



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:29 AM UTC

PDB ID : 5EJZ / pdb_00005ejz
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

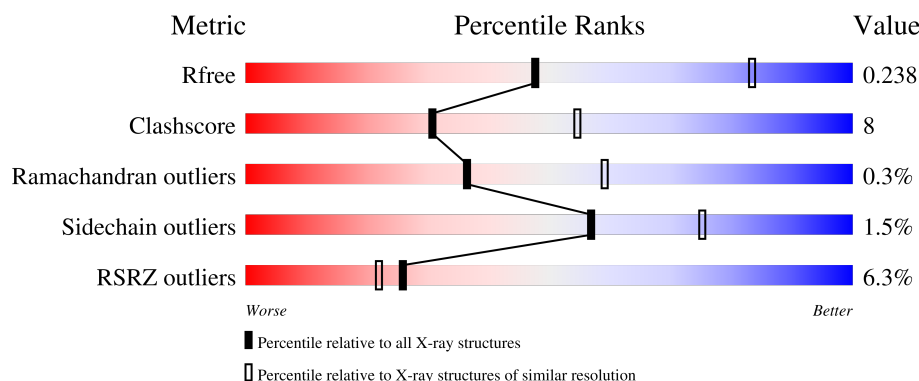
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

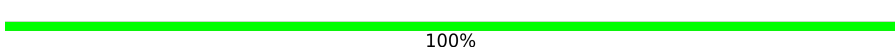
The reported resolution of this entry is 2.94 Å.

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}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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 $\leq 5\%$. 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	 6% 76% 14% • 9%
2	B	724	 5% 76% 14% • 10%
3	D	9	 100%
4	C	18	 50% 50%

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
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			

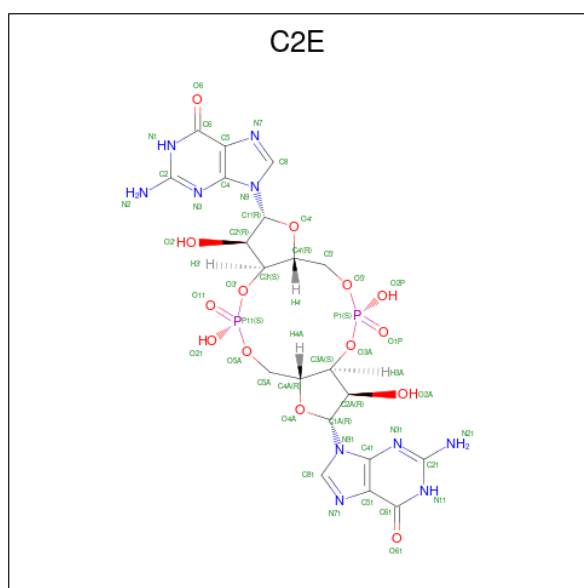
- Molecule 3 is a protein called poly(unk).

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

- [illegible]

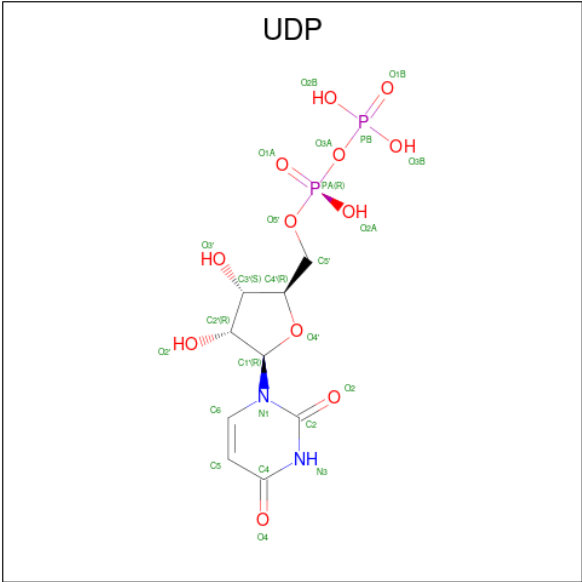
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	18	Total	C	F	O	0	0	0
			199	108	1	90			

- Molecule 5 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-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) (CCD ID: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$).



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

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $\text{C}_9\text{H}_{14}\text{N}_2\text{O}_{12}\text{P}_2$).

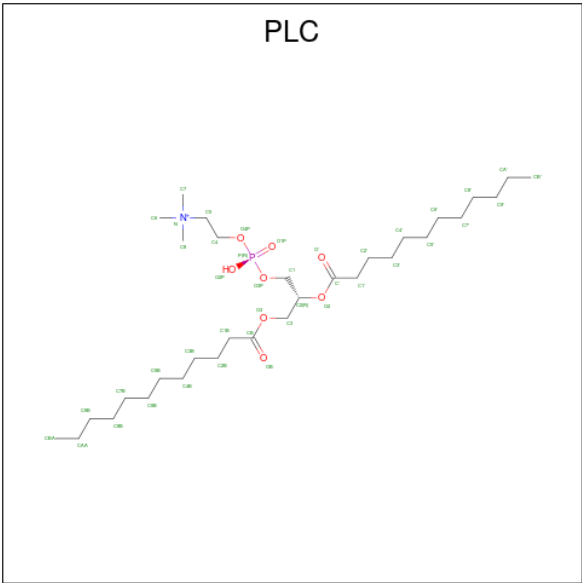


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

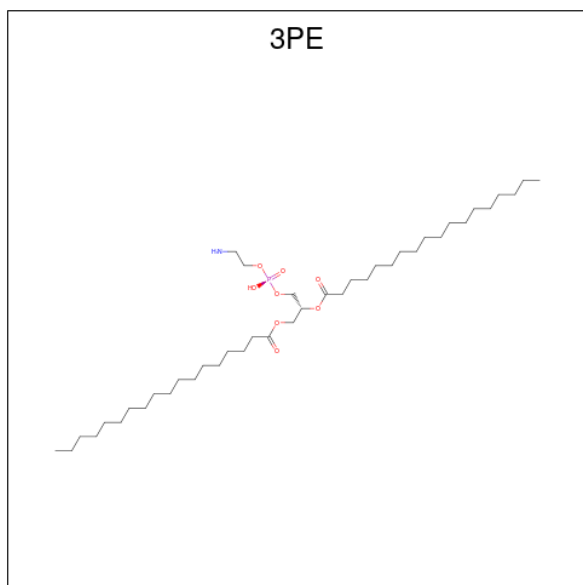
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		

- Molecule 8 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



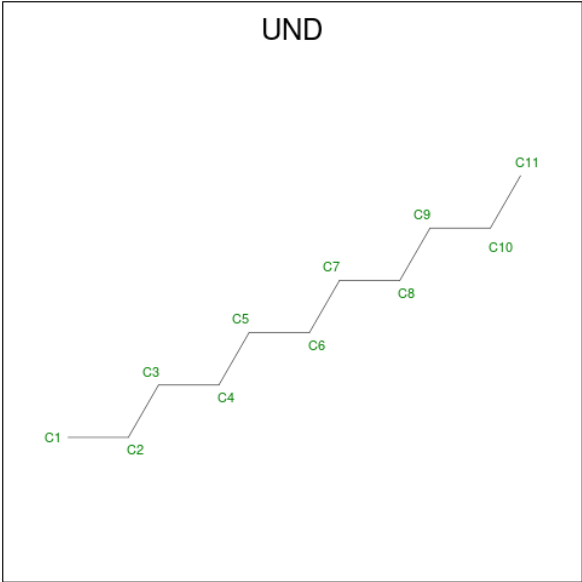
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			38	28	1	8	1		
8	B	1	Total	C				0	0
			9	9					
8	B	1	Total	C				0	0
			11	11					

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 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		

- Molecule 10 is UNDECANE (CCD ID: UND) (formula: $C_{11}H_{24}$).

