Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 10:39 am GMT

PDB ID	:	6GNF
Title	:	Granule Bound Starch Synthase from Cyanobacterium sp. CLg1 bound to acarbose and ADP
Authors	:	Cuesta-Seijo, J.A.; Nielsen, M.M.; Palcic, M.M.
Deposited on	:	2018-05-30
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

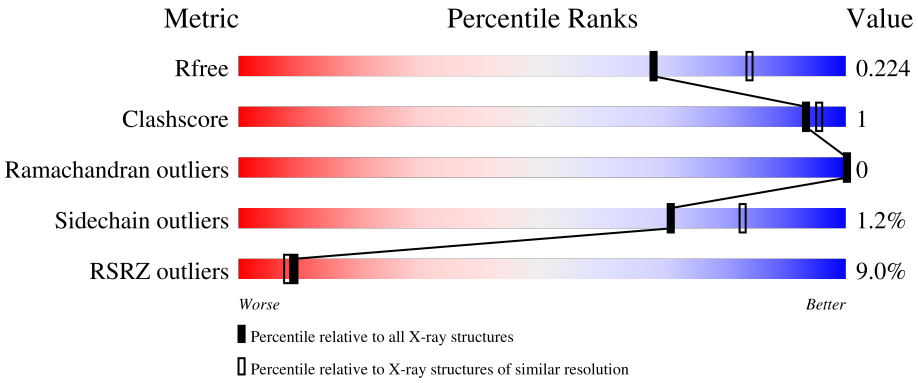
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	544	6% 93%
1	B	544	12% 86% 10%
1	C	544	6% 91% 6%
2	D	3	100%
2	E	3	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12463 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 Glycogen synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	2	0
			4076	2630	667	752	27			
1	B	492	Total	C	N	O	S	0	1	0
			3835	2476	632	700	27			
1	C	514	Total	C	N	O	S	0	0	0
			3995	2577	660	731	27			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP V5SNJ5
A	-18	GLY	-	expression tag	UNP V5SNJ5
A	-17	SER	-	expression tag	UNP V5SNJ5
A	-16	SER	-	expression tag	UNP V5SNJ5
A	-15	HIS	-	expression tag	UNP V5SNJ5
A	-14	HIS	-	expression tag	UNP V5SNJ5
A	-13	HIS	-	expression tag	UNP V5SNJ5
A	-12	HIS	-	expression tag	UNP V5SNJ5
A	-11	HIS	-	expression tag	UNP V5SNJ5
A	-10	HIS	-	expression tag	UNP V5SNJ5
A	-9	SER	-	expression tag	UNP V5SNJ5
A	-8	SER	-	expression tag	UNP V5SNJ5
A	-7	GLY	-	expression tag	UNP V5SNJ5
A	-6	LEU	-	expression tag	UNP V5SNJ5
A	-5	VAL	-	expression tag	UNP V5SNJ5
A	-4	PRO	-	expression tag	UNP V5SNJ5
A	-3	ARG	-	expression tag	UNP V5SNJ5
A	-2	GLY	-	expression tag	UNP V5SNJ5
A	-1	SER	-	expression tag	UNP V5SNJ5
A	0	HIS	-	expression tag	UNP V5SNJ5
B	-19	MET	-	initiating methionine	UNP V5SNJ5
B	-18	GLY	-	expression tag	UNP V5SNJ5
B	-17	SER	-	expression tag	UNP V5SNJ5

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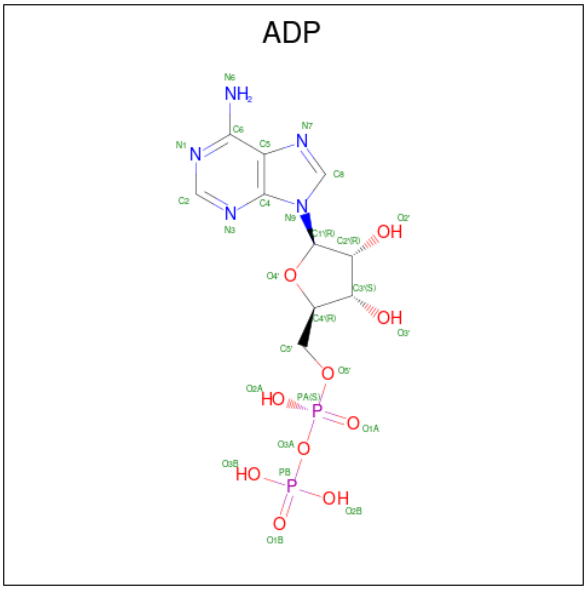
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP V5SNJ5
B	-15	HIS	-	expression tag	UNP V5SNJ5
B	-14	HIS	-	expression tag	UNP V5SNJ5
B	-13	HIS	-	expression tag	UNP V5SNJ5
B	-12	HIS	-	expression tag	UNP V5SNJ5
B	-11	HIS	-	expression tag	UNP V5SNJ5
B	-10	HIS	-	expression tag	UNP V5SNJ5
B	-9	SER	-	expression tag	UNP V5SNJ5
B	-8	SER	-	expression tag	UNP V5SNJ5
B	-7	GLY	-	expression tag	UNP V5SNJ5
B	-6	LEU	-	expression tag	UNP V5SNJ5
B	-5	VAL	-	expression tag	UNP V5SNJ5
B	-4	PRO	-	expression tag	UNP V5SNJ5
B	-3	ARG	-	expression tag	UNP V5SNJ5
B	-2	GLY	-	expression tag	UNP V5SNJ5
B	-1	SER	-	expression tag	UNP V5SNJ5
B	0	HIS	-	expression tag	UNP V5SNJ5
C	-19	MET	-	initiating methionine	UNP V5SNJ5
C	-18	GLY	-	expression tag	UNP V5SNJ5
C	-17	SER	-	expression tag	UNP V5SNJ5
C	-16	SER	-	expression tag	UNP V5SNJ5
C	-15	HIS	-	expression tag	UNP V5SNJ5
C	-14	HIS	-	expression tag	UNP V5SNJ5
C	-13	HIS	-	expression tag	UNP V5SNJ5
C	-12	HIS	-	expression tag	UNP V5SNJ5
C	-11	HIS	-	expression tag	UNP V5SNJ5
C	-10	HIS	-	expression tag	UNP V5SNJ5
C	-9	SER	-	expression tag	UNP V5SNJ5
C	-8	SER	-	expression tag	UNP V5SNJ5
C	-7	GLY	-	expression tag	UNP V5SNJ5
C	-6	LEU	-	expression tag	UNP V5SNJ5
C	-5	VAL	-	expression tag	UNP V5SNJ5
C	-4	PRO	-	expression tag	UNP V5SNJ5
C	-3	ARG	-	expression tag	UNP V5SNJ5
C	-2	GLY	-	expression tag	UNP V5SNJ5
C	-1	SER	-	expression tag	UNP V5SNJ5
C	0	HIS	-	expression tag	UNP V5SNJ5

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

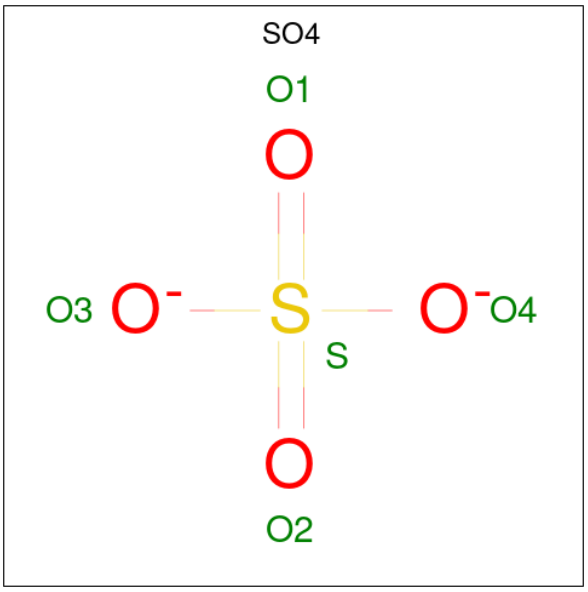
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	3	Total C N O 44 25 1 18	0	0	0
2	E	3	Total C N O 44 25 1 18	0	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



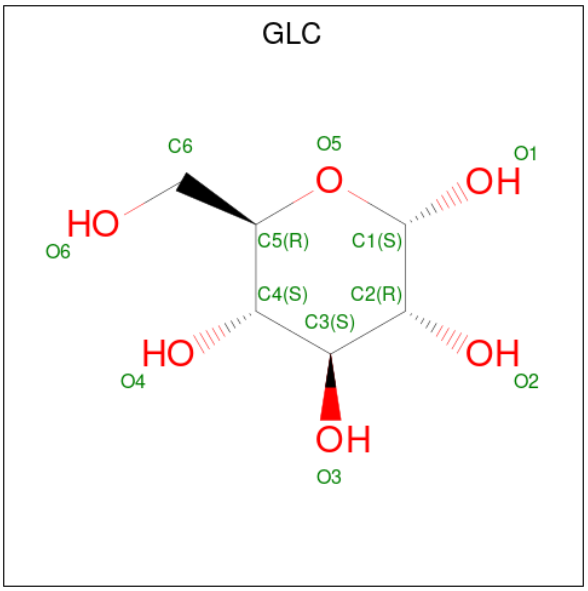
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0
3	C	1	Total C N O P 54 20 10 20 4	0	1

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 12 6 6	0	0

- Molecule 6 is water.

