



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:57 PM UTC

PDB ID : 4CFP / pdb_00004cfp
Title : Crystal structure of MltC in complex with tetrasaccharide at 2.15 Å resolution
Authors : Bernardo-Garcia, N.; Artola-Recolons, C.; Hermoso, J.A.
Deposited on : 2013-11-19
Resolution : 2.15 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

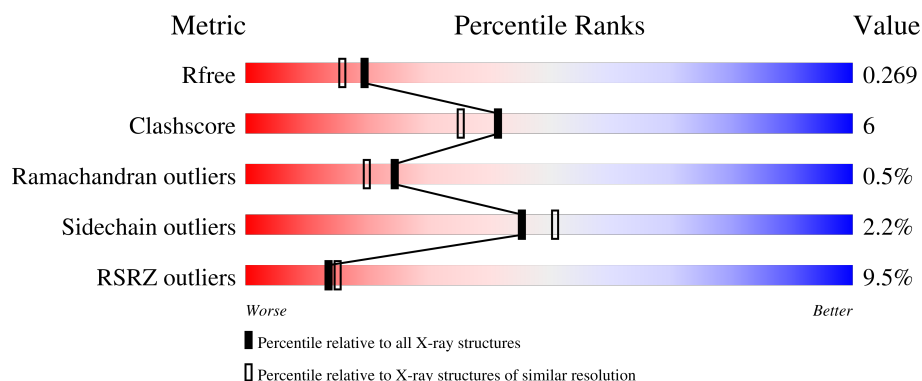
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	341	16% 76% 18% • •
1	B	341	2% 84% 11% • •
2	C	4	75% 25%
2	D	4	100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5525 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.

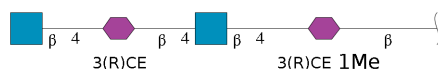
- Molecule 1 is a protein called MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2577	1616	461	492	8			
1	B	327	Total	C	N	O	S	0	0	0
			2577	1616	461	492	8			

There are 4 discrepancies between the modelled and reference sequences:

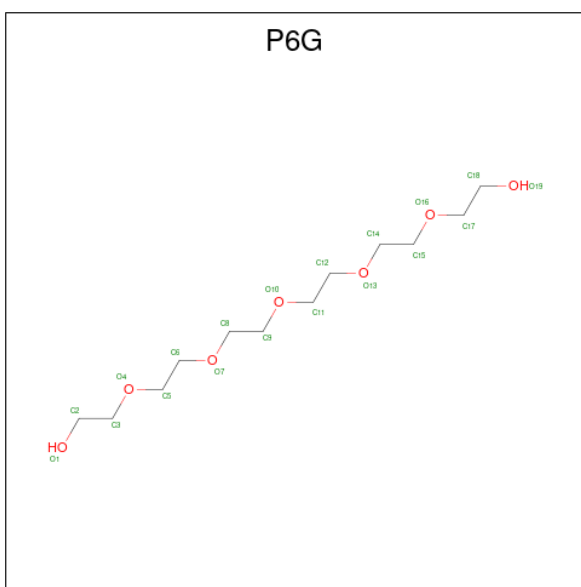
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP C5A0N2
A	217	GLN	GLU	engineered mutation	UNP C5A0N2
B	19	MET	-	expression tag	UNP C5A0N2
B	217	GLN	GLU	engineered mutation	UNP C5A0N2

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-3-O-[(1R)-1-carboxyethyl]-2-deoxy-beta-D-glucopyranoside.



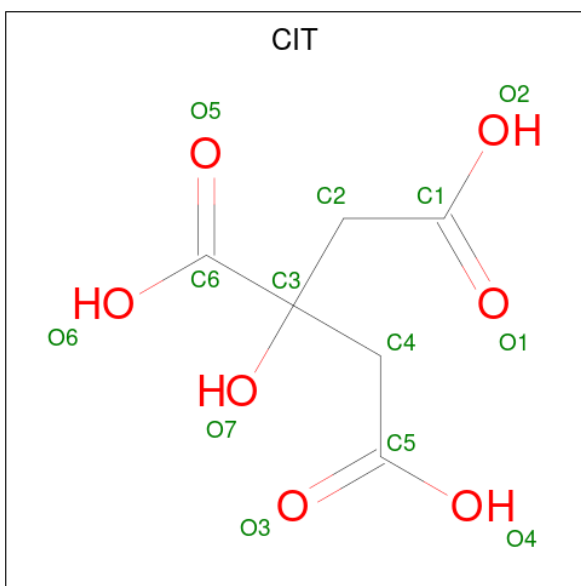
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			68	39	4	25			
2	D	4	Total	C	N	O	0	0	0
			68	39	4	25			

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		

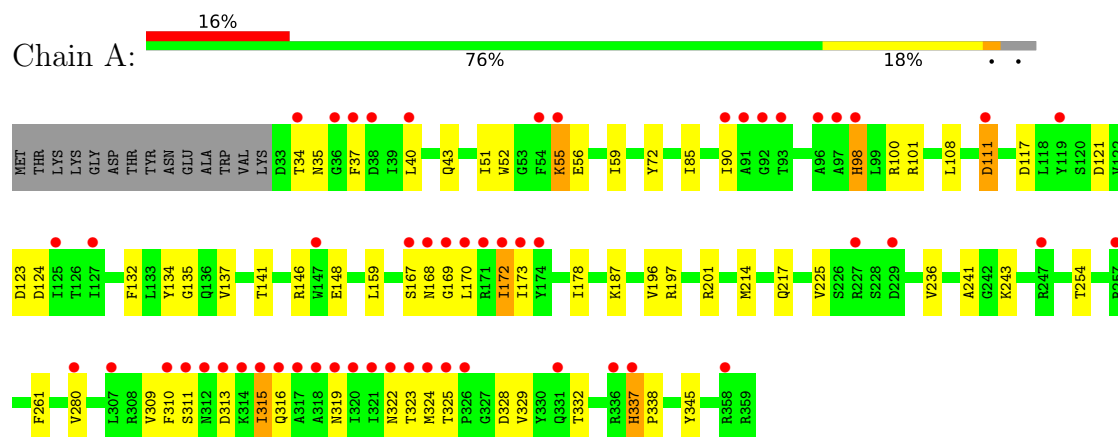
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	85	Total 85	O 85	0	0
5	B	118	Total 118	O 118	0	0

