wwPDB X-ray Structure Validation Summary Report (i)

Sep 20, 2023 – 09:19 AM EDT

PDB ID	:	5EIY
Title	:	Bacterial cellulose synthase bound to a substrate analogue
Authors	:	McNamara, J.T.; Zimmer, J.
Deposited on	:	2015-10-30
Resolution	:	2.95 Å(reported)

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

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

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

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

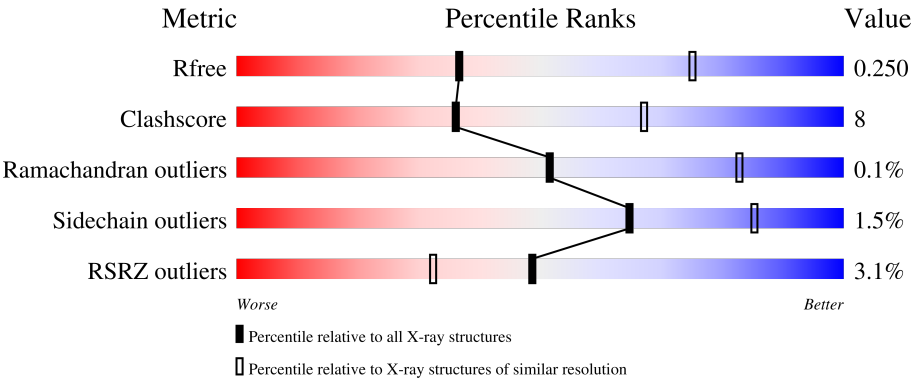
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	803	3% 73% 17% 9%
2	B	729	2% 77% 12% 10%
3	D	9	100%
4	C	17	71% 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	LDA	A	922	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 11144 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 Putative cellulose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5734	3721	1000	982	31	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q3J125
A	1	GLY	-	expression tag	UNP Q3J125
A	789	HIS	-	expression tag	UNP Q3J125
A	790	HIS	-	expression tag	UNP Q3J125
A	791	HIS	-	expression tag	UNP Q3J125
A	792	HIS	-	expression tag	UNP Q3J125
A	793	HIS	-	expression tag	UNP Q3J125
A	794	HIS	-	expression tag	UNP Q3J125
A	795	LYS	-	expression tag	UNP Q3J125
A	796	LEU	-	expression tag	UNP Q3J125
A	797	HIS	-	expression tag	UNP Q3J125
A	798	HIS	-	expression tag	UNP Q3J125
A	799	HIS	-	expression tag	UNP Q3J125
A	800	HIS	-	expression tag	UNP Q3J125
A	801	HIS	-	expression tag	UNP Q3J125
A	802	HIS	-	expression tag	UNP Q3J125

- Molecule 2 is a protein called Putative cellulose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	658	4946	3134	878	918	16	0	5	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	MET	-	initiating methionine	UNP Q3J126
B	-2	LYS	-	expression tag	UNP Q3J126
B	-1	TYR	-	expression tag	UNP Q3J126
B	0	LEU	-	expression tag	UNP Q3J126
B	1	LEU	-	expression tag	UNP Q3J126
B	2	PRO	-	expression tag	UNP Q3J126
B	3	THR	-	expression tag	UNP Q3J126
B	4	ALA	-	expression tag	UNP Q3J126
B	5	ALA	-	expression tag	UNP Q3J126
B	6	ALA	-	expression tag	UNP Q3J126
B	7	GLY	-	expression tag	UNP Q3J126
B	8	LEU	-	expression tag	UNP Q3J126
B	9	LEU	-	expression tag	UNP Q3J126
B	10	LEU	-	expression tag	UNP Q3J126
B	11	LEU	-	expression tag	UNP Q3J126
B	12	ALA	-	expression tag	UNP Q3J126
B	13	ALA	-	expression tag	UNP Q3J126
B	14	GLN	-	expression tag	UNP Q3J126
B	15	PRO	-	expression tag	UNP Q3J126
B	16	ALA	-	expression tag	UNP Q3J126
B	17	MET	-	expression tag	UNP Q3J126
B	18	ALA	-	expression tag	UNP Q3J126
B	19	MET	-	expression tag	UNP Q3J126
B	20	GLY	-	expression tag	UNP Q3J126

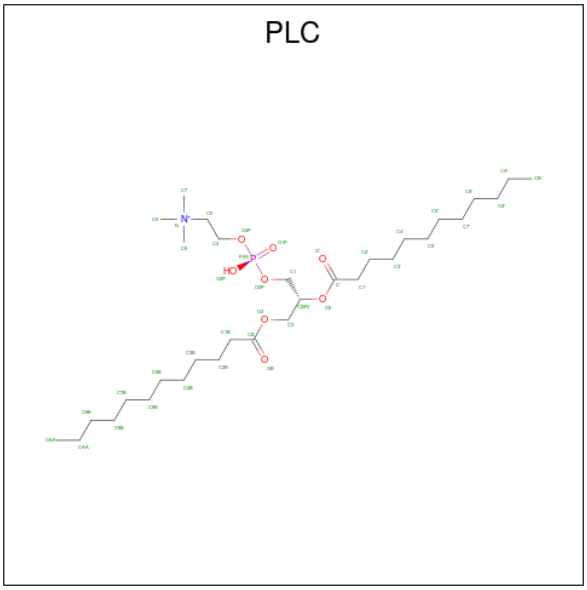
- Molecule 3 is a protein called poly(unk).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	9	Total	C	N	O	0	0	0
			45	27	9	9			

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.

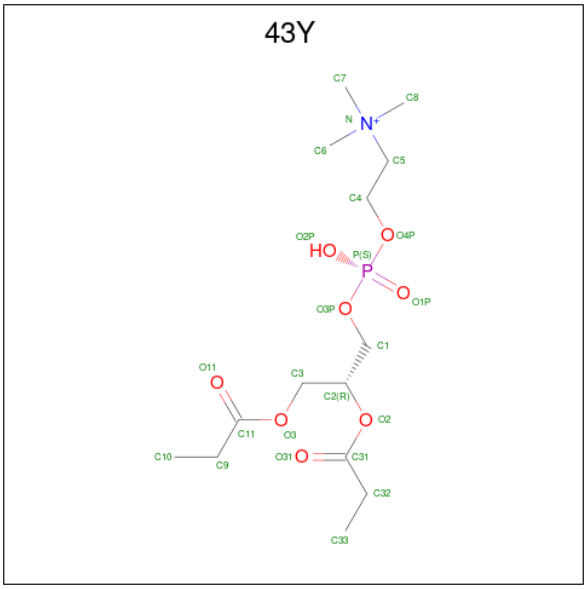
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	C	17	Total	C	O	0	0	0
			188	102	86			

- Molecule 5 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



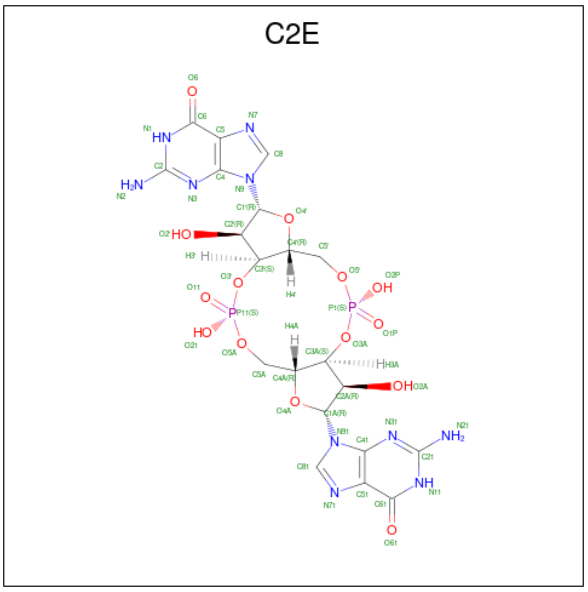
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

- Molecule 6 is [(2R)-3-[oxidanyl-[2-(trimethyl-$l^{4}-azanyl)ethoxy]phosphoryl]oxy-2-propanoyloxy-propyl] propanoate (three-letter code: 43Y) (formula: $C_{14}H_{29}NO_8P$).



