Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:08 PM UTC

PDB ID	:	1S4O / pdb_00001s4o
Title	:	Crystal structure of yeast alpha1,2-mannosyltransferase Kre2p/Mnt1p: binary complex with GDP/Mn
Authors	:	Lobsanov, Y.D.; Romero, P.A.; Sleno, B.; Yu, B.; Yip, P.; Herscovics, A.; Howell, P.L.
Deposited on	:	2004-01-16
Resolution	:	2.01 Å(reported)

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

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

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

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

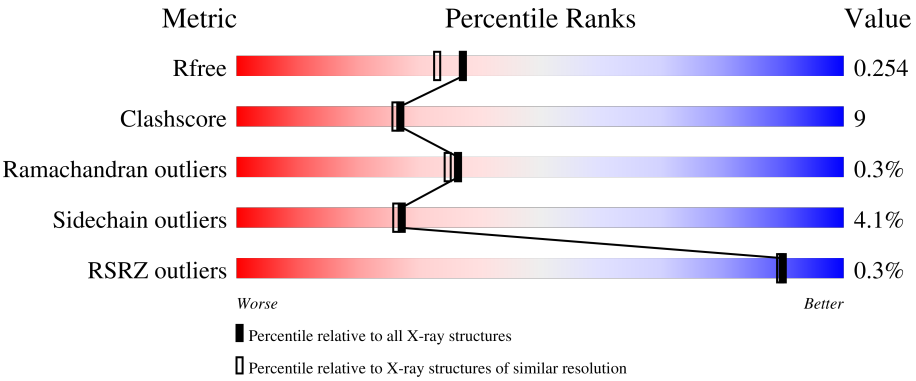
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

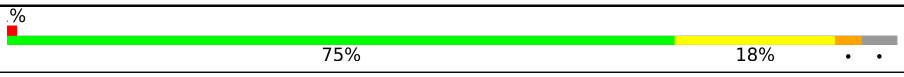
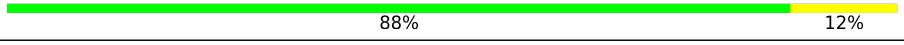
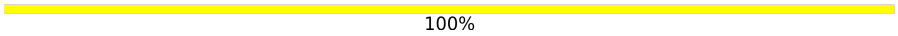
The reported resolution of this entry is 2.01 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	348	
1	B	348	
2	C	8	
3	D	2	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6452 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.

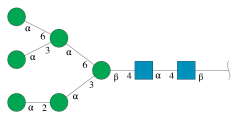
- Molecule 1 is a protein called Glycolipid 2-alpha-mannosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	1	0
			2836	1841	456	526	13			
1	B	335	Total	C	N	O	S	0	1	0
			2841	1845	457	526	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLU	-	cloning artifact	UNP P27809
A	96	PHE	-	cloning artifact	UNP P27809
B	95	GLU	-	cloning artifact	UNP P27809
B	96	PHE	-	cloning artifact	UNP P27809

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C N O 28 16 2 10	0	0	0

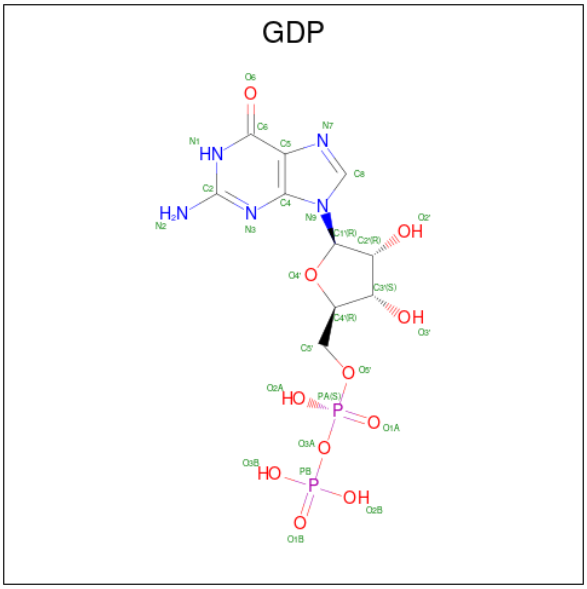
- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	B	1	Total Mn 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

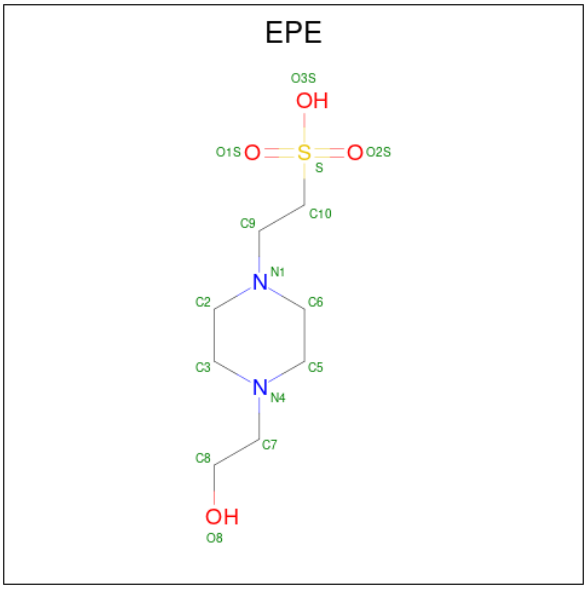
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	3	Total Cl 3 3	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P 28 10 5 11 2	0	0
6	B	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	282	Total	O	0	0
			282	282		
8	B	279	Total	O	0	0
			279	279		

3 Residue-property plots (i)

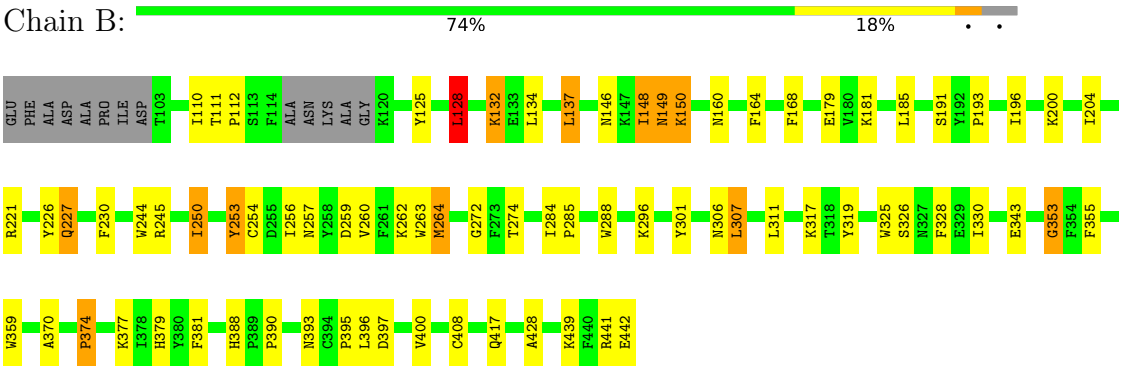
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glycolipid 2-alpha-mannosyltransferase