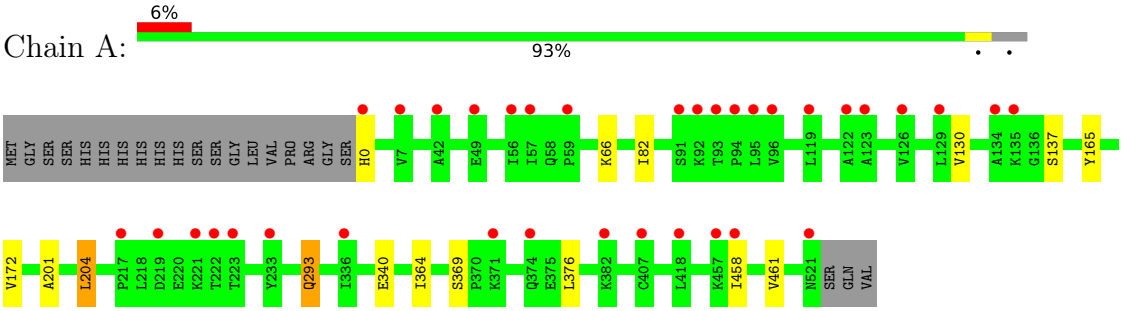
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	113	Total O 113 113	0	0
6	B	73	Total O 73 73	0	0
6	C	118	Total O 118 118	0	0

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.

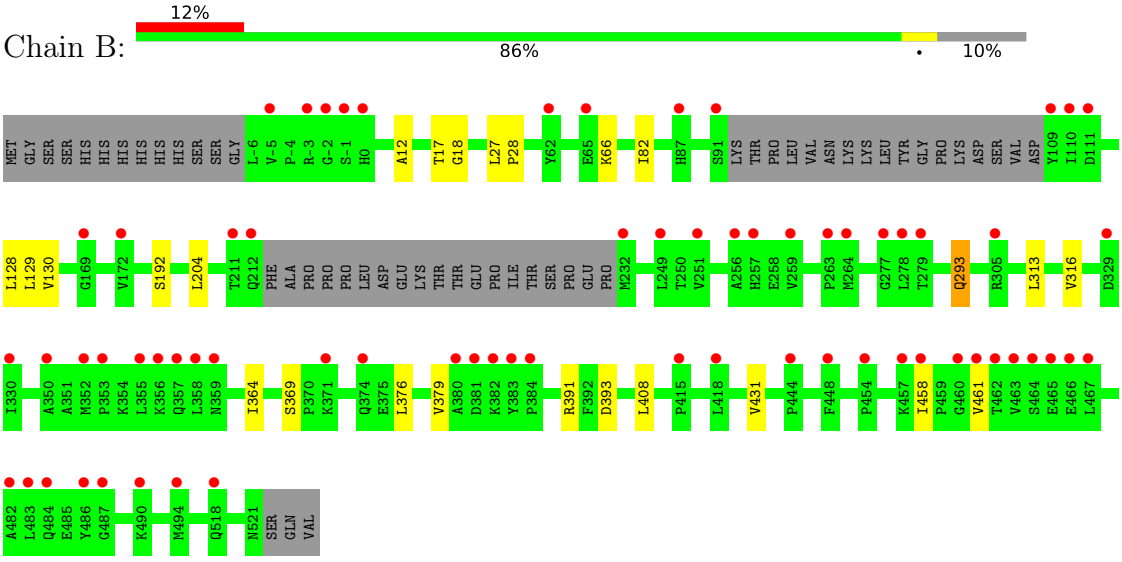
• Molecule 1: Glycogen synthase

Chain A:



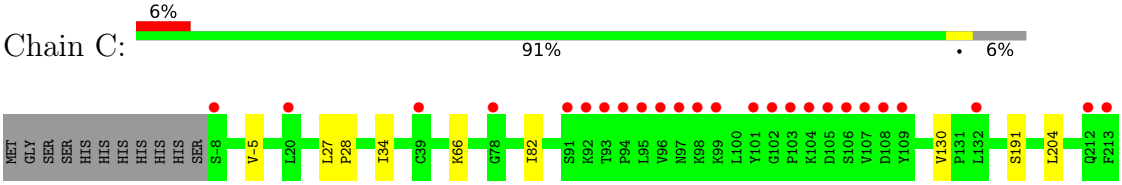
• Molecule 1: Glycogen synthase

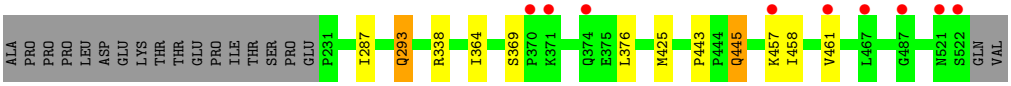
Chain B:



• Molecule 1: Glycogen synthase

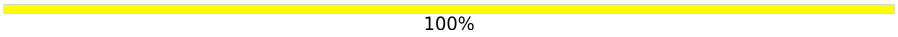
Chain C:





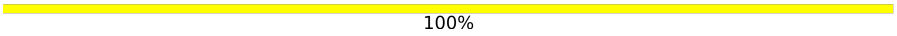
• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain D:



• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	194.26Å 132.65Å 123.69Å 90.00° 126.30° 90.00°	Depositor
Resolution (Å)	48.56 – 2.20 48.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.56-2.20) 95.6 (48.56-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.224 0.209 , 0.224	Depositor DCC
R_{free} test set	3647 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12463	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, BGC, AC1, ADP, SO4

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	0.34	0/4183	0.54	0/5682
1	B	0.34	0/3929	0.54	0/5328
1	C	0.36	0/4091	0.53	0/5548
All	All	0.35	0/12203	0.53	0/16558

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

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	4076	0	4101	8	0
1	B	3835	0	3855	14	0
1	C	3995	0	4022	11	0
2	D	44	0	30	0	0
2	E	44	0	30	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	54	0	24	4	0
4	A	20	0	0	0	0
4	B	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	15	0	0	1	0
5	B	12	0	12	0	0
6	A	113	0	0	2	0
6	B	73	0	0	1	0
6	C	118	0	0	1	0
All	All	12463	0	12098	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (35) 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:A:137:SER:HB3	6:A:701:HOH:O	1.81	0.81
3:C:601[A]:ADP:O1A	6:C:701:HOH:O	0.70	0.70
3:C:601[B]:ADP:O3B	3:C:601[B]:ADP:O2A	2.11	0.69
1:C:443:PRO:HB2	1:C:445:GLN:OE1	1.98	0.63
1:C:338:ARG:HG3	3:C:601[B]:ADP:O1A	1.98	0.63
1:B:17:THR:OG1	6:B:701:HOH:O	2.16	0.60
1:B:408:LEU:HD12	1:B:431:VAL:HG13	1.88	0.55
1:A:293:GLN:HE21	1:A:293:GLN:H	1.53	0.53
1:C:293:GLN:H	1:C:293:GLN:HE21	1.57	0.53
1:B:293:GLN:HE21	1:B:293:GLN:H	1.58	0.51
1:B:192:SER:N	4:B:603:SO4:O4	2.40	0.50
1:A:458:ILE:HG13	1:A:461:VAL:HB	1.97	0.47
1:B:12:ALA:HB2	1:B:17:THR:HG21	1.97	0.47
1:B:458:ILE:HG13	1:B:461:VAL:HB	1.97	0.47
3:C:601[B]:ADP:O3B	3:C:601[B]:ADP:H5'2	2.15	0.46
1:C:458:ILE:HG13	1:C:461:VAL:HB	1.97	0.46
1:B:82:ILE:HD12	1:B:130:VAL:HG11	1.99	0.45
1:C:82:ILE:HD12	1:C:130:VAL:HG11	1.98	0.45
1:A:82:ILE:HD12	1:A:130:VAL:HG11	1.98	0.45
1:B:364:ILE:HB	1:B:376:LEU:HD11	2.00	0.44
1:A:364:ILE:HB	1:A:376:LEU:HD11	2.00	0.44
1:A:172:VAL:HG12	6:A:712:HOH:O	2.17	0.44
1:C:34:ILE:HG22	1:C:34:ILE:O	2.18	0.43
1:C:191:SER:OG	4:C:604:SO4:O2	2.33	0.43
1:B:128:LEU:HB2	1:B:129:LEU:HD13	2.00	0.43
1:A:165:TYR:CE2	1:C:-5:VAL:HB	2.54	0.43
1:C:364:ILE:HB	1:C:376:LEU:HD11	2.00	0.42
1:B:17:THR:HG23	1:B:18:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LEU:HB3	1:C:28:PRO:HD3	2.02	0.42
1:B:27:LEU:HB3	1:B:28:PRO:HD3	2.02	0.41
1:C:287:ILE:HG23	1:C:425:MET:HE1	2.02	0.41
1:A:201:ALA:O	1:A:204:LEU:HB2	2.21	0.41
1:B:376:LEU:O	1:B:379:VAL:HG12	2.21	0.40
1:B:391:ARG:NH1	1:B:393:ASP:OD2	2.54	0.40
1:B:313:LEU:HA	1:B:316:VAL:HG22	2.03	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	522/544 (96%)	506 (97%)	16 (3%)	0	100	100
1	B	487/544 (90%)	472 (97%)	15 (3%)	0	100	100
1	C	510/544 (94%)	493 (97%)	17 (3%)	0	100	100
All	All	1519/1632 (93%)	1471 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	449/466 (96%)	443 (99%)	6 (1%)	69	81
1	B	418/466 (90%)	414 (99%)	4 (1%)	76	86
1	C	437/466 (94%)	431 (99%)	6 (1%)	67	80
All	All	1304/1398 (93%)	1288 (99%)	16 (1%)	71	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	66	LYS
1	A	204	LEU
1	A	293	GLN
1	A	340	GLU
1	A	369	SER
1	B	66	LYS
1	B	204	LEU
1	B	293	GLN
1	B	369	SER
1	C	66	LYS
1	C	204	LEU
1	C	293	GLN
1	C	369	SER
1	C	445	GLN
1	C	457	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	A	470	GLN
1	B	210	ASN
1	B	212	GLN
1	B	293	GLN
1	B	470	GLN
1	C	293	GLN
1	C	470	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
5	GLC	B	602	-	12,12,12	0.76	0	17,17,17	1.76	3 (17%)