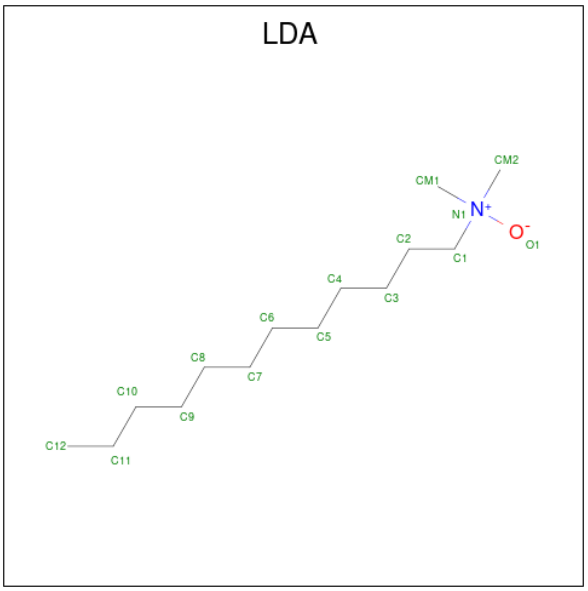
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			20	10	1	8	1		

- Molecule 7 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
7	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

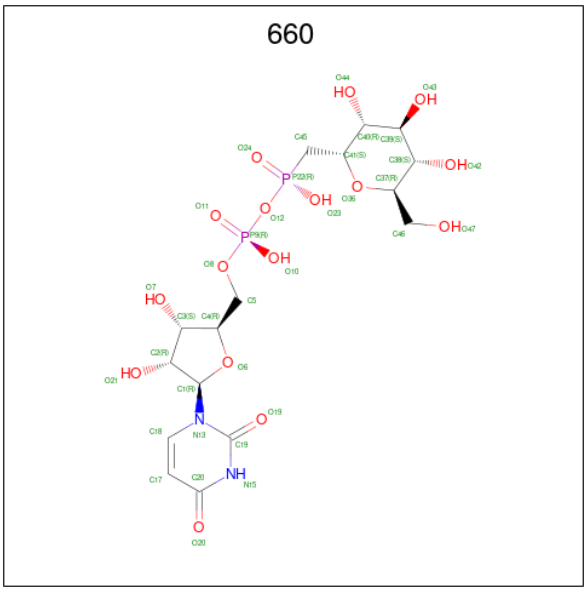


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 16 14 1 1	0	0
8	A	1	Total C N O 16 14 1 1	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Mg 1 1	0	0
9	B	1	Total Mg 1 1	0	0

- Molecule 10 is [[(2 {R},3 {S},4 {R},5 {R})-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-[[(2 {S},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]methyl]phosphinic acid (three-letter code: 660) (formula: $C_{16}H_{26}N_2O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			36	16	2	16	2		

- Molecule 11 is water.

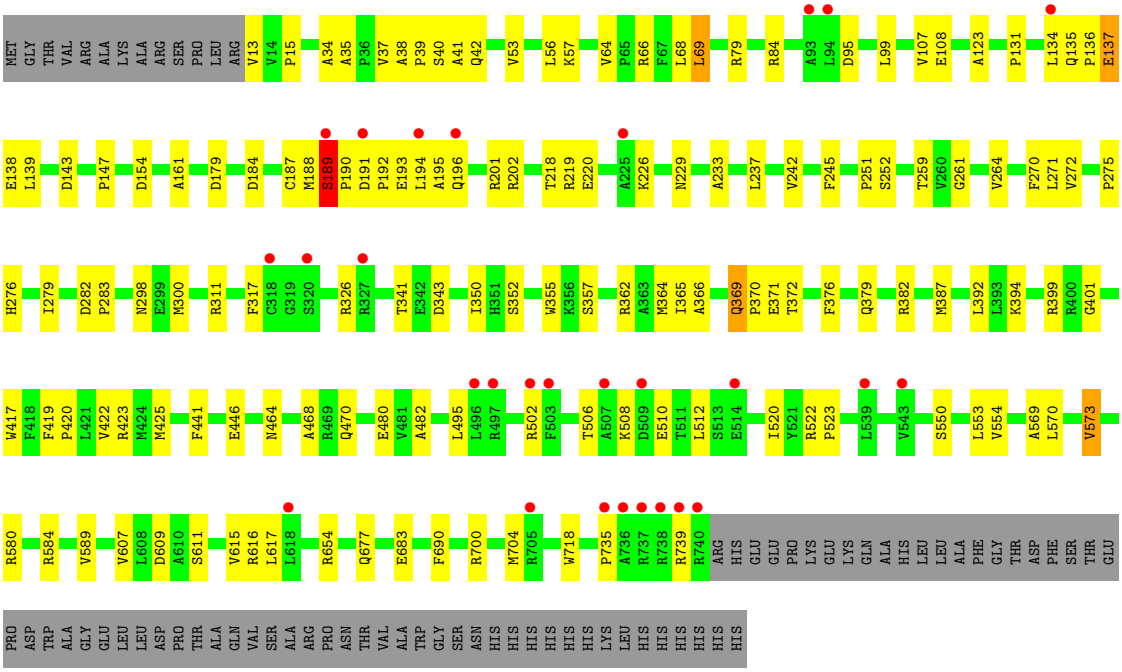
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	11	Total	O	0	0
			11	11		

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.

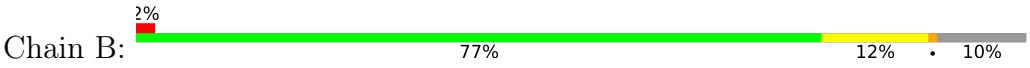
• Molecule 1: Putative cellulose synthase

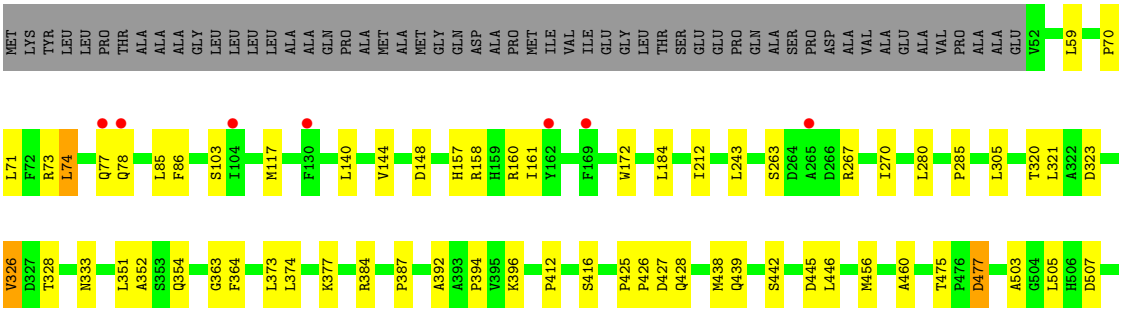
Chain A:

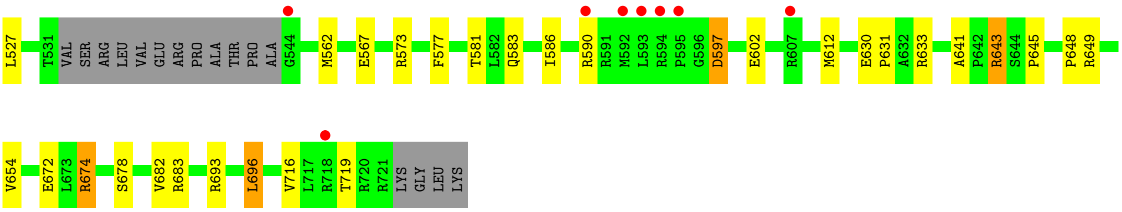


• Molecule 2: Putative cellulose synthase

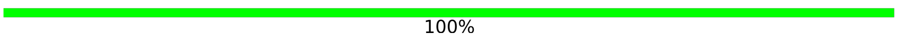
Chain B:







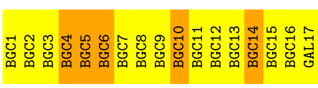
• Molecule 3: poly(unk)

Chain D:


There are no outlier residues recorded for this chain.

