



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2022 – 12:57 PM EDT

PDB ID : 8DCA  
Title : RNA ligase RtcB from *Pyrococcus horikoshii* in complex with Co<sup>2+</sup> and GTP  
Authors : Jacewicz, A.; Dantuluri, S.; Shuman, S.  
Deposited on : 2022-06-16  
Resolution : 2.43 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.31.2  
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) : 2.31.2

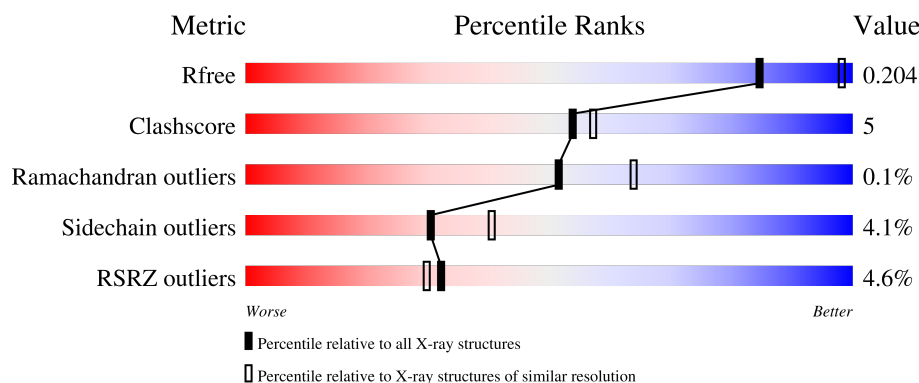
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	501	<div> <div>4%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
1	B	501	<div> <div>5%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7732 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 tRNA-splicing ligase RtcB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	1	0
			3774	2379	697	682	16			
1	B	481	Total	C	N	O	S	0	0	0
			3767	2375	694	681	17			

There are 40 discrepancies between the modelled and reference sequences:

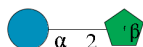
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O59245
A	-18	GLY	-	expression tag	UNP O59245
A	-17	SER	-	expression tag	UNP O59245
A	-16	SER	-	expression tag	UNP O59245
A	-15	HIS	-	expression tag	UNP O59245
A	-14	HIS	-	expression tag	UNP O59245
A	-13	HIS	-	expression tag	UNP O59245
A	-12	HIS	-	expression tag	UNP O59245
A	-11	HIS	-	expression tag	UNP O59245
A	-10	HIS	-	expression tag	UNP O59245
A	-9	SER	-	expression tag	UNP O59245
A	-8	SER	-	expression tag	UNP O59245
A	-7	GLY	-	expression tag	UNP O59245
A	-6	LEU	-	expression tag	UNP O59245
A	-5	VAL	-	expression tag	UNP O59245
A	-4	PRO	-	expression tag	UNP O59245
A	-3	ARG	-	expression tag	UNP O59245
A	-2	GLY	-	expression tag	UNP O59245
A	-1	SER	-	expression tag	UNP O59245
A	0	HIS	-	expression tag	UNP O59245
B	-19	MET	-	initiating methionine	UNP O59245
B	-18	GLY	-	expression tag	UNP O59245
B	-17	SER	-	expression tag	UNP O59245
B	-16	SER	-	expression tag	UNP O59245
B	-15	HIS	-	expression tag	UNP O59245

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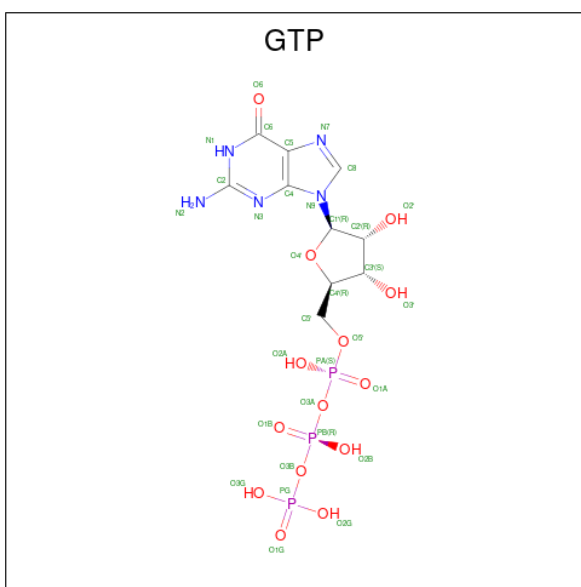
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP O59245
B	-13	HIS	-	expression tag	UNP O59245
B	-12	HIS	-	expression tag	UNP O59245
B	-11	HIS	-	expression tag	UNP O59245
B	-10	HIS	-	expression tag	UNP O59245
B	-9	SER	-	expression tag	UNP O59245
B	-8	SER	-	expression tag	UNP O59245
B	-7	GLY	-	expression tag	UNP O59245
B	-6	LEU	-	expression tag	UNP O59245
B	-5	VAL	-	expression tag	UNP O59245
B	-4	PRO	-	expression tag	UNP O59245
B	-3	ARG	-	expression tag	UNP O59245
B	-2	GLY	-	expression tag	UNP O59245
B	-1	SER	-	expression tag	UNP O59245
B	0	HIS	-	expression tag	UNP O59245

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



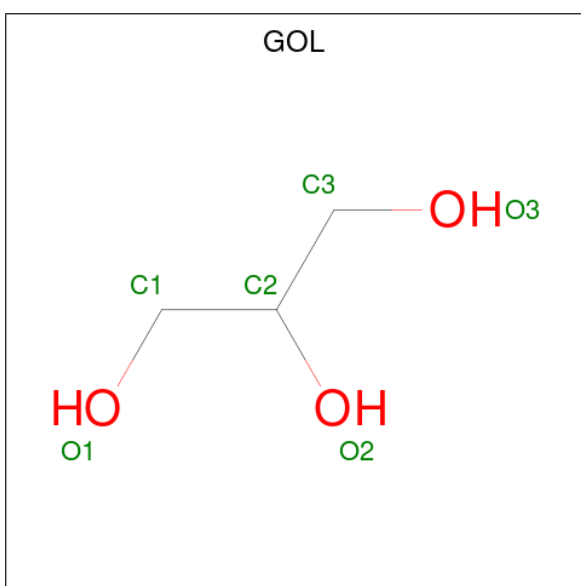
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	1	0	0
			23	12	11			
2	D	2	Total	C	O	2	0	0
			23	12	11			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	B	1	Total 32	C 10	N 5	O 14	P 3	1	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



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

- 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		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	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		

- Molecule 6 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Co 2	0	0
6	B	2	Total 2	Co 2	0	0

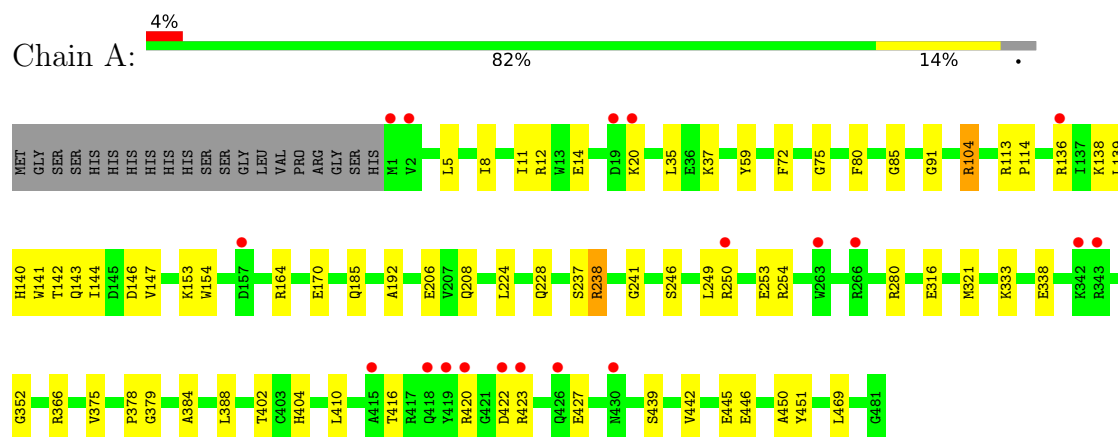
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total 6	O 6	0	0
7	B	5	Total 5	O 5	0	0

