O3A-PB-O1B	-2.11	99.50	111.19
3	C	401	GDP	O3B-PB-O2B	2.11	115.69	107.64



There are no chirality outliers.

All (11) torsion outliers are listed below:

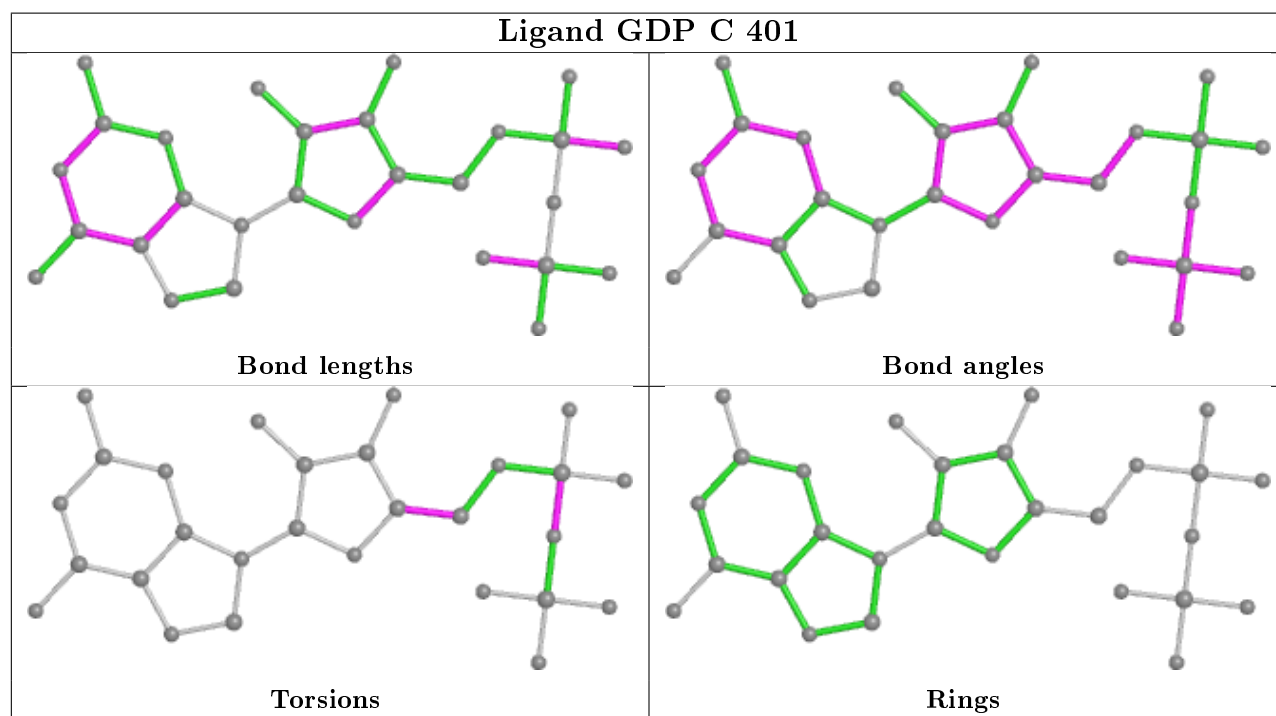
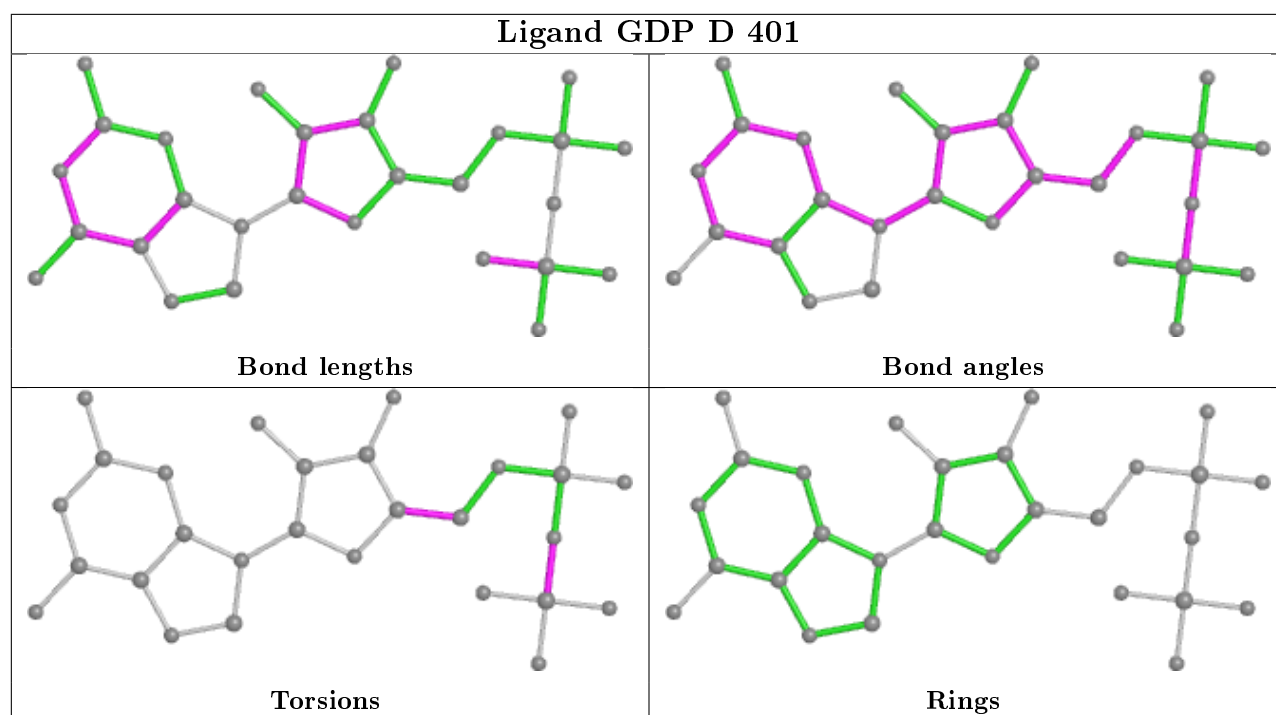
Mol	Chain	Res	Type	Atoms
3	D	401	GDP	PA-O3A-PB-O2B
3	D	401	GDP	PA-O3A-PB-O3B
3	D	401	GDP	O4'-C4'-C5'-O5'
3	C	401	GDP	O4'-C4'-C5'-O5'
3	A	401	GDP	O4'-C4'-C5'-O5'
3	B	401	GDP	O4'-C4'-C5'-O5'
3	D	401	GDP	C3'-C4'-C5'-O5'
3	C	401	GDP	PB-O3A-PA-O2A
3	D	401	GDP	PA-O3A-PB-O1B
3	A	401	GDP	PB-O3A-PA-O2A
3	B	401	GDP	PB-O3A-PA-O2A

