wwPDB X-ray Structure Validation Summary Report (i)

Sep 13, 2023 – 01:48 PM EDT

PDB ID	:	4RER
Title	:	Crystal structure of the phosphorylated human alpha1 beta2 gamma1 holo-AMPK complex bound to AMP and cyclodextrin
Authors	:	Zhou, X.E.; Ke, J.; Li, X.; Wang, L.; Gu, X.; de Waal, P.W.; Tan, M.H.E.; Wang, D.; Wu, D.; Xu, H.E.; Melcher, K.
Deposited on	:	2014-09-23
Resolution	:	4.05 Å(reported)

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

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

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

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

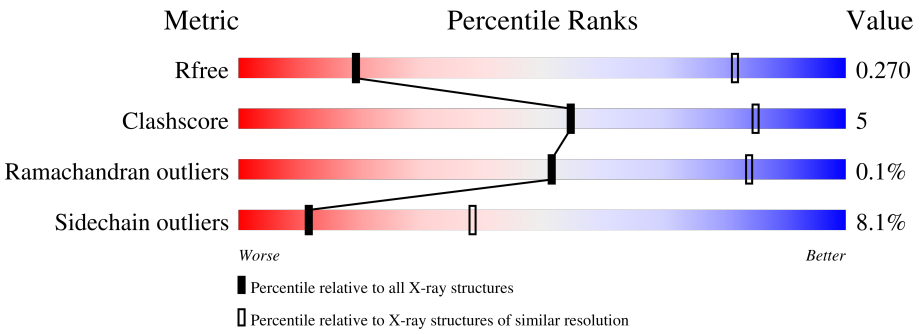
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.05 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	1105 (4.38-3.70)
Clashscore	141614	1005 (4.36-3.72)
Ramachandran outliers	138981	1125 (4.38-3.70)
Sidechain outliers	138945	1115 (4.38-3.70)

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%

Mol	Chain	Length	Quality of chain
1	A	540	68% 15% • 15%
2	B	197	72% 19% • 8%
3	G	304	81% 16% ••
4	C	7	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7798 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 5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	459	3725	2376	649	677	1	22	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	ARG	conflict	UNP Q13131
A	260	SER	THR	conflict	UNP Q13131
A	471	GLY	GLU	engineered mutation	UNP Q13131
A	474	ALA	GLU	engineered mutation	UNP Q13131
A	476	ALA	LYS	engineered mutation	UNP Q13131

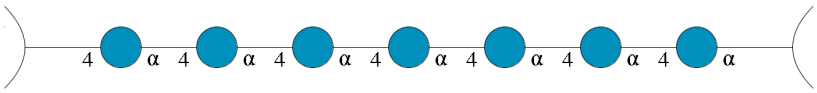
- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	B	181	1458	945	240	268	1	4	0	0	0

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

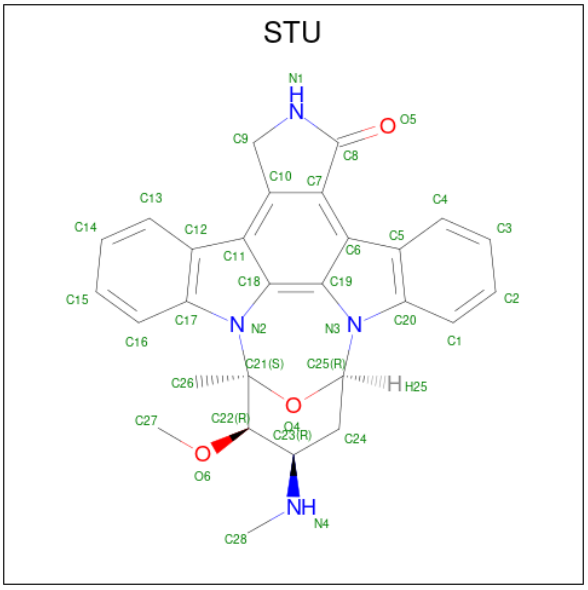
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	300	2419	1571	403	438	7	0	0	0

- Molecule 4 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).



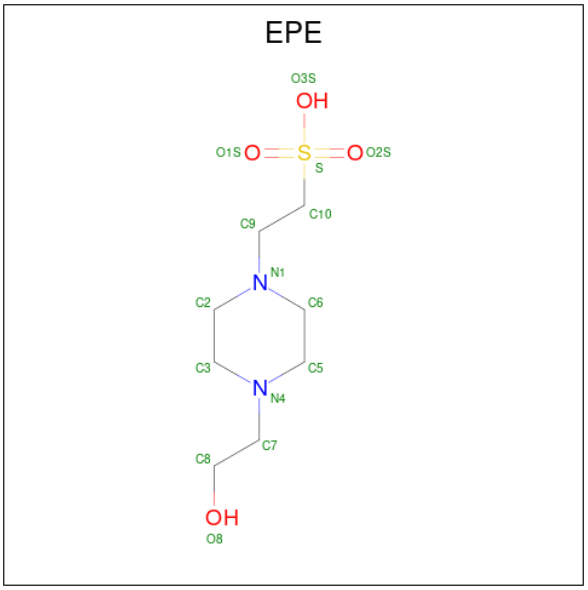
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
4	C	7	77	42	35	0	0	0

- Molecule 5 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



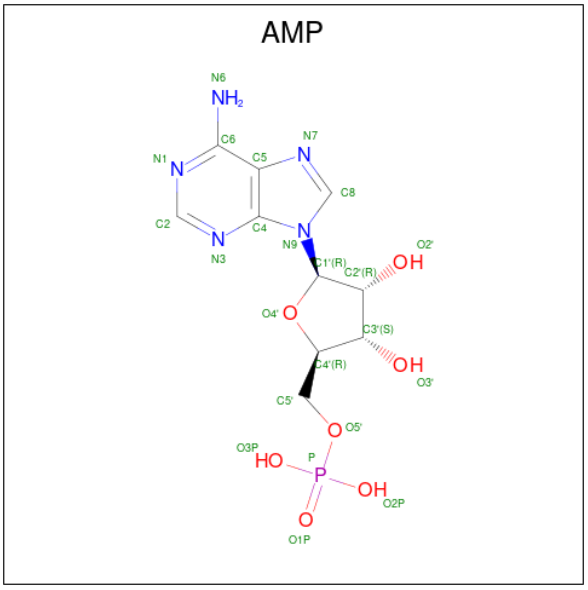
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	35	28	4	3	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	15	8	2	4	1	0	0