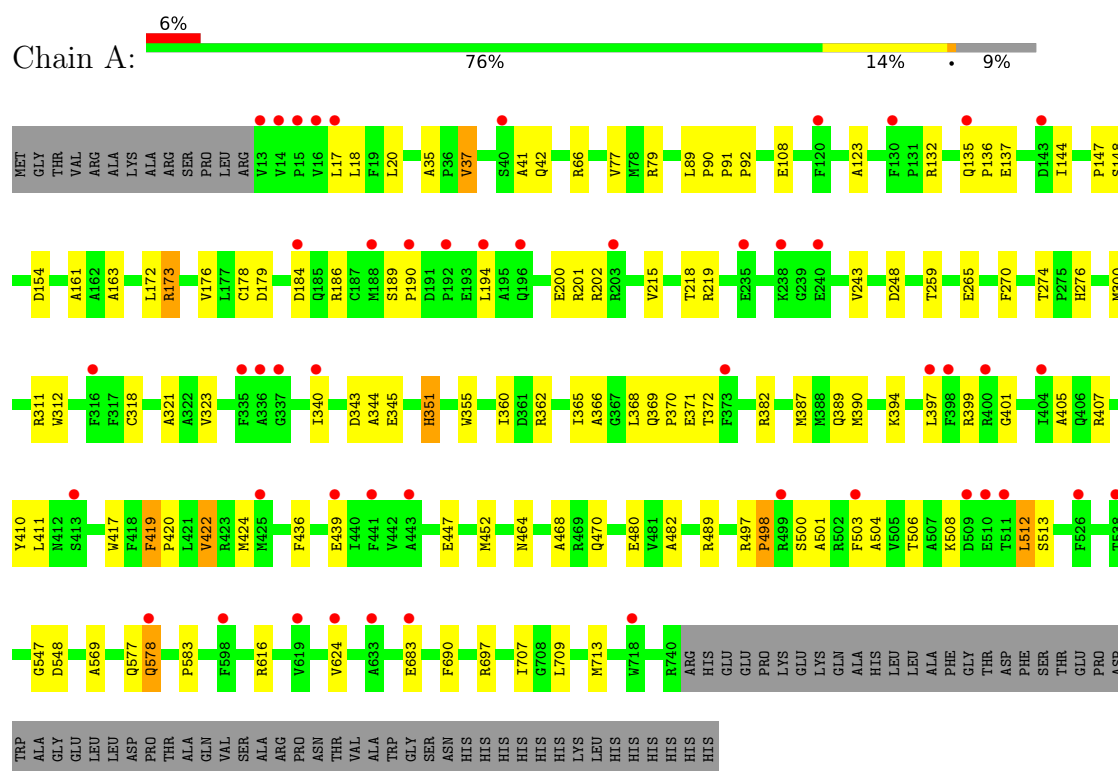


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	C	0	0
			11	11		

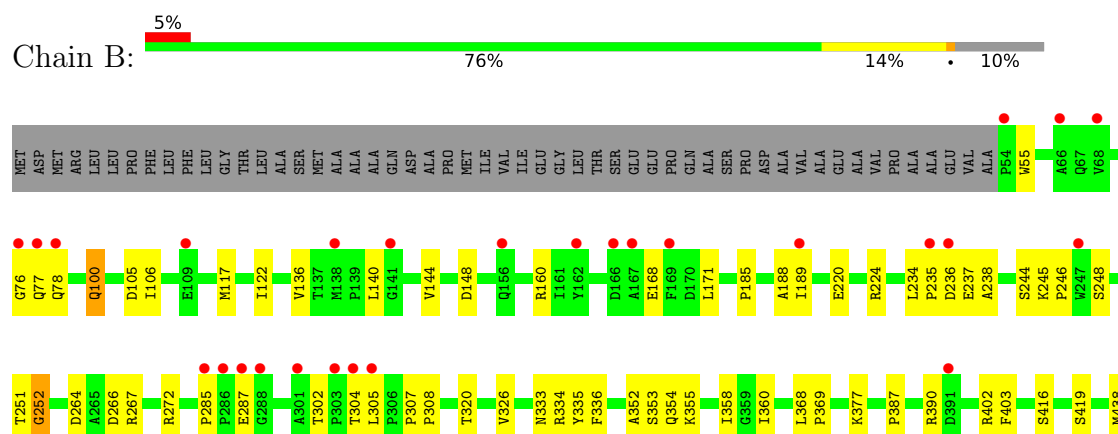
3 Residue-property plots

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

• Molecule 1: Putative cellulose synthase



• Molecule 2: Putative cellulose synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.27Å 216.84Å 221.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.35 – 2.94 34.35 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.35-2.94) 98.4 (34.35-2.94)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.206 , 0.233 0.211 , 0.238	Depositor DCC
R_{free} test set	3431 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLC, C2E, BGC, UND, UDP, MG, SHG, 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	0.32	0/5888	0.77	4/8007 (0.0%)
2	B	0.35	0/5006	0.82	4/6865 (0.1%)
All	All	0.34	0/10894	0.79	8/14872 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	514	ASN	N-CA-C	11.89	124.24	111.28
2	B	515	GLU	N-CA-C	7.26	119.77	108.96
1	A	172	LEU	N-CA-C	7.18	119.18	111.36
2	B	252	GLY	C-N-CD	5.37	132.41	120.60
2	B	100	GLN	N-CA-C	5.22	117.12	109.24
1	A	173	ARG	N-CA-C	5.16	117.90	109.59
1	A	419	PHE	CA-C-N	-5.13	114.32	119.56
1	A	419	PHE	C-N-CA	-5.13	114.32	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5739	0	5855	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4887	0	4966	92	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
10	B	11	0	24	2	0
All	All	11078	0	11181	184	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 (184) 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
2:B:77:GLN:CD	2:B:168:GLU:HB3	1.82	1.05
1:A:173:ARG:HD2	1:A:173:ARG:O	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
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
1:A:452:MET:HE2	4:C:11:BGC:O6	1.81	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:173:ARG:HD2	1:A:173:ARG:C	2.15	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
2:B:352:ALA:HB3	2:B:354:GLN:CD	2.16	0.69
1:A:345:GLU:CA	1:A:390:MET:HE1	2.22	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
2:B:77:GLN:O	2:B:78:GLN:HB3	1.95	0.67
2:B:516:GLU:HG2	2:B:600:LEU:CB	2.25	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
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
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:HE1	1.83	0.61
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	1.51	0.59
1:A:132:ARG:HG3	1:A:265:GLU:CD	2.27	0.59
1:A:259:THR:HG21	1:A:323:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:340:ILE:CG2	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
2:B:419:SER:HB3	2:B:438:MET:HE2	1.87	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
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:387:MET:HE2	4:C:17:BGC:H6C1	1.89	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: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
1:A:173:ARG:C	1:A:173:ARG:CD	2.80	0.53
2:B:352:ALA:CB	2:B:354:GLN:HE22	2.16	0.51
1:A:345:GLU:HB2	1:A:390:MET:HE1	1.92	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:OD1	1:A:154:ASP:N	2.43	0.51
1:A:300:MET:HA	1:A:470:GLN:HB3	1.92	0.51
1:A:345:GLU:HA	1:A:390:MET:CE	2.40	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
4:C:10:BGC:O3	4:C:11:BGC:O5	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:678:SER:O	2:B:682:VAL:HG23	2.12	0.49
2:B:77:GLN:N	2:B:77:GLN:OE1	2.45	0.49
2:B:77:GLN:OE1	2:B:168:GLU:O	2.30	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
1:A:506:THR:OG1	6:A:921:UDP:O2B	2.29	0.49
1:A:709:LEU:HG	1:A:713:MET:HE2	1.95	0.49
2:B:189:ILE:O	2:B:272:ARG:NH1	2.45	0.49
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
1:A:345:GLU:CB	1:A:390:MET:HE1	2.44	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
2:B:220:GLU:OE2	2:B:224:ARG:NH2	2.48	0.47
2:B:456:MET:HE2	2:B:456:MET:HB3	1.62	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
2:B:483:LEU:HA	2:B:486:MET:HE3	1.96	0.47
1:A:274:THR:OG1	1:A:321:ALA:O	2.23	0.46
1:A:37:VAL:HG13	1:A:41:ALA:HB3	1.98	0.46
1:A:389:GLN:NE2	1:A:498:PRO:O	2.49	0.46
2:B:77:GLN:CD	2:B:168:GLU:OE1	2.58	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
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
2:B:105:ASP:HA	2:B:160:ARG:HE	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:354:GLN:CD	2:B:354:GLN:H	2.17	0.44
2:B:505:LEU:HD21	2:B:527:LEU:HD12	2.00	0.44
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:HA	2:B:334:ARG:HD3	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:285:PRO:C	2:B:287:GLU:H	2.27	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:117:MET:HE2	2:B:122:ILE:HG21	2.02	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:390:MET:HE3	1:A:390:MET:HB2	1.71	0.41
1:A:312:TRP:HB3	1:A:405:ALA:HB1	2.02	0.41
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
2:B:387:PRO:HB3	4:C:5:BGC:H6	1.86	0.41
1:A:148:SER:HA	6:A:921:UDP:O2'	2.20	0.41
1:A:248:ASP:HB2	1:A:368:LEU:HG	2.02	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
1:A:547:GLY:O	4:C:7:BGC:O6	2.38	0.41
2:B:466:VAL:HG22	2:B:498:VAL:CG1	2.50	0.41
1:A:366:ALA:HB3	1:A:690:PHE:HD1	1.85	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:O	2:B:78:GLN:CG	2.70	0.40
2:B:701:MET:HE2	2:B:701:MET:HB3	2.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	727/803 (90%)	701 (96%)	24 (3%)	2 (0%)	36	59
2	B	651/724 (90%)	624 (96%)	25 (4%)	2 (0%)	36	59
All	All	1378/1527 (90%)	1325 (96%)	49 (4%)	4 (0%)	36	59

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%)	587 (98%)	12 (2%)	48	70
2	B	520/572 (91%)	515 (99%)	5 (1%)	68	81
All	All	1119/1233 (91%)	1102 (98%)	17 (2%)	57	75

