



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:09 PM BST

PDB ID : 5EJZ  
Title : Bacterial Cellulose Synthase Product-Bound State  
Authors : Morgan, J.L.W.; Zimmer, J.  
Deposited on : 2015-11-02  
Resolution : 2.94 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1  
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) : 2.13.1

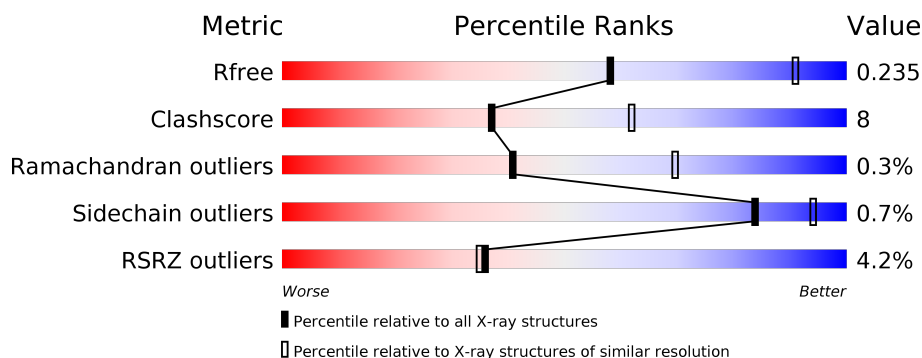
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	803	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>9%</div> </div> </div>
2	B	724	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>10%</div> </div> </div>
3	D	9	<div> <div></div> <div>100%</div> </div>
4	C	18	<div> <div></div> <div>50%</div> <div>50%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SHG	C	18	-	-	-	X
7	MG	A	922	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11078 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
1	A	728	Total	C	N	O	S	0	1	0
			5739	3725	1000	982	32			

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

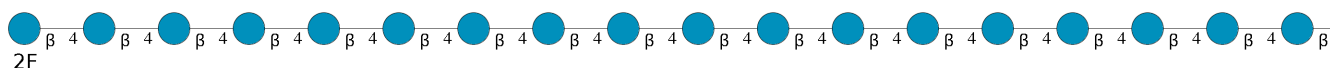
- Molecule 2 is a protein called Putative cellulose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	655	Total	C	N	O	S	0	0	0
			4887	3100	864	907	16			

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

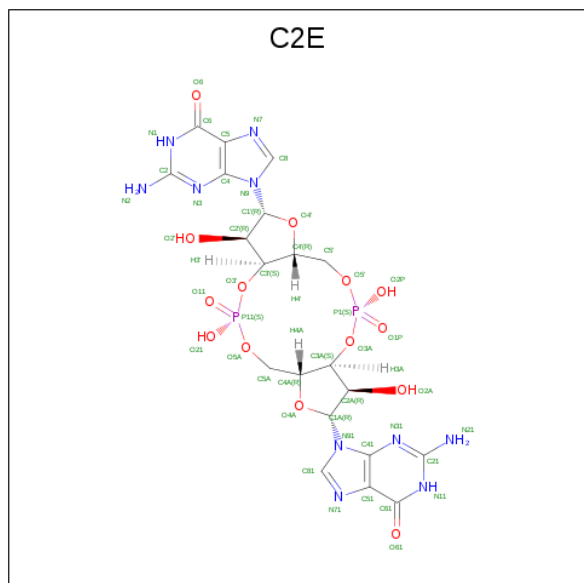
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	9	Total	C	N	O	0	0	0
			45	27	9	9			

- [illegible]



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	18	Total	C	F	O	0	0	0
			199	108	1	90			

- Molecule 5 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydro-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclodecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>14</sub>P<sub>2</sub>).



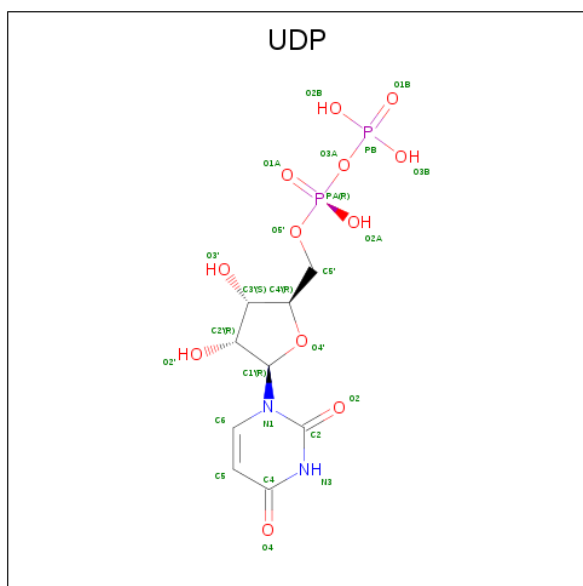
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

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

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).

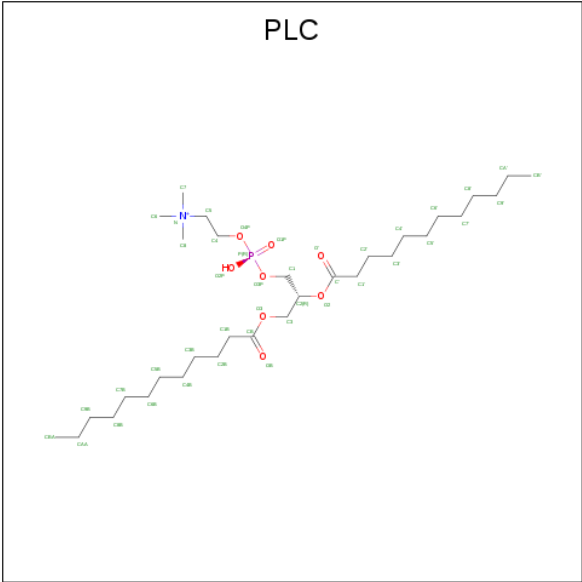


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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

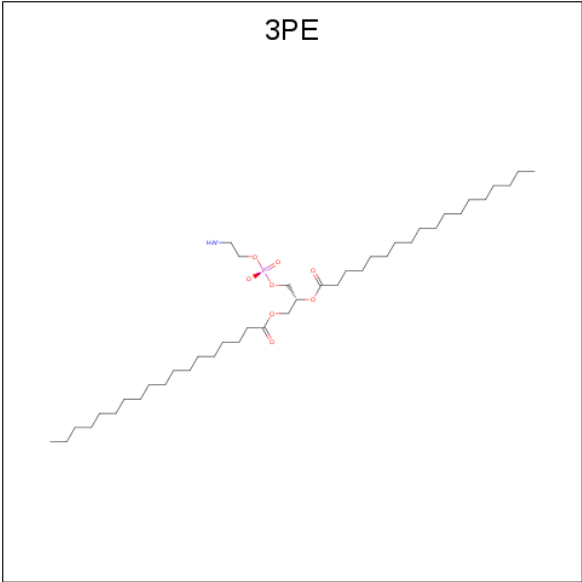
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		

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



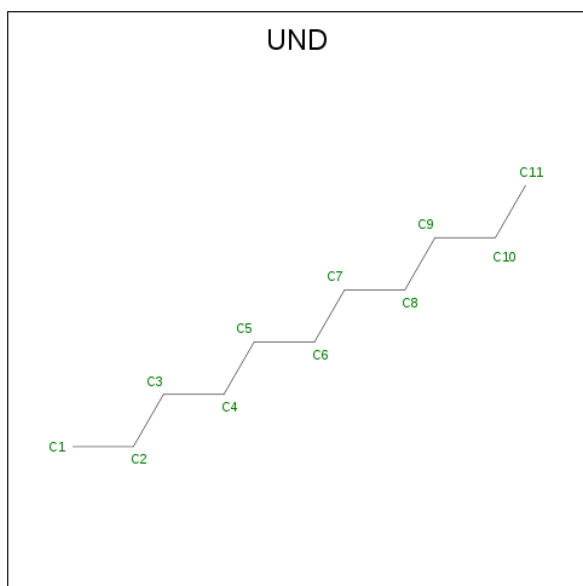
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			38	28	1	8	1		
8	B	1	Total	C				0	0
			9	9					
8	B	1	Total	C				0	0
			11	11					

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



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

- Molecule 10 is UNDECANE (three-letter code: UND) (formula:  $C_{11}H_{24}$ ).



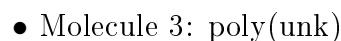
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	C	0	0
			11	11		





- Molecule 1: Putative cellulose synthase





There are no outlier residues recorded for this chain.

- [illegible]

BGC1
BGC2
BGC3
BGC4
BGC5
BGC6
BGC7
BGC8
BGC9
BGC10
BGC11
BGC12
BGC13
BGC14
BGC15
BGC16
BGC17
SHG18

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.27Å 216.84Å 221.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.35 – 2.94 38.70 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.35-2.94) 98.5 (38.70-2.94)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.206 , 0.233 0.210 , 0.235	Depositor DCC
$R_{free}$ test set	3431 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.0	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, BGC, C2E, UDP, PLC, SHG, UND, 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	0.23	0/5888	0.40	0/8007
2	B	0.24	0/5006	0.43	0/6865
All	All	0.23	0/10894	0.41	0/14872

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	89	0
2	B	4887	0	4966	85	0
3	D	45	0	13	0	0
4	C	199	0	163	14	0
5	A	92	0	44	1	0
6	A	25	0	11	4	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	38	0	53	2	0
8	B	20	0	38	1	0
9	A	20	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	11	0	24	2	0
All	All	11078	0	11181	174	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.