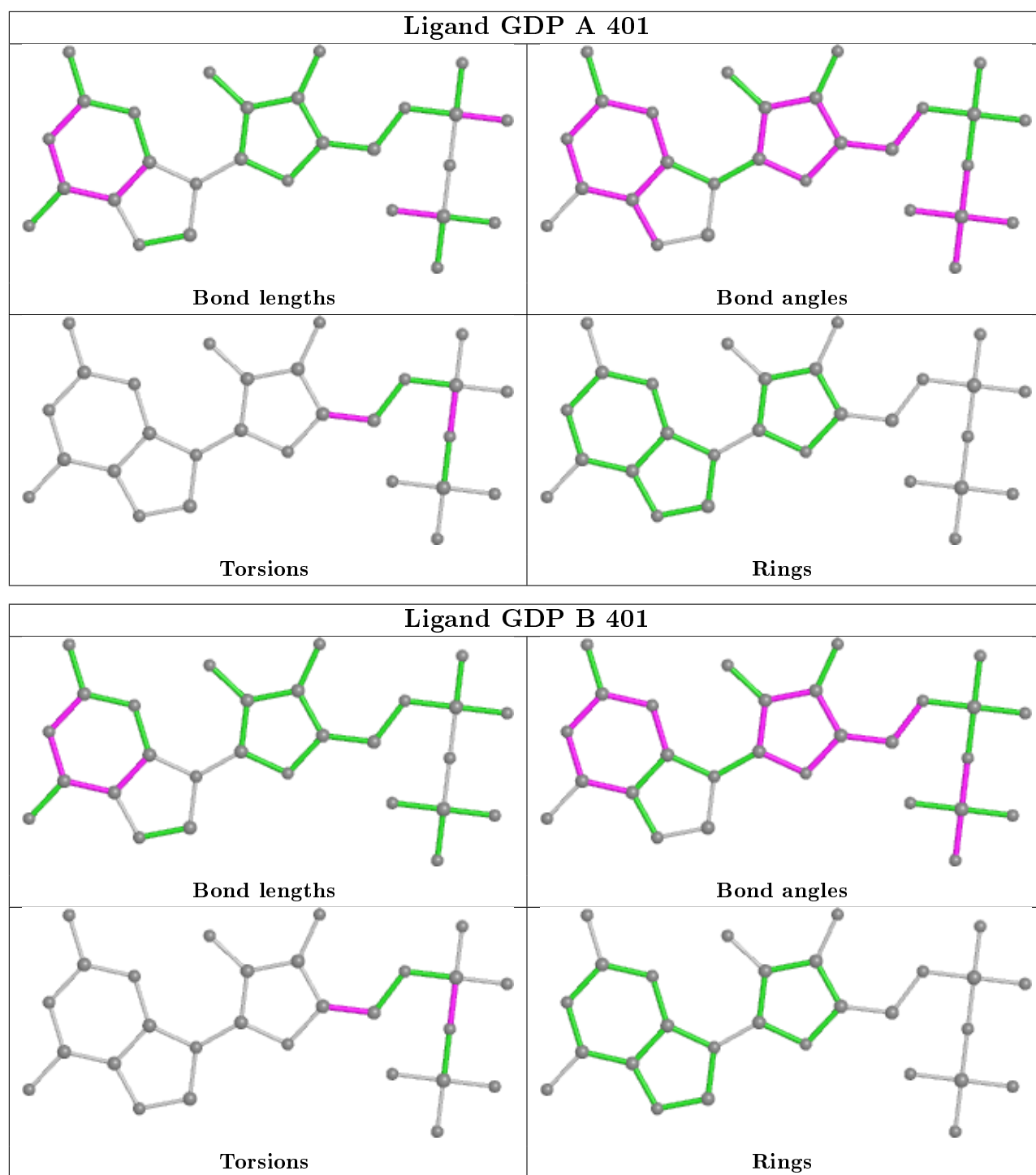
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	GDP	2	0
3	C	401	GDP	1	0
3	B	401	GDP	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	384/392 (97%)	-0.18	13 (3%) 45 52	27, 39, 69, 113	0
1	B	385/392 (98%)	-0.12	16 (4%) 36 43	27, 41, 71, 111	0
1	C	387/392 (98%)	-0.27	10 (2%) 56 63	31, 43, 74, 104	0
1	D	387/392 (98%)	-0.31	10 (2%) 56 63	26, 39, 65, 93	0
All	All	1543/1568 (98%)	-0.22	49 (3%) 47 54	26, 41, 69, 113	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	HIS	5.1
1	A	9	THR	3.7
1	B	38	LEU	3.7
1	B	142	ASP	3.7
1	C	205	ARG	3.7
1	D	381	GLY	3.5
1	D	17	THR	3.5
1	B	205	ARG	3.5
1	A	17	THR	3.4
1	B	381	GLY	3.3
1	B	105	VAL	3.2
1	B	17	THR	3.1
1	B	9	THR	3.0
1	B	103	ILE	3.0
1	C	105	VAL	2.9
1	C	142	ASP	2.9
1	A	18	ILE	2.8
1	D	103	ILE	2.8
1	A	105	VAL	2.7
1	C	9	THR	2.7
1	D	18	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	205	ARG	2.7
1	C	145	GLU	2.7
1	A	59	ARG	2.6
1	A	103	ILE	2.6
1	A	184	GLU	2.6
1	C	208	ASP	2.6
1	B	18	ILE	2.5
1	C	315	GLU	2.5
1	B	183	HIS	2.5
1	B	382	ARG	2.4
1	B	144	PRO	2.4
1	B	104	LEU	2.4
1	D	346	GLU	2.4
1	B	16	GLY	2.4
1	C	104	LEU	2.3
1	A	347	GLY	2.3
1	C	17	THR	2.3
1	B	102	ALA	2.3
1	A	346	GLU	2.2
1	D	105	VAL	2.2
1	A	16	GLY	2.1
1	D	59	ARG	2.1
1	D	249	SER	2.1
1	D	347	GLY	2.1
1	C	59	ARG	2.1
1	D	382	ARG	2.1
1	B	184	GLU	2.0
1	A	142	ASP	2.0