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	77	VAL

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Mol	Chain	Res	Type
1	A	137	GLU
1	A	200	GLU
1	A	351	HIS
1	A	365	ILE
1	A	422	VAL
1	A	489	ARG
1	A	512	LEU
1	A	578	GLN
1	A	624	VAL
1	A	707	ILE
2	B	326	VAL
2	B	402	ARG
2	B	448	VAL
2	B	456	MET
2	B	669	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	222	ASN
1	A	379	GLN
2	B	100	GLN
2	B	157	HIS
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	1.23	1 (8%)	17,17,17	1.48	4 (23%)
4	BGC	C	10	4	11,11,12	1.60	3 (27%)	15,15,17	1.46	1 (6%)
4	BGC	C	11	4	11,11,12	1.58	3 (27%)	15,15,17	1.05	1 (6%)
4	BGC	C	12	4	11,11,12	1.65	3 (27%)	15,15,17	0.68	0
4	BGC	C	13	4	11,11,12	1.52	2 (18%)	15,15,17	1.05	0
4	BGC	C	14	4	11,11,12	1.62	2 (18%)	15,15,17	1.45	2 (13%)
4	BGC	C	15	4	11,11,12	1.56	2 (18%)	15,15,17	1.47	3 (20%)
4	BGC	C	16	4	11,11,12	1.49	1 (9%)	15,15,17	1.98	4 (26%)
4	BGC	C	17	4	11,11,12	1.70	3 (27%)	15,15,17	0.85	0
4	SHG	C	18	4	11,11,12	1.63	1 (9%)	12,15,17	0.92	1 (8%)
4	BGC	C	2	4	11,11,12	1.71	3 (27%)	15,15,17	1.50	3 (20%)
4	BGC	C	3	4	11,11,12	1.63	2 (18%)	15,15,17	1.89	3 (20%)
4	BGC	C	4	4	11,11,12	1.65	3 (27%)	15,15,17	1.97	4 (26%)
4	BGC	C	5	4	11,11,12	1.55	2 (18%)	15,15,17	1.79	4 (26%)
4	BGC	C	6	4	11,11,12	2.05	3 (27%)	15,15,17	0.89	1 (6%)
4	BGC	C	7	4	11,11,12	1.67	3 (27%)	15,15,17	0.94	0
4	BGC	C	8	4	11,11,12	1.63	3 (27%)	15,15,17	1.62	4 (26%)
4	BGC	C	9	4	11,11,12	1.65	3 (27%)	15,15,17	1.15	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	2/2/19/22	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	6	BGC	O5-C1	5.28	1.52	1.43
4	C	14	BGC	O5-C1	4.20	1.50	1.43
4	C	9	BGC	O5-C1	4.20	1.50	1.43
4	C	4	BGC	O5-C1	4.19	1.50	1.43
4	C	18	SHG	O5-C1	4.17	1.50	1.43
4	C	12	BGC	O5-C1	4.15	1.50	1.43
4	C	3	BGC	O5-C1	4.14	1.50	1.43
4	C	7	BGC	O5-C1	4.10	1.50	1.43
4	C	17	BGC	O5-C1	4.08	1.50	1.43
4	C	2	BGC	O5-C1	4.08	1.50	1.43
4	C	8	BGC	O5-C1	4.04	1.50	1.43
4	C	11	BGC	O5-C1	3.93	1.50	1.43
4	C	10	BGC	O5-C1	3.88	1.50	1.43
4	C	16	BGC	O5-C1	3.84	1.50	1.43
4	C	15	BGC	O5-C1	3.80	1.50	1.43
4	C	5	BGC	O5-C1	3.75	1.50	1.43
4	C	13	BGC	O5-C1	3.59	1.49	1.43
4	C	1	BGC	O5-C1	3.18	1.50	1.42
4	C	6	BGC	C2-C3	-2.75	1.48	1.52
4	C	17	BGC	C2-C3	-2.74	1.48	1.52
4	C	6	BGC	O5-C5	2.70	1.48	1.43
4	C	2	BGC	C2-C3	-2.59	1.48	1.52
4	C	13	BGC	C2-C3	-2.41	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	10	BGC	C2-C3	-2.38	1.48	1.52
4	C	7	BGC	O5-C5	2.37	1.48	1.43
4	C	15	BGC	C2-C3	-2.36	1.48	1.52
4	C	2	BGC	O5-C5	2.34	1.48	1.43
4	C	7	BGC	C2-C3	-2.34	1.48	1.52
4	C	5	BGC	O2-C2	2.32	1.48	1.43
4	C	12	BGC	C2-C3	-2.29	1.49	1.52
4	C	11	BGC	C2-C3	-2.29	1.49	1.52
4	C	9	BGC	C2-C3	-2.27	1.49	1.52
4	C	3	BGC	C2-C3	-2.25	1.49	1.52
4	C	8	BGC	O5-C5	2.23	1.47	1.43
4	C	17	BGC	O5-C5	2.22	1.47	1.43
4	C	12	BGC	O5-C5	2.17	1.47	1.43
4	C	8	BGC	C2-C3	-2.15	1.49	1.52
4	C	14	BGC	C2-C3	-2.12	1.49	1.52
4	C	4	BGC	O5-C5	2.10	1.47	1.43
4	C	9	BGC	O5-C5	2.10	1.47	1.43
4	C	10	BGC	O5-C5	2.10	1.47	1.43
4	C	4	BGC	C2-C3	-2.04	1.49	1.52
4	C	11	BGC	O5-C5	2.03	1.47	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	16	BGC	C1-C2-C3	5.04	116.99	109.64
4	C	4	BGC	C1-C2-C3	4.70	116.49	109.64
4	C	3	BGC	C1-C2-C3	4.11	115.63	109.64
4	C	10	BGC	C1-C2-C3	4.10	115.62	109.64
4	C	5	BGC	C2-C3-C4	4.10	118.07	110.86
4	C	14	BGC	C1-C2-C3	3.92	115.35	109.64
4	C	4	BGC	C2-C3-C4	3.86	117.65	110.86
4	C	3	BGC	C2-C3-C4	3.67	117.31	110.86
4	C	5	BGC	C1-C2-C3	3.57	114.84	109.64
4	C	16	BGC	C2-C3-C4	3.37	116.80	110.86
4	C	1	BGC	C3-C4-C5	3.24	116.11	110.23
4	C	1	BGC	O5-C5-C4	3.21	115.49	109.70
4	C	2	BGC	C3-C4-C5	2.98	115.64	110.23
4	C	3	BGC	C3-C4-C5	2.89	115.47	110.23
4	C	8	BGC	C3-C4-C5	2.83	115.37	110.23
4	C	8	BGC	C2-C3-C4	2.83	115.84	110.86
4	C	15	BGC	C3-C4-C5	2.60	114.95	110.23
4	C	5	BGC	C1-O5-C5	-2.60	108.71	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5	BGC	O4-C4-C5	-2.56	103.01	109.32
4	C	8	BGC	C1-C2-C3	2.53	113.33	109.64
4	C	2	BGC	C2-C3-C4	2.51	115.27	110.86
4	C	18	SHG	C2-C3-C4	2.41	112.51	109.59
4	C	15	BGC	C2-C3-C4	2.40	115.09	110.86
4	C	9	BGC	C1-C2-C3	2.36	113.08	109.64
4	C	4	BGC	C6-C5-C4	-2.32	107.33	113.02
4	C	15	BGC	C1-O5-C5	-2.29	109.12	112.19
4	C	1	BGC	C4-C3-C2	2.26	114.80	110.83
4	C	4	BGC	C3-C4-C5	2.19	114.21	110.23
4	C	16	BGC	C1-O5-C5	-2.15	109.30	112.19
4	C	11	BGC	C3-C4-C5	2.09	114.02	110.23
4	C	16	BGC	C3-C4-C5	2.05	113.96	110.23
4	C	8	BGC	C1-O5-C5	-2.05	109.44	112.19
4	C	6	BGC	C1-C2-C3	2.03	112.60	109.64
4	C	1	BGC	C6-C5-C4	-2.02	108.07	113.02
4	C	14	BGC	C2-C3-C4	2.02	114.41	110.86
4	C	2	BGC	C6-C5-C4	-2.01	108.08	113.02

There are no chirality outliers.

