



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 05:01 PM BST

PDB ID : 6GNG
Title : Granule Bound Starch Synthase I from *Cyanophora paradoxa* bound to acarbose and ADP
Authors : Cuesta-Seijo, J.A.; Nielsen, M.M.; Palcic, M.M.
Deposited on : 2018-05-30
Resolution : 2.95 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 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 : 2.14.6
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) : 2.14.6

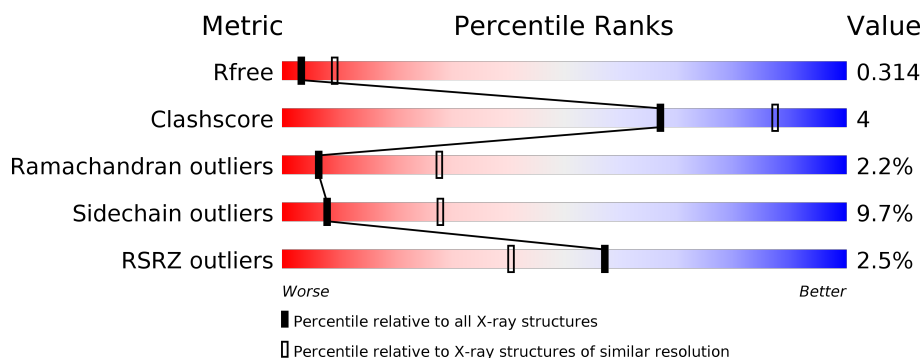
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	612	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	612	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>
2	C	3	<div> <div>33%</div> <div>67%</div> </div>
2	D	3	<div> <div>33%</div> <div>67%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8253 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 Granule-bound starch synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4051	2615	671	732	33			
1	B	526	Total	C	N	O	S	0	0	0
			4056	2618	672	733	33			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A8V967
A	-18	GLY	-	expression tag	UNP A8V967
A	-17	SER	-	expression tag	UNP A8V967
A	-16	SER	-	expression tag	UNP A8V967
A	-15	HIS	-	expression tag	UNP A8V967
A	-14	HIS	-	expression tag	UNP A8V967
A	-13	HIS	-	expression tag	UNP A8V967
A	-12	HIS	-	expression tag	UNP A8V967
A	-11	HIS	-	expression tag	UNP A8V967
A	-10	HIS	-	expression tag	UNP A8V967
A	-9	SER	-	expression tag	UNP A8V967
A	-8	SER	-	expression tag	UNP A8V967
A	-7	GLY	-	expression tag	UNP A8V967
A	-6	LEU	-	expression tag	UNP A8V967
A	-5	VAL	-	expression tag	UNP A8V967
A	-4	PRO	-	expression tag	UNP A8V967
A	-3	ARG	-	expression tag	UNP A8V967
A	-2	GLY	-	expression tag	UNP A8V967
A	-1	SER	-	expression tag	UNP A8V967
A	0	HIS	-	expression tag	UNP A8V967
B	-19	MET	-	initiating methionine	UNP A8V967
B	-18	GLY	-	expression tag	UNP A8V967
B	-17	SER	-	expression tag	UNP A8V967
B	-16	SER	-	expression tag	UNP A8V967
B	-15	HIS	-	expression tag	UNP A8V967

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP A8V967
B	-13	HIS	-	expression tag	UNP A8V967
B	-12	HIS	-	expression tag	UNP A8V967
B	-11	HIS	-	expression tag	UNP A8V967
B	-10	HIS	-	expression tag	UNP A8V967
B	-9	SER	-	expression tag	UNP A8V967
B	-8	SER	-	expression tag	UNP A8V967
B	-7	GLY	-	expression tag	UNP A8V967
B	-6	LEU	-	expression tag	UNP A8V967
B	-5	VAL	-	expression tag	UNP A8V967
B	-4	PRO	-	expression tag	UNP A8V967
B	-3	ARG	-	expression tag	UNP A8V967
B	-2	GLY	-	expression tag	UNP A8V967
B	-1	SER	-	expression tag	UNP A8V967
B	0	HIS	-	expression tag	UNP A8V967

- 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	C	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	D	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	2	Total	O	0	0
			2	2		


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.