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

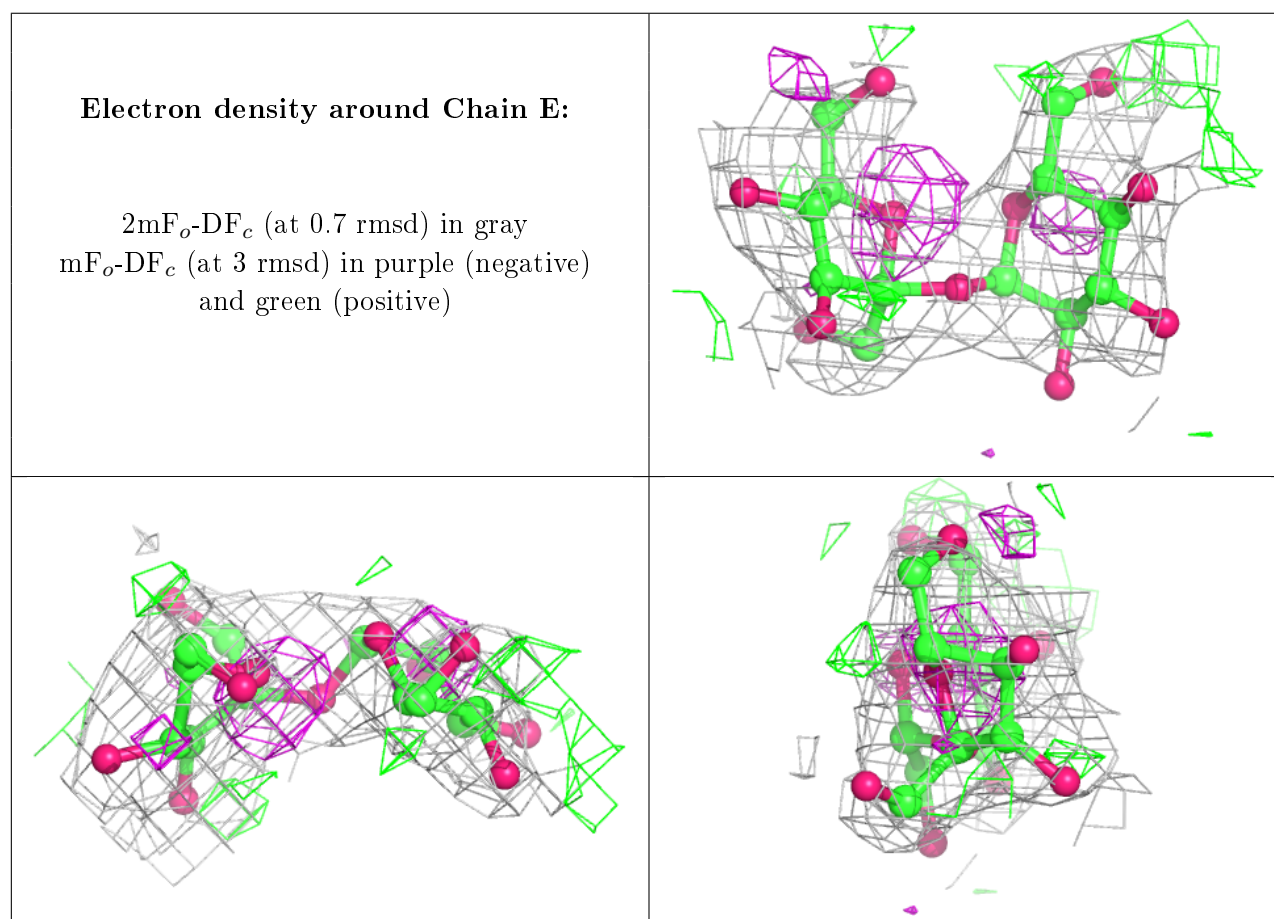
There are no non-standard protein/DNA/RNA residues in this entry.