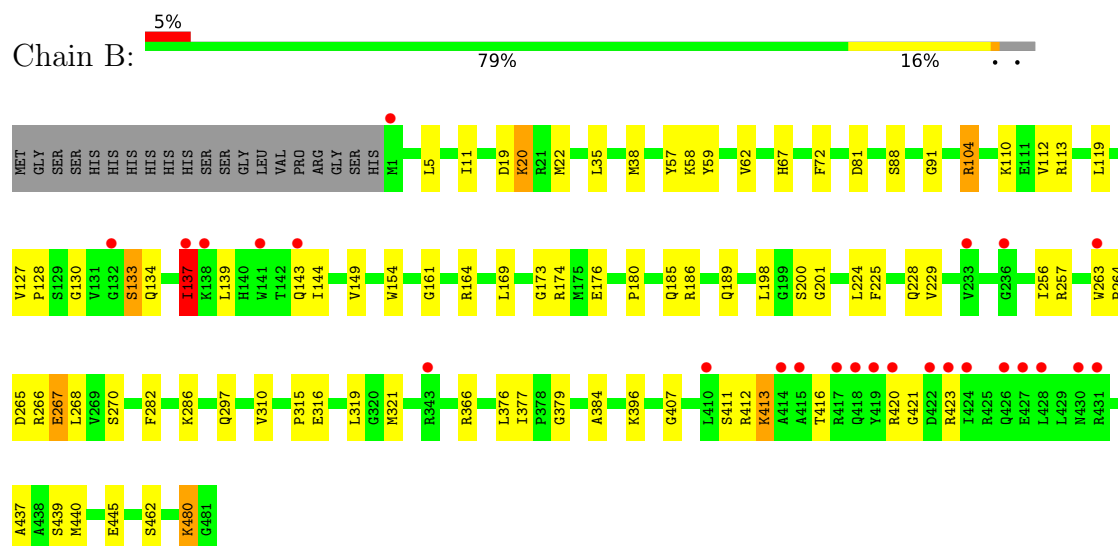
### 3 Residue-property plots

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.

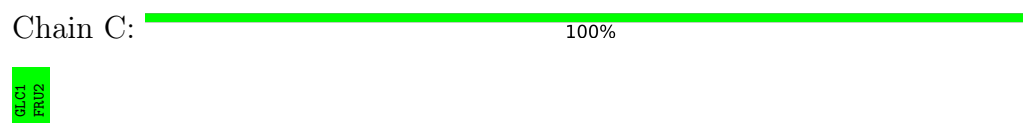
#### • Molecule 1: tRNA-splicing ligase RtcB



#### • Molecule 1: tRNA-splicing ligase RtcB



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





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

Chain D:  50% 50%

GLC1  
FRU2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.16Å 138.86Å 149.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.77 – 2.43 49.77 – 2.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.77-2.43) 100.0 (49.77-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.177 , 0.203 0.179 , 0.204	Depositor DCC
$R_{free}$ test set	3101 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.6	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.3	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	0.96	EDS
Total number of atoms	7732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: SO4, GTP, FRU, GOL, GLC, CO

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	0.42	0/3852	0.66	0/5197
1	B	0.43	0/3844	0.66	0/5185
All	All	0.42	0/7696	0.66	0/10382

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	3774	0	3793	35	0
1	B	3767	0	3794	46	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
3	A	32	0	12	0	0
3	B	32	0	12	1	0
4	A	6	0	8	0	0
5	A	35	0	0	1	0
5	B	25	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	6	0	0	0	0
7	B	5	0	0	1	0
All	All	7732	0	7661	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (81) 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:20:LYS:HD2	1:B:20:LYS:H	1.40	0.84
1:B:67:HIS:ND1	7:B:601:HOH:O	2.14	0.79
1:B:256:ILE:HD12	1:B:263:TRP:HZ3	1.50	0.77
1:B:256:ILE:HD12	1:B:263:TRP:CZ3	2.25	0.72
1:B:420:ARG:HH11	1:B:423:ARG:HH12	1.38	0.70
1:B:88:SER:HB2	1:B:270:SER:HB3	1.74	0.70
1:B:200:SER:OG	1:B:201:GLY:N	2.26	0.68
1:A:423:ARG:O	1:A:427:GLU:HG3	1.94	0.67
1:B:130:GLY:O	1:B:133:SER:OG	2.13	0.66
1:B:174:ARG:HH12	1:B:176:GLU:HG2	1.60	0.65
1:B:416:THR:HG23	1:B:445:GLU:HG3	1.77	0.65
1:B:421:GLY:HA3	1:B:440:MET:HG3	1.81	0.62
1:B:185:GLN:O	1:B:189:GLN:HG2	1.98	0.62
1:A:139:LEU:HD22	1:A:143:GLN:HB2	1.83	0.61
1:A:164:ARG:NH2	1:A:316:GLU:OE2	2.34	0.61
1:A:249:LEU:O	1:A:253:GLU:HG3	1.99	0.61
1:A:139:LEU:HD11	1:A:147:VAL:HG21	1.85	0.57
1:B:104:ARG:O	1:B:321:MET:HA	2.07	0.55
1:B:264:PRO:HG2	1:B:268:LEU:HD12	1.89	0.55
1:A:11:ILE:HD12	1:A:12:ARG:HG3	1.89	0.55
1:B:20:LYS:H	1:B:20:LYS:CD	2.11	0.54
1:B:5:LEU:HD13	1:B:35:LEU:HD21	1.87	0.54
1:A:238:ARG:HD2	5:A:504:SO4:O4	2.08	0.54
1:A:144:ILE:HD12	1:A:192:ALA:HB2	1.91	0.53
1:A:238:ARG:HB3	1:A:238:ARG:NH1	2.23	0.53
1:A:416:THR:HG23	1:A:445:GLU:HG3	1.90	0.53
1:A:8:ILE:HD11	1:A:14:GLU:HB2	1.89	0.53
1:B:72:PHE:CG	1:B:91:GLY:HA2	2.45	0.52
1:B:265:ASP:OD1	1:B:267:GLU:HG3	2.10	0.52
1:B:256:ILE:HG23	1:B:257:ARG:H	1.77	0.50
1:A:75:GLY:HA2	1:A:352:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG12	1:B:198:LEU:HG	1.94	0.50
1:B:128:PRO:HG2	1:B:134:GLN:O	2.12	0.49
1:B:266:ARG:HH11	1:B:266:ARG:HG2	1.77	0.49
1:B:149:VAL:HG23	1:B:180:PRO:HG3	1.93	0.49
1:B:19:ASP:O	1:B:22:MET:HG3	2.14	0.47
1:B:437:ALA:HA	1:B:480:LYS:O	2.14	0.47
1:A:140:HIS:O	1:A:142:THR:N	2.43	0.47
1:A:170:GLU:OE2	1:A:333:LYS:NZ	2.48	0.47
1:B:282:PHE:CE2	1:B:286:LYS:HE3	2.49	0.47
1:A:388:LEU:HD23	1:A:469:LEU:HA	1.96	0.47
1:A:72:PHE:CG	1:A:91:GLY:HA2	2.50	0.46
1:A:104:ARG:O	1:A:321:MET:HA	2.15	0.46
1:B:112:VAL:HG21	1:B:229:VAL:HG21	1.97	0.46
1:A:80:PHE:HB3	1:A:85:GLY:HA3	1.97	0.46
1:A:140:HIS:O	1:A:140:HIS:CG	2.68	0.46
1:B:164:ARG:NH2	1:B:316:GLU:OE1	2.49	0.46
1:A:379:GLY:HA3	1:A:384:ALA:O	2.17	0.45
1:A:378:PRO:HD2	1:A:404:HIS:O	2.16	0.45
1:B:411:SER:OG	1:B:413:LYS:HG3	2.16	0.45
1:B:412:ARG:NH1	1:B:445:GLU:HB3	2.32	0.44
1:A:141:TRP:O	1:A:144:ILE:HG22	2.17	0.44
1:B:315:PRO:HA	1:B:319:LEU:HB2	1.99	0.44
1:A:439:SER:OG	1:A:442:VAL:HG13	2.18	0.44
1:A:113:ARG:HB3	1:A:114:PRO:HD3	2.00	0.44
1:B:137:ILE:HG23	1:B:139:LEU:HD23	2.00	0.43
1:B:38:MET:HB2	1:B:38:MET:HE2	1.45	0.43
1:A:5:LEU:HD13	1:A:35:LEU:HD21	2.01	0.43
1:B:143:GLN:NE2	1:B:154:TRP:HE1	2.17	0.43
1:A:250:ARG:HH12	1:A:254:ARG:HH12	1.66	0.43
1:A:446:GLU:HG3	1:A:451:TYR:OH	2.18	0.43
1:B:225:PHE:CZ	1:B:228:GLN:HB2	2.53	0.43
1:A:375:VAL:HG11	1:A:402:THR:HG21	2.01	0.43
1:B:161:GLY:HA3	1:B:297:GLN:HE21	1.84	0.43
1:A:146:ASP:HB3	1:A:154:TRP:CD1	2.54	0.42
1:A:224:LEU:HA	1:A:228:GLN:OE1	2.19	0.42
1:A:113:ARG:HA	1:A:113:ARG:HD3	1.84	0.42
1:B:174:ARG:NH1	1:B:176:GLU:HG2	2.31	0.42
1:B:266:ARG:HG2	1:B:266:ARG:NH1	2.34	0.42
1:B:57:TYR:CE2	1:B:81:ASP:HB2	2.55	0.42
1:B:58:LYS:NZ	1:B:396:LYS:O	2.53	0.42
1:B:169:LEU:HD23	1:B:173:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LEU:HG	1:A:450:ALA:HA	2.02	0.41
1:B:376:LEU:O	1:B:377:ILE:HD13	2.21	0.41
1:A:206:GLU:HG2	1:A:208:GLN:HG3	2.03	0.41
1:B:224:LEU:HA	1:B:228:GLN:OE1	2.21	0.41
1:B:407:GLY:H	3:B:501:GTP:HO3'	1.67	0.41
1:A:237:SER:OG	1:A:241:GLY:HA3	2.21	0.41
1:B:379:GLY:HA3	1:B:384:ALA:O	2.21	0.41
1:B:119:LEU:HA	1:B:310:VAL:HG21	2.04	0.40
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/501 (96%)	458 (95%)	22 (5%)	0	100	100
1	B	479/501 (96%)	458 (96%)	20 (4%)	1 (0%)	47	57
All	All	959/1002 (96%)	916 (96%)	42 (4%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	137	ILE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/407 (96%)	375 (96%)	15 (4%)	33	43
1	B	390/407 (96%)	373 (96%)	17 (4%)	28	37
All	All	780/814 (96%)	748 (96%)	32 (4%)	30	40

