



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 18, 2021 – 12:13 PM JST

PDB ID : 7DDL  
Title : Crystal structures of Na<sup>+</sup>,K<sup>+</sup>-ATPase in complex with bufalin  
Authors : Ogawa, H.; Cornelius, F.; Kanai, R.; Motoyama, K.; Vilsen, B.; Toyoshima, C.  
Deposited on : 2020-10-29  
Resolution : 3.20 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 : 2.16  
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) : 2.16

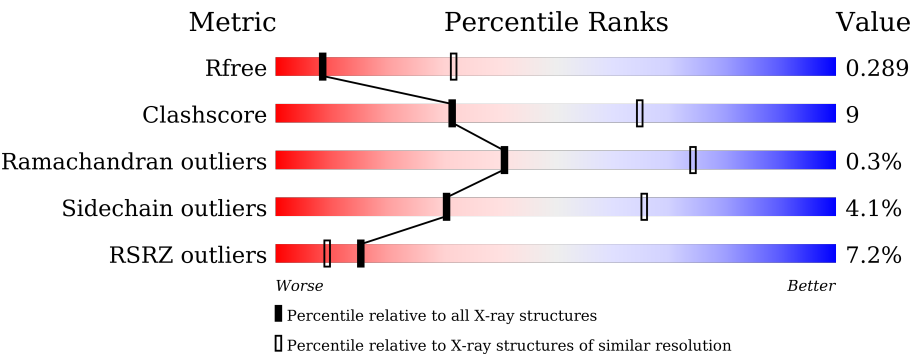
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1016	<div><div>9%</div><div>75%</div><div>22%</div><div>..</div></div>
1	C	1016	<div><div>5%</div><div>75%</div><div>21%</div><div>..</div></div>
2	B	303	<div><div>8%</div><div>71%</div><div>23%</div><div>..</div></div>
2	D	303	<div><div>7%</div><div>62%</div><div>30%</div><div>6%</div></div>
3	E	65	<div><div>37%</div><div>11%</div><div>51%</div></div>
3	G	65	<div><div>40%</div><div>9%</div><div>51%</div></div>

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Mol	Chain	Length	Quality of chain
4	F	2	 100%
4	H	2	 50% 50%
4	I	2	 50% 50%
4	J	2	 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
4	NAG	F	2	-	-	-	X
4	NAG	H	1	-	-	-	X
4	NAG	H	2	-	-	-	X
4	NAG	J	2	-	-	-	X
7	PCW	A	1106	-	-	-	X
7	PCW	A	1108	-	-	-	X
7	PCW	C	1107	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 21312 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			
1	C	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2386	1546	390	437	13			
2	D	285	Total	C	N	O	S	0	0	0
			2334	1514	383	424	13			

- Molecule 3 is a protein called FXYP domain-containing ion transport regulator.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	32	Total	C	N	O	0	0	0
			255	174	37	44			
3	E	32	Total	C	N	O	0	0	0
			255	174	37	44			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

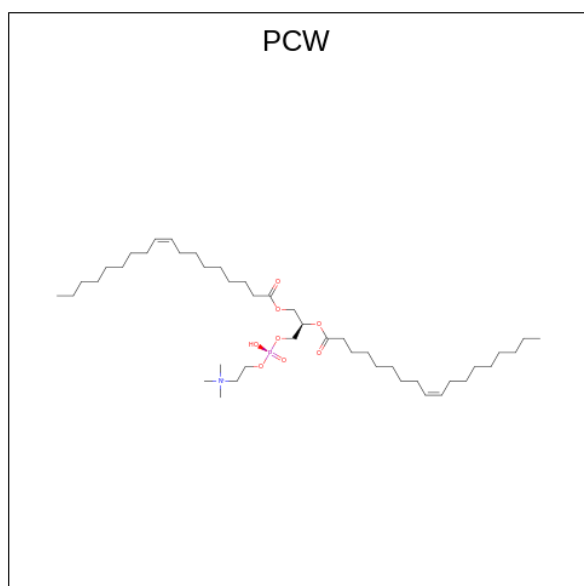
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

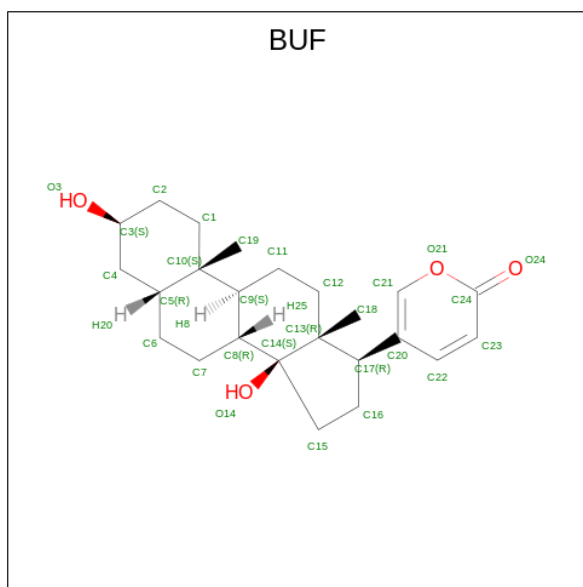
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



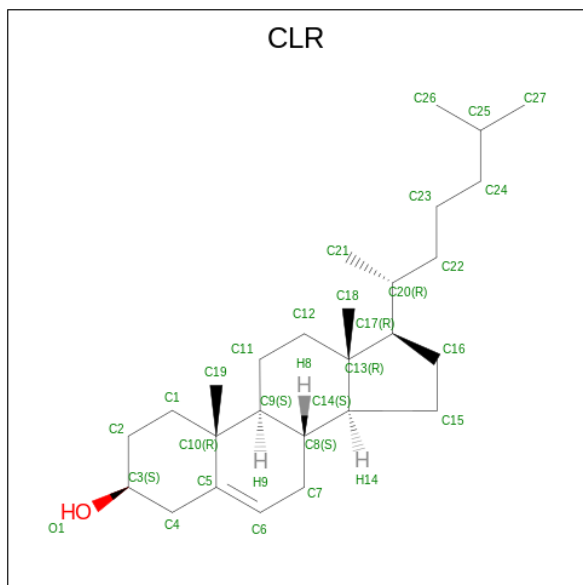
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	D	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

- Molecule 8 is bufalin (three-letter code: BUF) (formula:  $C_{24}H_{34}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			28	24	4		
8	C	1	Total	C	O	0	0
			28	24	4		

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			28	27	1		
9	B	1	Total	C	O	0	0
			28	27	1		
9	G	1	Total	C	O	0	0
			28	27	1		
9	C	1	Total	C	O	0	0
			28	27	1		
9	D	1	Total	C	O	0	0
			28	27	1		
9	E	1	Total	C	O	0	0
			28	27	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is water.

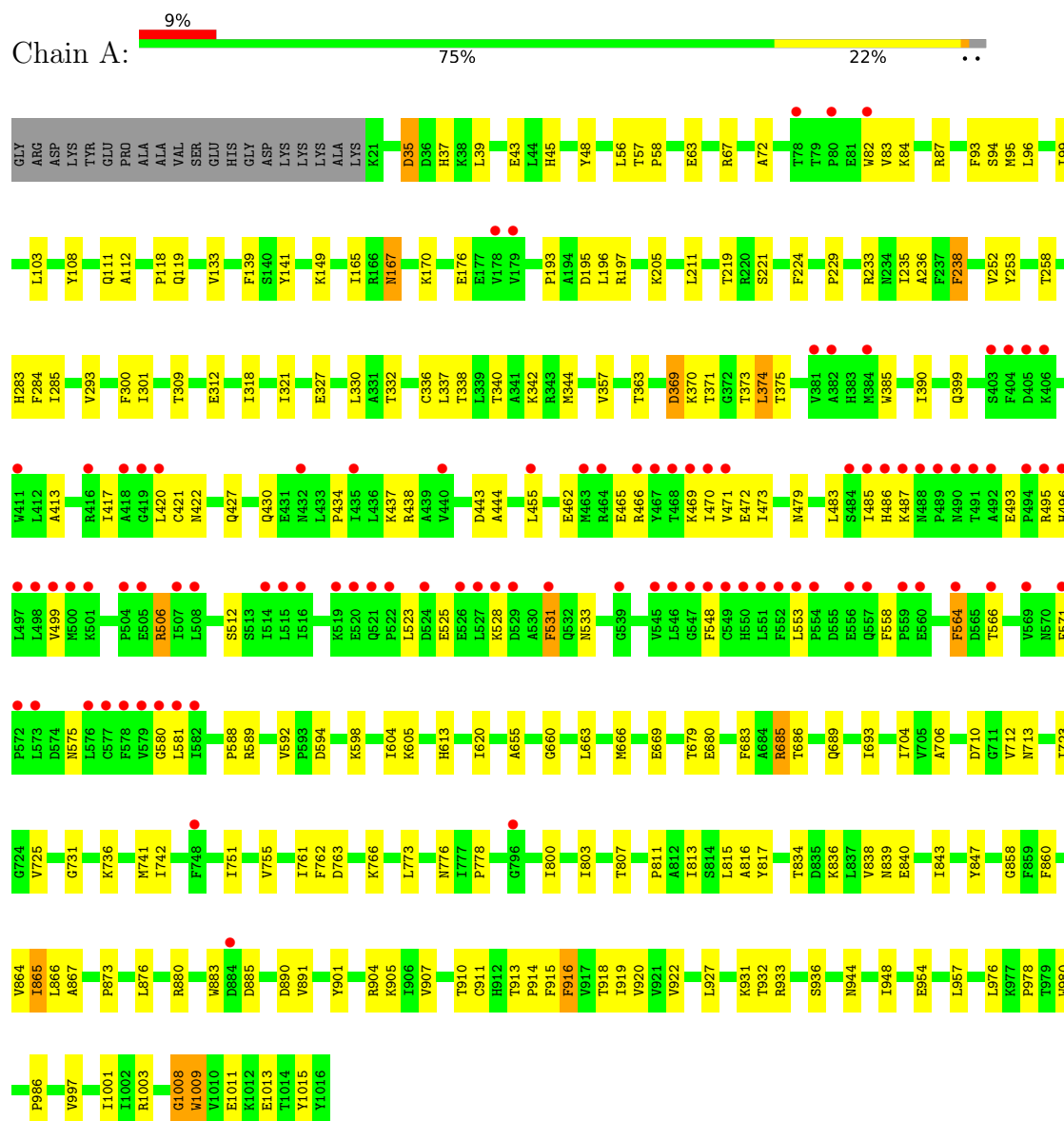
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	5	Total	O	0	0
			5	5		
11	C	5	Total	O	0	0
			5	5		



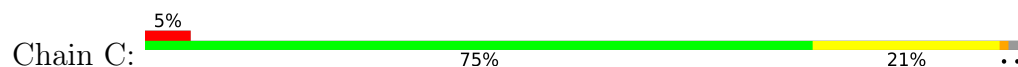
### 3 Residue-property plots

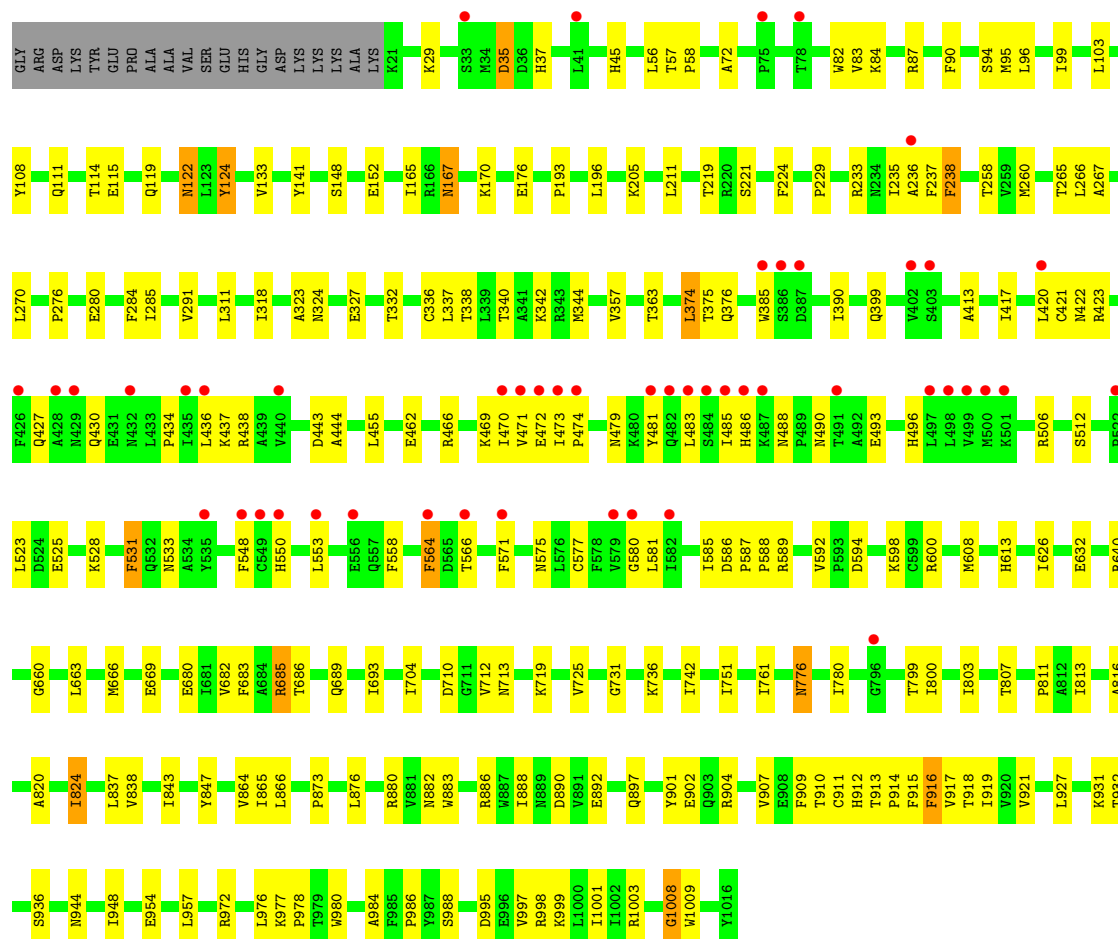
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sodium/potassium-transporting ATPase subunit alpha-1