All (29) 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	2	BGC	O5-C5-C6-O6
4	C	14	BGC	O5-C5-C6-O6
4	C	16	BGC	O5-C5-C6-O6
4	C	17	BGC	O5-C5-C6-O6
4	C	1	BGC	O5-C5-C6-O6
4	C	7	BGC	C4-C5-C6-O6
4	C	16	BGC	C4-C5-C6-O6
4	C	4	BGC	O5-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	8	BGC	C4-C5-C6-O6
4	C	17	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

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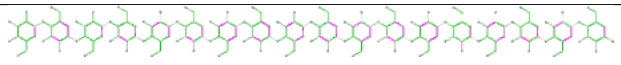
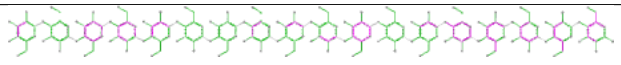
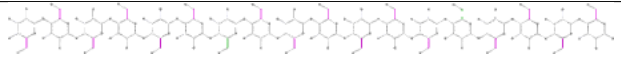
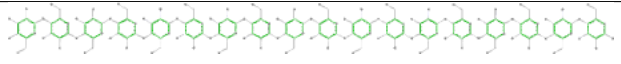
Mol	Chain	Res	Type	Atoms
4	C	13	BGC	C4-C5-C6-O6
4	C	9	BGC	O5-C5-C6-O6
4	C	10	BGC	O5-C5-C6-O6
4	C	13	BGC	O5-C5-C6-O6
4	C	6	BGC	O5-C5-C6-O6
4	C	3	BGC	O5-C5-C6-O6
4	C	15	BGC	C4-C5-C6-O6
4	C	1	BGC	C4-C5-C6-O6
4	C	15	BGC	O5-C5-C6-O6
4	C	9	BGC	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 14 short contacts:

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

Oligosaccharide Chain C	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.6 Ligand geometry [i](#)

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
8	PLC	B	803	-	8,8,41	0.31	0	7,7,49	0.78	0
5	C2E	A	919	-	52,52,52	1.15	5 (9%)	78,82,82	1.89	15 (19%)
8	PLC	B	804	-	10,10,41	0.30	0	9,9,49	0.81	0
5	C2E	A	920	-	52,52,52	1.16	6 (11%)	78,82,82	1.87	15 (19%)
8	PLC	A	923	-	37,37,41	1.13	4 (10%)	43,45,49	1.09	2 (4%)
9	3PE	A	924	-	19,19,50	1.39	4 (21%)	22,24,55	1.49	2 (9%)
6	UDP	A	921	7	25,26,26	1.11	2 (8%)	38,40,40	1.75	4 (10%)
10	UND	B	802	-	10,10,10	0.26	0	9,9,9	0.54	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
8	PLC	B	803	-	-	0/6/6/45	-
5	C2E	A	919	-	-	2/30/62/62	0/6/7/7
8	PLC	B	804	-	-	6/8/8/45	-
5	C2E	A	920	-	-	0/30/62/62	0/6/7/7
8	PLC	A	923	-	-	25/41/41/45	-
9	3PE	A	924	-	-	4/22/22/54	-
6	UDP	A	921	7	-	4/16/32/32	0/2/2/2
10	UND	B	802	-	-	1/8/8/8	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	919	C2E	C5-C4	3.14	1.47	1.38
5	A	920	C2E	C5-C4	3.14	1.47	1.38
5	A	920	C2E	C51-C41	3.12	1.47	1.38
5	A	919	C2E	C51-C41	3.04	1.47	1.38
9	A	924	3PE	O21-C2	-2.68	1.40	1.46
8	A	923	PLC	O2-C2	-2.60	1.40	1.46
6	A	921	UDP	PA-O3A	2.50	1.62	1.59
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	O3-CB	2.42	1.40	1.33
9	A	924	3PE	O21-C21	2.39	1.40	1.35
5	A	920	C2E	C6-N1	-2.38	1.34	1.38
5	A	919	C2E	C6-N1	-2.37	1.34	1.38
5	A	920	C2E	C61-N11	-2.35	1.34	1.38
5	A	919	C2E	C61-N11	-2.33	1.34	1.38
9	A	924	3PE	O31-C3	-2.16	1.40	1.45
8	A	923	PLC	O2-C'	2.16	1.40	1.34
8	A	923	PLC	O3-C3	-2.13	1.40	1.45
6	A	921	UDP	C5-C4	-2.08	1.39	1.43
5	A	920	C2E	C51-N71	-2.07	1.34	1.39
5	A	920	C2E	C5-N7	-2.04	1.35	1.39
5	A	919	C2E	C5-N7	-2.03	1.35	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	920	C2E	C51-C41-N31	-6.19	118.54	128.39
5	A	919	C2E	C5-C4-N3	-6.18	118.56	128.39
5	A	920	C2E	C5-C4-N3	-6.12	118.65	128.39
5	A	919	C2E	C51-C41-N31	-6.00	118.83	128.39
6	A	921	UDP	C4-N3-C2	-5.97	119.20	126.61
5	A	919	C2E	C21-N31-C41	5.02	120.95	112.30
5	A	919	C2E	C2-N3-C4	5.00	120.92	112.30
9	A	924	3PE	O21-C21-C22	4.99	119.98	111.09
5	A	920	C2E	C21-N31-C41	4.94	120.81	112.30
5	A	920	C2E	C2-N3-C4	4.87	120.70	112.30
5	A	919	C2E	N9-C4-N3	4.60	135.16	125.95
5	A	920	C2E	N9-C4-N3	4.51	134.96	125.95
5	A	920	C2E	N91-C41-N31	4.48	134.91	125.95
5	A	919	C2E	N91-C41-N31	4.44	134.84	125.95
6	A	921	UDP	C5-C4-N3	4.07	120.50	114.80
8	A	923	PLC	O2-C'-C1'	3.92	119.96	111.48
6	A	921	UDP	N3-C2-N1	3.61	119.59	114.89
5	A	919	C2E	C61-C51-N71	3.45	136.57	130.29
6	A	921	UDP	O4-C4-C5	-3.33	119.42	125.16
5	A	919	C2E	C6-C5-N7	3.29	136.27	130.29
5	A	920	C2E	C61-C51-N71	3.28	136.26	130.29
5	A	920	C2E	C6-C5-N7	3.23	136.17	130.29
9	A	924	3PE	O31-C31-C32	2.98	120.19	111.15
5	A	920	C2E	C41-C51-N71	-2.75	106.32	110.67
5	A	919	C2E	C41-C51-N71	-2.72	106.36	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	923	PLC	O3-CB-C1B	2.69	120.05	111.83
5	A	919	C2E	C4-C5-N7	-2.68	106.43	110.67
5	A	920	C2E	C4-C5-N7	-2.66	106.45	110.67
5	A	919	C2E	C3'-C2'-C1'	2.49	105.37	99.89
5	A	920	C2E	C2A-C1A-N91	-2.26	106.97	113.25
5	A	920	C2E	C3'-C2'-C1'	2.20	104.73	99.89
5	A	919	C2E	O61-C61-C51	-2.13	120.91	126.53
5	A	920	C2E	O61-C61-C51	-2.09	121.01	126.53
5	A	919	C2E	O6-C6-C5	-2.06	121.10	126.53
5	A	919	C2E	C81-N71-C51	2.05	107.91	104.26
5	A	920	C2E	O6-C6-C5	-2.02	121.20	126.53
5	A	920	C2E	C81-N71-C51	2.01	107.84	104.26
5	A	919	C2E	C8-N7-C5	2.00	107.82	104.26

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	921	UDP	C5'-O5'-PA-O2A
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	C1-O3P-P-O4P
8	A	923	PLC	C4-O4P-P-O1P
8	A	923	PLC	C4-O4P-P-O3P
9	A	924	3PE	C1-O11-P-O14
9	A	924	3PE	O13-C11-C12-N
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	C6B-C7B-C8B-C9B
8	A	923	PLC	CB-C1B-C2B-C3B
8	A	923	PLC	C1'-C2'-C3'-C4'
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	C1-C2-C3-O3
8	A	923	PLC	C4B-C5B-C6B-C7B
8	B	804	PLC	C8'-C9'-CA'-CB'
8	A	923	PLC	C8B-C9B-CAA-CBA

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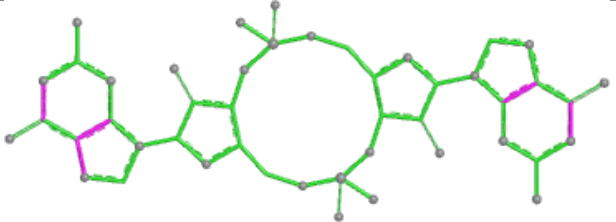
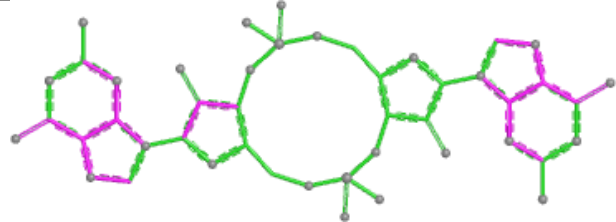
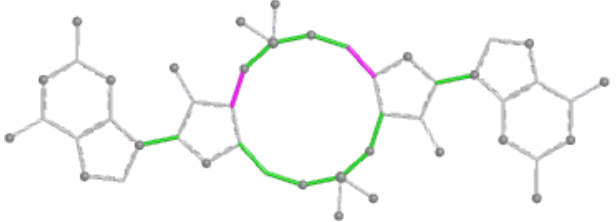
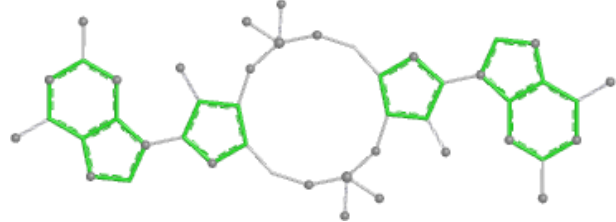
Mol	Chain	Res	Type	Atoms
10	B	802	UND	C7-C8-C9-C10
8	A	923	PLC	C1'-C'-O2-C2
8	A	923	PLC	C3B-C4B-C5B-C6B
8	A	923	PLC	O3P-C1-C2-C3
8	A	923	PLC	O'-C'-O2-C2
6	A	921	UDP	C5'-O5'-PA-O1A
6	A	921	UDP	C5'-O5'-PA-O3A
8	B	804	PLC	C3'-C4'-C5'-C6'
8	B	804	PLC	C2'-C3'-C4'-C5'
8	A	923	PLC	C'-C1'-C2'-C3'
5	A	919	C2E	O4A-C4A-C5A-O5A
8	A	923	PLC	C2B-C1B-CB-O3
8	B	804	PLC	C1'-C2'-C3'-C4'
8	A	923	PLC	OB-CB-O3-C3
8	A	923	PLC	C1B-CB-O3-C3
5	A	919	C2E	C2'-C3'-O3'-P11
8	A	923	PLC	C2B-C1B-CB-OB
6	A	921	UDP	C3'-C4'-C5'-O5'

There are no ring outliers.