Chain A:

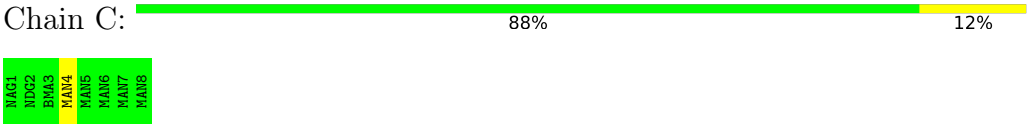
• Molecule 1: Glycolipid 2-alpha-mannosyltransferase

Chain B:



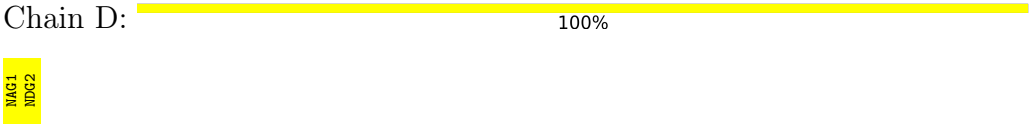
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 3: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.69Å 101.07Å 62.04Å 90.00° 98.81° 90.00°	Depositor
Resolution (Å)	52.42 – 2.01 52.42 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.6 (52.42-2.01) 95.6 (52.42-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.78 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.250 0.205 , 0.254	Depositor DCC
R_{free} test set	3313 reflections (6.96%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6452	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, MAN, CL, NAG, MN, NDG, GDP, BMA

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	0.56	1/2934 (0.0%)	0.98	16/3980 (0.4%)
1	B	0.56	1/2939 (0.0%)	0.97	12/3986 (0.3%)
All	All	0.56	2/5873 (0.0%)	0.98	28/7966 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	MET	SD-CE	-8.81	1.57	1.79
1	A	264	MET	SD-CE	-6.51	1.63	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	374	PRO	N-CA-C	-8.62	97.65	111.19
1	B	125	TYR	N-CA-C	-8.62	97.76	110.52
1	A	374	PRO	N-CA-C	-7.90	98.79	111.19
1	A	125	TYR	N-CA-C	-7.65	98.15	110.32
1	B	393	ASN	N-CA-C	-6.73	96.25	108.02
1	B	257	ASN	N-CA-C	6.60	120.25	112.72
1	A	234	HIS	N-CA-C	-6.59	101.21	110.50
1	A	257	ASN	N-CA-C	6.43	120.05	112.72
1	B	128	LEU	N-CA-C	-6.05	99.41	109.46
1	A	388	HIS	N-CA-C	-6.04	95.53	107.91
1	B	353	GLY	N-CA-C	5.69	120.84	113.27
1	B	149	ASN	N-CA-C	5.64	118.37	111.82
1	A	149	ASN	N-CA-C	5.60	118.15	111.71
1	B	230	PHE	N-CA-C	5.54	122.60	110.80
1	A	330	ILE	N-CA-C	-5.54	96.75	106.61
1	B	253	TYR	N-CA-C	5.45	118.15	111.82
1	A	393	ASN	N-CA-C	-5.45	98.48	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	LEU	CA-C-N	5.45	125.37	119.76
1	A	185	LEU	C-N-CA	5.45	125.37	119.76
1	A	217	SER	N-CA-C	5.42	117.54	109.25
1	B	134	LEU	N-CA-C	5.39	117.57	111.11
1	A	230	PHE	N-CA-C	5.38	122.25	110.80
1	A	281	GLU	N-CA-C	5.22	116.97	111.28
1	B	146	ASN	N-CA-C	5.19	116.94	111.28
1	A	391	TYR	N-CA-C	5.12	118.09	109.95
1	A	110	ILE	N-CA-C	5.11	116.21	111.81
1	B	110	ILE	N-CA-C	5.11	116.04	111.90
1	A	252	LEU	N-CA-C	-5.07	99.03	107.99

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	2836	0	2634	50	0
1	B	2841	0	2644	56	0
2	C	94	0	78	0	0
3	D	28	0	24	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	3	0	0	1	0
6	A	28	0	12	0	0
6	B	28	0	12	1	0
7	A	15	0	17	0	0
7	B	15	0	17	0	0
8	A	282	0	0	2	0
8	B	279	0	0	3	0
All	All	6452	0	5438	104	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 9.