All (174) 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)
2:B:77:GLN:NE2	2:B:168:GLU:CB	2.16	1.09
1:A:173:ARG:O	1:A:173:ARG:HD2	1.57	1.05
2:B:77:GLN:HG3	2:B:168:GLU:OE1	1.58	1.03
2:B:77:GLN:NE2	2:B:168:GLU:HB3	1.71	1.02
2:B:77:GLN:CD	2:B:168:GLU:HB3	1.82	1.00
1:A:340:ILE:CD1	1:A:501:ALA:HB3	1.92	0.99
1:A:340:ILE:HD13	1:A:501:ALA:HB1	1.46	0.97
1:A:340:ILE:CD1	1:A:501:ALA:CB	2.45	0.94
1:A:480:GLU:OE2	4:C:14:BGC:O6	1.86	0.92
2:B:352:ALA:HB3	2:B:354:GLN:HE22	1.36	0.90
2:B:77:GLN:NE2	2:B:168:GLU:HB2	1.85	0.89
1:A:340:ILE:HD13	1:A:501:ALA:CB	2.04	0.87
2:B:352:ALA:HB3	2:B:354:GLN:NE2	1.90	0.86
2:B:77:GLN:HE22	2:B:335:TYR:HB3	1.41	0.85
1:A:340:ILE:HD11	1:A:501:ALA:HB3	1.59	0.82
2:B:78:GLN:HG3	2:B:336:PHE:CD1	2.15	0.80
2:B:516:GLU:OE2	2:B:598:GLY:HA3	1.81	0.80
1:A:616:ARG:NH2	5:A:919:C2E:O61	2.15	0.80
2:B:516:GLU:CG	2:B:600:LEU:HB3	2.12	0.80
2:B:77:GLN:NE2	2:B:335:TYR:HB3	1.98	0.79
1:A:548:ASP:OD1	4:C:7:BGC:O6	2.01	0.79
2:B:77:GLN:NE2	2:B:168:GLU:OE1	2.18	0.76
2:B:77:GLN:CG	2:B:168:GLU:OE1	2.33	0.76
2:B:354:GLN:OE1	2:B:354:GLN:N	2.18	0.75
1:A:371:GLU:OE2	1:A:578:GLN:NE2	2.20	0.74
1:A:243:VAL:HG22	1:A:323:VAL:HG22	1.70	0.73
1:A:66:ARG:NH1	1:A:123:ALA:O	2.25	0.70
2:B:336:PHE:HB3	2:B:419:SER:OG	1.92	0.70
1:A:340:ILE:HG22	1:A:340:ILE:O	1.90	0.69
1:A:382:ARG:NH1	1:A:504:ALA:O	2.24	0.69
2:B:516:GLU:HG3	2:B:600:LEU:HB3	1.74	0.69
1:A:508:LYS:NZ	6:A:921:UDP:O2A	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:GLU:HG2	2:B:600:LEU:CB	2.25	0.67
2:B:77:GLN:O	2:B:78:GLN:HB3	1.95	0.67
1:A:399:ARG:O	1:A:407:ARG:NH1	2.27	0.67
2:B:352:ALA:HB3	2:B:354:GLN:OE1	1.95	0.67
2:B:77:GLN:HE22	2:B:168:GLU:HB2	1.56	0.67
2:B:251:THR:HG22	2:B:252:GLY:N	2.11	0.66
1:A:343:ASP:OD1	1:A:344:ALA:N	2.28	0.66
1:A:173:ARG:C	1:A:173:ARG:HD2	2.15	0.65
2:B:583:GLN:HA	2:B:586:ILE:HG12	1.79	0.65
2:B:482:THR:HG22	2:B:502:VAL:HB	1.78	0.65
1:A:108:GLU:OE2	4:C:12:BGC:O2	2.12	0.64
2:B:352:ALA:HB3	2:B:354:GLN:CD	2.16	0.64
1:A:186:ARG:HG2	1:A:194:LEU:HD21	1.79	0.64
2:B:387:PRO:HG3	4:C:5:BGC:O6	1.98	0.64
2:B:516:GLU:HG3	2:B:516:GLU:O	1.98	0.64
1:A:382:ARG:NH2	6:A:921:UDP:O2B	2.31	0.63
2:B:516:GLU:HG2	2:B:600:LEU:HB3	1.78	0.63
1:A:372:THR:HG22	1:A:512:LEU:HD21	1.79	0.63
1:A:369:GLN:HG3	1:A:370:PRO:HD2	1.81	0.62
2:B:245:LYS:HB3	2:B:246:PRO:HD2	1.82	0.62
1:A:340:ILE:HD11	1:A:501:ALA:CB	2.20	0.62
2:B:390:ARG:HH22	4:C:5:BGC:C6	2.13	0.62
2:B:390:ARG:HH22	4:C:5:BGC:H6C1	1.64	0.62
1:A:345:GLU:HA	1:A:390:MET:HE2	1.83	0.60
2:B:235:PRO:O	2:B:236:ASP:HB2	2.00	0.60
1:A:351:HIS:HD1	1:A:410:TYR:HH	1.48	0.60
1:A:382:ARG:HH22	1:A:506:THR:HG1	1.48	0.59
1:A:259:THR:HG21	1:A:323:VAL:HG21	1.84	0.59
2:B:78:GLN:HG3	2:B:336:PHE:HD1	1.63	0.59
2:B:100:GLN:HE21	2:B:136:VAL:HG23	1.68	0.59
2:B:148:ASP:HB3	2:B:305:LEU:HG	1.85	0.58
2:B:244:SER:OG	2:B:248:SER:HB3	2.03	0.58
1:A:340:ILE:CG2	1:A:340:ILE:O	2.52	0.58
1:A:343:ASP:OD2	4:C:17:BGC:H4	2.03	0.58
2:B:185:PRO:HG2	2:B:188:ALA:HB2	1.84	0.58
2:B:360:ILE:HA	2:B:444:THR:HG23	1.86	0.57
1:A:439:GLU:HB2	4:C:8:BGC:H6C2	1.87	0.56
1:A:394:LYS:O	1:A:399:ARG:NH1	2.38	0.56
2:B:244:SER:OG	2:B:248:SER:CB	2.53	0.56
1:A:512:LEU:HD12	1:A:578:GLN:HB3	1.87	0.56
2:B:106:ILE:HG22	2:B:171:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD22	1:A:583:PRO:HG2	1.88	0.55
1:A:35:ALA:O	1:A:79:ARG:NH2	2.40	0.55
1:A:179:ASP:OD1	1:A:201:ARG:NH1	2.40	0.55
1:A:184:ASP:HB3	1:A:202:ARG:HH12	1.72	0.55
1:A:132:ARG:HG3	1:A:265:GLU:CD	2.27	0.55
1:A:311:ARG:HH22	2:B:719:THR:HG23	1.71	0.54
2:B:77:GLN:HG3	2:B:333:ASN:HB3	1.90	0.54
1:A:482:ALA:HB2	1:A:569:ALA:HB1	1.90	0.53
1:A:135:GLN:HG3	1:A:136:PRO:HD2	1.90	0.53
1:A:340:ILE:HG23	1:A:503:PHE:HD1	1.74	0.53
1:A:218:THR:OG1	1:A:219:ARG:N	2.42	0.53
2:B:352:ALA:CB	2:B:354:GLN:HE22	2.16	0.51
1:A:419:PHE:HA	1:A:422:VAL:HG22	1.92	0.51
2:B:245:LYS:HB3	2:B:246:PRO:CD	2.39	0.51
1:A:497:ARG:HD2	1:A:500:SER:HB3	1.91	0.51
1:A:154:ASP:N	1:A:154:ASP:OD1	2.43	0.51
1:A:345:GLU:HA	1:A:390:MET:CE	2.40	0.51
1:A:300:MET:HA	1:A:470:GLN:HB3	1.92	0.51
2:B:587:GLN:O	2:B:591:ARG:HB2	2.10	0.51
1:A:362:ARG:HH12	1:A:697:ARG:HD2	1.75	0.50
1:A:176:VAL:HG22	1:A:215:VAL:HB	1.93	0.50