• Molecule 4: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.47Å 216.65Å 221.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.92 – 2.95 34.92 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.92-2.95) 99.8 (34.92-2.95)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.222 , 0.248 0.225 , 0.250	Depositor DCC
R_{free} test set	3482 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	75.5	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11144	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: BGC, GAL, 660, C2E, PLC, MG, LDA, 43Y

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	0.25	0/5880	0.45	1/7997 (0.0%)
2	B	0.22	0/5065	0.45	1/6945 (0.0%)
All	All	0.24	0/10945	0.45	2/14942 (0.0%)

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
2	B	0	3
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	SER	CB-CA-C	5.50	120.54	110.10
2	B	74	LEU	O-C-N	-5.19	114.40	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	GLN	Peptide
2	B	643	ARG	Sidechain
2	B	74	LEU	Mainchain

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	5734	0	5846	112	0
2	B	4946	0	5023	66	0
3	D	45	0	12	0	0
4	C	188	0	155	7	0
5	A	38	0	53	0	0
6	A	20	0	15	1	0
7	A	92	0	41	5	0
8	A	32	0	62	2	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	36	0	0	2	0
11	A	11	0	0	0	0
All	All	11144	0	11207	178	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 8.

The worst 5 of 178 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)
7:A:921:C2E:O4'	7:A:921:C2E:C4'	1.64	1.21
7:A:920:C2E:O4'	7:A:920:C2E:C4'	1.64	1.20
1:A:134:LEU:O	1:A:134:LEU:HD12	1.58	1.04
2:B:140:LEU:HB3	2:B:144:VAL:HG11	1.42	1.00
2:B:643:ARG:N	2:B:643:ARG:HD3	1.82	0.94

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	726/803 (90%)	700 (96%)	25 (3%)	1 (0%)	51 83
2	B	659/729 (90%)	646 (98%)	13 (2%)	0	100 100
All	All	1385/1532 (90%)	1346 (97%)	38 (3%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	SER

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	598/661 (90%)	590 (99%)	8 (1%)	69 87
2	B	525/573 (92%)	516 (98%)	9 (2%)	60 83
All	All	1123/1234 (91%)	1106 (98%)	17 (2%)	65 85

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	597	ASP
2	B	696	LEU
1	A	617	LEU
2	B	86	PHE
2	B	184	LEU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

17 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BGC	C	1	4	12,12,12	2.11	3 (25%)	17,17,17	1.68	4 (23%)
4	BGC	C	10	4	11,11,12	2.60	2 (18%)	15,15,17	1.92	4 (26%)
4	BGC	C	11	4	11,11,12	2.63	3 (27%)	15,15,17	1.23	2 (13%)
4	BGC	C	12	4	11,11,12	2.68	3 (27%)	15,15,17	1.23	2 (13%)
4	BGC	C	13	4	11,11,12	2.55	2 (18%)	15,15,17	1.38	2 (13%)
4	BGC	C	14	4	11,11,12	2.62	3 (27%)	15,15,17	1.97	2 (13%)
4	BGC	C	15	4	11,11,12	2.62	4 (36%)	15,15,17	1.39	2 (13%)
4	BGC	C	16	4	11,11,12	2.72	3 (27%)	15,15,17	1.85	4 (26%)
4	GAL	C	17	4	11,11,12	0.58	0	15,15,17	0.90	0
4	BGC	C	2	4	11,11,12	2.62	4 (36%)	15,15,17	1.84	4 (26%)
4	BGC	C	3	4	11,11,12	2.66	2 (18%)	15,15,17	2.31	5 (33%)
4	BGC	C	4	4	11,11,12	2.70	5 (45%)	15,15,17	2.14	5 (33%)
4	BGC	C	5	4	11,11,12	2.55	3 (27%)	15,15,17	2.14	4 (26%)
4	BGC	C	6	4	11,11,12	2.93	5 (45%)	15,15,17	1.01	1 (6%)
4	BGC	C	7	4	11,11,12	2.66	4 (36%)	15,15,17	1.35	2 (13%)
4	BGC	C	8	4	11,11,12	2.52	4 (36%)	15,15,17	1.95	5 (33%)
4	BGC	C	9	4	11,11,12	2.61	1 (9%)	15,15,17	1.58	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	C	1	4	-	2/2/22/22	0/1/1/1
4	BGC	C	10	4	-	1/2/19/22	0/1/1/1
4	BGC	C	11	4	-	0/2/19/22	0/1/1/1
4	BGC	C	12	4	-	0/2/19/22	0/1/1/1
4	BGC	C	13	4	-	1/2/19/22	0/1/1/1
4	BGC	C	14	4	-	0/2/19/22	0/1/1/1
4	BGC	C	15	4	-	2/2/19/22	0/1/1/1
4	BGC	C	16	4	-	2/2/19/22	0/1/1/1
4	GAL	C	17	4	-	2/2/19/22	0/1/1/1
4	BGC	C	2	4	-	2/2/19/22	0/1/1/1
4	BGC	C	3	4	-	1/2/19/22	0/1/1/1
4	BGC	C	4	4	-	2/2/19/22	0/1/1/1
4	BGC	C	5	4	-	0/2/19/22	0/1/1/1
4	BGC	C	6	4	-	1/2/19/22	0/1/1/1
4	BGC	C	7	4	-	2/2/19/22	0/1/1/1
4	BGC	C	8	4	-	2/2/19/22	0/1/1/1
4	BGC	C	9	4	-	0/2/19/22	0/1/1/1

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	6	BGC	O5-C1	8.00	1.56	1.43
4	C	12	BGC	O5-C1	7.34	1.55	1.43
4	C	7	BGC	O5-C1	7.34	1.55	1.43
4	C	3	BGC	O5-C1	7.30	1.55	1.43
4	C	4	BGC	O5-C1	7.27	1.55	1.43

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	14	BGC	C1-C2-C3	6.19	117.28	109.67
4	C	5	BGC	C1-C2-C3	5.58	116.52	109.67
4	C	3	BGC	C1-C2-C3	5.22	116.08	109.67
4	C	10	BGC	C1-C2-C3	5.02	115.84	109.67
4	C	4	BGC	C2-C3-C4	4.78	119.17	110.89

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	16	BGC	O5-C5-C6-O6

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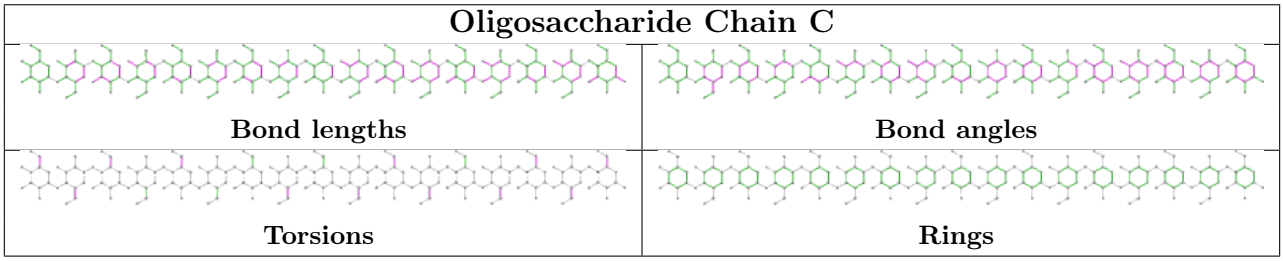
Mol	Chain	Res	Type	Atoms
4	C	4	BGC	O5-C5-C6-O6
4	C	7	BGC	O5-C5-C6-O6
4	C	2	BGC	O5-C5-C6-O6
4	C	16	BGC	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5	BGC	1	0
4	C	10	BGC	1	0
4	C	14	BGC	1	0
4	C	17	GAL	1	0
4	C	6	BGC	3	0
4	C	4	BGC	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

