wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2024 – 07:13 AM EDT

PDB ID	:	4P00
Title	:	Bacterial Cellulose Synthase in complex with cyclic-di-GMP and UDP
Authors	:	Morgan, J.L.W.; McNamara, J.T.; Zimmer, J.
Deposited on	:	2014-02-19
Resolution	:	3.20 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:

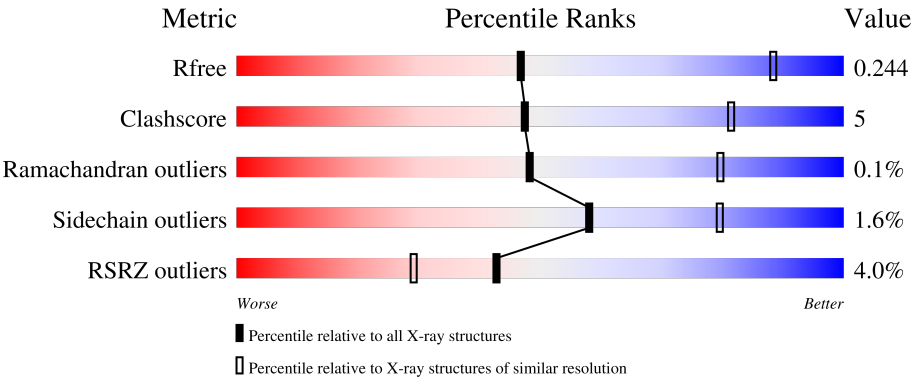
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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%, 77%, 13%, 9%
2	B	724	4%, 78%, 12%, 10%
3	D	9	100%
4	C	17	41%, 41%, 18%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 11070 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 Cellulose Synthase A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5739	3725	1000	982	32	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	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

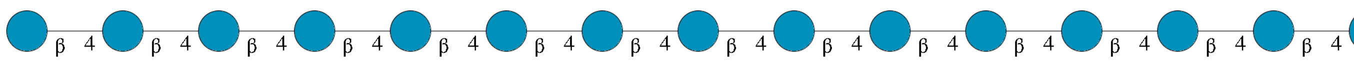
- Molecule 2 is a protein called Cellulose Synthase B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	655	4923	3120	872	915	16	0	5	0

- Molecule 3 is a protein called unidentified peptide.

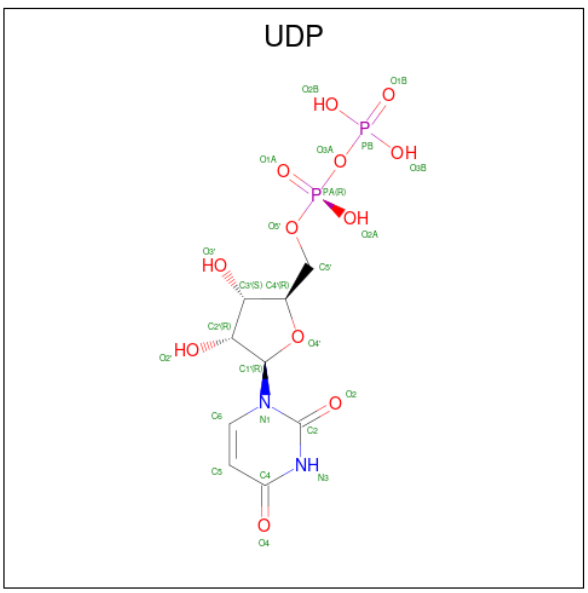
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	9	45	27	9	9	0	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
4	C	17	187	102	85	0	0	0

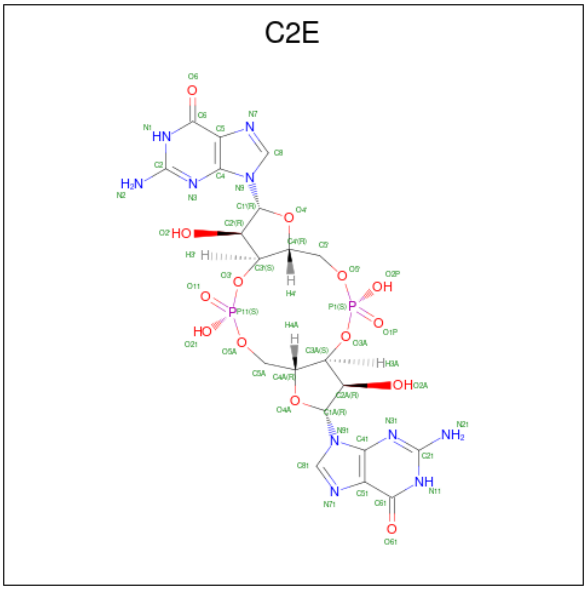
- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	25	9	2	12	2	0	0

- Molecule 6 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:

$C_{20}H_{24}N_{10}O_{14}P_2$).

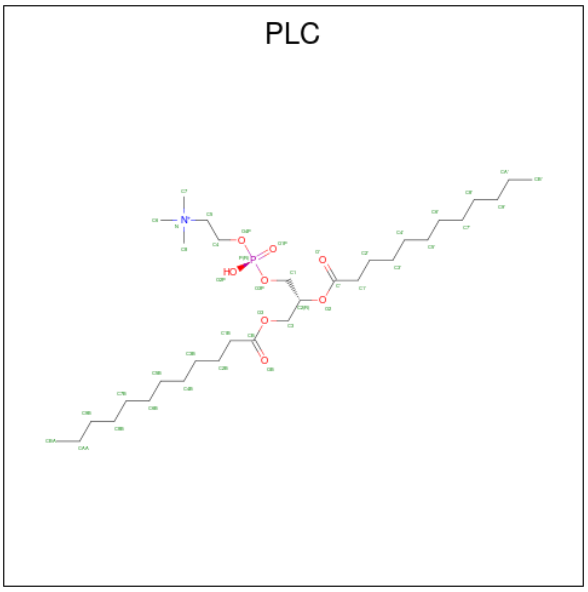


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
6	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

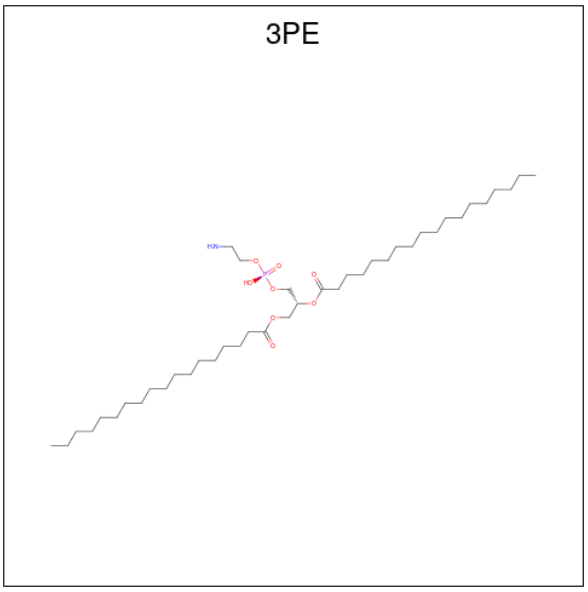
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

