



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 AM UTC

PDB ID : 5EJ1 / pdb_00005ej1
Title : Pre-translocation state of bacterial cellulose synthase
Authors : Moragn, J.L.W.; Zimmer, J.
Deposited on : 2015-10-30
Resolution : 3.40 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

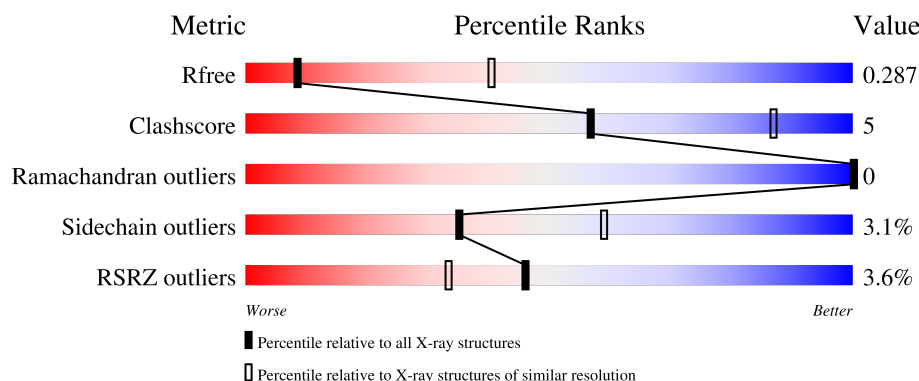
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	728	4% 84% 14% .
2	B	669	3% 89% 8% ..
3	D	7	100%
4	C	18	56% 44%

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 2 is a protein called Putative cellulose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	657	Total	C	N	O	S	0	0	0
			4899	3108	866	909	16			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	0	0	0
			35	21	7	7			

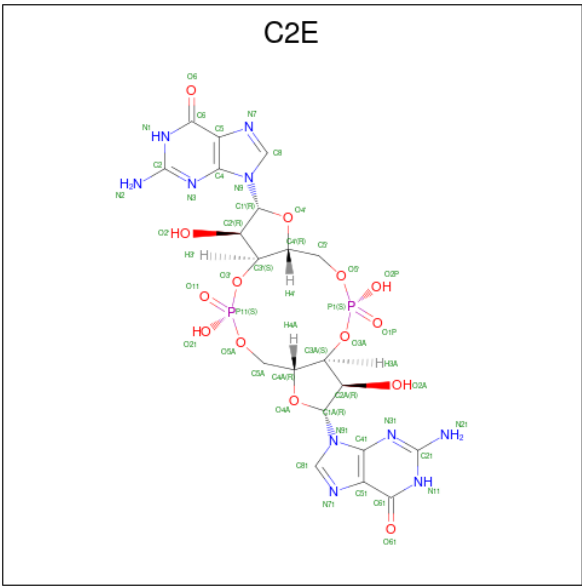
- [illegible]



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	C	18	Total	C	O	0	0	0
			199	108	91			

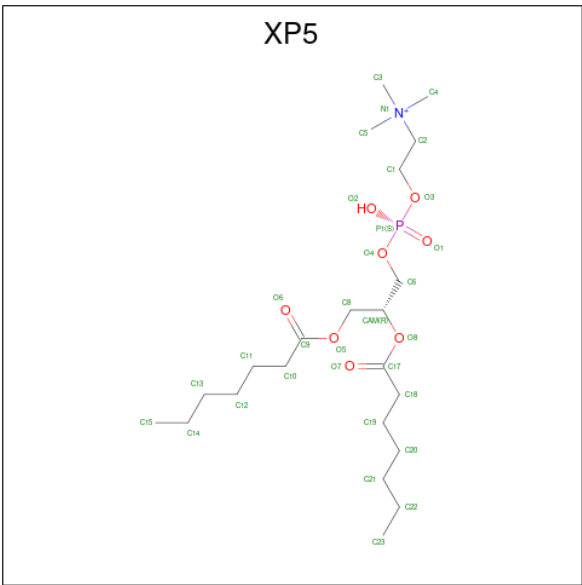
- Molecule 5 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-i][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-

diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (CCD ID: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).



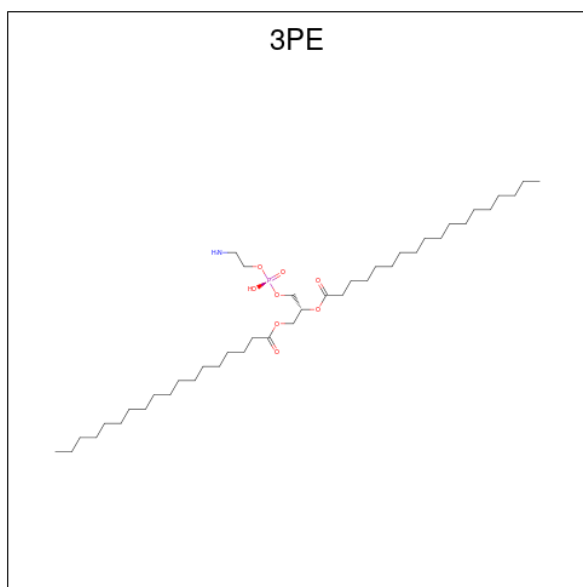
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 46	C 20	N 10	O 14	P 2	0	0
5	A	1	Total 46	C 20	N 10	O 14	P 2	0	0

- Molecule 6 is (4S,7R)-7-(heptanoyloxy)-4-hydroxy-N,N,N-trimethyl-10-oxo-3,5,9-trioxa-4-phosphahehexadecan-1-aminium 4-oxide (CCD ID: XP5) (formula: C₂₂H₄₅NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			22	13	1	7	1		
6	B	1	Total	C	N	O	P	0	0
			19	10	1	7	1		

- Molecule 7 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).

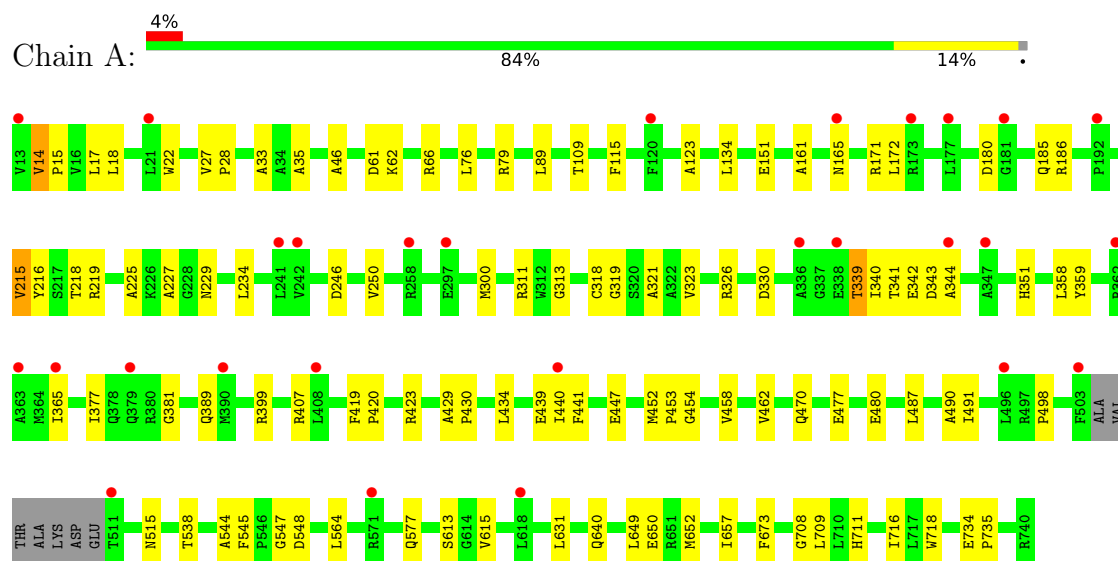


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			20	10	1	8	1		
7	A	1	Total	C				0	0
			8	8					

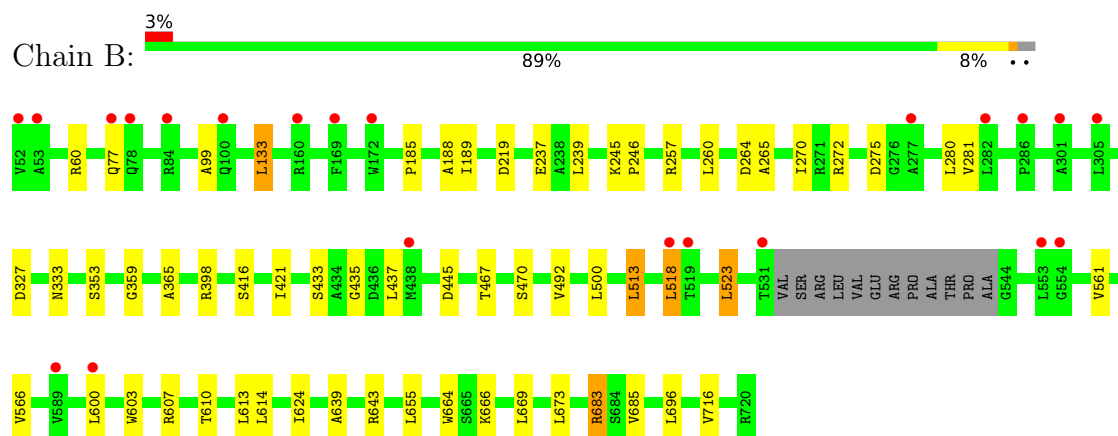
3 Residue-property plots

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



• Molecule 3: poly(unk)



There are no outlier residues recorded for this chain.

