



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:17 PM UTC

PDB ID : 6GNG / pdb_00006gng
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.

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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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

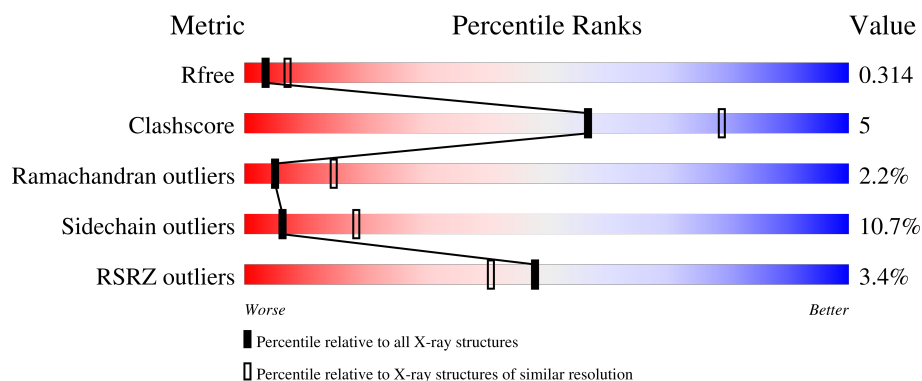
1 Overall quality at a glance

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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 $\leq 5\%$. 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	4% 67% 17% • 14%
1	B	612	2% 69% 15% • 14%
2	C	3	33% 67%
2	D	3	33% 67%

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

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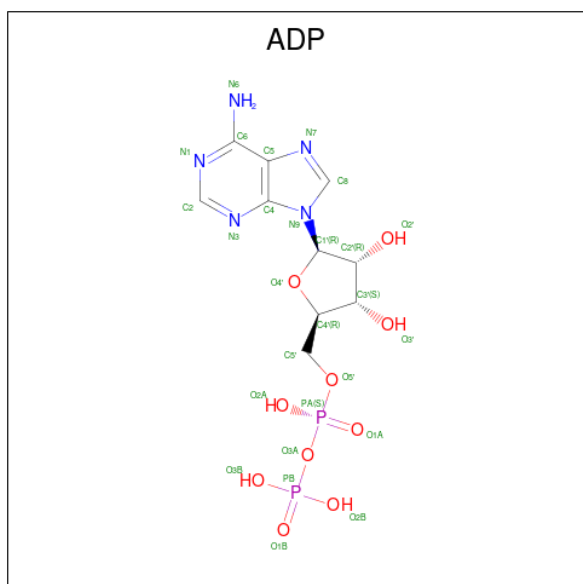
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP A8V967
B	-13	HIS	-	expression tag	UNP A8V967
B	-12	HIS	-	expression tag	UNP A8V967
B	-11	HIS	-	expression tag	UNP A8V967
B	-10	HIS	-	expression tag	UNP A8V967
B	-9	SER	-	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			

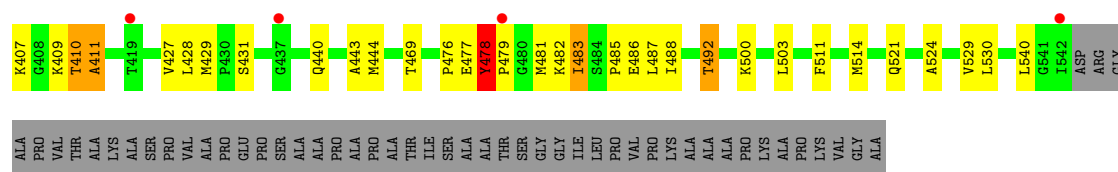
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	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		



- 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:



- 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:



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 20.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	90.5 (20.00-2.95) 90.5 (20.00-2.95)	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)	0.30 , 54.2	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, ADP, BGC, AC1

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	0.64	0/4154	0.90	3/5624 (0.1%)
1	B	0.64	0/4159	0.92	3/5631 (0.1%)
All	All	0.64	0/8313	0.91	6/11255 (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 (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	TYR	CA-CB-CG	7.22	126.90	113.90
1	A	478	TYR	CA-CB-CG	7.03	126.56	113.90
1	B	478	TYR	CB-CA-C	5.64	121.29	110.17
1	A	117	ASN	N-CA-C	-5.45	101.97	110.42
1	B	483	ILE	N-CA-C	5.33	120.42	109.34
1	A	478	TYR	CB-CA-C	5.02	120.06	110.17