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	37	LYS
1	A	59	TYR
1	A	104	ARG
1	A	136	ARG
1	A	138	LYS
1	A	153	LYS
1	A	185	GLN
1	A	238	ARG
1	A	246	SER
1	A	280	ARG
1	A	338	GLU
1	A	366	ARG
1	A	420	ARG
1	A	422	ASP
1	B	11	ILE
1	B	20	LYS
1	B	59	TYR
1	B	62	VAL
1	B	104	ARG
1	B	110	LYS
1	B	113	ARG
1	B	133	SER
1	B	137	ILE
1	B	144	ILE
1	B	186	ARG
1	B	267	GLU
1	B	366	ARG
1	B	413	LYS
1	B	439	SER
1	B	462	SER
1	B	480	LYS

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

sidechains are listed below:

Mol	Chain	Res	Type
1	B	418	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 ⓘ

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	$\# Z  > 2$
2	GLC	C	1	2	11,11,12	0.63	0	15,15,17	1.08	0
2	FRU	C	2	2	11,12,12	0.45	0	10,18,18	0.68	0
2	GLC	D	1	2	11,11,12	0.62	0	15,15,17	1.03	1 (6%)
2	FRU	D	2	2	11,12,12	0.58	0	10,18,18	0.62	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
2	GLC	C	1	2	-	2/2/19/22	0/1/1/1
2	FRU	C	2	2	-	3/5/24/24	0/1/1/1
2	GLC	D	1	2	-	2/2/19/22	0/1/1/1
2	FRU	D	2	2	-	2/5/24/24	0/1/1/1



There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	O5-C1-C2	-2.59	106.77	110.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

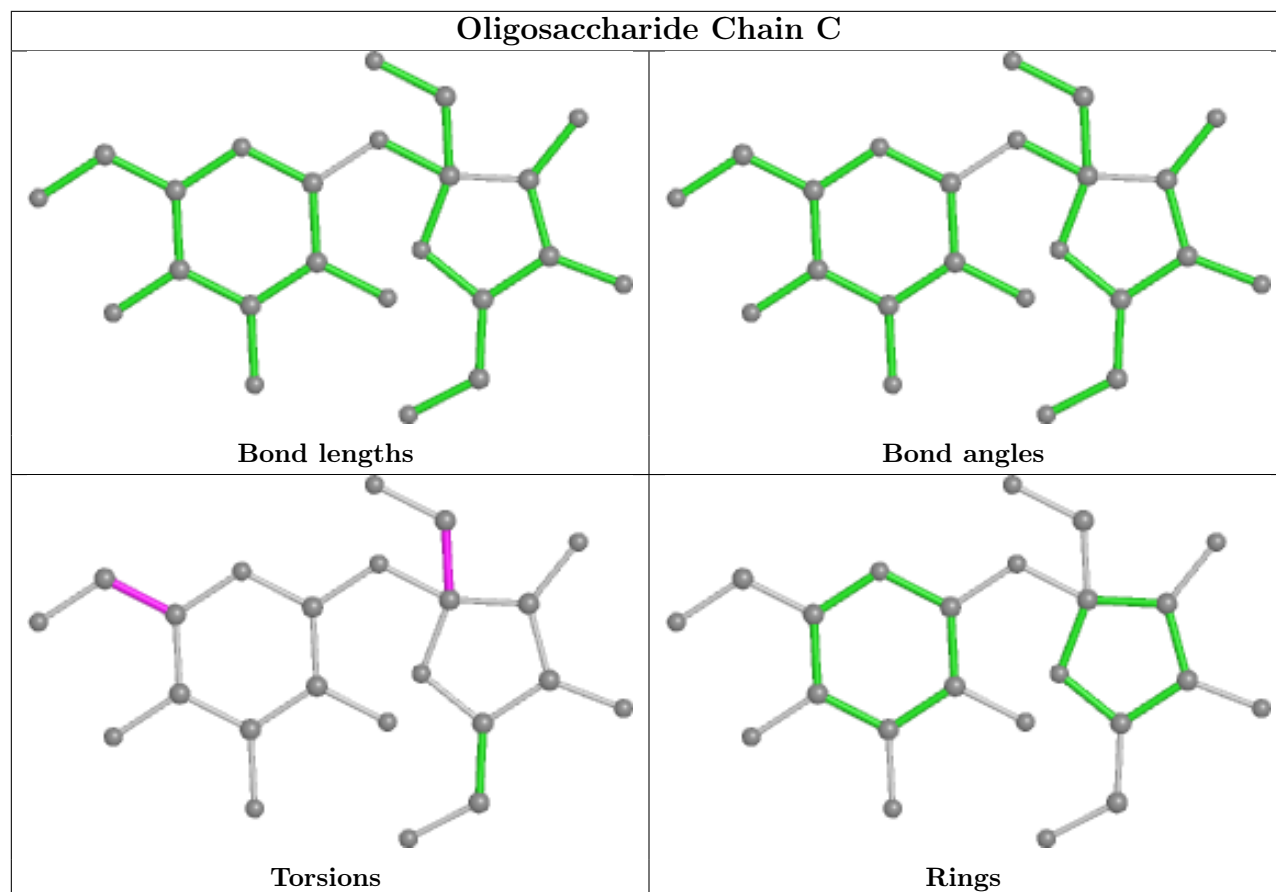
Mol	Chain	Res	Type	Atoms
2	C	2	FRU	O1-C1-C2-C3
2	C	2	FRU	O1-C1-C2-O2
2	C	1	GLC	O5-C5-C6-O6
2	D	2	FRU	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	D	2	FRU	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	C	2	FRU	O1-C1-C2-O5

There are no ring outliers.