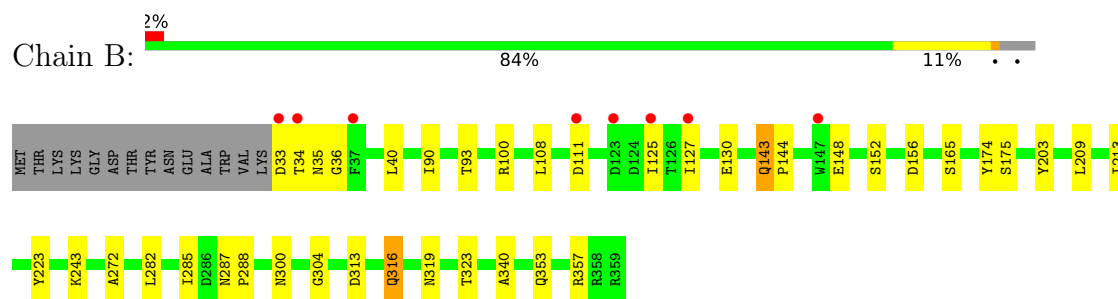
3 Residue-property plots

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.

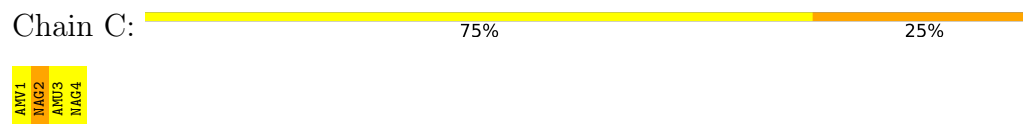
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE C



• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE C



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-3-O-[(1R)-1-carboxyethyl]-2-deoxy-beta-D-glucopyranoside



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-3-O-[(1R)-1-carboxyethyl]-2-deoxy-beta-D-glucopyranoside



ANY1
NAG2
AND3
NAG4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.51Å 114.33Å 61.77Å 90.00° 93.28° 90.00°	Depositor
Resolution (Å)	49.43 – 2.15 49.43 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.43-2.15) 94.8 (49.43-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.191 , 0.268 0.198 , 0.269	Depositor DCC
R_{free} test set	1858 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5525	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: CIT, NAG, P6G, AMV, AMU

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	0.52	0/2628	0.92	7/3559 (0.2%)
1	B	0.53	0/2628	0.86	4/3559 (0.1%)
All	All	0.53	0/5256	0.89	11/7118 (0.2%)