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
5	GLC	B	602	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	602	GLC	O5-C1-C2	3.92	117.28	110.28
5	B	602	GLC	C1-C2-C3	3.40	117.37	110.31
5	B	602	GLC	C1-O5-C5	3.04	119.39	113.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

6 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	BGC	D	1	2	12,12,12	0.54	0	17,17,17	1.02	1 (5%)
2	GLC	D	2	2	11,11,12	0.44	0	15,15,17	0.99	1 (6%)
2	AC1	D	3	2	21,22,23	0.80	1 (4%)	22,32,34	1.34	4 (18%)
2	BGC	E	1	2	12,12,12	0.50	0	17,17,17	0.85	1 (5%)
2	GLC	E	2	2	11,11,12	0.52	0	15,15,17	1.07	1 (6%)
2	AC1	E	3	2	21,22,23	0.95	1 (4%)	22,32,34	1.63	5 (22%)

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	BGC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	AC1	D	3	2	-	1/6/43/46	0/2/2/2
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	AC1	E	3	2	-	1/6/43/46	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	AC1	C2B-C1B	2.48	1.56	1.52
2	E	3	AC1	C4A-C5B	-2.21	1.49	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	GLC	C1-O5-C5	3.61	117.09	112.19
2	D	3	AC1	O2B-C2B-C3B	-3.08	103.22	110.35
2	E	3	AC1	C2B-C3B-C4A	3.03	114.99	110.18
2	E	3	AC1	O3B-C3B-C4A	-2.90	104.15	109.68
2	E	3	AC1	C7B-C1B-N4A	2.81	114.89	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	AC1	O6B-C6B-C5B	-2.36	106.84	112.50
2	D	3	AC1	O2B-C2B-C1B	2.31	113.76	109.12
2	E	3	AC1	O2B-C2B-C3B	-2.30	105.04	110.35
2	E	3	AC1	C1-C2-C3	2.22	112.40	109.67
2	D	1	BGC	O5-C5-C4	2.16	113.62	109.69
2	E	1	BGC	C3-C4-C5	2.13	114.04	110.24
2	D	2	GLC	O5-C5-C6	2.06	110.43	107.20
2	D	3	AC1	O4-C4A-C3B	-2.04	106.31	110.53

There are no chirality outliers.

All (6) torsion outliers are listed below:

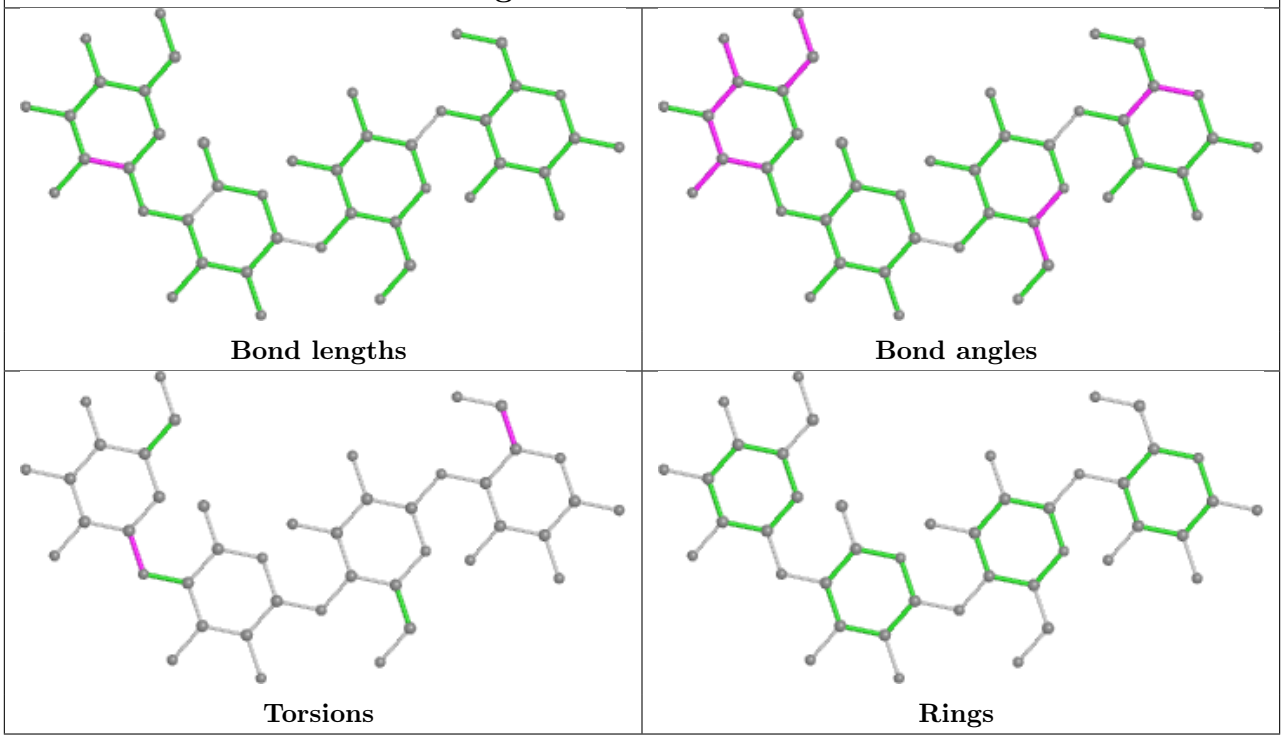
Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C7B-C1B-N4A-C4
2	E	3	AC1	C7B-C1B-N4A-C4
2	E	2	GLC	O5-C5-C6-O6
2	D	1	BGC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	D	1	BGC	O5-C5-C6-O6

There are no ring outliers.