- Molecule 8 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



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

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



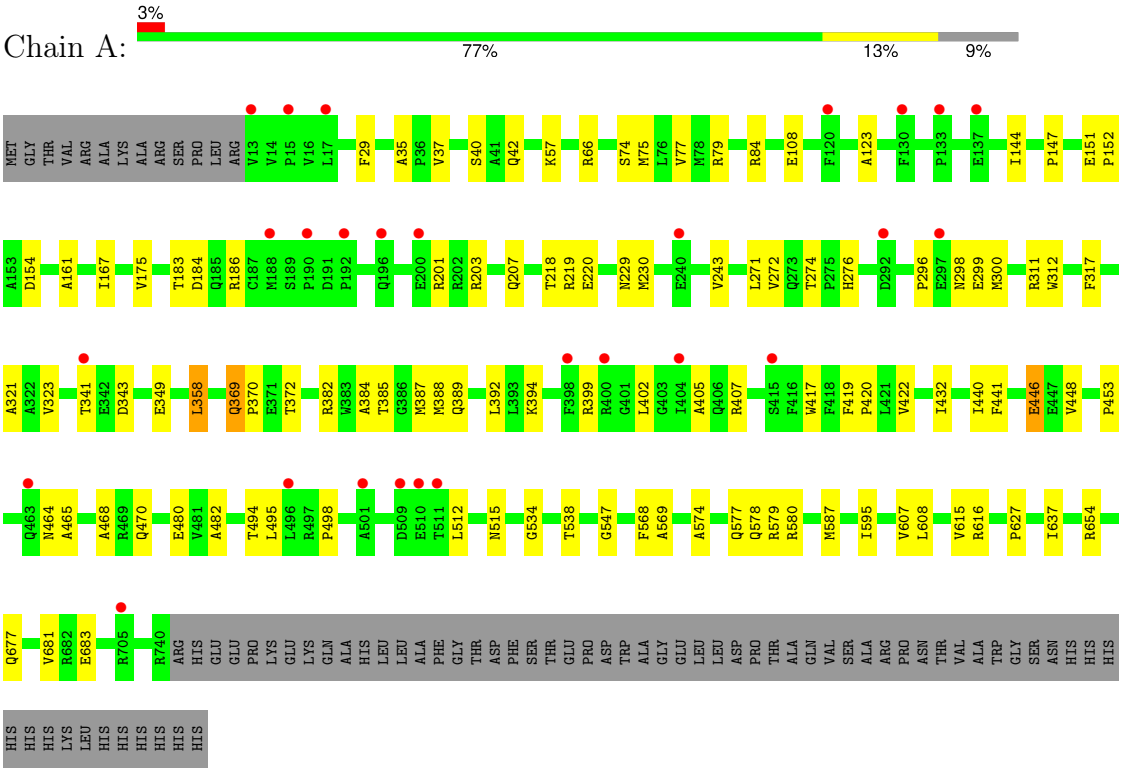
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			20	10	1	8	1		

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.

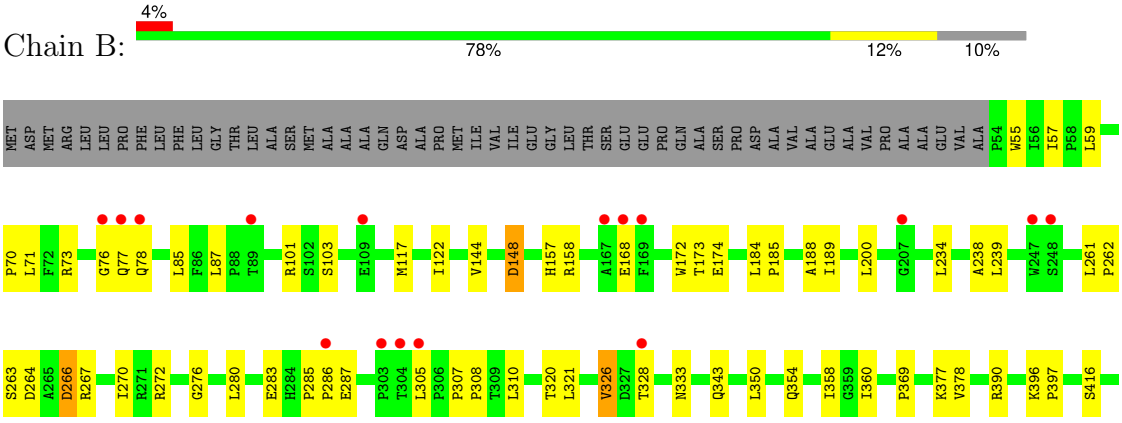
• Molecule 1: Cellulose Synthase A subunit

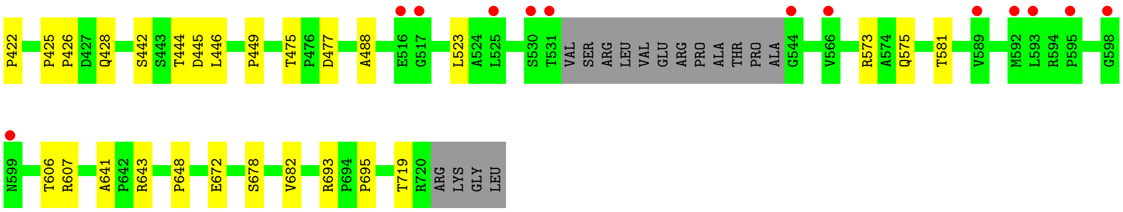
Chain A:



• Molecule 2: Cellulose Synthase B subunit

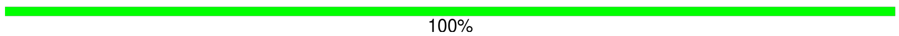
Chain B:





• Molecule 3: unidentified peptide

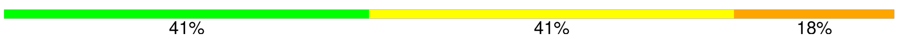
Chain D:

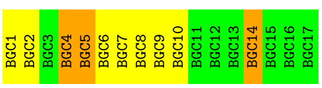


There are no outlier residues recorded for this chain.