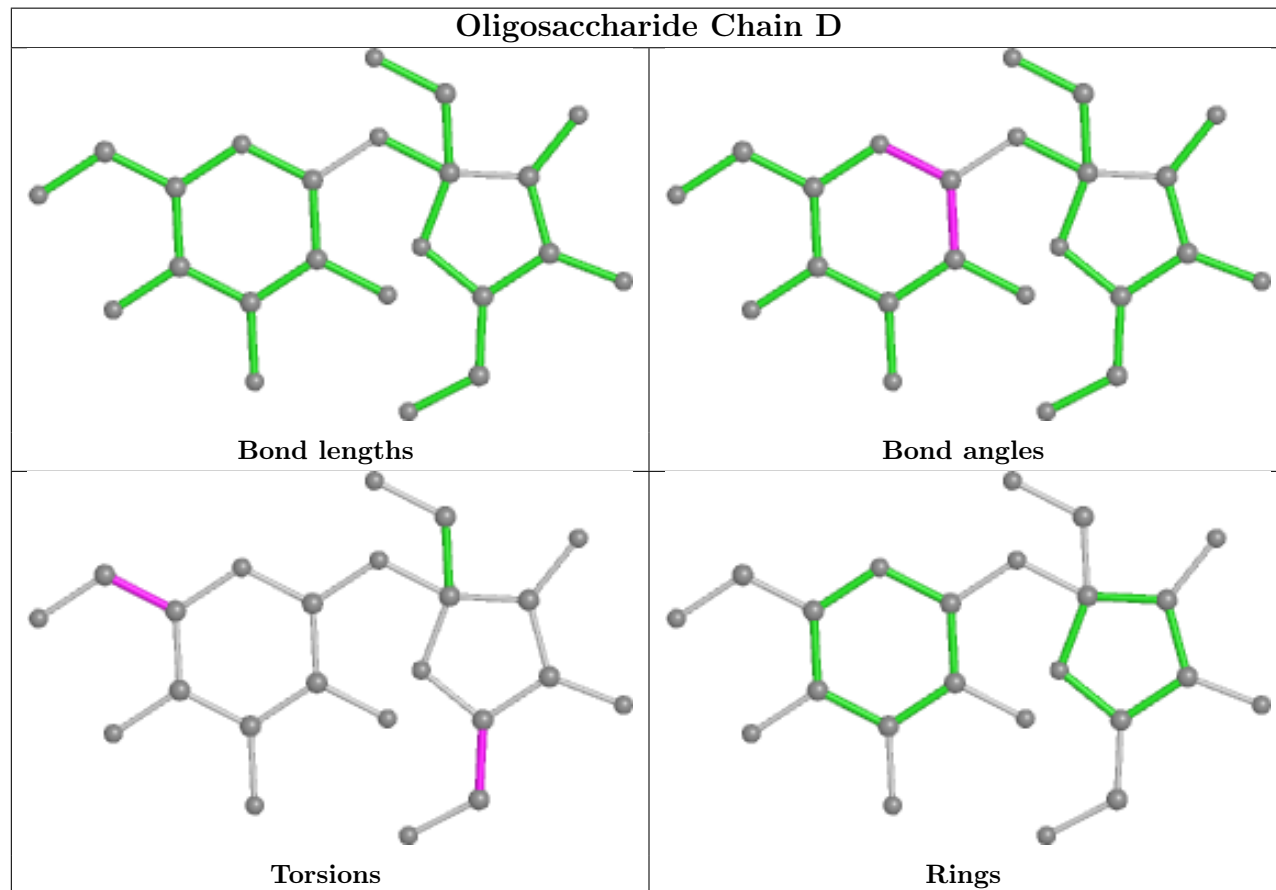
No monomer is involved in short contacts.

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

## Oligosaccharide Chain C



## Oligosaccharide Chain D



## 5.6 Ligand geometry

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	509	-	4,4,4	0.18	0	6,6,6	0.22	0
3	GTP	A	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.60	6 (18%)
5	SO4	A	504	-	4,4,4	0.15	0	6,6,6	0.38	0
5	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.57	0
5	SO4	B	502	-	4,4,4	0.19	0	6,6,6	0.50	0
5	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.21	0
3	GTP	B	501	6	26,34,34	1.08	2 (7%)	32,54,54	1.82	9 (28%)
5	SO4	B	505	-	4,4,4	0.25	0	6,6,6	0.24	0
5	SO4	B	506	-	4,4,4	0.09	0	6,6,6	0.21	0
5	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.50	0
5	SO4	A	508	-	4,4,4	0.19	0	6,6,6	0.16	0
5	SO4	B	504	-	4,4,4	0.13	0	6,6,6	0.17	0
5	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.69	0
5	SO4	A	507	-	4,4,4	0.16	0	6,6,6	0.12	0
4	GOL	A	502	-	5,5,5	1.09	0	5,5,5	0.78	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	GTP	B	501	6	-	4/18/38/38	0/3/3/3
3	GTP	A	501	6	-	8/18/38/38	0/3/3/3
4	GOL	A	502	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GTP	C5-C6	-4.08	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	GTP	C5-C6	-3.57	1.40	1.47
3	A	501	GTP	C2-N3	2.23	1.38	1.33
3	B	501	GTP	C2-N3	2.04	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	GTP	PA-O3A-PB	-4.45	117.56	132.83
3	A	501	GTP	PB-O3B-PG	-4.43	117.63	132.83
3	B	501	GTP	PB-O3B-PG	-4.36	117.88	132.83
3	A	501	GTP	PA-O3A-PB	-3.32	121.44	132.83
3	B	501	GTP	C8-N7-C5	3.26	109.21	102.99
3	A	501	GTP	C5-C6-N1	3.19	119.58	113.95
3	A	501	GTP	C8-N7-C5	3.03	108.77	102.99
3	B	501	GTP	C3'-C2'-C1'	2.92	105.38	100.98
3	B	501	GTP	O3G-PG-O3B	2.78	113.95	104.64
3	A	501	GTP	C2-N1-C6	-2.65	120.22	125.10
3	B	501	GTP	C5-C6-N1	2.55	118.45	113.95
3	B	501	GTP	C2-N1-C6	-2.42	120.64	125.10
3	B	501	GTP	C5'-C4'-C3'	-2.27	106.67	115.18
3	B	501	GTP	N2-C2-N1	2.07	121.11	116.71
3	A	501	GTP	O6-C6-C5	-2.03	120.40	124.37

There are no chirality outliers.

All (12) torsion outliers are listed below:

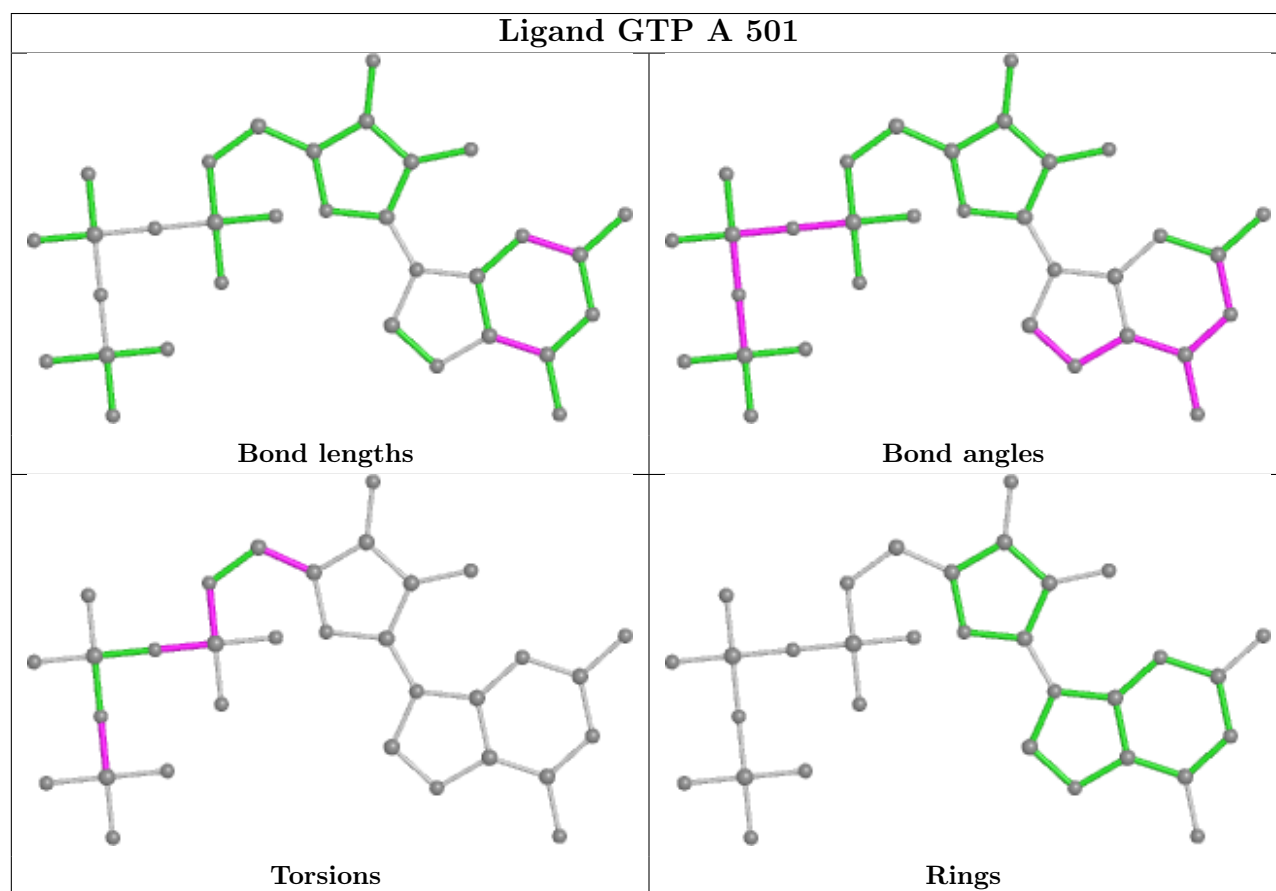
Mol	Chain	Res	Type	Atoms
3	A	501	GTP	C5'-O5'-PA-O3A
3	A	501	GTP	C5'-O5'-PA-O1A
3	B	501	GTP	C3'-C4'-C5'-O5'
3	B	501	GTP	O4'-C4'-C5'-O5'
3	A	501	GTP	PB-O3B-PG-O3G
3	A	501	GTP	C3'-C4'-C5'-O5'
3	A	501	GTP	O4'-C4'-C5'-O5'
3	A	501	GTP	PB-O3B-PG-O2G
3	A	501	GTP	PB-O3A-PA-O1A
3	A	501	GTP	PB-O3A-PA-O2A
3	B	501	GTP	PB-O3A-PA-O1A
3	B	501	GTP	PB-O3A-PA-O2A