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
7	C2E	A	920	-	44,52,52	4.58	30 (68%)	52,82,82	1.61	14 (26%)
8	LDA	A	922	-	12,15,15	2.10	1 (8%)	14,17,17	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	43Y	A	902	-	19,19,23	1.36	3 (15%)	22,24,31	1.48	2 (9%)
8	LDA	A	923	-	12,15,15	2.09	1 (8%)	14,17,17	0.58	0
5	PLC	A	901	-	37,37,41	1.11	4 (10%)	43,45,49	1.03	2 (4%)
7	C2E	A	921	-	44,52,52	4.58	31 (70%)	52,82,82	1.62	14 (26%)
10	660	A	925	-	36,38,38	2.39	13 (36%)	49,58,58	1.60	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	C2E	A	920	-	-	7/22/62/62	0/6/7/7
8	LDA	A	922	-	-	5/13/13/13	-
6	43Y	A	902	-	-	6/22/22/27	-
8	LDA	A	923	-	-	8/13/13/13	-
5	PLC	A	901	-	-	23/41/41/45	-
7	C2E	A	921	-	-	3/22/62/62	0/6/7/7
10	660	A	925	-	-	7/20/59/59	0/3/3/3

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	920	C2E	C2A-C3A	-13.85	1.22	1.52
7	A	921	C2E	C2A-C3A	-13.76	1.22	1.52
7	A	921	C2E	C3'-C4'	-9.87	1.26	1.52
7	A	920	C2E	C3'-C4'	-9.69	1.26	1.52
7	A	920	C2E	O4'-C4'	8.81	1.64	1.45

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	925	660	C20-N15-C19	-5.20	119.72	126.58
6	A	902	43Y	O2-C31-C32	4.84	120.00	111.09
10	A	925	660	N15-C19-N13	4.16	120.41	114.89
5	A	901	PLC	O2-C'-C1'	3.49	119.03	111.50
7	A	920	C2E	C51-C61-N11	3.47	120.09	113.95

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

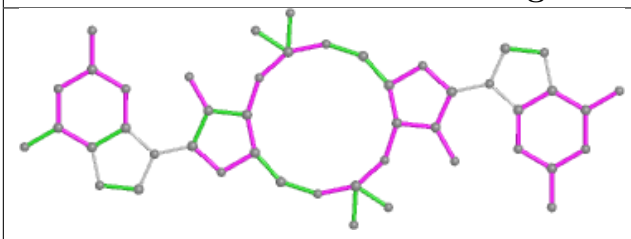
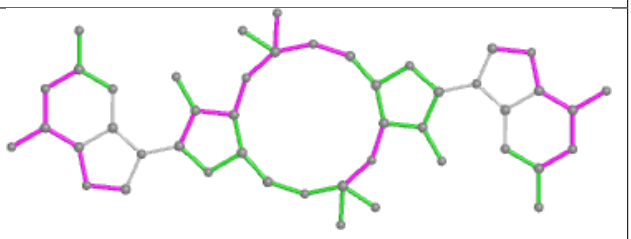
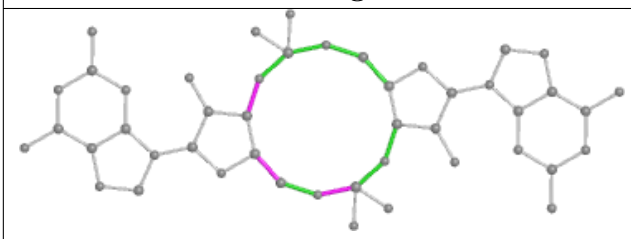
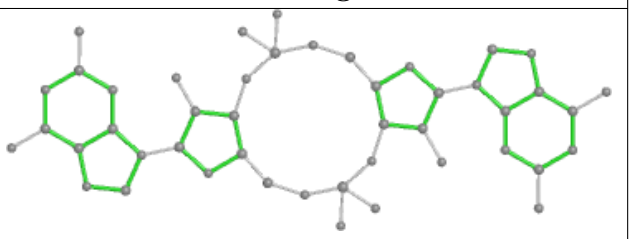
Mol	Chain	Res	Type	Atoms
5	A	901	PLC	O3P-C1-C2-O2
5	A	901	PLC	O4P-C4-C5-N
6	A	902	43Y	C1-O3P-P-O1P
7	A	920	C2E	C5'-O5'-P1-O1P
7	A	921	C2E	C5A-O5A-P11-O11

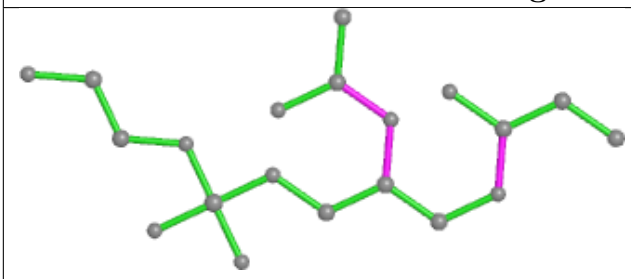
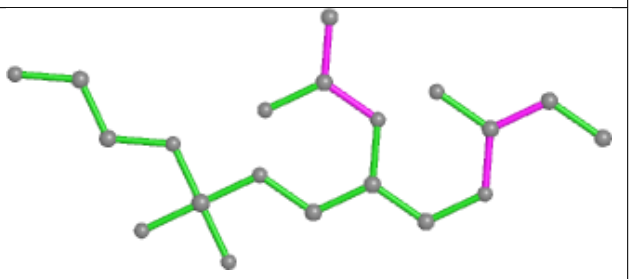
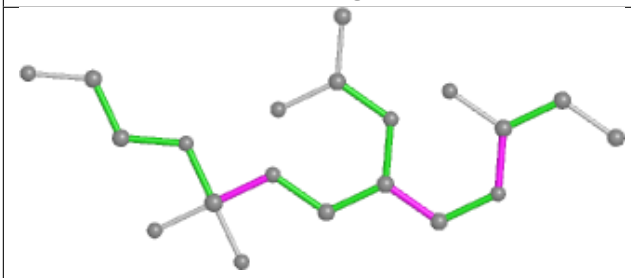
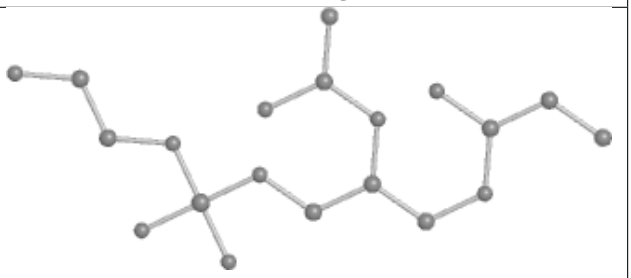
There are no ring outliers.