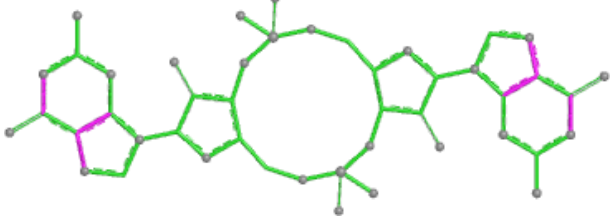
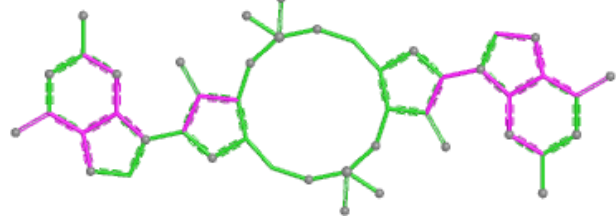
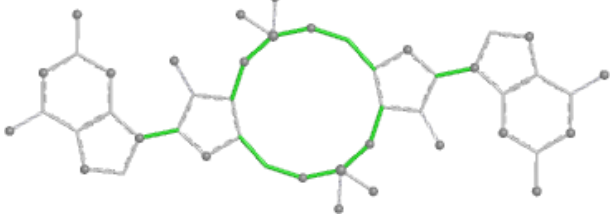
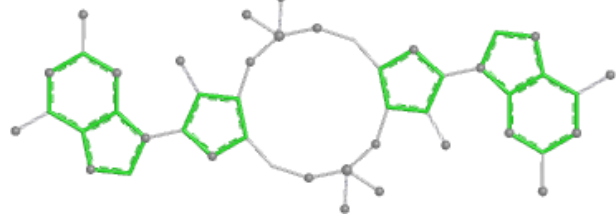
5 monomers are involved in 9 short contacts:

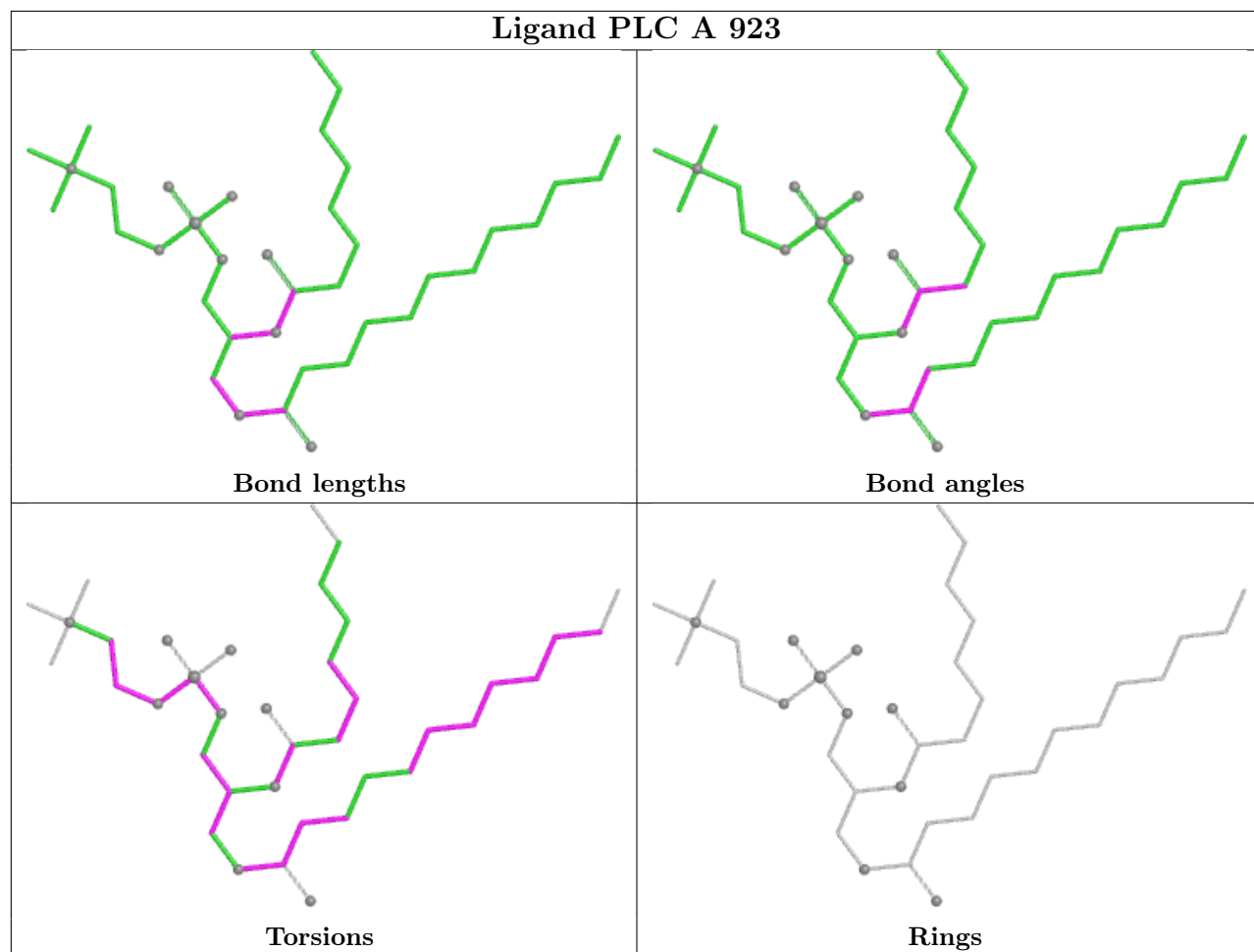
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	803	PLC	1	0
5	A	919	C2E	1	0
8	A	923	PLC	2	0
6	A	921	UDP	4	0
10	B	802	UND	2	0

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 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.