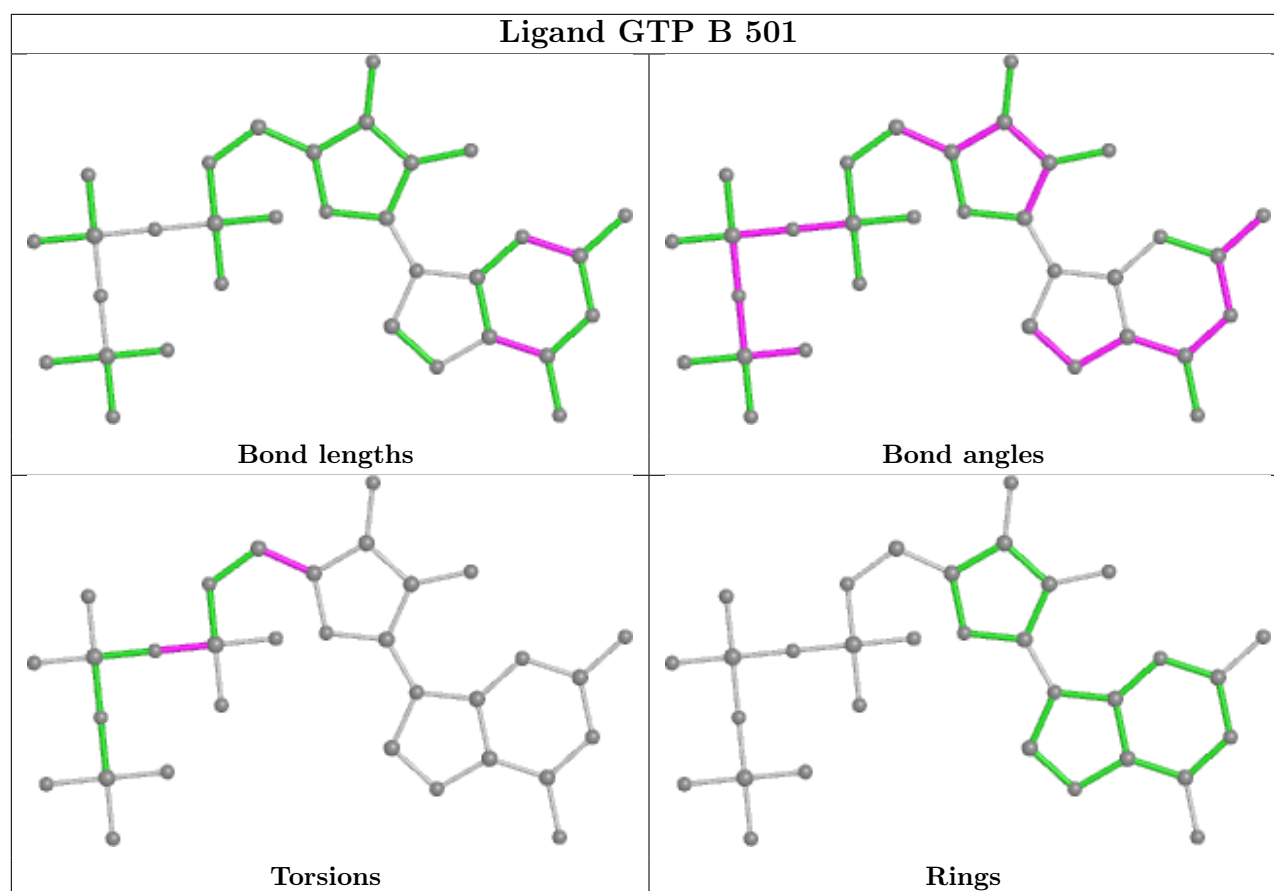
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	SO4	1	0
3	B	501	GTP	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	481/501 (96%)	0.15	19 (3%)	38 35	53, 73, 109, 152	0
1	B	481/501 (96%)	0.16	25 (5%)	27 24	53, 72, 110, 143	1 (0%)
All	All	962/1002 (96%)	0.16	44 (4%)	32 30	53, 72, 110, 152	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	TRP	5.6
1	B	138	LYS	4.6
1	B	415	ALA	4.4
1	A	419	TYR	4.3
1	A	263	TRP	4.0
1	B	428	LEU	3.9
1	B	423	ARG	3.8
1	B	424	ILE	3.7
1	A	423	ARG	3.5
1	B	417	ARG	3.4
1	A	422	ASP	3.3
1	B	143	GLN	3.2
1	A	136	ARG	3.2
1	A	415	ALA	3.1
1	B	422	ASP	3.1
1	A	343	ARG	2.9
1	B	426	GLN	2.7
1	B	427	GLU	2.7
1	B	410	LEU	2.7
1	B	420	ARG	2.6
1	A	1	MET	2.6
1	A	266	ARG	2.6
1	A	430	ASN	2.5
1	A	20	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	137	ILE	2.5
1	B	414	ALA	2.4
1	A	342	LYS	2.3
1	B	343	ARG	2.3
1	B	431	ARG	2.3
1	A	19	ASP	2.3
1	B	418	GLN	2.3
1	B	419	TYR	2.3
1	B	236	GLY	2.2
1	A	2	VAL	2.2
1	B	233	VAL	2.2
1	B	141	TRP	2.2
1	B	1	MET	2.2
1	A	418	GLN	2.2
1	B	430	ASN	2.2
1	B	132	GLY	2.2
1	A	157	ASP	2.1
1	A	420	ARG	2.1
1	A	250	ARG	2.1
1	A	426	GLN	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.

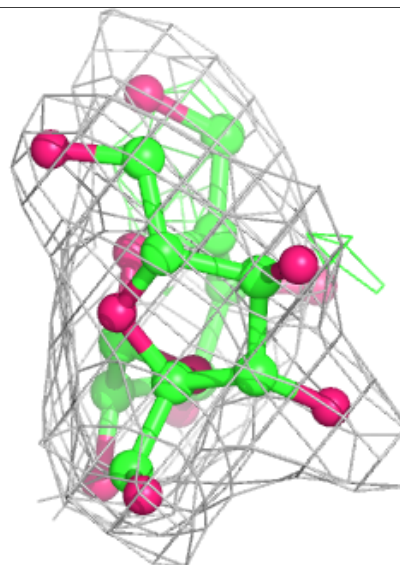
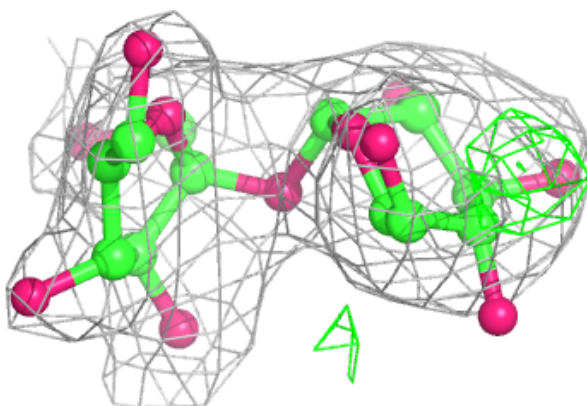
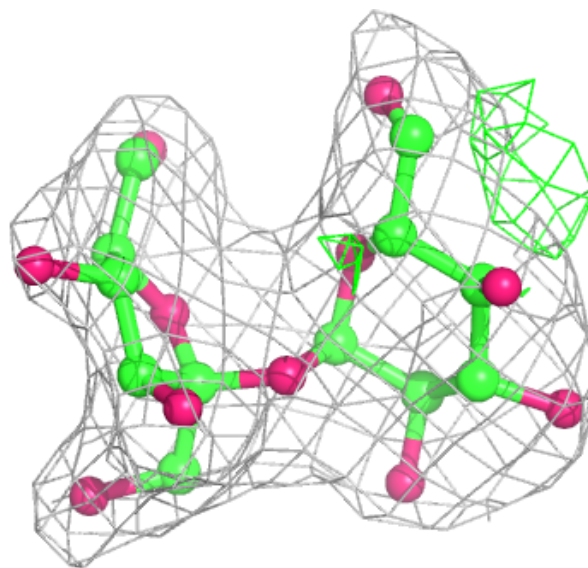
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FRU	D	2	12/12	0.90	0.30	76,81,93,93	5
2	FRU	C	2	12/12	0.91	0.15	76,79,85,88	6
2	GLC	D	1	11/12	0.92	0.23	78,87,92,93	5
2	GLC	C	1	11/12	0.93	0.18	76,82,88,96	6