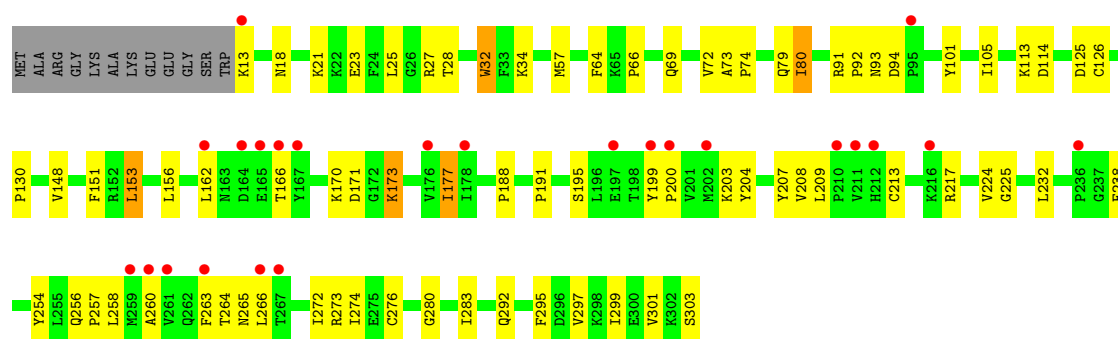


- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1



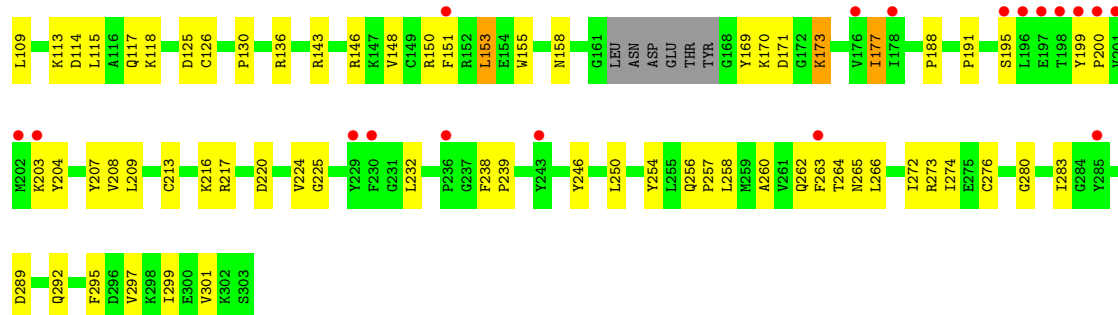


• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1





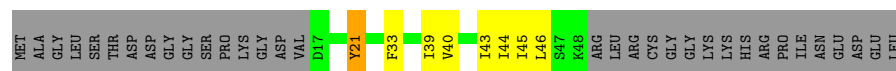
- Molecule 3: FXYP domain-containing ion transport regulator

Chain G: 40% 9% 51%



- Molecule 3: FXYP domain-containing ion transport regulator

Chain E: 37% 11% 51%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.72Å 117.65Å 492.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 3.20 49.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	41.9 (14.99-3.20) 42.5 (49.95-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.241 , 0.281 0.250 , 0.289	Depositor DCC
$R_{free}$ test set	2020 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	21312	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, NAG, NA, PCW, PHD, BUF, CLR

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	0.29	0/7867	0.53	1/10674 (0.0%)
1	C	0.29	0/7867	0.53	1/10674 (0.0%)
2	B	0.28	0/2449	0.54	0/3301
2	D	0.29	0/2395	0.54	0/3225
3	E	0.31	0/261	0.51	0/354
3	G	0.30	0/261	0.47	0/354
All	All	0.29	0/21100	0.53	2/28582 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	GLY	N-CA-C	5.18	126.05	113.10
1	C	1008	GLY	N-CA-C	5.04	125.69	113.10

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	7730	0	7777	147	0
1	C	7730	0	7777	132	0
2	B	2386	0	2361	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2334	0	2317	60	0
3	E	255	0	259	5	0
3	G	255	0	259	3	0
4	F	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	1	0
4	J	28	0	25	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	132	0	108	9	0
7	C	88	0	72	3	0
7	D	22	0	18	0	0
8	A	28	0	34	2	0
8	C	28	0	34	1	0
9	A	28	0	46	1	0
9	B	28	0	46	0	0
9	C	28	0	46	1	0
9	D	28	0	46	2	0
9	E	28	0	46	3	0
9	G	28	0	46	2	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	A	5	0	0	0	0
11	C	5	0	0	0	0
All	All	21312	0	21418	384	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 9.