- Chain A:

- [illegible]

ALA
THR
SER
GLY
GLY
ILE
LEU
PRO
VAL
PRO
LYS
ALA
ALA
ALA
PRO
LYS
ALA
PRO
LYS
VAL
GLY
ALA

- 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 C:  33% 67%

BC1
GLC2
AC13

- 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:  33% 67%

BC1
GLC2
AC13

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.30Å 106.10Å 175.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.95 19.95 – 2.95	Depositor EDS
% Data completeness (in resolution range)	90.5 (20.00-2.95) 90.9 (19.95-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.272 , 0.303 0.285 , 0.314	Depositor DCC
R_{free} test set	760 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8253	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.45	0/4154	0.70	3/5624 (0.1%)
1	B	0.46	0/4159	0.70	4/5631 (0.1%)
All	All	0.45	0/8313	0.70	7/11255 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	TYR	CA-CB-CG	7.10	126.90	113.40
1	A	206	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	478	TYR	CA-CB-CG	6.92	126.56	113.40
1	A	206	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	540	LEU	CA-CB-CG	5.83	128.71	115.30
1	B	478	TYR	CB-CA-C	5.44	121.29	110.40
1	B	206	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	477	GLU	Peptide
1	A	478	TYR	Peptide
1	B	477	GLU	Peptide
1	B	478	TYR	Peptide

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	4051	0	4059	34	0
1	B	4056	0	4061	30	0
2	C	44	0	30	0	0
2	D	44	0	30	0	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	8253	0	8204	64	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 4.

All (64) 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:305:ILE:HD12	1:B:524:ALA:HB2	1.78	0.65
1:A:305:ILE:HD12	1:A:524:ALA:HB2	1.78	0.64
1:B:224:ASP:OD2	1:B:262:HIS:NE2	2.32	0.62
1:A:485:PRO:HG2	1:A:488:ILE:HD12	1.82	0.61
1:B:369:ALA:HB2	1:B:492:THR:HG23	1.85	0.58
1:A:374:VAL:HG12	1:A:379:ALA:O	2.05	0.56
1:A:224:ASP:OD2	1:A:262:HIS:NE2	2.29	0.55
1:B:98:ASP:HB3	1:B:151:LEU:HD13	1.90	0.54
1:A:98:ASP:HB3	1:A:151:LEU:HD13	1.90	0.54
1:A:202:ILE:HA	1:A:285:VAL:HG21	1.91	0.53
1:A:417:GLU:OE1	3:A:602:ADP:O2'	2.22	0.53
1:A:268:THR:HB	1:A:296:ILE:HD11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:N	1:A:326:ASP:OD1	2.44	0.51
1:B:268:THR:HB	1:B:296:ILE:HD11	1.91	0.51
1:A:374:VAL:HG21	1:A:402:PHE:CD1	2.44	0.51
1:B:112:TRP:HA	1:B:112:TRP:CE3	2.45	0.51
1:A:177:ILE:HD11	1:A:221:ALA:HB1	1.92	0.51
1:B:202:ILE:HA	1:B:285:VAL:HG21	1.92	0.50
1:A:350:LEU:HD11	1:A:382:VAL:HG23	1.95	0.48
1:A:329:LYS:HE2	1:A:515:ARG:NH1	2.28	0.48
1:B:177:ILE:HD11	1:B:221:ALA:HB1	1.95	0.48
1:A:261:ILE:HD11	1:A:290:TYR:CE1	2.49	0.48
1:A:60:GLN:O	1:A:101:PHE:HA	2.14	0.47
1:B:112:TRP:HA	1:B:112:TRP:HE3	1.79	0.47
1:B:60:GLN:O	1:B:101:PHE:HA	2.14	0.47
1:B:350:LEU:HD11	1:B:382:VAL:HG23	1.96	0.47
1:A:383:CYS:HB3	1:A:395:PHE:CE2	2.50	0.46
1:A:429:MET:SD	1:A:440:GLN:HB3	2.55	0.46
1:B:383:CYS:HB3	1:B:395:PHE:CE2	2.51	0.46
1:B:429:MET:SD	1:B:440:GLN:HB3	2.55	0.46
1:B:49:LEU:HD23	1:B:529:VAL:HG13	1.97	0.45
1:B:427:VAL:HG11	1:B:443:ALA:CB	2.46	0.45
1:A:164:ILE:HD13	1:A:165:PHE:N	2.32	0.45
1:A:237:ASP:OD1	1:A:238:GLY:N	2.50	0.45
1:B:167:CYS:SG	1:B:175:VAL:HG22	2.57	0.44
1:B:237:ASP:OD1	1:B:238:GLY:N	2.50	0.44
1:B:260:PHE:CE2	1:B:287:LEU:HD23	2.53	0.44
1:B:377:LEU:HD11	1:B:500:LYS:HA	2.00	0.44
1:A:427:VAL:HG23	1:A:448:ALA:HB1	2.01	0.43
1:A:410:THR:O	1:A:411:ALA:HB3	2.18	0.43
1:B:170:TRP:HA	1:B:173:ALA:HB2	2.01	0.43
1:A:377:LEU:HD11	1:A:500:LYS:HA	2.01	0.43
1:A:49:LEU:HD23	1:A:529:VAL:HG13	2.00	0.43
1:B:326:ASP:N	1:B:326:ASP:OD1	2.50	0.43
1:B:410:THR:O	1:B:411:ALA:HB3	2.18	0.43
1:B:179:LEU:HD11	1:B:189:TYR:HB3	1.99	0.43
1:A:260:PHE:CE2	1:A:287:LEU:HD23	2.54	0.43
1:A:260:PHE:HE2	1:A:287:LEU:HD23	1.84	0.42
1:B:129:PRO:HA	1:B:236:LEU:HD23	2.01	0.42
1:A:45:LEU:HB3	1:A:46:PRO:HD3	2.00	0.42
1:A:351:ILE:HD11	1:A:503:LEU:HD11	2.02	0.42
1:A:170:TRP:HA	1:A:173:ALA:HB2	2.02	0.42
1:B:317:VAL:HG21	1:B:335:VAL:HG21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PRO:HA	1:A:159:TYR:HB2	2.02	0.42
1:A:179:LEU:HD11	1:A:189:TYR:HB3	2.01	0.42
1:A:196:PHE:CZ	1:A:256:LEU:CD1	3.03	0.42
1:A:468:PHE:CE2	1:A:514:MET:CE	3.03	0.42
1:B:146:PRO:HA	1:B:159:TYR:HB2	2.01	0.41
1:A:167:CYS:SG	1:A:175:VAL:HG22	2.59	0.41
1:B:196:PHE:CZ	1:B:256:LEU:CD1	3.04	0.41
1:A:485:PRO:O	1:A:487:LEU:N	2.54	0.41
1:B:260:PHE:HE2	1:B:287:LEU:HD23	1.84	0.41
1:B:45:LEU:HB3	1:B:46:PRO:HD3	2.01	0.41
1:B:485:PRO:HG2	1:B:488:ILE:HD12	2.02	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	523/612 (86%)	474 (91%)	35 (7%)	14 (3%)	5	23
1	B	524/612 (86%)	477 (91%)	38 (7%)	9 (2%)	9	34
All	All	1047/1224 (86%)	951 (91%)	73 (7%)	23 (2%)	6	28