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



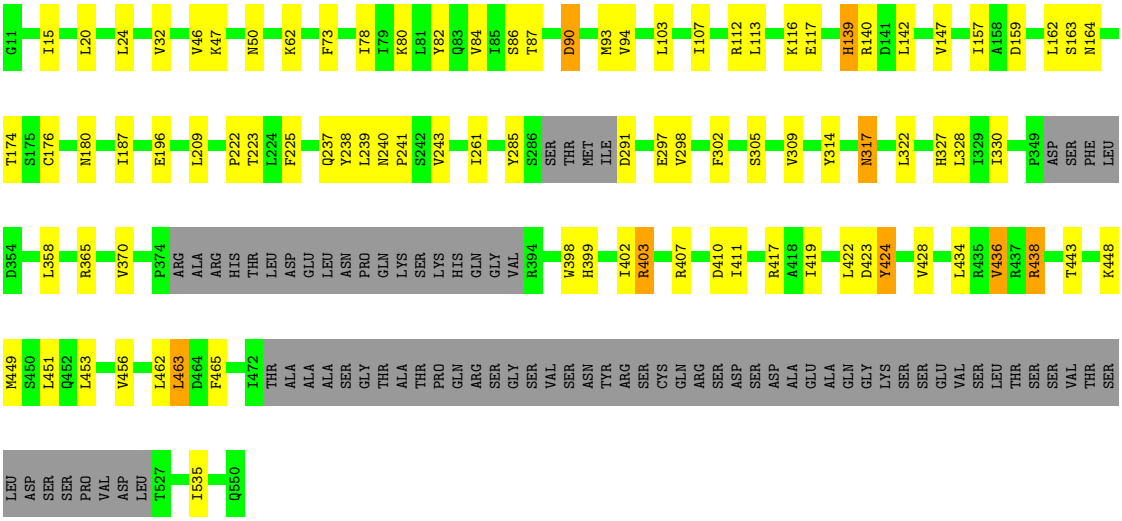
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	G	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
7	G	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
7	G	1	23	10	5	7	1	0	0

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. 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. 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.

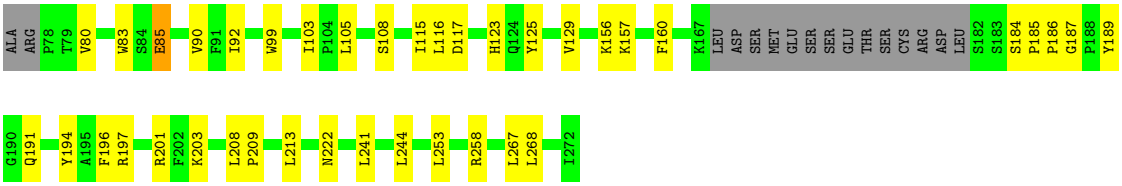
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1

Chain A:



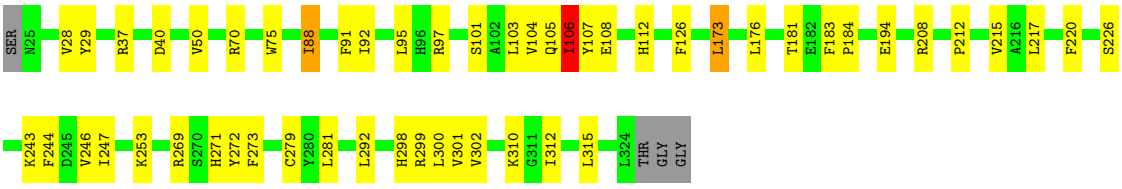
- Molecule 2: 5'-AMP-activated protein kinase subunit beta-2

Chain B:



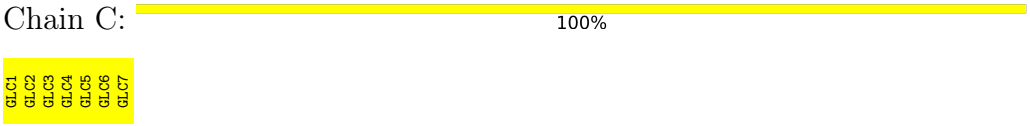
- Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1

Chain G:



- Molecule 4: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	132.57Å 132.57Å 195.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.66 – 4.05 39.66 – 4.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.66-4.05) 99.1 (39.66-4.05)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.224 , 0.260 0.239 , 0.270	Depositor DCC
R_{free} test set	1213 reflections (7.32%)	wwPDB-VP
Wilson B-factor (Å^2)	122.7	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 119.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7798	wwPDB-VP
Average B, all atoms (Å^2)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: STU, AMP, EPE, TPO, GLC, SEP

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	0.30	0/3800	0.48	1/5132 (0.0%)
2	B	0.31	0/1491	0.54	1/2027 (0.0%)
3	G	0.28	0/2470	0.46	0/3353
All	All	0.30	0/7761	0.49	2/10512 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	187	GLY	C-N-CD	5.84	140.66	128.40
1	A	291	ASP	CB-CG-OD2	5.20	122.98	118.30

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	3725	0	3716	41	0
2	B	1458	0	1446	16	0
3	G	2419	0	2483	26	0
4	C	77	0	61	0	0
5	A	35	0	26	3	0
6	A	15	0	17	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	69	0	36	1	0
All	All	7798	0	7785	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.