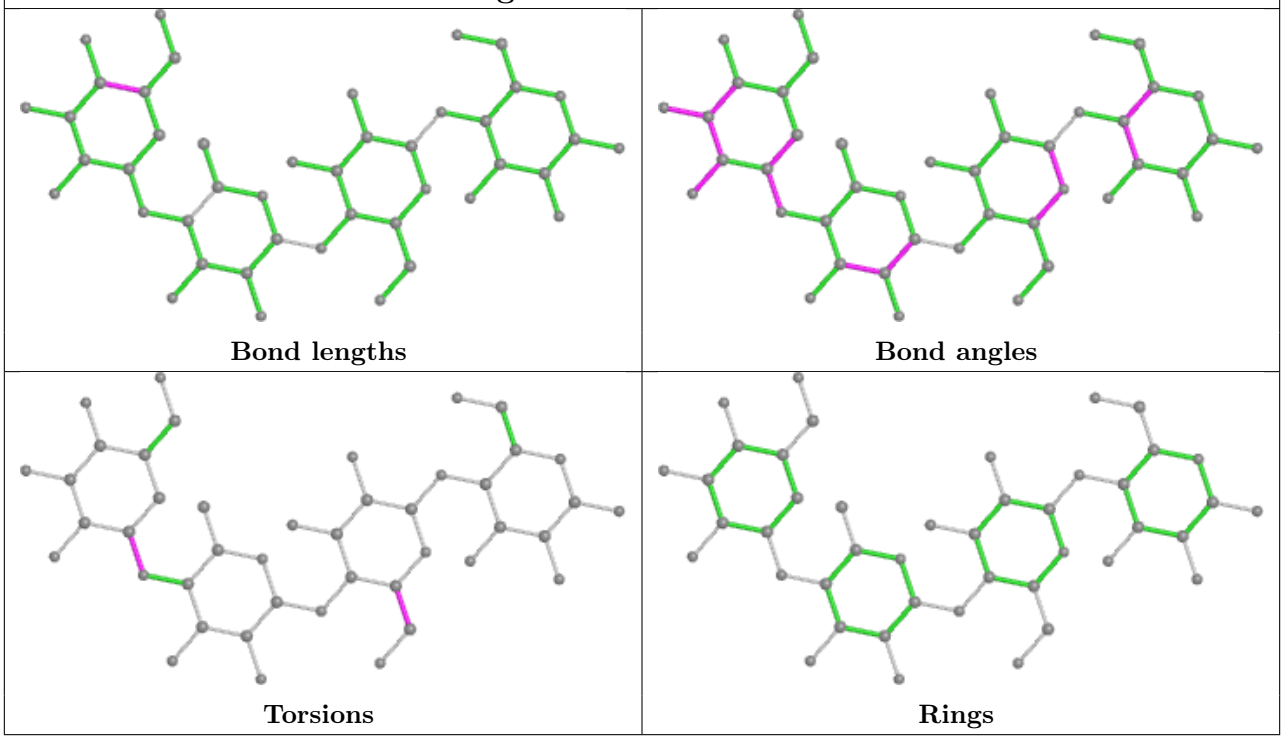
No monomer is involved in short contacts.

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

Oligosaccharide Chain D



Oligosaccharide Chain E



5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	604	-	4,4,4	0.35	0	6,6,6	0.18	0
3	ADP	C	601[B]	-	24,29,29	0.96	1 (4%)	29,45,45	1.52	4 (13%)
4	SO4	B	604	-	4,4,4	0.35	0	6,6,6	0.11	0
4	SO4	A	603	-	4,4,4	0.39	0	6,6,6	0.20	0
3	ADP	B	601	-	24,29,29	1.04	1 (4%)	29,45,45	1.28	3 (10%)
3	ADP	C	601[A]	-	24,29,29	0.95	1 (4%)	29,45,45	1.40	4 (13%)
3	ADP	A	601	-	24,29,29	0.97	1 (4%)	29,45,45	1.40	5 (17%)
4	SO4	C	604	-	4,4,4	0.42	0	6,6,6	0.23	0
4	SO4	C	605	-	4,4,4	0.31	0	6,6,6	0.14	0
4	SO4	B	603	-	4,4,4	0.39	0	6,6,6	0.34	0
4	SO4	A	606	-	4,4,4	0.36	0	6,6,6	0.17	0
5	GLC	B	602	-	12,12,12	0.76	0	17,17,17	1.76	3 (17%)
4	SO4	A	605	-	4,4,4	0.36	0	6,6,6	0.25	0
4	SO4	C	603	-	4,4,4	0.45	0	6,6,6	0.26	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	ADP	C	601[B]	-	-	6/12/32/32	0/3/3/3
3	ADP	B	601	-	-	4/12/32/32	0/3/3/3
3	ADP	C	601[A]	-	-	4/12/32/32	0/3/3/3
3	ADP	A	601	-	-	5/12/32/32	0/3/3/3
5	GLC	B	602	-	-	0/2/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	ADP	C5-C4	2.63	1.47	1.40
3	A	601	ADP	C5-C4	2.49	1.47	1.40
3	C	601[A]	ADP	C5-C4	2.37	1.47	1.40
3	C	601[B]	ADP	C5-C4	2.34	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	601[B]	ADP	PA-O3A-PB	-4.76	116.48	132.83
3	A	601	ADP	N3-C2-N1	-3.97	122.48	128.68
5	B	602	GLC	O5-C1-C2	3.92	117.28	110.28
3	C	601[A]	ADP	N3-C2-N1	-3.75	122.81	128.68
3	C	601[B]	ADP	N3-C2-N1	-3.69	122.91	128.68
5	B	602	GLC	C1-C2-C3	3.40	117.37	110.31
3	B	601	ADP	PA-O3A-PB	-3.23	121.75	132.83
3	B	601	ADP	N3-C2-N1	-3.13	123.79	128.68
5	B	602	GLC	C1-O5-C5	3.04	119.39	113.66
3	C	601[A]	ADP	PA-O3A-PB	-2.98	122.59	132.83
3	A	601	ADP	C4-C5-N7	-2.63	106.66	109.40
3	B	601	ADP	C4-C5-N7	-2.59	106.70	109.40
3	C	601[A]	ADP	C4-C5-N7	-2.39	106.91	109.40
3	C	601[B]	ADP	C4-C5-N7	-2.31	107.00	109.40
3	C	601[B]	ADP	C2-N1-C6	2.17	122.47	118.75
3	A	601	ADP	C3'-C2'-C1'	2.15	104.21	100.98
3	A	601	ADP	C2-N1-C6	2.07	122.30	118.75
3	A	601	ADP	O3B-PB-O2B	2.07	115.54	107.64
3	C	601[A]	ADP	O3B-PB-O2B	2.00	115.29	107.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ADP	PA-O3A-PB-O2B
3	C	601[A]	ADP	PA-O3A-PB-O3B
3	C	601[B]	ADP	PA-O3A-PB-O3B
3	B	601	ADP	O4'-C4'-C5'-O5'
3	B	601	ADP	C3'-C4'-C5'-O5'
3	C	601[B]	ADP	O4'-C4'-C5'-O5'
3	C	601[B]	ADP	C3'-C4'-C5'-O5'
3	B	601	ADP	PB-O3A-PA-O1A
3	A	601	ADP	C5'-O5'-PA-O3A
3	C	601[A]	ADP	O4'-C4'-C5'-O5'
3	A	601	ADP	O4'-C4'-C5'-O5'
3	C	601[B]	ADP	PA-O3A-PB-O1B
3	A	601	ADP	PA-O3A-PB-O3B
3	C	601[A]	ADP	PA-O3A-PB-O2B
3	C	601[B]	ADP	PA-O3A-PB-O2B
3	B	601	ADP	PB-O3A-PA-O2A
3	C	601[B]	ADP	C5'-O5'-PA-O1A

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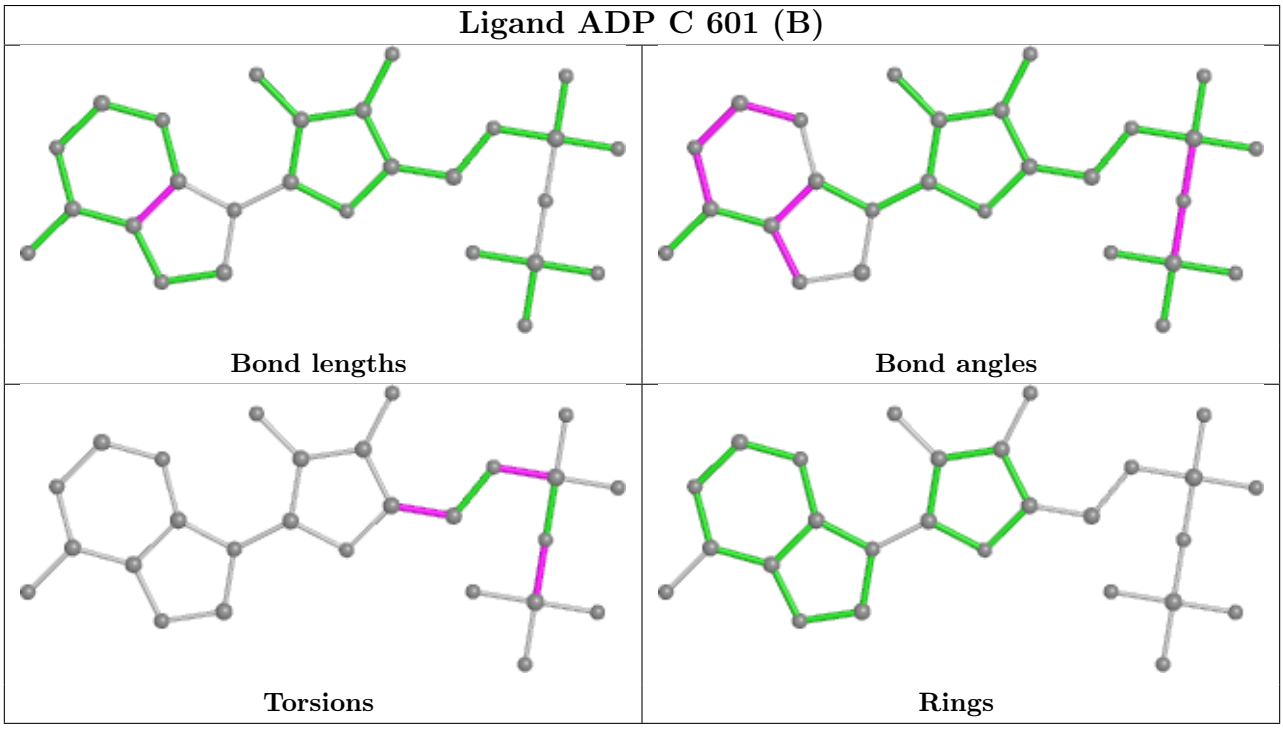
Mol	Chain	Res	Type	Atoms
3	C	601[A]	ADP	C3'-C4'-C5'-O5'
3	A	601	ADP	PA-O3A-PB-O1B

There are no ring outliers.