2:B:320:THR:HA	2:B:445:ASP:HA	1.94	0.50
2:B:264:ASP:OD1	2:B:267:ARG:NH2	2.45	0.50
2:B:302:THR:O	2:B:304:THR:HG23	2.12	0.49
2:B:678:SER:O	2:B:682:VAL:HG23	2.12	0.49
2:B:77:GLN:OE1	2:B:168:GLU:O	2.30	0.49
2:B:77:GLN:N	2:B:77:GLN:OE1	2.45	0.49
1:A:436:PHE:HA	8:A:923:PLC:H1'2	1.95	0.49
1:A:161:ALA:HB1	1:A:683:GLU:HG2	1.93	0.49
2:B:189:ILE:O	2:B:272:ARG:NH1	2.45	0.49
1:A:173:ARG:C	1:A:173:ARG:CD	2.80	0.48
2:B:224:ARG:HD3	2:B:469:ALA:HA	1.95	0.48
2:B:575:GLN:HE21	10:B:802:UND:H21	1.78	0.48
2:B:514:ASN:O	2:B:515:GLU:HG3	2.14	0.48
2:B:238:ALA:HB2	2:B:488:ALA:HB2	1.94	0.48
2:B:516:GLU:HG2	2:B:600:LEU:HB2	1.94	0.48
1:A:512:LEU:O	1:A:578:GLN:O	2.31	0.48
2:B:140:LEU:HB3	2:B:144:VAL:HB	1.96	0.47
10:B:802:UND:H42	8:B:803:PLC:H4'2	1.95	0.47
1:A:362:ARG:NH1	1:A:697:ARG:HD2	2.29	0.47
1:A:419:PHE:CD2	1:A:420:PRO:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:GLU:OE2	2:B:224:ARG:NH2	2.48	0.47
2:B:251:THR:CG2	2:B:252:GLY:N	2.78	0.47
2:B:353:SER:O	2:B:355:LYS:HD2	2.13	0.47
1:A:270:PHE:HB3	1:A:355:TRP:HB3	1.96	0.47
1:A:274:THR:OG1	1:A:321:ALA:O	2.23	0.46
1:A:389:GLN:NE2	1:A:498:PRO:O	2.49	0.46
1:A:37:VAL:HG13	1:A:41:ALA:HB3	1.98	0.46
1:A:387:MET:HG3	1:A:417:TRP:CD1	2.50	0.46
1:A:464:ASN:O	1:A:468:ALA:HB2	2.16	0.46
2:B:377:LYS:HB2	2:B:416:SER:HB2	1.98	0.46
1:A:18:LEU:HD22	2:B:711:ILE:HG23	1.97	0.46
1:A:397:LEU:HD21	1:A:411:LEU:HD13	1.96	0.46
2:B:358:ILE:HG13	2:B:403:PHE:HE2	1.80	0.46
1:A:147:PRO:HA	1:A:178:CYS:HB2	1.98	0.46
1:A:452:MET:HE2	4:C:11:BGC:O6	2.15	0.45
2:B:466:VAL:HG13	2:B:470:SER:OG	2.17	0.45
2:B:617:GLU:HG3	2:B:620:LYS:HB2	1.98	0.45
1:A:390:MET:HE3	1:A:390:MET:HB2	1.61	0.45
2:B:105:ASP:HA	2:B:160:ARG:HE	1.81	0.45
4:C:10:BGC:O3	4:C:11:BGC:O5	2.25	0.45
2:B:251:THR:HG22	2:B:252:GLY:H	1.82	0.45
2:B:456:MET:O	2:B:458:ASP:N	2.49	0.45
1:A:42:GLN:OE1	1:A:79:ARG:NH1	2.51	0.44
2:B:76:GLY:N	2:B:171:LEU:O	2.40	0.44
2:B:505:LEU:HD21	2:B:527:LEU:HD12	2.00	0.44
1:A:452:MET:HE2	1:A:558:TRP:HE1	1.83	0.43
1:A:452:MET:CE	4:C:11:BGC:O6	2.67	0.43
2:B:612:MET:HG2	2:B:654:VAL:HG22	2.01	0.43
1:A:274:THR:HG22	1:A:360:ILE:HG23	1.99	0.43
1:A:345:GLU:HB2	1:A:390:MET:CE	2.49	0.43
2:B:55:TRP:CE3	2:B:189:ILE:HG13	2.54	0.43
2:B:334:ARG:HD3	2:B:334:ARG:HA	1.84	0.43
1:A:276:HIS:HE1	1:A:318:CYS:HB3	1.84	0.42
1:A:513:SER:O	1:A:577:GLN:HG3	2.18	0.42
2:B:387:PRO:HB3	4:C:5:BGC:H6	1.85	0.42
2:B:307:PRO:HA	2:B:308:PRO:HD3	1.85	0.42
1:A:189:SER:HA	1:A:190:PRO:HD3	1.92	0.42
2:B:266:ASP:OD1	2:B:285:PRO:HD3	2.20	0.42
1:A:91:PRO:HA	1:A:92:PRO:HD3	1.90	0.41
1:A:312:TRP:HB3	1:A:405:ALA:HB1	2.02	0.41
2:B:77:GLN:CD	2:B:168:GLU:OE1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:ALA:HB2	2:B:576:THR:HG23	2.01	0.41
2:B:234:LEU:HB3	2:B:237:GLU:HB2	2.01	0.41
1:A:144:ILE:HG21	1:A:163:ALA:HB1	2.03	0.41
1:A:248:ASP:HB2	1:A:368:LEU:HG	2.02	0.41
1:A:148:SER:HA	6:A:921:UDP:O2'	2.20	0.41
1:A:447:GLU:OE2	2:B:355:LYS:NZ	2.53	0.41
2:B:368:LEU:HA	2:B:369:PRO:HD3	1.84	0.41
2:B:448:VAL:HA	2:B:449:PRO:HD3	1.89	0.41
1:A:186:ARG:HG2	1:A:194:LEU:CD2	2.50	0.41
2:B:466:VAL:HG22	2:B:498:VAL:CG1	2.50	0.41
1:A:547:GLY:O	4:C:7:BGC:O6	2.38	0.41
1:A:366:ALA:HB3	1:A:690:PHE:HD1	1.85	0.41
1:A:151:GLU:OE2	6:A:921:UDP:O2'	2.32	0.41
1:A:420:PRO:O	1:A:424:MET:HG2	2.21	0.41
1:A:497:ARG:HD2	1:A:500:SER:CB	2.50	0.41
8:A:923:PLC:H71	4:C:6:BGC:O3	2.21	0.41
1:A:17:LEU:HD23	1:A:20:LEU:HD12	2.02	0.40
1:A:89:LEU:HA	1:A:90:PRO:HD2	1.91	0.40
2:B:78:GLN:CG	2:B:78:GLN:O	2.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	727/803 (90%)	701 (96%)	24 (3%)	2 (0%)	41 69
2	B	651/724 (90%)	624 (96%)	25 (4%)	2 (0%)	41 69
All	All	1378/1527 (90%)	1325 (96%)	49 (4%)	4 (0%)	41 69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	498	PRO
2	B	457	ALA
1	A	401	GLY
2	B	493	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	599/661 (91%)	594 (99%)	5 (1%)	81	93
2	B	520/572 (91%)	517 (99%)	3 (1%)	86	95
All	All	1119/1233 (91%)	1111 (99%)	8 (1%)	84	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	77	VAL
1	A	325	ARG
1	A	512	LEU
1	A	578	GLN
2	B	326	VAL
2	B	669	LEU
2	B	693	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
2	B	77	GLN
2	B	100	GLN
2	B	514	ASN
2	B	575	GLN