All (104) 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:250:ILE:HD11	1:B:388:HIS:HD2	1.48	0.79
1:B:374:PRO:HG2	1:B:377:LYS:HG2	1.63	0.79
1:B:227:GLN:HA	1:B:227:GLN:HE21	1.50	0.74
1:B:193:PRO:HG2	1:B:196:ILE:HG12	1.71	0.72
1:B:264:MET:HE3	1:B:381:PHE:HZ	1.55	0.72
1:A:174:LYS:HB2	1:A:174:LYS:NZ	2.04	0.71
1:B:150:LYS:NZ	1:B:150:LYS:HB3	2.05	0.71
1:B:264:MET:HE3	1:B:381:PHE:CZ	2.26	0.70
1:B:263:TRP:CZ3	1:B:264:MET:HE2	2.26	0.69
1:A:174:LYS:HB2	1:A:174:LYS:HZ2	1.57	0.68
1:A:227:GLN:HE21	1:A:227:GLN:HA	1.60	0.67
1:B:353:GLY:HA3	1:B:359:TRP:CE2	2.31	0.65
1:A:285:PRO:HD2	1:A:357:GLU:OE1	1.99	0.63
1:A:300:GLU:H	1:A:300:GLU:CD	2.08	0.61
1:B:307:LEU:HD22	1:B:428:ALA:HB1	1.82	0.61
1:B:263:TRP:HZ3	1:B:264:MET:HE2	1.66	0.60
1:A:353:GLY:HA3	1:A:359:TRP:CE2	2.37	0.59
1:A:264:MET:HE2	1:A:269:LYS:HB2	1.84	0.59
1:A:250:ILE:HD11	1:A:388:HIS:HD2	1.68	0.58
1:B:374:PRO:HG2	1:B:377:LYS:CG	2.32	0.57
1:B:397:ASP:OD2	1:B:400:VAL:HG23	2.05	0.57
1:B:253:TYR:CG	1:B:408:CYS:HB3	2.40	0.57
1:A:250:ILE:HD11	1:A:388:HIS:CD2	2.40	0.56
1:B:250:ILE:HD11	1:B:388:HIS:CD2	2.34	0.56
1:A:253:TYR:CG	1:A:408:CYS:HB3	2.41	0.55
1:B:253:TYR:CD2	1:B:408:CYS:HB3	2.42	0.55
1:A:187:LYS:HG2	8:A:1120:HOH:O	2.06	0.54
1:A:200:LYS:O	1:A:204:ILE:HG12	2.06	0.54
1:B:288:TRP:CG	1:B:319:TYR:HB2	2.43	0.54
1:B:284:ILE:N	1:B:285:PRO:HD3	2.23	0.54
1:B:288:TRP:CD2	1:B:319:TYR:HB2	2.43	0.53
1:B:185:LEU:HD22	1:B:226:TYR:CZ	2.43	0.53
1:A:253:TYR:CD2	1:A:408:CYS:HB3	2.44	0.52
1:A:288:TRP:CD2	1:A:319:TYR:HB2	2.44	0.52
1:B:191:SER:HB2	5:B:704:CL:CL	2.47	0.52
1:B:263:TRP:HZ3	1:B:264:MET:CE	2.23	0.52
1:A:193:PRO:HD2	1:A:196:ILE:HG13	1.92	0.51
1:A:411:GLY:H	1:B:132:LYS:NZ	2.09	0.51
1:B:263:TRP:CZ3	1:B:264:MET:CE	2.92	0.51
1:A:283:THR:CG2	1:A:284:ILE:HG23	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:TRP:CE3	1:B:264:MET:HE2	2.45	0.50
1:A:284:ILE:N	1:A:285:PRO:HD3	2.26	0.50
1:A:212:TYR:CE1	1:A:215:GLY:HA2	2.47	0.50
1:B:137:LEU:HD12	1:B:168:PHE:CZ	2.47	0.50
1:B:200:LYS:O	1:B:204:ILE:HG12	2.12	0.50
1:A:280:TYR:O	1:A:283:THR:HB	2.12	0.49
1:A:295:ILE:HD11	1:A:372:PHE:HE1	1.78	0.49
1:B:353:GLY:HA3	1:B:359:TRP:CD2	2.47	0.49
1:B:160:ASN:HB2	1:B:164:PHE:CZ	2.47	0.49
1:A:253:TYR:CE2	1:A:387:HIS:HB2	2.48	0.49
1:A:137:LEU:HD12	1:A:168:PHE:CZ	2.48	0.49
1:A:328:PHE:CD1	1:A:328:PHE:C	2.91	0.48
1:B:150:LYS:HB3	1:B:150:LYS:HZ3	1.74	0.48
1:B:179:GLU:OE2	1:B:181:LYS:HE2	2.12	0.48
1:A:238:GLU:HG2	8:A:1150:HOH:O	2.13	0.48
1:B:417:GLN:NE2	8:B:1094:HOH:O	2.44	0.48
1:A:129:VAL:HG22	1:A:130:ARG:N	2.29	0.47
1:A:411:GLY:H	1:B:132:LYS:HZ2	1.62	0.46
1:A:353:GLY:HA3	1:A:359:TRP:CD2	2.51	0.46
1:B:353:GLY:HA3	1:B:359:TRP:CZ2	2.51	0.46
1:B:301:TYR:CE2	1:B:343:GLU:OE1	2.68	0.46
1:B:441:ARG:NH2	8:B:908:HOH:O	2.47	0.46
1:A:325:TRP:CZ3	1:A:388:HIS:HB3	2.51	0.46
1:B:185:LEU:HD22	1:B:226:TYR:OH	2.16	0.46
1:B:311:LEU:HD11	1:B:370:ALA:HB3	1.98	0.46
1:B:221:ARG:HD3	1:B:355:PHE:HA	1.98	0.46
1:A:235:GLU:O	1:A:238:GLU:HG2	2.16	0.45
1:B:260:VAL:HG11	1:B:330:ILE:HD13	1.97	0.45
1:A:174:LYS:NZ	1:A:174:LYS:CB	2.78	0.44
1:B:128:LEU:HD22	6:B:801:GDP:N3	2.32	0.44
1:B:111:THR:N	1:B:112:PRO:HD2	2.33	0.44
1:B:328:PHE:C	1:B:328:PHE:CD1	2.95	0.44
1:A:332:ASN:OD1	1:A:334:ASN:HB2	2.18	0.44
1:A:274:THR:HG23	1:A:328:PHE:CE1	2.52	0.44
1:A:297:LYS:HB2	1:A:297:LYS:NZ	2.33	0.44
1:A:160:ASN:HB2	1:A:164:PHE:CZ	2.53	0.43
1:B:306:ASN:HB2	1:B:370:ALA:O	2.19	0.43
1:A:425:TYR:CZ	1:A:429:GLN:HG3	2.54	0.43
1:B:274:THR:HG23	1:B:328:PHE:CE1	2.53	0.43
1:A:263:TRP:CZ3	1:A:264:MET:HE3	2.54	0.43
1:A:283:THR:HG23	1:A:284:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLY:HA2	1:B:379:HIS:O	2.19	0.43
1:B:301:TYR:HE2	1:B:343:GLU:OE1	2.00	0.43
1:B:148:ILE:HD12	1:B:256:ILE:HG21	1.99	0.43
1:A:244:TRP:C	1:A:244:TRP:CD1	2.95	0.43
1:A:288:TRP:CG	1:A:319:TYR:HB2	2.54	0.42
1:B:148:ILE:HG23	1:B:149:ASN:N	2.34	0.42
1:B:193:PRO:HG2	1:B:196:ILE:CG1	2.47	0.42
1:B:245:ARG:HD3	1:B:326:SER:O	2.19	0.42
1:A:244:TRP:HA	1:A:329:GLU:O	2.20	0.41
1:A:389:PRO:HA	1:A:390:PRO:HA	1.78	0.41
1:A:251:LYS:HB2	1:A:387:HIS:HB3	2.03	0.41
1:A:264:MET:CE	1:A:269:LYS:HB2	2.49	0.41
1:B:439:LYS:O	1:B:442:GLU:HG3	2.20	0.41
1:A:250:ILE:HG23	1:A:251:LYS:N	2.35	0.41
1:A:281:GLU:C	1:A:283:THR:N	2.79	0.41
1:B:244:TRP:C	1:B:244:TRP:CD1	2.99	0.41
1:B:150:LYS:NZ	1:B:150:LYS:CB	2.80	0.41
1:A:320:ASN:O	1:A:321:LEU:HB2	2.21	0.40
1:A:396:LEU:HD12	1:A:434:PRO:HG3	2.04	0.40
1:A:124:CYS:O	1:A:243:TYR:HA	2.21	0.40
1:B:259:ASP:HB3	1:B:262:LYS:HE3	2.04	0.40
1:A:283:THR:HG22	1:A:284:ILE:HG23	2.03	0.40
1:B:112:PRO:HG2	8:B:1107:HOH:O	2.21	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	332/348 (95%)	321 (97%)	10 (3%)	1 (0%)	36	35
1	B	332/348 (95%)	320 (96%)	11 (3%)	1 (0%)	36	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	664/696 (95%)	641 (96%)	21 (3%)	2 (0%)	36 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	ILE
1	A	148	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	304/313 (97%)	293 (96%)	11 (4%)	31 31
1	B	305/313 (97%)	291 (95%)	14 (5%)	24 22
All	All	609/626 (97%)	584 (96%)	25 (4%)	27 26