All (384) 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:80:ILE:HG12	2:B:177:ILE:HG12	1.59	0.84
1:A:430:GLN:HG3	1:A:438:ARG:HB2	1.59	0.82
2:D:80:ILE:HG12	2:D:177:ILE:HG12	1.61	0.82
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.64	0.80
1:A:375:THR:HA	1:A:588:PRO:HA	1.65	0.78
1:A:901:TYR:HA	1:A:904:ARG:HE	1.48	0.77
1:C:375:THR:HA	1:C:588:PRO:HA	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:THR:HB	1:A:954:GLU:HG3	1.68	0.76
1:C:807:THR:HB	1:C:954:GLU:HG3	1.67	0.75
1:C:430:GLN:HG3	1:C:438:ARG:HB2	1.69	0.74
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.70	0.72
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.72	0.72
1:A:978:PRO:HB3	9:G:101:CLR:H192	1.71	0.72
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.72	0.72
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.73	0.71
2:D:204:TYR:HE1	2:D:207:TYR:HB2	1.55	0.71
1:C:978:PRO:HB3	9:E:101:CLR:H192	1.73	0.70
2:D:177:ILE:HA	2:D:260:ALA:HA	1.73	0.70
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.73	0.69
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.73	0.69
1:A:96:LEU:HD22	1:A:285:ILE:HG23	1.74	0.68
1:C:96:LEU:HD22	1:C:285:ILE:HG23	1.75	0.67
2:D:80:ILE:HD11	2:D:177:ILE:H	1.59	0.67
1:C:108:TYR:HA	1:C:111:GLN:HE21	1.60	0.67
1:C:986:PRO:HB3	9:C:1104:CLR:H213	1.75	0.67
1:A:84:LYS:HG3	1:A:141:TYR:HE1	1.60	0.66
1:C:221:SER:H	1:C:233:ARG:HB3	1.60	0.66
1:C:901:TYR:HA	1:C:904:ARG:HE	1.61	0.65
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.79	0.65
1:C:385:TRP:HE3	1:C:580:GLY:HA2	1.63	0.64
1:A:891:VAL:HG21	1:A:904:ARG:NH1	2.13	0.63
1:A:385:TRP:HB3	1:A:581:LEU:H	1.64	0.63
2:B:204:TYR:HE1	2:B:207:TYR:HB2	1.64	0.63
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.81	0.62
1:A:119:GLN:HE22	8:A:1121:BUF:H20	1.64	0.62
1:A:385:TRP:HE3	1:A:580:GLY:HA2	1.64	0.61
1:A:512:SER:HB2	1:A:575:ASN:HA	1.82	0.61
2:D:102:VAL:HG13	2:D:169:TYR:HD2	1.66	0.61
1:C:108:TYR:HB2	1:C:122:ASN:HB3	1.83	0.61
1:C:434:PRO:HG2	1:C:437:LYS:HB2	1.83	0.61
1:A:558:PHE:HB3	1:A:564:PHE:HE2	1.66	0.61
1:A:283:HIS:CE1	7:A:1105:PCW:H42	2.35	0.60
1:C:385:TRP:HB3	1:C:581:LEU:H	1.66	0.60
1:A:1009:TRP:HZ2	2:B:34:LYS:HB3	1.67	0.60
1:A:907:VAL:O	1:A:911:CYS:HB2	2.02	0.60
1:C:558:PHE:HB3	1:C:564:PHE:HE2	1.67	0.60
1:C:663:LEU:HA	1:C:666:MET:HG3	1.84	0.60
2:B:177:ILE:HA	2:B:260:ALA:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ILE:HD11	2:B:177:ILE:H	1.67	0.60
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.84	0.59
1:A:913:THR:HB	1:A:976:LEU:HD21	1.84	0.59
1:C:907:VAL:HA	1:C:910:THR:HG22	1.84	0.59
1:A:434:PRO:HG2	1:A:437:LYS:HB2	1.84	0.59
1:C:72:ALA:HB2	1:C:176:GLU:HG2	1.84	0.59
1:A:883:TRP:HA	1:A:904:ARG:NH1	2.17	0.59
2:B:225:GLY:HA3	2:B:265:ASN:HB3	1.85	0.58
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.84	0.58
1:C:238:PHE:HD2	1:C:258:THR:HG21	1.69	0.58
1:A:907:VAL:HA	1:A:910:THR:HG22	1.86	0.58
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.86	0.58
1:A:663:LEU:HA	1:A:666:MET:HG3	1.86	0.57
2:D:35:ILE:HG21	9:D:501:CLR:H22	1.87	0.57
1:A:238:PHE:HD2	1:A:258:THR:HG21	1.70	0.57
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.87	0.57
1:A:363:THR:HA	1:A:704:ILE:HB	1.87	0.57
7:C:1105:PCW:H82	2:D:16:ILE:HD13	1.87	0.57
2:D:130:PRO:HB3	2:D:239:PRO:HB3	1.86	0.57
1:A:736:LYS:HG3	1:A:742:ILE:HD12	1.87	0.56
1:C:594:ASP:O	1:C:598:LYS:HG2	2.05	0.56
1:A:839:ASN:HA	7:A:1105:PCW:H52	1.88	0.56
1:A:836:LYS:HB2	7:A:1105:PCW:H83	1.88	0.56
1:A:84:LYS:HG3	1:A:141:TYR:CE1	2.40	0.56
1:C:332:THR:HA	1:C:813:ILE:HD11	1.86	0.56
2:D:17:TRP:O	2:D:24:PHE:HA	2.06	0.55
2:D:173:LYS:HB3	2:D:262:GLN:HE21	1.71	0.55
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.86	0.55
1:C:683:PHE:HB3	1:C:686:THR:HG21	1.89	0.55
1:A:205:LYS:HA	1:A:219:THR:HA	1.87	0.55
1:C:114:THR:HG21	1:C:311:LEU:HD13	1.88	0.55
1:C:589:ARG:HB2	1:C:592:VAL:HG23	1.89	0.55
1:C:803:ILE:HG12	1:C:916:PHE:HD2	1.72	0.55
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.89	0.55
2:D:66:PRO:HG2	2:D:69:GLN:HG2	1.89	0.55
2:B:276:CYS:HB2	2:B:295:PHE:HD2	1.72	0.55
1:A:344:MET:HG3	1:A:357:VAL:HG23	1.89	0.55
1:C:469:LYS:HA	1:C:486:HIS:HD2	1.72	0.54
1:C:843:ILE:HG23	1:C:847:TYR:HD2	1.71	0.54
2:D:191:PRO:HD3	2:D:280:GLY:HA2	1.87	0.54
1:A:473:ILE:HB	1:A:483:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:TRP:HD1	1:C:390:ILE:HD13	1.73	0.54
1:A:683:PHE:HB3	1:A:686:THR:HG21	1.89	0.54
1:A:221:SER:H	1:A:233:ARG:HB3	1.71	0.54
1:C:399:GLN:HE21	1:C:436:LEU:HD11	1.72	0.54
1:A:83:VAL:O	1:A:87:ARG:HG2	2.07	0.54
1:C:336:CYS:SG	1:C:816:ALA:HB2	2.48	0.54
2:D:225:GLY:HA3	2:D:265:ASN:HB3	1.89	0.54
2:B:266:LEU:HD22	2:B:272:ILE:HD11	1.90	0.53
2:D:27:ARG:HG3	2:D:32:TRP:CD1	2.43	0.53
1:C:421:CYS:O	1:C:422:ASN:ND2	2.41	0.53
1:C:103:LEU:HB3	1:C:318:ILE:HG23	1.90	0.53
1:C:613:HIS:CE1	1:C:685:ARG:HH21	2.27	0.53
1:A:332:THR:HA	1:A:813:ILE:HD11	1.90	0.53
1:C:291:VAL:HG23	1:C:324:ASN:HD21	1.74	0.53
1:A:338:THR:O	1:A:342:LYS:HG2	2.08	0.53
1:A:803:ILE:HG12	1:A:916:PHE:HD2	1.74	0.53
2:D:276:CYS:HB2	2:D:295:PHE:HD2	1.74	0.53
1:A:867:ALA:HB2	1:A:873:PRO:HD3	1.91	0.53
2:D:18:ASN:HA	2:D:23:GLU:O	2.08	0.53
1:A:493:GLU:OE1	1:A:495:ARG:NH2	2.41	0.52
1:A:594:ASP:O	1:A:598:LYS:HG2	2.08	0.52
1:C:470:ILE:HB	1:C:485:ILE:HG23	1.92	0.52
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.92	0.52
2:D:115:LEU:HD13	2:D:118:LYS:HD2	1.89	0.52
1:A:763:ASP:OD2	1:A:933:ARG:NH1	2.43	0.52
2:D:136:ARG:O	2:D:146:ARG:NH1	2.43	0.52
2:D:224:VAL:HG21	2:D:274:ILE:HD11	1.91	0.52
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.91	0.51
1:C:340:THR:O	1:C:344:MET:HG2	2.11	0.51
1:C:995:ASP:OD1	1:C:998:ARG:NH1	2.43	0.51
1:C:205:LYS:HA	1:C:219:THR:HA	1.92	0.51
2:D:217:ARG:NH1	2:D:220:ASP:OD2	2.43	0.51
2:B:191:PRO:HD3	2:B:280:GLY:HA2	1.92	0.51
1:C:553:LEU:HD11	1:C:571:PHE:HD1	1.74	0.51
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.91	0.51
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.92	0.51
1:C:84:LYS:HG3	1:C:141:TYR:HE1	1.76	0.51
1:A:479:ASN:HA	1:A:506:ARG:HD3	1.94	0.50
1:A:978:PRO:HB2	7:C:1108:PCW:H31	1.94	0.50
1:C:907:VAL:O	1:C:911:CYS:HB2	2.11	0.50
1:C:799:THR:HG21	1:C:912:HIS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:913:THR:HB	1:C:976:LEU:HD21	1.93	0.50
1:C:363:THR:HA	1:C:704:ILE:HB	1.92	0.50
2:D:130:PRO:HD3	2:D:232:LEU:HD12	1.92	0.50
3:E:39:ILE:O	3:E:43:ILE:HG12	2.11	0.50
1:A:370:LYS:HA	1:A:374:LEU:HB2	1.92	0.50
1:A:340:THR:O	1:A:344:MET:HG2	2.11	0.50
1:A:63:GLU:O	1:A:67:ARG:HB2	2.12	0.50
1:C:165:ILE:HG12	1:C:170:LYS:HG2	1.94	0.50
1:C:469:LYS:HD3	1:C:472:GLU:HB3	1.94	0.50
1:A:885:ASP:O	1:A:904:ARG:NH2	2.44	0.50
2:B:80:ILE:HB	2:B:105:ILE:HD12	1.94	0.50
2:D:80:ILE:HD12	2:D:105:ILE:HD12	1.94	0.49
1:A:284:PHE:HE1	1:A:773:LEU:HD11	1.76	0.49
3:E:33:PHE:CZ	9:E:101:CLR:H151	2.47	0.49
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.47	0.49
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.94	0.49
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.47	0.49
2:D:217:ARG:HH12	2:D:273:ARG:HD2	1.76	0.49
1:A:843:ILE:HG23	1:A:847:TYR:HD2	1.76	0.49
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.95	0.49
2:D:213:CYS:HA	2:D:276:CYS:HA	1.95	0.49
2:B:91:ARG:HG2	2:B:93:ASN:H	1.77	0.49
1:C:512:SER:HB2	1:C:575:ASN:HA	1.95	0.49
2:B:101:TYR:O	2:B:105:ILE:HG12	2.13	0.49
1:C:873:PRO:HA	1:C:876:LEU:HD12	1.93	0.49
2:D:224:VAL:HG22	2:D:272:ILE:HD12	1.94	0.49
1:A:469:LYS:HA	1:A:486:HIS:HD2	1.78	0.49
1:C:776:ASN:HB3	1:C:847:TYR:HE1	1.77	0.49
1:C:488:ASN:ND2	1:C:493:GLU:O	2.46	0.48
1:C:84:LYS:HG3	1:C:141:TYR:CE1	2.48	0.48
2:D:263:PHE:HB3	2:D:266:LEU:HD21	1.94	0.48
2:D:91:ARG:HG2	2:D:93:ASN:H	1.78	0.48
1:A:94:SER:HB3	1:A:133:VAL:HG13	1.94	0.48
1:A:800:ILE:HG21	8:A:1121:BUF:H33	1.95	0.48
1:A:93:PHE:HB3	1:A:330:LEU:HD13	1.94	0.48
1:C:83:VAL:O	1:C:87:ARG:HG2	2.14	0.48
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.95	0.48
1:A:762:PHE:CE1	1:A:766:LYS:HE3	2.49	0.48
1:A:72:ALA:HB2	1:A:176:GLU:HG2	1.96	0.48
1:A:385:TRP:HD1	1:A:390:ILE:HD13	1.78	0.48
2:D:101:TYR:O	2:D:105:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:VAL:HG21	2:B:274:ILE:HD11	1.95	0.48
1:C:94:SER:HB3	1:C:133:VAL:HG13	1.95	0.48
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.95	0.47
2:D:266:LEU:HD22	2:D:272:ILE:HD11	1.95	0.47
1:A:689:GLN:O	1:A:693:ILE:HG12	2.15	0.47
2:D:39:TYR:CZ	9:D:501:CLR:H191	2.49	0.47
1:A:149:LYS:HG3	7:A:1108:PCW:H41	1.95	0.47
2:D:27:ARG:NH1	2:D:31:SER:OG	2.47	0.47
1:A:370:LYS:HZ2	1:A:620:ILE:HG13	1.79	0.47
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.94	0.47
2:B:217:ARG:HH12	2:B:273:ARG:HD2	1.78	0.47
1:C:890:ASP:OD1	1:C:890:ASP:N	2.46	0.47
2:B:80:ILE:HD12	2:B:105:ILE:HD12	1.96	0.47
1:C:689:GLN:O	1:C:693:ILE:HG12	2.14	0.47
2:D:92:PRO:HG3	2:D:301:VAL:HG12	1.96	0.47
1:A:834:THR:O	7:A:1105:PCW:H81	2.14	0.47
1:A:112:ALA:HA	1:A:118:PRO:HG2	1.96	0.47
2:B:66:PRO:HG2	2:B:69:GLN:HG2	1.95	0.47
1:C:124:TYR:CZ	7:C:1107:PCW:H2	2.49	0.47
1:C:918:THR:HG23	1:C:984:ALA:HB2	1.97	0.47
3:G:45:ILE:HD12	3:G:46:LEU:HG	1.95	0.47
1:A:470:ILE:HG22	1:A:471:VAL:HG23	1.97	0.47
2:B:213:CYS:HA	2:B:276:CYS:HA	1.96	0.47
3:E:45:ILE:HD12	3:E:46:LEU:HG	1.97	0.47
1:A:713:ASN:N	1:A:713:ASN:OD1	2.48	0.47
2:D:117:GLN:O	2:D:150:ARG:NH1	2.47	0.47
2:D:27:ARG:HG3	2:D:32:TRP:HD1	1.79	0.47
1:A:976:LEU:HB3	1:A:980:TRP:HD1	1.80	0.47
1:C:58:PRO:HD3	1:C:167:ASN:HB2	1.96	0.47
1:A:421:CYS:O	1:A:422:ASN:ND2	2.48	0.46
1:A:710:ASP:HB2	1:A:731:GLY:HA2	1.96	0.46
1:A:211:LEU:HA	1:A:712:VAL:HG22	1.98	0.46
1:A:284:PHE:CD1	1:A:838:VAL:HG21	2.50	0.46
1:C:915:PHE:O	1:C:919:ILE:HG12	2.15	0.46
1:C:932:THR:HG1	1:C:999:LYS:HZ2	1.56	0.46
2:D:151:PHE:HE2	2:D:258:LEU:HB2	1.80	0.46
1:A:300:PHE:HD2	1:A:301:ILE:HD12	1.79	0.46
1:C:385:TRP:CH2	1:C:531:PHE:HB2	2.50	0.46
1:A:443:ASP:OD1	1:A:444:ALA:N	2.49	0.46
1:C:977:LYS:HD2	1:C:980:TRP:CZ2	2.50	0.46
1:A:815:LEU:HD12	1:A:815:LEU:HA	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:PRO:HG3	2:B:301:VAL:HG12	1.98	0.46
1:A:470:ILE:HB	1:A:485:ILE:HG23	1.98	0.46
2:B:173:LYS:HG3	2:B:264:THR:O	2.16	0.46
1:C:883:TRP:HA	1:C:904:ARG:HH11	1.81	0.46
2:B:92:PRO:HD2	2:B:303:SER:HA	1.97	0.46
1:C:909:PHE:HB3	1:C:972:ARG:O	2.16	0.46
2:D:173:LYS:HG3	2:D:264:THR:O	2.16	0.46
2:D:239:PRO:HD2	2:D:257:PRO:HB3	1.97	0.46
1:A:336:CYS:SG	1:A:816:ALA:HB2	2.56	0.45
1:A:725:VAL:HG13	1:A:741:MET:HE3	1.98	0.45
1:A:890:ASP:N	1:A:890:ASP:OD1	2.49	0.45
1:A:864:VAL:HG12	1:A:980:TRP:HZ3	1.82	0.45
2:B:27:ARG:HG3	2:B:32:TRP:CD1	2.51	0.45
1:C:944:ASN:O	1:C:948:ILE:HG12	2.16	0.45
2:B:204:TYR:O	2:B:208:VAL:HG12	2.16	0.45
3:G:40:VAL:O	3:G:44:ILE:HG12	2.17	0.45
1:C:284:PHE:CD1	1:C:838:VAL:HG21	2.51	0.45
1:A:883:TRP:CH2	1:A:904:ARG:HB2	2.52	0.45
1:C:276:PRO:O	1:C:280:GLU:HG2	2.16	0.45
1:C:95:MET:O	1:C:99:ILE:HG23	2.16	0.45
2:B:130:PRO:HD3	2:B:232:LEU:HD12	1.99	0.45
1:C:443:ASP:OD1	1:C:444:ALA:N	2.50	0.45
1:A:817:TYR:HB2	1:A:944:ASN:HD21	1.82	0.45
1:C:196:LEU:HB2	1:C:236:ALA:HB3	1.99	0.45
1:A:660:GLY:HA3	1:A:685:ARG:O	2.17	0.45
1:C:473:ILE:HB	1:C:483:LEU:HG	1.97	0.45
2:D:153:LEU:H	2:D:153:LEU:HD12	1.82	0.45
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.81	0.45
1:C:608:MET:HB3	1:C:682:VAL:HG22	1.99	0.45
1:A:196:LEU:HB2	1:A:236:ALA:HB3	1.99	0.45
1:A:525:GLU:HA	1:A:528:LYS:HB3	1.98	0.45
1:C:997:VAL:O	1:C:1001:ILE:HG12	2.17	0.45
2:D:204:TYR:O	2:D:208:VAL:HG12	2.17	0.45
1:A:413:ALA:O	1:A:417:ILE:HG13	2.17	0.44
1:C:525:GLU:HA	1:C:528:LYS:HB3	1.98	0.44
2:D:216:LYS:H	2:D:220:ASP:HB2	1.82	0.44
1:C:337:LEU:HA	1:C:761:ILE:HD11	1.99	0.44
1:C:866:LEU:HA	1:C:866:LEU:HD23	1.86	0.44
1:C:931:LYS:HG2	1:C:932:THR:HG23	1.98	0.44
3:G:33:PHE:CZ	9:G:101:CLR:H151	2.52	0.44
1:C:267:ALA:O	1:C:719:LYS:NZ	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:PHE:O	1:C:94:SER:HB2	2.18	0.44
1:A:165:ILE:HG12	1:A:170:LYS:HG2	1.99	0.44
1:A:39:LEU:HD22	1:A:43:GLU:HG2	1.99	0.44
1:A:807:THR:HG22	1:A:957:LEU:HD12	2.00	0.44
2:B:263:PHE:HB3	2:B:266:LEU:HD21	2.00	0.44
1:C:344:MET:HG3	1:C:357:VAL:HG23	2.00	0.44
1:C:462:GLU:O	1:C:466:ARG:HB2	2.18	0.44
1:A:462:GLU:HA	1:A:465:GLU:HG2	2.00	0.44
2:D:280:GLY:HA3	2:D:283:ILE:HD13	1.98	0.44
2:B:156:LEU:HD13	2:B:260:ALA:HB2	2.00	0.44
1:A:399:GLN:CD	1:A:455:LEU:HD21	2.38	0.44
1:C:470:ILE:HG22	1:C:471:VAL:HG23	1.99	0.44
1:C:710:ASP:HB2	1:C:731:GLY:HA2	2.00	0.44
1:A:911:CYS:C	1:A:914:PRO:HD2	2.39	0.44
1:A:865:ILE:HD12	1:A:914:PRO:HG3	2.00	0.43
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.53	0.43
1:A:95:MET:O	1:A:99:ILE:HG23	2.17	0.43
1:C:911:CYS:C	1:C:914:PRO:HD2	2.39	0.43
1:A:669:GLU:N	1:A:669:GLU:OE1	2.45	0.43
2:B:280:GLY:HA3	2:B:283:ILE:HD13	2.01	0.43
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.83	0.43
1:A:427:GLN:HB2	1:A:430:GLN:OE1	2.19	0.43
1:C:660:GLY:HA3	1:C:685:ARG:O	2.18	0.43
1:C:892:GLU:HA	1:C:897:GLN:O	2.19	0.43
2:D:246:TYR:O	2:D:250:LEU:HB2	2.18	0.43
7:A:1108:PCW:H42	7:A:1108:PCW:H73	1.79	0.43
1:A:496:HIS:HB2	1:A:553:LEU:HB2	2.01	0.43
1:C:496:HIS:HB2	1:C:553:LEU:HB2	1.99	0.43
1:A:417:ILE:HG22	1:A:548:PHE:HD2	1.83	0.43
1:A:997:VAL:O	1:A:1001:ILE:HG12	2.18	0.43
1:C:148:SER:O	1:C:152:GLU:HG2	2.18	0.43
1:A:139:PHE:HD1	7:A:1110:PCW:H2	1.84	0.43
1:A:48:TYR:HE2	1:A:252:VAL:HG22	1.83	0.43
1:A:866:LEU:HA	1:A:866:LEU:HD23	1.88	0.43
1:A:865:ILE:CD1	1:A:914:PRO:HG3	2.49	0.43
1:C:35:ASP:HB2	1:C:229:PRO:HG3	2.01	0.43
1:C:29:LYS:NZ	1:C:265:THR:HB	2.34	0.43
1:A:918:THR:O	1:A:922:VAL:HG22	2.19	0.43
2:B:21:LYS:HA	2:B:21:LYS:HD2	1.78	0.43
1:C:813:ILE:HD13	1:C:813:ILE:HA	1.82	0.43
1:A:35:ASP:HB2	1:A:229:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:PRO:HB2	1:A:919:ILE:HD11	2.01	0.43
2:B:74:PRO:HG2	2:B:292:GLN:OE1	2.19	0.43
1:C:882:ASN:O	1:C:904:ARG:NH1	2.49	0.43
1:A:309:THR:HG23	1:A:312:GLU:H	1.84	0.42
1:A:931:LYS:HG2	1:A:932:THR:HG23	2.01	0.42
1:C:713:ASN:OD1	1:C:713:ASN:N	2.51	0.42
1:A:337:LEU:HD23	1:A:761:ILE:HD13	2.00	0.42
1:C:479:ASN:O	1:C:481:TYR:HD1	2.02	0.42
1:A:986:PRO:HB3	9:A:1104:CLR:H213	2.01	0.42
2:D:109:LEU:HD23	2:D:153:LEU:HD23	2.01	0.42
1:C:820:ALA:HB2	1:C:824:ILE:HD11	2.02	0.42
1:A:1009:TRP:CZ3	1:A:1013:GLU:HG3	2.55	0.42
1:A:471:VAL:HG21	1:A:564:PHE:O	2.19	0.42
2:D:155:TRP:CD2	2:D:232:LEU:HD22	2.54	0.42
2:B:18:ASN:HA	2:B:23:GLU:O	2.19	0.42
1:A:1009:TRP:CZ2	2:B:34:LYS:HB3	2.49	0.42
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.55	0.42
1:A:103:LEU:HB3	1:A:318:ILE:HG23	2.02	0.42
1:A:149:LYS:HA	1:A:149:LYS:HD3	1.90	0.42
1:A:421:CYS:HB2	1:A:499:VAL:HG23	2.01	0.42
1:C:550:HIS:O	1:C:577:CYS:HB3	2.19	0.42
1:A:553:LEU:HD11	1:A:571:PHE:HD1	1.84	0.42
1:C:323:ALA:HB1	1:C:780:ILE:HG12	2.02	0.42
1:C:585:ILE:O	1:C:587:PRO:HD3	2.19	0.42
1:C:669:GLU:N	1:C:669:GLU:OE1	2.46	0.42
1:A:883:TRP:O	1:A:904:ARG:NH1	2.53	0.42
2:B:151:PHE:HE2	2:B:258:LEU:HB2	1.84	0.42
1:C:399:GLN:CD	1:C:455:LEU:HD21	2.40	0.42
1:C:417:ILE:HG22	1:C:548:PHE:HD2	1.84	0.42
1:C:374:LEU:HA	1:C:374:LEU:HD12	1.90	0.42
1:C:427:GLN:HB2	1:C:430:GLN:OE1	2.20	0.42
1:C:280:GLU:HB3	1:C:837:LEU:HB2	2.02	0.42
1:C:902:GLU:HB2	2:D:289:ASP:OD2	2.20	0.42
2:D:74:PRO:HG2	2:D:292:GLN:OE1	2.19	0.42
2:D:80:ILE:HB	2:D:105:ILE:HD12	2.02	0.42
1:A:58:PRO:HD3	1:A:167:ASN:HB2	2.00	0.41
1:A:915:PHE:O	1:A:919:ILE:HG12	2.20	0.41
1:A:93:PHE:CD1	1:A:330:LEU:HB2	2.55	0.41
1:A:139:PHE:CD1	7:A:1110:PCW:H2	2.55	0.41
1:A:905:LYS:HA	1:A:905:LYS:HD3	1.91	0.41
1:C:800:ILE:HG21	8:C:1121:BUF:H33	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:ILE:O	1:C:904:ARG:NH2	2.52	0.41
1:C:266:LEU:O	1:C:270:LEU:HG	2.20	0.41
1:C:413:ALA:O	1:C:417:ILE:HG13	2.20	0.41
1:C:374:LEU:HD21	1:C:626:ILE:HD11	2.01	0.41
1:C:632:GLU:OE1	1:C:640:ARG:NH1	2.54	0.41
1:C:280:GLU:HB3	1:C:837:LEU:CB	2.49	0.41
1:A:936:SER:HB2	1:A:1003:ARG:CZ	2.51	0.41
1:C:111:GLN:O	1:C:115:GLU:HG2	2.20	0.41
1:C:488:ASN:HD21	1:C:490:ASN:HB2	1.85	0.41
1:C:807:THR:HG22	1:C:957:LEU:HD12	2.01	0.41
1:C:917:VAL:O	1:C:921:VAL:HG23	2.20	0.41
1:A:605:LYS:HE3	1:A:679:THR:O	2.21	0.41
2:B:91:ARG:HD2	2:B:94:ASP:HB2	2.02	0.41
1:C:736:LYS:HG3	1:C:742:ILE:HD12	2.02	0.41
1:C:936:SER:HB2	1:C:1003:ARG:CZ	2.50	0.41
2:D:143:ARG:HD2	2:D:146:ARG:NH1	2.36	0.41
9:E:101:CLR:H231	9:E:101:CLR:H211	1.72	0.41
1:A:858:GLY:HA2	1:A:918:THR:HG21	2.03	0.41
1:C:423:ARG:NH1	1:C:474:PRO:HB3	2.36	0.41
1:C:600:ARG:NH2	1:C:680:GLU:HG2	2.35	0.41
1:C:886:ARG:HG3	1:C:901:TYR:CE2	2.55	0.41
1:C:921:VAL:HG12	1:C:988:SER:OG	2.21	0.41
2:D:80:ILE:HD12	2:D:81:PRO:HD3	2.03	0.41
1:A:613:HIS:CE1	1:A:685:ARG:HH21	2.38	0.41
1:A:920:VAL:HG13	1:A:954:GLU:HG2	2.03	0.41
1:A:944:ASN:O	1:A:948:ILE:HG12	2.21	0.41
1:C:211:LEU:HD13	1:C:237:PHE:HB3	2.01	0.41
2:D:21:LYS:HA	2:D:21:LYS:HD2	1.84	0.41
2:D:80:ILE:HG13	2:D:80:ILE:H	1.49	0.41
3:E:40:VAL:O	3:E:44:ILE:HG12	2.21	0.41
1:A:1011:GLU:O	1:A:1015:TYR:HB3	2.21	0.40
1:A:293:VAL:HG12	1:A:321:ILE:HD13	2.03	0.40
1:C:376:GLN:HE21	1:C:589:ARG:HA	1.86	0.40
7:A:1109:PCW:H73	3:E:21:TYR:CE1	2.56	0.40
1:A:108:TYR:HA	1:A:111:GLN:HE21	1.85	0.40
2:D:158:ASN:OD1	4:I:1:NAG:N2	2.54	0.40
1:A:197:ARG:HB2	1:A:252:VAL:HG23	2.02	0.40
1:A:462:GLU:O	1:A:466:ARG:HB2	2.22	0.40
1:A:469:LYS:HD3	1:A:472:GLU:HB3	2.03	0.40
1:A:655:ALA:HA	1:A:680:GLU:O	2.21	0.40
1:C:338:THR:O	1:C:342:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ILE:HD11	1:A:487:LYS:HE2	2.02	0.40
1:A:706:ALA:HA	1:A:723:ILE:O	2.21	0.40
1:A:860:PHE:O	1:A:864:VAL:HG23	2.22	0.40
1:C:685:ARG:HB3	1:C:685:ARG:HH11	1.86	0.40
1:C:260:MET:HE1	1:C:712:VAL:HG11	2.04	0.40
1:A:369:PHD:O	1:A:373:THR:HB	2.22	0.40
1:A:369:PHD:OP1	1:A:371:THR:N	2.49	0.40
1:A:385:TRP:CH2	1:A:531:PHE:HB2	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	993/1016 (98%)	923 (93%)	68 (7%)	2 (0%)	47	79
1	C	993/1016 (98%)	925 (93%)	66 (7%)	2 (0%)	47	79
2	B	289/303 (95%)	260 (90%)	27 (9%)	2 (1%)	22	61
2	D	281/303 (93%)	256 (91%)	23 (8%)	2 (1%)	22	61
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
3	G	30/65 (46%)	29 (97%)	1 (3%)	0	100	100
All	All	2616/2768 (94%)	2421 (92%)	187 (7%)	8 (0%)	41	74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	PRO
2	D	200	PRO
2	B	199	TYR
2	D	199	TYR