### 5.3.3 RNA ⓘ

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 ⓘ

18 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	1.22	1 (8%)	17,17,17	1.49	4 (23%)
4	BGC	C	10	4	11,11,12	1.65	3 (27%)	15,15,17	1.65	1 (6%)
4	BGC	C	11	4	11,11,12	1.64	2 (18%)	15,15,17	1.10	1 (6%)
4	BGC	C	12	4	11,11,12	1.71	3 (27%)	15,15,17	0.78	0
4	BGC	C	13	4	11,11,12	1.57	2 (18%)	15,15,17	1.09	1 (6%)
4	BGC	C	14	4	11,11,12	1.67	2 (18%)	15,15,17	1.69	3 (20%)
4	BGC	C	15	4	11,11,12	1.61	2 (18%)	15,15,17	1.54	4 (26%)
4	BGC	C	16	4	11,11,12	1.54	1 (9%)	15,15,17	2.20	4 (26%)
4	BGC	C	17	4	11,11,12	1.76	3 (27%)	15,15,17	0.88	0
4	SHG	C	18	4	11,11,12	1.67	1 (9%)	10,15,17	0.63	0
4	BGC	C	2	4	11,11,12	1.77	3 (27%)	15,15,17	1.56	4 (26%)
4	BGC	C	3	4	11,11,12	1.69	2 (18%)	15,15,17	2.02	3 (20%)
4	BGC	C	4	4	11,11,12	1.70	3 (27%)	15,15,17	2.15	5 (33%)
4	BGC	C	5	4	11,11,12	1.60	2 (18%)	15,15,17	1.91	4 (26%)
4	BGC	C	6	4	11,11,12	2.12	3 (27%)	15,15,17	1.00	1 (6%)
4	BGC	C	7	4	11,11,12	1.73	3 (27%)	15,15,17	0.97	0
4	BGC	C	8	4	11,11,12	1.68	3 (27%)	15,15,17	1.70	4 (26%)
4	BGC	C	9	4	11,11,12	1.71	3 (27%)	15,15,17	1.28	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	-	2/2/19/22	0/1/1/1
4	BGC	C	12	4	-	0/2/19/22	0/1/1/1
4	BGC	C	13	4	-	2/2/19/22	0/1/1/1
4	BGC	C	14	4	-	2/2/19/22	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	BGC	C	17	4	-	2/2/19/22	0/1/1/1
4	SHG	C	18	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	-	1/2/19/22	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	6	BGC	O5-C1	5.54	1.52	1.43
4	C	14	BGC	O5-C1	4.40	1.50	1.43
4	C	9	BGC	O5-C1	4.40	1.50	1.43
4	C	4	BGC	O5-C1	4.39	1.50	1.43
4	C	18	SHG	O5-C1	4.37	1.50	1.43
4	C	12	BGC	O5-C1	4.35	1.50	1.43
4	C	3	BGC	O5-C1	4.34	1.50	1.43
4	C	7	BGC	O5-C1	4.29	1.50	1.43
4	C	17	BGC	O5-C1	4.28	1.50	1.43
4	C	2	BGC	O5-C1	4.27	1.50	1.43
4	C	8	BGC	O5-C1	4.23	1.50	1.43
4	C	11	BGC	O5-C1	4.11	1.50	1.43
4	C	10	BGC	O5-C1	4.06	1.50	1.43
4	C	16	BGC	O5-C1	4.02	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	15	BGC	O5-C1	3.99	1.50	1.43
4	C	5	BGC	O5-C1	3.93	1.50	1.43
4	C	13	BGC	O5-C1	3.76	1.49	1.43
4	C	1	BGC	O5-C1	3.10	1.50	1.42
4	C	6	BGC	C2-C3	-2.88	1.48	1.52
4	C	17	BGC	C2-C3	-2.87	1.48	1.52
4	C	2	BGC	C2-C3	-2.71	1.48	1.52
4	C	6	BGC	O5-C5	2.59	1.48	1.43
4	C	13	BGC	C2-C3	-2.53	1.48	1.52
4	C	10	BGC	C2-C3	-2.49	1.48	1.52
4	C	15	BGC	C2-C3	-2.47	1.48	1.52
4	C	7	BGC	C2-C3	-2.45	1.48	1.52
4	C	12	BGC	C2-C3	-2.40	1.49	1.52
4	C	11	BGC	C2-C3	-2.40	1.49	1.52
4	C	9	BGC	C2-C3	-2.38	1.49	1.52
4	C	3	BGC	C2-C3	-2.36	1.49	1.52
4	C	5	BGC	O2-C2	2.29	1.48	1.43
4	C	7	BGC	O5-C5	2.27	1.48	1.43
4	C	8	BGC	C2-C3	-2.26	1.49	1.52
4	C	2	BGC	O5-C5	2.24	1.48	1.43
4	C	14	BGC	C2-C3	-2.22	1.49	1.52
4	C	4	BGC	C2-C3	-2.14	1.49	1.52
4	C	8	BGC	O5-C5	2.13	1.47	1.43
4	C	17	BGC	O5-C5	2.12	1.47	1.43
4	C	12	BGC	O5-C5	2.08	1.47	1.43
4	C	4	BGC	O5-C5	2.02	1.47	1.43
4	C	9	BGC	O5-C5	2.01	1.47	1.43
4	C	10	BGC	O5-C5	2.01	1.47	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	16	BGC	C1-C2-C3	5.96	116.99	109.67
4	C	4	BGC	C1-C2-C3	5.55	116.49	109.67
4	C	3	BGC	C1-C2-C3	4.85	115.63	109.67
4	C	10	BGC	C1-C2-C3	4.84	115.62	109.67
4	C	14	BGC	C1-C2-C3	4.63	115.35	109.67
4	C	5	BGC	C1-C2-C3	4.21	114.84	109.67
4	C	5	BGC	C2-C3-C4	4.15	118.07	110.89
4	C	4	BGC	C2-C3-C4	3.90	117.65	110.89
4	C	3	BGC	C2-C3-C4	3.71	117.31	110.89
4	C	16	BGC	C2-C3-C4	3.41	116.80	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	BGC	C3-C4-C5	3.29	116.11	110.24
4	C	1	BGC	O5-C5-C4	3.19	115.49	109.69
4	C	2	BGC	C3-C4-C5	3.03	115.64	110.24
4	C	8	BGC	C1-C2-C3	2.98	113.33	109.67
4	C	3	BGC	C3-C4-C5	2.93	115.47	110.24
4	C	8	BGC	C3-C4-C5	2.88	115.37	110.24
4	C	8	BGC	C2-C3-C4	2.86	115.84	110.89
4	C	9	BGC	C1-C2-C3	2.78	113.08	109.67
4	C	15	BGC	C3-C4-C5	2.64	114.95	110.24
4	C	5	BGC	C1-O5-C5	-2.57	108.71	112.19
4	C	5	BGC	O4-C4-C5	-2.53	103.01	109.30
4	C	2	BGC	C2-C3-C4	2.53	115.27	110.89
4	C	15	BGC	C2-C3-C4	2.42	115.09	110.89
4	C	4	BGC	C6-C5-C4	-2.42	107.33	113.00
4	C	14	BGC	O5-C1-C2	2.40	114.47	110.77
4	C	6	BGC	C1-C2-C3	2.38	112.60	109.67
4	C	15	BGC	C1-C2-C3	2.34	112.54	109.67
4	C	1	BGC	C4-C3-C2	2.28	114.80	110.82
4	C	15	BGC	C1-O5-C5	-2.27	109.12	112.19
4	C	4	BGC	C3-C4-C5	2.22	114.21	110.24
4	C	16	BGC	C1-O5-C5	-2.13	109.30	112.19
4	C	11	BGC	C3-C4-C5	2.12	114.02	110.24
4	C	1	BGC	C6-C5-C4	-2.11	108.07	113.00
4	C	2	BGC	C6-C5-C4	-2.10	108.08	113.00
4	C	16	BGC	C3-C4-C5	2.08	113.96	110.24
4	C	8	BGC	C1-O5-C5	-2.03	109.44	112.19
4	C	14	BGC	C2-C3-C4	2.03	114.41	110.89
4	C	2	BGC	C1-C2-C3	2.02	112.15	109.67
4	C	4	BGC	O3-C3-C4	-2.01	105.69	110.35
4	C	13	BGC	C6-C5-C4	-2.00	108.31	113.00

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	7	BGC	O5-C5-C6-O6
4	C	18	SHG	C4-C5-C6-O6
4	C	17	BGC	O5-C5-C6-O6
4	C	16	BGC	O5-C5-C6-O6
4	C	2	BGC	O5-C5-C6-O6
4	C	14	BGC	O5-C5-C6-O6
4	C	1	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	7	BGC	C4-C5-C6-O6
4	C	4	BGC	O5-C5-C6-O6
4	C	16	BGC	C4-C5-C6-O6
4	C	8	BGC	O5-C5-C6-O6
4	C	18	SHG	O5-C5-C6-O6
4	C	14	BGC	C4-C5-C6-O6
4	C	11	BGC	O5-C5-C6-O6
4	C	17	BGC	C4-C5-C6-O6
4	C	8	BGC	C4-C5-C6-O6
4	C	11	BGC	C4-C5-C6-O6
4	C	4	BGC	C4-C5-C6-O6
4	C	2	BGC	C4-C5-C6-O6
4	C	13	BGC	C4-C5-C6-O6
4	C	9	BGC	O5-C5-C6-O6
4	C	13	BGC	O5-C5-C6-O6
4	C	10	BGC	O5-C5-C6-O6
4	C	6	BGC	O5-C5-C6-O6
4	C	3	BGC	O5-C5-C6-O6
4	C	15	BGC	C4-C5-C6-O6
4	C	1	BGC	C4-C5-C6-O6
4	C	15	BGC	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	10	BGC	1	0
4	C	17	BGC	1	0
4	C	6	BGC	1	0
4	C	14	BGC	1	0
4	C	11	BGC	3	0
4	C	12	BGC	1	0
4	C	7	BGC	2	0
4	C	8	BGC	1	0
4	C	5	BGC	4	0

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
9	3PE	A	924	-	19,19,50	1.36	4 (21%)	22,24,55	1.49	2 (9%)
8	PLC	B	804	-	10,10,41	0.30	0	9,9,49	0.80	0
5	C2E	A	920	-	44,52,52	1.23	4 (9%)	54,82,82	1.84	13 (24%)
8	PLC	A	923	-	37,37,41	1.11	4 (10%)	43,45,49	1.08	2 (4%)
10	UND	B	802	-	10,10,10	0.26	0	9,9,9	0.54	0
5	C2E	A	919	-	44,52,52	1.23	4 (9%)	54,82,82	1.89	13 (24%)
8	PLC	B	803	-	8,8,41	0.30	0	7,7,49	0.77	0
6	UDP	A	921	7	20,26,26	1.22	1 (5%)	25,40,40	1.15	2 (8%)

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
9	3PE	A	924	-	-	5/22/22/54	-
8	PLC	B	804	-	-	6/8/8/45	-
5	C2E	A	920	-	-	0/22/62/62	0/6/7/7
8	PLC	A	923	-	-	25/41/41/45	-
10	UND	B	802	-	-	1/8/8/8	-
5	C2E	A	919	-	-	2/22/62/62	0/6/7/7
8	PLC	B	803	-	-	0/6/6/45	-
6	UDP	A	921	7	-	3/14/32/32	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	919	C2E	C6-C5	4.32	1.48	1.41
5	A	919	C2E	C61-C51	4.21	1.48	1.41
5	A	920	C2E	C6-C5	4.20	1.48	1.41
5	A	920	C2E	C61-C51	4.14	1.48	1.41
6	A	921	UDP	C4-N3	3.26	1.38	1.33
9	A	924	3PE	O21-C2	-2.52	1.40	1.46
9	A	924	3PE	O31-C31	2.45	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	923	PLC	O2-C2	-2.44	1.40	1.46
5	A	919	C2E	C5-C4	2.44	1.47	1.40
5	A	920	C2E	C5-C4	2.44	1.47	1.40
8	A	923	PLC	O3-CB	2.43	1.40	1.33
5	A	920	C2E	C51-C41	2.41	1.47	1.40
9	A	924	3PE	O21-C21	2.34	1.40	1.35
5	A	919	C2E	C51-C41	2.33	1.47	1.40
8	A	923	PLC	O2-C'	2.15	1.40	1.34
9	A	924	3PE	O31-C3	-2.11	1.40	1.45
8	A	923	PLC	O3-C3	-2.08	1.40	1.45