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	166	GLU
1	A	174	LYS
1	A	227	GLN
1	A	237	LEU
1	A	250	ILE
1	A	283	THR
1	A	287	LEU
1	A	297	LYS
1	A	325	TRP
1	A	390	PRO
1	B	128	LEU
1	B	132	LYS
1	B	137	LEU
1	B	150	LYS
1	B	227	GLN

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Mol	Chain	Res	Type
1	B	250	ILE
1	B	254	CYS
1	B	296	LYS
1	B	307	LEU
1	B	317	LYS
1	B	325	TRP
1	B	390	PRO
1	B	395	PRO
1	B	396	LEU

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

Mol	Chain	Res	Type
1	A	227	GLN
1	A	402	ASN
1	A	417	GLN
1	B	189	HIS
1	B	227	GLN
1	B	334	ASN
1	B	393	ASN
1	B	417	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)

10 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	NAG	C	1	1,2	14,14,15	0.57	0	17,19,21	0.75	0
2	NDG	C	2	2	14,14,15	0.71	0	17,19,21	0.65	0
2	BMA	C	3	2	11,11,12	0.52	0	15,15,17	0.51	0
2	MAN	C	4	2	11,11,12	0.52	0	15,15,17	0.60	1 (6%)
2	MAN	C	5	2	11,11,12	0.49	0	15,15,17	0.52	0
2	MAN	C	6	2	11,11,12	0.61	0	15,15,17	0.60	0
2	MAN	C	7	2	11,11,12	0.57	0	15,15,17	0.55	0
2	MAN	C	8	2	11,11,12	0.45	0	15,15,17	0.54	0
3	NAG	D	1	3,1	14,14,15	0.63	0	17,19,21	0.80	1 (5%)
3	NDG	D	2	3	14,14,15	0.58	0	17,19,21	0.85	1 (5%)

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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NDG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
2	MAN	C	8	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NDG	D	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	NAG	C2-N2-C7	-2.54	119.50	122.90
3	D	2	NDG	C2-N2-C7	-2.34	119.77	122.90
2	C	4	MAN	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

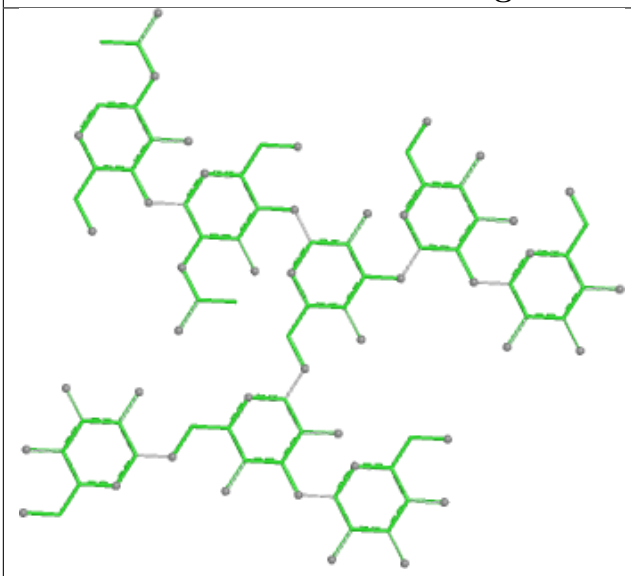
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NDG	C8-C7-N2-C2
3	D	2	NDG	O7-C7-N2-C2
2	C	5	MAN	C4-C5-C6-O6
2	C	8	MAN	O5-C5-C6-O6
2	C	2	NDG	O5-C5-C6-O6
2	C	2	NDG	C4-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
2	C	8	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
3	D	2	NDG	C4-C5-C6-O6
3	D	2	NDG	O5-C5-C6-O6

There are no ring outliers.

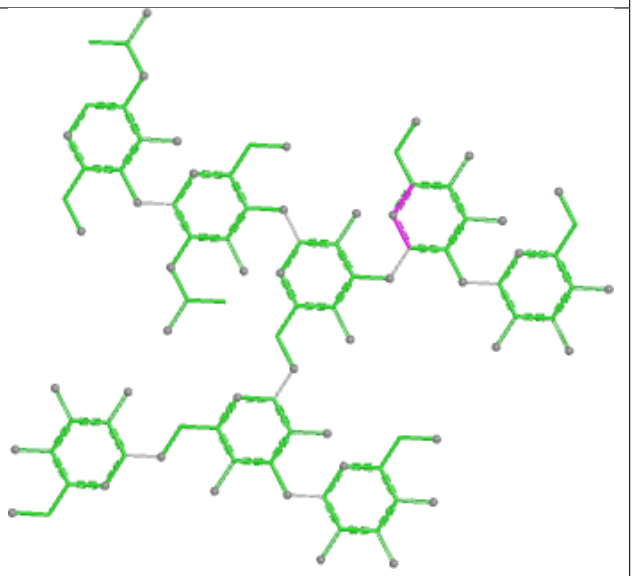
No monomer is involved in short contacts.