• Molecule 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-(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	67.49Å 216.79Å 219.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 3.20 48.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.98-3.20) 98.2 (48.98-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.208 , 0.238 0.217 , 0.244	Depositor DCC
R_{free} test set	2715 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	70.0	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11070	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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, PLC, UDP, C2E, MG, 3PE

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	0.21	0/5888	0.37	0/8007
2	B	0.20	0/5042	0.40	0/6913
All	All	0.21	0/10930	0.38	0/14920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5739	0	5855	64	0
2	B	4923	0	4997	51	0
3	D	45	0	12	0	0
4	C	187	0	154	9	0
5	A	25	0	11	1	0
6	A	92	0	44	11	0
7	A	1	0	0	0	0
8	A	38	0	53	1	0
9	A	20	0	14	1	0
All	All	11070	0	11140	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 122 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)
6:A:920:C2E:H81	6:A:920:C2E:H511	1.21	1.11
6:A:920:C2E:H81	6:A:920:C2E:C5A	1.93	0.98
1:A:578:GLN:OE1	6:A:920:C2E:N2	1.99	0.94
2:B:390:ARG:NH2	4:C:5:BGC:O6	2.05	0.88
1:A:57:LYS:NZ	9:A:923:3PE:O12	2.16	0.78

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	727/803 (90%)	689 (95%)	36 (5%)	2 (0%)	37 69
2	B	656/724 (91%)	632 (96%)	24 (4%)	0	100 100
All	All	1383/1527 (91%)	1321 (96%)	60 (4%)	2 (0%)	48 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	574	ALA
1	A	167	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	599/661 (91%)	591 (99%)	8 (1%)	65 83
2	B	523/572 (91%)	513 (98%)	10 (2%)	52 76
All	All	1122/1233 (91%)	1104 (98%)	18 (2%)	58 79

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	523	LEU
2	B	672	GLU
2	B	643	ARG
2	B	87	LEU
2	B	378	VAL

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	11,11,12	0.29	0	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BGC	C	10	4	11,11,12	0.31	0	15,15,17	0.76	1 (6%)
4	BGC	C	11	4	11,11,12	0.28	0	15,15,17	0.55	0
4	BGC	C	12	4	11,11,12	0.29	0	15,15,17	0.70	0
4	BGC	C	13	4	11,11,12	0.30	0	15,15,17	0.56	0
4	BGC	C	14	4	11,11,12	0.32	0	15,15,17	1.14	1 (6%)
4	BGC	C	15	4	11,11,12	0.30	0	15,15,17	0.72	0
4	BGC	C	16	4	11,11,12	0.28	0	15,15,17	0.66	0
4	BGC	C	17	4	11,11,12	0.25	0	15,15,17	0.58	0
4	BGC	C	2	4	11,11,12	0.33	0	15,15,17	0.83	0
4	BGC	C	3	4	11,11,12	0.29	0	15,15,17	0.69	0
4	BGC	C	4	4	11,11,12	0.37	0	15,15,17	1.10	1 (6%)
4	BGC	C	5	4	11,11,12	0.43	0	15,15,17	1.46	2 (13%)
4	BGC	C	6	4	11,11,12	0.26	0	15,15,17	0.59	0
4	BGC	C	7	4	11,11,12	0.26	0	15,15,17	0.75	0
4	BGC	C	8	4	11,11,12	0.35	0	15,15,17	1.05	1 (6%)
4	BGC	C	9	4	11,11,12	0.29	0	15,15,17	0.64	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
4	BGC	C	1	4	-	0/2/19/22	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	-	0/2/19/22	0/1/1/1
4	BGC	C	14	4	-	0/2/19/22	0/1/1/1
4	BGC	C	15	4	-	0/2/19/22	0/1/1/1
4	BGC	C	16	4	-	1/2/19/22	0/1/1/1
4	BGC	C	17	4	-	0/2/19/22	0/1/1/1
4	BGC	C	2	4	-	1/2/19/22	0/1/1/1
4	BGC	C	3	4	-	1/2/19/22	0/1/1/1
4	BGC	C	4	4	-	0/2/19/22	0/1/1/1
4	BGC	C	5	4	-	1/2/19/22	0/1/1/1
4	BGC	C	6	4	-	2/2/19/22	0/1/1/1
4	BGC	C	7	4	-	2/2/19/22	0/1/1/1
4	BGC	C	8	4	-	0/2/19/22	0/1/1/1
4	BGC	C	9	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	5	BGC	C1-C2-C3	3.82	115.20	109.64
4	C	14	BGC	C1-C2-C3	3.53	114.79	109.64
4	C	4	BGC	C1-C2-C3	3.15	114.23	109.64
4	C	5	BGC	C2-C3-C4	2.51	115.28	110.86
4	C	10	BGC	C1-C2-C3	2.26	112.93	109.64

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

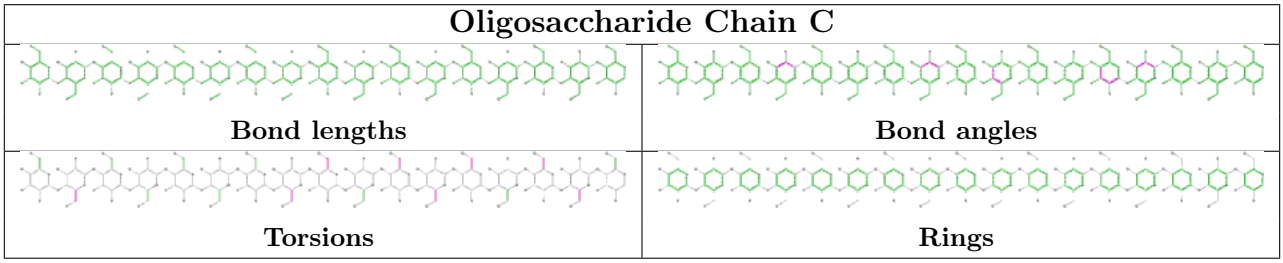
Mol	Chain	Res	Type	Atoms
4	C	6	BGC	O5-C5-C6-O6
4	C	6	BGC	C4-C5-C6-O6
4	C	9	BGC	O5-C5-C6-O6
4	C	9	BGC	C4-C5-C6-O6
4	C	7	BGC	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	BGC	1	0
4	C	4	BGC	2	0
4	C	7	BGC	1	0
4	C	5	BGC	4	0
4	C	2	BGC	1	0
4	C	14	BGC	1	0
4	C	6	BGC	2	0
4	C	9	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 (i)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	C2E	A	920	-	44,52,52	0.96	3 (6%)	50,82,82	1.15	5 (10%)
8	PLC	A	922	-	37,37,41	1.12	2 (5%)	43,45,49	1.12	3 (6%)
9	3PE	A	923	-	19,19,50	1.60	2 (10%)	22,24,55	1.65	4 (18%)
6	C2E	A	919	-	44,52,52	0.97	4 (9%)	50,82,82	1.20	6 (12%)
5	UDP	A	918	7	25,26,26	1.01	1 (4%)	38,40,40	1.61	5 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	C2E	A	920	-	-	11/22/62/62	0/6/7/7
8	PLC	A	922	-	-	21/41/41/45	-
9	3PE	A	923	-	-	3/22/22/54	-
6	C2E	A	919	-	-	7/22/62/62	0/6/7/7
5	UDP	A	918	7	-	7/16/32/32	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	923	3PE	O21-C21	4.81	1.45	1.35
9	A	923	3PE	O31-C31	4.31	1.45	1.33
8	A	922	PLC	O3-CB	4.31	1.45	1.33
8	A	922	PLC	O2-C'	4.13	1.46	1.34
6	A	920	C2E	C61-N11	-2.32	1.34	1.37