## 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.

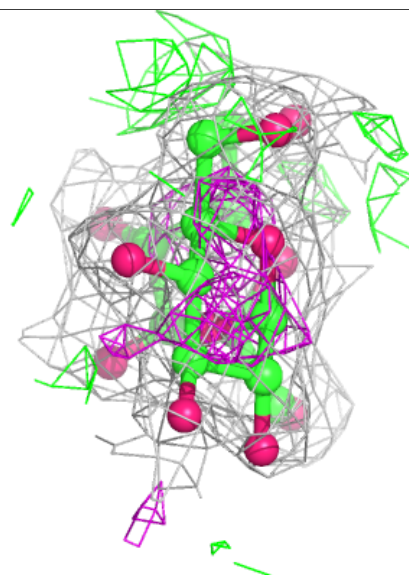
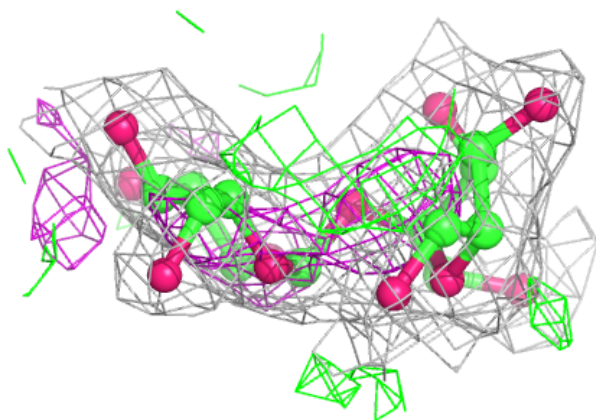
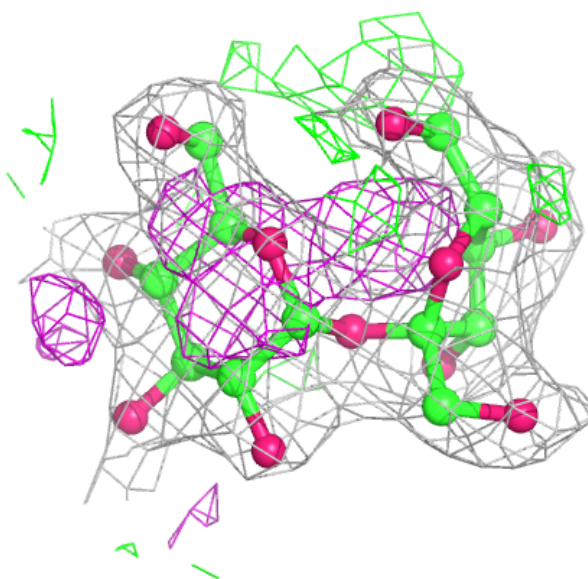
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FRU	E	2	12/12	0.75	0.22	88,93,97,98	0
2	GLC	E	1	11/12	0.78	0.24	79,94,99,103	0
2	FRU	G	2	12/12	0.81	0.35	82,97,101,102	0
2	FRU	F	2	12/12	0.84	0.17	78,92,97,99	0
2	FRU	H	2	12/12	0.87	0.18	49,73,77,79	0
2	GLC	F	1	11/12	0.89	0.22	55,70,79,84	0
2	GLC	G	1	11/12	0.91	0.17	57,80,85,87	0
2	GLC	H	1	11/12	0.94	0.17	48,64,74,74	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.



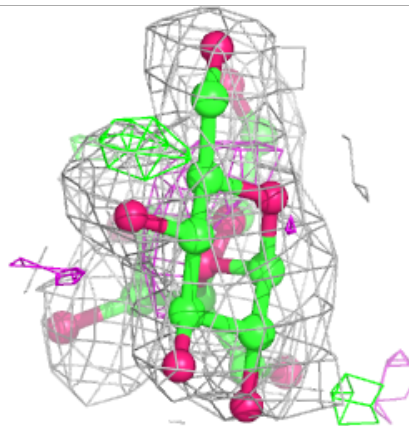
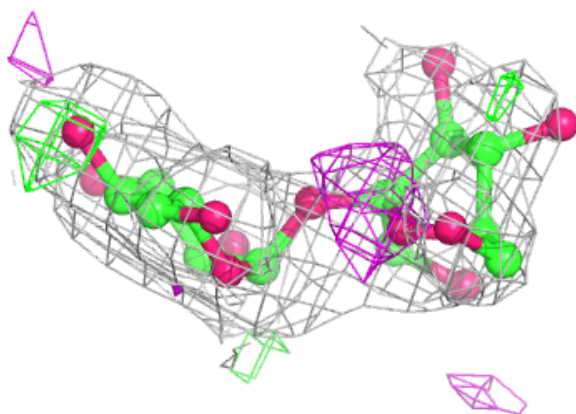
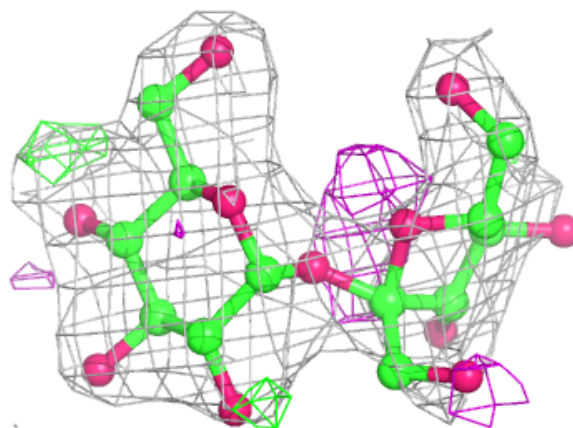
**Electron density around Chain F:**