The worst 5 of 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:A:424:TYR:CD2	1:A:438:ARG:HB3	2.12	0.85
1:A:32:VAL:HG12	1:A:47:LYS:HA	1.76	0.68
3:G:101:SER:HB3	3:G:104:VAL:HG22	1.75	0.66
3:G:301:VAL:HG12	3:G:312:ILE:HG12	1.80	0.64
3:G:173:LEU:HD12	3:G:315:LEU:HD22	1.80	0.64

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	448/540 (83%)	426 (95%)	22 (5%)	0	100	100
2	B	176/197 (89%)	165 (94%)	11 (6%)	0	100	100
3	G	298/304 (98%)	285 (96%)	12 (4%)	1 (0%)	41	75
All	All	922/1041 (89%)	876 (95%)	45 (5%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	106	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	414/484 (86%)	379 (92%)	35 (8%)	10	37
2	B	166/181 (92%)	150 (90%)	16 (10%)	8	30
3	G	275/278 (99%)	257 (94%)	18 (6%)	17	45
All	All	855/943 (91%)	786 (92%)	69 (8%)	11	38

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	107	TYR
3	G	112	HIS
3	G	253	LYS
1	A	370	VAL
1	A	358	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	SEP	B	108	2	8,9,10	1.54	1 (12%)	8,12,14	0.97	0
1	TPO	A	174	1	8,10,11	1.02	0	10,14,16	1.72	2 (20%)

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	SEP	B	108	2	-	0/5/8/10	-
1	TPO	A	174	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	108	SEP	P-O1P	3.33	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	174	TPO	P-OG1-CB	-4.49	109.65	123.21
1	A	174	TPO	CG2-CB-CA	-2.35	108.53	113.16

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)

7 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GLC	C	1	4	11,11,12	2.21	5 (45%)	15,15,17	1.33	3 (20%)
4	GLC	C	2	4	11,11,12	1.34	1 (9%)	15,15,17	1.04	1 (6%)
4	GLC	C	3	4	11,11,12	1.85	5 (45%)	15,15,17	1.21	2 (13%)
4	GLC	C	4	4	11,11,12	1.21	1 (9%)	15,15,17	1.33	2 (13%)
4	GLC	C	5	4	11,11,12	2.09	6 (54%)	15,15,17	1.51	4 (26%)
4	GLC	C	6	4	11,11,12	1.81	4 (36%)	15,15,17	2.18	5 (33%)
4	GLC	C	7	4	11,11,12	1.48	2 (18%)	15,15,17	1.87	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	C	1	4	-	2/2/19/22	0/1/1/1
4	GLC	C	2	4	-	0/2/19/22	0/1/1/1
4	GLC	C	3	4	-	0/2/19/22	0/1/1/1
4	GLC	C	4	4	-	2/2/19/22	0/1/1/1
4	GLC	C	5	4	-	2/2/19/22	0/1/1/1
4	GLC	C	6	4	-	2/2/19/22	0/1/1/1
4	GLC	C	7	4	-	2/2/19/22	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	GLC	O5-C5	3.90	1.51	1.43
4	C	1	GLC	C4-C3	-3.74	1.42	1.52
4	C	5	GLC	O2-C2	-3.73	1.35	1.43
4	C	6	GLC	O2-C2	-3.44	1.36	1.43
4	C	3	GLC	C4-C3	-3.41	1.43	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	6	GLC	C1-O5-C5	5.79	120.03	112.19
4	C	7	GLC	C1-O5-C5	4.97	118.92	112.19
4	C	5	GLC	C3-C4-C5	3.03	115.64	110.24
4	C	6	GLC	C3-C4-C5	2.96	115.52	110.24
4	C	5	GLC	C2-C3-C4	2.83	115.79	110.89

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

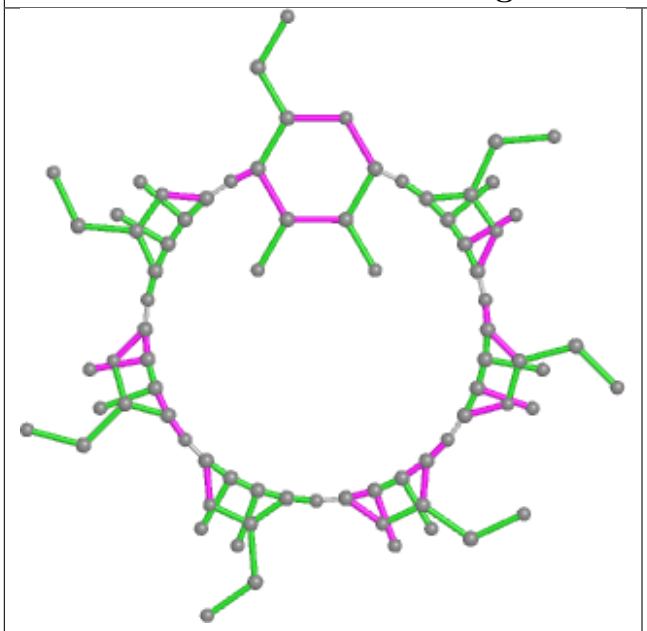
Mol	Chain	Res	Type	Atoms
4	C	4	GLC	O5-C5-C6-O6
4	C	6	GLC	O5-C5-C6-O6
4	C	7	GLC	O5-C5-C6-O6
4	C	4	GLC	C4-C5-C6-O6
4	C	5	GLC	C4-C5-C6-O6

There are no ring outliers.

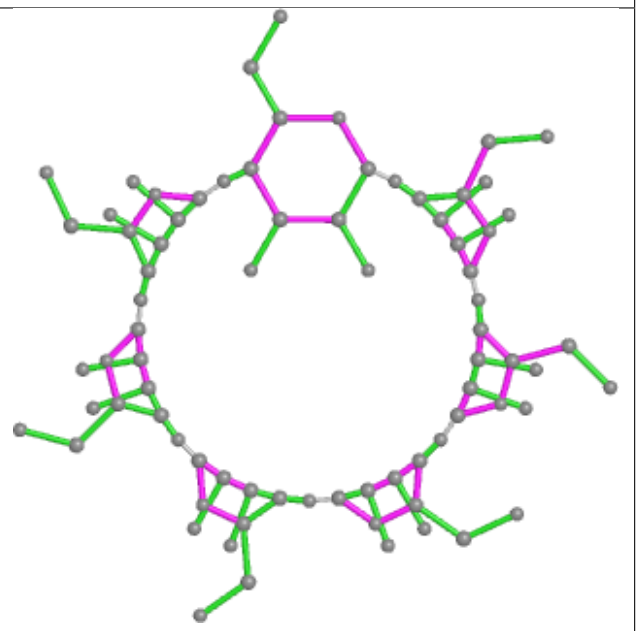
No monomer is involved in short contacts.