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

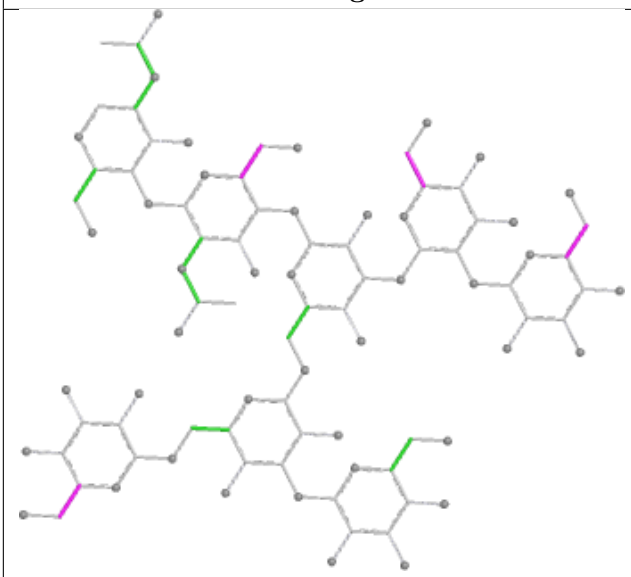
Oligosaccharide Chain C



Bond lengths



Bond angles



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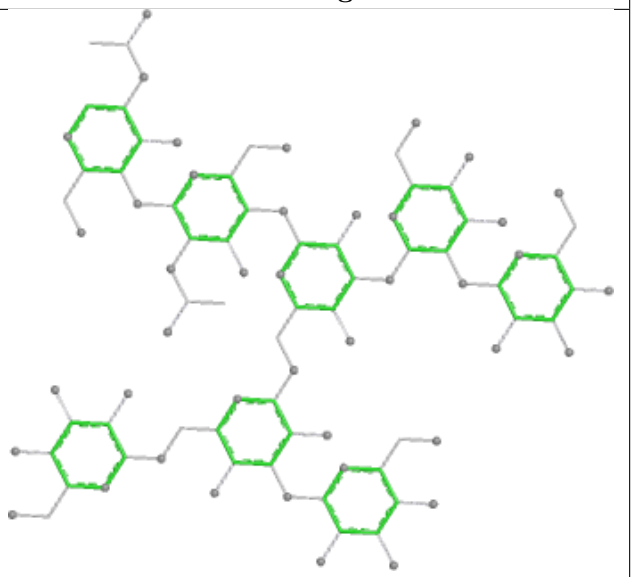
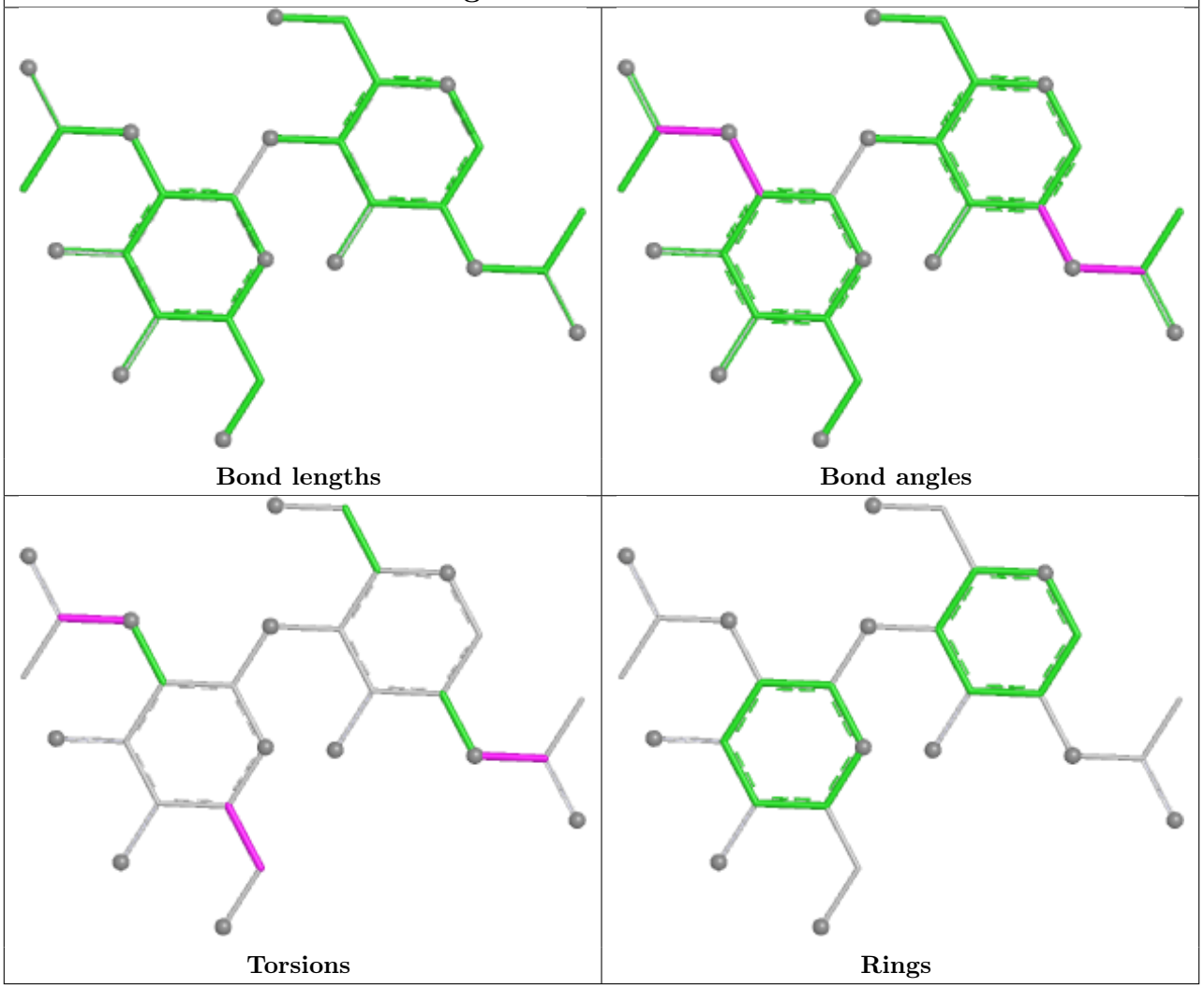


Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GDP	B	801	4	29,30,30	1.15	2 (6%)	45,47,47	0.84	2 (4%)
7	EPE	B	902	-	15,15,15	1.13	1 (6%)	19,20,20	0.79	0
6	GDP	A	800	4	29,30,30	0.98	2 (6%)	45,47,47	0.82	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EPE	A	901	-	15,15,15	1.03	0	19,20,20	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	B	801	4	-	0/16/32/32	0/3/3/3
7	EPE	B	902	-	-	2/9/19/19	0/1/1/1
6	GDP	A	800	4	-	0/16/32/32	0/3/3/3
7	EPE	A	901	-	-	2/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	801	GDP	PA-O3A	-3.48	1.55	1.59
6	A	800	GDP	C1'-N9	3.34	1.57	1.47
6	B	801	GDP	C1'-N9	2.78	1.55	1.47
7	B	902	EPE	C6-N1	2.13	1.52	1.46
6	A	800	GDP	O3'-C3'	2.02	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	800	GDP	O3'-C3'-C4'	-2.74	103.21	111.08
6	B	801	GDP	O3'-C3'-C4'	-2.66	103.44	111.08
6	B	801	GDP	O2'-C2'-C1'	2.05	117.15	110.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	901	EPE	C10-C9-N1-C2
7	A	901	EPE	C10-C9-N1-C6
7	B	902	EPE	C10-C9-N1-C2
7	B	902	EPE	C10-C9-N1-C6