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	478	TYR
1	A	479	PRO
1	A	481	MET
1	A	486	GLU
1	A	487	LEU
1	B	478	TYR
1	B	479	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	483	ILE
1	B	486	GLU
1	A	115	THR
1	B	115	THR
1	A	489	ALA
1	A	19	LYS
1	A	492	THR
1	A	411	ALA
1	B	411	ALA
1	A	484	SER
1	B	114	ILE
1	B	476	PRO
1	B	492	THR
1	A	114	ILE
1	A	476	PRO
1	A	116	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/489 (87%)	383 (90%)	43 (10%)	7	26
1	B	426/489 (87%)	386 (91%)	40 (9%)	8	29
All	All	852/978 (87%)	769 (90%)	83 (10%)	8	28

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	21	THR
1	A	40	ASP
1	A	60	GLN
1	A	99	ARG
1	A	108	LEU
1	A	112	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	115	THR
1	A	119	LEU
1	A	123	LYS
1	A	138	MET
1	A	157	THR
1	A	164	ILE
1	A	169	ASP
1	A	175	VAL
1	A	186	ARG
1	A	188	LEU
1	A	197	LEU
1	A	223	LYS
1	A	241	GLU
1	A	244	ILE
1	A	248	LYS
1	A	252	MET
1	A	265	ARG
1	A	282	ARG
1	A	286	GLU
1	A	287	LEU
1	A	305	ILE
1	A	316	LEU
1	A	326	ASP
1	A	366	MET
1	A	386	SER
1	A	410	THR
1	A	416	GLU
1	A	453	SER
1	A	459	LYS
1	A	469	THR
1	A	471	GLU
1	A	478	TYR
1	A	487	LEU
1	A	509	LYS
1	A	522	ASP
1	A	540	LEU
1	B	20	LEU
1	B	21	THR
1	B	40	ASP
1	B	60	GLN
1	B	83	LYS
1	B	95	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	99	ARG
1	B	108	LEU
1	B	110	LYS
1	B	112	TRP
1	B	119	LEU
1	B	138	MET
1	B	157	THR
1	B	169	ASP
1	B	175	VAL
1	B	188	LEU
1	B	197	LEU
1	B	242	GLN
1	B	244	ILE
1	B	265	ARG
1	B	282	ARG
1	B	287	LEU
1	B	305	ILE
1	B	316	LEU
1	B	327	GLU
1	B	359	ASP
1	B	366	MET
1	B	386	SER
1	B	390	ASP
1	B	407	LYS
1	B	409	LYS
1	B	431	SER
1	B	469	THR
1	B	478	TYR
1	B	481	MET
1	B	482	LYS
1	B	487	LEU
1	B	503	LEU
1	B	530	LEU
1	B	540	LEU