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

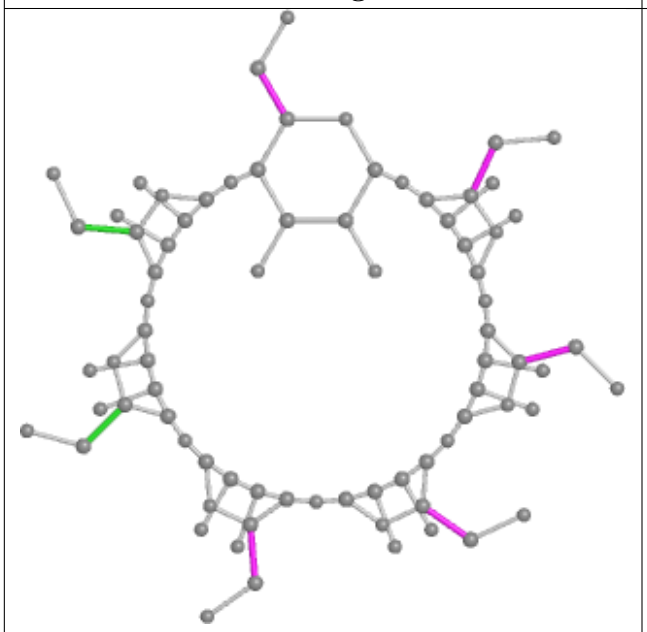
Oligosaccharide Chain C



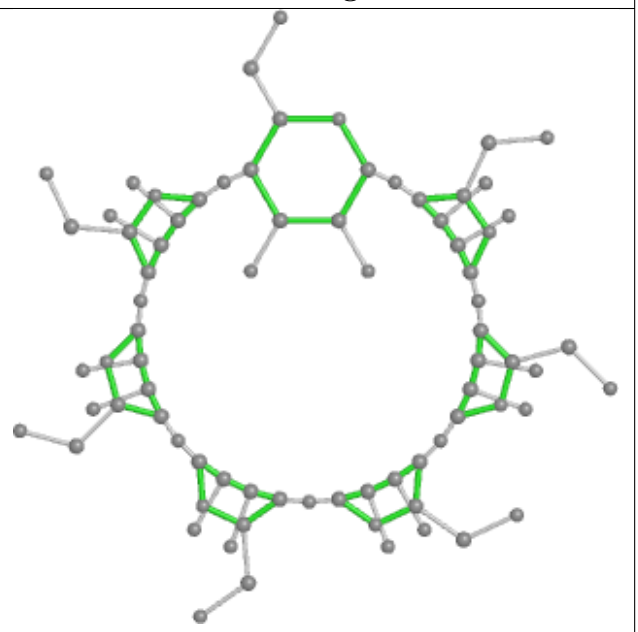
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
7	AMP	G	403	-	22,25,25	1.34	3 (13%)	25,38,38	1.13	3 (12%)
6	EPE	A	602	-	15,15,15	0.66	0	18,20,20	1.57	4 (22%)
7	AMP	G	401	-	22,25,25	1.37	3 (13%)	25,38,38	1.29	4 (16%)
5	STU	A	601	-	30,42,42	1.08	2 (6%)	31,68,68	2.10	6 (19%)
7	AMP	G	402	-	22,25,25	1.32	3 (13%)	25,38,38	1.23	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AMP	G	403	-	-	0/6/26/26	0/3/3/3
6	EPE	A	602	-	-	2/9/19/19	0/1/1/1
7	AMP	G	401	-	-	0/6/26/26	0/3/3/3
5	STU	A	601	-	-	2/4/42/42	-
7	AMP	G	402	-	-	0/6/26/26	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	401	AMP	C6-N6	4.14	1.49	1.34
7	G	403	AMP	C6-N6	4.07	1.48	1.34
7	G	402	AMP	C6-N6	4.06	1.48	1.34
5	A	601	STU	O4-C25	-3.11	1.38	1.43
7	G	401	AMP	P-O1P	3.01	1.60	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	STU	C9-N1-C8	-5.20	108.85	113.85
5	A	601	STU	C26-C21-C22	-4.66	103.57	112.64
5	A	601	STU	C10-C9-N1	4.22	106.05	101.76
5	A	601	STU	C27-O6-C22	-4.22	107.17	114.44
7	G	402	AMP	N3-C2-N1	-3.92	122.55	128.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	STU	C22-C23-N4-C28
6	A	602	EPE	C8-C7-N4-C5
5	A	601	STU	C24-C23-N4-C28
6	A	602	EPE	C10-C9-N1-C6