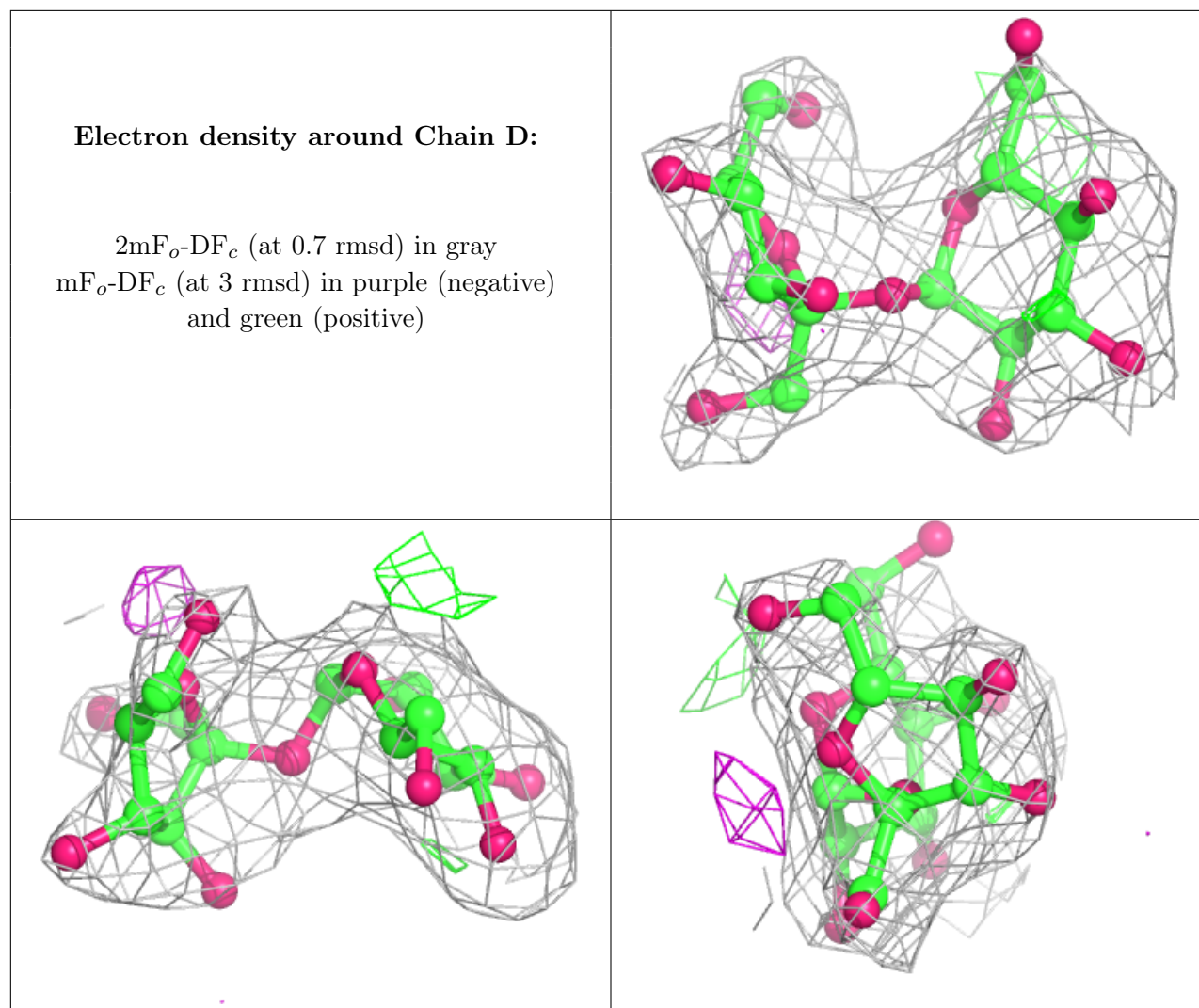
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain C:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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.

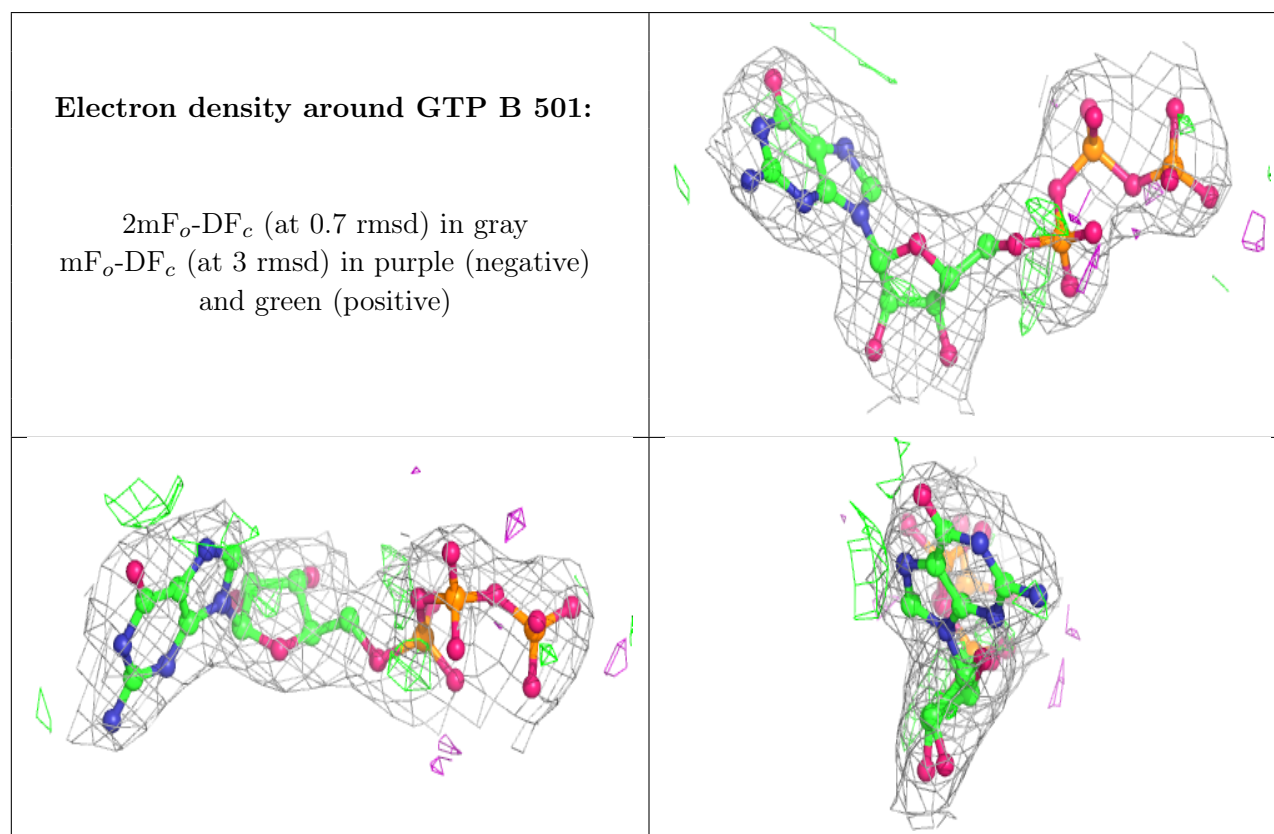
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	502	6/6	0.71	0.20	75,90,94,96	0
5	SO4	B	505	5/5	0.83	0.16	93,95,104,106	2
5	SO4	A	506	5/5	0.88	0.17	75,77,78,78	3
5	SO4	A	508	5/5	0.89	0.24	83,85,90,102	3
5	SO4	A	509	5/5	0.90	0.35	90,91,96,101	3
5	SO4	A	507	5/5	0.90	0.15	96,99,107,108	2
5	SO4	A	505	5/5	0.95	0.13	72,85,87,94	2
3	GTP	B	501	32/32	0.95	0.22	53,69,75,83	16