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	919	C2E	C21-N31-C41	4.90	120.95	115.36
5	A	919	C2E	C2-N3-C4	4.87	120.92	115.36
9	A	924	3PE	O21-C21-C22	4.83	119.98	111.09
5	A	920	C2E	C21-N31-C41	4.77	120.81	115.36
5	A	920	C2E	C2-N3-C4	4.67	120.70	115.36
5	A	920	C2E	C5-C6-N1	-3.98	117.99	123.43
8	A	923	PLC	O2-C'-C1'	3.92	119.96	111.50
5	A	920	C2E	C51-C61-N11	-3.92	118.07	123.43
5	A	919	C2E	C61-C51-C41	-3.90	117.07	120.80
5	A	919	C2E	C5-C6-N1	-3.87	118.14	123.43
5	A	919	C2E	C51-C61-N11	-3.81	118.21	123.43
5	A	920	C2E	C6-N1-C2	3.80	121.96	115.93
5	A	919	C2E	C61-N11-C21	3.78	121.93	115.93
5	A	919	C2E	C6-N1-C2	3.72	121.84	115.93
5	A	920	C2E	C61-N11-C21	3.69	121.79	115.93
5	A	919	C2E	C6-C5-C4	-3.67	117.30	120.80
5	A	920	C2E	C6-C5-C4	-3.58	117.38	120.80
5	A	920	C2E	C61-C51-C41	-3.54	117.42	120.80
9	A	924	3PE	O31-C31-C32	3.36	120.19	111.38
5	A	919	C2E	N31-C21-N11	-3.17	123.00	127.22
5	A	919	C2E	N3-C2-N1	-2.99	123.24	127.22
5	A	920	C2E	C41-C51-N71	-2.96	106.32	109.40
5	A	920	C2E	N3-C2-N1	-2.92	123.32	127.22
5	A	919	C2E	C41-C51-N71	-2.92	106.36	109.40
5	A	920	C2E	N31-C21-N11	-2.89	123.36	127.22
6	A	921	UDP	PA-O3A-PB	-2.86	123.00	132.83
5	A	919	C2E	C4-C5-N7	-2.85	106.43	109.40
5	A	920	C2E	C4-C5-N7	-2.83	106.45	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	923	PLC	O3-CB-C1B	2.59	120.05	111.91
6	A	921	UDP	C3'-C2'-C1'	2.53	104.78	100.98
5	A	919	C2E	C3'-C2'-C1'	2.47	105.37	99.89
5	A	920	C2E	C3'-C2'-C1'	2.19	104.73	99.89

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	924	3PE	C1-O11-P-O14
9	A	924	3PE	O13-C11-C12-N
8	A	923	PLC	O3P-C1-C2-O2
8	A	923	PLC	O4P-C4-C5-N
8	A	923	PLC	C5-C4-O4P-P
8	A	923	PLC	C1-O3P-P-O1P
8	A	923	PLC	C4-O4P-P-O1P
6	A	921	UDP	C5'-O5'-PA-O2A
6	A	921	UDP	C5'-O5'-PA-O3A
9	A	924	3PE	O32-C31-O31-C3
9	A	924	3PE	C32-C31-O31-C3
8	A	923	PLC	O2-C2-C3-O3
8	A	923	PLC	C1-O3P-P-O4P
8	A	923	PLC	C4-O4P-P-O3P
8	A	923	PLC	C6B-C7B-C8B-C9B
8	A	923	PLC	C1'-C2'-C3'-C4'
8	A	923	PLC	CB-C1B-C2B-C3B
8	A	923	PLC	C5B-C6B-C7B-C8B
8	A	923	PLC	C7B-C8B-C9B-CAA
8	B	804	PLC	C5'-C6'-C7'-C8'
8	B	804	PLC	C7'-C8'-C9'-CA'
8	A	923	PLC	C4B-C5B-C6B-C7B
8	A	923	PLC	C1-C2-C3-O3
8	B	804	PLC	C8'-C9'-CA'-CB'
8	A	923	PLC	C8B-C9B-CAA-CBA
10	B	802	UND	C7-C8-C9-C10
8	A	923	PLC	C1'-C'-O2-C2
8	A	923	PLC	C3B-C4B-C5B-C6B
8	A	923	PLC	O'-C'-O2-C2
9	A	924	3PE	C1-O11-P-O13
6	A	921	UDP	C5'-O5'-PA-O1A
8	A	923	PLC	O3P-C1-C2-C3
8	B	804	PLC	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
8	A	923	PLC	C'-C1'-C2'-C3'
8	B	804	PLC	C2'-C3'-C4'-C5'
8	A	923	PLC	C2B-C1B-CB-O3
8	B	804	PLC	C1'-C2'-C3'-C4'
8	A	923	PLC	C1B-CB-O3-C3
8	A	923	PLC	OB-CB-O3-C3
5	A	919	C2E	O4A-C4A-C5A-O5A
8	A	923	PLC	C2B-C1B-CB-OB
5	A	919	C2E	C2'-C3'-O3'-P11

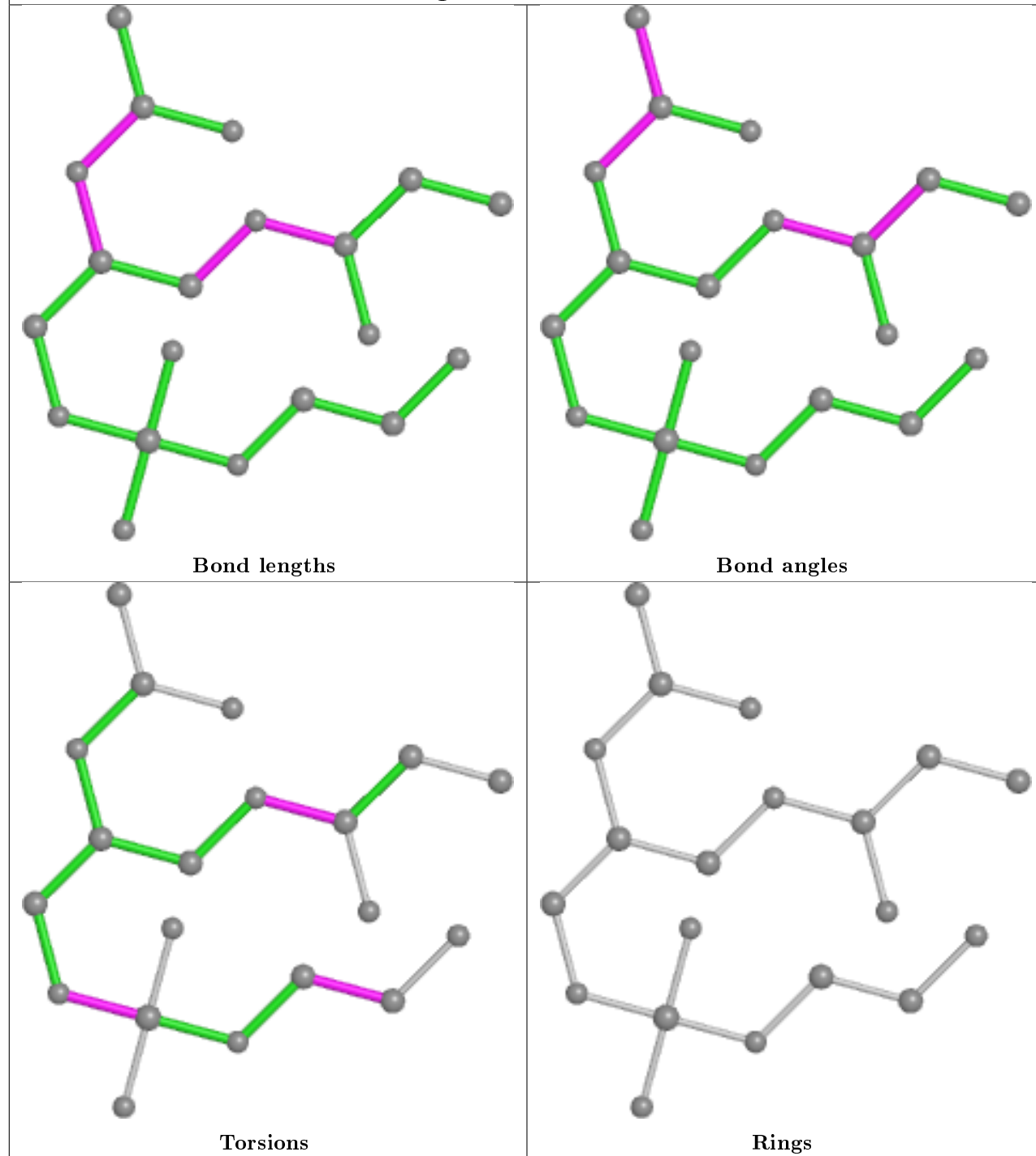
There are no ring outliers.