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Mol	Chain	Res	Type
1	C	193	PRO
1	A	193	PRO
1	A	1008	GLY
1	C	1008	GLY

### 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	846/861 (98%)	824 (97%)	22 (3%)	46	76
1	C	846/861 (98%)	820 (97%)	26 (3%)	40	72
2	B	261/269 (97%)	239 (92%)	22 (8%)	11	39
2	D	255/269 (95%)	235 (92%)	20 (8%)	12	43
3	E	26/52 (50%)	25 (96%)	1 (4%)	33	67
3	G	26/52 (50%)	25 (96%)	1 (4%)	33	67
All	All	2260/2364 (96%)	2168 (96%)	92 (4%)	30	66

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	45	HIS
1	A	56	LEU
1	A	57	THR
1	A	82	TRP
1	A	167	ASN
1	A	224	PHE
1	A	238	PHE
1	A	327	GLU
1	A	374	LEU
1	A	506	ARG
1	A	523	LEU
1	A	531	PHE
1	A	533	ASN

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Mol	Chain	Res	Type
1	A	564	PHE
1	A	566	THR
1	A	685	ARG
1	A	776	ASN
1	A	840	GLU
1	A	865	ILE
1	A	916	PHE
1	A	1009	TRP
2	B	13	LYS
2	B	25	LEU
2	B	28	THR
2	B	32	TRP
2	B	64	PHE
2	B	72	VAL
2	B	80	ILE
2	B	114	ASP
2	B	125	ASP
2	B	126	CYS
2	B	153	LEU
2	B	162	LEU
2	B	166	THR
2	B	170	LYS
2	B	171	ASP
2	B	173	LYS
2	B	177	ILE
2	B	195	SER
2	B	203	LYS
2	B	256	GLN
2	B	297	VAL
2	B	299	ILE
3	G	21	TYR
1	C	35	ASP
1	C	45	HIS
1	C	56	LEU
1	C	57	THR
1	C	82	TRP
1	C	119	GLN
1	C	122	ASN
1	C	124	TYR
1	C	167	ASN
1	C	224	PHE
1	C	238	PHE

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Mol	Chain	Res	Type
1	C	327	GLU
1	C	374	LEU
1	C	506	ARG
1	C	523	LEU
1	C	531	PHE
1	C	533	ASN
1	C	564	PHE
1	C	566	THR
1	C	586	ASP
1	C	685	ARG
1	C	776	ASN
1	C	824	ILE
1	C	865	ILE
1	C	916	PHE
1	C	1009	TRP
2	D	13	LYS
2	D	25	LEU
2	D	28	THR
2	D	32	TRP
2	D	64	PHE
2	D	72	VAL
2	D	80	ILE
2	D	114	ASP
2	D	125	ASP
2	D	126	CYS
2	D	153	LEU
2	D	170	LYS
2	D	171	ASP
2	D	173	LYS
2	D	177	ILE
2	D	195	SER
2	D	203	LYS
2	D	256	GLN
2	D	297	VAL
2	D	299	ILE
3	E	21	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	119	GLN

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Mol	Chain	Res	Type
1	A	122	ASN
1	A	427	GLN
1	A	613	HIS
1	A	776	ASN
1	A	898	GLN
1	C	111	GLN
1	C	119	GLN
1	C	122	ASN
1	C	324	ASN
1	C	376	GLN
1	C	399	GLN
1	C	613	HIS
1	C	897	GLN
2	D	262	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	PHD	A	369	1,5	9,11,12	0.93	0	10,15,17	1.20	1 (10%)
1	PHD	C	369	1,5	9,11,12	0.92	0	10,15,17	0.97	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
1	PHD	A	369	1,5	-	1/8/11/13	-
1	PHD	C	369	1,5	-	2/8/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	PHD	OD1-CG-CB	2.51	118.02	111.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	369	PHD	CA-CB-CG-OD1
1	C	369	PHD	CA-CB-CG-OD1
1	C	369	PHD	CA-CB-CG-OD2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	369	PHD	2	0

## 5.5 Carbohydrates [i](#)

8 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	NAG	F	1	2,4	14,14,15	0.34	0	17,19,21	0.43	0
4	NAG	F	2	4	14,14,15	0.31	0	17,19,21	0.51	0
4	NAG	H	1	2,4	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
4	NAG	H	2	4	14,14,15	0.35	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	I	1	2,4	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	I	2	4	14,14,15	0.27	0	17,19,21	0.52	0
4	NAG	J	1	2,4	14,14,15	0.61	1 (7%)	17,19,21	0.62	0
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	-2.40	1.39	1.43
4	J	1	NAG	O5-C1	-2.07	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

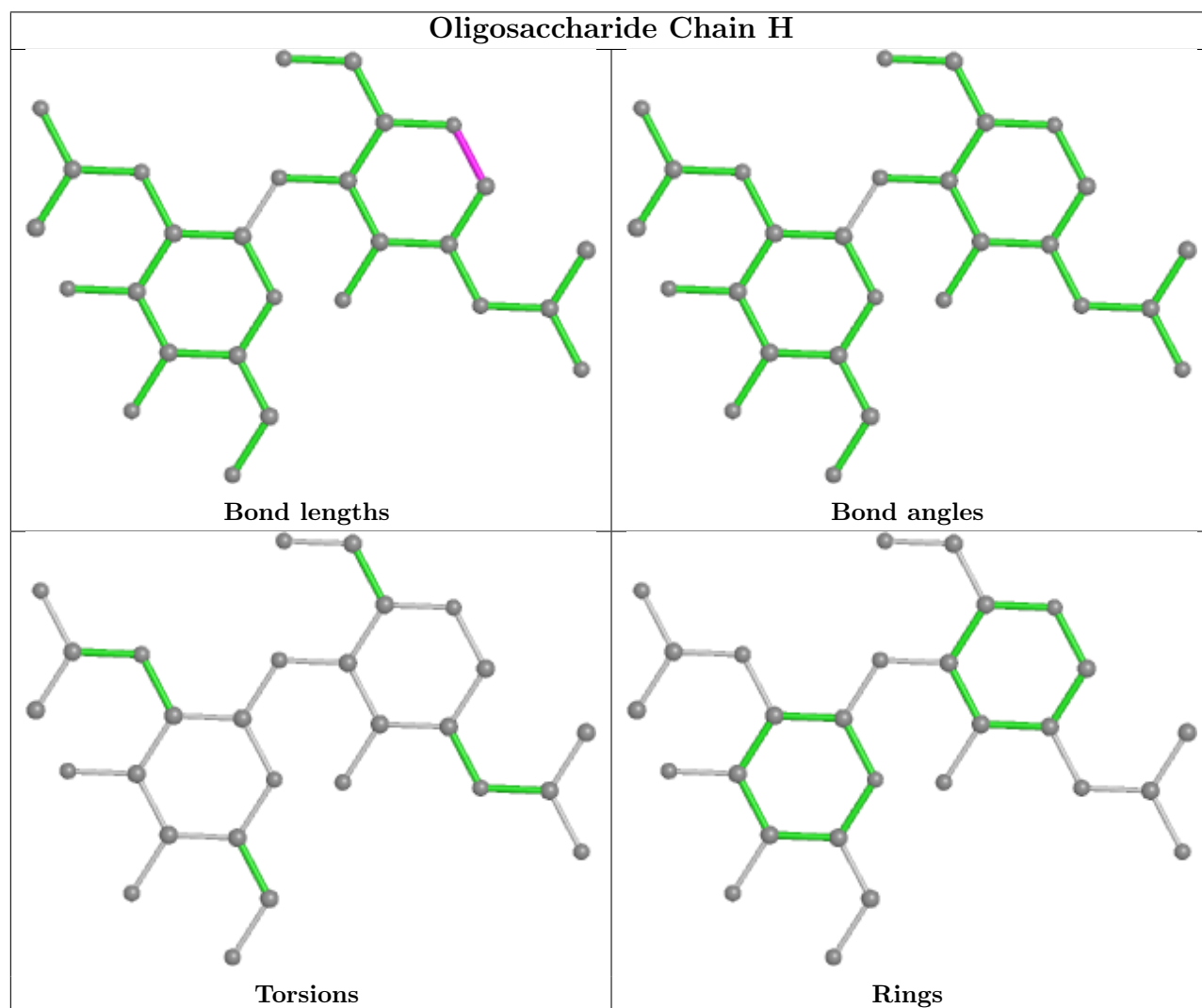
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6

There are no ring outliers.