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	918	UDP	C4-N3-C2	-5.48	119.81	126.61
9	A	923	3PE	O21-C21-C22	5.16	120.29	111.09
8	A	922	PLC	O2-C'-C1'	4.08	120.30	111.48
5	A	918	UDP	N3-C2-N1	3.96	120.05	114.89
5	A	918	UDP	C5-C4-N3	3.31	119.43	114.80

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	919	C2E	C5'-O5'-P1-O1P
6	A	920	C2E	C5'-O5'-P1-O1P
6	A	920	C2E	O4'-C4'-C5'-O5'
6	A	920	C2E	C5A-O5A-P11-O3'
6	A	920	C2E	C5A-O5A-P11-O21

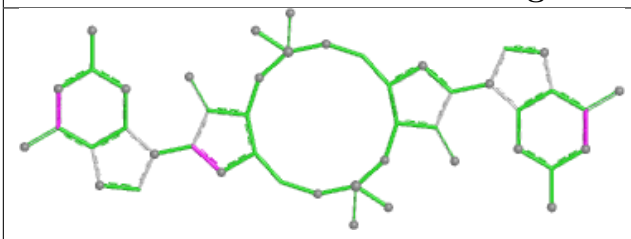
There are no ring outliers.

5 monomers are involved in 14 short contacts:

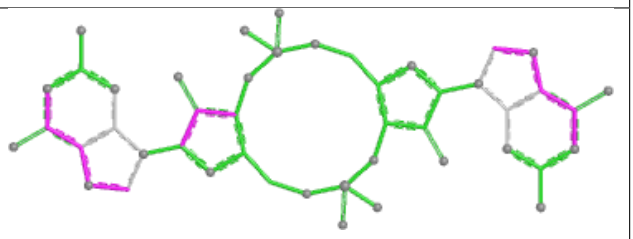
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	920	C2E	9	0
8	A	922	PLC	1	0
9	A	923	3PE	1	0
6	A	919	C2E	3	0
5	A	918	UDP	1	0

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.