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	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	337	HIS	CA-C-N	6.75	128.28	119.84
1	A	337	HIS	C-N-CA	6.75	128.28	119.84
1	A	98	HIS	CB-CA-C	6.16	119.38	109.27
1	A	337	HIS	CB-CA-C	5.79	117.85	110.16
1	B	175	SER	N-CA-C	5.74	117.57	108.79
1	B	90	ILE	N-CA-C	-5.33	107.52	112.43
1	A	309	VAL	N-CA-C	-5.17	105.79	113.39
1	B	143	GLN	CA-C-N	5.16	125.08	119.76
1	B	143	GLN	C-N-CA	5.16	125.08	119.76
1	A	172	ILE	N-CA-C	5.16	116.00	108.58
1	A	315	ILE	N-CA-C	5.03	115.18	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	HIS	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	2577	0	2547	48	0
1	B	2577	0	2547	18	0
2	C	68	0	59	2	0
2	D	68	0	59	4	0
3	A	19	0	26	3	0
4	B	13	0	5	1	0
5	A	85	0	0	0	0
5	B	118	0	0	1	0
All	All	5525	0	5243	68	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 6.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:SER:HB2	1:A:172:ILE:HD12	1.61	0.83
1:A:55:LYS:HE3	1:A:168:ASN:HB2	1.60	0.82
1:B:100:ARG:NH1	1:B:156:ASP:OD1	2.22	0.73
1:A:111:ASP:HB3	1:A:132:PHE:HB2	1.74	0.69
1:A:197:ARG:HB3	1:A:201:ARG:HH12	1.58	0.69
1:A:236:VAL:HA	2:C:2:NAG:H83	1.77	0.67
1:A:90:ILE:HG22	1:A:173:ILE:HG12	1.77	0.66
1:A:337:HIS:HD2	1:A:338:PRO:CD	2.09	0.66
1:A:319:ASN:O	1:A:323:THR:HG23	2.00	0.61
1:A:337:HIS:CD2	1:A:338:PRO:HD2	2.35	0.61
1:A:337:HIS:CD2	1:A:338:PRO:CD	2.84	0.60
1:B:340:ALA:HB3	4:B:1364:CIT:H22	1.84	0.59
1:A:187:LYS:HD2	3:A:1365:P6G:H121	1.84	0.59
1:A:51:ILE:HD12	1:A:72:TYR:HB2	1.86	0.58
1:A:101:ARG:NH2	1:A:123:ASP:OD2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:HG13	1:A:316:GLN:N	2.19	0.56
1:B:353:GLN:O	1:B:357:ARG:HG3	2.07	0.55
2:D:3:AMU:H111	2:D:4:NAG:O6	2.09	0.53
1:A:40:LEU:HA	1:A:43:GLN:HB2	1.91	0.53
1:A:217:GLN:NE2	1:A:345:TYR:HE2	2.06	0.53
1:A:168:ASN:OD1	1:A:170:LEU:N	2.41	0.52
1:A:324:MET:HB2	1:A:328:ASP:HB2	1.90	0.52
1:B:304:GLY:HA3	2:D:3:AMU:H112	1.91	0.52
1:A:319:ASN:HA	1:A:322:ASN:HB2	1.92	0.51
1:B:300:ASN:O	2:D:1:AMV:H111	2.10	0.51
1:A:117:ASP:N	1:A:124:ASP:OD2	2.42	0.50
1:B:35:ASN:ND2	5:B:2001:HOH:O	2.44	0.50
1:A:241:ALA:HB3	2:C:2:NAG:H82	1.94	0.49
1:B:282:LEU:HB3	1:B:285:ILE:HD12	1.93	0.49
1:A:313:ASP:OD2	1:A:315:ILE:HG12	2.12	0.49
1:A:337:HIS:HD2	1:A:338:PRO:N	2.11	0.49
1:B:313:ASP:HB3	1:B:316:GLN:HB2	1.95	0.48
1:A:225:VAL:CG1	1:A:261:PHE:HZ	2.27	0.46
1:A:197:ARG:HB3	1:A:201:ARG:NH1	2.26	0.46
1:A:100:ARG:HB2	1:A:159:LEU:HD11	1.96	0.46
1:A:337:HIS:CD2	1:A:337:HIS:C	2.93	0.46
1:B:319:ASN:O	1:B:323:THR:HG23	2.15	0.46
1:A:134:TYR:CE1	1:A:146:ARG:HB2	2.51	0.45
1:A:324:MET:HB2	1:A:328:ASP:CB	2.47	0.45
1:A:325:THR:O	1:A:328:ASP:HB2	2.16	0.45
1:A:196:VAL:CG2	1:A:214:MET:HE1	2.46	0.45
1:A:337:HIS:HD2	1:A:338:PRO:CG	2.29	0.45
1:B:36:GLY:O	1:B:40:LEU:HG	2.17	0.45
1:B:111:ASP:HA	1:B:223:TYR:OH	2.18	0.44
1:B:203:TYR:CZ	1:B:272:ALA:HB2	2.52	0.44
1:A:187:LYS:NZ	3:A:1365:P6G:O7	2.50	0.44
1:A:337:HIS:CD2	1:A:338:PRO:HG2	2.52	0.44
1:B:33:ASP:CG	1:B:34:THR:H	2.25	0.44
1:A:167:SER:C	1:A:169:GLY:H	2.26	0.43
1:B:108:LEU:HD11	1:B:148:GLU:HA	2.00	0.43
1:B:165:SER:HB3	1:B:174:TYR:CD1	2.53	0.43
1:A:337:HIS:HD2	1:A:338:PRO:HG2	1.84	0.43
1:B:287:ASN:HA	1:B:288:PRO:HD3	1.86	0.43
1:A:35:ASN:C	1:A:37:PHE:N	2.76	0.43
1:A:90:ILE:CG2	1:A:173:ILE:HG12	2.48	0.43
1:A:108:LEU:HD11	1:A:148:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:TYR:CE1	1:A:121:ASP:HB3	2.54	0.42
1:A:135:GLY:HA2	3:A:1365:P6G:H32	2.01	0.42
1:A:85:ILE:HB	1:A:178:ILE:HB	2.01	0.42
1:A:52:TRP:HB3	1:A:56:GLU:HB2	2.02	0.42
1:B:143:GLN:HA	1:B:144:PRO:HD3	1.90	0.41
1:B:209:LEU:O	1:B:213:ILE:HG12	2.20	0.41
1:A:310:PHE:O	1:A:311:SER:HB2	2.21	0.41
2:D:1:AMV:H9	2:D:2:NAG:O5	2.21	0.41
1:A:35:ASN:C	1:A:37:PHE:H	2.28	0.41
1:A:325:THR:O	1:A:329:VAL:HG23	2.20	0.40
1:A:225:VAL:HG13	1:A:261:PHE:HZ	1.86	0.40
1:A:243:LYS:HD3	1:A:254:THR:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	325/341 (95%)	306 (94%)	17 (5%)	2 (1%)	21	15
1	B	325/341 (95%)	320 (98%)	4 (1%)	1 (0%)	36	34
All	All	650/682 (95%)	626 (96%)	21 (3%)	3 (0%)	24	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ASP
1	A	280	VAL
1	B	125	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	279/291 (96%)	273 (98%)	6 (2%)	45	51
1	B	279/291 (96%)	273 (98%)	6 (2%)	45	51
All	All	558/582 (96%)	546 (98%)	12 (2%)	45	51

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	55	LYS
1	A	59	ILE
1	A	137	VAL
1	A	141	THR
1	A	332	THR
1	B	93	THR
1	B	127	ILE
1	B	130	GLU
1	B	152	SER
1	B	243	LYS
1	B	316	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	HIS
1	A	215	GLN
1	A	337	HIS
1	B	161	ASN
1	B	190	HIS
1	B	249	GLN