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

Chain C:  56% 44%

BGC1	BGC2	BGC3	BGC4	BGC5	BGC6	BGC7	BGC8	BGC9	BGC10	BGC11	BGC12	BGC13	BGC14	BGC15	BGC16	BGC17	BGC18
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.36Å 218.23Å 220.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 – 3.40 24.86 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.86-3.40) 99.5 (24.86-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.233 , 0.277 0.242 , 0.287	Depositor DCC
R_{free} test set	2300 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	120.9	Xtriage
Anisotropy	0.798	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10978	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C2E, 3PE, BGC, XP5

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	0.35	0/5829	0.73	5/7926 (0.1%)
2	B	0.35	0/5018	0.69	1/6883 (0.0%)
All	All	0.35	0/10847	0.71	6/14809 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ILE	N-CA-C	-8.86	104.72	111.90
1	A	14	VAL	CB-CA-C	-6.26	107.72	114.35
1	A	339	THR	N-CA-C	5.79	117.86	108.08
1	A	225	ALA	CB-CA-C	-5.54	110.17	116.54
2	B	518	LEU	CB-CA-C	-5.42	108.74	115.89
1	A	339	THR	CB-CA-C	-5.15	110.66	116.63

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	5684	0	5796	67	0
2	B	4899	0	4979	31	0
3	D	35	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	199	0	164	13	0
5	A	92	0	41	7	0
6	A	22	0	25	0	0
6	B	19	0	19	1	0
7	A	28	0	29	4	0
All	All	10978	0	11064	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (101) 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)
5:A:920:C2E:O4'	5:A:920:C2E:C4'	1.64	1.14
5:A:919:C2E:C4'	5:A:919:C2E:O4'	1.63	1.07
2:B:566:VAL:HG21	4:C:5:BGC:O2	1.69	0.93
2:B:513:LEU:HD21	2:B:523:LEU:HD22	1.61	0.83
1:A:319:GLY:HA3	4:C:18:BGC:H5	1.69	0.75
1:A:66:ARG:NH1	1:A:123:ALA:O	2.21	0.72
2:B:513:LEU:CD2	2:B:523:LEU:HD22	2.20	0.71
1:A:76:LEU:HD21	1:A:454:GLY:C	2.15	0.69
1:A:318:CYS:O	4:C:18:BGC:H5	1.95	0.67
1:A:480:GLU:OE1	4:C:14:BGC:O6	2.16	0.63
1:A:326:ARG:NH1	1:A:330:ASP:OD1	2.32	0.62
2:B:566:VAL:CG2	4:C:5:BGC:O2	2.46	0.61
1:A:341:THR:O	1:A:341:THR:HG23	2.00	0.61
1:A:161:ALA:O	1:A:165:ASN:ND2	2.33	0.60
2:B:60:ARG:NE	2:B:237:GLU:OE1	2.33	0.60
2:B:513:LEU:CD2	2:B:523:LEU:CD2	2.79	0.60
1:A:318:CYS:O	4:C:18:BGC:C5	2.52	0.58
2:B:264:ASP:OD1	2:B:265:ALA:N	2.37	0.57
2:B:639:ALA:O	2:B:643:ARG:NH2	2.37	0.57
1:A:718:TRP:HE3	7:A:923:3PE:H2D1	1.69	0.57
5:A:920:C2E:H81	5:A:920:C2E:H512	1.85	0.57
1:A:547:GLY:HA3	4:C:6:BGC:H2	1.86	0.56
2:B:513:LEU:HD23	2:B:523:LEU:CD2	2.36	0.56
1:A:76:LEU:HD21	1:A:454:GLY:O	2.06	0.56
1:A:341:THR:O	1:A:341:THR:CG2	2.54	0.55
2:B:398:ARG:NH2	2:B:445:ASP:OD1	2.39	0.55
2:B:77:GLN:NE2	2:B:333:ASN:OD1	2.39	0.55
1:A:447:GLU:OE2	2:B:353:SER:OG	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ASN:OD1	1:A:577:GLN:N	2.40	0.53
1:A:613:SER:HG	5:A:919:C2E:HO2A	1.55	0.53
2:B:467:THR:O	2:B:470:SER:OG	2.26	0.53
2:B:257:ARG:NH1	2:B:275:ASP:OD2	2.43	0.52
1:A:61:ASP:OD1	1:A:62:LYS:N	2.44	0.51
1:A:711:HIS:HB2	7:A:922:3PE:H122	1.92	0.51
2:B:603:TRP:O	2:B:607:ARG:NH1	2.44	0.51
5:A:920:C2E:H81	5:A:920:C2E:C5A	2.41	0.50
2:B:245:LYS:HB3	2:B:246:PRO:HD2	1.93	0.50
2:B:433:SER:OG	2:B:435:GLY:O	2.27	0.50
2:B:683:ARG:HE	6:B:801:XP5:H53C	1.76	0.50
1:A:313:GLY:O	1:A:351:HIS:NE2	2.44	0.50
1:A:487:LEU:O	1:A:490:ALA:N	2.43	0.50
1:A:300:MET:HA	1:A:470:GLN:HB3	1.93	0.49
1:A:640:GLN:NE2	1:A:650:GLU:OE2	2.46	0.49
2:B:365:ALA:N	2:B:437:LEU:O	2.46	0.49
1:A:14:VAL:N	1:A:15:PRO:HD2	2.28	0.49
2:B:189:ILE:O	2:B:272:ARG:NH1	2.46	0.48
1:A:46:ALA:HA	1:A:76:LEU:HD13	1.94	0.48
1:A:389:GLN:NE2	1:A:498:PRO:O	2.47	0.48
1:A:423:ARG:NH1	4:C:12:BGC:O6	2.47	0.47
1:A:477:GLU:N	1:A:477:GLU:OE1	2.44	0.47
2:B:664:TRP:CH2	2:B:666:LYS:HA	2.49	0.47
1:A:76:LEU:HD23	1:A:458:VAL:HG22	1.95	0.47
1:A:439:GLU:HB2	4:C:8:BGC:H6C2	1.96	0.47
1:A:14:VAL:O	1:A:17:LEU:N	2.45	0.47
1:A:708:GLY:HA3	7:A:922:3PE:H111	1.97	0.47
2:B:610:THR:N	2:B:655:LEU:O	2.45	0.47
1:A:246:ASP:OD2	4:C:18:BGC:O6	2.29	0.46
1:A:76:LEU:HD23	1:A:458:VAL:CG2	2.45	0.46
1:A:18:LEU:O	1:A:22:TRP:N	2.47	0.46
2:B:185:PRO:HG2	2:B:188:ALA:HB2	1.98	0.45
1:A:115:PHE:HE1	1:A:462:VAL:HG11	1.81	0.45
2:B:600:LEU:HD12	2:B:600:LEU:N	2.32	0.44
1:A:377:ILE:O	1:A:381:GLY:N	2.48	0.44
1:A:76:LEU:CD2	1:A:454:GLY:O	2.65	0.44
1:A:709:LEU:N	7:A:922:3PE:O14	2.46	0.44
1:A:180:ASP:OD1	1:A:229:ASN:ND2	2.49	0.43
1:A:441:PHE:HB3	4:C:9:BGC:H3	2.01	0.43
1:A:548:ASP:OD1	4:C:7:BGC:O6	2.28	0.43
1:A:734:GLU:N	1:A:735:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:HA	1:A:79:ARG:HD2	2.02	0.42
1:A:180:ASP:O	1:A:186:ARG:NE	2.52	0.42
5:A:920:C2E:H511	5:A:920:C2E:H3'	2.02	0.42
1:A:419:PHE:N	1:A:420:PRO:CD	2.83	0.42
1:A:35:ALA:O	1:A:79:ARG:NH2	2.50	0.42
1:A:452:MET:HB3	1:A:453:PRO:HD3	2.01	0.42
1:A:343:ASP:OD1	1:A:344:ALA:N	2.52	0.42
1:A:399:ARG:O	1:A:407:ARG:NH2	2.53	0.42
1:A:434:LEU:HD22	1:A:538:THR:HG22	2.02	0.41
1:A:311:ARG:NH2	2:B:716:VAL:O	2.53	0.41
1:A:358:LEU:HD13	1:A:359:TYR:N	2.35	0.41
2:B:99:ALA:HB1	2:B:133:LEU:HD11	2.01	0.41
1:A:171:ARG:HG3	1:A:172:LEU:HD22	2.02	0.41
1:A:151:GLU:OE1	1:A:151:GLU:N	2.52	0.41
1:A:227:ALA:HB2	1:A:342:GLU:HB2	2.02	0.41
1:A:429:ALA:HB3	1:A:430:PRO:HD3	2.02	0.41
1:A:215:VAL:HG12	1:A:216:TYR:H	1.84	0.41
2:B:270:ILE:HG22	2:B:280:LEU:HA	2.01	0.41
2:B:359:GLY:HA3	2:B:398:ARG:NH2	2.36	0.41
1:A:218:THR:HG22	1:A:219:ARG:N	2.35	0.41
1:A:419:PHE:CD1	1:A:419:PHE:C	2.99	0.41
1:A:613:SER:OG	5:A:919:C2E:O2A	2.28	0.41
2:B:327:ASP:OD1	2:B:327:ASP:N	2.51	0.41
1:A:321:ALA:HB2	1:A:365:ILE:HG13	2.02	0.41
1:A:544:ALA:C	1:A:545:PHE:HD1	2.29	0.41
2:B:600:LEU:HG	2:B:664:TRP:CH2	2.56	0.41
1:A:439:GLU:CG	4:C:8:BGC:H6C2	2.51	0.40
1:A:487:LEU:O	1:A:491:ILE:N	2.54	0.40
2:B:219:ASP:OD1	2:B:219:ASP:N	2.51	0.40
1:A:234:LEU:O	1:A:326:ARG:NH2	2.54	0.40
1:A:27:VAL:N	1:A:28:PRO:HD2	2.37	0.40
1:A:615:VAL:HG23	1:A:673:PHE:CZ	2.57	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	717/728 (98%)	683 (95%)	34 (5%)	0	100	100
2	B	653/669 (98%)	638 (98%)	15 (2%)	0	100	100
All	All	1370/1397 (98%)	1321 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	593/598 (99%)	578 (98%)	15 (2%)	42	62
2	B	521/531 (98%)	501 (96%)	20 (4%)	29	54
All	All	1114/1129 (99%)	1079 (97%)	35 (3%)	35	59