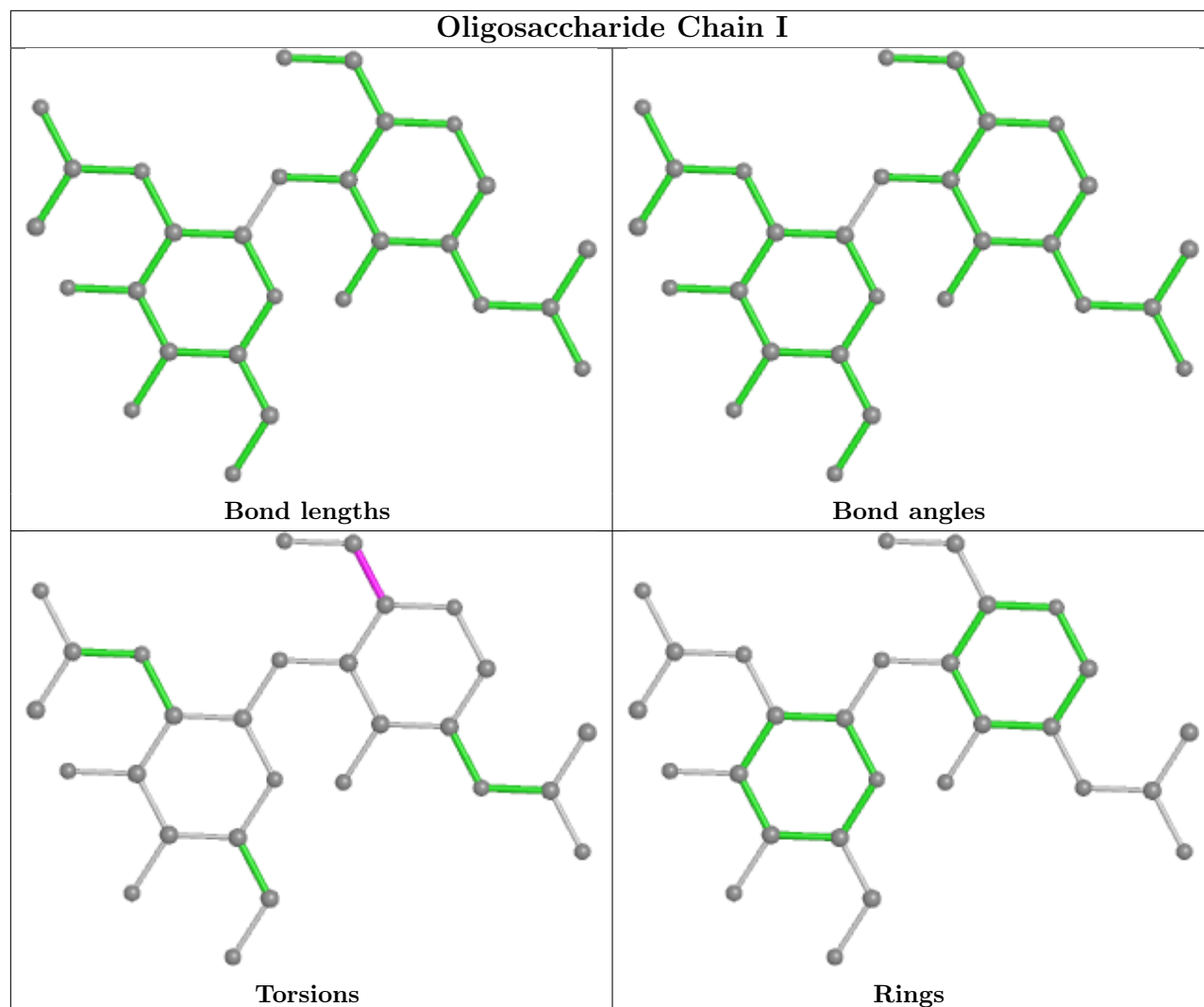
1 monomer is involved in 1 short contact:

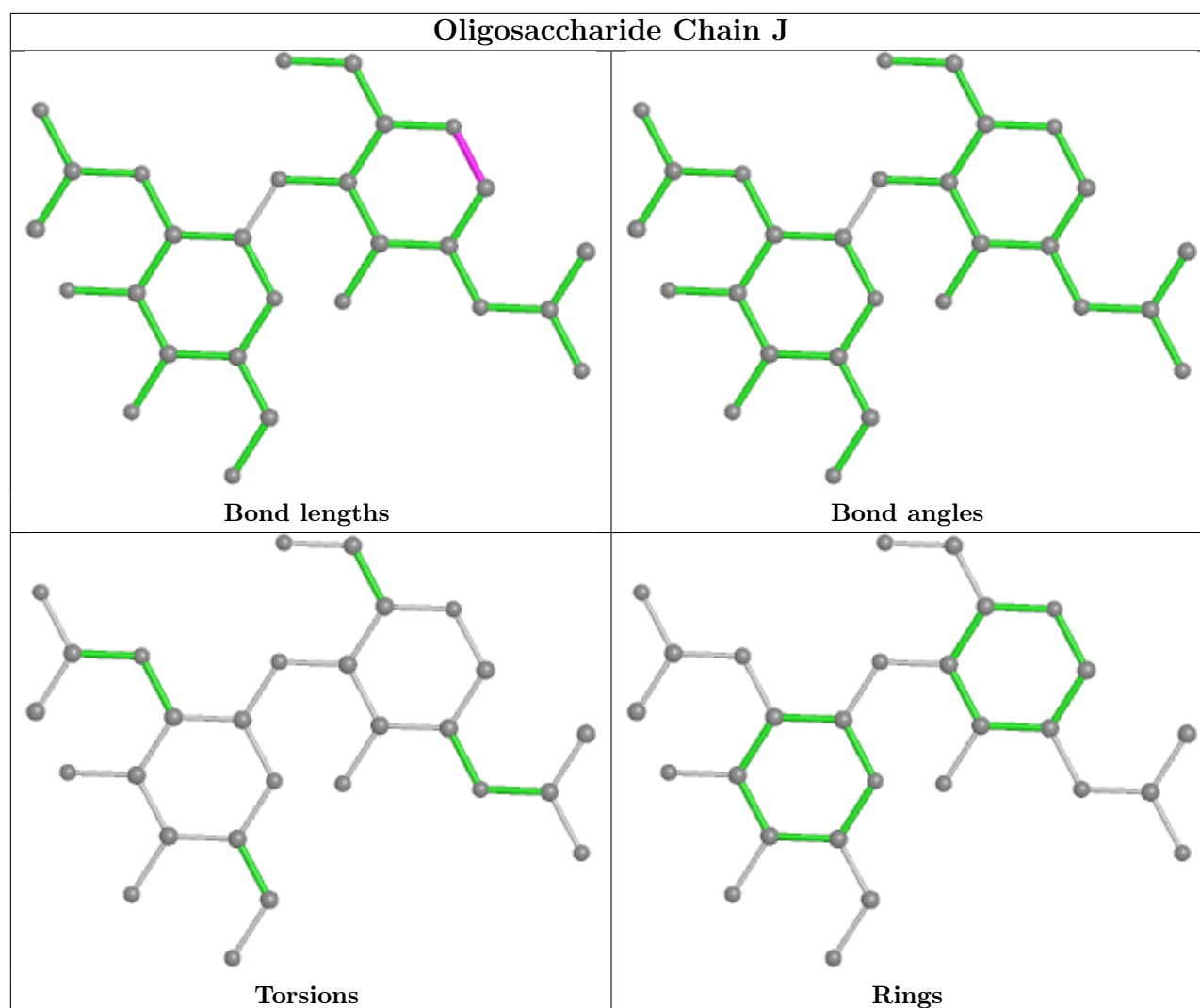
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 6 are monoatomic - leaving 21 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	CLR	A	1104	-	31,31,31	1.72	9 (29%)	48,48,48	1.57	11 (22%)
8	BUF	A	1121	-	28,32,32	1.53	5 (17%)	46,52,52	1.58	8 (17%)
7	PCW	C	1105	-	21,21,53	1.69	6 (28%)	27,29,61	1.27	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	B	401	2	14,14,15	0.27	0	17,19,21	0.45	0
7	PCW	C	1106	-	21,21,53	1.69	5 (23%)	27,29,61	1.19	2 (7%)
7	PCW	A	1106	-	21,21,53	1.66	6 (28%)	27,29,61	1.15	1 (3%)
9	CLR	E	101	-	31,31,31	1.78	8 (25%)	48,48,48	1.58	10 (20%)
9	CLR	D	501	-	31,31,31	2.07	12 (38%)	48,48,48	1.46	8 (16%)
9	CLR	G	101	-	31,31,31	1.65	7 (22%)	48,48,48	1.67	13 (27%)
10	NAG	D	401	2	14,14,15	0.32	0	17,19,21	0.53	0
7	PCW	A	1108	-	21,21,53	1.70	6 (28%)	27,29,61	1.19	1 (3%)
9	CLR	B	501	-	31,31,31	1.86	10 (32%)	48,48,48	1.52	11 (22%)
7	PCW	D	402	-	21,21,53	1.67	6 (28%)	27,29,61	1.23	1 (3%)
7	PCW	A	1109	-	21,21,53	1.72	6 (28%)	27,29,61	1.33	2 (7%)
7	PCW	C	1108	-	21,21,53	1.70	5 (23%)	27,29,61	1.41	3 (11%)
7	PCW	A	1110	-	21,21,53	1.70	5 (23%)	27,29,61	1.24	1 (3%)
7	PCW	A	1107	-	21,21,53	1.68	6 (28%)	27,29,61	1.23	2 (7%)
9	CLR	C	1104	-	31,31,31	1.74	8 (25%)	48,48,48	1.54	11 (22%)
7	PCW	C	1107	-	21,21,53	1.75	5 (23%)	27,29,61	1.26	2 (7%)
8	BUF	C	1121	-	28,32,32	1.52	6 (21%)	46,52,52	1.64	9 (19%)
7	PCW	A	1105	-	21,21,53	1.67	4 (19%)	27,29,61	1.21	1 (3%)

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	CLR	A	1104	-	-	4/10/68/68	0/4/4/4
8	BUF	A	1121	-	-	0/4/68/68	0/5/5/5
7	PCW	C	1105	-	-	10/23/23/57	-
10	NAG	B	401	2	-	1/6/23/26	0/1/1/1
7	PCW	C	1106	-	-	14/23/23/57	-
7	PCW	A	1106	-	-	10/23/23/57	-
9	CLR	E	101	-	-	3/10/68/68	0/4/4/4
9	CLR	D	501	-	-	0/10/68/68	0/4/4/4
9	CLR	G	101	-	-	3/10/68/68	0/4/4/4
10	NAG	D	401	2	-	4/6/23/26	0/1/1/1
7	PCW	A	1108	-	-	10/23/23/57	-
9	CLR	B	501	-	-	0/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	D	402	-	-	7/23/23/57	-
7	PCW	A	1109	-	-	14/23/23/57	-
7	PCW	C	1108	-	-	10/23/23/57	-
7	PCW	A	1110	-	-	7/23/23/57	-
7	PCW	A	1107	-	-	10/23/23/57	-
9	CLR	C	1104	-	-	4/10/68/68	0/4/4/4
7	PCW	C	1107	-	-	11/23/23/57	-
8	BUF	C	1121	-	-	0/4/68/68	0/5/5/5
7	PCW	A	1105	-	-	17/23/23/57	-