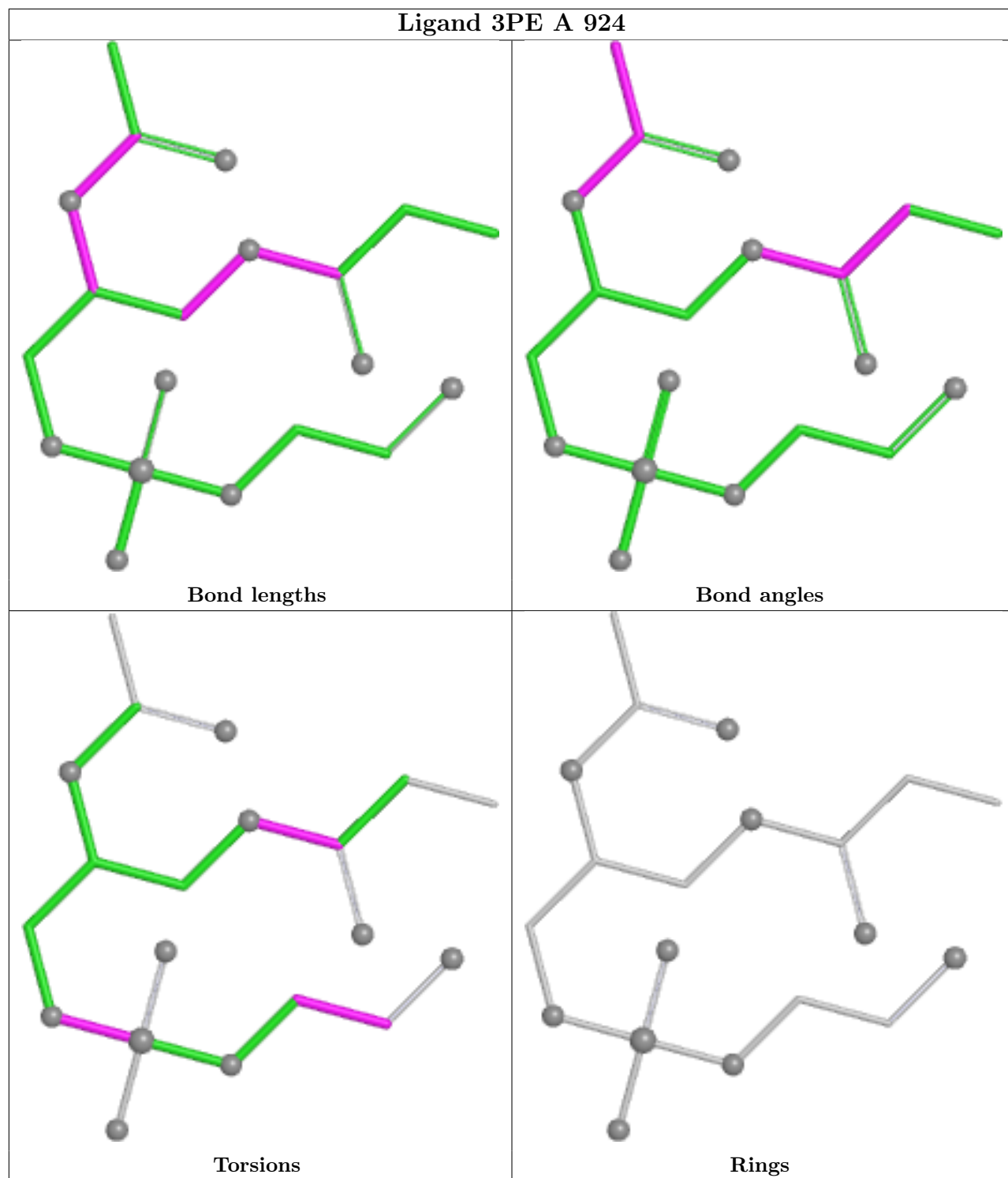
Ligand C2E A 919	
	
Bond lengths	Bond angles
	
Torsions	Rings

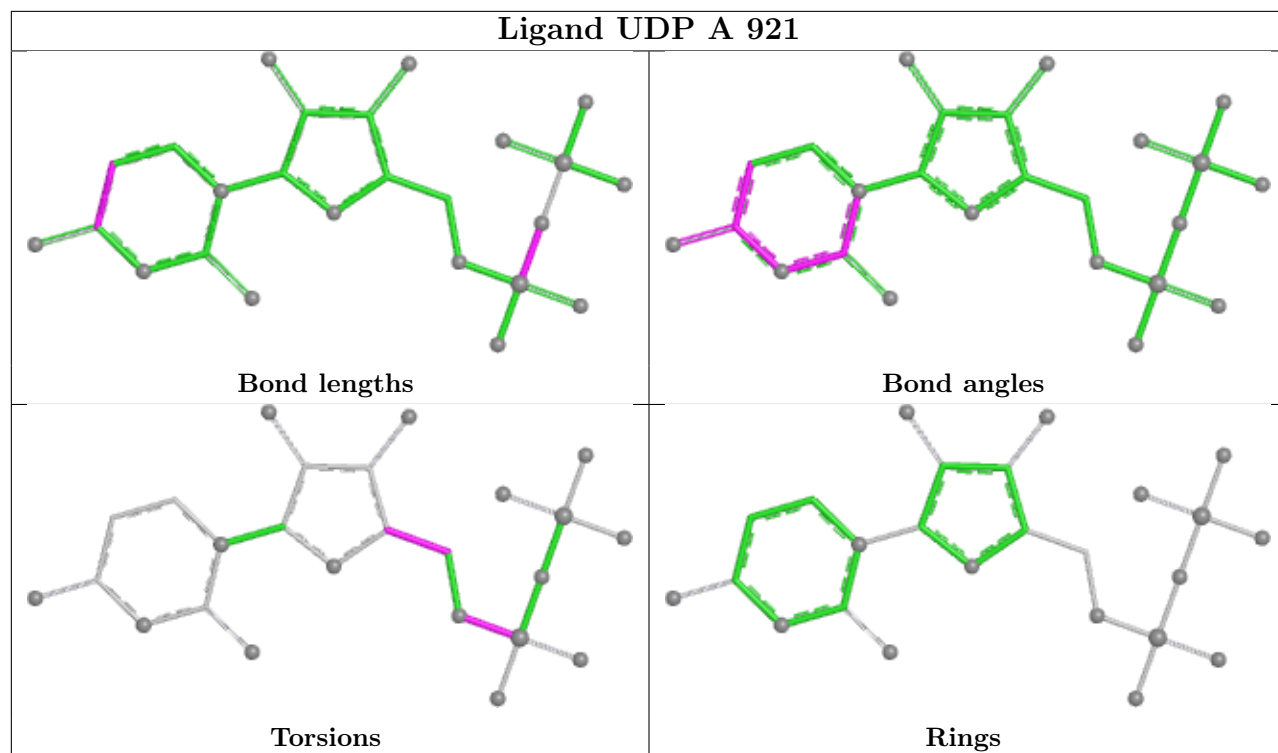
Ligand PLC B 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand C2E A 920	
	
Bond lengths	Bond angles
	
Torsions	Rings



Ligand 3PE A 924





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	728/803 (90%)	0.58	49 (6%) 24 21	47, 79, 133, 176	1 (0%)
2	B	655/724 (90%)	0.49	38 (5%) 29 23	49, 72, 116, 161	0
3	D	0/9	-	-	-	-
All	All	1383/1536 (90%)	0.54	87 (6%) 26 22	47, 75, 126, 176	1 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	77	GLN	8.0
2	B	640	MET	5.7
2	B	169	PHE	5.6
1	A	509	ASP	5.3
2	B	78	GLN	5.1
1	A	13	VAL	4.9
1	A	188	MET	4.7
1	A	120	PHE	4.5
2	B	304	THR	4.4
1	A	16	VAL	4.3
2	B	54	PRO	4.1
2	B	305	LEU	4.0
2	B	286	PRO	4.0
1	A	203	ARG	3.8
2	B	167	ALA	3.8
2	B	109	GLU	3.7
1	A	439	GLU	3.6
2	B	515	GLU	3.6
1	A	15	PRO	3.5
2	B	288	GLY	3.4
2	B	66	ALA	3.4
2	B	531	THR	3.3
1	A	14	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	624	VAL	3.3
1	A	510	GLU	3.3
2	B	156	GLN	3.3
1	A	413	SER	3.3
2	B	516	GLU	3.2
1	A	130	PHE	3.1
1	A	184	ASP	3.0
1	A	335	PHE	2.9
2	B	247	TRP	2.9
1	A	240	GLU	2.8
1	A	194	LEU	2.8
2	B	76	GLY	2.7
1	A	619	VAL	2.7
1	A	17	LEU	2.7
1	A	633	ALA	2.7
2	B	141	GLY	2.7
1	A	718	TRP	2.7
1	A	192	PRO	2.6
1	A	337	GLY	2.6
1	A	511	THR	2.6
1	A	196	GLN	2.6
1	A	683	GLU	2.6
2	B	593	LEU	2.6
1	A	340	ILE	2.6
1	A	135	GLN	2.6
1	A	190	PRO	2.5
2	B	287	GLU	2.5
1	A	425[A]	MET	2.5
1	A	598	PHE	2.5
1	A	499	ARG	2.5
1	A	443	ALA	2.5
1	A	578	GLN	2.5
2	B	68	VAL	2.4
2	B	162	TYR	2.4
1	A	40	SER	2.4
1	A	538	THR	2.4
2	B	590	ARG	2.4
2	B	301	ALA	2.4
2	B	138	MET	2.4
2	B	235	PRO	2.4
1	A	400	ARG	2.4
1	A	398	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	373	PHE	2.3
1	A	235	GLU	2.3
2	B	303	PRO	2.3
2	B	592	MET	2.2
1	A	336	ALA	2.2
1	A	397	LEU	2.2
1	A	404	ILE	2.2
1	A	143	ASP	2.2
2	B	494	ASP	2.2
2	B	466	VAL	2.2
2	B	285	PRO	2.1
2	B	189	ILE	2.1
2	B	166	ASP	2.1
2	B	391	ASP	2.1
2	B	718	ARG	2.1
2	B	544	GLY	2.1
1	A	441	PHE	2.1
1	A	503	PHE	2.1
1	A	238	LYS	2.0
1	A	316	PHE	2.0
1	A	526	PHE	2.0
2	B	236	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