5 monomers are involved in 9 short contacts:

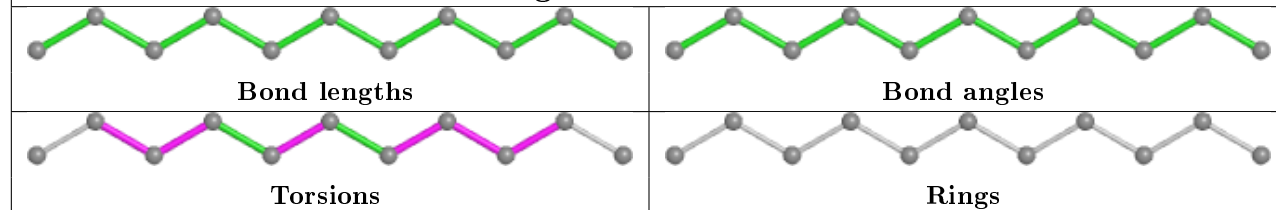
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	923	PLC	2	0
10	B	802	UND	2	0
5	A	919	C2E	1	0
8	B	803	PLC	1	0
6	A	921	UDP	4	0

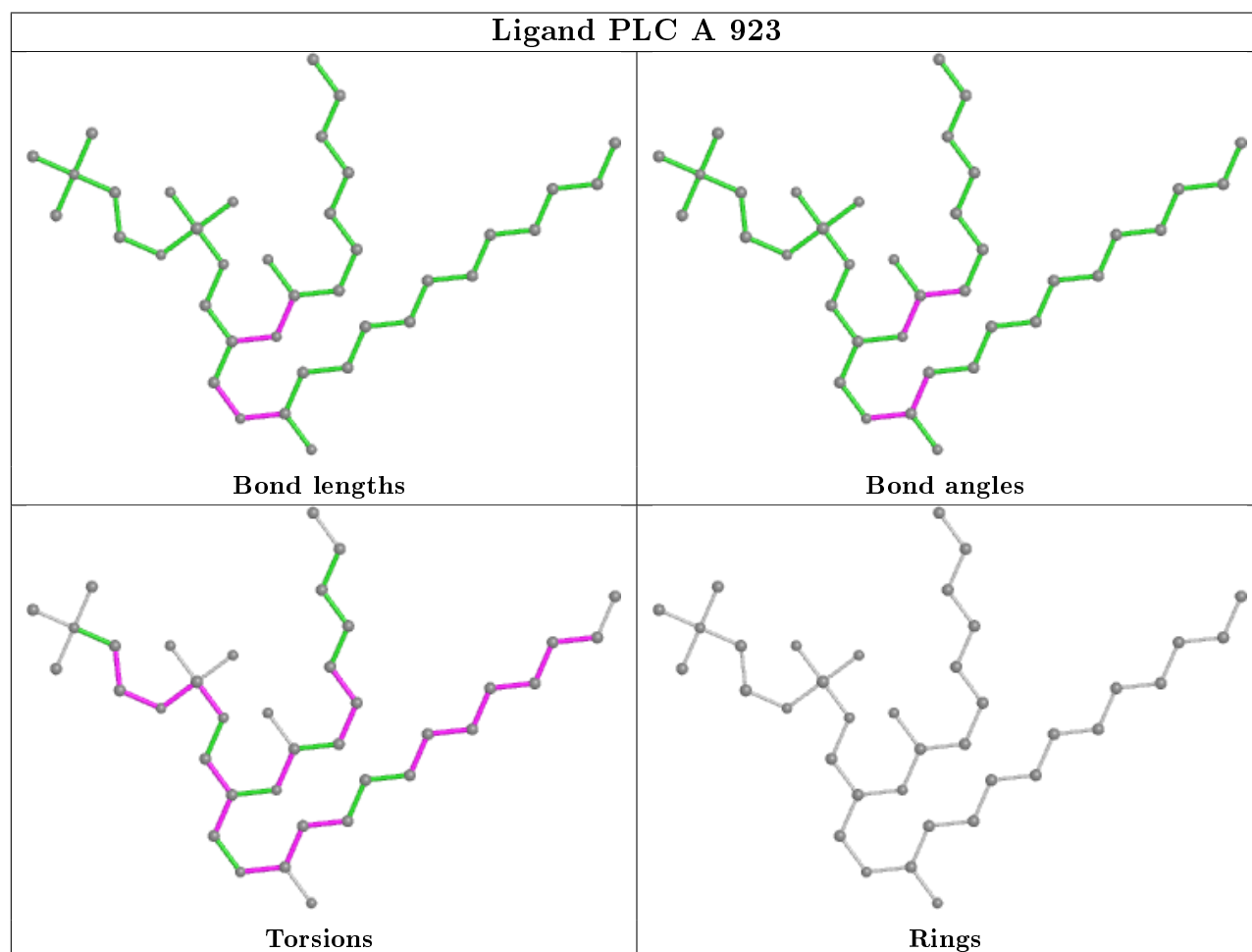
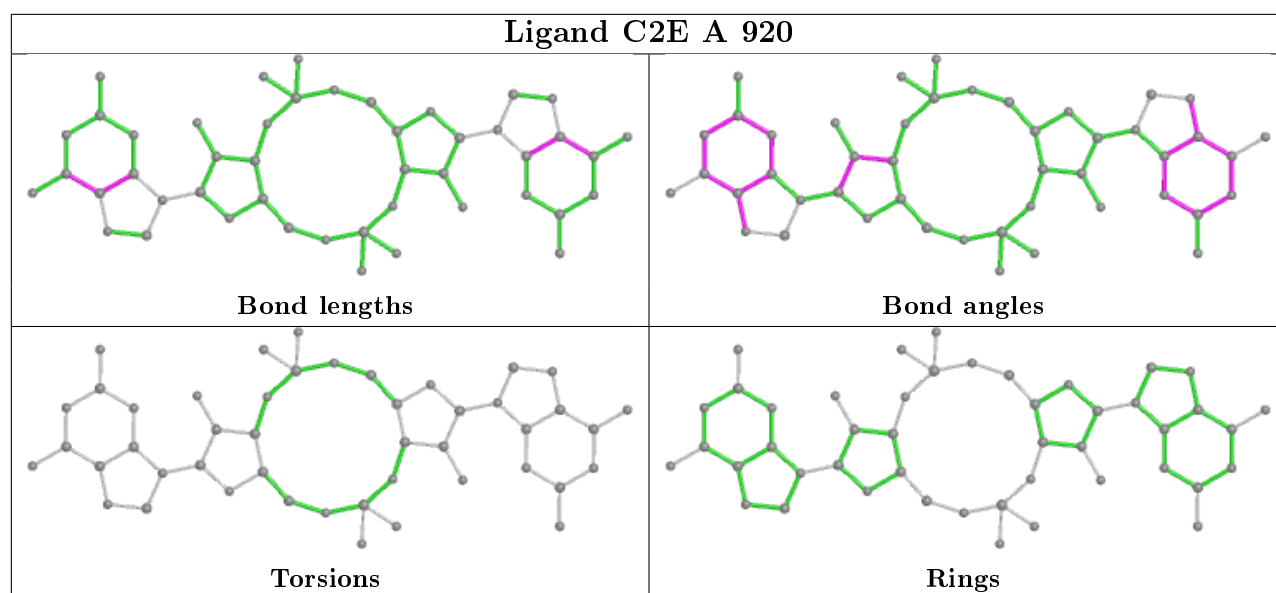
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