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 [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	4051	0	4059	39	0
1	B	4056	0	4061	36	0
2	C	44	0	30	0	0
2	D	44	0	30	0	0
3	A	27	0	12	0	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	75	0

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

All (75) 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:B:366:MET:HE1	1:B:428:LEU:HD23	1.81	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:A:340:MET:HE1	1:A:409:LYS:HG3	1.89	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:MET:HE1	1:B:428:LEU:CD2	2.39	0.53
1:B:444:MET:HE3	1:B:521:GLN:HE22	1.75	0.52
1:A:444:MET:HE3	1:A:521:GLN:HE22	1.74	0.51
1:A:268:THR:HB	1:A:296:ILE:HD11	1.92	0.51
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:A:231:PHE:O	1:A:252:MET:HE1	2.10	0.51
1:B:202:ILE:HA	1:B:285:VAL:HG21	1.92	0.50
1:A:329:LYS:HE2	1:A:515:ARG:NH1	2.28	0.48
1:A:350:LEU:HD11	1:A:382:VAL:HG23	1.95	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:A:444:MET:HE3	1:A:521:GLN:NE2	2.30	0.46
1:B:429:MET:SD	1:B:440:GLN:HB3	2.55	0.46
1:B:444:MET:HE3	1:B:521:GLN:NE2	2.30	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:A:340:MET:HE3	1:A:407:LYS:HD3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:146:PRO:HA	1:A:159:TYR:HB2	2.02	0.42
1:B:353:PHE:CD1	1:B:366:MET:HE3	2.55	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:45:LEU:HB3	1:B:46:PRO:HD3	2.01	0.41
1:B:260:PHE:HE2	1:B:287:LEU:HD23	1.84	0.41
1:B:485:PRO:HG2	1:B:488:ILE:HD12	2.02	0.40
1:A:525:TRP:O	1:A:526:LYS:C	2.65	0.40
1:B:511:PHE:HA	1:B:514:MET:HE3	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	523/612 (86%)	474 (91%)	35 (7%)	14 (3%)	4	11
1	B	524/612 (86%)	477 (91%)	38 (7%)	9 (2%)	7	20
All	All	1047/1224 (86%)	951 (91%)	73 (7%)	23 (2%)	5	15

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
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%)	382 (90%)	44 (10%)	7	19
1	B	426/489 (87%)	379 (89%)	47 (11%)	6	17
All	All	852/978 (87%)	761 (89%)	91 (11%)	6	18

All (91) 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	57	MET
1	A	60	GLN
1	A	92	ILE
1	A	108	LEU
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	167	CYS
1	A	169	ASP
1	A	175	VAL
1	A	186	ARG
1	A	188	LEU
1	A	197	LEU
1	A	206	ARG
1	A	223	LYS
1	A	241	GLU
1	A	242	GLN
1	A	244	ILE
1	A	248	LYS
1	A	286	GLU
1	A	287	LEU
1	A	305	ILE
1	A	316	LEU
1	A	326	ASP
1	A	359	ASP
1	A	366	MET
1	A	377	LEU
1	A	386	SER
1	A	410	THR
1	A	459	LYS
1	A	465	GLU
1	A	469	THR
1	A	471	GLU
1	A	478	TYR
1	A	487	LEU
1	A	509	LYS
1	A	530	LEU

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Mol	Chain	Res	Type
1	A	540	LEU
1	B	20	LEU
1	B	21	THR
1	B	40	ASP
1	B	57	MET
1	B	60	GLN
1	B	84	LEU
1	B	92	ILE
1	B	95	LYS
1	B	108	LEU
1	B	110	LYS
1	B	112	TRP
1	B	115	THR
1	B	119	LEU
1	B	138	MET
1	B	157	THR
1	B	167	CYS
1	B	169	ASP
1	B	175	VAL
1	B	188	LEU
1	B	197	LEU
1	B	241	GLU
1	B	242	GLN
1	B	244	ILE
1	B	245	ILE
1	B	282	ARG
1	B	287	LEU
1	B	289	LYS
1	B	305	ILE
1	B	316	LEU
1	B	327	GLU
1	B	359	ASP
1	B	366	MET
1	B	377	LEU
1	B	386	SER
1	B	390	ASP
1	B	407	LYS
1	B	409	LYS
1	B	410	THR
1	B	431	SER
1	B	469	THR
1	B	478	TYR