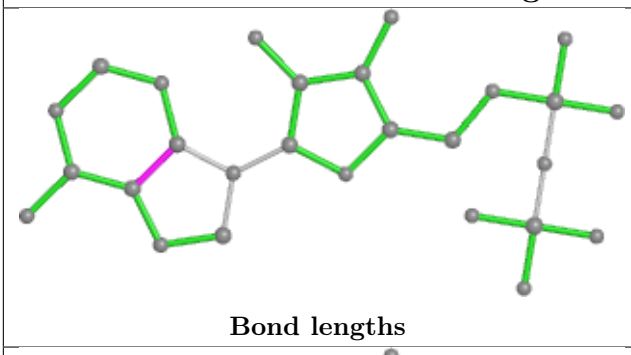
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601[B]	ADP	3	0
3	C	601[A]	ADP	1	0
4	C	604	SO4	1	0
4	B	603	SO4	1	0

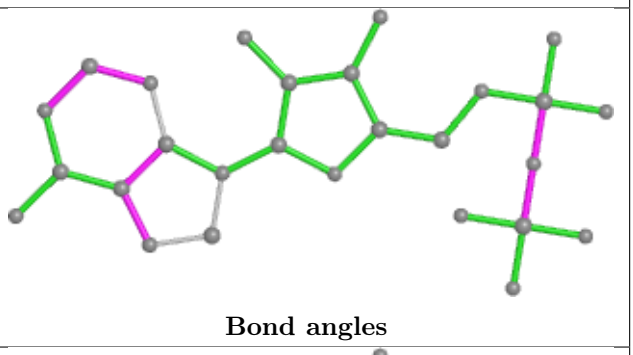
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



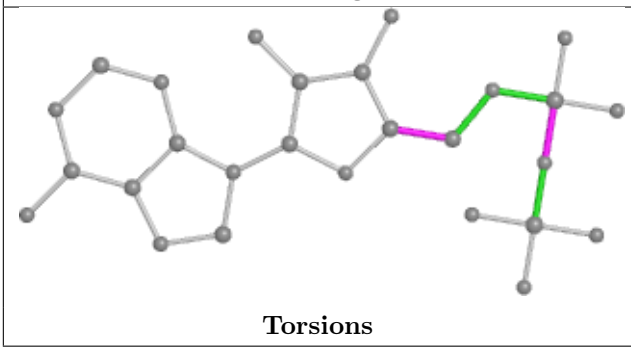
Ligand ADP B 601



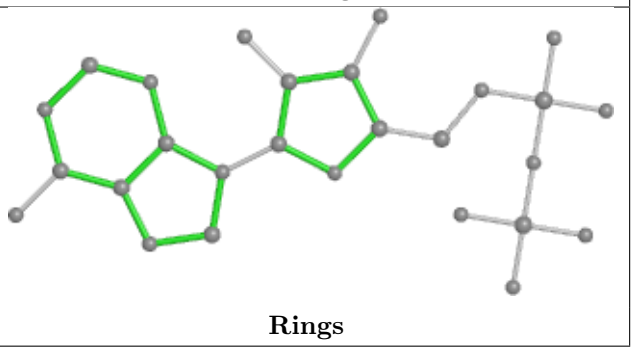
Bond lengths



Bond angles

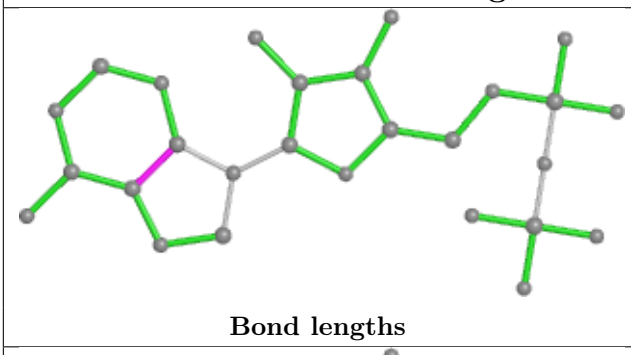


Torsions

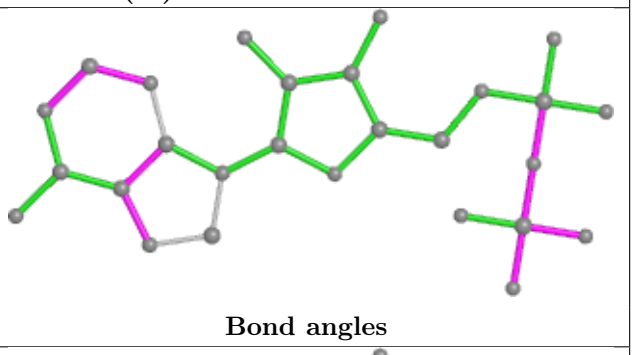


Rings

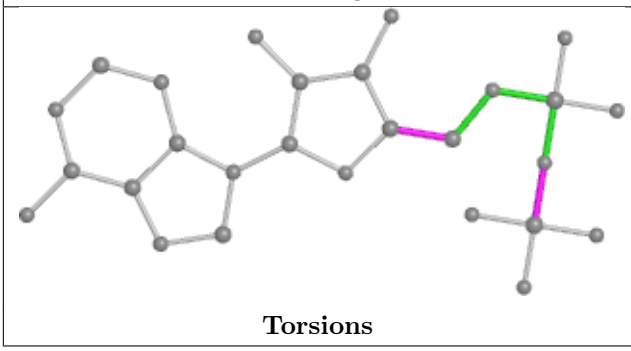
Ligand ADP C 601 (A)