5.3.3 RNA [i](#)

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 ⓘ

8 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	AMV	C	1	2	21,21,21	1.44	1 (4%)	25,29,29	1.26	3 (12%)
2	NAG	C	2	2	14,14,15	1.25	1 (7%)	17,19,21	2.35	5 (29%)
2	AMU	C	3	2	19,19,20	1.67	4 (21%)	23,26,28	1.46	3 (13%)
2	NAG	C	4	2	14,14,15	1.15	1 (7%)	17,19,21	1.38	3 (17%)
2	AMV	D	1	2	21,21,21	1.50	4 (19%)	25,29,29	1.92	7 (28%)
2	NAG	D	2	2	14,14,15	1.54	3 (21%)	17,19,21	1.16	0
2	AMU	D	3	2	19,19,20	1.80	4 (21%)	23,26,28	1.53	5 (21%)
2	NAG	D	4	2	14,14,15	1.16	2 (14%)	17,19,21	1.33	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	AMV	C	1	2	-	7/16/36/36	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	AMU	C	3	2	-	0/14/31/34	0/1/1/1
2	NAG	C	4	2	-	0/6/23/26	0/1/1/1
2	AMV	D	1	2	-	8/16/36/36	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	AMU	D	3	2	-	4/14/31/34	0/1/1/1
2	NAG	D	4	2	-	1/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	AMV	C7-N2	3.58	1.45	1.34
2	D	1	AMV	C7-N2	3.53	1.45	1.34
2	D	2	NAG	C7-N2	3.32	1.45	1.34
2	D	3	AMU	O5-C1	-3.29	1.38	1.43
2	C	3	AMU	C7-N2	3.24	1.44	1.34
2	C	3	AMU	C2-N2	-3.07	1.41	1.46
2	D	3	AMU	C2-N2	-3.04	1.41	1.46
2	D	3	AMU	C3-C2	2.92	1.56	1.52
2	C	4	NAG	C7-N2	2.90	1.43	1.34
2	C	2	NAG	C7-N2	2.89	1.43	1.34
2	D	4	NAG	C7-N2	2.87	1.43	1.34
2	C	3	AMU	C3-C2	2.79	1.56	1.52
2	D	3	AMU	C7-N2	2.79	1.43	1.34
2	D	1	AMV	C1-C2	-2.73	1.48	1.53
2	C	3	AMU	O5-C1	-2.66	1.39	1.43
2	D	2	NAG	O5-C1	-2.52	1.39	1.43
2	D	2	NAG	C2-N2	-2.41	1.42	1.46
2	D	4	NAG	C2-N2	-2.36	1.42	1.46
2	D	1	AMV	C8-C7	2.23	1.55	1.50
2	D	1	AMV	O3-C3	-2.07	1.38	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	4.56	118.30	112.19
2	D	1	AMV	O3-C9-C11	4.37	119.71	107.54
2	C	2	NAG	O5-C1-C2	-4.29	104.66	111.29
2	C	2	NAG	C4-C3-C2	-4.28	104.75	111.02
2	D	1	AMV	O3-C3-C4	4.20	117.92	107.23
2	C	2	NAG	C8-C7-N2	4.07	122.86	116.12
2	C	3	AMU	C1-O5-C5	3.91	117.43	112.19
2	D	3	AMU	C11-C9-C10	-3.64	102.60	109.42
2	D	4	NAG	C1-O5-C5	3.48	116.85	112.19
2	D	1	AMV	C1-C2-C3	-3.38	103.79	109.92
2	D	1	AMV	O5-C1-C2	-3.18	104.59	110.59
2	C	3	AMU	C1-C2-N2	-2.98	105.74	110.43
2	D	1	AMV	C3-C4-C5	-2.95	103.27	109.57
2	C	4	NAG	O5-C1-C2	-2.63	107.23	111.29
2	D	3	AMU	C1-C2-N2	-2.36	106.71	110.43
2	D	1	AMV	C3-C2-N2	2.32	114.60	110.91
2	C	4	NAG	C8-C7-N2	2.30	119.93	116.12
2	D	3	AMU	C1-O5-C5	2.26	115.22	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	AMU	C8-C7-N2	2.22	119.80	116.12
2	C	3	AMU	O5-C1-C2	-2.18	107.91	111.29
2	C	2	NAG	O7-C7-C8	-2.16	118.20	122.05
2	C	1	AMV	C3-C2-N2	2.16	114.34	110.91
2	D	3	AMU	C3-C4-C5	2.15	114.15	109.57
2	C	4	NAG	O5-C5-C6	2.13	111.80	107.66
2	D	1	AMV	O1-C1-C2	2.13	111.36	108.13
2	C	1	AMV	O5-C1-C2	-2.13	106.58	110.59
2	C	1	AMV	C1-C2-C3	-2.10	106.12	109.92

There are no chirality outliers.

All (24) torsion outliers are listed below:

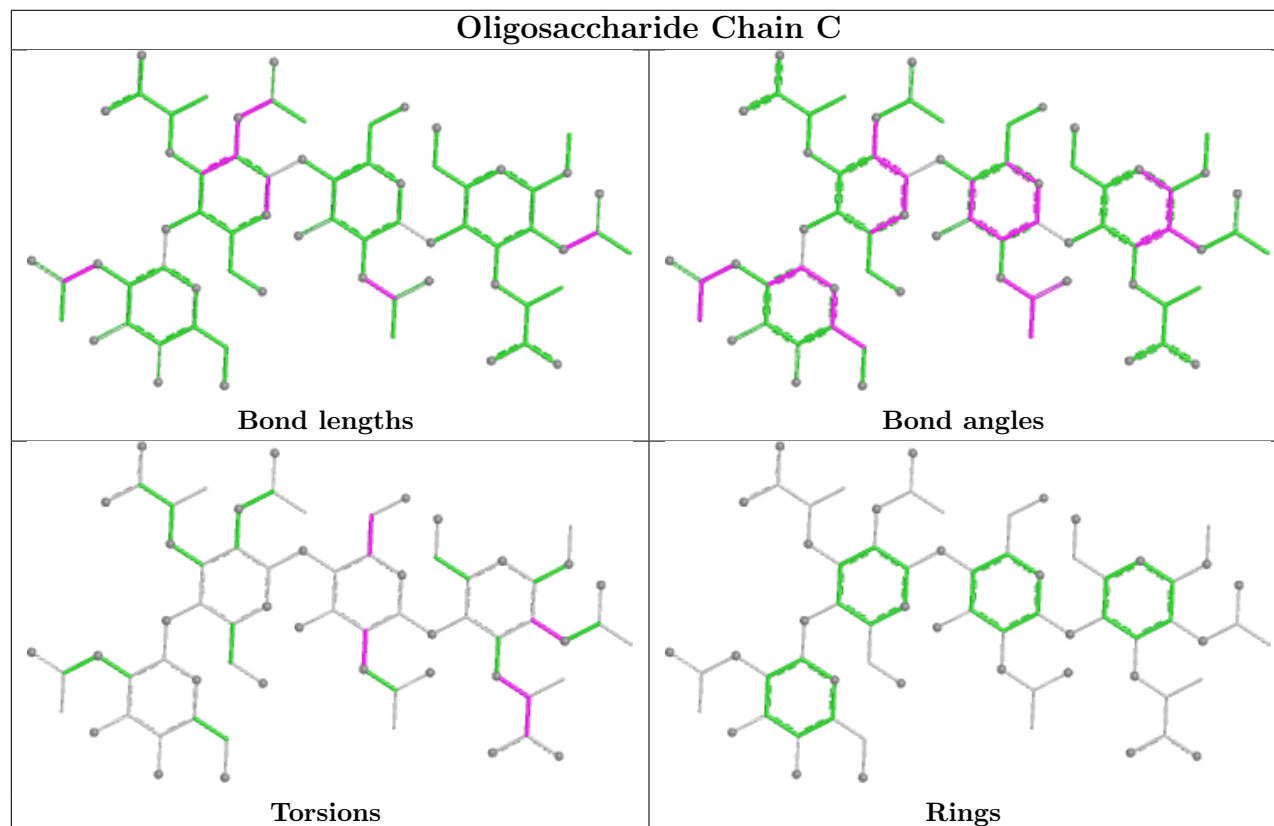
Mol	Chain	Res	Type	Atoms
2	C	1	AMV	O11-C10-C9-C11
2	C	1	AMV	OXT-C10-C9-C11
2	C	1	AMV	O11-C10-C9-O3
2	C	1	AMV	OXT-C10-C9-O3
2	D	1	AMV	C11-C9-O3-C3
2	D	3	AMU	O10-C10-C9-C11
2	D	3	AMU	O11-C10-C9-C11
2	D	3	AMU	O10-C10-C9-O3
2	D	3	AMU	O11-C10-C9-O3
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	1	AMV	O5-C1-O1-C12
2	D	1	AMV	O11-C10-C9-C11
2	D	1	AMV	OXT-C10-C9-C11
2	D	1	AMV	C3-C2-N2-C7
2	C	2	NAG	O5-C5-C6-O6
2	C	1	AMV	C1-C2-N2-C7
2	D	1	AMV	C2-C1-O1-C12
2	C	2	NAG	C3-C2-N2-C7
2	D	4	NAG	C4-C5-C6-O6
2	C	1	AMV	C3-C2-N2-C7
2	D	1	AMV	C1-C2-N2-C7
2	C	1	AMV	C11-C9-O3-C3
2	D	1	AMV	C4-C3-O3-C9

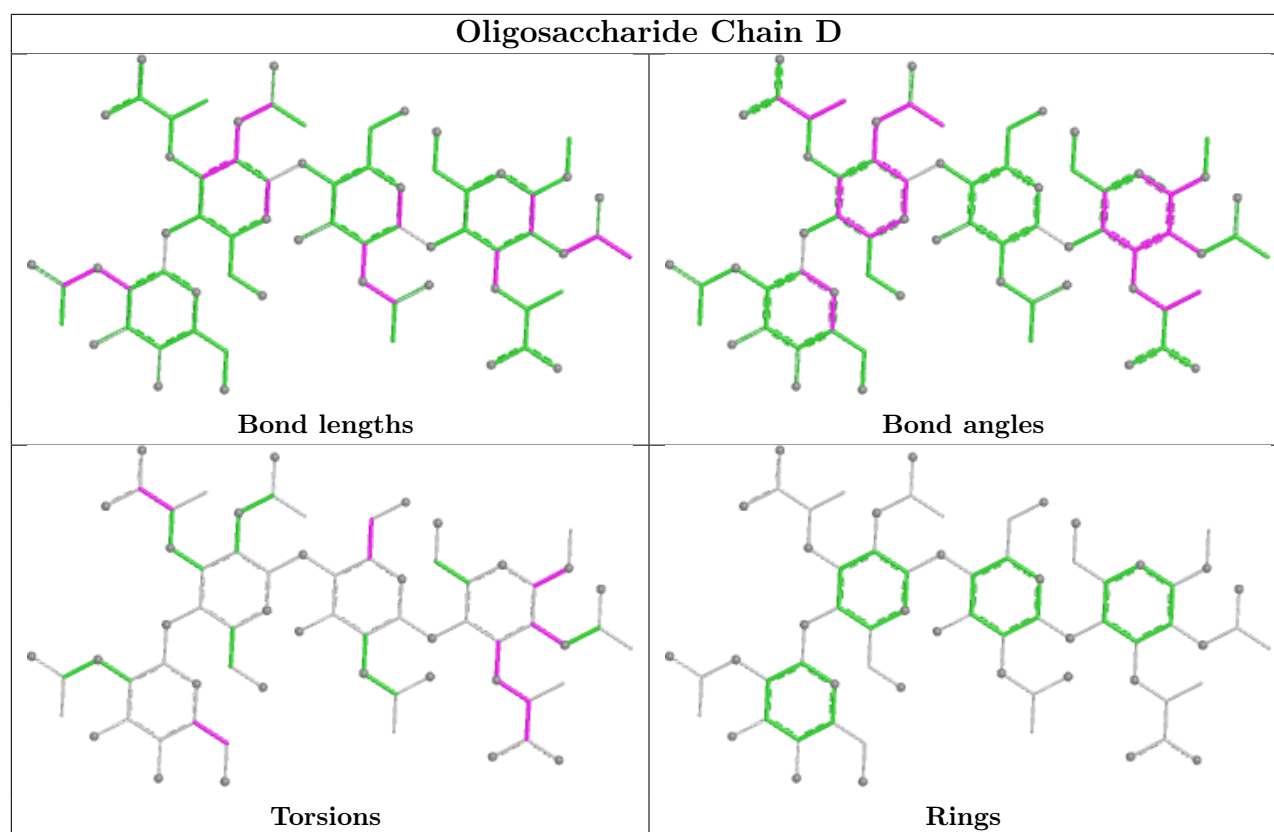
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0
2	D	3	AMU	2	0
2	D	2	NAG	1	0
2	D	1	AMV	2	0
2	D	4	NAG	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 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	P6G	A	1365	-	18,18,18	0.75	0	17,17,17	0.30	0
4	CIT	B	1364	-	12,12,12	1.11	0	17,17,17	1.70	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P6G	A	1365	-	-	9/16/16/16	-
4	CIT	B	1364	-	-	7/16/16/16	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1364	CIT	O6-C6-C3	3.70	120.23	113.14
4	B	1364	CIT	O2-C1-C2	2.59	122.55	114.35
4	B	1364	CIT	C3-C4-C5	-2.18	107.96	113.92