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	109	THR
1	A	134	LEU
1	A	185	GLN
1	A	215	VAL
1	A	250	VAL
1	A	323	VAL
1	A	339	THR
1	A	440	ILE
1	A	564	LEU
1	A	631	LEU
1	A	649	LEU
1	A	652	MET
1	A	657	ILE

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Mol	Chain	Res	Type
1	A	716	ILE
2	B	133	LEU
2	B	239	LEU
2	B	260	LEU
2	B	281	VAL
2	B	416	SER
2	B	421	ILE
2	B	492	VAL
2	B	500	LEU
2	B	513	LEU
2	B	518	LEU
2	B	523	LEU
2	B	561	VAL
2	B	613	LEU
2	B	614	LEU
2	B	624	ILE
2	B	669	LEU
2	B	673	LEU
2	B	683	ARG
2	B	685	VAL
2	B	696	LEU

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

Mol	Chain	Res	Type
1	A	196	GLN
1	A	224	HIS
1	A	276	HIS
1	A	306	HIS
1	A	412	ASN
2	B	579	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	1.71	3 (27%)	15,15,17	1.57	3 (20%)
4	BGC	C	11	4	11,11,12	1.56	2 (18%)	15,15,17	1.02	0
4	BGC	C	12	4	11,11,12	1.65	3 (27%)	15,15,17	0.76	0
4	BGC	C	13	4	11,11,12	1.57	2 (18%)	15,15,17	1.10	0
4	BGC	C	14	4	11,11,12	1.57	2 (18%)	15,15,17	1.28	1 (6%)
4	BGC	C	15	4	11,11,12	1.59	3 (27%)	15,15,17	1.41	3 (20%)
4	BGC	C	16	4	11,11,12	1.50	1 (9%)	15,15,17	1.86	3 (20%)
4	BGC	C	17	4	11,11,12	1.71	3 (27%)	15,15,17	0.92	0
4	BGC	C	18	4	11,11,12	1.62	2 (18%)	15,15,17	0.93	0
4	BGC	C	2	4	11,11,12	1.70	3 (27%)	15,15,17	1.50	3 (20%)
4	BGC	C	3	4	11,11,12	1.64	3 (27%)	15,15,17	1.89	3 (20%)
4	BGC	C	4	4	11,11,12	1.66	3 (27%)	15,15,17	1.98	5 (33%)
4	BGC	C	5	4	11,11,12	1.56	2 (18%)	15,15,17	1.79	4 (26%)
4	BGC	C	6	4	11,11,12	2.06	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	1.62	3 (27%)	15,15,17	1.61	4 (26%)
4	BGC	C	9	4	11,11,12	1.61	2 (18%)	15,15,17	1.13	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

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

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	6	BGC	O5-C1	5.27	1.52	1.43
4	C	10	BGC	O5-C1	4.24	1.50	1.43
4	C	4	BGC	O5-C1	4.18	1.50	1.43
4	C	9	BGC	O5-C1	4.18	1.50	1.43
4	C	12	BGC	O5-C1	4.14	1.50	1.43
4	C	7	BGC	O5-C1	4.13	1.50	1.43
4	C	3	BGC	O5-C1	4.13	1.50	1.43
4	C	18	BGC	O5-C1	4.12	1.50	1.43
4	C	17	BGC	O5-C1	4.11	1.50	1.43
4	C	14	BGC	O5-C1	4.05	1.50	1.43
4	C	2	BGC	O5-C1	4.03	1.50	1.43
4	C	8	BGC	O5-C1	3.99	1.50	1.43
4	C	11	BGC	O5-C1	3.93	1.50	1.43
4	C	15	BGC	O5-C1	3.87	1.50	1.43
4	C	16	BGC	O5-C1	3.84	1.50	1.43
4	C	13	BGC	O5-C1	3.82	1.50	1.43
4	C	5	BGC	O5-C1	3.75	1.50	1.43
4	C	1	BGC	O5-C1	3.18	1.50	1.42
4	C	6	BGC	C2-C3	-2.81	1.48	1.52
4	C	6	BGC	O5-C5	2.71	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	17	BGC	C2-C3	-2.62	1.48	1.52
4	C	2	BGC	C2-C3	-2.59	1.48	1.52
4	C	13	BGC	C2-C3	-2.39	1.48	1.52
4	C	12	BGC	C2-C3	-2.36	1.48	1.52
4	C	5	BGC	O2-C2	2.36	1.48	1.43
4	C	7	BGC	O5-C5	2.35	1.48	1.43
4	C	15	BGC	C2-C3	-2.34	1.48	1.52
4	C	10	BGC	C2-C3	-2.33	1.48	1.52
4	C	2	BGC	O5-C5	2.32	1.48	1.43
4	C	7	BGC	C2-C3	-2.29	1.49	1.52
4	C	17	BGC	O5-C5	2.29	1.47	1.43
4	C	3	BGC	C2-C3	-2.28	1.49	1.52
4	C	8	BGC	O5-C5	2.24	1.47	1.43
4	C	18	BGC	C2-C3	-2.23	1.49	1.52
4	C	10	BGC	O5-C5	2.22	1.47	1.43
4	C	4	BGC	O5-C5	2.16	1.47	1.43
4	C	12	BGC	O5-C5	2.14	1.47	1.43
4	C	15	BGC	O5-C5	2.12	1.47	1.43
4	C	8	BGC	C2-C3	-2.12	1.49	1.52
4	C	9	BGC	C2-C3	-2.09	1.49	1.52
4	C	14	BGC	C2-C3	-2.07	1.49	1.52
4	C	4	BGC	C2-C3	-2.06	1.49	1.52
4	C	3	BGC	O5-C5	2.05	1.47	1.43
4	C	11	BGC	C2-C3	-2.05	1.49	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	4	BGC	C1-C2-C3	4.70	116.49	109.64
4	C	16	BGC	C1-C2-C3	4.64	116.39	109.64
4	C	10	BGC	C1-C2-C3	4.27	115.86	109.64
4	C	3	BGC	C1-C2-C3	4.13	115.65	109.64
4	C	5	BGC	C2-C3-C4	4.08	118.03	110.86
4	C	4	BGC	C2-C3-C4	3.87	117.66	110.86
4	C	3	BGC	C2-C3-C4	3.69	117.35	110.86
4	C	14	BGC	C1-C2-C3	3.63	114.93	109.64
4	C	5	BGC	C1-C2-C3	3.59	114.88	109.64
4	C	16	BGC	C2-C3-C4	3.29	116.65	110.86
4	C	1	BGC	C3-C4-C5	3.25	116.12	110.23
4	C	1	BGC	O5-C5-C4	3.20	115.47	109.70
4	C	9	BGC	C1-C2-C3	3.08	114.14	109.64
4	C	2	BGC	C3-C4-C5	3.00	115.67	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	BGC	C3-C4-C5	2.90	115.48	110.23
4	C	8	BGC	C3-C4-C5	2.82	115.35	110.23
4	C	8	BGC	C2-C3-C4	2.80	115.79	110.86
4	C	15	BGC	C3-C4-C5	2.70	115.13	110.23
4	C	5	BGC	C1-O5-C5	-2.61	108.69	112.19
4	C	5	BGC	O4-C4-C5	-2.57	102.98	109.32
4	C	2	BGC	C2-C3-C4	2.52	115.30	110.86
4	C	8	BGC	C1-C2-C3	2.52	113.31	109.64
4	C	4	BGC	C6-C5-C4	-2.31	107.34	113.02
4	C	1	BGC	C4-C3-C2	2.25	114.78	110.83
4	C	16	BGC	C3-C4-C5	2.24	114.29	110.23
4	C	10	BGC	C2-C3-C4	2.19	114.72	110.86
4	C	4	BGC	C3-C4-C5	2.19	114.21	110.23
4	C	15	BGC	C2-C3-C4	2.15	114.64	110.86
4	C	10	BGC	O3-C3-C2	-2.07	105.83	110.05
4	C	8	BGC	C1-O5-C5	-2.07	109.42	112.19
4	C	6	BGC	C1-C2-C3	2.02	112.59	109.64
4	C	15	BGC	C1-O5-C5	-2.01	109.49	112.19
4	C	4	BGC	O3-C3-C4	-2.01	105.64	110.38
4	C	2	BGC	C6-C5-C4	-2.00	108.10	113.02
4	C	1	BGC	C6-C5-C4	-2.00	108.11	113.02