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

Mol	Chain	Res	Type
1	A	199	HIS
1	A	521	GLN
1	B	191	ASN
1	B	521	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 ⓘ

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	C	1	2	12,12,12	0.50	0	17,17,17	0.97	0
2	GLC	C	2	2	11,11,12	0.55	0	15,15,17	1.80	2 (13%)
2	AC1	C	3	2	21,22,23	1.08	2 (9%)	22,32,34	1.47	5 (22%)
2	BGC	D	1	2	12,12,12	0.53	0	17,17,17	0.94	0
2	GLC	D	2	2	11,11,12	0.29	0	15,15,17	2.05	1 (6%)
2	AC1	D	3	2	21,22,23	0.92	1 (4%)	22,32,34	1.19	2 (9%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	AC1	C1B-C7B	2.75	1.54	1.50
2	D	3	AC1	C1B-C7B	2.15	1.53	1.50
2	C	3	AC1	C2B-C1B	2.15	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C1-O5-C5	7.03	121.72	112.19
2	C	2	GLC	C1-O5-C5	5.94	120.24	112.19
2	C	3	AC1	C7B-C1B-N4A	3.44	115.84	110.68
2	C	3	AC1	O5-C1-C2	-2.76	106.51	110.77
2	D	3	AC1	C1-C2-C3	2.63	112.89	109.67
2	C	2	GLC	O5-C1-C2	2.43	114.52	110.77
2	C	3	AC1	C2-C3-C4	-2.41	108.51	110.63
2	C	3	AC1	O2B-C2B-C1B	2.37	113.87	109.12
2	D	3	AC1	O3-C3-C2	-2.37	105.46	109.99
2	C	3	AC1	O3-C3-C4	2.23	114.15	109.66

There are no chirality outliers.

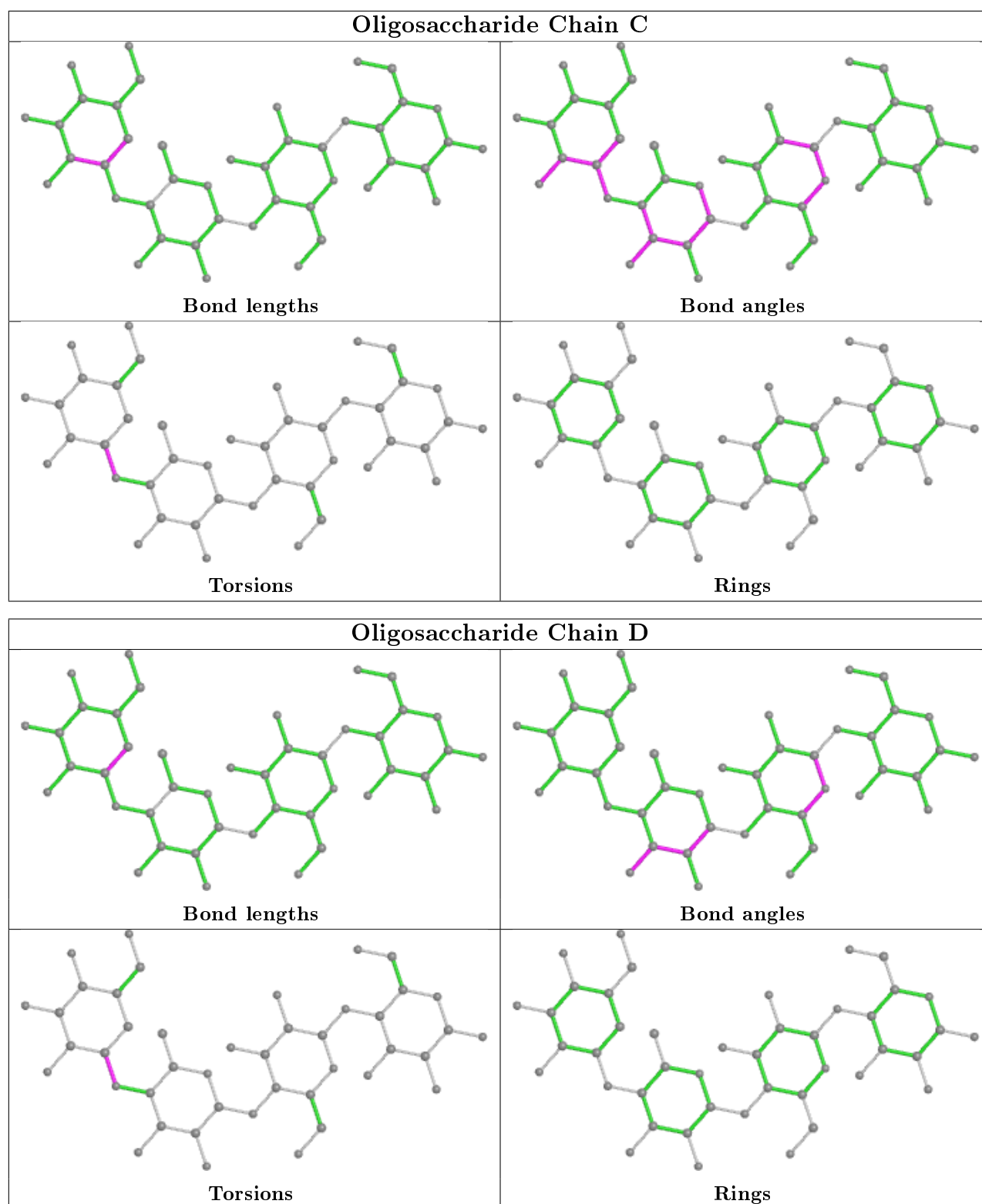
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C7B-C1B-N4A-C4
2	C	3	AC1	C7B-C1B-N4A-C4