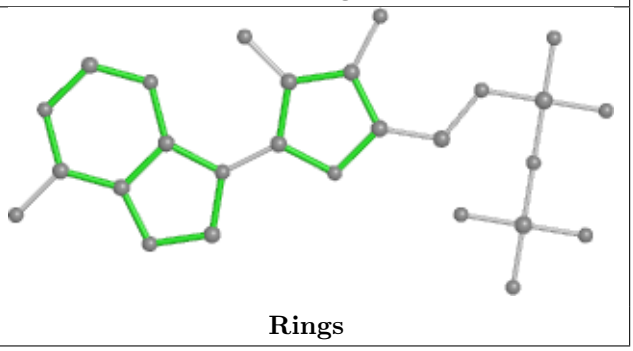
Bond lengths



Bond angles

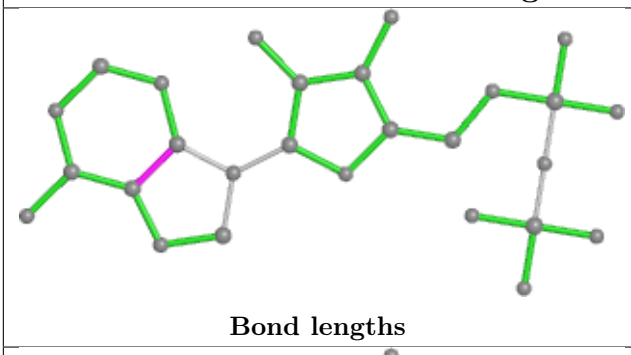


Torsions

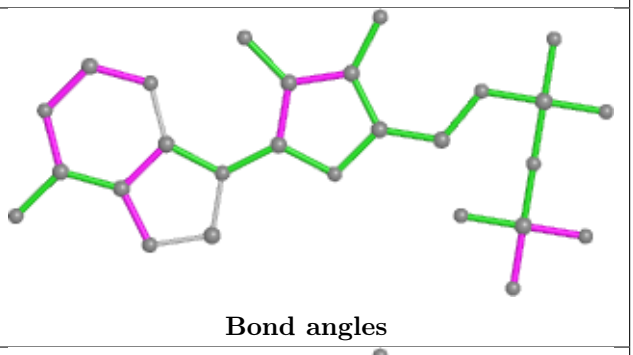


Rings

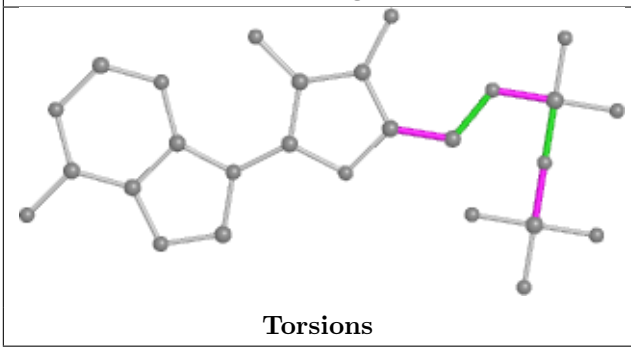
Ligand ADP A 601



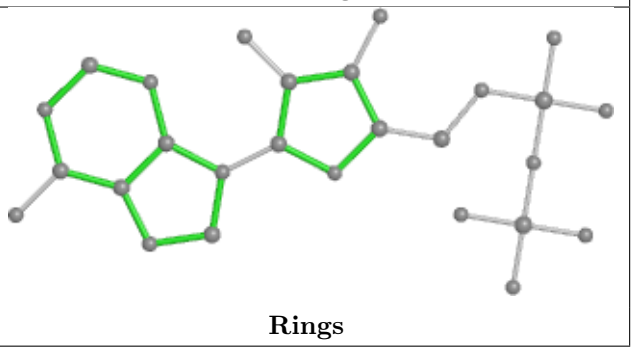
Bond lengths



Bond angles



Torsions



Rings

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	522/544 (95%)	0.41	35 (6%) 17 16	40, 68, 109, 132	0
1	B	492/544 (90%)	0.72	68 (13%) 2 2	43, 80, 143, 188	0
1	C	514/544 (94%)	0.41	34 (6%) 18 17	40, 62, 116, 153	0
All	All	1528/1632 (93%)	0.51	137 (8%) 9 8	40, 70, 129, 188	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	213	PHE	8.7
1	C	96	VAL	8.5
1	C	103	PRO	8.0
1	C	94	PRO	7.6
1	C	107	VAL	7.6
1	C	95	LEU	7.1
1	C	108	ASP	7.0
1	B	383	TYR	6.8
1	C	522	SER	6.6
1	C	104	LYS	6.5
1	B	109	TYR	6.2
1	C	106	SER	6.2
1	B	458	ILE	6.2
1	A	91	SER	6.1
1	C	105	ASP	6.0
1	B	-1	SER	5.8
1	B	448	PHE	5.8
1	A	96	VAL	5.6
1	B	457	LYS	5.5
1	C	91	SER	5.3
1	C	93	THR	5.1
1	A	135	LYS	5.0
1	B	487	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	350	ALA	4.7
1	A	95	LEU	4.6
1	B	461	VAL	4.5
1	B	0	HIS	4.3
1	B	464	SER	4.3
1	B	374	GLN	4.3
1	B	111	ASP	4.3
1	B	352	MET	4.1
1	C	461	VAL	4.1
1	B	257	HIS	4.1
1	B	110	ILE	4.0
1	C	97	ASN	4.0
1	B	358	LEU	4.0
1	B	466	GLU	3.9
1	C	102	GLY	3.9
1	A	371	LYS	3.9
1	C	99	LYS	3.8
1	B	212	GLN	3.7
1	B	463	VAL	3.7
1	C	457	LYS	3.6
1	B	263	PRO	3.5
1	A	219	ASP	3.5
1	B	382	LYS	3.5
1	C	101	TYR	3.4
1	B	169	GLY	3.4
1	A	233	TYR	3.4
1	B	232	MET	3.4
1	B	264	MET	3.3
1	B	467	LEU	3.3
1	A	457	LYS	3.3
1	B	278	LEU	3.3
1	C	371	LYS	3.3
1	B	462	THR	3.2
1	B	482	ALA	3.2
1	B	381	ASP	3.2
1	B	371	LYS	3.2
1	A	217	PRO	3.2
1	B	454	PRO	3.2
1	C	-8	SER	3.1
1	A	223	THR	3.1
1	C	109	TYR	3.1
1	B	359	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	92	LYS	3.0
1	B	380	ALA	2.9
1	C	212	GLN	2.9
1	C	98	LYS	2.9
1	C	521	ASN	2.9
1	B	460	GLY	2.9
1	C	374	GLN	2.9
1	A	94	PRO	2.8
1	C	370	PRO	2.8
1	A	222	THR	2.8
1	A	129	LEU	2.8
1	B	355	LEU	2.8
1	B	357	GLN	2.8
1	B	384	PRO	2.8
1	A	374	GLN	2.8
1	A	407	CYS	2.8
1	A	221	LYS	2.7
1	A	57	ILE	2.7
1	A	123	ALA	2.7
1	B	91	SER	2.6
1	C	487	GLY	2.6
1	A	126	VAL	2.6
1	B	484	GLN	2.6
1	A	122	ALA	2.6
1	B	486	TYR	2.6
1	B	279	THR	2.6
1	B	490	LYS	2.6
1	A	7	VAL	2.6
1	B	483	LEU	2.5
1	A	458	ILE	2.5
1	A	418	LEU	2.5
1	B	259	VAL	2.5
1	A	382	LYS	2.5
1	B	251	VAL	2.5
1	A	93	THR	2.5
1	B	65	GLU	2.4
1	B	330	ILE	2.4
1	A	119	LEU	2.4
1	C	39	CYS	2.4
1	C	467	LEU	2.4
1	B	211	THR	2.3
1	B	518	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	-2	GLY	2.3
1	B	256	ALA	2.3
1	A	49	GLU	2.3
1	A	56	ILE	2.3
1	B	277	GLY	2.3
1	B	305	ARG	2.2
1	C	78	GLY	2.2
1	B	356	LYS	2.2
1	B	465	GLU	2.2
1	A	42	ALA	2.2
1	B	329	ASP	2.1
1	C	20	LEU	2.1
1	B	-3	ARG	2.1
1	B	249	LEU	2.1
1	B	-5	VAL	2.1
1	A	521	ASN	2.1
1	B	415	PRO	2.1
1	A	92	LYS	2.1
1	B	62	TYR	2.1
1	A	59	PRO	2.1
1	B	418	LEU	2.1
1	C	132	LEU	2.0
1	A	134	ALA	2.0
1	B	172	VAL	2.0
1	B	444	PRO	2.0
1	A	0	HIS	2.0
1	B	87	HIS	2.0
1	A	336	ILE	2.0
1	B	494	MET	2.0
1	B	353	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GLC	B	602	12/12	0.95	0.17	47,58,59,63	0

6.3 Carbohydrates (i)

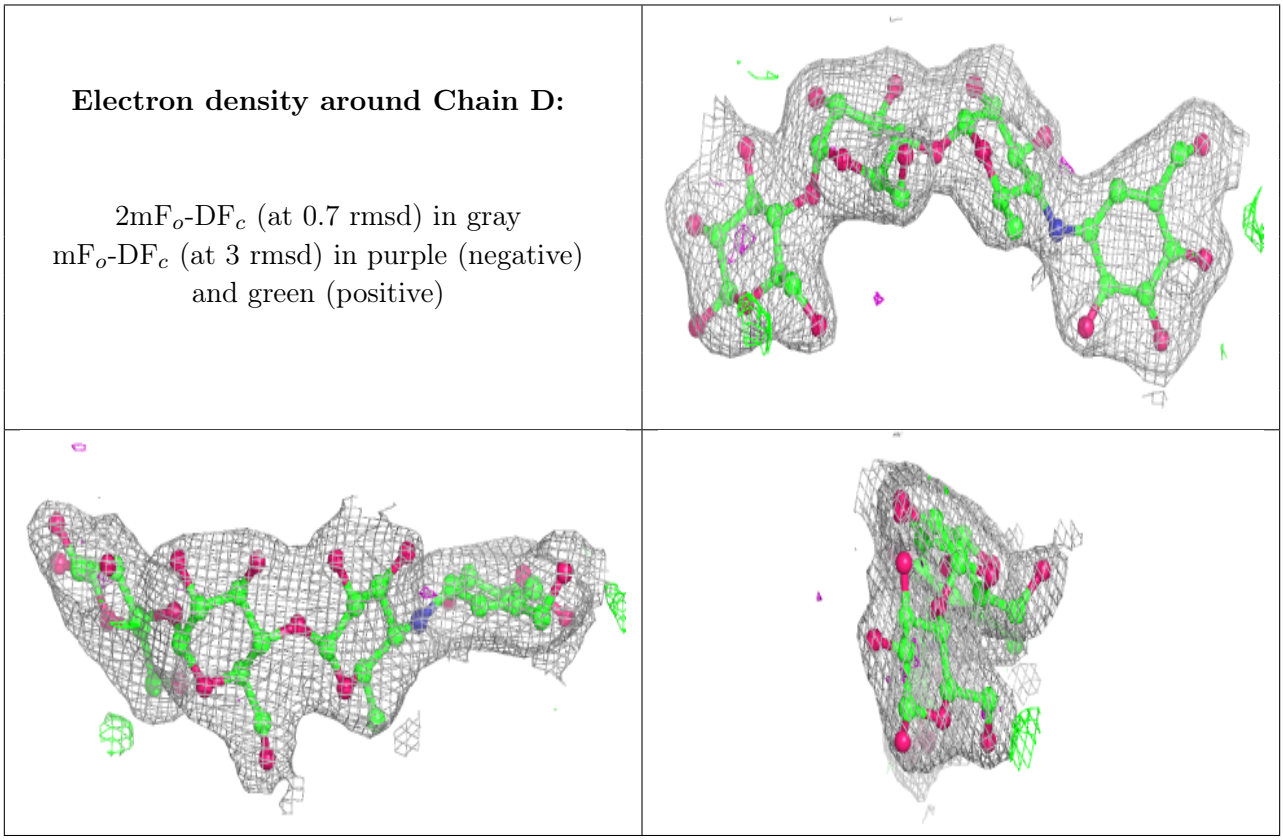
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