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	7	BGC	O5-C5-C6-O6
4	C	18	BGC	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	11	BGC	O5-C5-C6-O6
4	C	1	BGC	O5-C5-C6-O6
4	C	7	BGC	C4-C5-C6-O6
4	C	17	BGC	O5-C5-C6-O6
4	C	4	BGC	O5-C5-C6-O6
4	C	8	BGC	O5-C5-C6-O6
4	C	18	BGC	O5-C5-C6-O6
4	C	14	BGC	C4-C5-C6-O6
4	C	16	BGC	C4-C5-C6-O6
4	C	11	BGC	C4-C5-C6-O6
4	C	17	BGC	C4-C5-C6-O6

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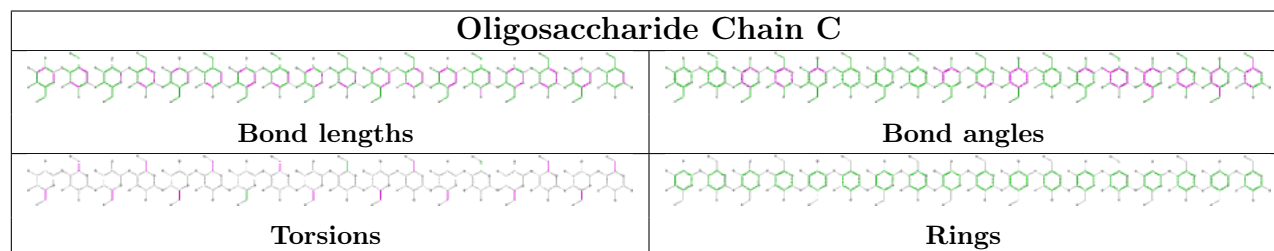
Mol	Chain	Res	Type	Atoms
4	C	8	BGC	C4-C5-C6-O6
4	C	4	BGC	C4-C5-C6-O6
4	C	13	BGC	O5-C5-C6-O6
4	C	13	BGC	C4-C5-C6-O6
4	C	2	BGC	C4-C5-C6-O6
4	C	15	BGC	C4-C5-C6-O6
4	C	15	BGC	O5-C5-C6-O6
4	C	6	BGC	O5-C5-C6-O6
4	C	10	BGC	O5-C5-C6-O6
4	C	3	BGC	O5-C5-C6-O6
4	C	1	BGC	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	7	BGC	1	0
4	C	9	BGC	1	0
4	C	14	BGC	1	0
4	C	8	BGC	2	0
4	C	12	BGC	1	0
4	C	6	BGC	1	0
4	C	5	BGC	2	0
4	C	18	BGC	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 oligosaccharide.



5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	XP5	B	801	-	18,18,31	1.25	1 (5%)	23,25,39	0.78	1 (4%)
5	C2E	A	919	-	52,52,52	3.92	32 (61%)	78,82,82	2.01	24 (30%)
7	3PE	A	922	-	19,19,50	1.38	4 (21%)	22,24,55	1.63	3 (13%)
5	C2E	A	920	-	52,52,52	3.92	31 (59%)	78,82,82	1.98	25 (32%)
6	XP5	A	921	-	21,21,31	1.27	2 (9%)	26,28,39	1.11	1 (3%)
7	3PE	A	923	-	7,7,50	0.31	0	6,6,55	0.80	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
6	XP5	B	801	-	-	5/19/19/35	-
5	C2E	A	919	-	-	3/30/62/62	0/6/7/7
7	3PE	A	922	-	-	10/22/22/54	-
5	C2E	A	920	-	-	8/30/62/62	0/6/7/7
6	XP5	A	921	-	-	7/24/24/35	-
7	3PE	A	923	-	-	3/5/5/54	-

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	919	C2E	C3'-C4'	-10.93	1.24	1.52
5	A	920	C2E	C3'-C4'	-10.76	1.25	1.52
5	A	919	C2E	O4A-C1A	9.09	1.63	1.42
5	A	920	C2E	O4A-C1A	9.02	1.62	1.42
5	A	920	C2E	O4'-C4'	8.58	1.64	1.45
5	A	919	C2E	O4'-C4'	8.45	1.63	1.45
5	A	920	C2E	C2A-C1A	-7.43	1.30	1.53
5	A	919	C2E	C2A-C1A	-7.32	1.30	1.53
5	A	919	C2E	C4-N3	6.91	1.50	1.34
5	A	920	C2E	C4-N3	6.88	1.50	1.34
5	A	920	C2E	C41-N31	6.59	1.49	1.34
5	A	919	C2E	C41-N31	6.52	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	919	C2E	C2-N3	6.24	1.48	1.33
5	A	920	C2E	C2-N3	6.09	1.47	1.33
5	A	919	C2E	O4A-C4A	-6.06	1.31	1.45
5	A	920	C2E	O4A-C4A	-5.93	1.31	1.45
5	A	919	C2E	C2-N2	5.76	1.47	1.34
5	A	920	C2E	C2-N2	5.64	1.47	1.34
5	A	920	C2E	C21-N31	5.55	1.46	1.33
5	A	919	C2E	C21-N31	5.48	1.46	1.33
5	A	920	C2E	P11-O3'	5.02	1.74	1.59
5	A	919	C2E	P11-O3'	4.98	1.74	1.59
5	A	919	C2E	O4'-C1'	-4.83	1.30	1.42
5	A	920	C2E	O4'-C1'	-4.82	1.30	1.42
5	A	920	C2E	C21-N21	4.60	1.44	1.34
5	A	919	C2E	C21-N21	4.46	1.44	1.34
5	A	919	C2E	P1-O3A	4.36	1.72	1.59
5	A	920	C2E	P1-O3A	4.34	1.72	1.59
5	A	920	C2E	O3'-C3'	3.63	1.56	1.44
5	A	919	C2E	O3'-C3'	3.52	1.56	1.44
5	A	920	C2E	O2A-C2A	3.37	1.51	1.43
5	A	920	C2E	C21-N11	3.33	1.45	1.37
5	A	919	C2E	O2A-C2A	3.30	1.51	1.43
5	A	920	C2E	P1-O5'	3.30	1.72	1.59
5	A	919	C2E	P1-O5'	3.20	1.71	1.59
5	A	919	C2E	C21-N11	3.17	1.45	1.37
5	A	919	C2E	C6-N1	3.16	1.44	1.38
5	A	919	C2E	C2-N1	2.94	1.44	1.37
5	A	920	C2E	C6-N1	2.93	1.44	1.38
5	A	920	C2E	C51-N71	-2.87	1.33	1.39
5	A	920	C2E	C2-N1	2.82	1.44	1.37
5	A	919	C2E	O3A-C3A	-2.82	1.34	1.44
5	A	920	C2E	O3A-C3A	-2.81	1.34	1.44
5	A	919	C2E	C5-C6	2.77	1.54	1.44
5	A	920	C2E	C5-C6	2.73	1.54	1.44
6	A	921	XP5	O8-CAM	-2.70	1.40	1.46
5	A	919	C2E	C51-N71	-2.65	1.33	1.39
5	A	919	C2E	P11-O5A	2.62	1.69	1.59
5	A	919	C2E	O2'-C2'	-2.61	1.36	1.43
5	A	920	C2E	P11-O5A	2.57	1.69	1.59
5	A	920	C2E	C2'-C3'	2.55	1.58	1.53
7	A	922	3PE	O21-C2	-2.55	1.40	1.46
5	A	919	C2E	C51-C61	2.54	1.53	1.44
5	A	919	C2E	C2'-C3'	2.54	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	920	C2E	O2'-C2'	-2.53	1.36	1.43
5	A	920	C2E	C51-C61	2.49	1.53	1.44
7	A	922	3PE	O31-C31	2.46	1.40	1.33
7	A	922	3PE	O21-C21	2.39	1.40	1.35
5	A	920	C2E	C61-N11	2.37	1.43	1.38
5	A	919	C2E	C61-N11	2.30	1.43	1.38
5	A	920	C2E	C41-N91	-2.27	1.32	1.38
5	A	919	C2E	C41-N91	-2.25	1.32	1.38
5	A	920	C2E	O6-C6	-2.18	1.19	1.23
6	B	801	XP5	O5-C8	-2.13	1.40	1.45
6	A	921	XP5	O8-C17	2.12	1.40	1.34
7	A	922	3PE	O31-C3	-2.11	1.40	1.45
5	A	920	C2E	C5A-C4A	2.10	1.57	1.51
5	A	919	C2E	C5A-C4A	2.07	1.57	1.51
5	A	919	C2E	O6-C6	-2.02	1.19	1.23
5	A	919	C2E	C5-N7	-2.02	1.35	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	922	3PE	O21-C21-C22	5.32	120.57	111.09
5	A	919	C2E	C51-C41-N31	-4.76	120.81	128.39
5	A	920	C2E	C51-C41-N31	-4.76	120.81	128.39
5	A	920	C2E	C1'-N9-C4	-4.66	112.71	126.49
5	A	919	C2E	C1'-N9-C4	-4.65	112.75	126.49
5	A	920	C2E	C5-C4-N3	-4.62	121.03	128.39
5	A	919	C2E	C5-C4-N3	-4.60	121.06	128.39
5	A	919	C2E	C21-N31-C41	4.24	119.60	112.30
5	A	920	C2E	C2-N3-C4	4.22	119.57	112.30
5	A	920	C2E	C21-N31-C41	4.22	119.56	112.30
5	A	919	C2E	C2-N3-C4	4.21	119.55	112.30
6	A	921	XP5	O8-C17-C18	3.97	120.06	111.48
5	A	919	C2E	N91-C81-N71	-3.93	106.12	113.40
5	A	920	C2E	N91-C81-N71	-3.80	106.35	113.40
5	A	920	C2E	N9-C8-N7	-3.73	106.48	113.40
5	A	919	C2E	N9-C8-N7	-3.70	106.53	113.40
5	A	920	C2E	N91-C41-N31	3.70	133.35	125.95
5	A	920	C2E	C1'-N9-C8	3.63	137.04	126.73
5	A	919	C2E	C1'-N9-C8	3.62	137.01	126.73
5	A	919	C2E	N91-C41-N31	3.57	133.09	125.95
5	A	919	C2E	N9-C4-N3	3.23	132.40	125.95
5	A	920	C2E	N9-C4-N3	3.21	132.38	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	919	C2E	C3A-C2A-C1A	3.03	106.56	99.89
7	A	922	3PE	O31-C31-C32	3.03	120.33	111.15
5	A	920	C2E	C21-N11-C61	-2.95	119.76	125.11
5	A	919	C2E	C21-N11-C61	-2.95	119.77	125.11
5	A	919	C2E	C2-N1-C6	-2.87	119.91	125.11
5	A	920	C2E	C2-N1-C6	-2.79	120.05	125.11
7	A	922	3PE	C2-O21-C21	-2.77	112.96	117.85
5	A	919	C2E	C51-C61-N11	2.67	120.05	113.25
5	A	920	C2E	C51-C61-N11	2.65	120.01	113.25
5	A	919	C2E	O21-P11-O3'	2.64	117.44	106.70
5	A	920	C2E	O61-C61-C51	-2.61	119.64	126.53
5	A	919	C2E	C5-C6-N1	2.61	119.90	113.25
5	A	920	C2E	C5-C6-N1	2.61	119.90	113.25
5	A	919	C2E	C3'-C2'-C1'	2.61	105.63	99.89
5	A	919	C2E	C81-N91-C41	2.61	110.91	106.03
5	A	920	C2E	C3A-C2A-C1A	2.59	105.58	99.89
5	A	919	C2E	O6-C6-C5	-2.56	119.77	126.53
5	A	920	C2E	C81-N91-C41	2.53	110.77	106.03
5	A	919	C2E	O61-C61-C51	-2.52	119.87	126.53
5	A	920	C2E	O6-C6-C5	-2.52	119.88	126.53
5	A	920	C2E	O21-P11-O3'	2.50	116.88	106.70
5	A	919	C2E	C81-N71-C51	2.35	108.44	104.26
5	A	919	C2E	C8-N7-C5	2.34	108.44	104.26
5	A	920	C2E	C8-N7-C5	2.33	108.42	104.26
5	A	920	C2E	C3'-C2'-C1'	2.32	105.00	99.89
5	A	920	C2E	C81-N71-C51	2.27	108.30	104.26
5	A	920	C2E	C8-N9-C4	2.25	110.25	106.03
5	A	919	C2E	C8-N9-C4	2.25	110.23	106.03
5	A	920	C2E	O21-P11-O5A	2.20	117.53	107.57
5	A	920	C2E	P11-O5A-C5A	-2.14	109.11	121.35
5	A	919	C2E	O21-P11-O5A	2.09	117.06	107.57
6	B	801	XP5	C1-C2-N1	-2.05	109.23	115.82