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

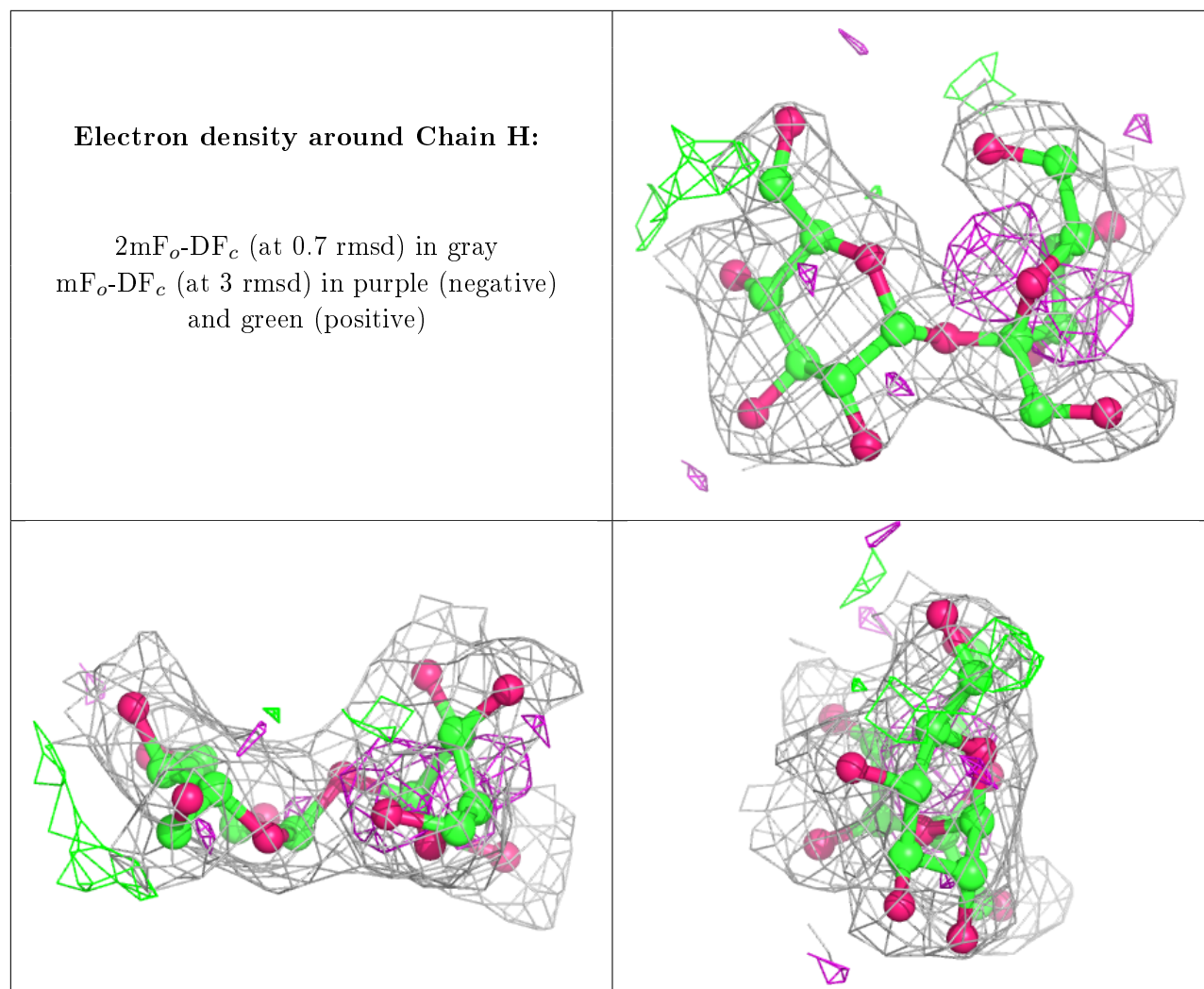


**Electron density around Chain G:**

$2mF_o-DF_c$  (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
5	SO4	D	407	5/5	0.79	0.21	120,122,123,124	5
5	SO4	D	404	5/5	0.81	0.16	122,123,124,126	0
5	SO4	C	405	5/5	0.82	0.28	133,133,134,135	0
5	SO4	C	407	5/5	0.83	0.31	112,112,114,115	5
5	SO4	B	406	5/5	0.84	0.30	123,124,125,125	5
5	SO4	C	406	5/5	0.86	0.16	126,128,130,131	0
5	SO4	D	405	5/5	0.86	0.25	100,104,105,106	5
5	SO4	B	407	5/5	0.88	0.24	83,87,90,91	5
5	SO4	D	406	5/5	0.91	0.29	78,82,85,86	5