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	CLR	C10-C9	4.26	1.63	1.56
8	A	1121	BUF	C23-C24	4.18	1.45	1.37
8	C	1121	BUF	C23-C24	4.09	1.45	1.37
7	C	1107	PCW	O2-C31	4.01	1.44	1.35
9	E	101	CLR	C10-C9	3.97	1.62	1.56
9	D	501	CLR	C13-C14	3.94	1.62	1.55
9	D	501	CLR	C4-C3	3.86	1.58	1.52
7	A	1110	PCW	O2-C31	3.74	1.43	1.35
9	E	101	CLR	C16-C17	3.72	1.62	1.54
7	A	1105	PCW	O2-C31	3.71	1.43	1.35
7	C	1106	PCW	O2-C31	3.70	1.43	1.35
7	A	1108	PCW	O2-C31	3.69	1.43	1.35
7	C	1105	PCW	O2-C31	3.69	1.43	1.35
7	A	1109	PCW	O2-C31	3.64	1.43	1.35
8	A	1121	BUF	C22-C20	3.61	1.44	1.39
7	C	1108	PCW	O2-C31	3.61	1.43	1.35
7	D	402	PCW	O2-C31	3.61	1.43	1.35
7	A	1107	PCW	O2-C31	3.59	1.43	1.35
9	G	101	CLR	C16-C17	3.55	1.61	1.54
8	C	1121	BUF	C22-C20	3.55	1.44	1.39
9	D	501	CLR	C10-C9	3.54	1.62	1.56
9	G	101	CLR	C10-C5	3.46	1.59	1.52
9	D	501	CLR	C16-C17	3.41	1.61	1.54
7	A	1106	PCW	O2-C31	3.39	1.42	1.35
9	B	501	CLR	C16-C17	3.38	1.61	1.54
9	C	1104	CLR	C10-C9	3.36	1.61	1.56
9	E	101	CLR	C13-C14	3.30	1.61	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	CLR	C13-C14	3.29	1.61	1.55
9	G	101	CLR	C13-C14	3.21	1.61	1.55
9	A	1104	CLR	C10-C5	3.14	1.59	1.52
9	D	501	CLR	C13-C17	3.11	1.60	1.55
9	C	1104	CLR	C16-C17	3.10	1.60	1.54
9	C	1104	CLR	C11-C9	3.07	1.58	1.53
9	B	501	CLR	C12-C11	3.06	1.59	1.53
9	B	501	CLR	C12-C13	3.06	1.59	1.54
9	G	101	CLR	C10-C9	3.06	1.61	1.56
9	C	1104	CLR	C12-C11	3.06	1.59	1.53
9	A	1104	CLR	C4-C3	3.05	1.57	1.52
8	A	1121	BUF	C13-C17	-2.97	1.54	1.58
9	D	501	CLR	C12-C11	2.95	1.59	1.53
9	A	1104	CLR	C12-C11	2.93	1.59	1.53
9	C	1104	CLR	C4-C3	2.88	1.57	1.52
9	A	1104	CLR	C11-C9	2.82	1.58	1.53
9	C	1104	CLR	C13-C14	2.81	1.60	1.55
9	A	1104	CLR	C16-C17	2.81	1.60	1.54
9	D	501	CLR	C16-C15	2.80	1.61	1.54
9	E	101	CLR	C10-C5	2.70	1.58	1.52
9	B	501	CLR	C13-C17	2.68	1.60	1.55
8	C	1121	BUF	C13-C17	-2.67	1.55	1.58
9	A	1104	CLR	C10-C9	2.64	1.60	1.56
9	A	1104	CLR	C13-C14	2.63	1.60	1.55
7	A	1109	PCW	C6-N	-2.63	1.42	1.50
9	E	101	CLR	C12-C13	2.62	1.58	1.54
9	B	501	CLR	C10-C5	2.60	1.58	1.52
9	E	101	CLR	C12-C11	2.59	1.58	1.53
7	A	1105	PCW	C6-N	-2.58	1.42	1.50
8	C	1121	BUF	C14-C8	2.57	1.57	1.54
9	E	101	CLR	C13-C17	2.55	1.59	1.55
9	D	501	CLR	C4-C5	2.51	1.57	1.51
7	A	1110	PCW	C7-N	-2.49	1.42	1.50
9	B	501	CLR	C4-C3	2.48	1.56	1.52
7	A	1105	PCW	C8-N	-2.48	1.42	1.50
9	D	501	CLR	C22-C20	2.48	1.60	1.54
7	C	1108	PCW	C7-N	-2.48	1.42	1.50
7	C	1105	PCW	C6-N	-2.47	1.42	1.50
7	C	1106	PCW	C7-N	-2.47	1.42	1.50
7	D	402	PCW	C6-N	-2.47	1.42	1.50
7	A	1107	PCW	C7-N	-2.46	1.42	1.50
7	A	1106	PCW	C6-N	-2.46	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1107	PCW	C6-N	-2.46	1.42	1.50
7	A	1108	PCW	C7-N	-2.46	1.42	1.50
7	A	1109	PCW	C7-N	-2.46	1.42	1.50
7	A	1110	PCW	C6-N	-2.45	1.42	1.50
7	A	1108	PCW	C6-N	-2.45	1.42	1.50
7	C	1108	PCW	C6-N	-2.44	1.42	1.50
7	C	1107	PCW	C7-N	-2.44	1.42	1.50
7	A	1106	PCW	C7-N	-2.43	1.42	1.50
7	D	402	PCW	C7-N	-2.43	1.42	1.50
9	C	1104	CLR	C10-C5	2.43	1.57	1.52
7	C	1105	PCW	C7-N	-2.43	1.42	1.50
7	A	1107	PCW	C6-N	-2.39	1.43	1.50
7	C	1106	PCW	C6-N	-2.38	1.43	1.50
9	A	1104	CLR	C16-C15	2.37	1.60	1.54
7	C	1107	PCW	P-O3P	2.37	1.68	1.59
7	A	1105	PCW	C7-N	-2.34	1.43	1.50
9	D	501	CLR	C12-C13	2.33	1.58	1.54
9	D	501	CLR	C7-C8	2.29	1.57	1.53
9	B	501	CLR	C16-C15	2.28	1.60	1.54
9	G	101	CLR	C12-C11	2.26	1.58	1.53
9	E	101	CLR	C4-C3	2.26	1.56	1.52
8	A	1121	BUF	C14-C8	2.25	1.57	1.54
8	C	1121	BUF	C23-C22	-2.19	1.34	1.38
7	A	1106	PCW	O2-C2	-2.19	1.41	1.46
9	A	1104	CLR	C12-C13	2.18	1.58	1.54
7	C	1106	PCW	P-O3P	2.17	1.68	1.59
7	A	1108	PCW	P-O3P	2.17	1.68	1.59
7	C	1108	PCW	O2-C2	-2.16	1.41	1.46
7	A	1110	PCW	P-O3P	2.16	1.68	1.59
7	A	1109	PCW	P-O3P	2.16	1.68	1.59
8	C	1121	BUF	O14-C14	-2.16	1.40	1.44
7	C	1108	PCW	P-O3P	2.14	1.68	1.59
9	G	101	CLR	C12-C13	2.13	1.58	1.54
9	D	501	CLR	C11-C9	2.13	1.57	1.53
8	A	1121	BUF	O14-C14	-2.12	1.40	1.44
9	G	101	CLR	C13-C17	2.12	1.59	1.55
7	A	1107	PCW	O2-C2	-2.11	1.41	1.46
7	A	1107	PCW	P-O3P	2.11	1.67	1.59
7	A	1109	PCW	O2-C2	-2.11	1.41	1.46
7	C	1105	PCW	P-O3P	2.09	1.67	1.59
7	C	1105	PCW	O2-C2	-2.08	1.41	1.46
9	B	501	CLR	C22-C20	2.05	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1109	PCW	C8-N	-2.05	1.44	1.50
9	C	1104	CLR	C16-C15	2.04	1.59	1.54
7	C	1105	PCW	C8-N	-2.04	1.44	1.50
7	C	1106	PCW	C8-N	-2.04	1.44	1.50
7	D	402	PCW	C8-N	-2.03	1.44	1.50
7	A	1107	PCW	C8-N	-2.03	1.44	1.50
7	A	1110	PCW	C8-N	-2.03	1.44	1.50
7	A	1106	PCW	P-O3P	2.03	1.67	1.59
7	A	1108	PCW	C8-N	-2.02	1.44	1.50
7	A	1106	PCW	C8-N	-2.02	1.44	1.50
7	D	402	PCW	P-O3P	2.02	1.67	1.59
7	A	1108	PCW	O2-C2	-2.01	1.41	1.46
7	D	402	PCW	O2-C2	-2.00	1.41	1.46
7	C	1107	PCW	C8-N	-2.00	1.44	1.50

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1108	PCW	O2-C31-C32	5.25	120.74	111.09
7	A	1109	PCW	O2-C31-C32	5.08	120.43	111.09
7	A	1110	PCW	O2-C31-C32	4.98	120.25	111.09
7	C	1105	PCW	O2-C31-C32	4.98	120.25	111.09
7	D	402	PCW	O2-C31-C32	4.94	120.19	111.09
7	C	1107	PCW	O2-C31-C32	4.91	120.13	111.09
7	C	1106	PCW	O2-C31-C32	4.81	119.95	111.09
8	C	1121	BUF	C15-C16-C17	4.77	108.70	103.17
7	A	1108	PCW	O2-C31-C32	4.72	119.78	111.09
7	A	1107	PCW	O2-C31-C32	4.72	119.77	111.09
7	A	1105	PCW	O2-C31-C32	4.69	119.72	111.09
7	A	1106	PCW	O2-C31-C32	4.57	119.50	111.09
8	A	1121	BUF	C15-C16-C17	4.56	108.46	103.17
9	G	101	CLR	C17-C13-C14	-4.14	95.17	100.07
8	C	1121	BUF	C18-C13-C17	-4.00	111.72	115.99
9	C	1104	CLR	C8-C7-C6	-3.99	107.00	112.73
9	A	1104	CLR	C8-C7-C6	-3.96	107.04	112.73
8	A	1121	BUF	C18-C13-C17	-3.84	111.89	115.99
9	D	501	CLR	C8-C7-C6	-3.63	107.52	112.73
9	E	101	CLR	C17-C13-C14	-3.50	95.93	100.07
9	G	101	CLR	C2-C3-C4	-3.35	105.71	110.31
9	B	501	CLR	C8-C7-C6	-3.28	108.03	112.73
9	G	101	CLR	C22-C20-C17	-3.25	103.58	110.28
8	C	1121	BUF	C12-C13-C14	3.18	112.82	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	101	CLR	C2-C3-C4	-3.15	105.99	110.31
9	B	501	CLR	C2-C3-C4	-3.11	106.04	110.31
7	C	1108	PCW	C2-O2-C31	-3.00	112.30	117.90
9	G	101	CLR	C8-C7-C6	-3.00	108.43	112.73
8	A	1121	BUF	C12-C13-C14	2.99	112.58	108.97
8	C	1121	BUF	C18-C13-C12	2.90	113.84	109.73
9	E	101	CLR	C22-C20-C17	-2.89	104.31	110.28
9	D	501	CLR	C3-C4-C5	2.88	116.91	112.03
8	A	1121	BUF	C18-C13-C12	2.76	113.64	109.73
9	E	101	CLR	C8-C7-C6	-2.72	108.82	112.73
9	A	1104	CLR	C2-C3-C4	-2.71	106.58	110.31
9	G	101	CLR	C4-C5-C6	-2.63	116.82	120.61
9	G	101	CLR	C16-C17-C20	-2.57	108.16	112.15
9	A	1104	CLR	C15-C14-C8	-2.57	114.85	119.08
9	C	1104	CLR	C15-C14-C8	-2.54	114.89	119.08
9	A	1104	CLR	C13-C17-C20	-2.53	115.52	119.49
9	E	101	CLR	C16-C17-C20	-2.50	108.28	112.15
9	A	1104	CLR	C3-C4-C5	2.46	116.20	112.03
9	E	101	CLR	C4-C5-C6	-2.46	117.07	120.61
9	C	1104	CLR	C2-C3-C4	-2.44	106.96	110.31
7	A	1109	PCW	C2-O2-C31	-2.41	113.40	117.90
9	G	101	CLR	O1-C3-C2	2.41	116.31	110.16
9	A	1104	CLR	C15-C14-C13	2.40	106.74	103.84
9	A	1104	CLR	C18-C13-C12	2.38	114.34	110.59
8	A	1121	BUF	C14-C13-C17	2.36	106.27	103.56
8	C	1121	BUF	C9-C10-C5	2.35	111.88	108.58
9	D	501	CLR	C16-C17-C20	-2.35	108.51	112.15
9	C	1104	CLR	C16-C17-C20	-2.33	108.54	112.15
9	D	501	CLR	C18-C13-C12	2.32	114.25	110.59
9	B	501	CLR	C22-C20-C17	-2.31	105.52	110.28
9	B	501	CLR	C16-C17-C20	-2.31	108.57	112.15
9	G	101	CLR	C18-C13-C12	2.31	114.23	110.59
9	B	501	CLR	C18-C13-C12	2.30	114.23	110.59
9	C	1104	CLR	C3-C4-C5	2.30	115.93	112.03
9	D	501	CLR	C17-C13-C14	-2.28	97.37	100.07
9	C	1104	CLR	C13-C17-C20	-2.28	115.92	119.49
9	B	501	CLR	C17-C13-C14	-2.28	97.38	100.07
9	D	501	CLR	C2-C3-C4	-2.27	107.19	110.31
9	E	101	CLR	C18-C13-C12	2.27	114.17	110.59
9	G	101	CLR	C7-C8-C14	-2.26	107.63	110.91
9	B	501	CLR	C11-C9-C10	2.26	116.05	113.08
9	B	501	CLR	C4-C5-C10	-2.25	113.43	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	CLR	C4-C5-C6	-2.23	117.39	120.61
9	B	501	CLR	O1-C3-C2	2.22	115.81	110.16
8	C	1121	BUF	C22-C23-C24	2.21	121.20	118.45
9	A	1104	CLR	O1-C3-C2	2.20	115.77	110.16
9	A	1104	CLR	C16-C17-C20	-2.20	108.74	112.15
9	D	501	CLR	C22-C20-C17	-2.20	105.74	110.28
9	E	101	CLR	O1-C3-C2	2.20	115.75	110.16
9	C	1104	CLR	C22-C20-C17	-2.19	105.75	110.28
9	D	501	CLR	C21-C20-C17	2.19	116.27	112.92
7	A	1107	PCW	C2-O2-C31	-2.19	113.82	117.90
9	E	101	CLR	C21-C20-C17	2.19	116.27	112.92
7	C	1107	PCW	C2-O2-C31	2.19	121.97	117.90
9	G	101	CLR	C13-C14-C8	2.18	117.61	114.38
8	A	1121	BUF	C1-C2-C3	-2.18	107.67	110.47
9	C	1104	CLR	C15-C14-C13	2.13	106.41	103.84
8	C	1121	BUF	C14-C13-C17	2.12	105.98	103.56
8	A	1121	BUF	C9-C10-C5	2.11	111.55	108.58
9	B	501	CLR	C21-C20-C17	2.11	116.16	112.92
9	A	1104	CLR	C12-C13-C14	-2.11	104.00	107.27
9	G	101	CLR	C15-C14-C8	-2.11	115.61	119.08
9	C	1104	CLR	C12-C13-C14	-2.09	104.03	107.27
9	G	101	CLR	C21-C20-C17	2.08	116.11	112.92
9	C	1104	CLR	C18-C13-C12	2.08	113.87	110.59
9	C	1104	CLR	C21-C20-C17	2.06	116.08	112.92
8	C	1121	BUF	C7-C6-C5	2.06	115.97	111.84
9	E	101	CLR	C11-C9-C10	2.06	115.79	113.08
8	C	1121	BUF	C1-C2-C3	-2.03	107.86	110.47
8	A	1121	BUF	C22-C23-C24	2.03	120.97	118.45
9	G	101	CLR	C24-C23-C22	-2.02	103.94	113.24
7	C	1108	PCW	C3-O3-C11	-2.02	112.04	117.10
9	A	1104	CLR	C22-C20-C17	-2.01	106.14	110.28
7	C	1106	PCW	O3-C11-C12	2.01	121.12	112.38