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Mol	Chain	Res	Type
1	B	481	MET
1	B	482	LYS
1	B	487	LEU
1	B	503	LEU
1	B	530	LEU
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	199	HIS
1	A	242	GLN
1	A	521	GLN
1	B	51	GLN
1	B	117	ASN
1	B	190	GLN
1	B	191	ASN
1	B	199	HIS
1	B	301	ASN
1	B	332	ASN
1	B	521	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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	C	1	2	12,12,12	0.50	0	17,17,17	0.97	0
2	GLC	C	2	2	11,11,12	0.53	0	15,15,17	1.75	1 (6%)
2	AC1	C	3	2	21,22,23	1.06	2 (9%)	22,32,34	1.41	4 (18%)
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	2.04	1 (6%)
2	AC1	D	3	2	21,22,23	0.92	1 (4%)	22,32,34	1.17	3 (13%)

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	C	3	AC1	C2B-C1B	2.14	1.55	1.53
2	D	3	AC1	C1B-C7B	2.14	1.53	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C1-O5-C5	7.11	121.72	112.19
2	C	2	GLC	C1-O5-C5	6.01	120.24	112.19
2	C	3	AC1	C7B-C1B-N4A	3.51	115.84	110.68
2	C	3	AC1	C3B-C4A-C5B	-2.69	107.44	111.67
2	D	3	AC1	C3B-C4A-C5B	-2.56	107.65	111.67
2	C	3	AC1	O2B-C2B-C1B	2.44	113.87	109.08
2	C	3	AC1	O3-C3-C4	2.30	114.15	109.58
2	D	3	AC1	O3-C3-C2	-2.25	105.46	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	AC1	C1-C2-C3	2.23	112.89	109.64

There are no chirality outliers.

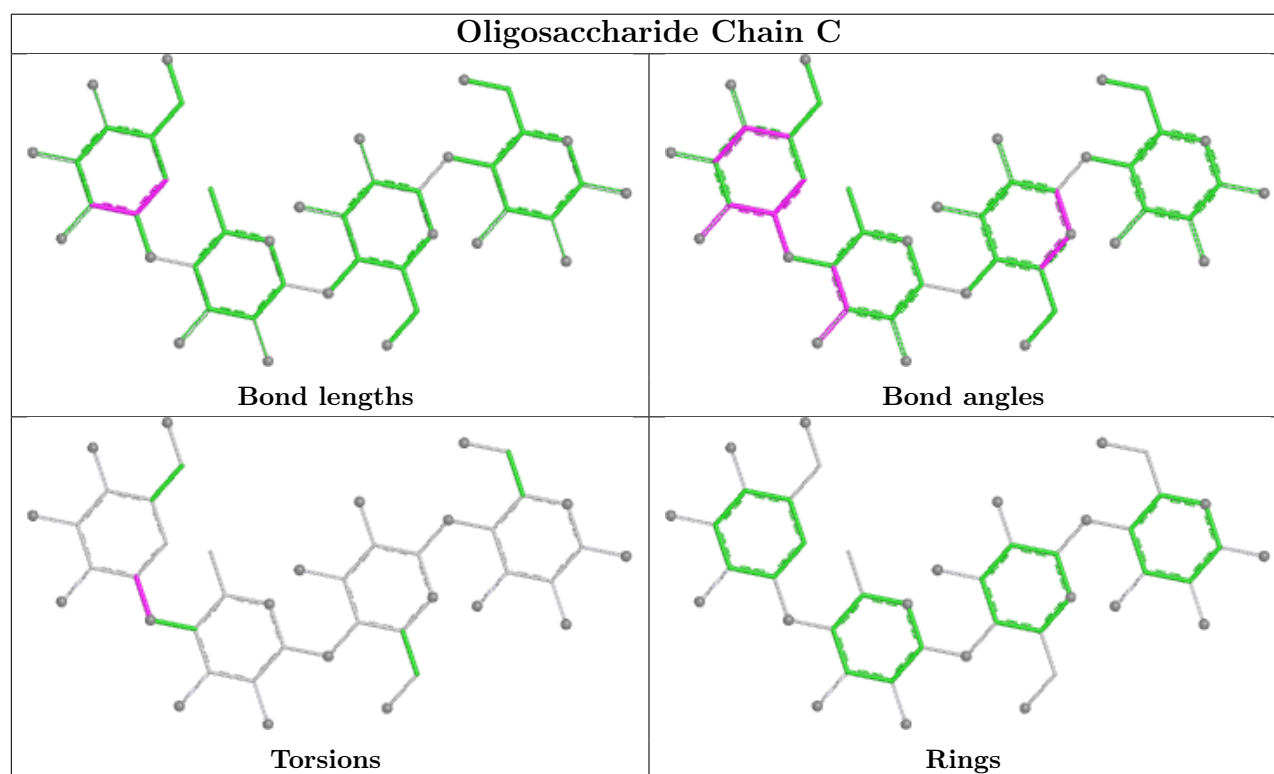
All (2) torsion outliers are listed below:

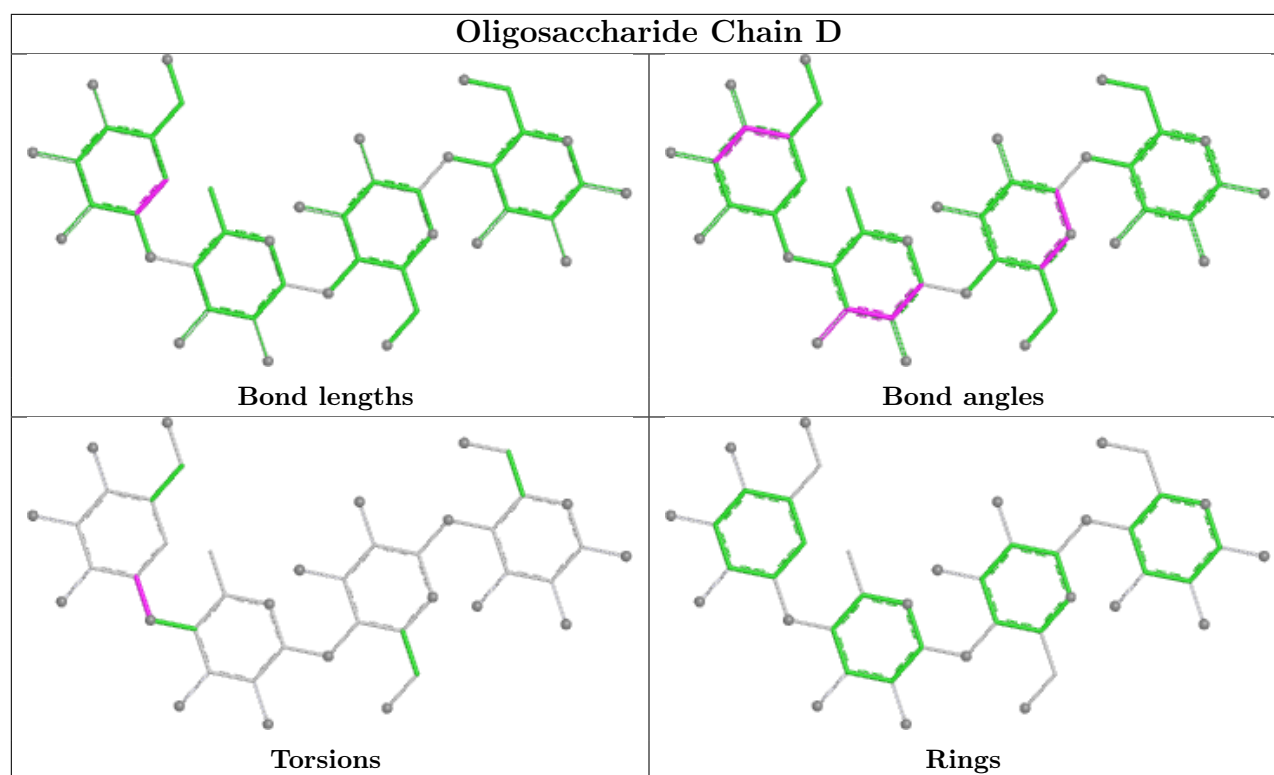
Mol	Chain	Res	Type	Atoms
2	C	3	AC1	C7B-C1B-N4A-C4
2	D	3	AC1	C7B-C1B-N4A-C4

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	A	602	-	28,29,29	1.43	4 (14%)	43,45,45	2.06	16 (37%)
3	ADP	B	602	-	28,29,29	1.49	3 (10%)	43,45,45	2.01	12 (27%)