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.



5.6 Ligand geometry [i](#)

2 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$
3	ADP	B	602	-	24,29,29	1.07	1 (4%)	29,45,45	1.51	5 (17%)
3	ADP	A	602	-	24,29,29	1.11	3 (12%)	29,45,45	1.68	6 (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
3	ADP	B	602	-	-	4/12/32/32	0/3/3/3
3	ADP	A	602	-	-	6/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ADP	O4'-C1'	2.73	1.44	1.41
3	B	602	ADP	C5-C4	2.48	1.47	1.40
3	A	602	ADP	C2-N3	2.21	1.35	1.32
3	A	602	ADP	C5-C4	2.17	1.46	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ADP	N3-C2-N1	-4.37	121.85	128.68
3	B	602	ADP	N3-C2-N1	-4.31	121.95	128.68
3	B	602	ADP	C4-C5-N7	-3.27	106.00	109.40
3	A	602	ADP	PA-O3A-PB	-3.24	121.69	132.83
3	A	602	ADP	C1'-N9-C4	-3.01	121.35	126.64
3	A	602	ADP	C3'-C2'-C1'	2.97	105.45	100.98
3	B	602	ADP	C1'-N9-C4	-2.80	121.72	126.64
3	B	602	ADP	PA-O3A-PB	-2.55	124.09	132.83
3	A	602	ADP	N6-C6-N1	2.31	123.36	118.57
3	A	602	ADP	O3B-PB-O2B	2.25	116.24	107.64
3	B	602	ADP	C2-N1-C6	2.07	122.30	118.75

There are no chirality outliers.

All (10) torsion outliers are listed below:

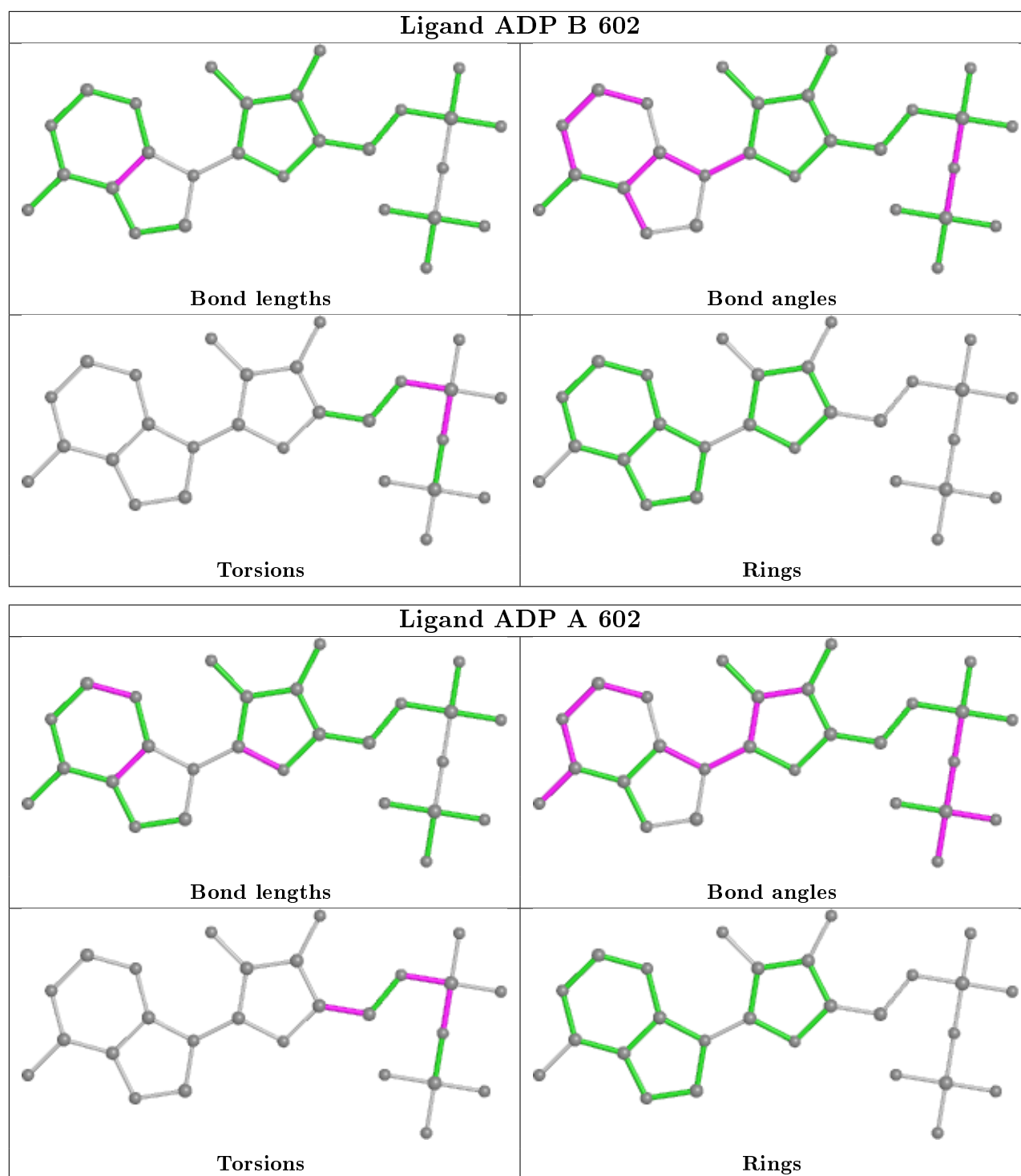
Mol	Chain	Res	Type	Atoms
3	B	602	ADP	PB-O3A-PA-O5'
3	B	602	ADP	C5'-O5'-PA-O1A
3	B	602	ADP	C5'-O5'-PA-O2A
3	A	602	ADP	C5'-O5'-PA-O1A
3	A	602	ADP	C5'-O5'-PA-O2A
3	A	602	ADP	C3'-C4'-C5'-O5'
3	A	602	ADP	O4'-C4'-C5'-O5'
3	B	602	ADP	C5'-O5'-PA-O3A
3	A	602	ADP	PB-O3A-PA-O5'
3	A	602	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	ADP	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 ⓘ

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, 95th 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	525/612 (85%)	0.31	16 (3%)	50 34	40, 64, 94, 126	0
1	B	526/612 (85%)	0.24	10 (1%)	66 49	34, 57, 89, 120	0
All	All	1051/1224 (85%)	0.28	26 (2%)	57 40	34, 61, 92, 126	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	542	ILE	6.0
1	A	113	GLY	3.7
1	B	486	GLU	3.5
1	A	247	LEU	3.4
1	B	239	ILE	3.4
1	A	114	ILE	3.4
1	A	112	TRP	3.4
1	B	112	TRP	3.1
1	B	114	ILE	3.1
1	B	113	GLY	3.0
1	B	479	PRO	3.0
1	A	415	LYS	3.0
1	A	542	ILE	2.8
1	A	483	ILE	2.7
1	A	482	LYS	2.6
1	A	246	SER	2.5
1	A	477	GLU	2.4
1	B	190	GLN	2.3
1	A	326	ASP	2.3
1	A	479	PRO	2.3
1	A	486	GLU	2.2
1	B	326	ASP	2.2
1	A	478	TYR	2.2
1	A	322	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	19	LYS	2.2
1	B	17	GLU	2.1

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](#)