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1365	P6G	O10-C11-C12-O13
3	A	1365	P6G	O4-C5-C6-O7
3	A	1365	P6G	O13-C14-C15-O16
3	A	1365	P6G	C2-C3-O4-C5
3	A	1365	P6G	C9-C8-O7-C6
4	B	1364	CIT	C2-C3-C6-O5
4	B	1364	CIT	C4-C3-C6-O5
3	A	1365	P6G	O16-C17-C18-O19
3	A	1365	P6G	C14-C15-O16-C17
4	B	1364	CIT	C2-C3-C6-O6
4	B	1364	CIT	C4-C3-C6-O6
3	A	1365	P6G	C15-C14-O13-C12
4	B	1364	CIT	O2-C1-C2-C3
4	B	1364	CIT	O7-C3-C6-O5
4	B	1364	CIT	O1-C1-C2-C3
3	A	1365	P6G	O1-C2-C3-O4

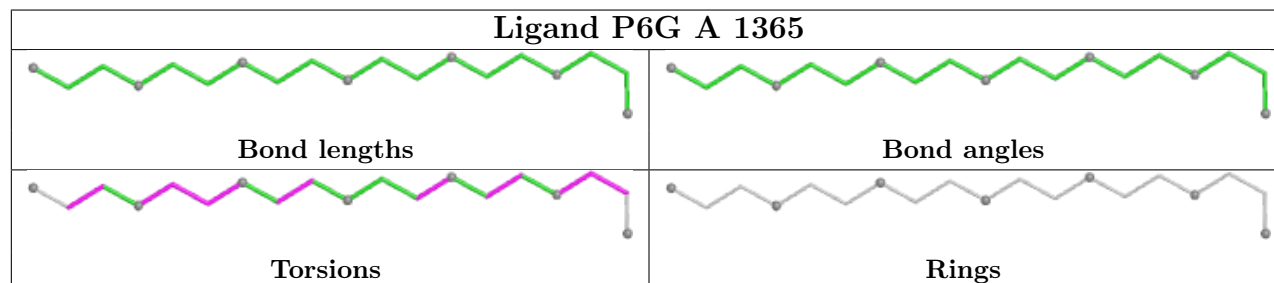
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1365	P6G	3	0
4	B	1364	CIT	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	327/341 (95%)	0.81	54 (16%) 4 5	21, 44, 97, 140	0
1	B	327/341 (95%)	0.06	8 (2%) 59 63	17, 31, 60, 97	0
All	All	654/682 (95%)	0.43	62 (9%) 14 15	17, 36, 87, 140	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	GLY	6.0
1	A	323	THR	5.3
1	A	315	ILE	5.3
1	A	320	ILE	4.9
1	A	317	ALA	4.8
1	A	91	ALA	4.8
1	A	90	ILE	4.6
1	A	316	GLN	4.6
1	A	93	THR	4.5
1	A	54	PHE	4.3
1	A	172	ILE	4.1
1	A	92	GLY	4.0
1	B	147	TRP	3.9
1	A	170	LEU	3.8
1	A	40	LEU	3.8
1	A	98	HIS	3.8
1	A	311	SER	3.5
1	A	174	TYR	3.4
1	A	318	ALA	3.3
1	A	34	THR	3.2
1	A	247	ARG	3.2
1	A	227	ARG	3.2
1	A	337	HIS	3.2
1	A	319	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	167	SER	3.1
1	A	324	MET	3.0
1	A	171	ARG	3.0
1	A	310	PHE	2.9
1	A	322	ASN	2.9
1	A	313	ASP	2.8
1	A	37	PHE	2.8
1	A	55	LYS	2.8
1	A	127	ILE	2.7
1	A	314	LYS	2.6
1	A	325	THR	2.6
1	A	307	LEU	2.6
1	A	229	ASP	2.6
1	B	34	THR	2.5
1	A	36	GLY	2.5
1	A	326	PRO	2.5
1	A	147	TRP	2.5
1	A	331	GLN	2.4
1	A	97	ALA	2.4
1	A	312	ASN	2.4
1	A	119	TYR	2.4
1	A	38	ASP	2.4
1	A	321	ILE	2.4
1	B	125	ILE	2.4
1	B	37	PHE	2.3
1	A	125	ILE	2.3
1	B	127	ILE	2.3
1	A	168	ASN	2.3
1	A	96	ALA	2.3
1	A	173	ILE	2.2
1	A	358	ARG	2.2
1	A	111	ASP	2.1
1	B	33	ASP	2.1
1	B	111	ASP	2.1
1	A	257	ARG	2.1
1	A	336	ARG	2.1
1	A	280	VAL	2.1
1	B	123	ASP	2.0