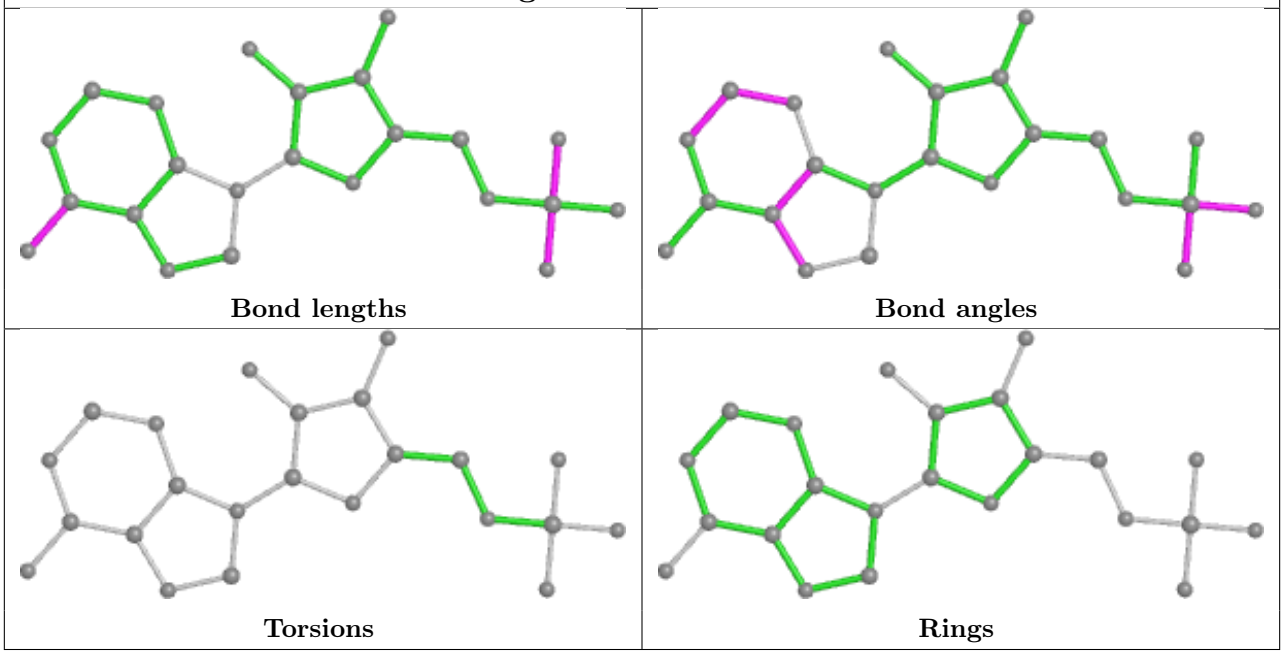
There are no ring outliers.

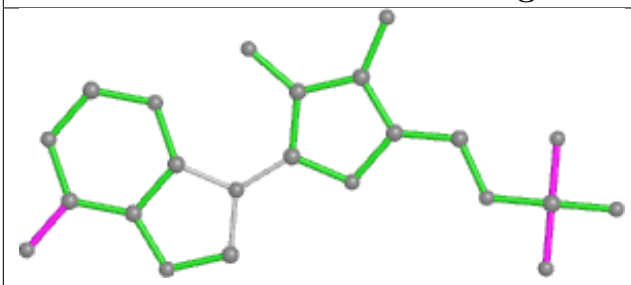
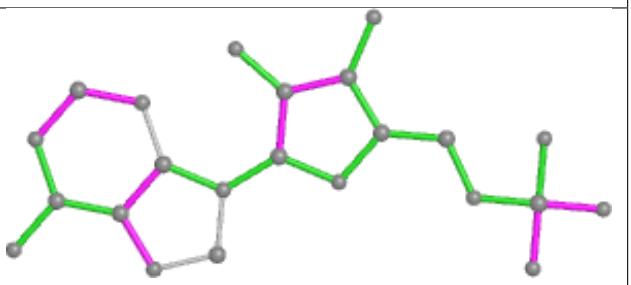
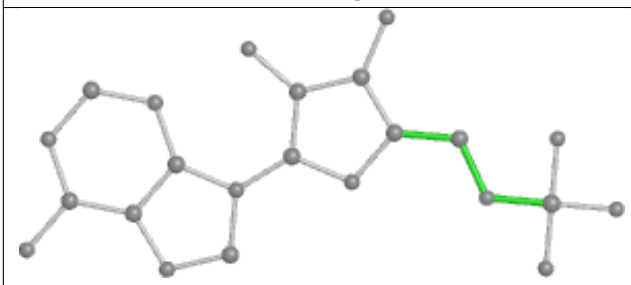
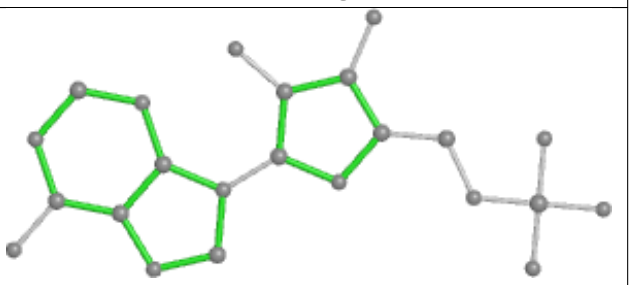
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	EPE	1	0
5	A	601	STU	3	0
7	G	402	AMP	1	0

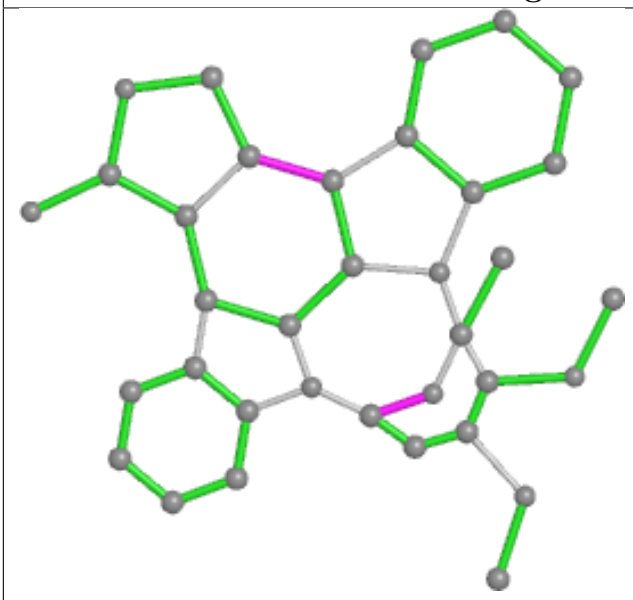
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 AMP G 403