5 monomers are involved in 10 short contacts:

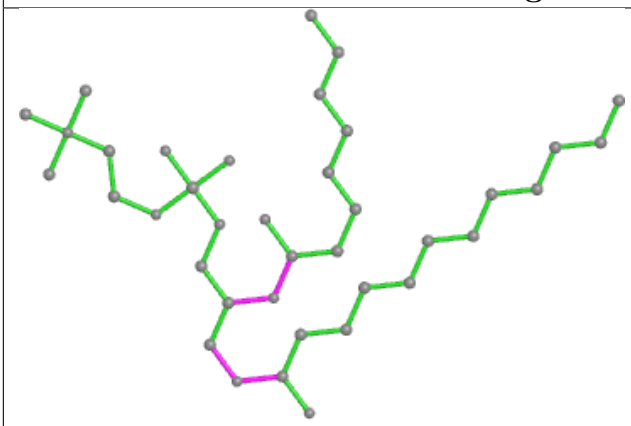
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	920	C2E	2	0
6	A	902	43Y	1	0
8	A	923	LDA	2	0
7	A	921	C2E	4	0
10	A	925	660	2	0

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.

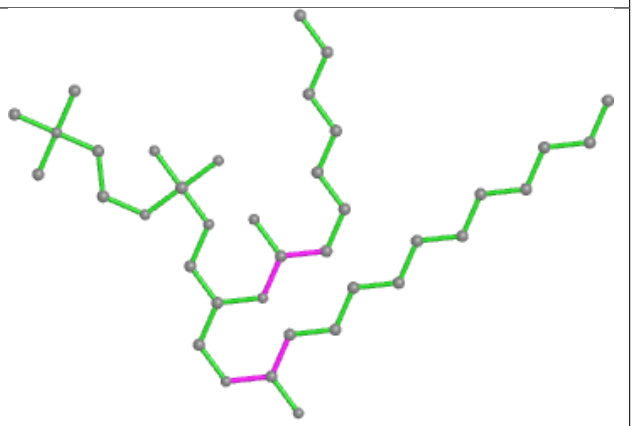
Ligand C2E A 920	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 43Y A 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