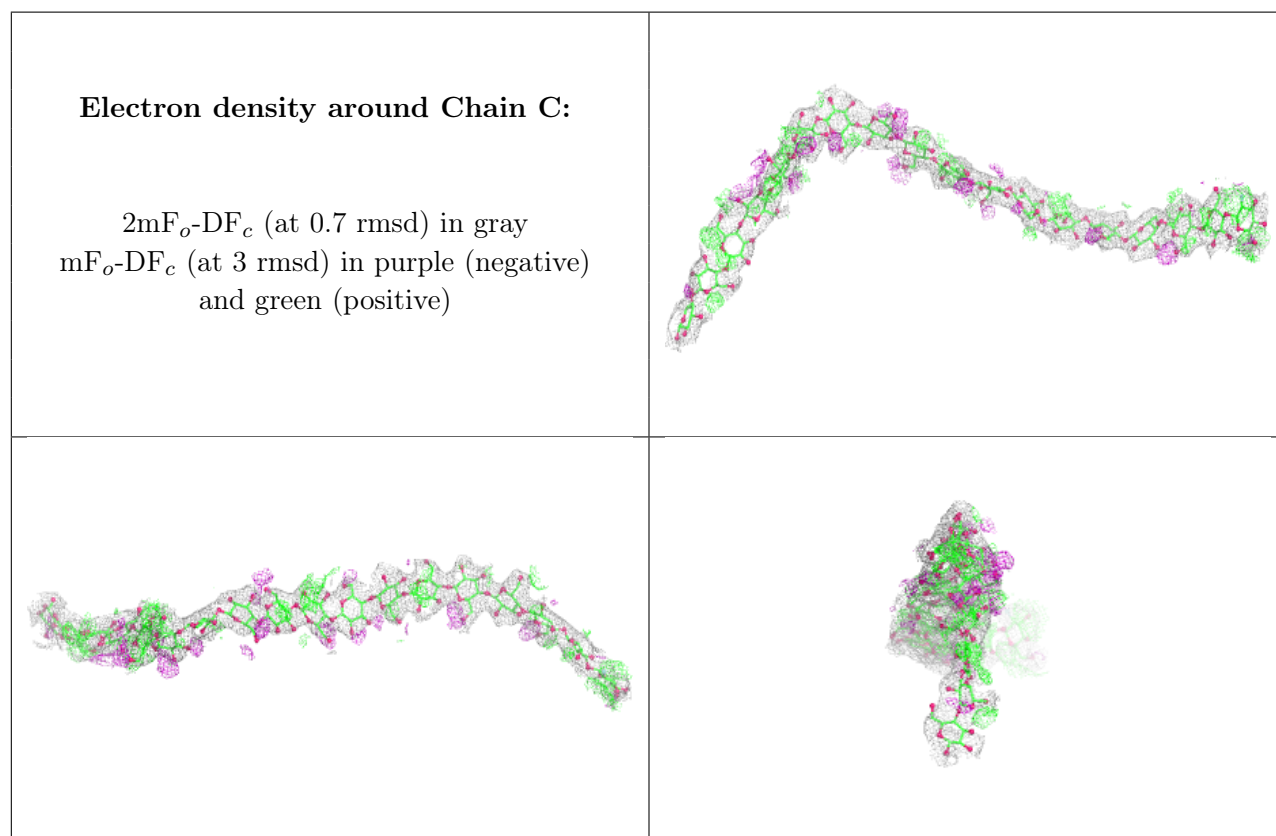
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BGC	C	1	12/12	-	-	120,132,137,143	0
4	BGC	C	2	11/12	-	-	100,107,112,112	0
4	BGC	C	3	11/12	-	-	81,91,107,109	0
4	BGC	C	4	11/12	-	-	56,67,86,93	0
4	BGC	C	5	11/12	-	-	49,52,86,113	0
4	BGC	C	6	11/12	-	-	50,58,80,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BGC	C	7	11/12	-	-	49,57,76,89	0
4	BGC	C	8	11/12	-	-	67,85,116,135	0
4	BGC	C	9	11/12	-	-	84,91,101,106	0
4	BGC	C	10	11/12	-	-	65,96,113,131	0
4	BGC	C	11	11/12	-	-	77,86,100,103	0
4	BGC	C	12	11/12	-	-	64,80,89,94	0
4	BGC	C	13	11/12	-	-	66,71,88,92	0
4	BGC	C	14	11/12	-	-	57,74,80,87	0
4	BGC	C	15	11/12	-	-	62,76,87,89	0
4	BGC	C	16	11/12	-	-	69,75,90,100	0
4	BGC	C	17	11/12	-	-	77,82,98,99	0
4	SHG	C	18	11/12	-	-	100,108,125,138	0

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



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

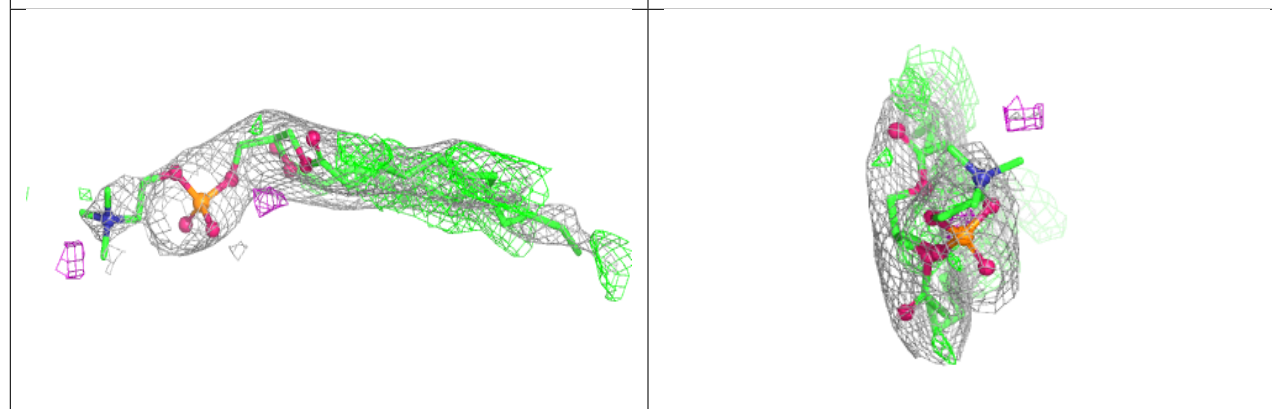
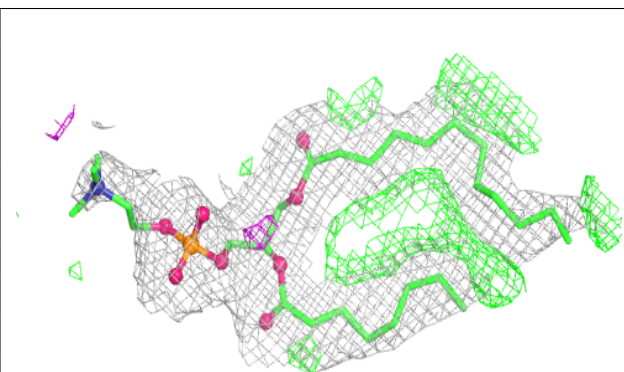
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	A	922	1/1	0.36	0.60	98,98,98,98	0
10	UND	B	802	11/11	0.72	0.37	63,68,80,82	0
8	PLC	A	923	38/42	0.74	0.31	87,124,155,157	0
8	PLC	B	803	9/42	0.80	0.33	49,77,87,92	0
9	3PE	A	924	20/51	0.83	0.18	87,105,115,120	0
8	PLC	B	804	11/42	0.84	0.30	72,83,94,97	0
7	MG	B	801	1/1	0.88	0.12	61,61,61,61	0
5	C2E	A	920	46/46	0.91	0.09	49,74,90,101	0
6	UDP	A	921	25/25	0.93	0.10	77,102,116,116	0
5	C2E	A	919	46/46	0.94	0.09	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.

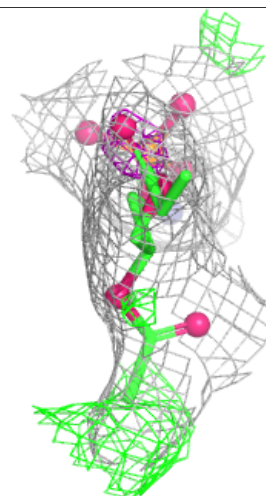
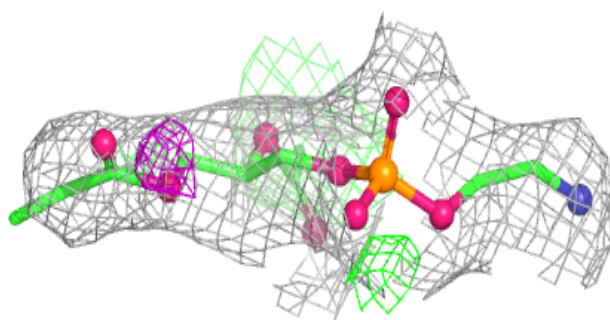
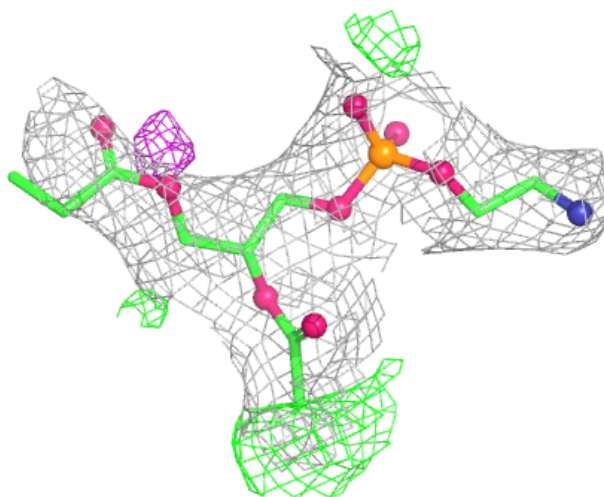
Electron density around PLC A 923:

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



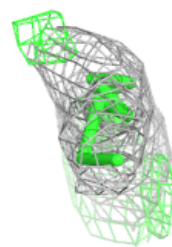
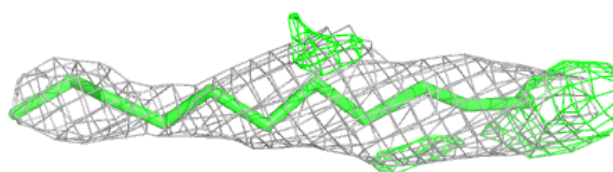
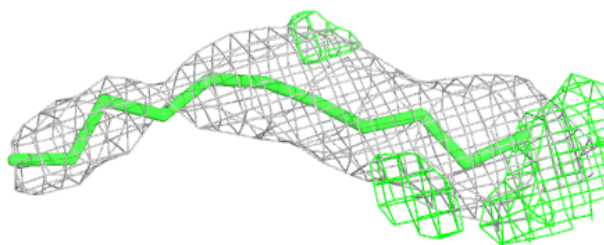
Electron density around 3PE A 924:

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



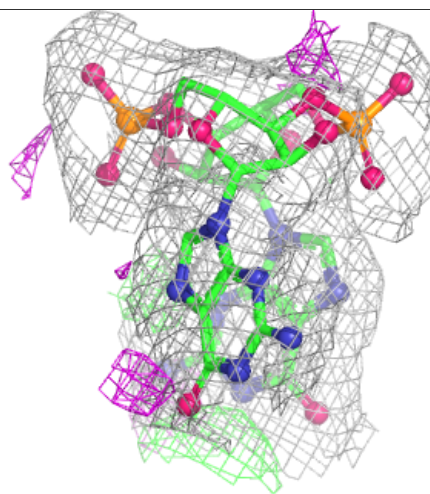
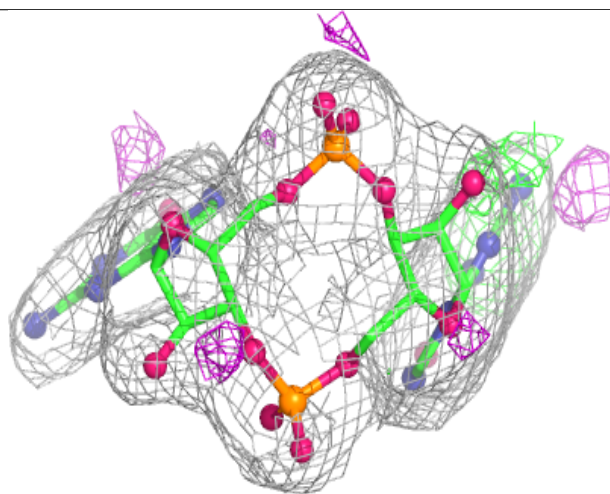
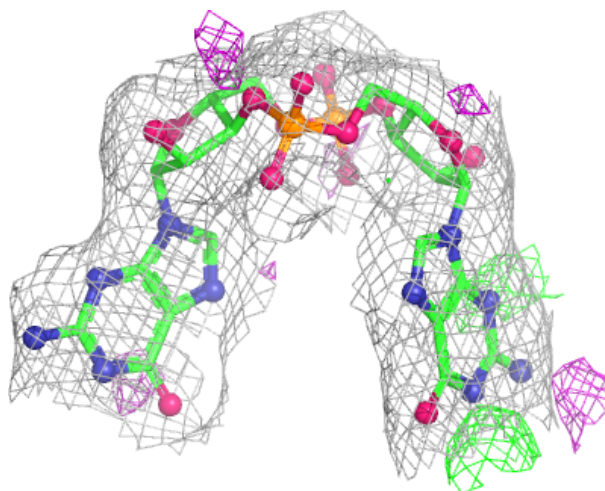
Electron density around PLC B 804:

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



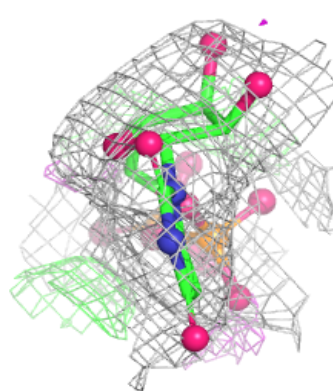
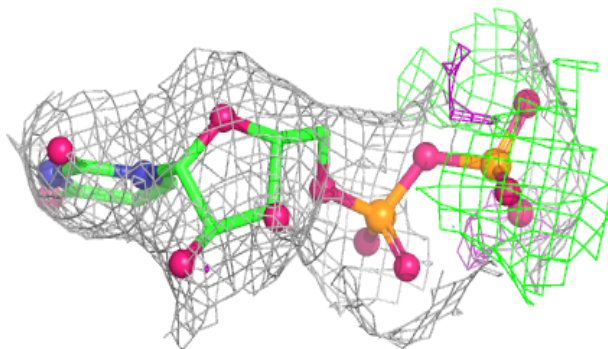
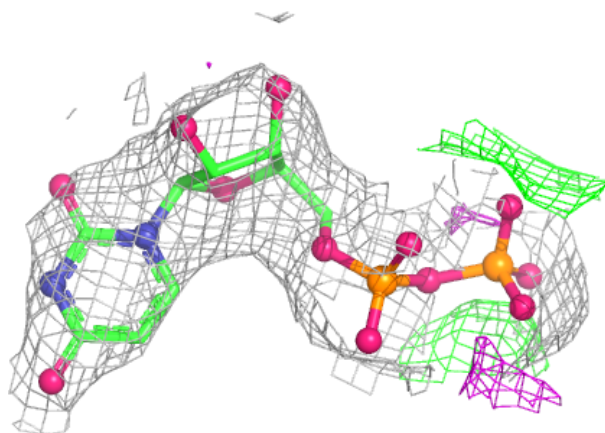
Electron density around C2E A 920:

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



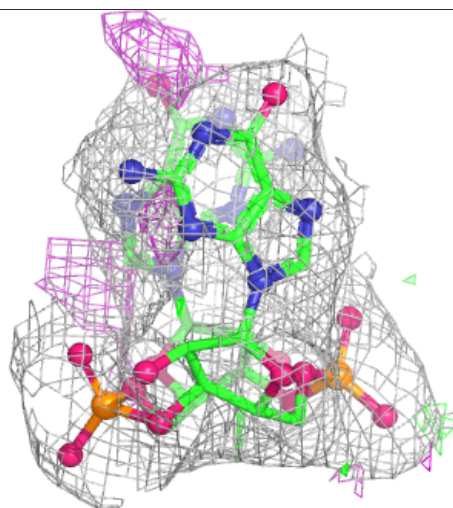
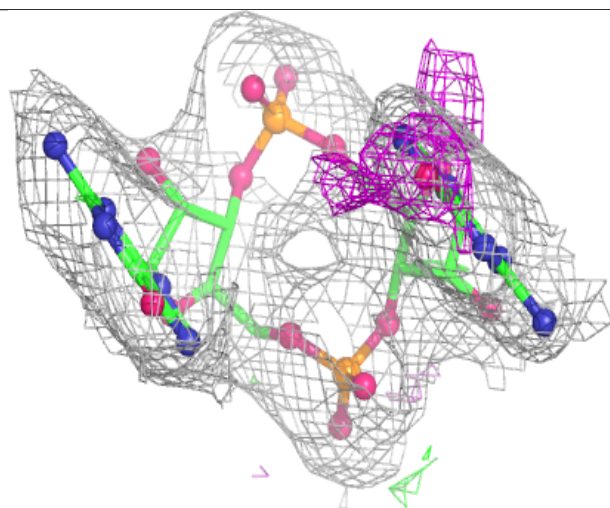
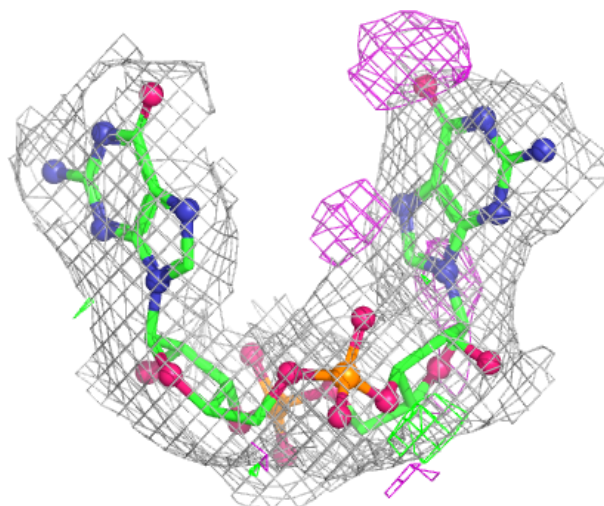
Electron density around UDP A 921:

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



Electron density around C2E A 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 [i](#)

There are no such residues in this entry.