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	A	602	-	-	10/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	602	-	-	4/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ADP	C5-C4	4.71	1.47	1.39
3	A	602	ADP	C5-C4	4.25	1.46	1.39
3	B	602	ADP	C5-C6	3.32	1.50	1.41
3	B	602	ADP	C8-N7	2.71	1.36	1.31
3	A	602	ADP	C5-N7	-2.67	1.34	1.39
3	A	602	ADP	C5-C6	2.51	1.48	1.41
3	A	602	ADP	C8-N7	2.12	1.35	1.31

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ADP	C5-C4-N3	-5.51	119.12	126.72
3	B	602	ADP	C5-C4-N3	-5.46	119.19	126.72
3	A	602	ADP	N3-C4-N9	4.84	135.39	127.17
3	A	602	ADP	N3-C2-N1	-4.45	121.85	128.58
3	B	602	ADP	N3-C2-N1	-4.38	121.95	128.58
3	B	602	ADP	C2-N3-C4	4.27	122.27	111.83
3	A	602	ADP	C2-N3-C4	4.07	121.77	111.83
3	B	602	ADP	N3-C4-N9	4.02	134.00	127.17
3	B	602	ADP	C4-C5-N7	-4.01	106.00	110.58
3	B	602	ADP	C6-C5-N7	3.38	138.60	132.09
3	A	602	ADP	C4-N9-C8	3.18	109.08	105.74
3	B	602	ADP	C5-N7-C8	2.98	108.13	103.45
3	B	602	ADP	C4-N9-C8	2.87	108.75	105.74
3	A	602	ADP	C4-C5-N7	-2.69	107.50	110.58
3	B	602	ADP	N9-C8-N7	-2.56	110.31	113.94
3	A	602	ADP	C5-N7-C8	2.48	107.35	103.45
3	A	602	ADP	C2'-C1'-N9	2.39	119.23	113.30
3	A	602	ADP	N9-C8-N7	-2.37	110.57	113.94
3	A	602	ADP	C4-N9-C1'	-2.26	121.35	126.63
3	A	602	ADP	O3B-PB-O2B	2.25	116.24	107.80
3	A	602	ADP	N6-C6-N1	2.24	123.36	118.38
3	B	602	ADP	C2-N1-C6	2.17	122.30	118.73
3	A	602	ADP	C5-C6-N6	-2.12	118.03	123.29
3	B	602	ADP	C2'-C1'-N9	2.12	118.56	113.30
3	A	602	ADP	C3'-C2'-C1'	2.11	105.45	101.46
3	B	602	ADP	C4-N9-C1'	-2.10	121.72	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ADP	C2'-C3'-C4'	2.01	106.50	102.61
3	A	602	ADP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