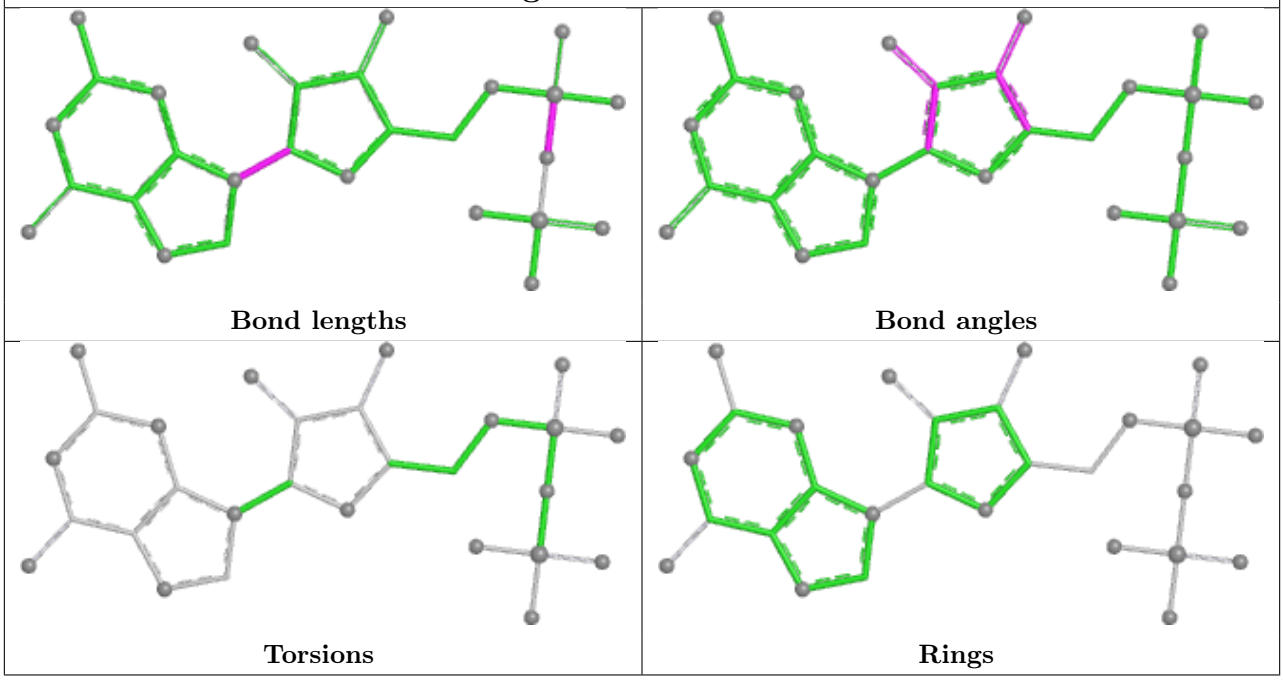
There are no ring outliers.

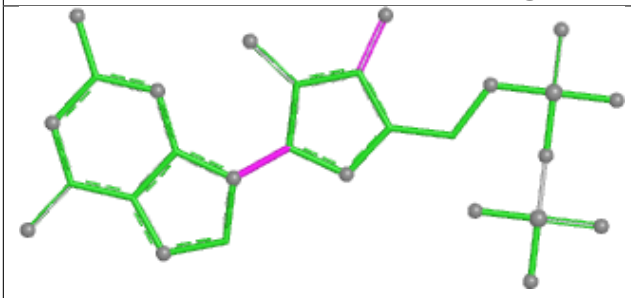
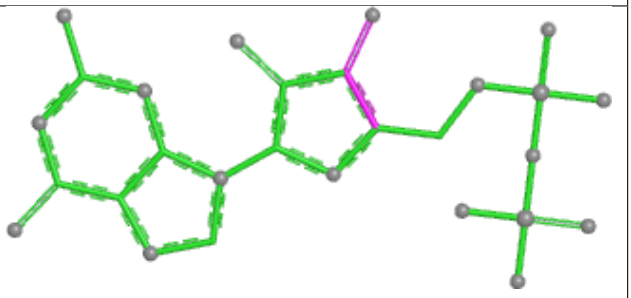
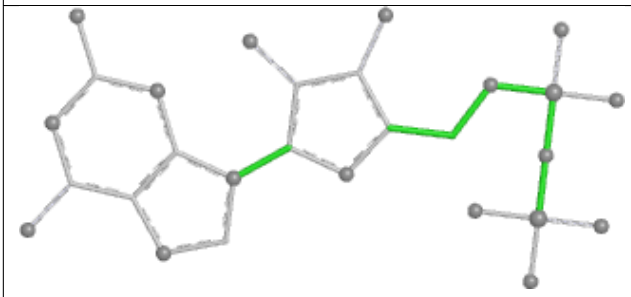
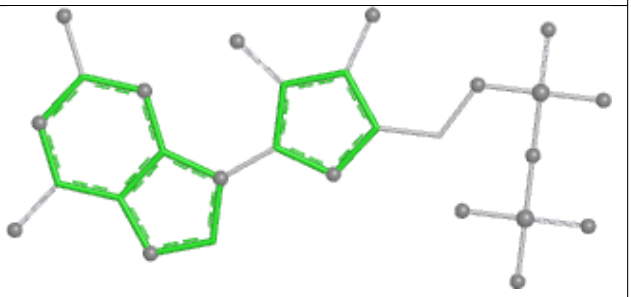
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	801	GDP	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 GDP B 801



Ligand GDP A 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/348 (96%)	-0.23	2 (0%) 85 85	12, 23, 34, 49	1 (0%)
1	B	335/348 (96%)	-0.23	0 100 100	11, 22, 33, 38	1 (0%)
All	All	670/696 (96%)	-0.23	2 (0%) 90 89	11, 22, 34, 49	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	PHE	2.2
1	A	119	GLY	2.2

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NDG	D	2	14/15	0.63	0.18	53,56,58,60	0
2	MAN	C	5	11/12	0.77	0.13	45,46,47,50	11
2	MAN	C	8	11/12	0.78	0.14	38,41,43,46	11
2	MAN	C	4	11/12	0.83	0.11	37,41,42,43	10
2	MAN	C	7	11/12	0.86	0.11	29,32,33,34	10
3	NAG	D	1	14/15	0.88	0.11	39,41,43,49	0
2	NAG	C	1	14/15	0.88	0.12	31,32,34,34	0