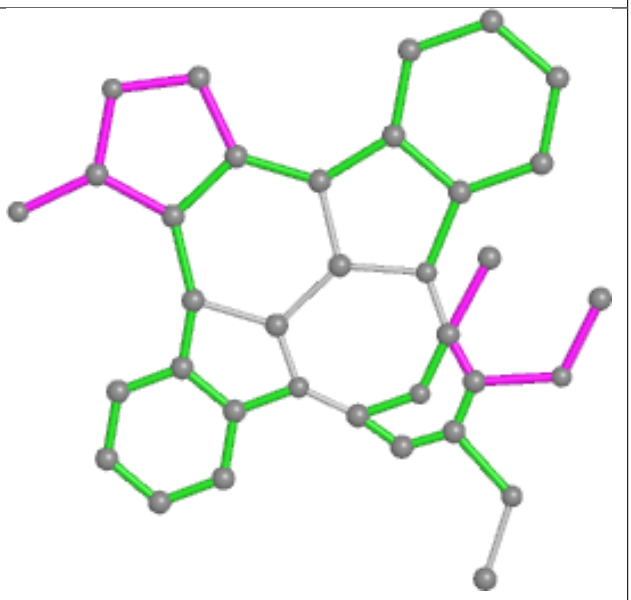


Ligand AMP G 401	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

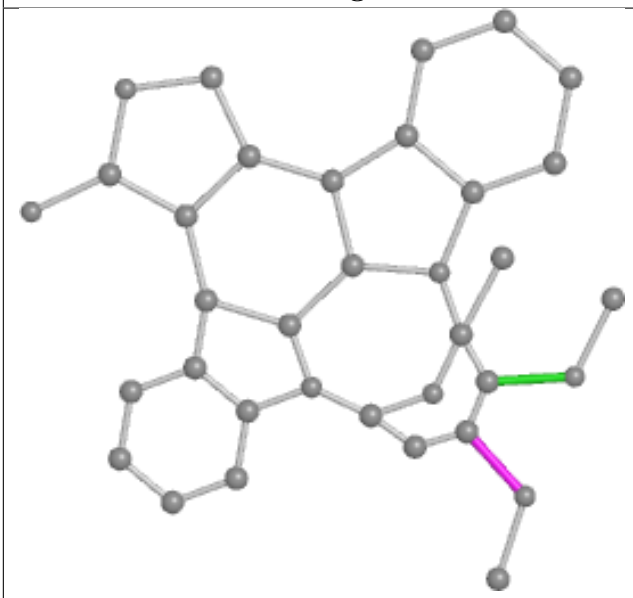
Ligand STU A 601



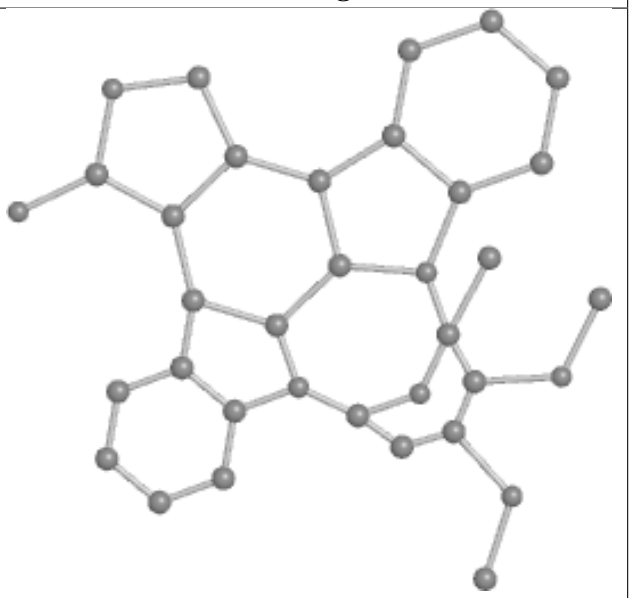
Bond lengths



Bond angles

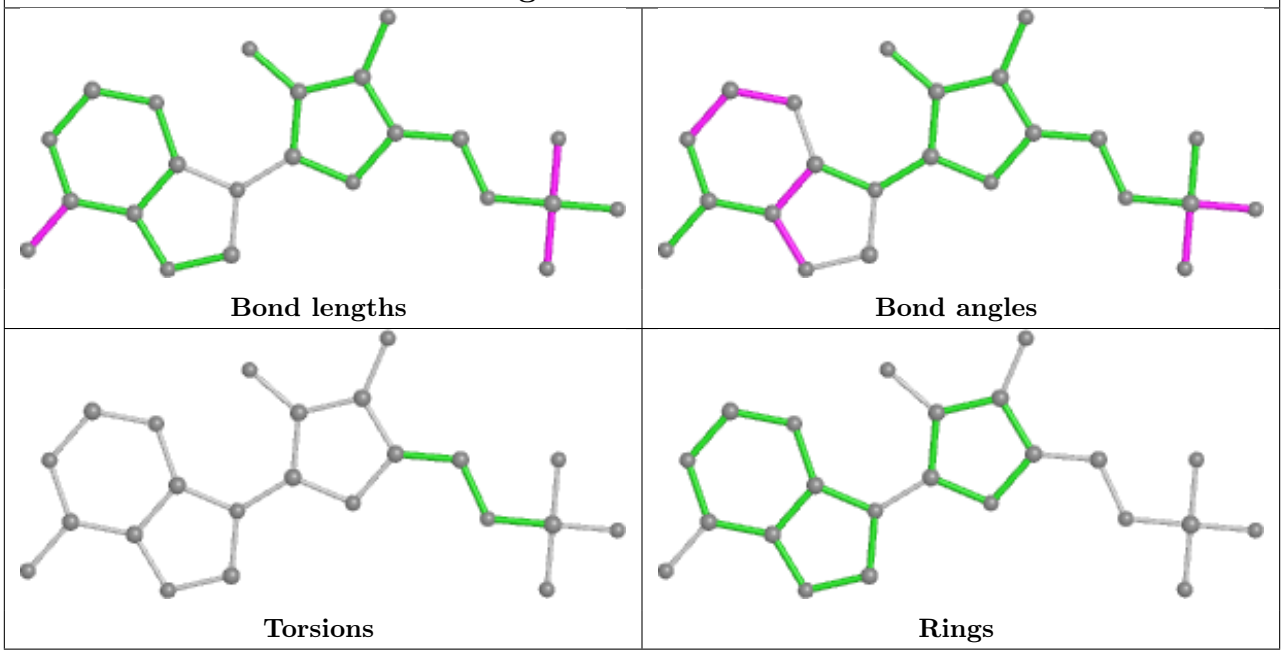


Torsions



Rings

Ligand AMP G 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

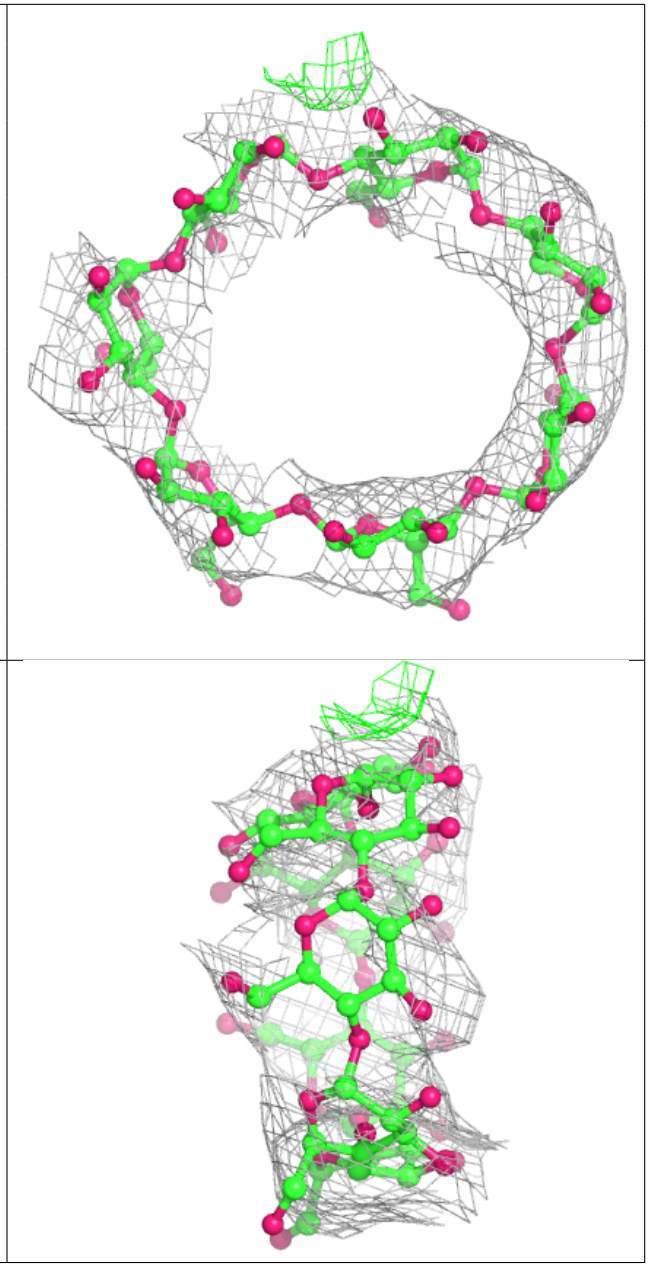