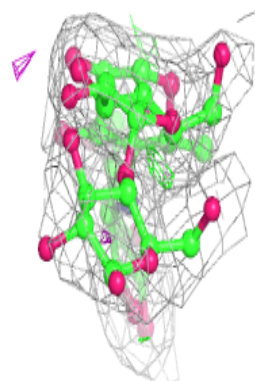
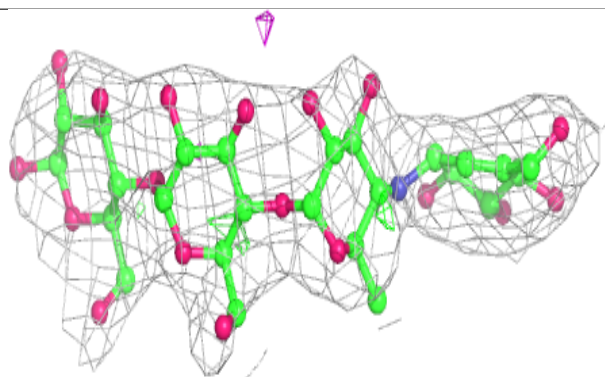
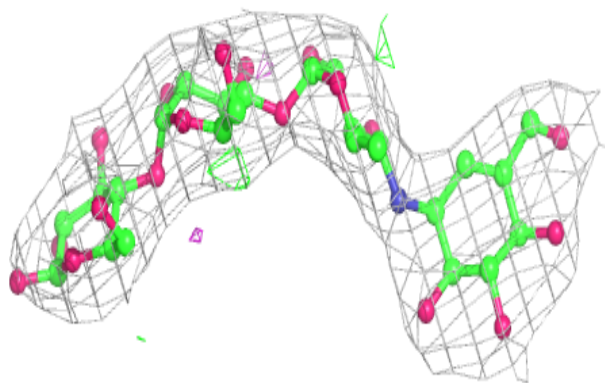
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	D	1	12/12	0.92	0.20	49,55,60,61	0
2	BGC	C	1	12/12	0.93	0.15	46,52,56,60	0
2	AC1	D	3	21/22	0.93	0.18	43,52,55,56	0
2	AC1	C	3	21/22	0.93	0.16	28,33,40,41	0
2	GLC	C	2	11/12	0.94	0.17	36,40,44,44	0
2	GLC	D	2	11/12	0.96	0.16	44,47,49,49	0

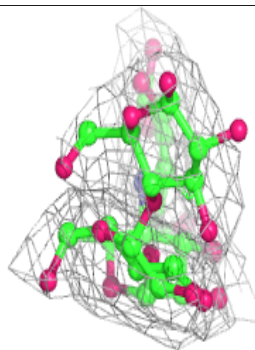
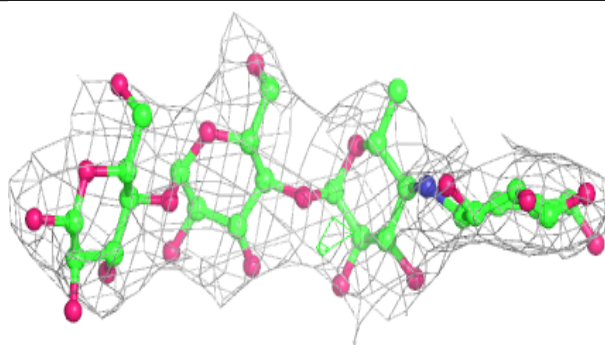
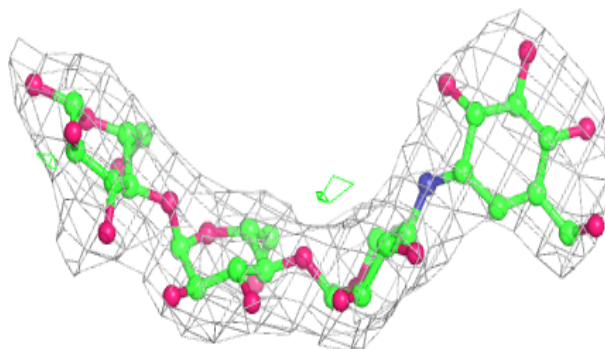
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