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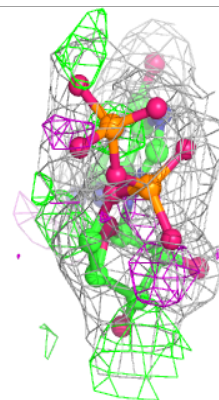
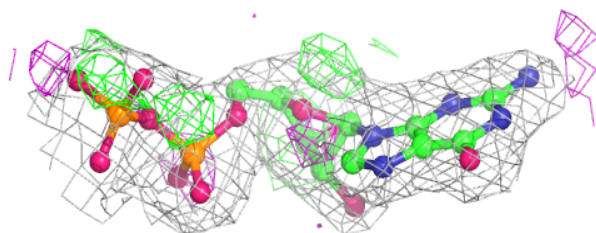
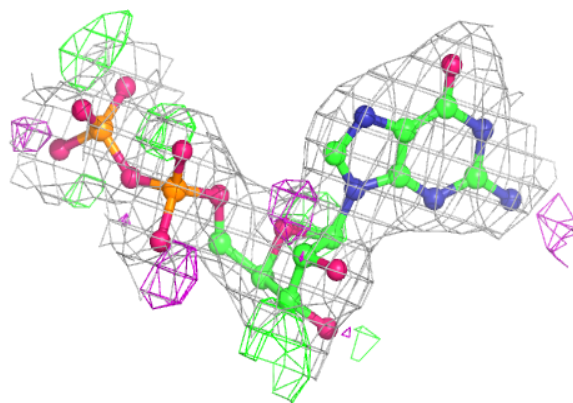
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	404	5/5	0.92	0.26	63,64,67,68	5
5	SO4	C	408	5/5	0.92	0.13	94,99,100,101	0
5	SO4	B	405	5/5	0.94	0.15	67,70,70,74	5
5	SO4	D	409	5/5	0.94	0.13	78,85,88,90	0
5	SO4	B	408	5/5	0.94	0.10	95,97,100,102	0
5	SO4	C	404	5/5	0.94	0.13	61,67,70,71	5
4	MG	D	402	1/1	0.94	0.11	38,38,38,38	0
3	GDP	C	401	28/28	0.95	0.13	37,46,53,67	0
3	GDP	D	401	28/28	0.95	0.14	34,48,53,72	0
5	SO4	D	408	5/5	0.95	0.15	55,55,59,60	5
3	GDP	B	401	28/28	0.95	0.12	36,44,51,60	0
5	SO4	D	403	5/5	0.96	0.14	57,63,67,68	5
3	GDP	A	401	28/28	0.96	0.14	25,38,43,57	0
5	SO4	C	403	5/5	0.97	0.16	75,81,84,88	0
5	SO4	B	403	5/5	0.97	0.12	58,61,64,66	5
5	SO4	A	404	5/5	0.97	0.10	66,67,68,71	5
4	MG	C	402	1/1	0.98	0.12	37,37,37,37	0
5	SO4	A	403	5/5	0.98	0.09	64,66,69,70	5
4	MG	B	402	1/1	0.99	0.12	37,37,37,37	0
4	MG	A	402	1/1	0.99	0.14	31,31,31,31	0

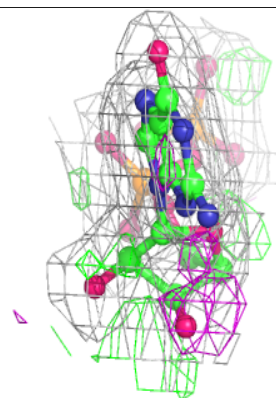
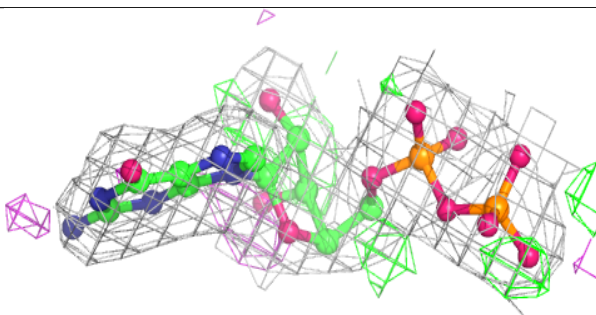
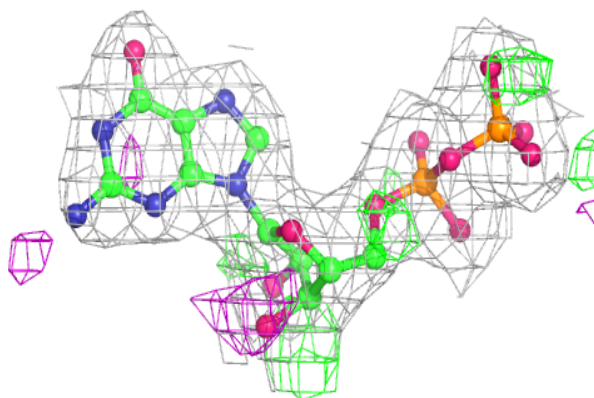
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GDP C 401:**