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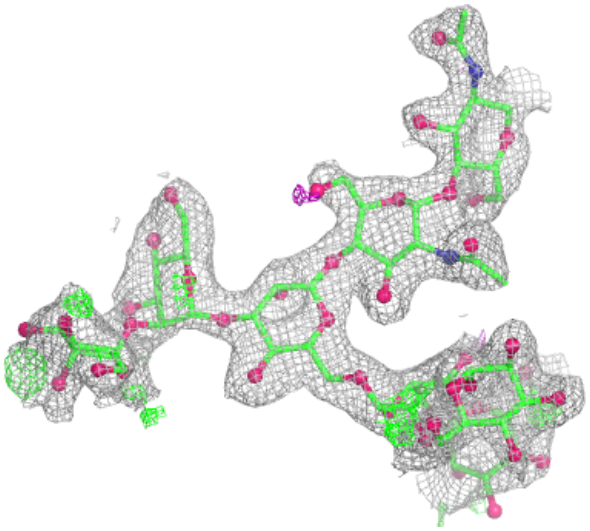
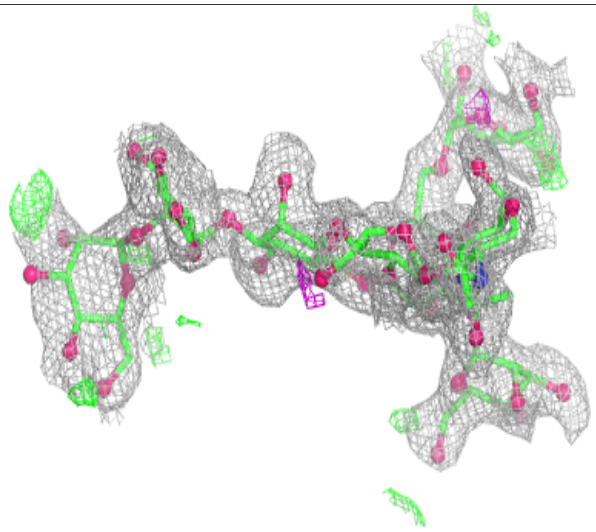
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NDG	C	2	14/15	0.89	0.11	30,32,36,40	0
2	BMA	C	3	11/12	0.94	0.09	25,27,29,34	11
2	MAN	C	6	11/12	0.95	0.09	24,27,30,34	11

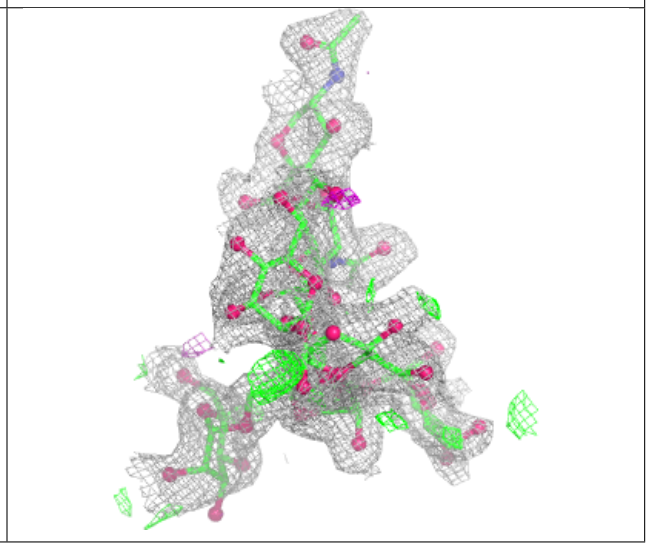
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

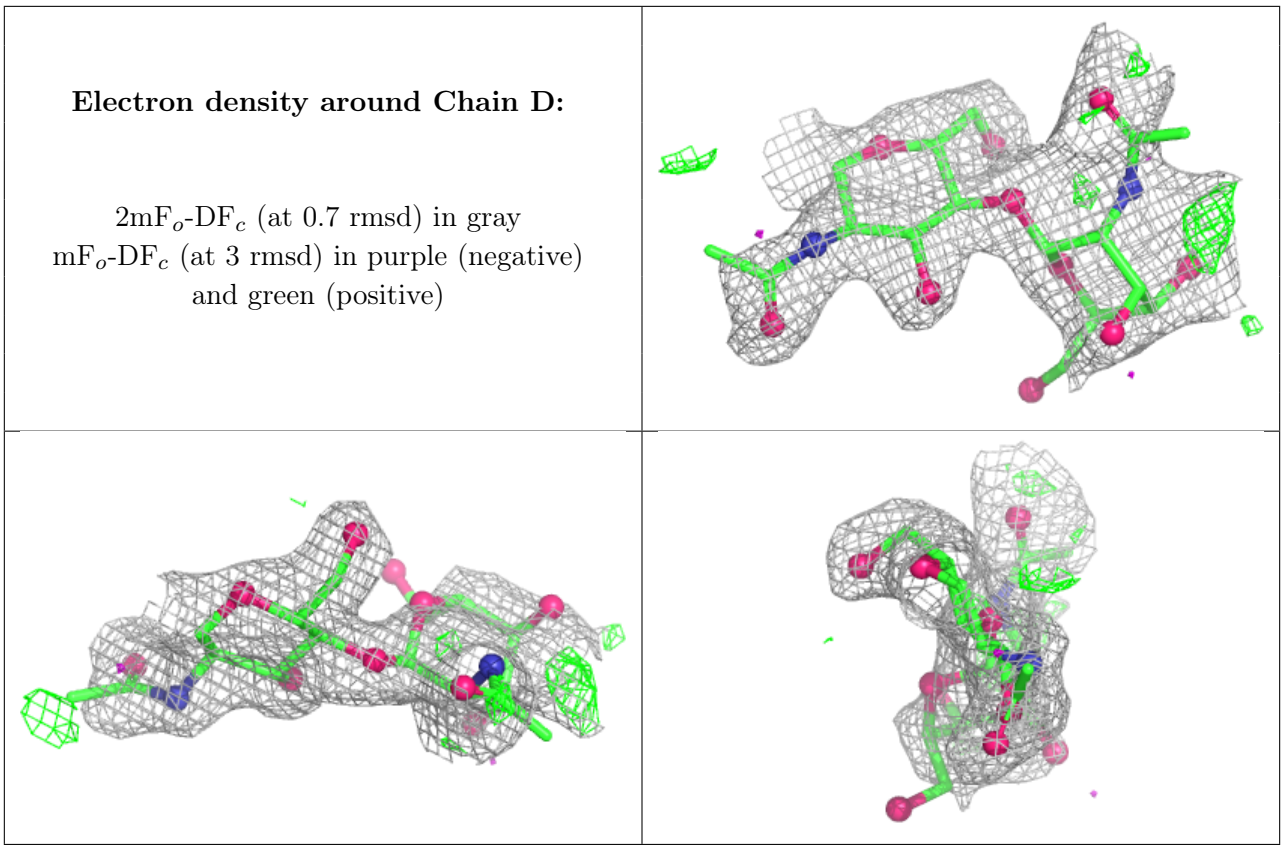






Electron density around Chain D:

$2mF_o$-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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