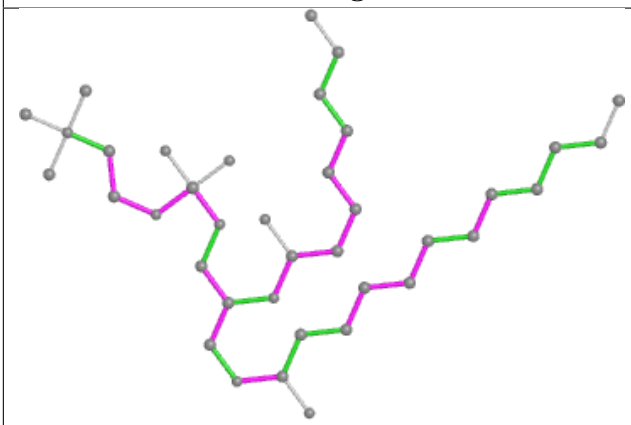
Ligand PLC A 901



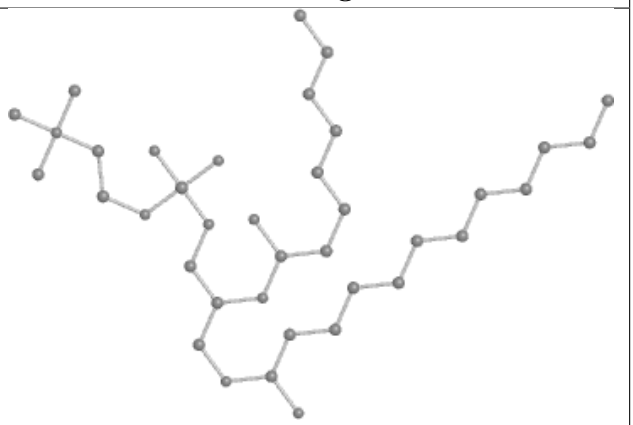
Bond lengths



Bond angles

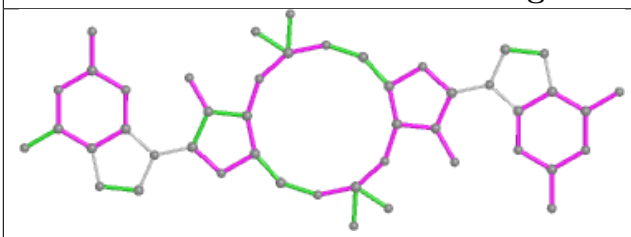


Torsions

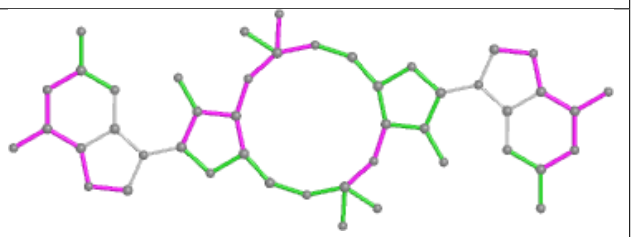


Rings

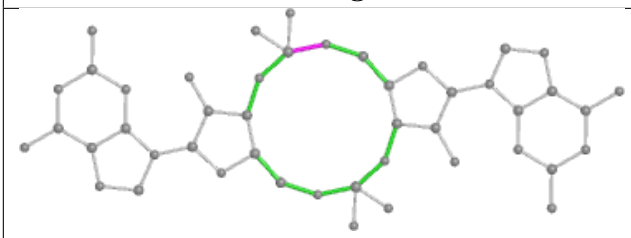
Ligand C2E A 921



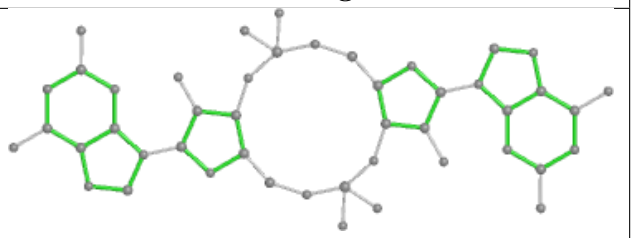
Bond lengths



Bond angles

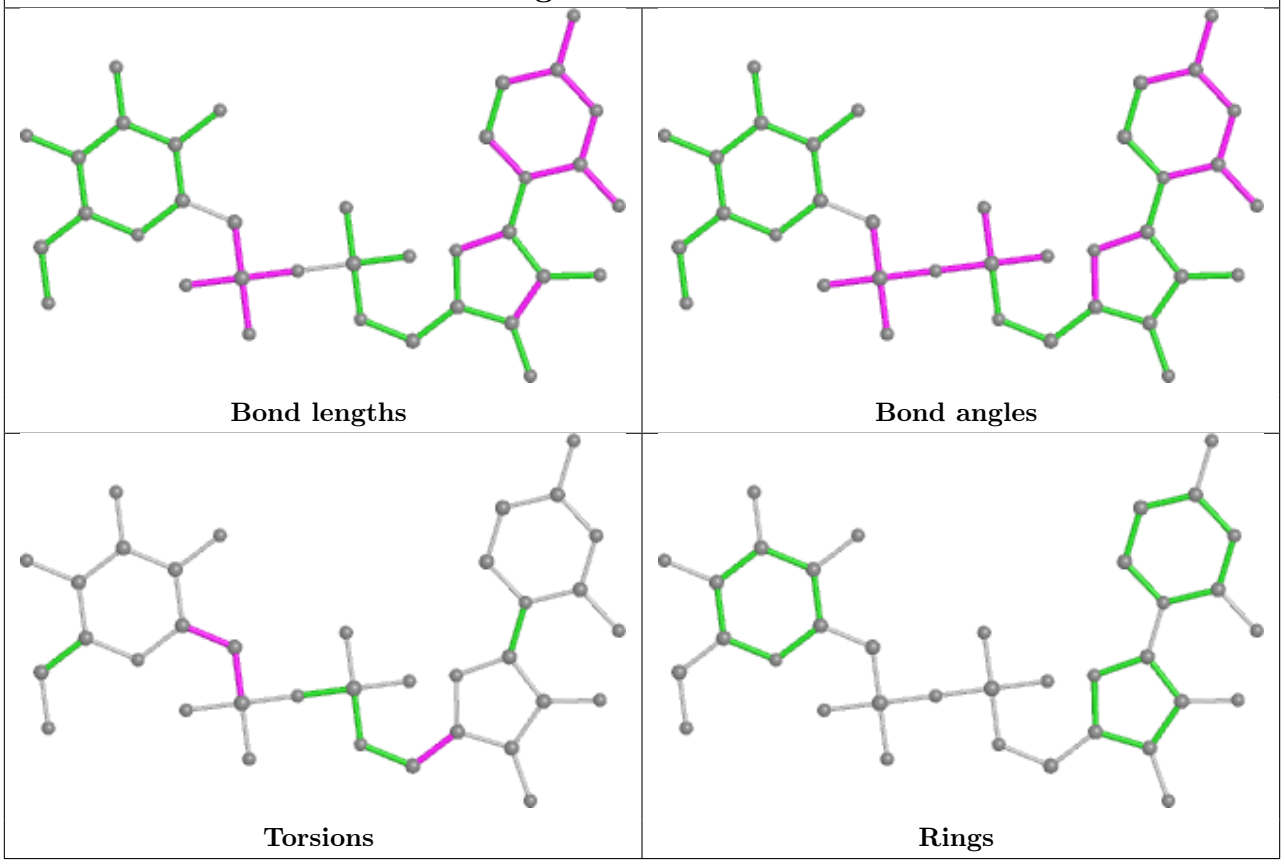


Torsions



Rings

Ligand 660 A 925



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, 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	728/803 (90%)	0.06	28 (3%)	40	26	47, 80, 140, 234	0
2	B	658/729 (90%)	-0.09	15 (2%)	60	43	47, 74, 123, 188	0
3	D	0/9	-	-			-	-
All	All	1386/1541 (89%)	-0.01	43 (3%)	49	32	47, 77, 132, 234	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	ARG	5.5
1	A	496	LEU	5.0
2	B	77[A]	GLN	4.8
1	A	509	ASP	3.9
1	A	318	CYS	3.8

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
4	BGC	C	1	12/12	0.73	0.34	161,171,185,205	0
4	BGC	C	2	11/12	0.83	0.25	105,120,134,148	0
4	BGC	C	6	11/12	0.88	0.19	53,63,85,108	0
4	BGC	C	3	11/12	0.90	0.20	92,109,121,126	0

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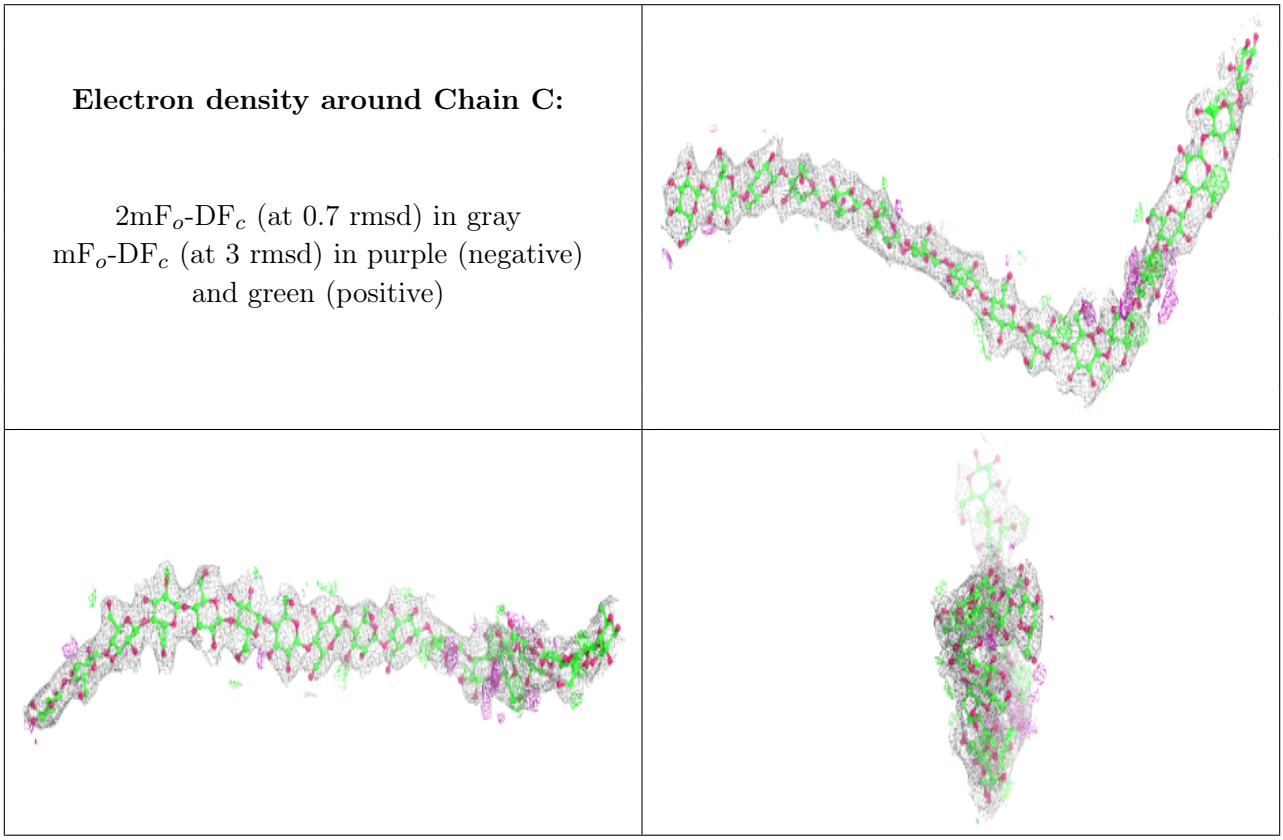
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BGC	C	7	11/12	0.90	0.17	49,65,72,81	0
4	BGC	C	5	11/12	0.93	0.18	49,55,64,105	0
4	BGC	C	8	11/12	0.93	0.21	72,76,97,117	0
4	BGC	C	4	11/12	0.94	0.19	56,69,114,142	0
4	BGC	C	14	11/12	0.94	0.28	65,81,86,87	0
4	BGC	C	13	11/12	0.95	0.30	63,80,85,85	0
4	BGC	C	12	11/12	0.96	0.23	63,73,83,87	0
4	BGC	C	10	11/12	0.96	0.23	71,77,92,98	0
4	BGC	C	11	11/12	0.96	0.20	82,89,93,95	0
4	GAL	C	17	11/12	0.96	0.33	65,80,96,98	0
4	BGC	C	15	11/12	0.97	0.26	59,68,73,73	0
4	BGC	C	16	11/12	0.97	0.30	59,69,86,93	0
4	BGC	C	9	11/12	0.97	0.20	69,74,79,88	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)