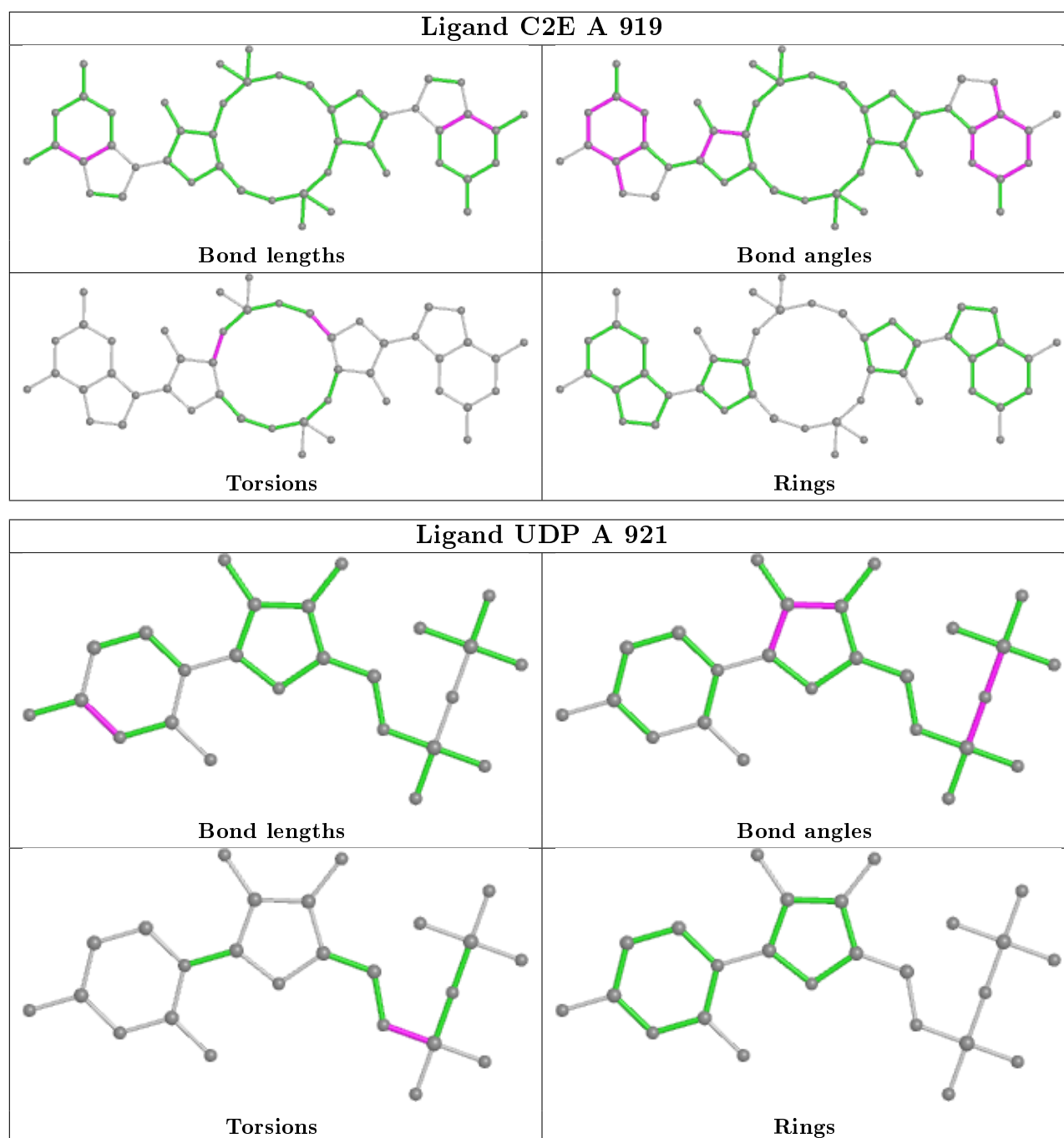
## Ligand 3PE A 924



## Ligand PLC B 804







## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	728/803 (90%)	0.20	42 (5%) 23 21	55, 79, 133, 176	0
2	B	655/724 (90%)	-0.13	16 (2%) 59 59	49, 72, 116, 161	0
3	D	0/9	-	-	-	-
All	All	1383/1536 (90%)	0.05	58 (4%) 36 35	49, 75, 126, 176	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	VAL	5.3
1	A	13	VAL	5.2
1	A	15	PRO	4.3
2	B	77	GLN	4.2
1	A	318	CYS	4.1
1	A	499	ARG	3.7
1	A	188	MET	3.7
2	B	593	LEU	3.6
2	B	78	GLN	3.5
2	B	595	PRO	3.5
2	B	594	ARG	3.5
1	A	398	PHE	3.4
1	A	192	PRO	3.4
1	A	739	ARG	3.3
1	A	496	LEU	3.3
1	A	221	ARG	3.2
1	A	393	LEU	3.1
1	A	502	ARG	3.1
1	A	17	LEU	3.1
1	A	134	LEU	3.0
1	A	740	ARG	2.9
1	A	94	LEU	2.9
2	B	590	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	187	CYS	2.8
2	B	169	PHE	2.8
1	A	514	GLU	2.7
1	A	497	ARG	2.7
2	B	531	THR	2.7
1	A	543	VAL	2.7
1	A	14	VAL	2.7
1	A	264	VAL	2.6
1	A	735	PRO	2.6
2	B	130	PHE	2.6
1	A	620	ARG	2.6
2	B	544	GLY	2.6
1	A	498	PRO	2.6
1	A	335	PHE	2.6
2	B	589	VAL	2.6
1	A	19	PHE	2.5
1	A	194	LEU	2.5
1	A	501	ALA	2.5
1	A	737	ARG	2.4
1	A	137	GLU	2.4
1	A	738	ARG	2.4
1	A	706	PRO	2.4
2	B	592	MET	2.3
1	A	120	PHE	2.3
1	A	705	ARG	2.3
1	A	319	GLY	2.3
2	B	494	ASP	2.3
1	A	297	GLU	2.2
1	A	235	GLU	2.2
1	A	20	LEU	2.1
2	B	131	GLY	2.1
2	B	596	GLY	2.1
2	B	247	TRP	2.1
1	A	400	ARG	2.0
1	A	240	GLU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SHG	C	18	11/12	0.78	0.41	100,108,125,138	0
4	BGC	C	1	12/12	0.82	0.31	120,132,137,143	0
4	BGC	C	2	11/12	0.88	0.18	100,107,112,112	0
4	BGC	C	8	11/12	0.90	0.25	67,85,116,135	0
4	BGC	C	17	11/12	0.91	0.40	77,82,98,99	0
4	BGC	C	3	11/12	0.91	0.14	81,91,107,109	0
4	BGC	C	5	11/12	0.92	0.21	49,52,86,113	0
4	BGC	C	6	11/12	0.92	0.22	50,58,80,103	0
4	BGC	C	16	11/12	0.92	0.38	69,75,90,100	0
4	BGC	C	15	11/12	0.93	0.32	62,76,87,89	0
4	BGC	C	10	11/12	0.93	0.26	65,96,113,131	0
4	BGC	C	13	11/12	0.94	0.29	66,71,88,92	0
4	BGC	C	14	11/12	0.94	0.28	57,74,80,87	0
4	BGC	C	9	11/12	0.94	0.23	84,91,101,106	0
4	BGC	C	4	11/12	0.95	0.18	56,67,86,93	0
4	BGC	C	7	11/12	0.95	0.14	49,57,76,89	0
4	BGC	C	12	11/12	0.96	0.26	64,80,89,94	0
4	BGC	C	11	11/12	0.97	0.20	77,86,100,103	0

### 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<sup>th</sup> 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.

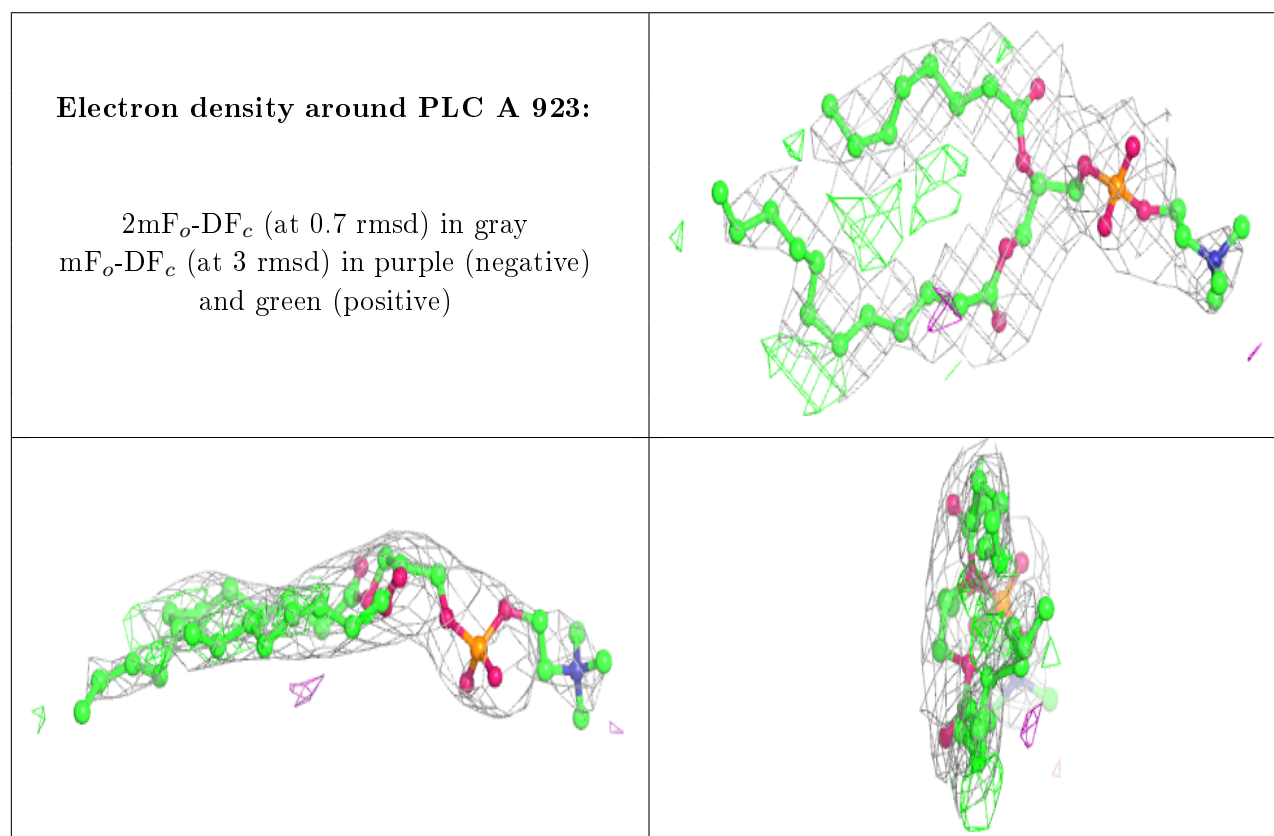
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	MG	A	922	1/1	0.73	0.93	98,98,98,98	0
7	MG	B	801	1/1	0.81	0.13	61,61,61,61	0
8	PLC	A	923	38/42	0.83	0.46	87,124,155,157	0
8	PLC	B	804	11/42	0.85	0.42	72,83,94,97	0
10	UND	B	802	11/11	0.87	0.37	63,68,80,82	0
9	3PE	A	924	20/51	0.91	0.26	87,105,115,120	0
8	PLC	B	803	9/42	0.91	0.26	49,77,87,92	0
6	UDP	A	921	25/25	0.94	0.18	77,102,116,116	0
5	C2E	A	920	46/46	0.95	0.13	49,74,90,101	0

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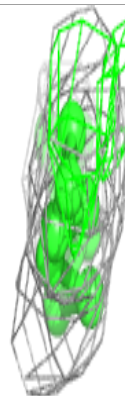
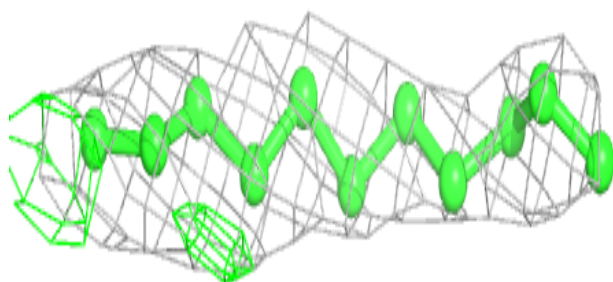
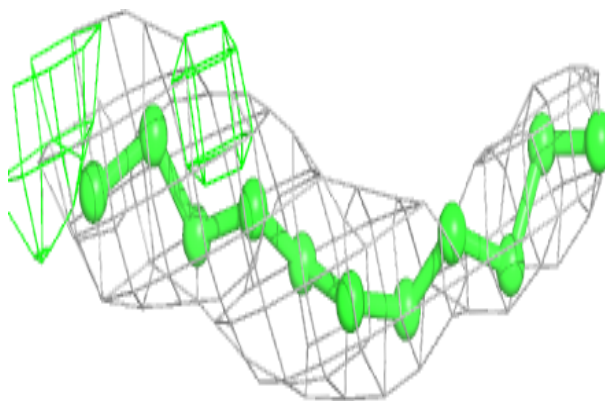
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	C2E	A	919	46/46	0.96	0.14	49,68,83,95	0

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.