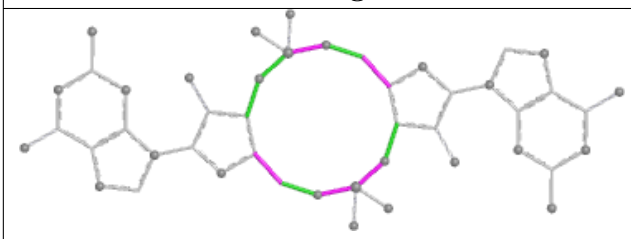
Ligand C2E A 920



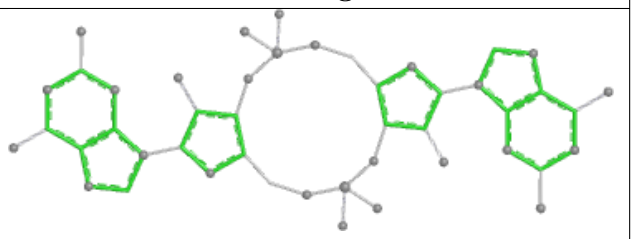
Bond lengths



Bond angles

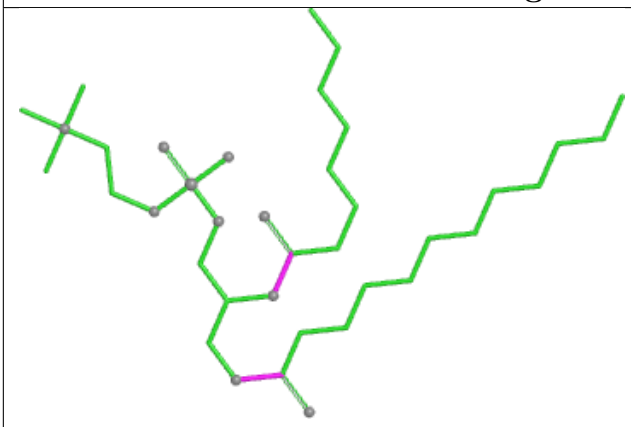


Torsions

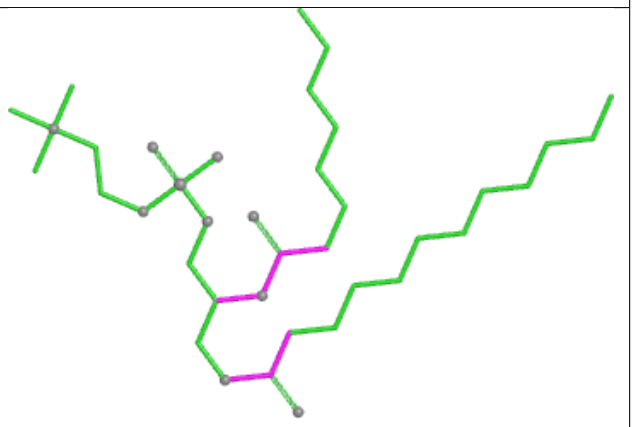


Rings

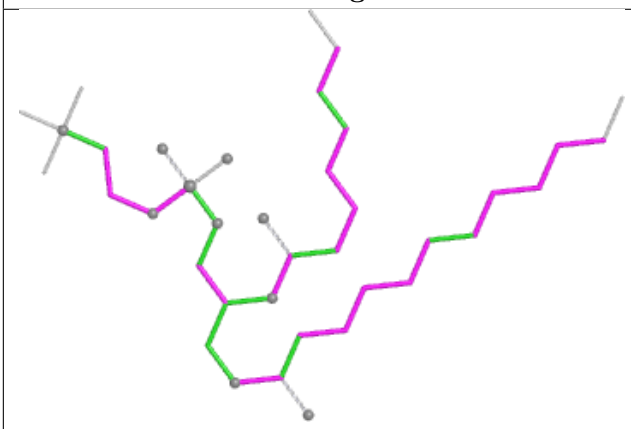
Ligand PLC A 922



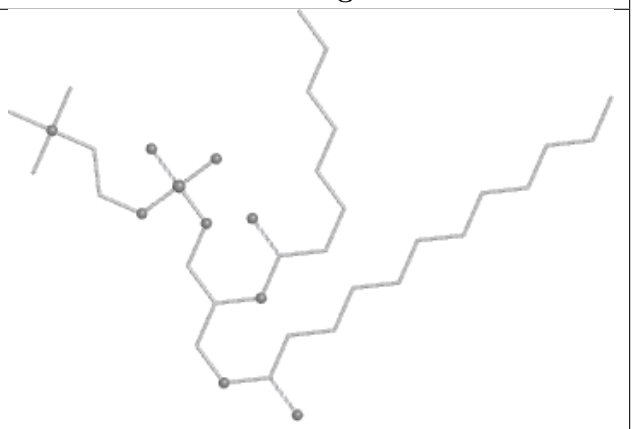
Bond lengths



Bond angles

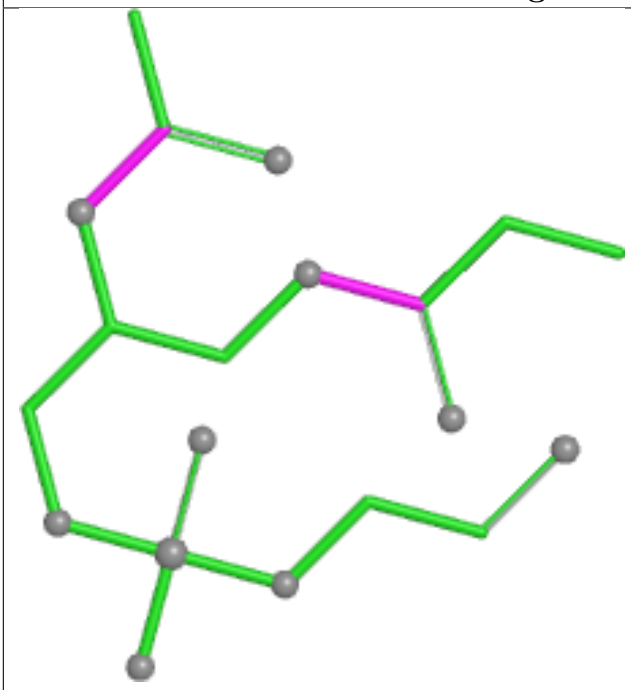


Torsions

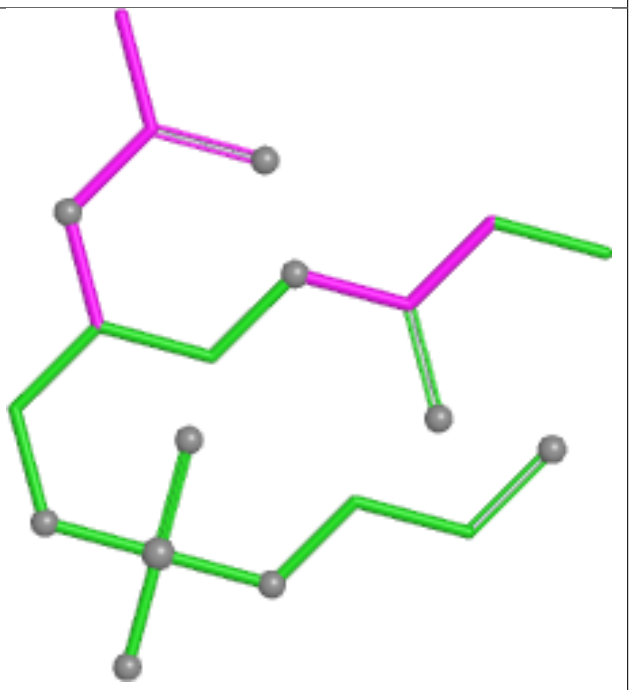


Rings

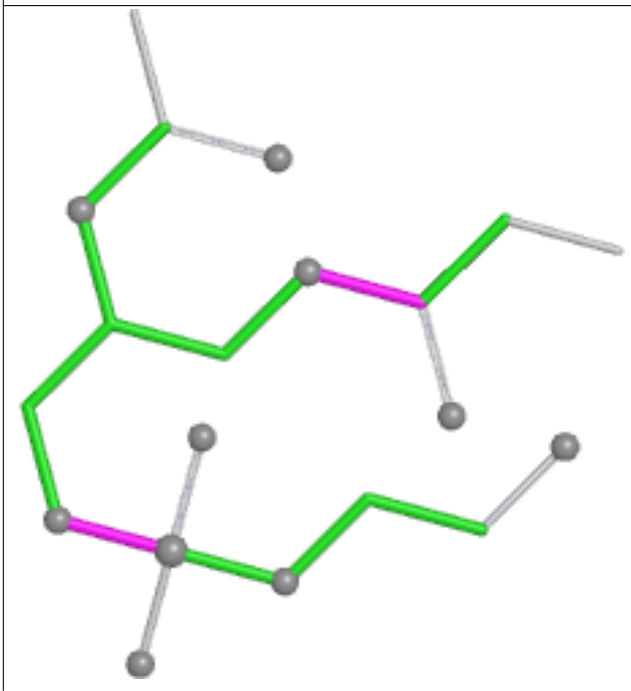
Ligand 3PE A 923



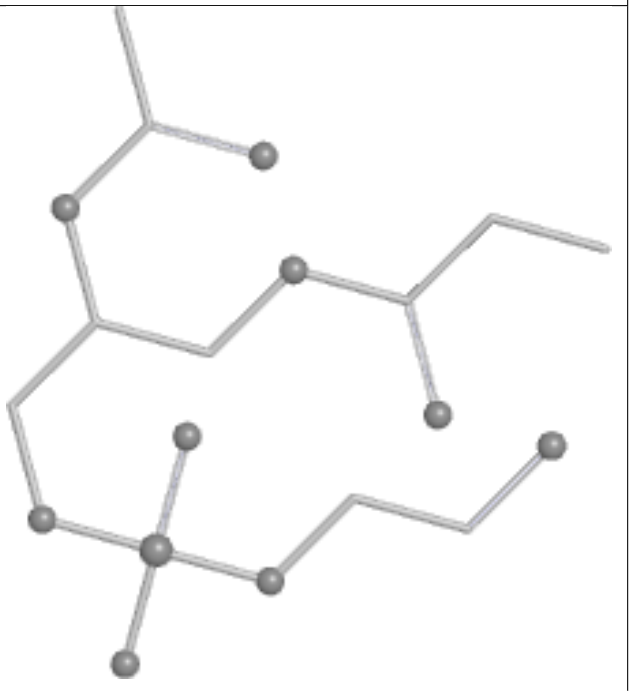
Bond lengths



Bond angles

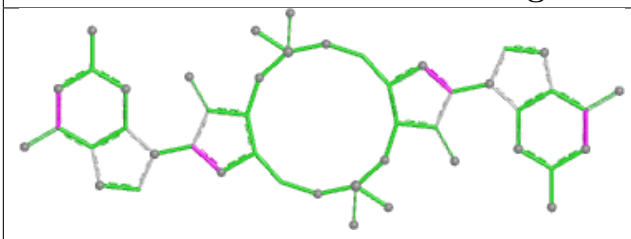


Torsions

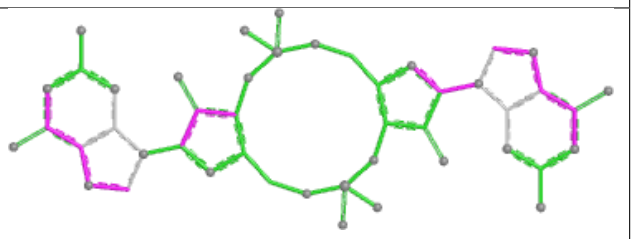


Rings

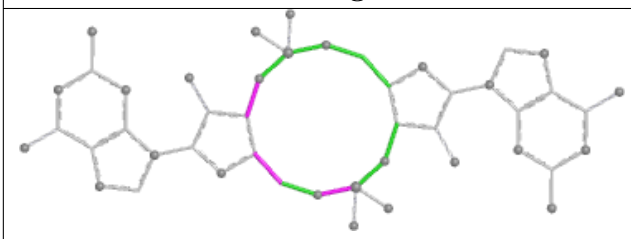
Ligand C2E A 919



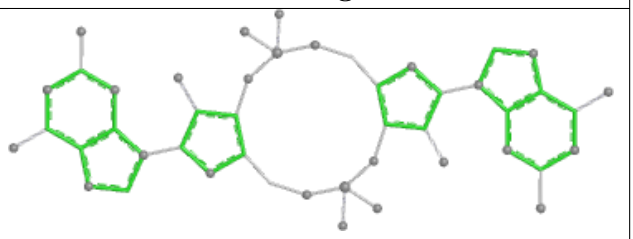
Bond lengths



Bond angles

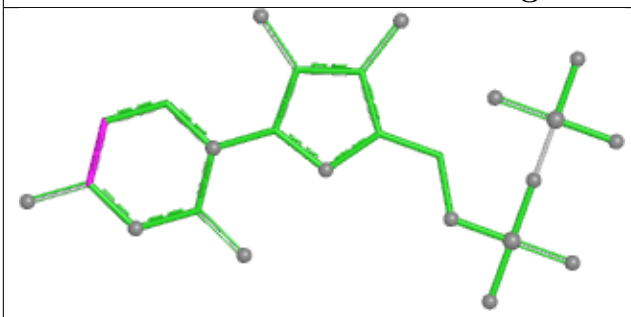


Torsions

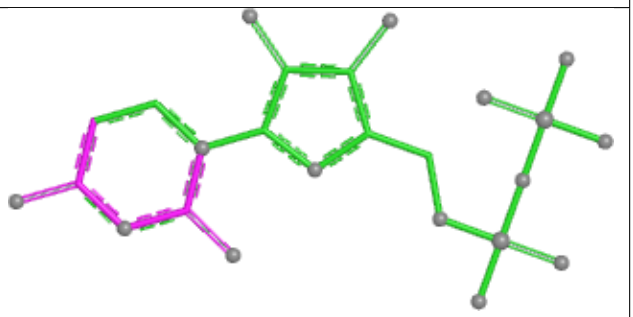


Rings

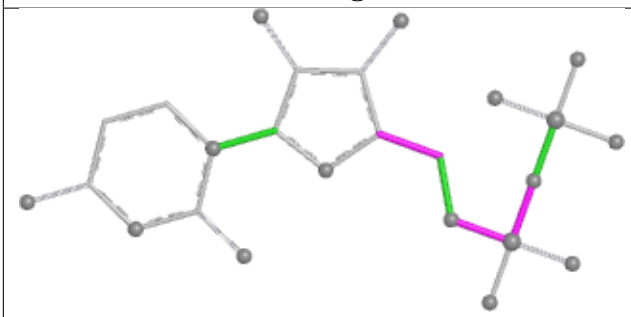
Ligand UDP A 918