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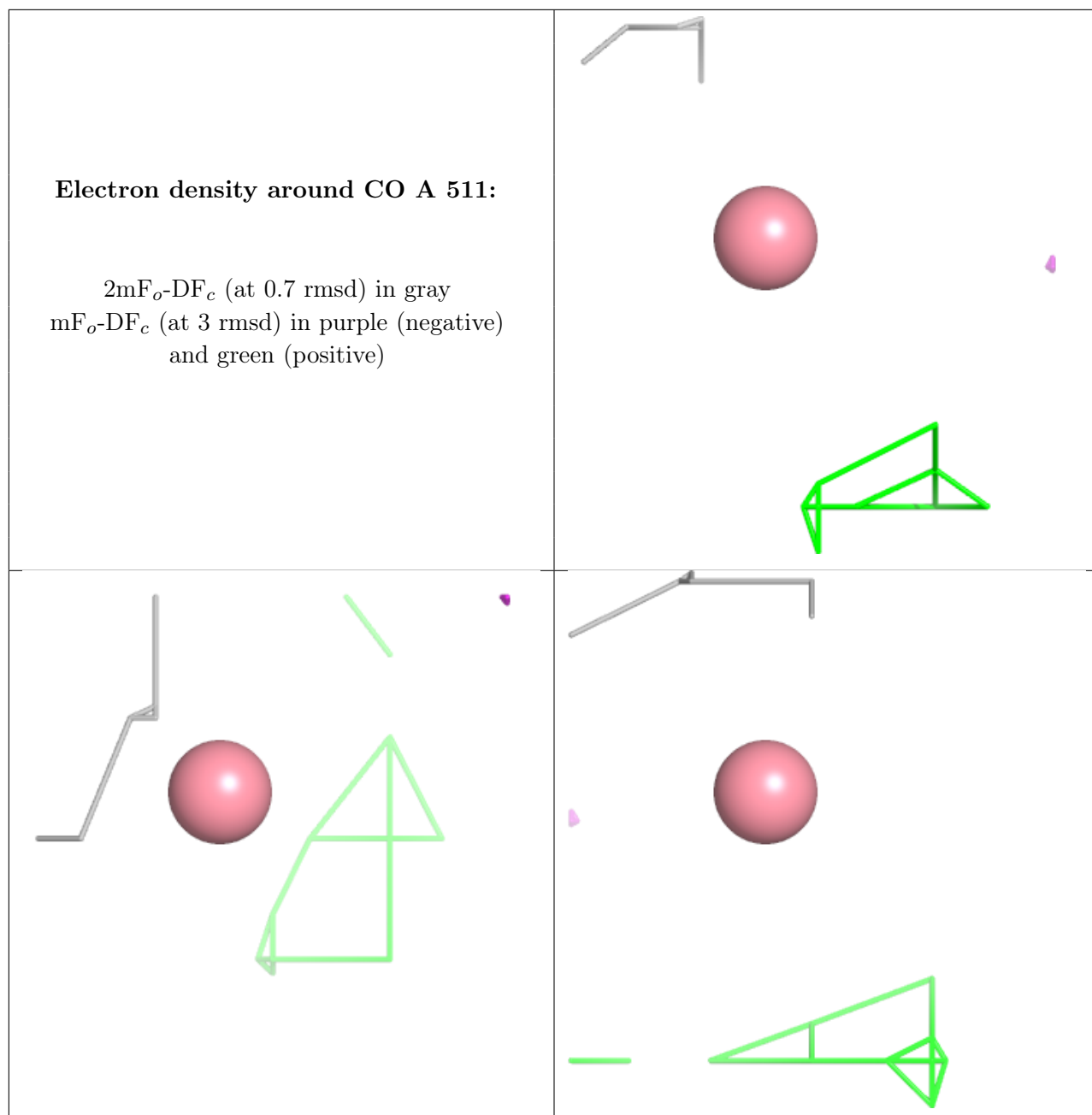
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	506	5/5	0.95	0.38	87,90,93,96	3
5	SO4	B	504	5/5	0.96	0.08	82,87,91,91	3
5	SO4	B	503	5/5	0.97	0.34	66,68,73,77	2
5	SO4	A	504	5/5	0.97	0.36	66,66,76,83	3
5	SO4	A	503	5/5	0.97	0.23	67,68,74,78	3
5	SO4	B	502	5/5	0.97	0.24	57,58,68,78	3
6	CO	A	511	1/1	0.97	0.13	70,70,70,70	1
6	CO	B	507	1/1	0.97	0.15	72,72,72,72	1
6	CO	B	508	1/1	0.97	0.12	77,77,77,77	0
3	GTP	A	501	32/32	0.98	0.24	49,67,72,76	18
6	CO	A	510	1/1	0.99	0.12	71,71,71,71	1

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.