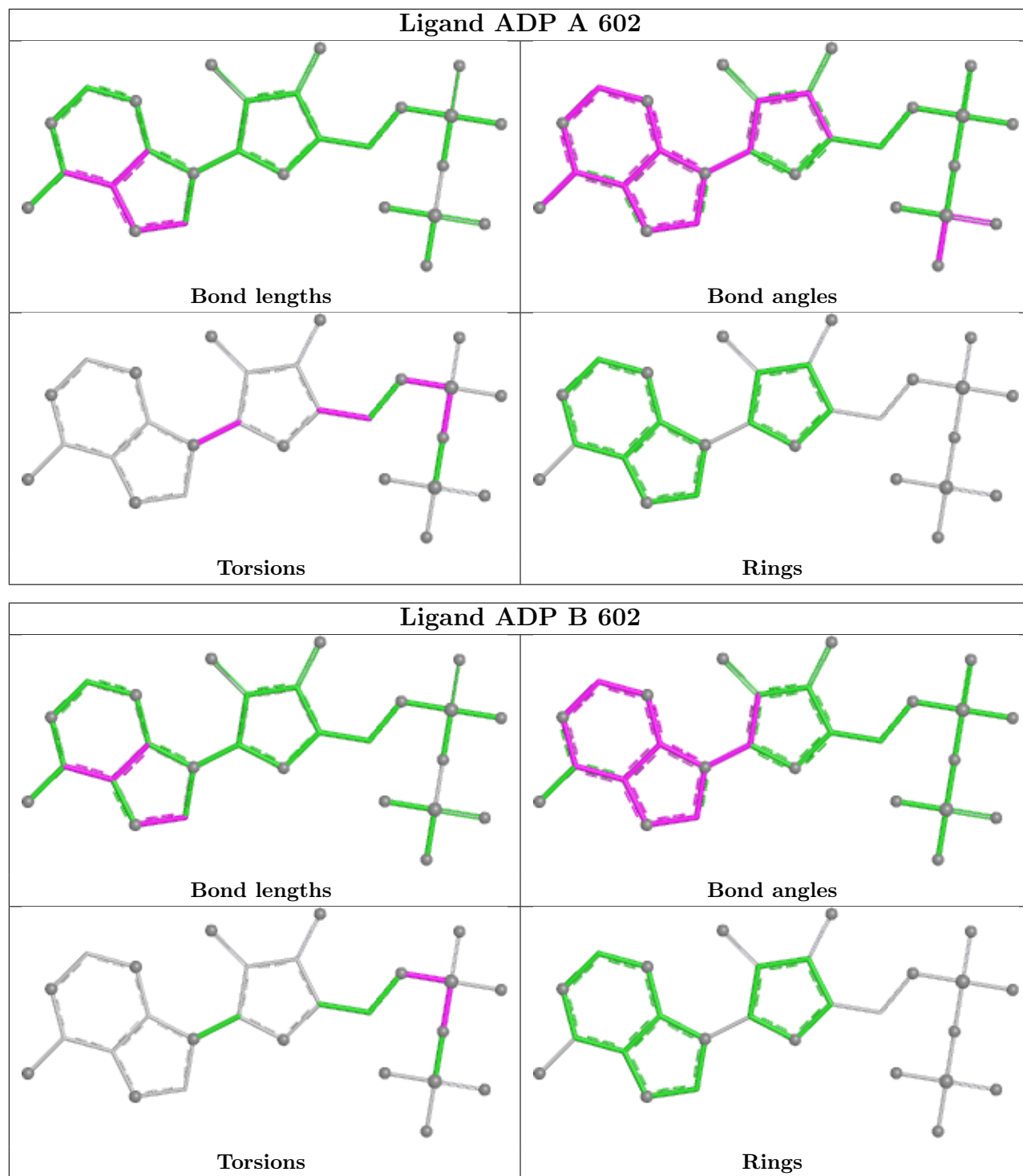
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	ADP	C5'-O5'-PA-O1A
3	A	602	ADP	C5'-O5'-PA-O2A
3	A	602	ADP	C5'-O5'-PA-O3A
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	B	602	ADP	C5'-O5'-PA-O3A
3	A	602	ADP	C3'-C4'-C5'-O5'
3	A	602	ADP	O4'-C4'-C5'-O5'
3	A	602	ADP	C2'-C1'-N9-C8
3	A	602	ADP	C2'-C1'-N9-C4
3	A	602	ADP	PB-O3A-PA-O5'
3	A	602	ADP	O4'-C1'-N9-C8
3	A	602	ADP	PB-O3A-PA-O2A

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 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%)	0.70	24 (4%) 37 31	40, 64, 94, 126	0
1	B	526/612 (85%)	0.65	12 (2%) 61 53	34, 57, 89, 120	0
All	All	1051/1224 (85%)	0.67	36 (3%) 48 41	34, 61, 92, 126	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	479	PRO	4.7
1	B	437	GLY	3.8
1	A	479	PRO	3.4
1	B	391	MET	3.1
1	A	322	ALA	3.0
1	A	472	GLU	2.9
1	A	112	TRP	2.9
1	B	542	ILE	2.6
1	A	415	LYS	2.6
1	A	115	THR	2.5
1	A	489	ALA	2.5
1	A	466	CYS	2.5
1	B	246	SER	2.5
1	A	41	VAL	2.4
1	A	113	GLY	2.4
1	A	89	PHE	2.4
1	B	419	THR	2.4
1	B	378	GLY	2.3
1	A	465	GLU	2.3
1	A	298	GLY	2.3
1	A	480	GLY	2.2
1	A	490	LYS	2.2
1	A	483	ILE	2.2
1	B	302	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	502	ALA	2.2
1	A	180	LYS	2.1
1	B	148	ARG	2.1
1	A	314	LYS	2.1
1	B	365	CYS	2.1
1	A	449	VAL	2.1
1	B	149	ILE	2.1
1	A	377	LEU	2.0
1	B	89	PHE	2.0
1	A	393	ALA	2.0
1	A	417	GLU	2.0
1	A	478	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