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1108	PCW	C4-O4P-P-O1P
7	A	1107	PCW	C4-O4P-P-O2P
7	C	1105	PCW	O4P-C4-C5-N
7	C	1105	PCW	C1-O3P-P-O1P
7	C	1105	PCW	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
7	C	1105	PCW	C1-O3P-P-O4P
7	D	402	PCW	C32-C31-O2-C2
7	D	402	PCW	O31-C31-O2-C2
7	A	1109	PCW	C32-C31-O2-C2
7	A	1109	PCW	C4-O4P-P-O1P
7	C	1106	PCW	C32-C31-O2-C2
7	C	1106	PCW	C4-O4P-P-O2P
7	C	1107	PCW	C32-C31-O2-C2
7	C	1107	PCW	C1-O3P-P-O1P
7	C	1107	PCW	C1-O3P-P-O2P
7	C	1107	PCW	C1-O3P-P-O4P
7	C	1107	PCW	C4-O4P-P-O1P
7	C	1107	PCW	C4-O4P-P-O2P
7	C	1107	PCW	C4-O4P-P-O3P
7	C	1108	PCW	C4-O4P-P-O2P
7	A	1106	PCW	C1-O3P-P-O2P
7	C	1105	PCW	C32-C31-O2-C2
7	A	1105	PCW	C32-C31-O2-C2
7	A	1110	PCW	C32-C31-O2-C2
7	A	1107	PCW	C32-C31-O2-C2
7	C	1108	PCW	C32-C31-O2-C2
7	A	1105	PCW	O31-C31-O2-C2
7	A	1106	PCW	C32-C31-O2-C2
7	C	1105	PCW	O31-C31-O2-C2
7	A	1110	PCW	O31-C31-O2-C2
7	C	1107	PCW	O31-C31-O2-C2
7	A	1110	PCW	O11-C11-O3-C3
7	A	1109	PCW	O31-C31-O2-C2
7	C	1106	PCW	O31-C31-O2-C2
7	A	1108	PCW	C32-C31-O2-C2
7	C	1105	PCW	O11-C11-O3-C3
7	A	1107	PCW	C12-C11-O3-C3
7	C	1105	PCW	C12-C11-O3-C3
7	A	1110	PCW	C12-C11-O3-C3
7	A	1107	PCW	O31-C31-O2-C2
7	C	1108	PCW	O31-C31-O2-C2
7	A	1109	PCW	O11-C11-O3-C3
10	D	401	NAG	O5-C5-C6-O6
7	C	1108	PCW	O11-C11-O3-C3
7	A	1105	PCW	O11-C11-O3-C3
7	C	1107	PCW	C12-C11-O3-C3
7	C	1108	PCW	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
9	E	101	CLR	C21-C20-C22-C23
7	A	1106	PCW	O31-C31-O2-C2
7	A	1105	PCW	C4-C5-N-C7
7	A	1109	PCW	C12-C11-O3-C3
10	D	401	NAG	C8-C7-N2-C2
10	D	401	NAG	O7-C7-N2-C2
10	D	401	NAG	C4-C5-C6-O6
9	G	101	CLR	C21-C20-C22-C23
7	A	1105	PCW	C12-C11-O3-C3
9	C	1104	CLR	C20-C22-C23-C24
7	A	1107	PCW	O11-C11-O3-C3
7	A	1105	PCW	C4-C5-N-C6
7	C	1107	PCW	O11-C11-O3-C3
7	A	1108	PCW	C4-O4P-P-O3P
7	A	1109	PCW	C4-O4P-P-O3P
7	A	1110	PCW	C4-O4P-P-O3P
7	A	1108	PCW	O31-C31-O2-C2
9	C	1104	CLR	C23-C24-C25-C26
7	C	1106	PCW	C12-C11-O3-C3
9	E	101	CLR	C20-C22-C23-C24
7	A	1105	PCW	C4-C5-N-C8
9	C	1104	CLR	C23-C24-C25-C27
9	E	101	CLR	C22-C23-C24-C25
7	C	1106	PCW	O11-C11-O3-C3
9	A	1104	CLR	C20-C22-C23-C24
7	A	1109	PCW	C1-O3P-P-O4P
7	C	1106	PCW	C4-O4P-P-O3P
7	A	1106	PCW	C1-O3P-P-O4P
7	A	1109	PCW	O3P-C1-C2-C3
7	C	1108	PCW	O3P-C1-C2-C3
7	A	1105	PCW	O3P-C1-C2-C3
7	A	1107	PCW	C1-C2-C3-O3
9	G	101	CLR	C22-C23-C24-C25
7	D	402	PCW	C12-C11-O3-C3
7	A	1106	PCW	O2-C2-C3-O3
7	A	1108	PCW	C1-C2-C3-O3
9	G	101	CLR	C20-C22-C23-C24
7	C	1108	PCW	C4-O4P-P-O3P
10	B	401	NAG	O5-C5-C6-O6
7	A	1105	PCW	O2-C2-C3-O3
7	C	1106	PCW	O3P-C1-C2-C3
7	A	1105	PCW	C3-C2-O2-C31

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Mol	Chain	Res	Type	Atoms
9	A	1104	CLR	C13-C17-C20-C21
7	A	1109	PCW	O3P-C1-C2-O2
9	C	1104	CLR	C13-C17-C20-C21
7	A	1107	PCW	C4-O4P-P-O3P
7	A	1105	PCW	C4-O4P-P-O3P
7	A	1108	PCW	C4-O4P-P-O2P
7	A	1109	PCW	C1-O3P-P-O1P
7	A	1109	PCW	C4-O4P-P-O2P
7	C	1106	PCW	C4-C5-N-C6
7	A	1110	PCW	C4-O4P-P-O2P
7	C	1106	PCW	O3P-C1-C2-O2
7	A	1105	PCW	O3P-C1-C2-O2
7	A	1108	PCW	O4P-C4-C5-N
7	A	1107	PCW	O4P-C4-C5-N
7	D	402	PCW	O4P-C4-C5-N
7	A	1109	PCW	O4P-C4-C5-N
7	C	1106	PCW	O4P-C4-C5-N
7	C	1107	PCW	O4P-C4-C5-N
7	C	1108	PCW	O4P-C4-C5-N
7	A	1106	PCW	O4P-C4-C5-N
7	A	1105	PCW	O4P-C4-C5-N
7	A	1110	PCW	O4P-C4-C5-N
7	A	1108	PCW	O2-C2-C3-O3
7	A	1107	PCW	O2-C2-C3-O3
7	C	1108	PCW	O3P-C1-C2-O2
7	C	1106	PCW	C4-C5-N-C8
7	A	1108	PCW	C1-O3P-P-O4P
7	A	1107	PCW	C1-O3P-P-O4P
7	C	1105	PCW	C4-O4P-P-O3P
7	D	402	PCW	C1-O3P-P-O4P
7	D	402	PCW	C4-O4P-P-O3P
7	C	1106	PCW	C1-O3P-P-O4P
7	C	1108	PCW	C1-O3P-P-O4P
7	A	1106	PCW	C4-O4P-P-O3P
7	A	1105	PCW	C1-O3P-P-O4P
7	A	1106	PCW	C12-C11-O3-C3
7	A	1106	PCW	C1-C2-C3-O3
7	D	402	PCW	O11-C11-O3-C3
9	A	1104	CLR	C23-C24-C25-C26
7	C	1106	PCW	C4-C5-N-C7
7	A	1109	PCW	O2-C2-C3-O3
9	A	1104	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
7	A	1105	PCW	C1-C2-C3-O3
7	C	1106	PCW	C1-C2-C3-O3
7	A	1108	PCW	C1-O3P-P-O2P
7	C	1105	PCW	C4-O4P-P-O2P
7	A	1109	PCW	C1-O3P-P-O2P
7	A	1106	PCW	C4-O4P-P-O2P
7	A	1105	PCW	C4-O4P-P-O2P
7	A	1105	PCW	C5-C4-O4P-P

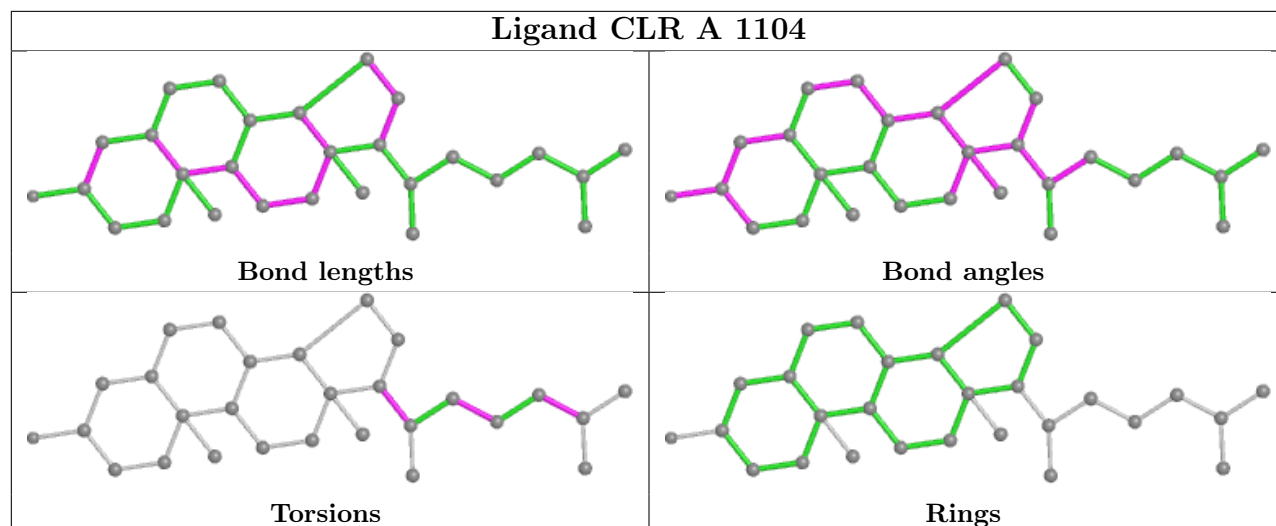
There are no ring outliers.

14 monomers are involved in 24 short contacts:

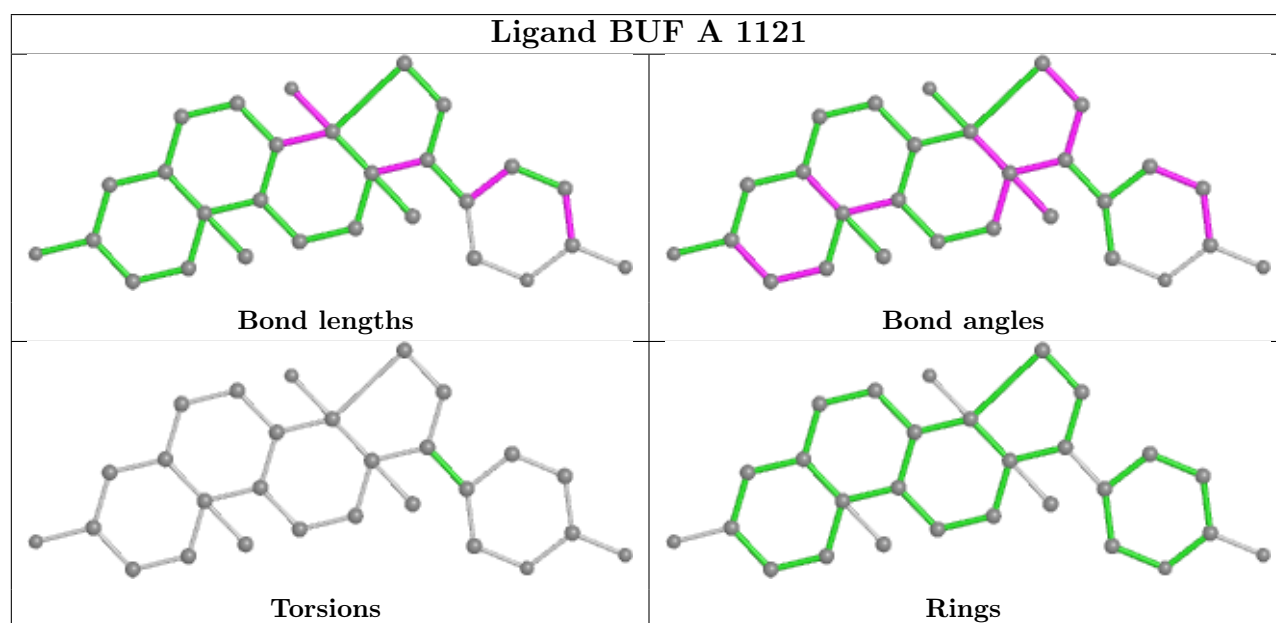
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1104	CLR	1	0
8	A	1121	BUF	2	0
7	C	1105	PCW	1	0
9	E	101	CLR	3	0
9	D	501	CLR	2	0
9	G	101	CLR	2	0
7	A	1108	PCW	2	0
7	A	1109	PCW	1	0
7	C	1108	PCW	1	0
7	A	1110	PCW	2	0
9	C	1104	CLR	1	0
7	C	1107	PCW	1	0
8	C	1121	BUF	1	0
7	A	1105	PCW	4	0

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.