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,

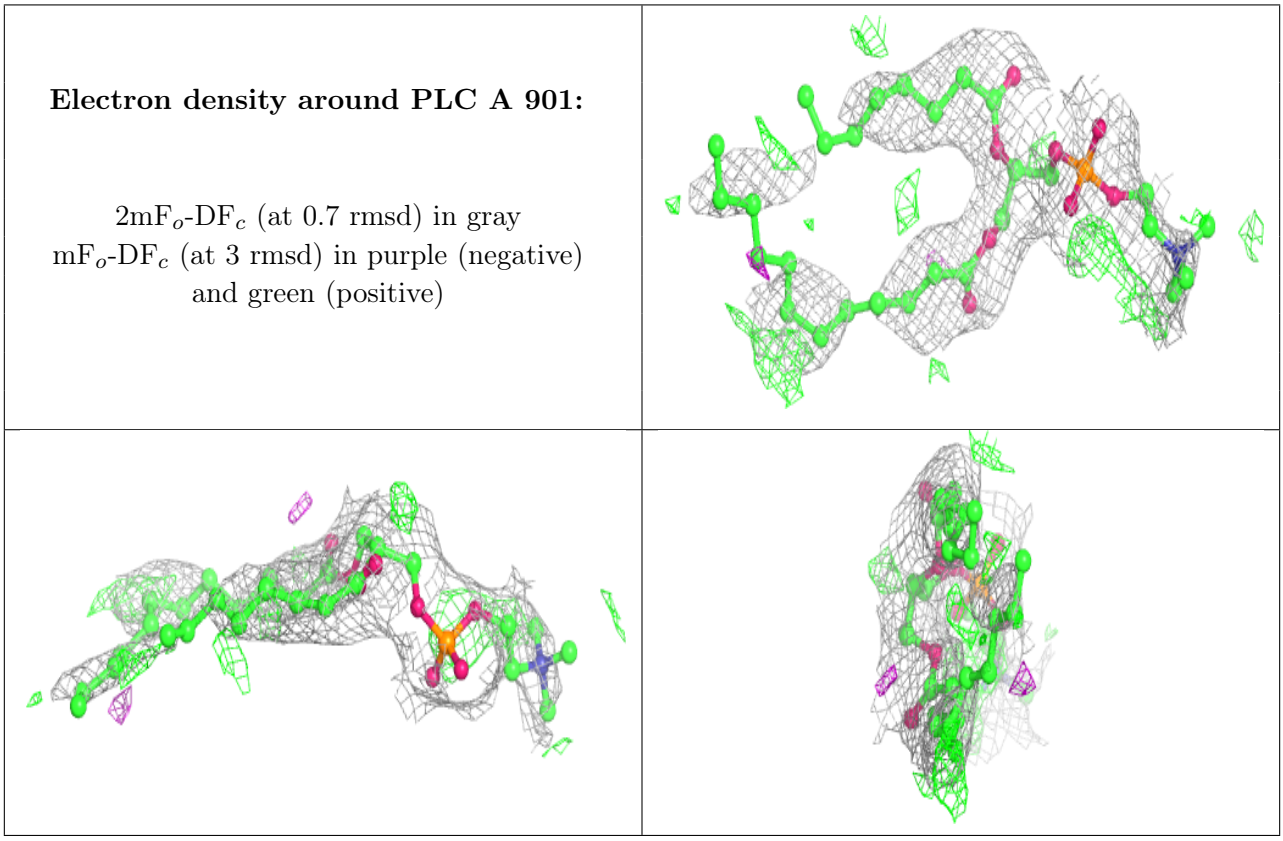
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	LDA	A	922	16/16	0.61	0.48	52,67,83,85	16
8	LDA	A	923	16/16	0.62	0.28	76,91,111,119	16
9	MG	B	801	1/1	0.73	0.19	54,54,54,54	0
5	PLC	A	901	38/42	0.82	0.42	106,129,151,152	0
9	MG	A	924	1/1	0.88	1.45	83,83,83,83	0
10	660	A	925	36/36	0.92	0.33	67,78,89,95	36
6	43Y	A	902	20/24	0.93	0.27	88,105,122,129	0
7	C2E	A	921	46/46	0.95	0.12	53,76,86,95	0
7	C2E	A	920	46/46	0.96	0.13	51,67,82,82	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.

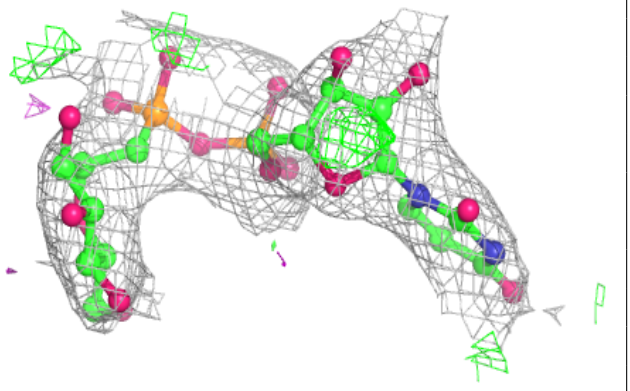
Electron density around PLC A 901:

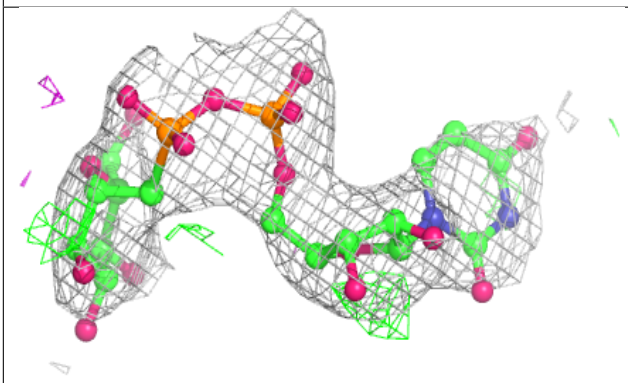
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

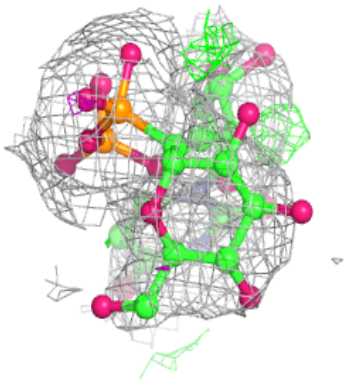


Electron density around 660 A 925:

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

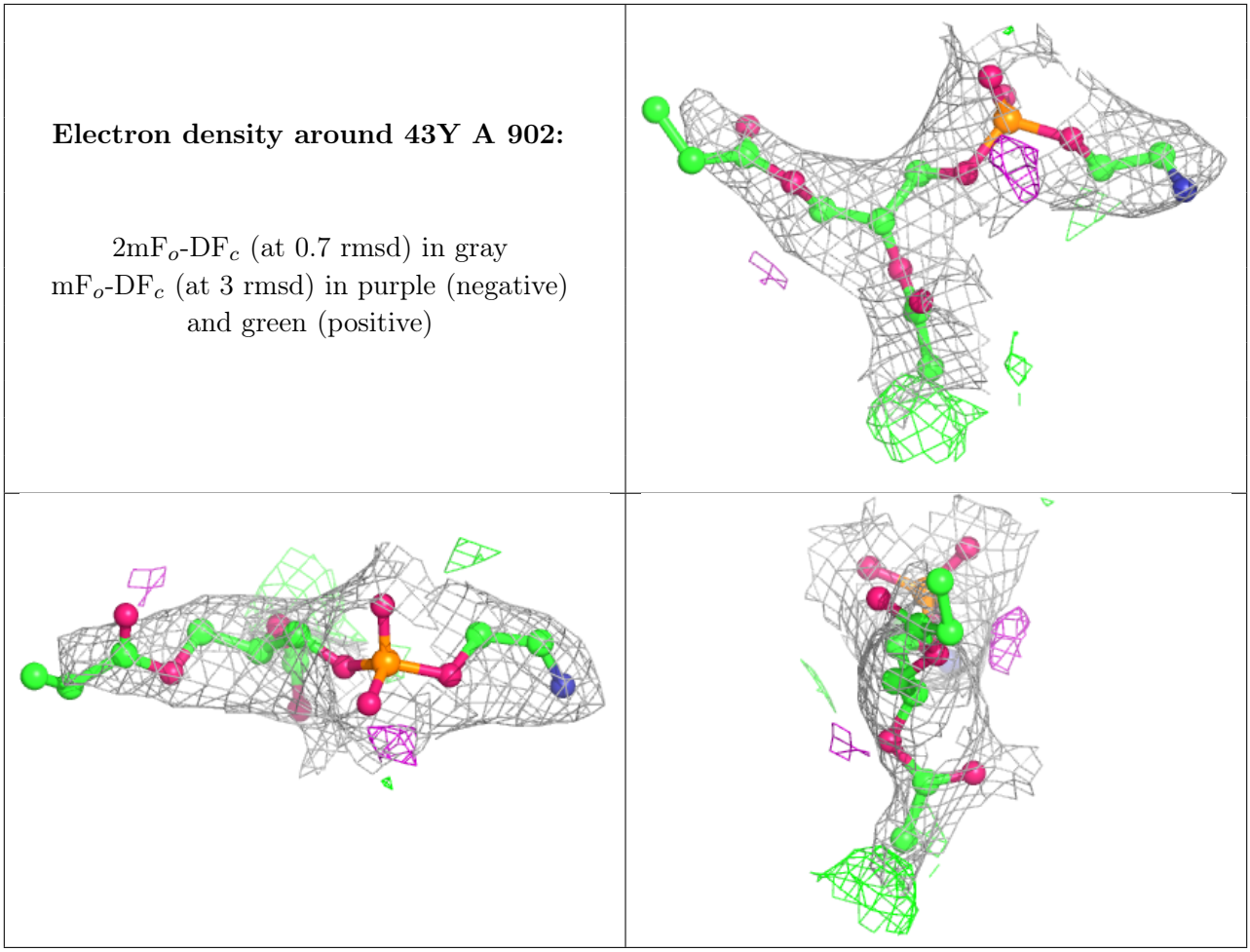






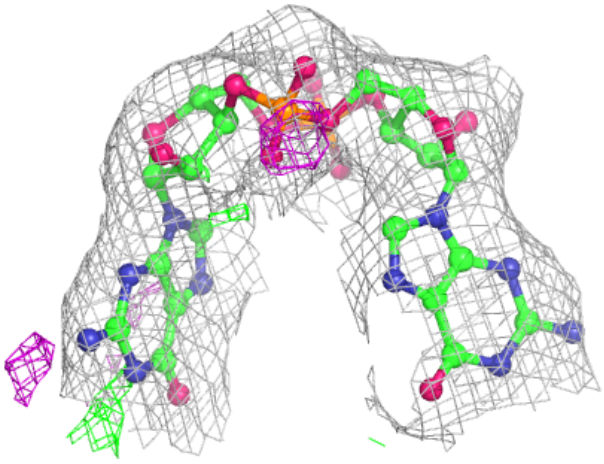
Electron density around 43Y A 902:

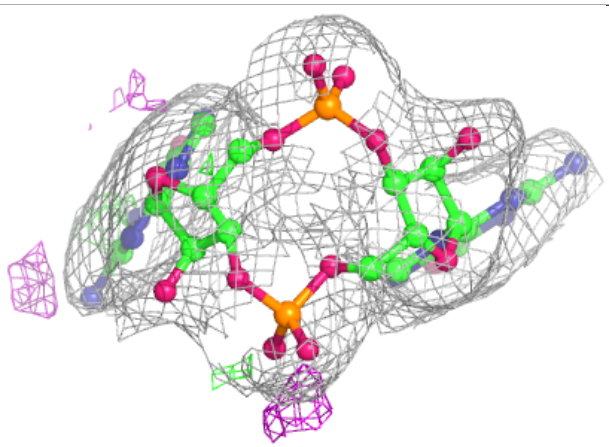
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

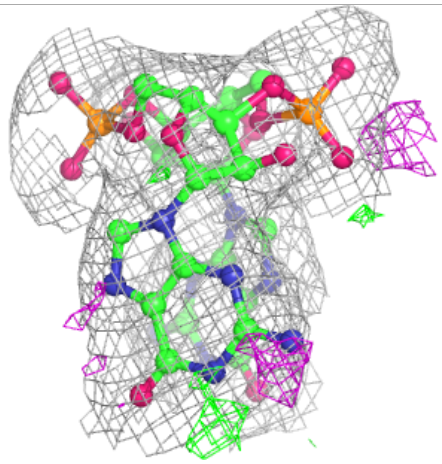


Electron density around C2E A 921:

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

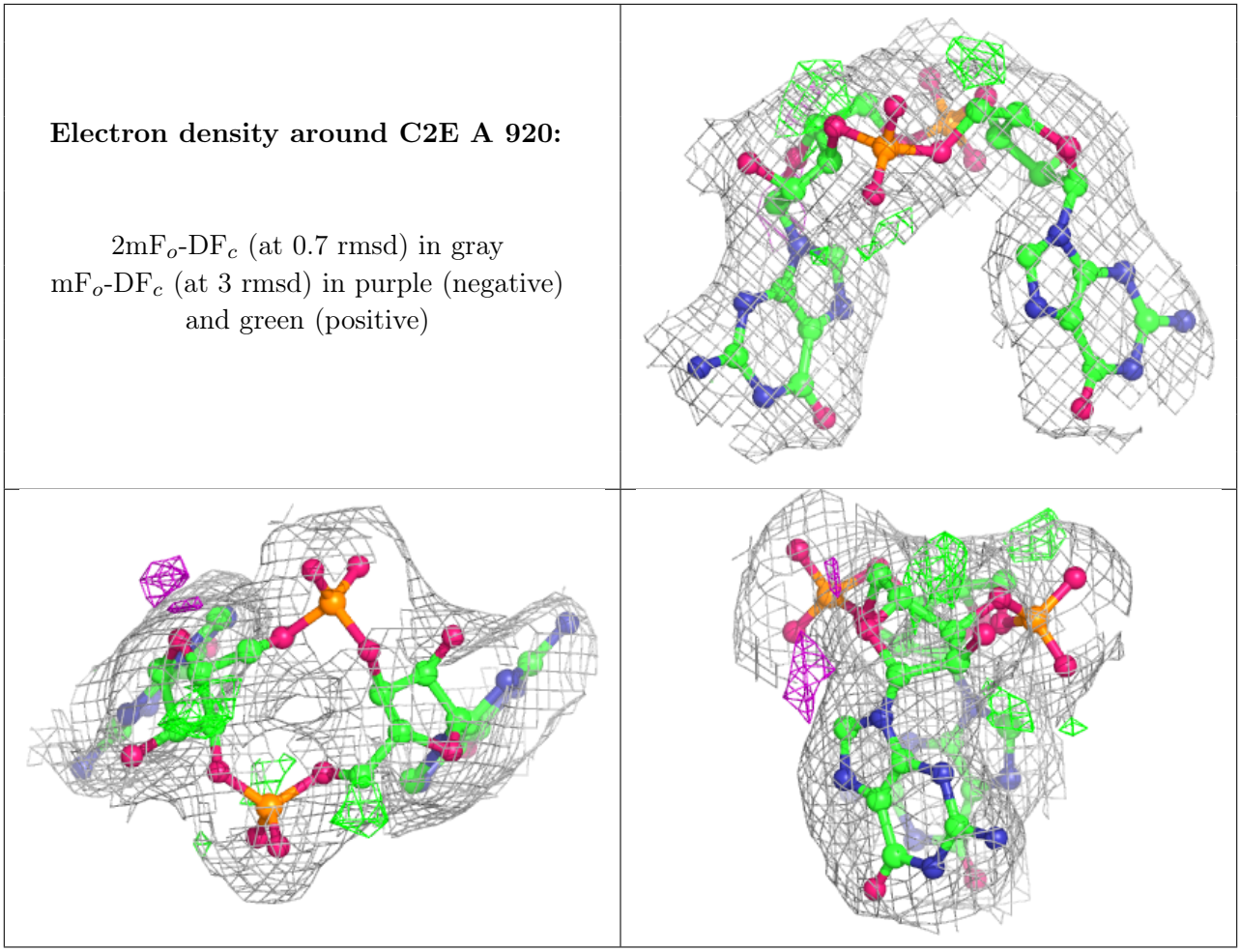






Electron density around C2E A 920:

$2mF_o$-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.