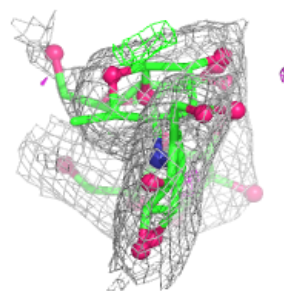
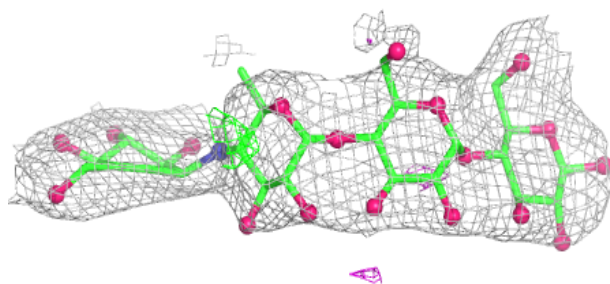
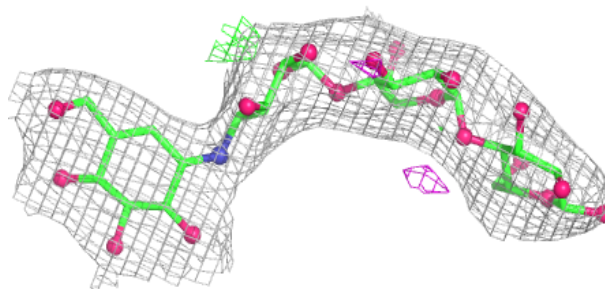
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	C	2	11/12	0.89	0.13	36,40,44,44	0
2	BGC	C	1	12/12	0.90	0.09	46,52,56,60	0
2	AC1	C	3	21/22	0.91	0.10	28,33,40,41	0
2	BGC	D	1	12/12	0.91	0.10	49,55,60,61	0
2	GLC	D	2	11/12	0.91	0.12	44,47,49,49	0
2	AC1	D	3	21/22	0.91	0.13	43,52,55,56	0

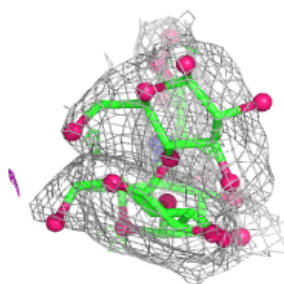
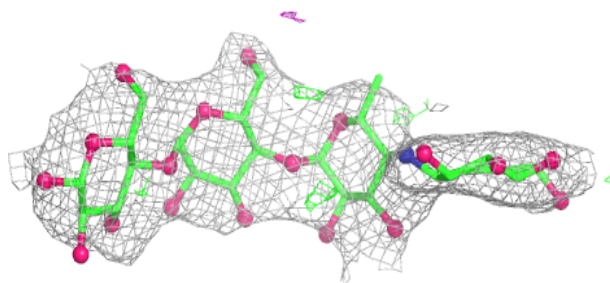
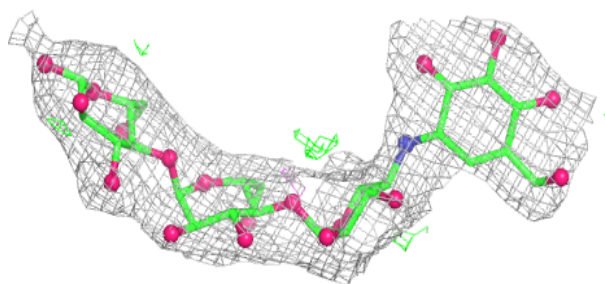
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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