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

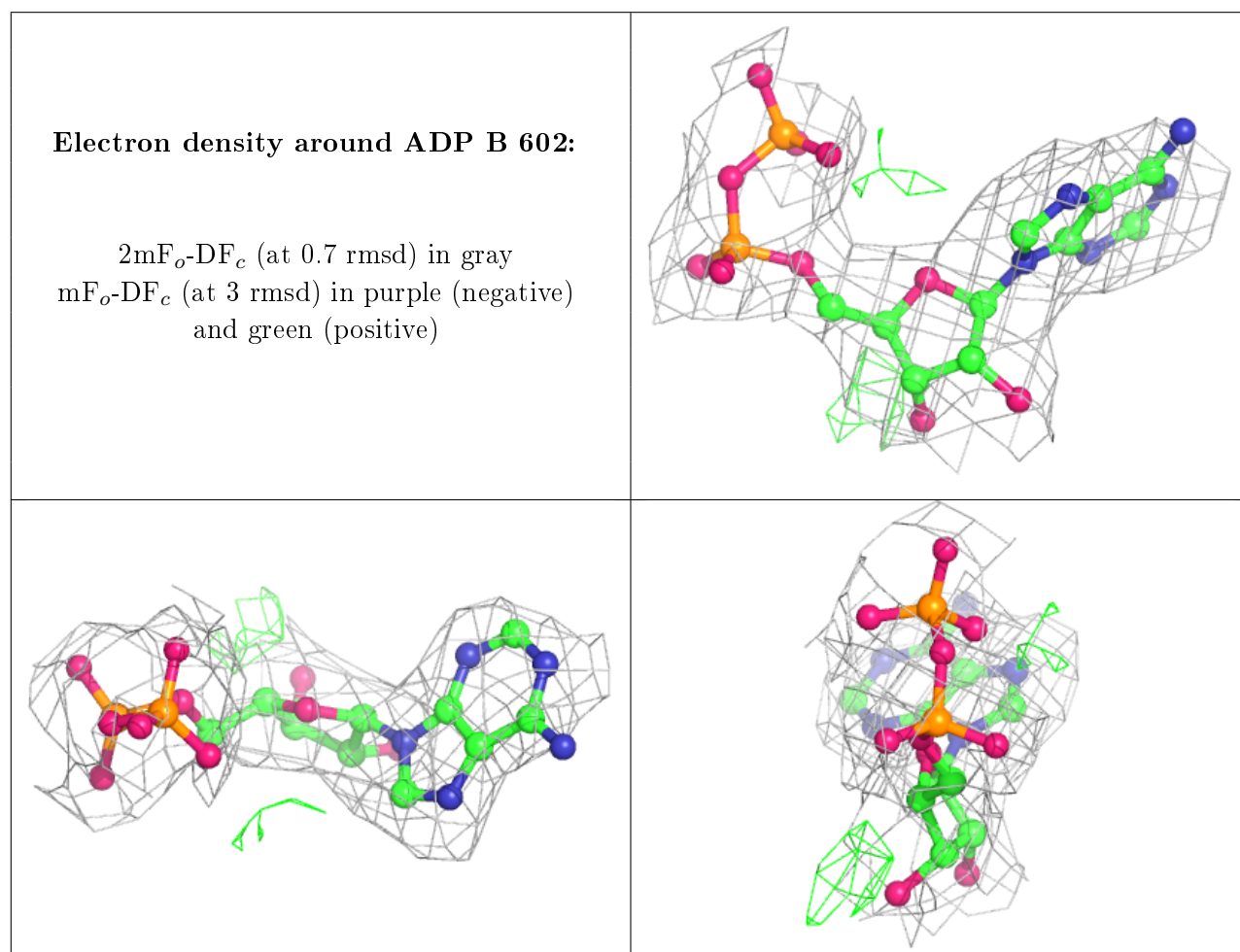


6.4 Ligands ⓘ

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, 95th 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.

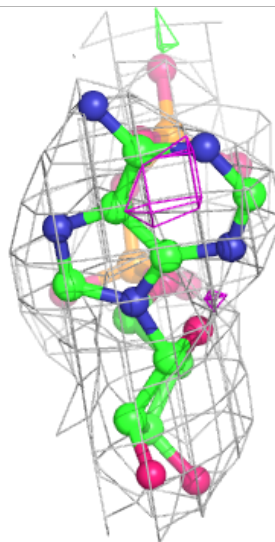
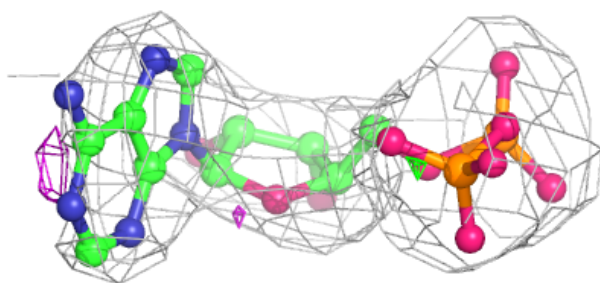
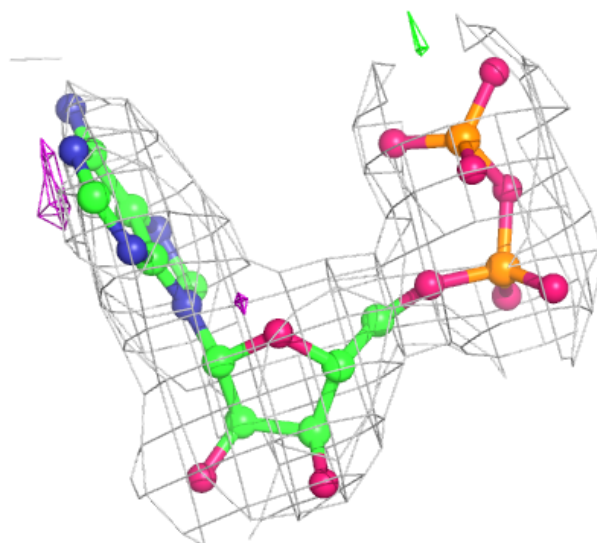
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	B	602	27/27	0.94	0.16	44,64,67,68	0
3	ADP	A	602	27/27	0.95	0.15	47,63,73,74	0

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 A 602:

$2mF_o-DF_c$ (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.