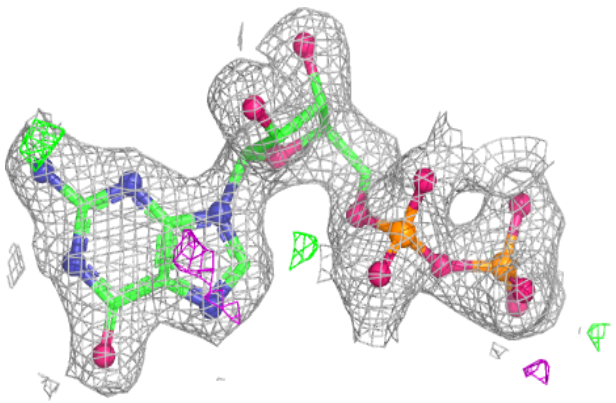
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EPE	B	902	15/15	0.81	0.18	64,68,69,69	0
7	EPE	A	901	15/15	0.87	0.15	41,52,54,54	0
5	CL	B	704	1/1	0.94	0.09	45,45,45,45	0
6	GDP	A	800	28/28	0.97	0.06	19,22,25,25	0
6	GDP	B	801	28/28	0.97	0.06	18,24,28,29	0
5	CL	B	703	1/1	0.98	0.09	35,35,35,35	0
5	CL	A	708	1/1	0.98	0.10	39,39,39,39	0
5	CL	B	702	1/1	0.98	0.07	29,29,29,29	0
4	MN	A	601	1/1	0.99	0.01	21,21,21,21	0
4	MN	B	602	1/1	0.99	0.02	23,23,23,23	0

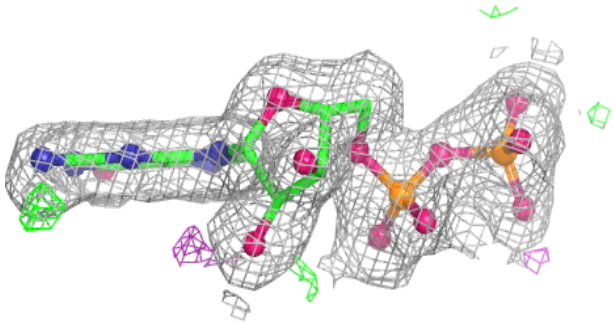
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

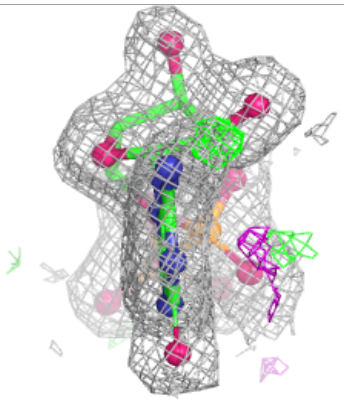
orientation to approximate a three-dimensional view.

Electron density around GDP A 800:

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

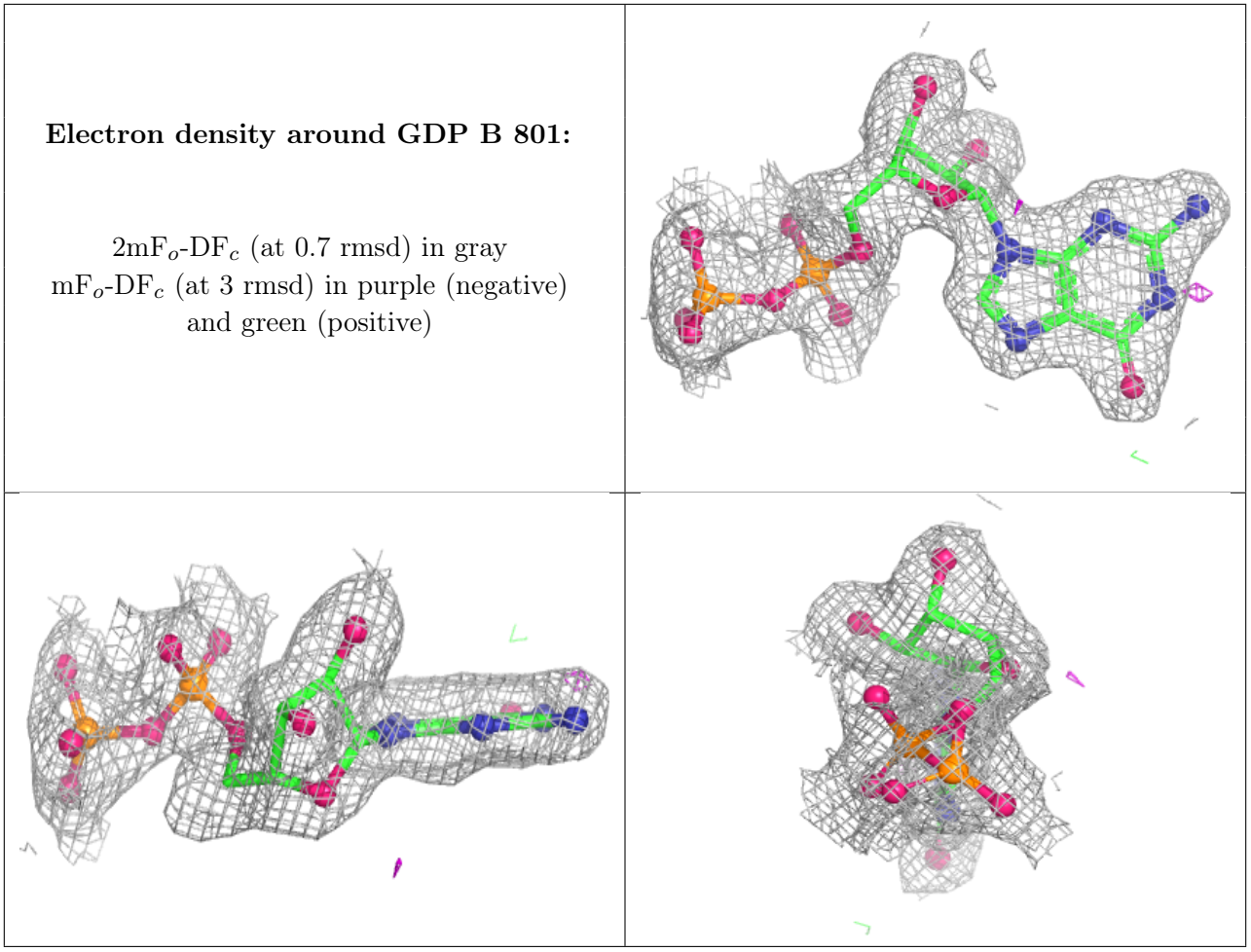






Electron density around GDP B 801:

$2mF_o$-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.