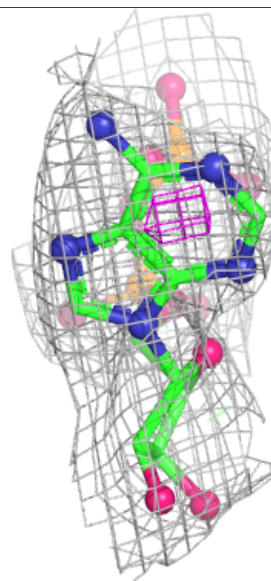
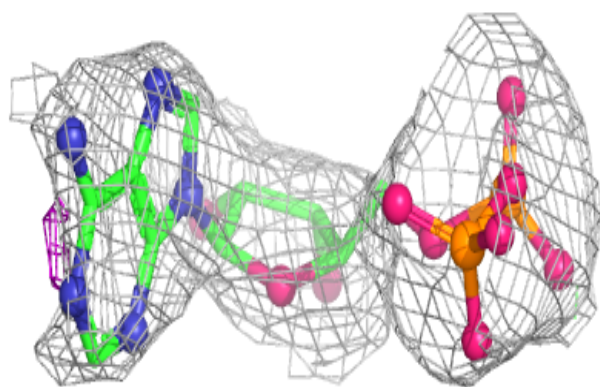
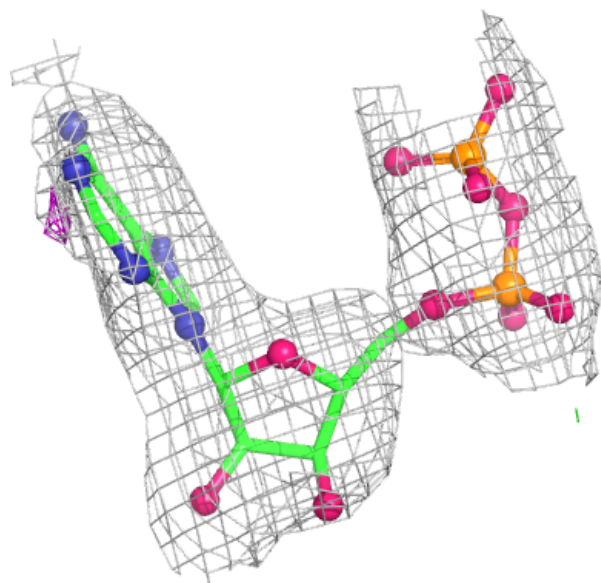
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	602	27/27	0.93	0.11	47,63,73,74	0
3	ADP	B	602	27/27	0.93	0.10	44,64,67,68	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.

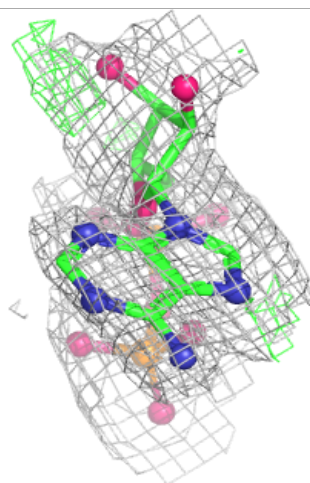
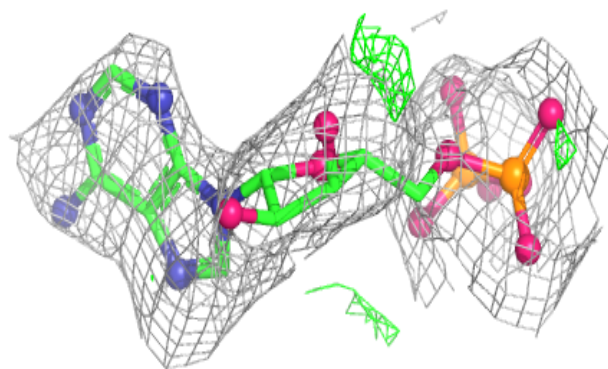
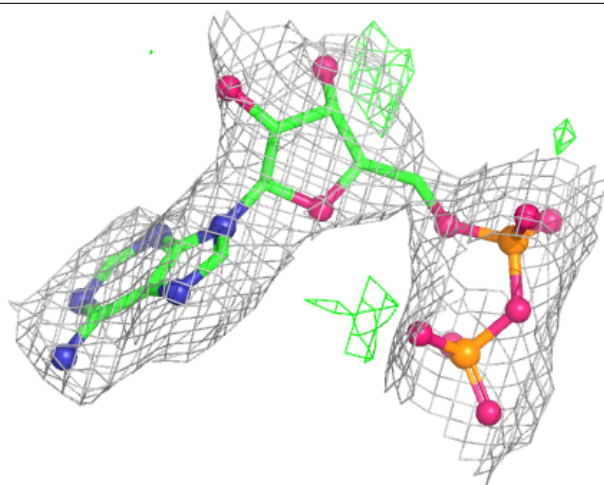
Electron density around ADP A 602:

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



Electron density around ADP B 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.