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

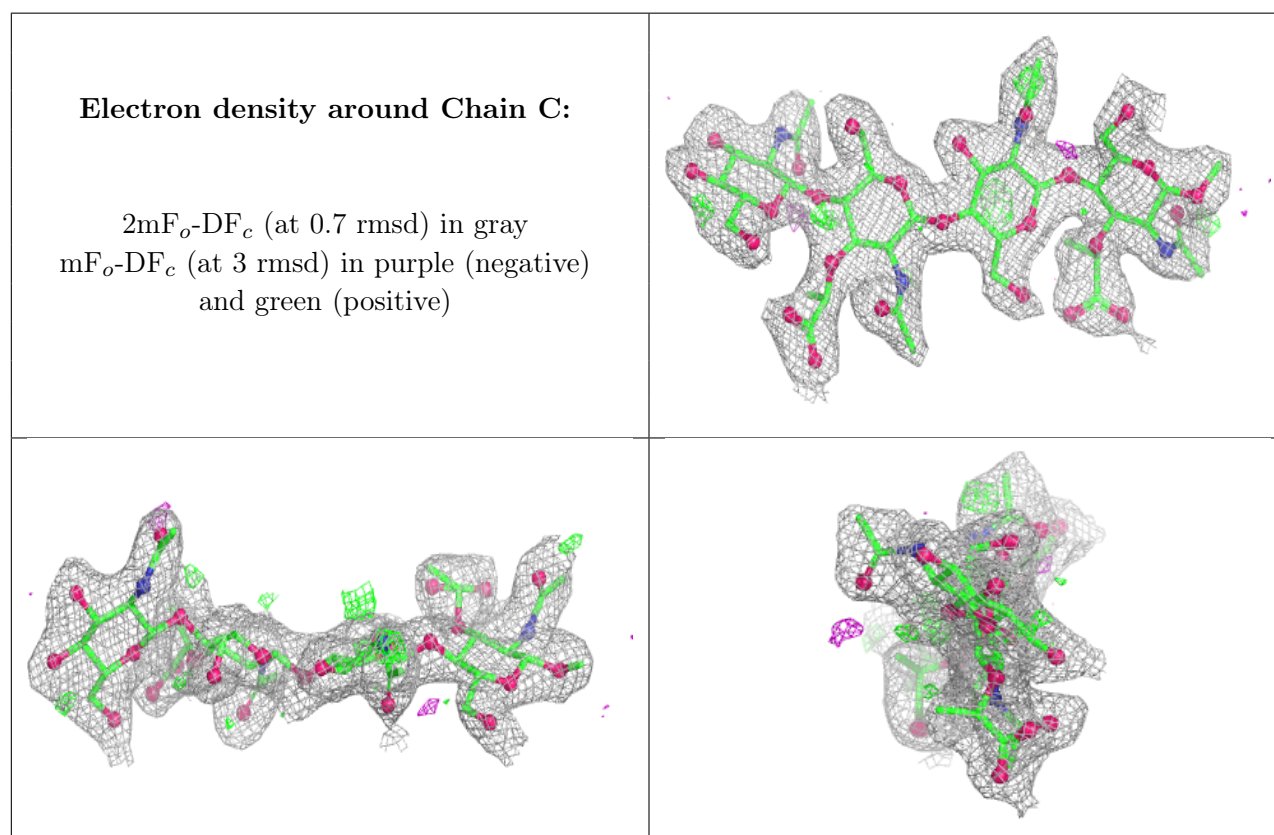
There are no non-standard protein/DNA/RNA residues in this entry.