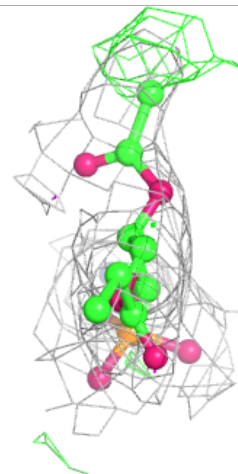
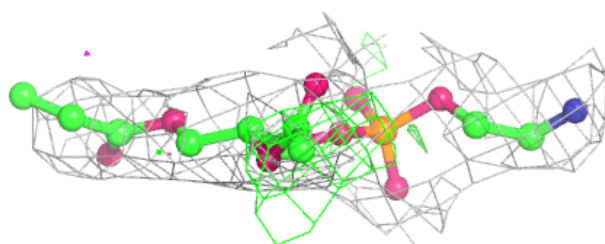
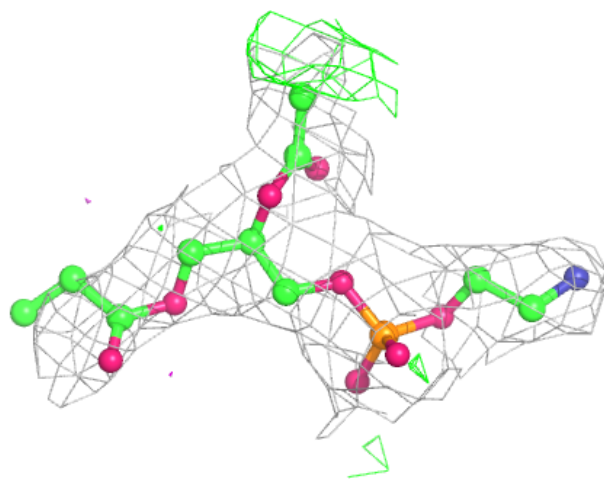
**Electron density around PLC B 804:**

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



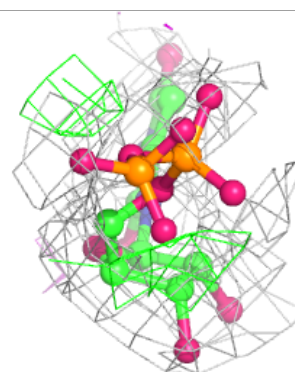
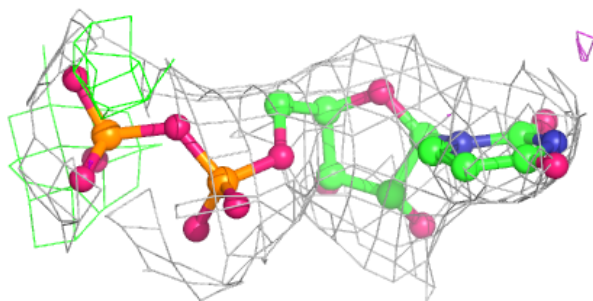
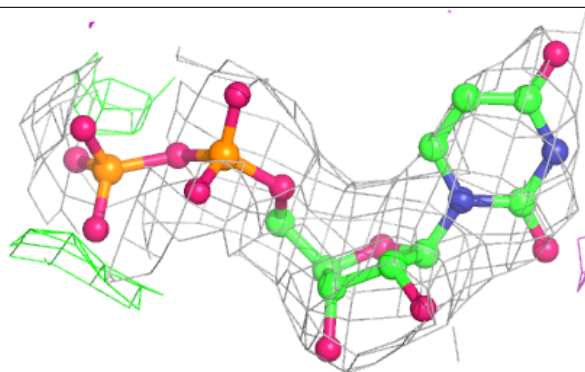
**Electron density around 3PE A 924:**

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



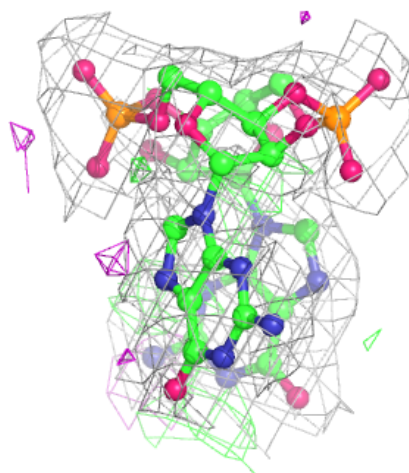
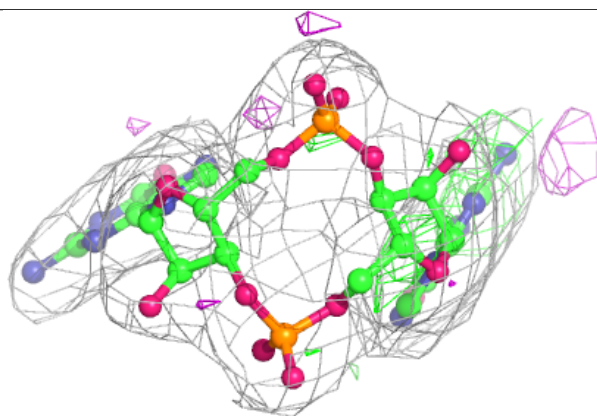
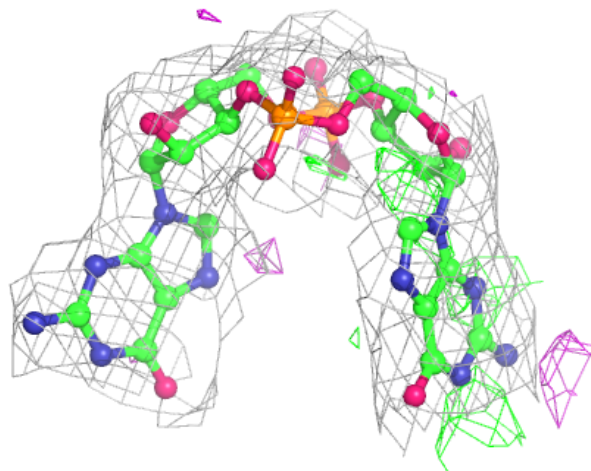
**Electron density around UDP A 921:**

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



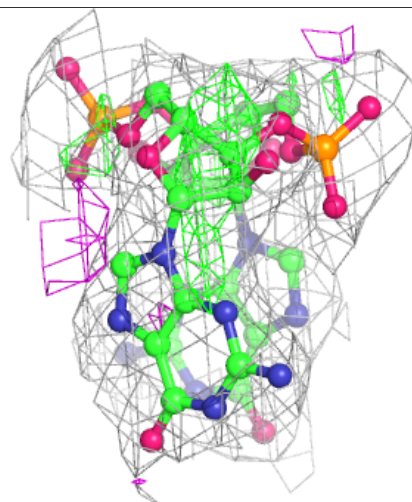
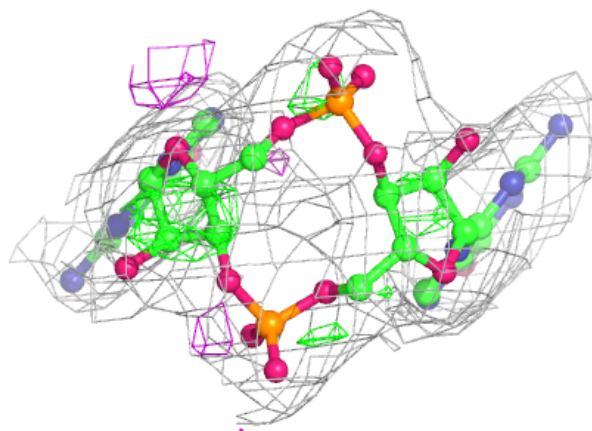
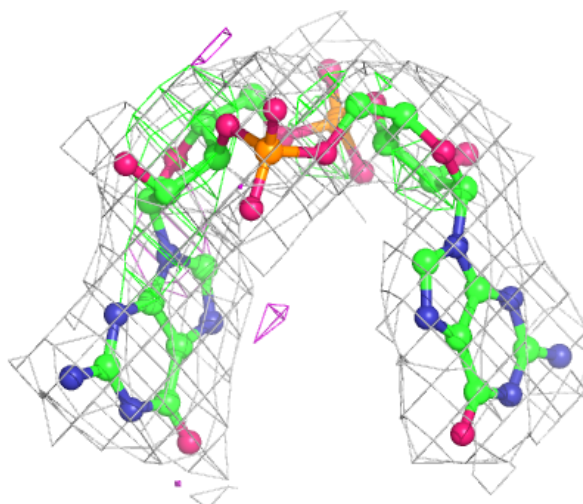
**Electron density around C2E A 920:**

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



**Electron density around C2E A 919:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.