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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)



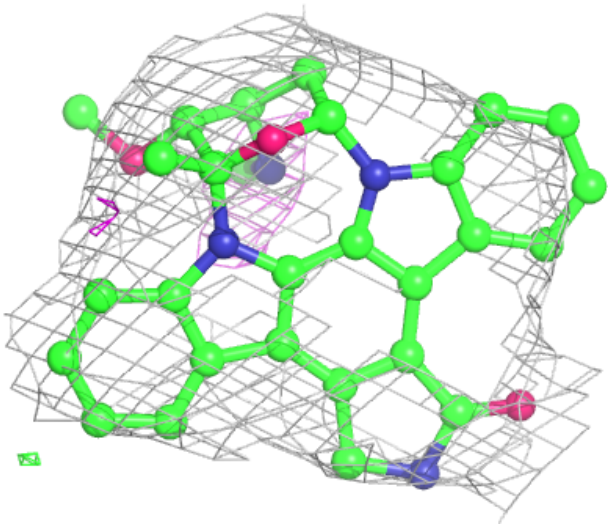
6.4 Ligands (i)

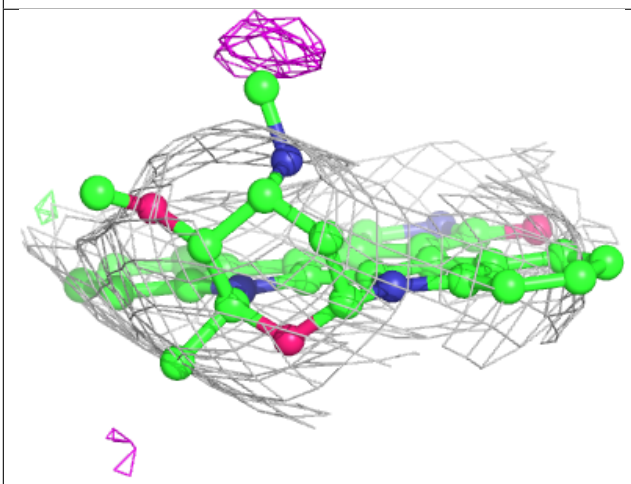
Unable to reproduce the depositors R factor - this section is therefore empty.

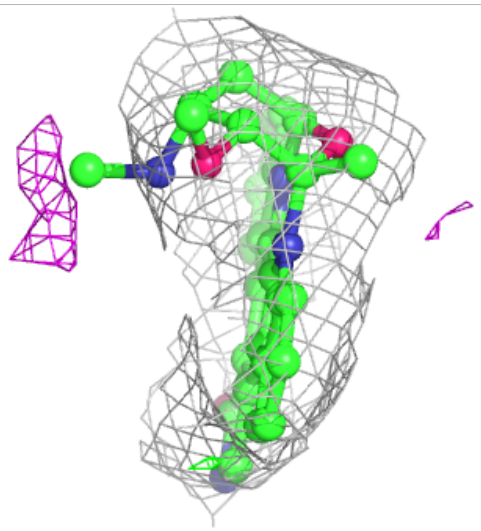
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STU 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)