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	920	C2E	C5'-O5'-P1-O1P
5	A	920	C2E	C5A-O5A-P11-O3'
5	A	920	C2E	C5A-O5A-P11-O21
5	A	920	C2E	C5A-O5A-P11-O11
5	A	920	C2E	O4A-C4A-C5A-O5A

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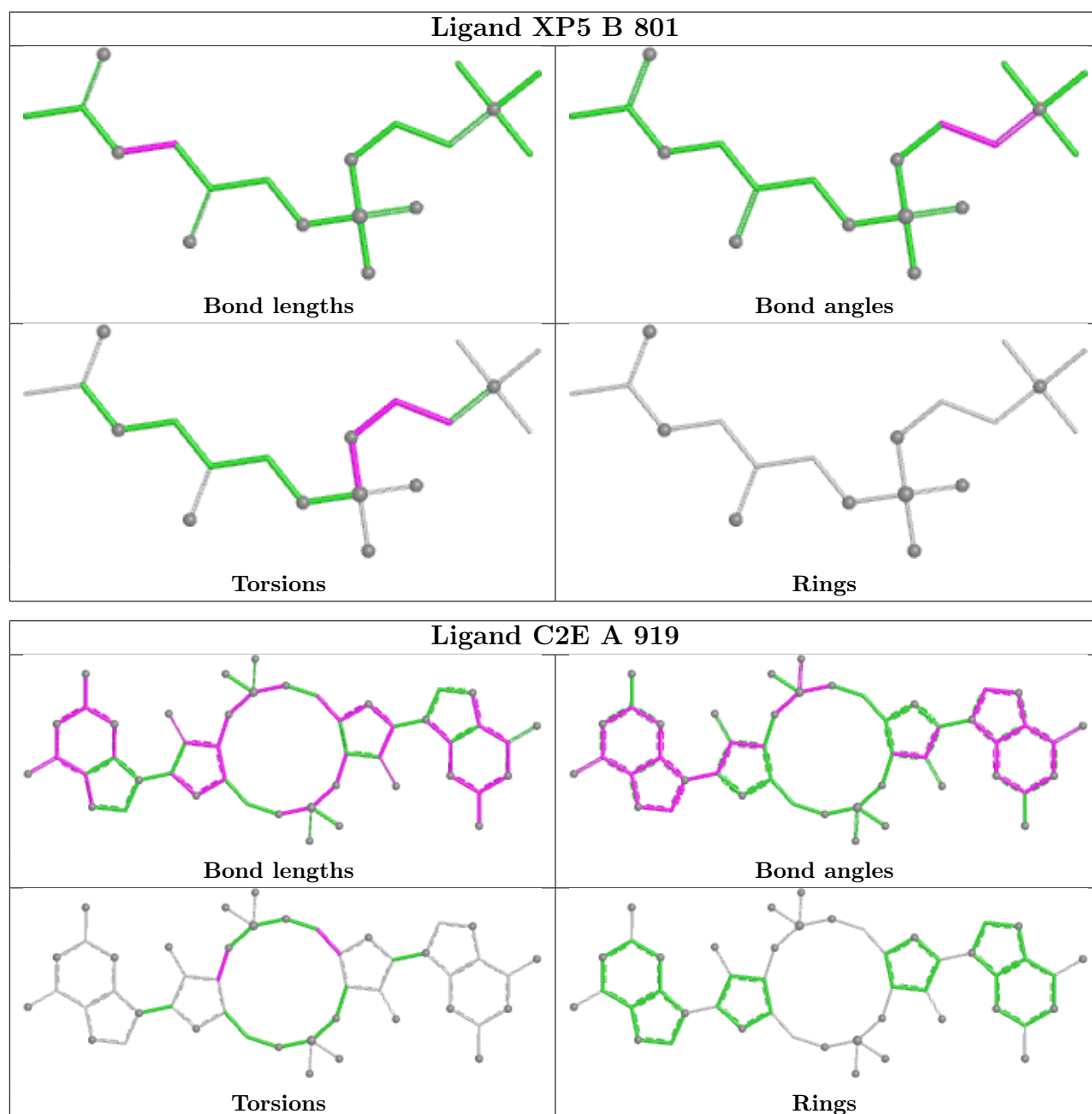
Mol	Chain	Res	Type	Atoms
5	A	920	C2E	C3A-C4A-C5A-O5A
6	A	921	XP5	C1-O3-P1-O1
6	A	921	XP5	C1-O3-P1-O4
6	A	921	XP5	C2-C1-O3-P1
6	A	921	XP5	O3-C1-C2-N1
6	B	801	XP5	C1-O3-P1-O2
6	B	801	XP5	O3-C1-C2-N1
7	A	922	3PE	C1-O11-P-O12
7	A	922	3PE	C1-O11-P-O13
7	A	922	3PE	C1-O11-P-O14
7	A	922	3PE	C11-O13-P-O11
7	A	922	3PE	O13-C11-C12-N
7	A	922	3PE	C22-C21-O21-C2
7	A	922	3PE	O22-C21-O21-C2
7	A	923	3PE	C2D-C2E-C2F-C2G
5	A	919	C2E	C2'-C3'-O3'-P11
7	A	923	3PE	C2C-C2D-C2E-C2F
6	B	801	XP5	C2-C1-O3-P1
7	A	923	3PE	C2F-C2G-C2H-C2I
7	A	922	3PE	O11-C1-C2-O21
5	A	920	C2E	C5'-O5'-P1-O2P
5	A	920	C2E	C5'-O5'-P1-O3A
6	B	801	XP5	C1-O3-P1-O1
6	B	801	XP5	C1-O3-P1-O4
7	A	922	3PE	C11-O13-P-O14
6	A	921	XP5	O5-C8-CAM-C6
7	A	922	3PE	O11-C1-C2-C3
6	A	921	XP5	O5-C8-CAM-O8
5	A	919	C2E	O4A-C4A-C5A-O5A
5	A	919	C2E	C4'-C3'-O3'-P11
6	A	921	XP5	O8-C17-C18-C19

There are no ring outliers.