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

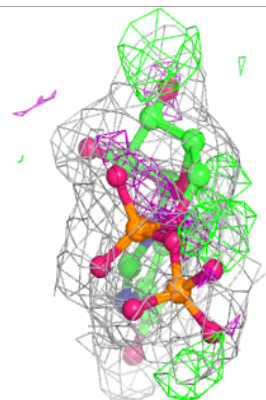
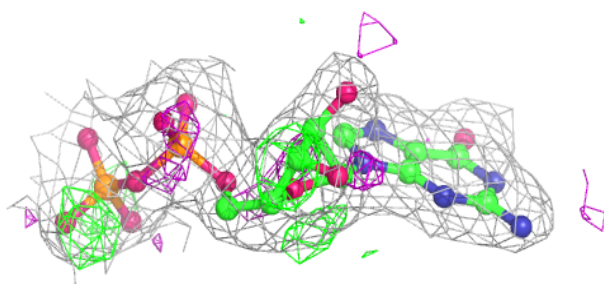
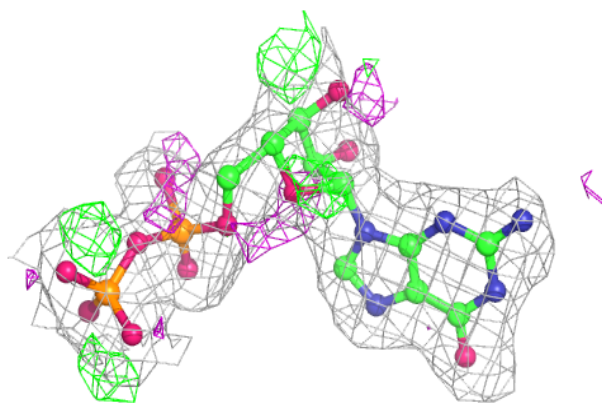
**Electron density around GDP D 401:**

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

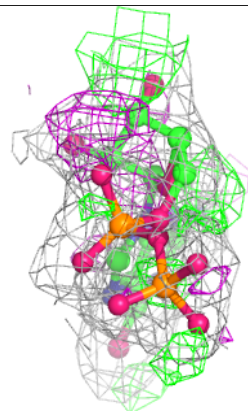
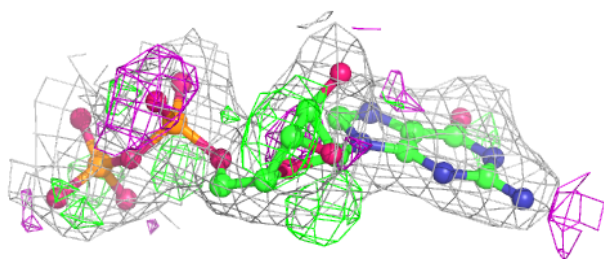
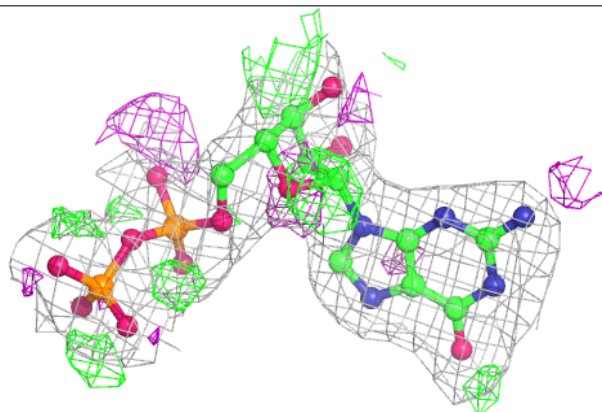


**Electron density around GDP B 401:**

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

**Electron density around GDP A 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.