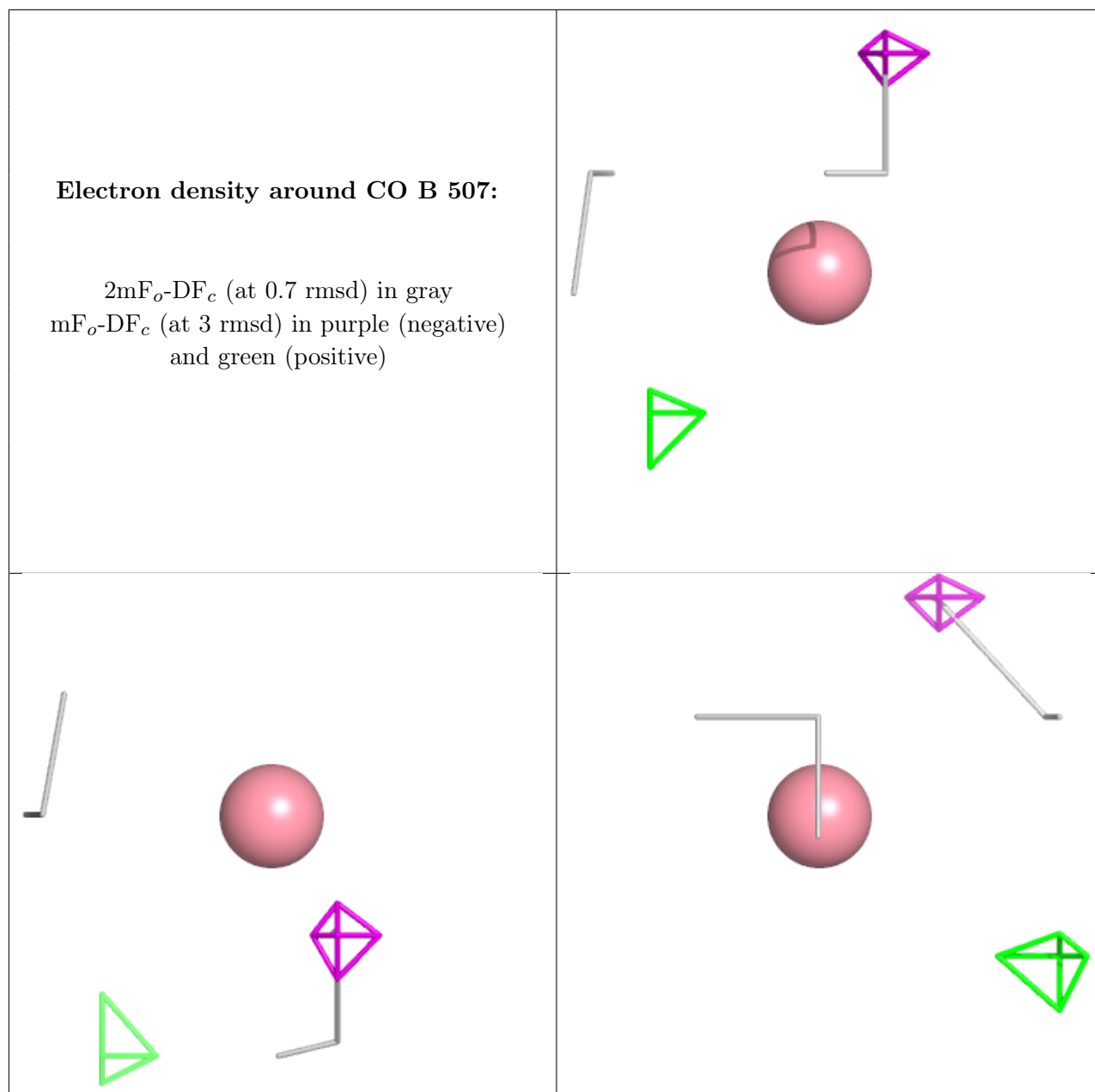
**Electron density around CO A 511:**

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



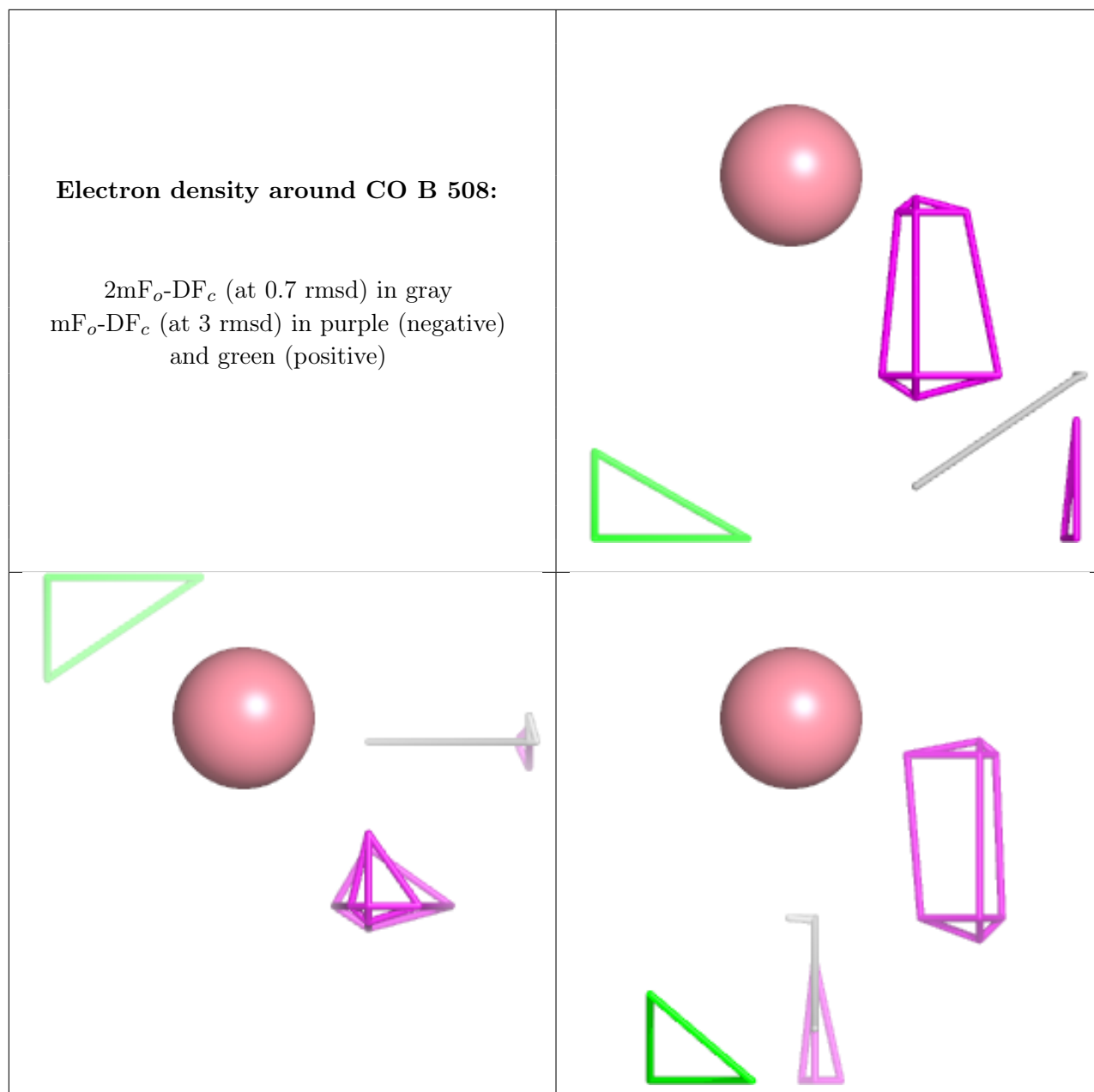
**Electron density around CO B 507:**

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



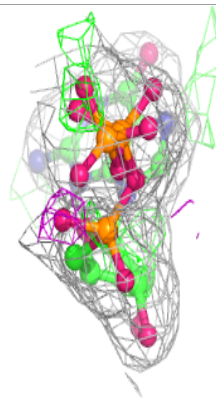
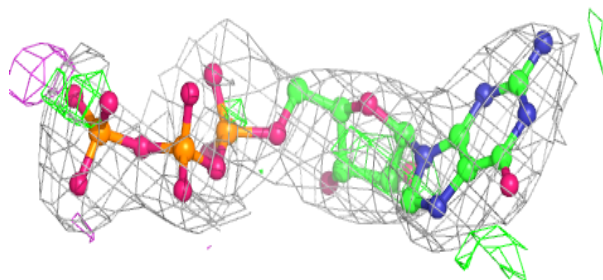
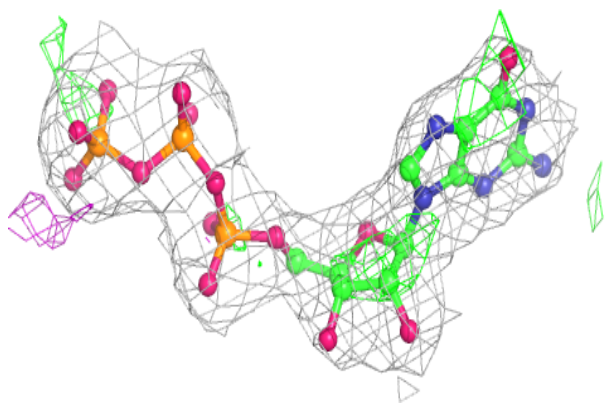
**Electron density around CO B 508:**

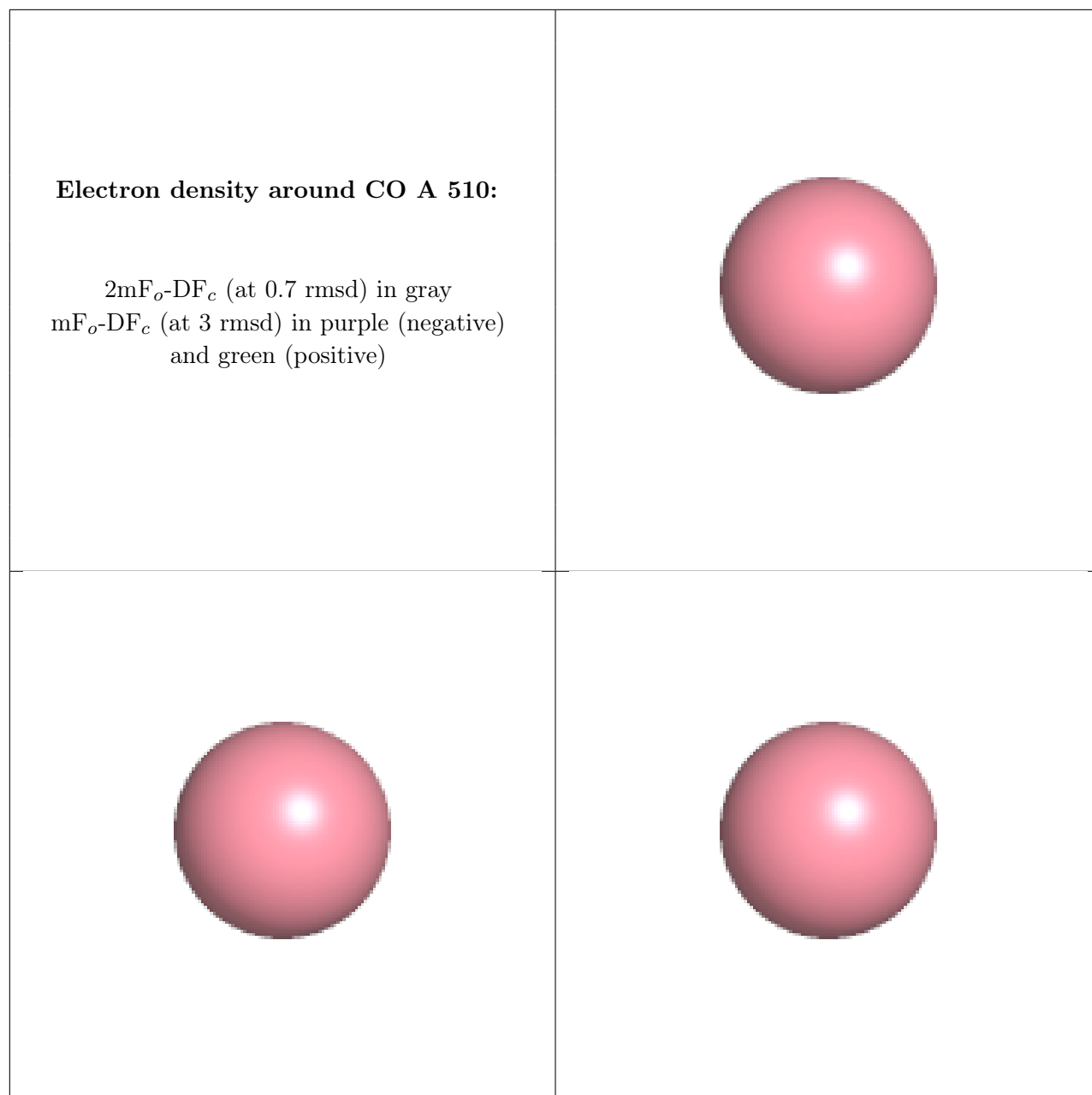
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GTP A 501:**

$2mF_o-DF_c$  (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.