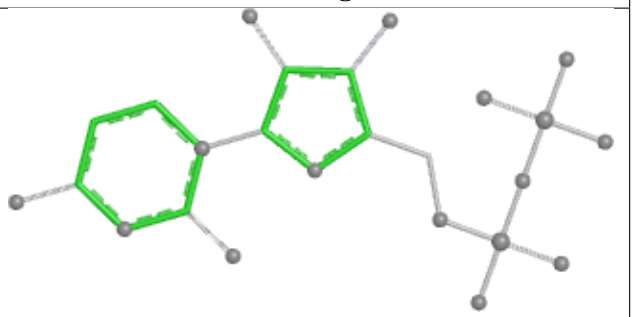
Bond lengths



Bond angles



Torsions



Rings

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%)	0.15	27 (3%)	45	31	42, 69, 116, 196	1 (0%)
2	B	655/724 (90%)	0.16	29 (4%)	39	27	32, 63, 112, 169	5 (0%)
3	D	0/9	-	-			-	-
All	All	1383/1536 (90%)	0.15	56 (4%)	43	29	32, 67, 115, 196	6 (0%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	77[A]	GLN	9.7
2	B	78[A]	GLN	9.2
2	B	304	THR	5.3
2	B	169	PHE	4.8
2	B	328	THR	4.7

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

SUGAR-RSR INFOmissingINFO

6.4 Ligands

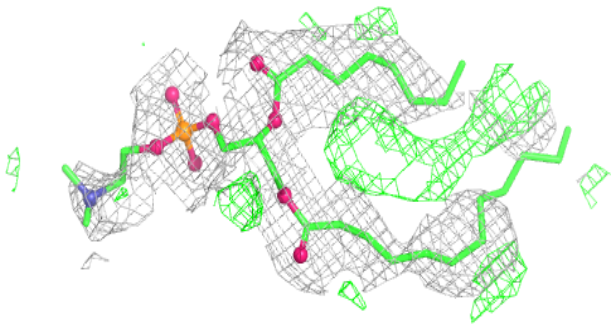
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

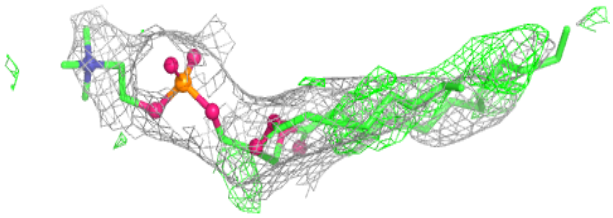
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PLC	A	922	38/42	0.84	0.28	87,120,154,168	0
9	3PE	A	923	20/51	0.86	0.18	71,90,113,120	0
5	UDP	A	918	25/25	0.93	0.13	54,80,92,126	0
6	C2E	A	920	46/46	0.94	0.08	35,56,70,91	0
7	MG	A	921	1/1	0.94	0.26	36,36,36,36	0
6	C2E	A	919	46/46	0.96	0.08	31,51,63,76	0