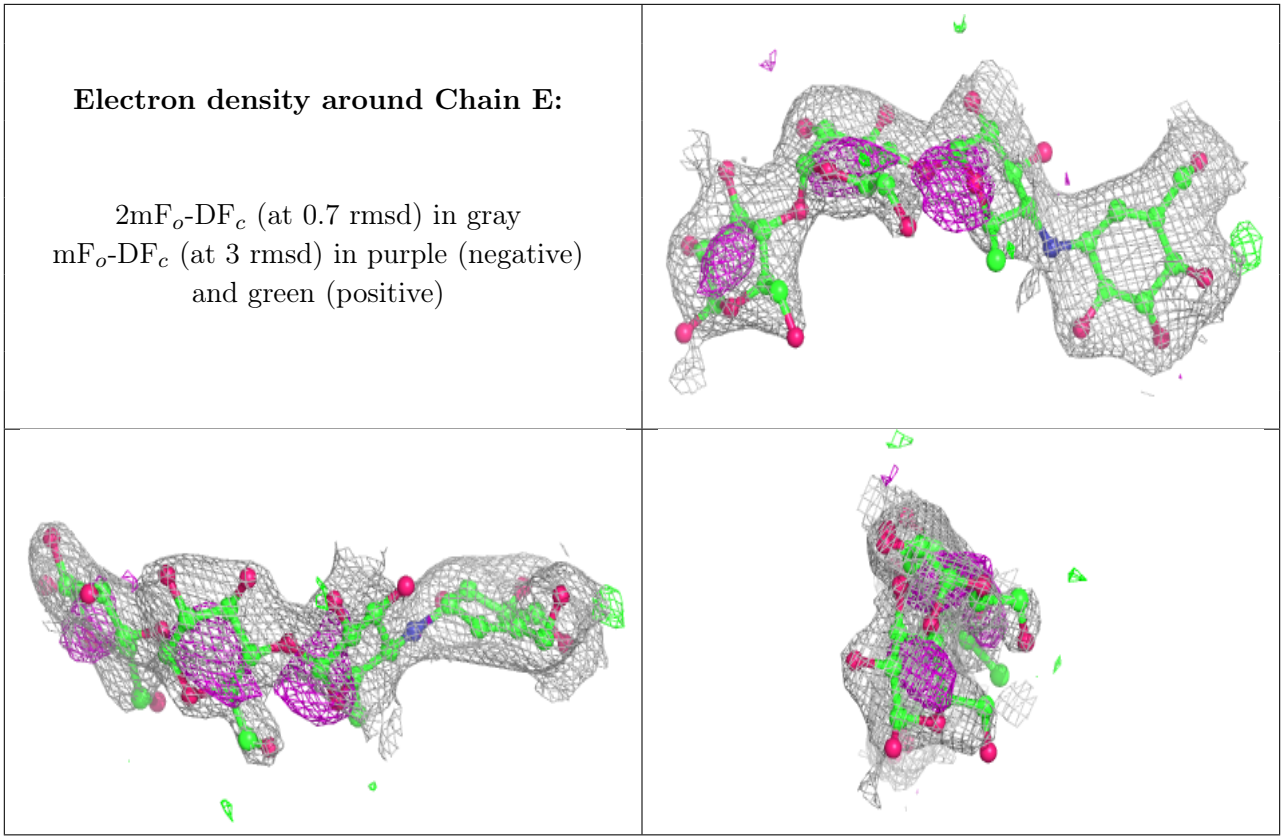
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	E	2	11/12	0.74	0.25	98,109,120,121	0
2	BGC	E	1	12/12	0.79	0.27	112,124,126,127	0
2	AC1	E	3	21/22	0.90	0.20	41,50,94,100	0
2	BGC	D	1	12/12	0.91	0.12	64,73,75,81	0
2	AC1	D	3	21/22	0.94	0.20	44,51,62,64	0
2	GLC	D	2	11/12	0.97	0.12	56,61,62,63	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 D:

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





6.4 Ligands

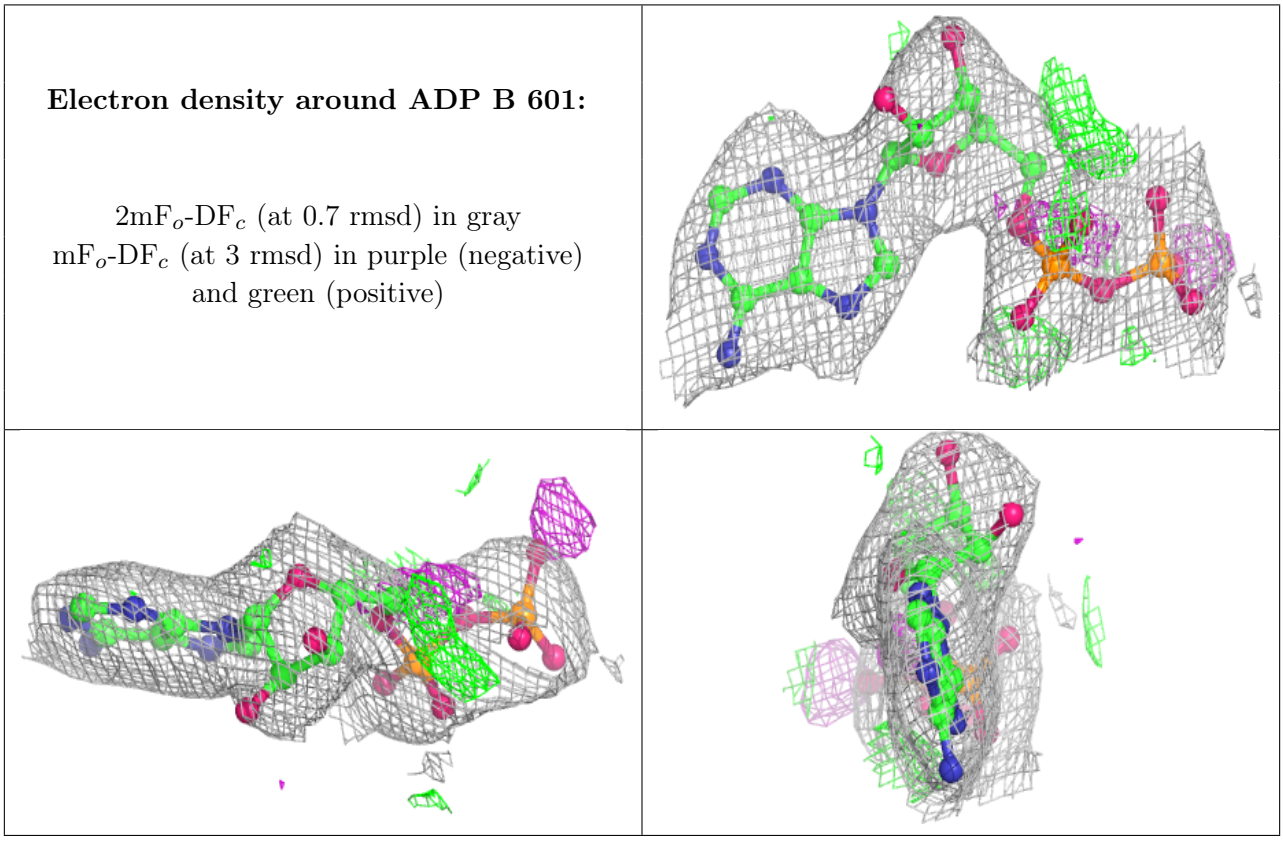
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	604	5/5	0.75	0.30	129,133,136,144	0
4	SO4	B	603	5/5	0.78	0.25	88,97,98,104	0
4	SO4	C	605	5/5	0.83	0.19	115,119,127,130	0
4	SO4	A	604	5/5	0.87	0.23	110,112,117,122	0
4	SO4	C	603	5/5	0.89	0.12	74,81,87,91	0
4	SO4	C	604	5/5	0.90	0.17	78,85,88,93	0
4	SO4	A	606	5/5	0.90	0.19	114,117,127,128	0
4	SO4	A	605	5/5	0.91	0.25	99,101,103,106	0
3	ADP	B	601	27/27	0.95	0.14	55,73,84,87	0
3	ADP	C	601[A]	27/27	0.95	0.15	55,74,75,76	27
3	ADP	C	601[B]	27/27	0.95	0.15	52,58,61,64	27
4	SO4	A	603	5/5	0.95	0.14	82,84,88,94	0
5	GLC	B	602	12/12	0.95	0.17	47,58,59,63	0
3	ADP	A	601	27/27	0.96	0.17	60,72,84,85	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.