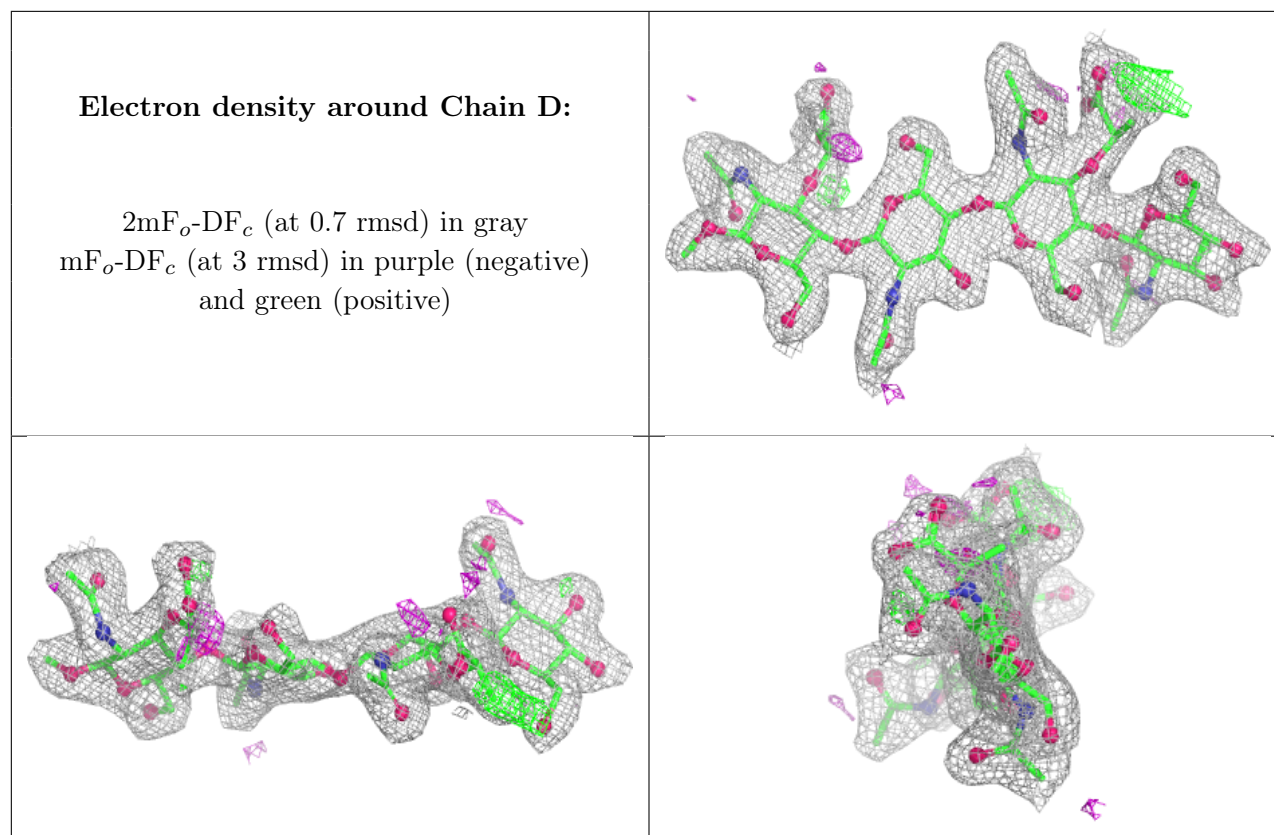
6.3 Carbohydrates ⓘ

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	NAG	C	4	14/15	0.86	0.10	38,44,48,49	0
2	AMU	C	3	19/20	0.90	0.09	26,33,53,57	0
2	NAG	C	2	14/15	0.90	0.11	20,33,45,52	0
2	AMU	D	3	19/20	0.91	0.10	16,24,57,66	0
2	AMV	C	1	21/21	0.92	0.11	15,36,54,59	0
2	AMV	D	1	21/21	0.93	0.10	16,25,54,56	0
2	NAG	D	4	14/15	0.93	0.08	21,27,39,41	0
2	NAG	D	2	14/15	0.95	0.07	9,27,32,41	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.



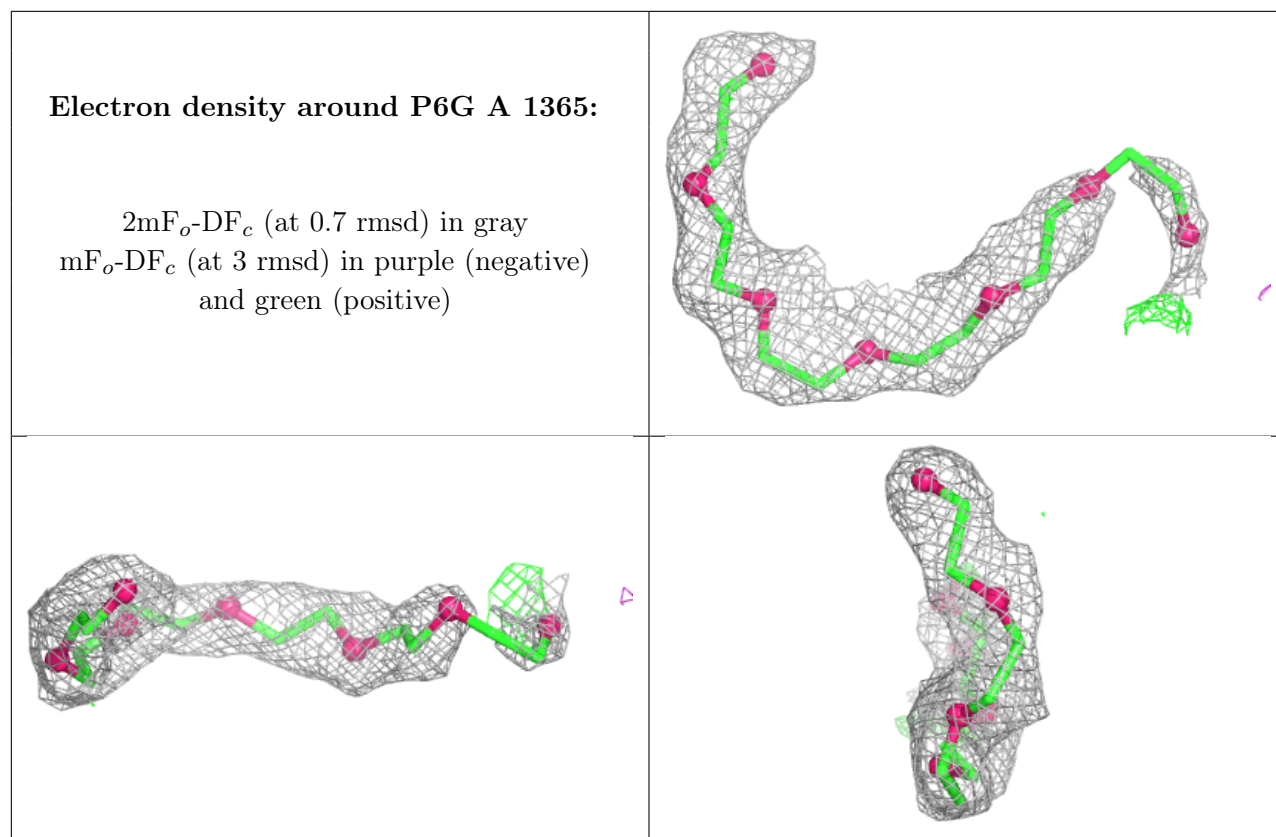


6.4 Ligands [i](#)

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(Å ²)	Q<0.9
4	CIT	B	1364	13/13	0.78	0.15	57,71,85,86	0
3	P6G	A	1365	19/19	0.83	0.15	43,55,74,76	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.