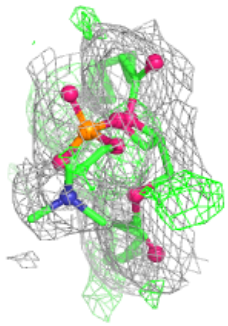
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLC A 922:

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

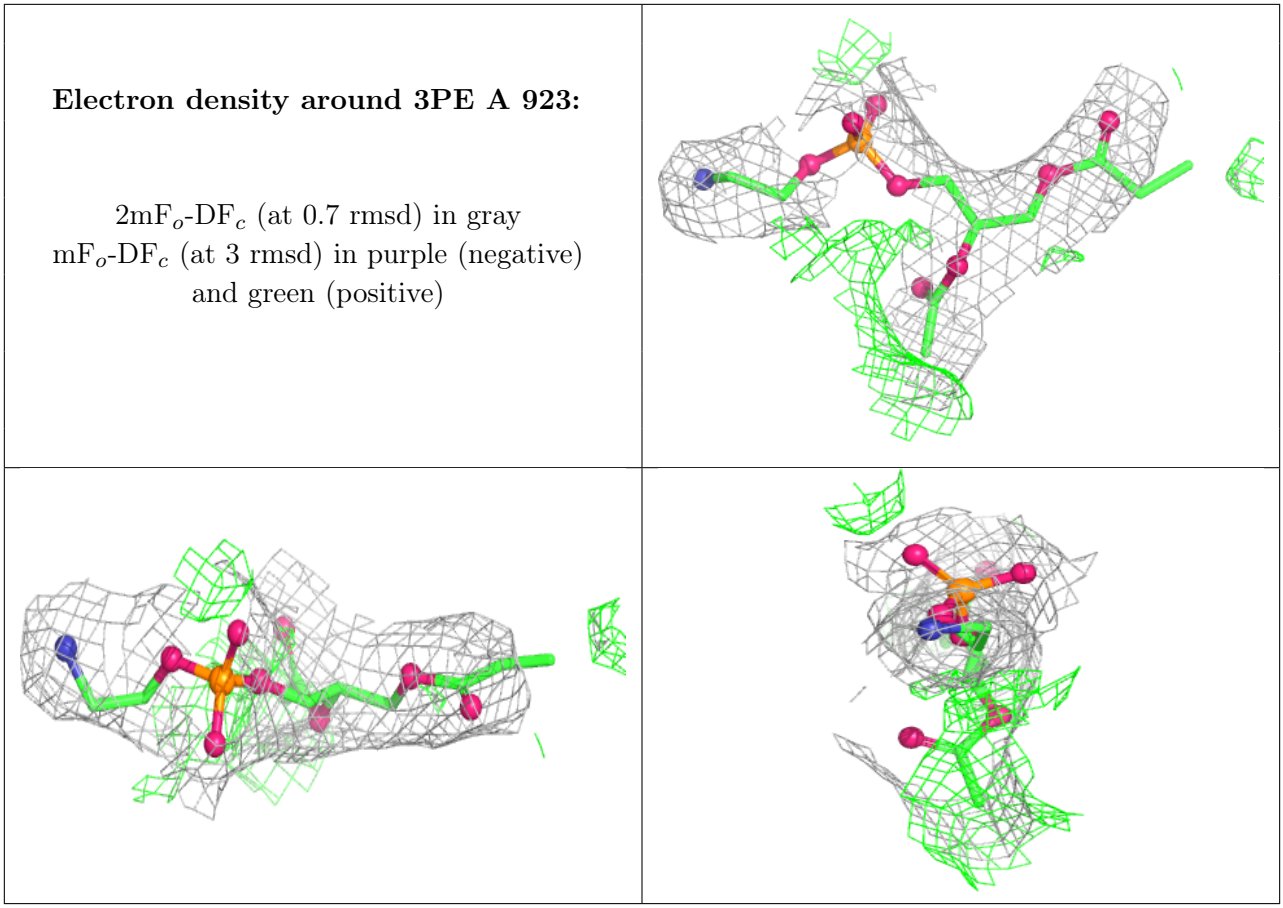






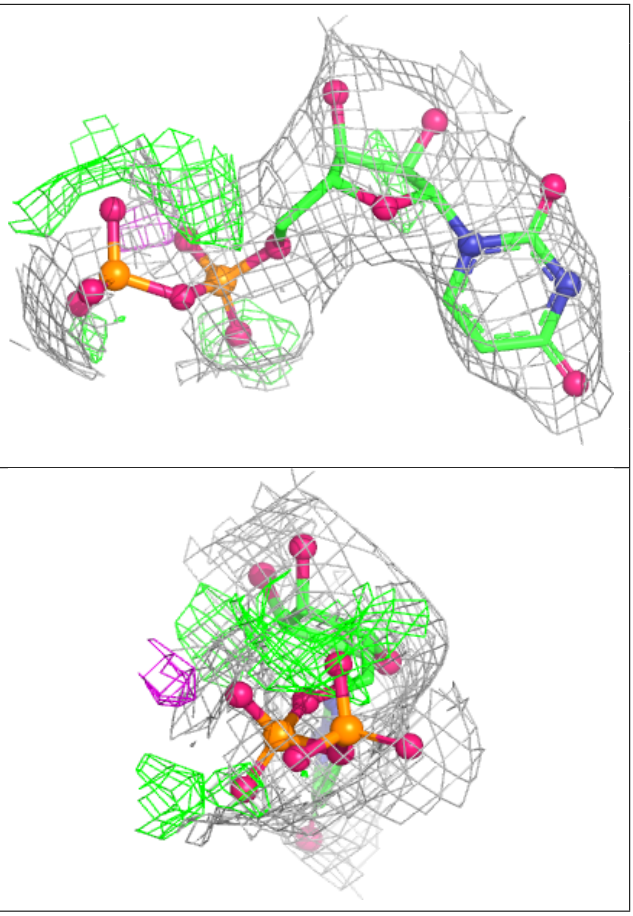
Electron density around 3PE A 923:

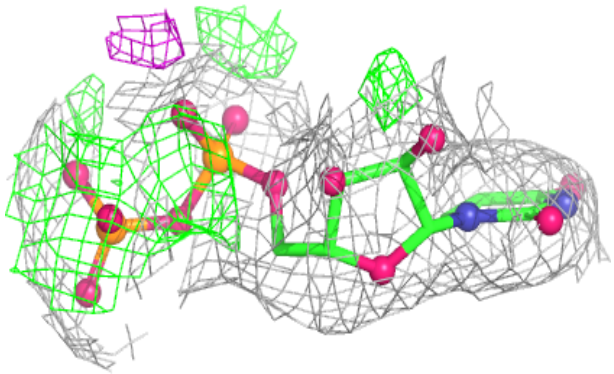
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around UDP A 918:

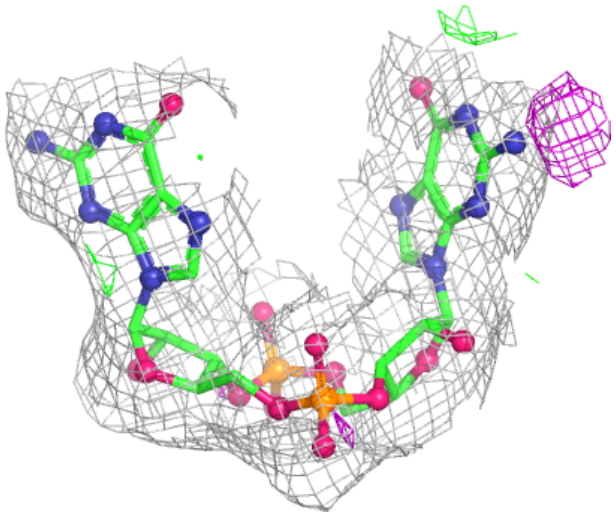
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

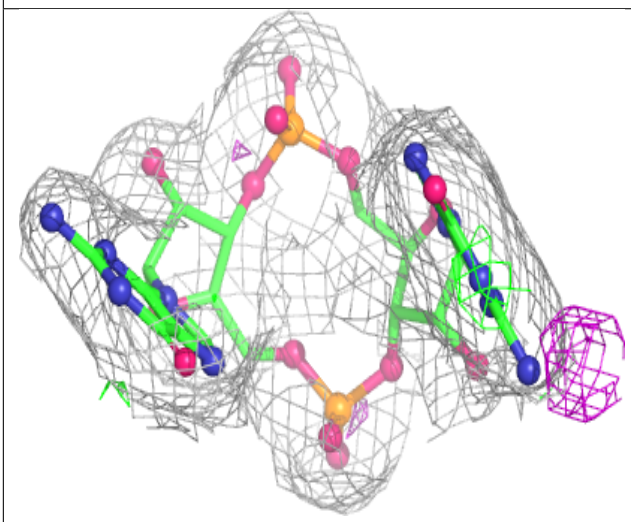


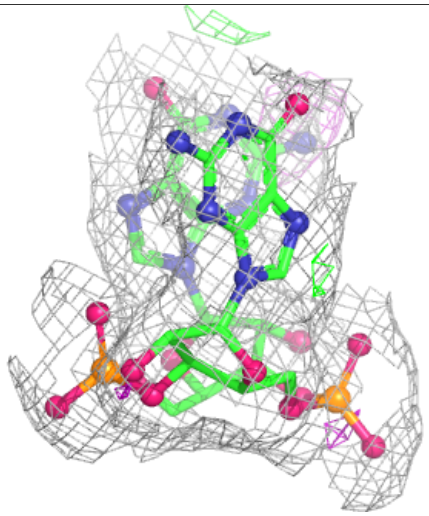


Electron density around C2E A 920:

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







Electron density around C2E A 919:

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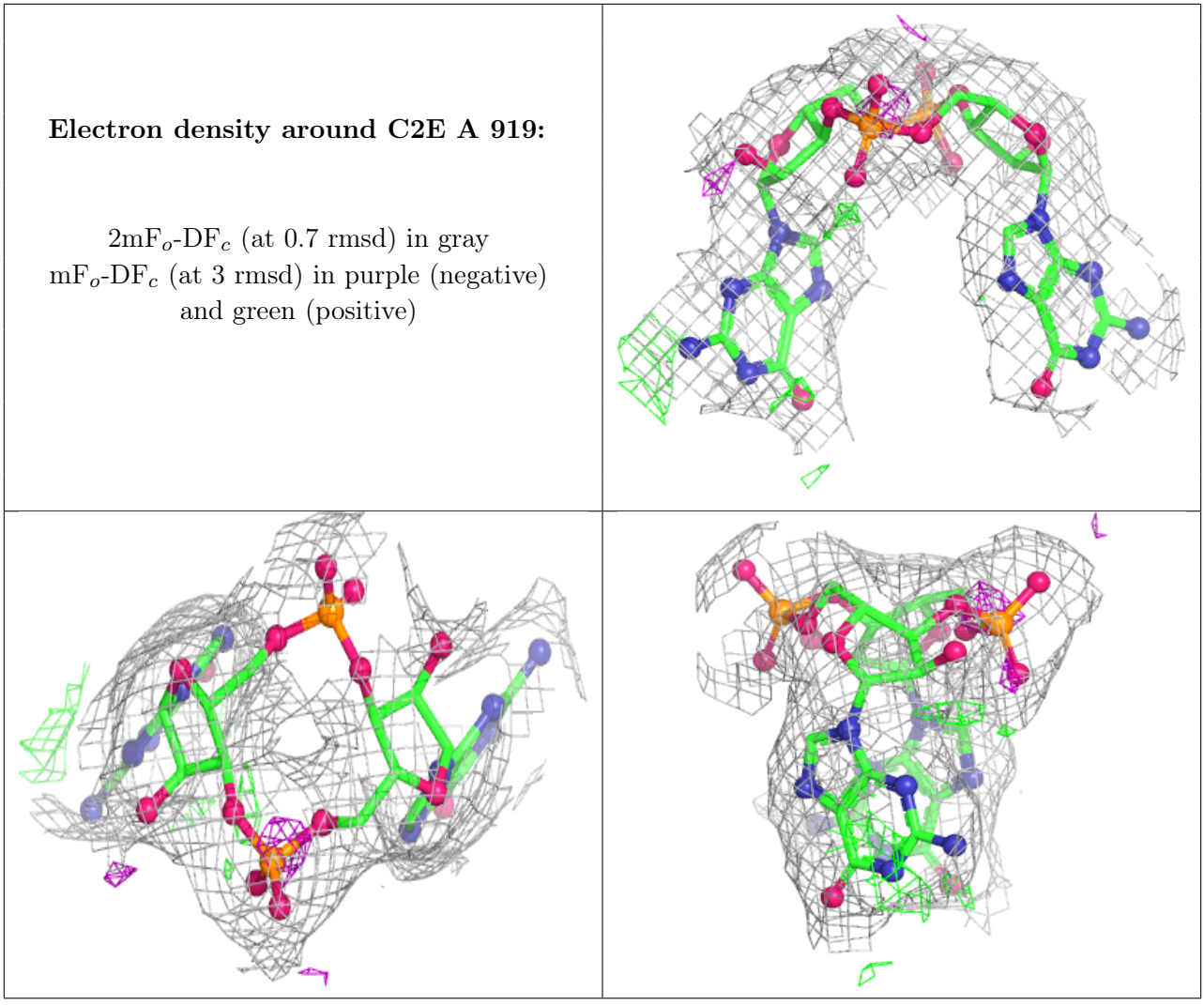
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.