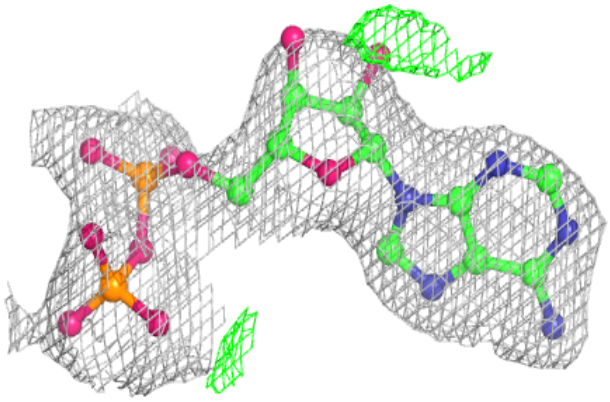
Electron density around ADP B 601:

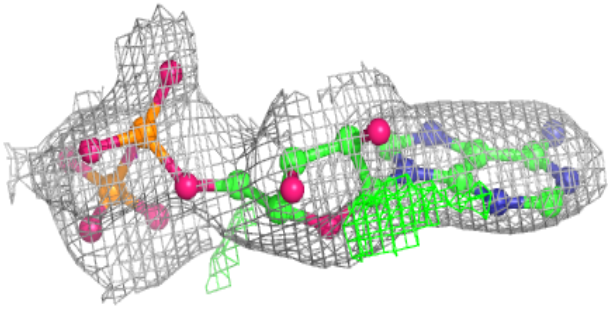
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

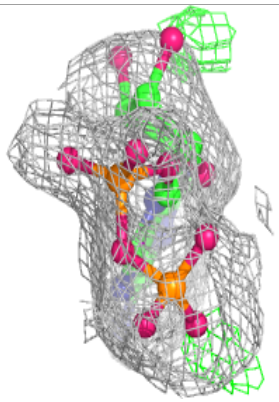


Electron density around ADP C 601 (A):

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

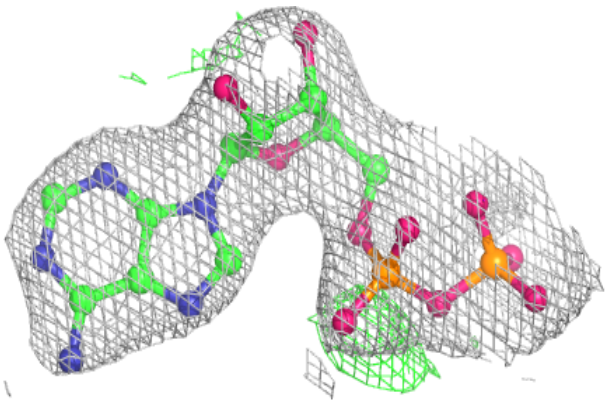


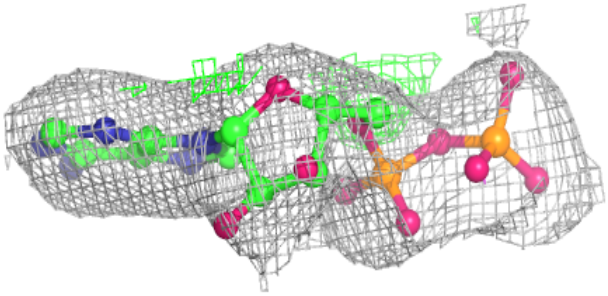


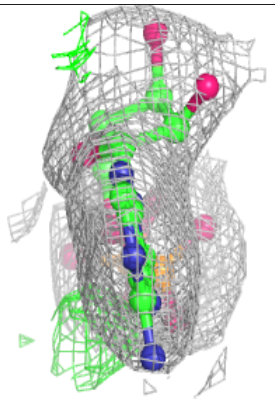


Electron density around ADP C 601 (B):

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

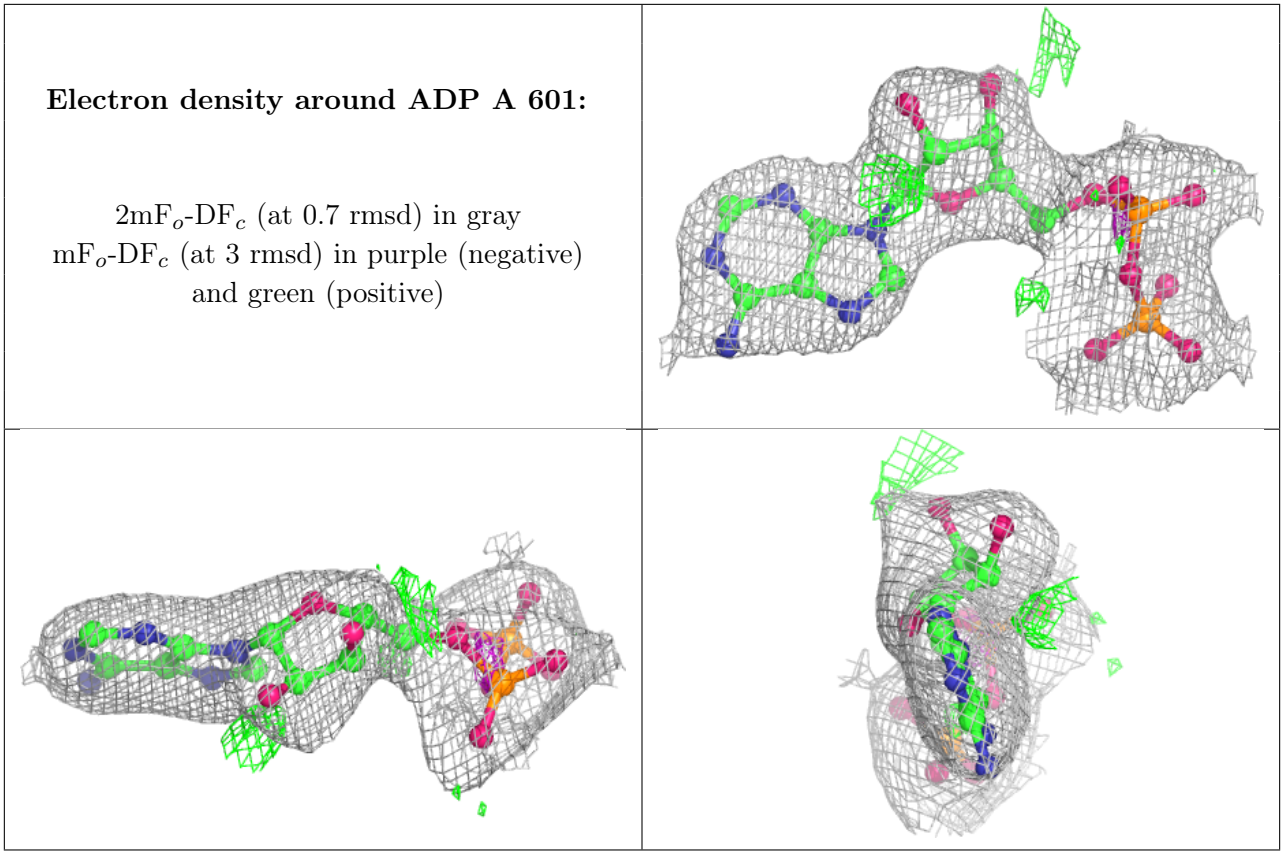






Electron density around ADP A 601:

$2mF_o$-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.