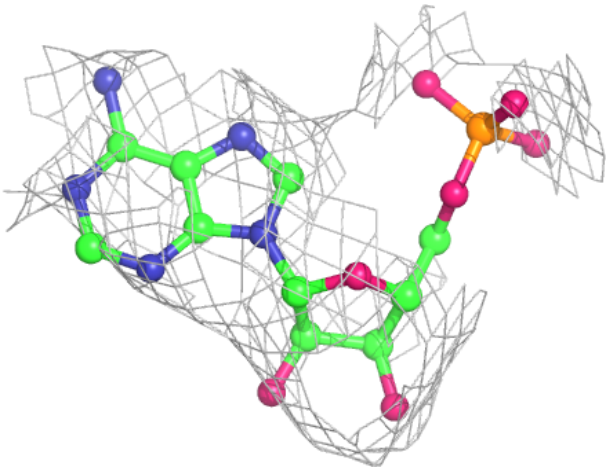


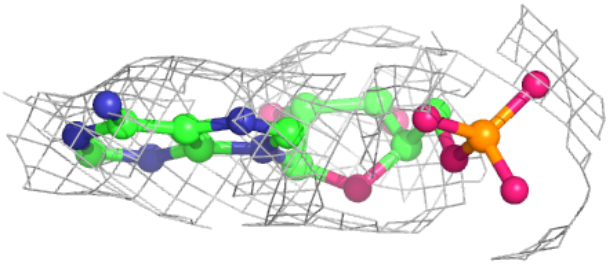


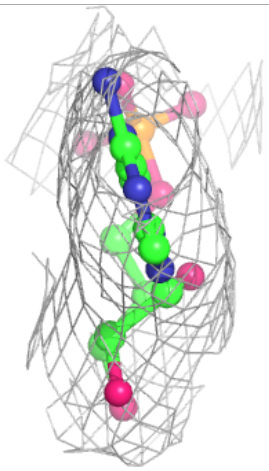


Electron density around AMP G 401:

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

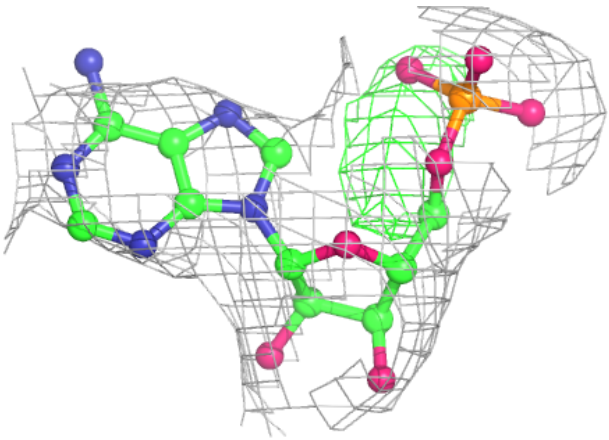


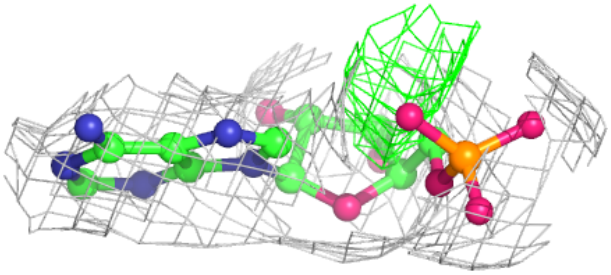


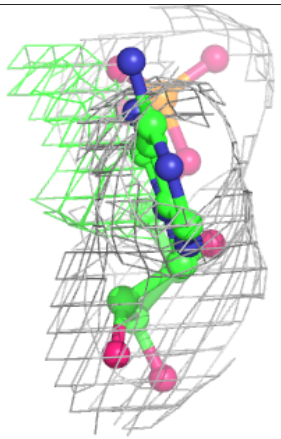


Electron density around AMP G 402:

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

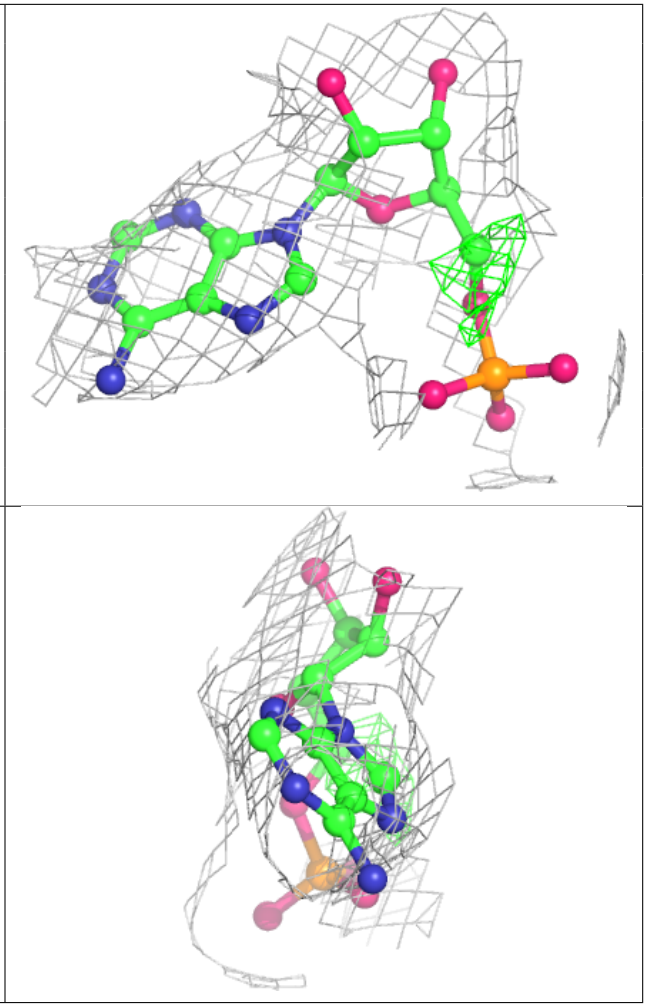






Electron density around AMP G 403:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.