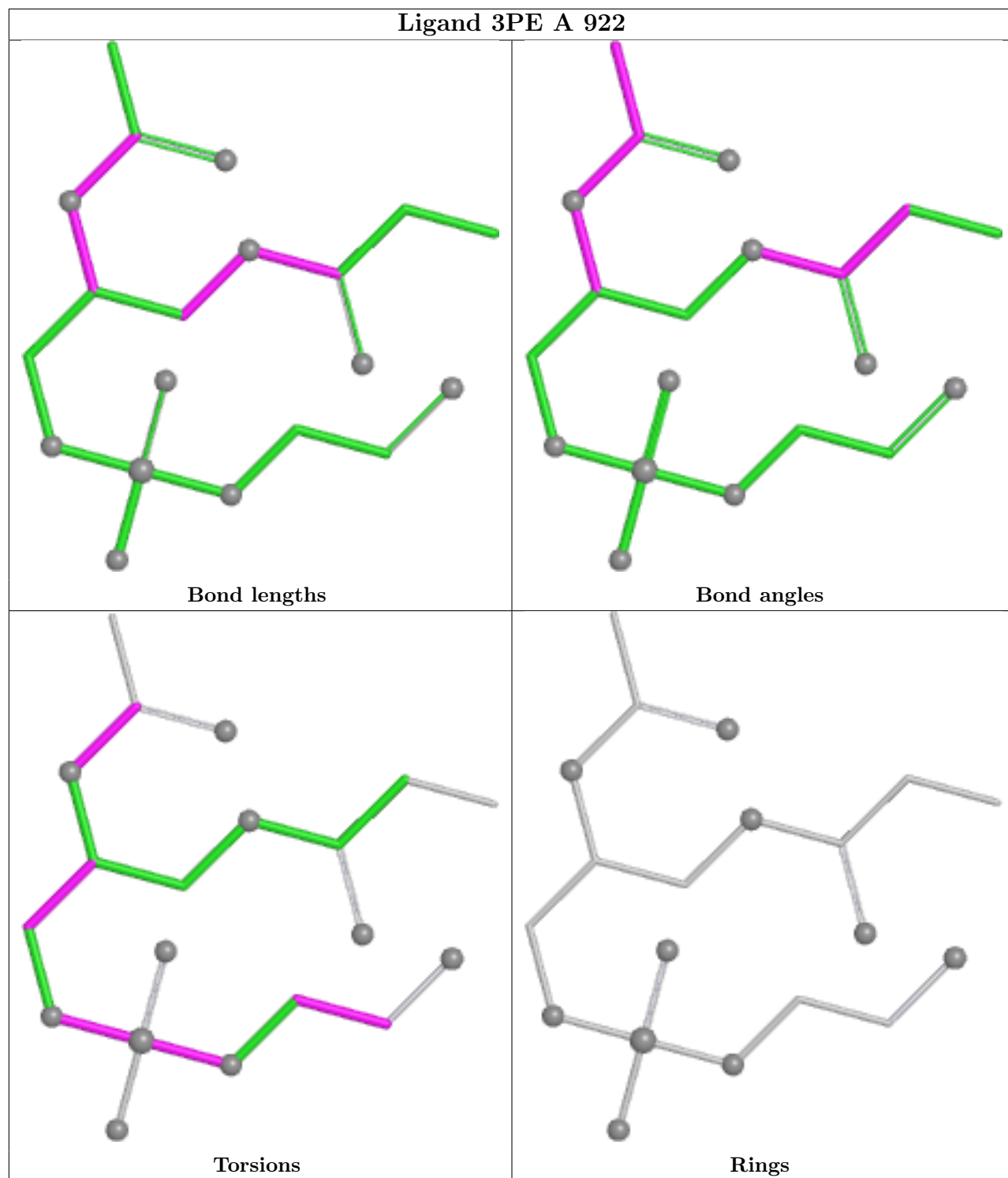
5 monomers are involved in 12 short contacts:

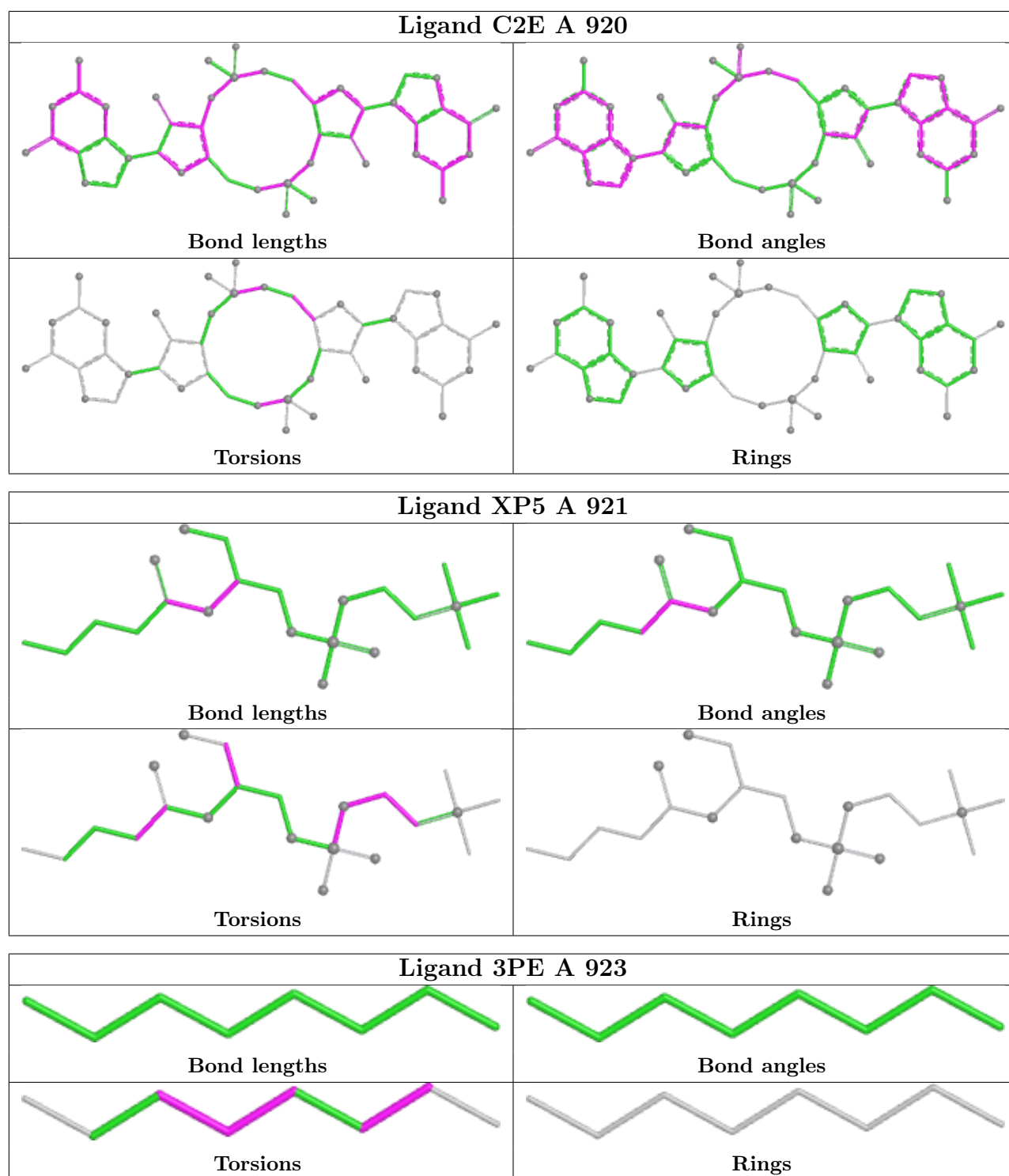
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	801	XP5	1	0
5	A	919	C2E	3	0
7	A	922	3PE	3	0
5	A	920	C2E	4	0
7	A	923	3PE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand 3PE A 922





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	173:UNK	C	175:UNK	N	4.64

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	721/728 (99%)	0.14	28 (3%) 43 31	95, 145, 232, 335	0
2	B	657/669 (98%)	0.11	22 (3%) 49 36	93, 139, 213, 325	0
3	D	0/7	-	-	-	-
All	All	1378/1404 (98%)	0.13	50 (3%) 46 33	93, 142, 227, 335	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	LEU	4.6
2	B	589	VAL	4.1
2	B	518	LEU	3.9
2	B	78	GLN	3.9
1	A	362	ARG	3.8
2	B	531	THR	3.4
2	B	160	ARG	3.4
2	B	84	ARG	3.3
1	A	408	LEU	3.3
1	A	258	ARG	3.2
2	B	100	GLN	3.2
2	B	305	LEU	3.2
2	B	52	VAL	3.0
2	B	600	LEU	2.9
2	B	282	LEU	2.9
1	A	177	LEU	2.9
1	A	297	GLU	2.7
1	A	344	ALA	2.7
2	B	169	PHE	2.6
1	A	173	ARG	2.6
2	B	53	ALA	2.5
1	A	181	GLY	2.5
1	A	21	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	365	ILE	2.5
2	B	438	MET	2.4
1	A	242	VAL	2.4
1	A	503	PHE	2.4
2	B	554	GLY	2.4
1	A	336	ALA	2.3
2	B	301	ALA	2.3
1	A	511	THR	2.3
1	A	120	PHE	2.3
1	A	379	GLN	2.3
1	A	571	ARG	2.3
1	A	338	GLU	2.2
2	B	286	PRO	2.2
2	B	77	GLN	2.2
2	B	277	ALA	2.2
1	A	13	VAL	2.2
1	A	363	ALA	2.2
1	A	192	PRO	2.2
2	B	519	THR	2.1
1	A	390	MET	2.1
1	A	347	ALA	2.1
1	A	241	LEU	2.1
2	B	553	LEU	2.1
1	A	165	ASN	2.0
1	A	618	LEU	2.0
2	B	172	TRP	2.0
1	A	440	ILE	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.

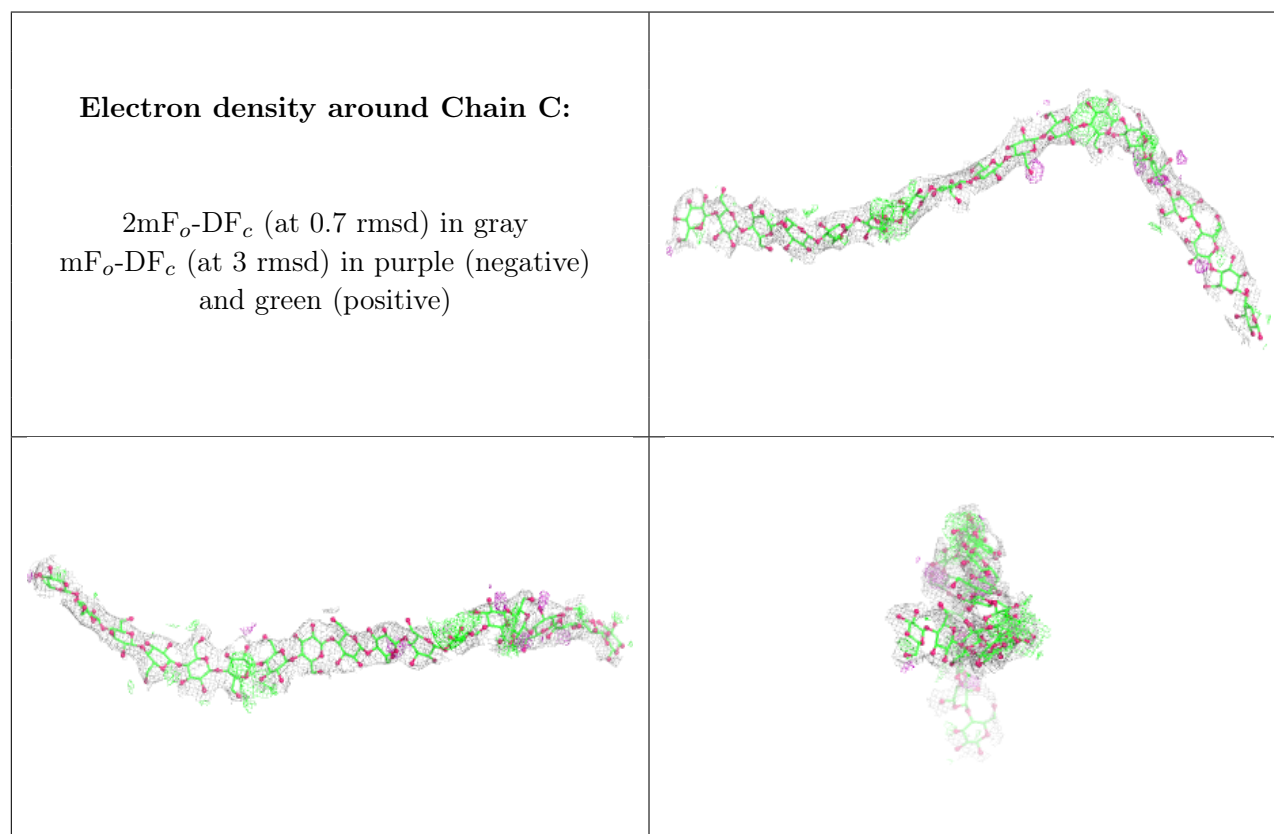
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BGC	C	1	12/12	-	-	267,272,285,306	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BGC	C	2	11/12	-	-	185,200,214,230	0
4	BGC	C	3	11/12	-	-	181,200,213,215	0
4	BGC	C	4	11/12	-	-	119,127,169,194	0
4	BGC	C	5	11/12	-	-	111,114,128,173	0
4	BGC	C	6	11/12	-	-	149,158,183,204	0
4	BGC	C	7	11/12	-	-	118,136,142,154	0
4	BGC	C	8	11/12	-	-	153,158,185,206	0
4	BGC	C	9	11/12	-	-	112,117,123,127	0
4	BGC	C	10	11/12	-	-	117,125,144,150	0
4	BGC	C	11	11/12	-	-	136,138,142,142	0
4	BGC	C	12	11/12	-	-	150,155,158,161	0
4	BGC	C	13	11/12	-	-	148,153,155,155	0
4	BGC	C	14	11/12	-	-	132,133,134,134	0
4	BGC	C	15	11/12	-	-	146,146,147,148	0
4	BGC	C	16	11/12	-	-	168,168,169,170	0
4	BGC	C	17	11/12	-	-	142,144,146,147	0
4	BGC	C	18	11/12	-	-	160,161,162,163	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 ⓘ

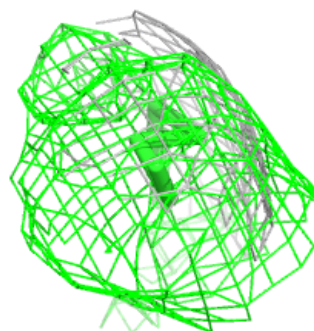
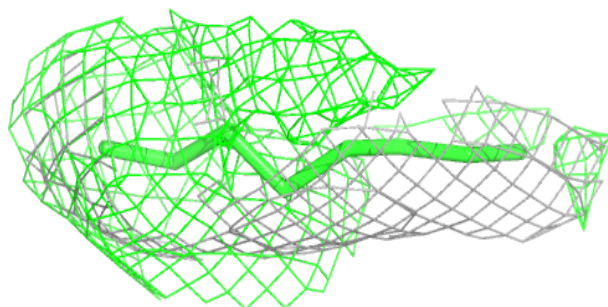
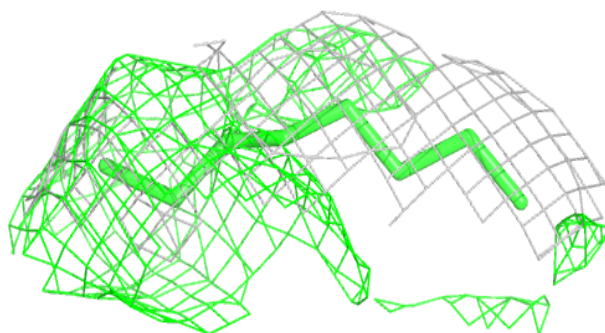
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	3PE	A	923	8/51	0.60	0.34	118,120,122,123	0
6	XP5	B	801	19/32	0.67	0.20	208,212,214,215	0
7	3PE	A	922	20/51	0.73	0.15	162,167,172,172	0
6	XP5	A	921	22/32	0.77	0.18	215,221,227,228	0
5	C2E	A	920	46/46	0.90	0.08	143,147,150,151	0
5	C2E	A	919	46/46	0.93	0.07	133,138,143,144	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.

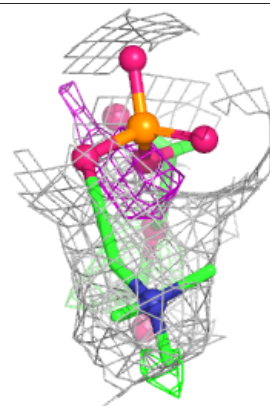
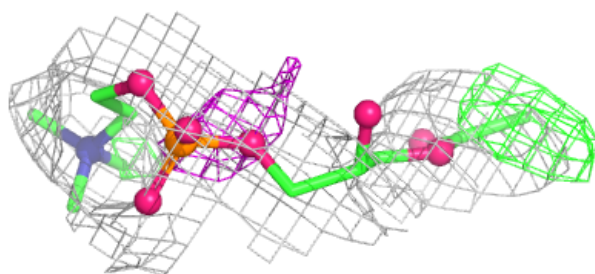
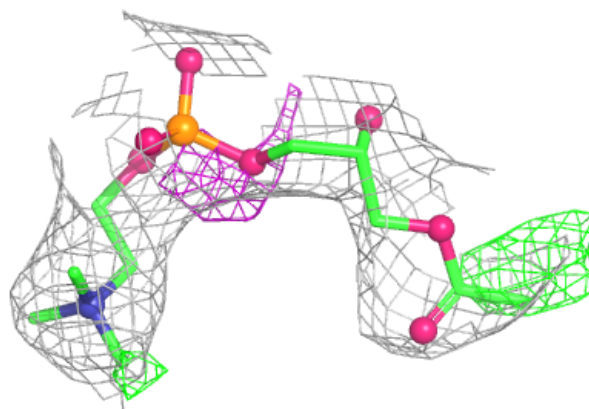
Electron density around 3PE A 923:

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



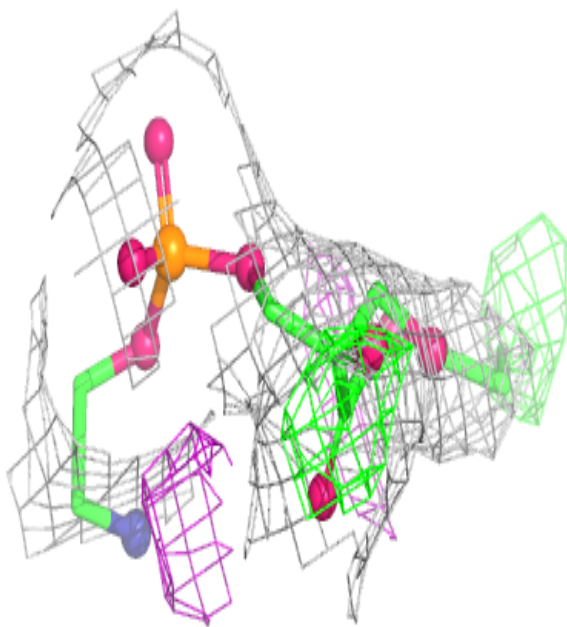
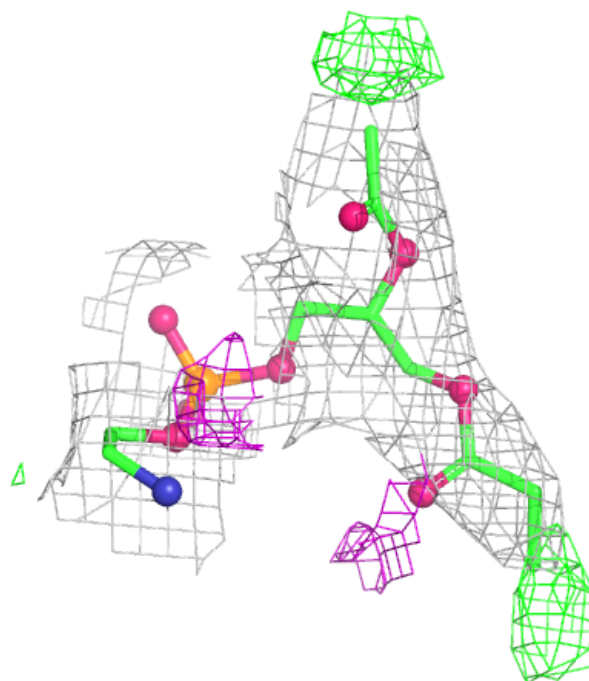
Electron density around XP5 B 801:

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



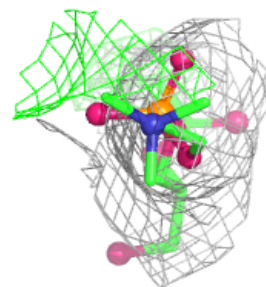
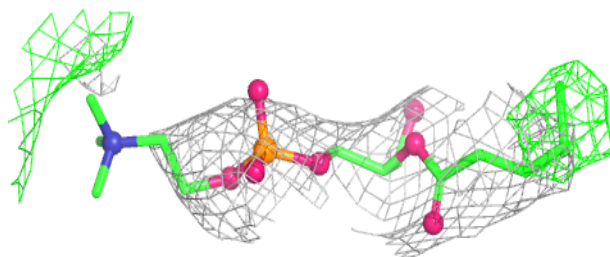
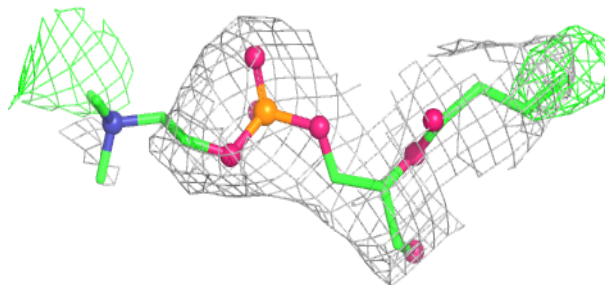
Electron density around 3PE A 922:

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



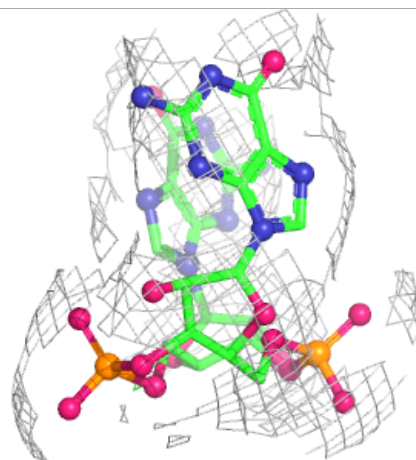
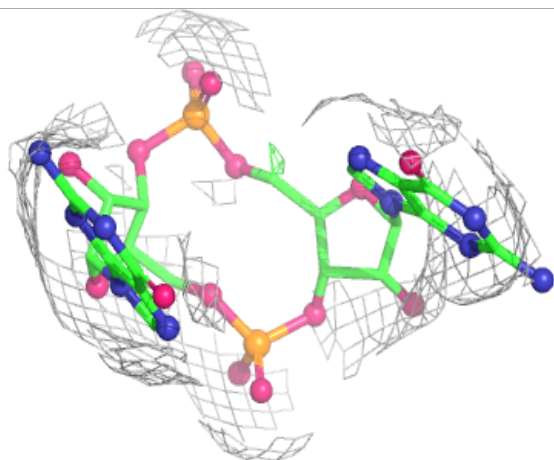
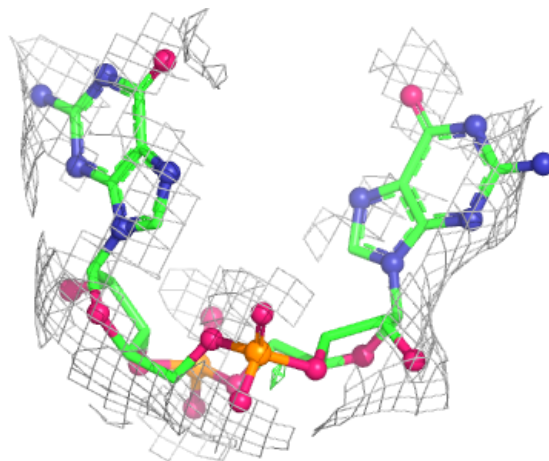
Electron density around XP5 A 921:

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



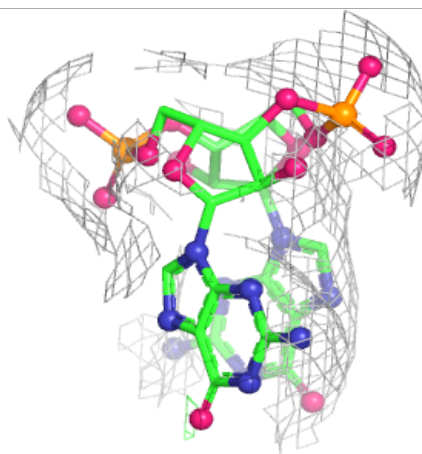
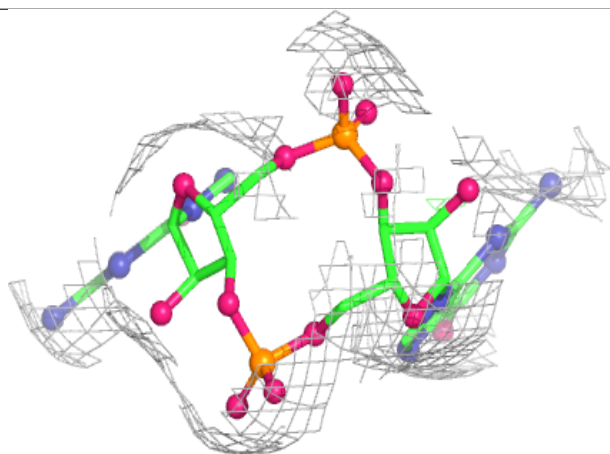
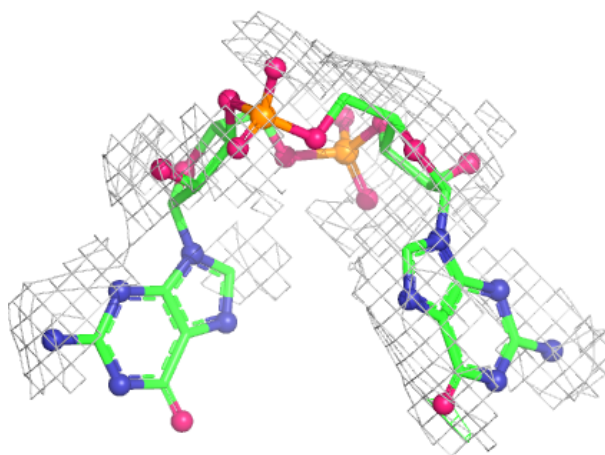
Electron density around C2E A 920:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.