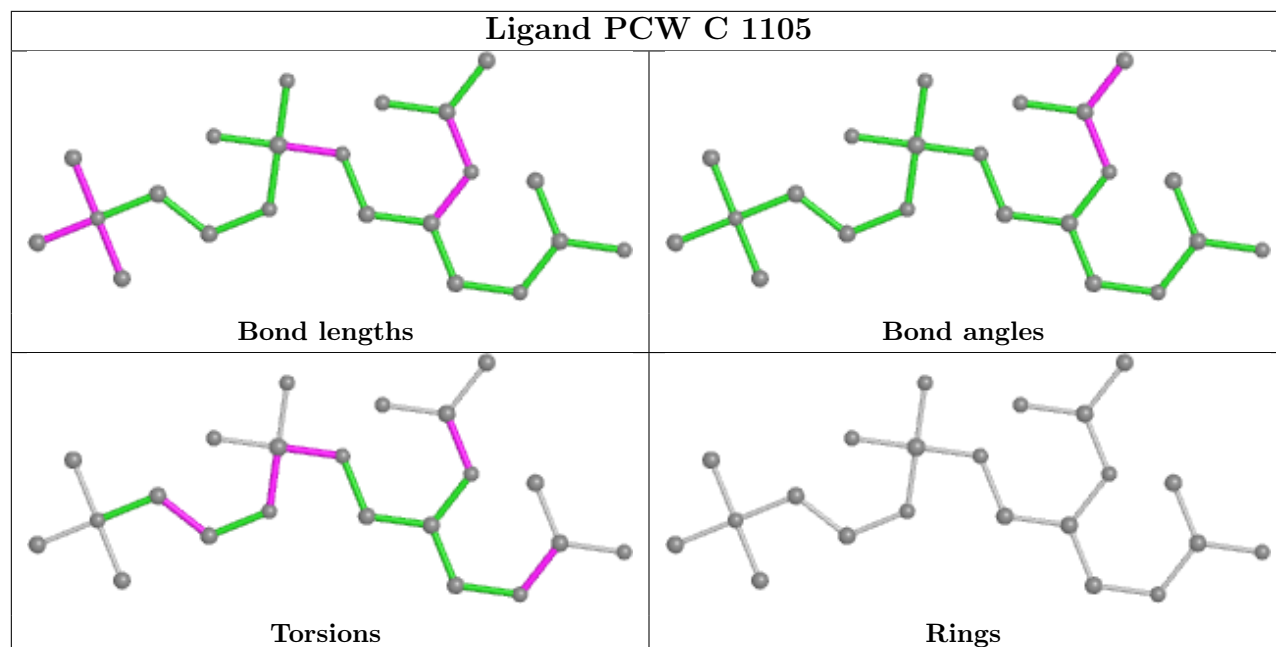
## Ligand CLR A 1104



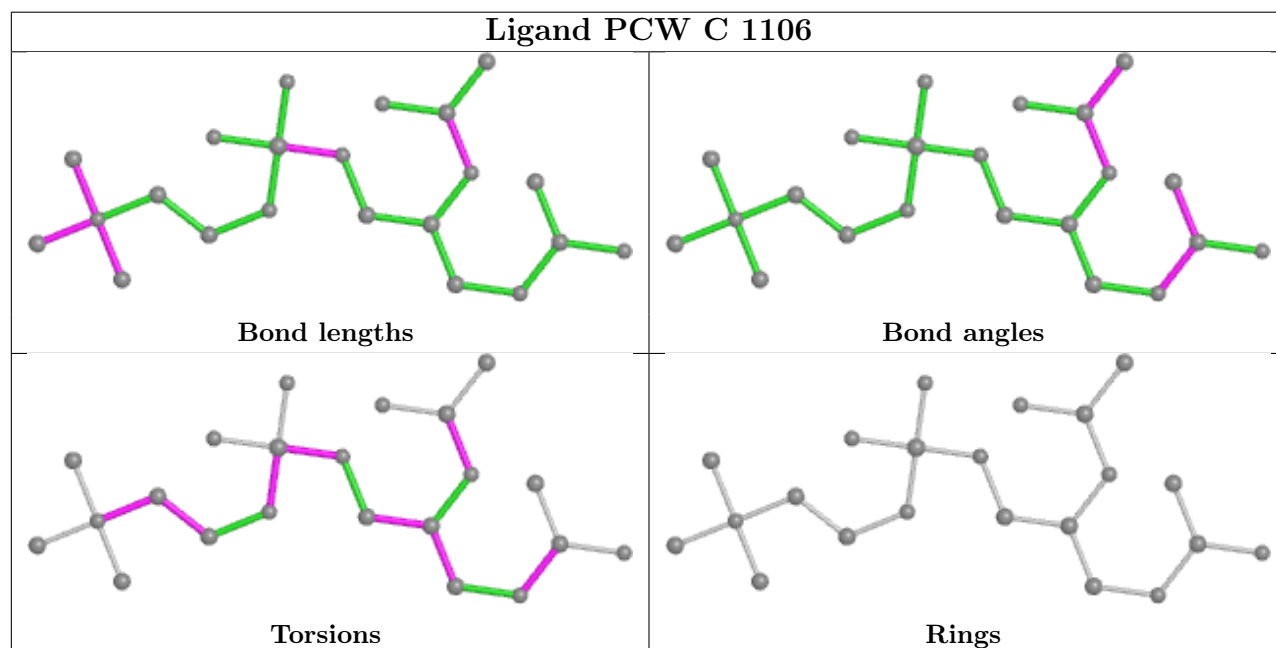
## Ligand BUF A 1121



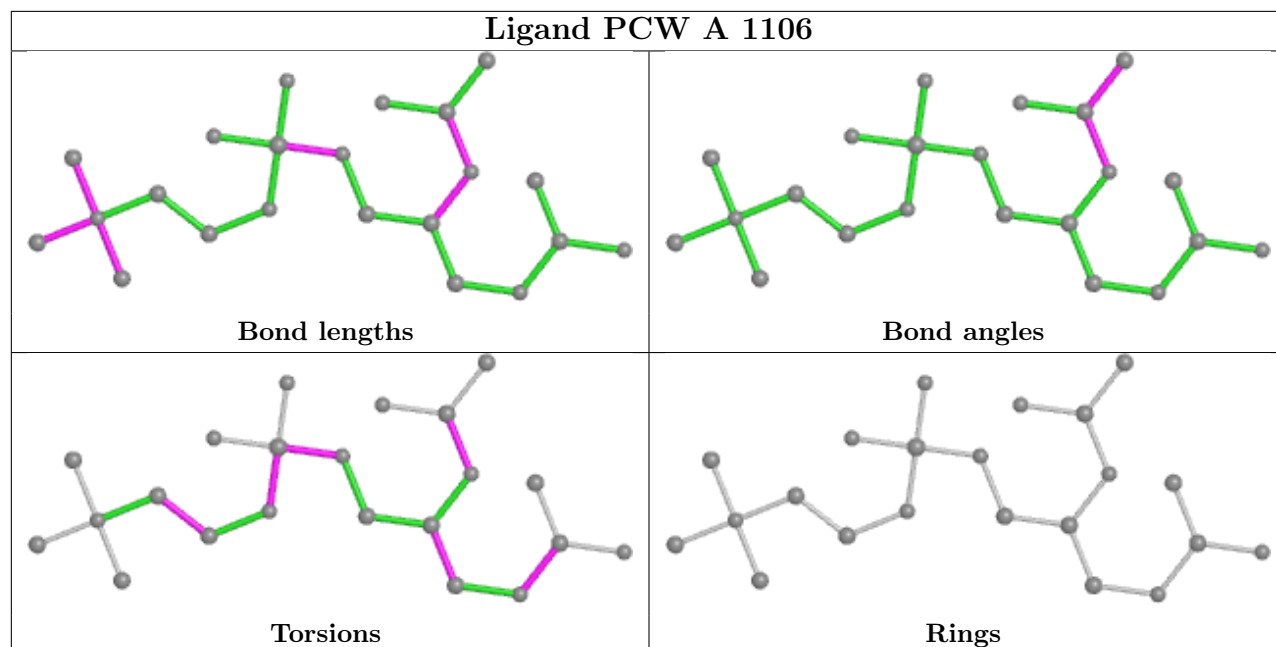
## Ligand PCW C 1105



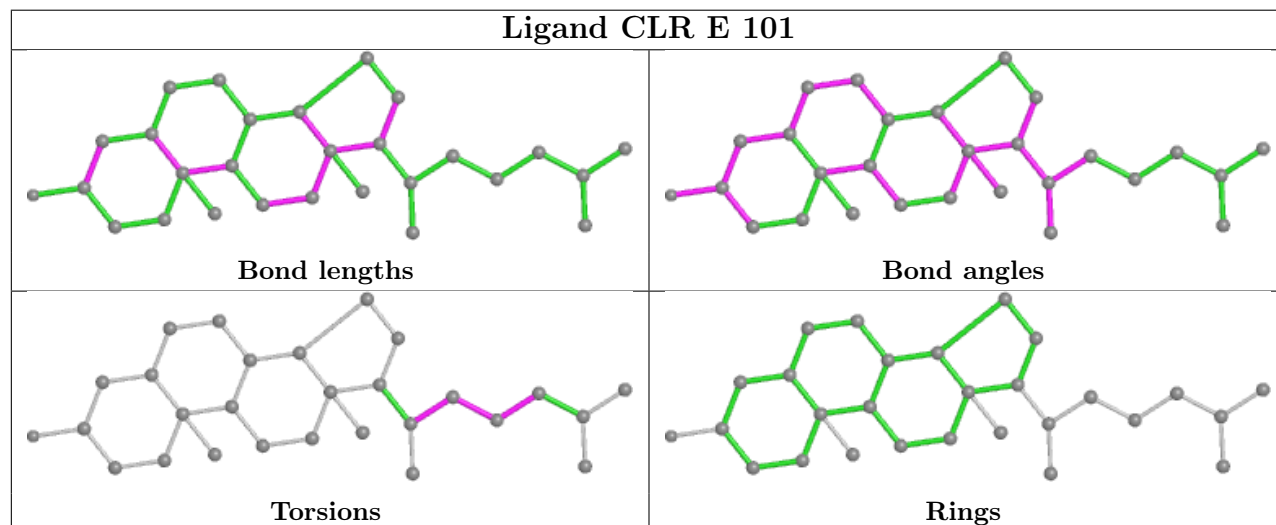
## Ligand PCW C 1106



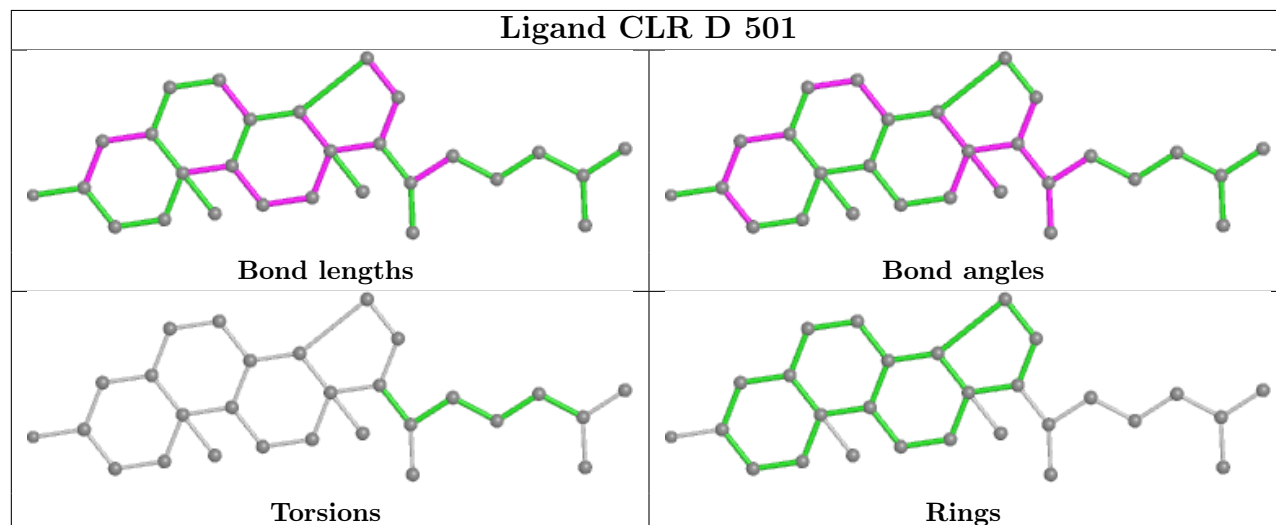
## Ligand PCW A 1106



## Ligand CLR E 101

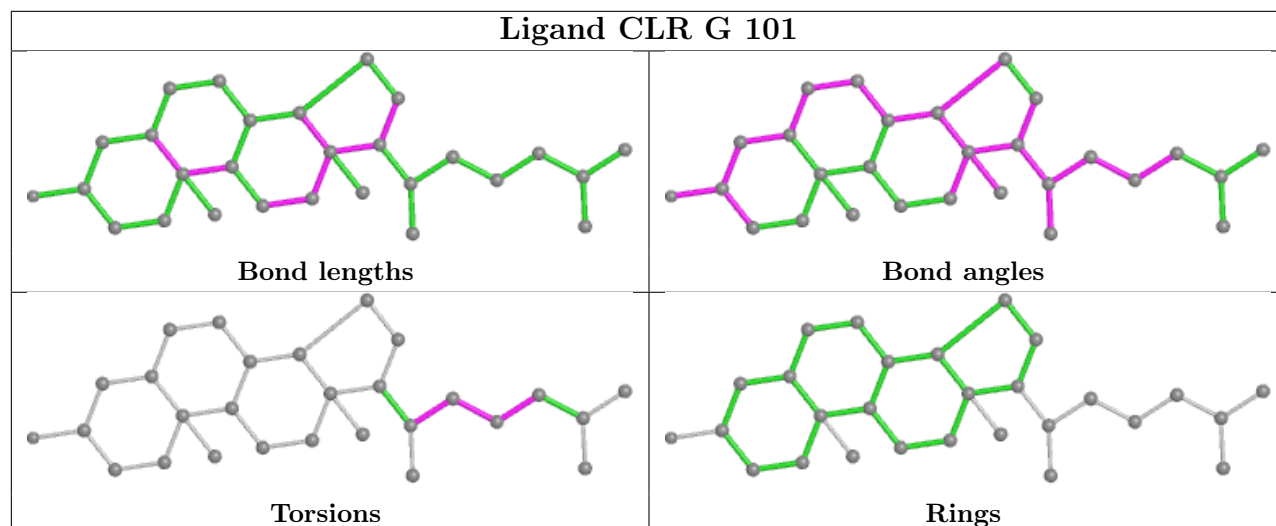


## Ligand CLR D 501

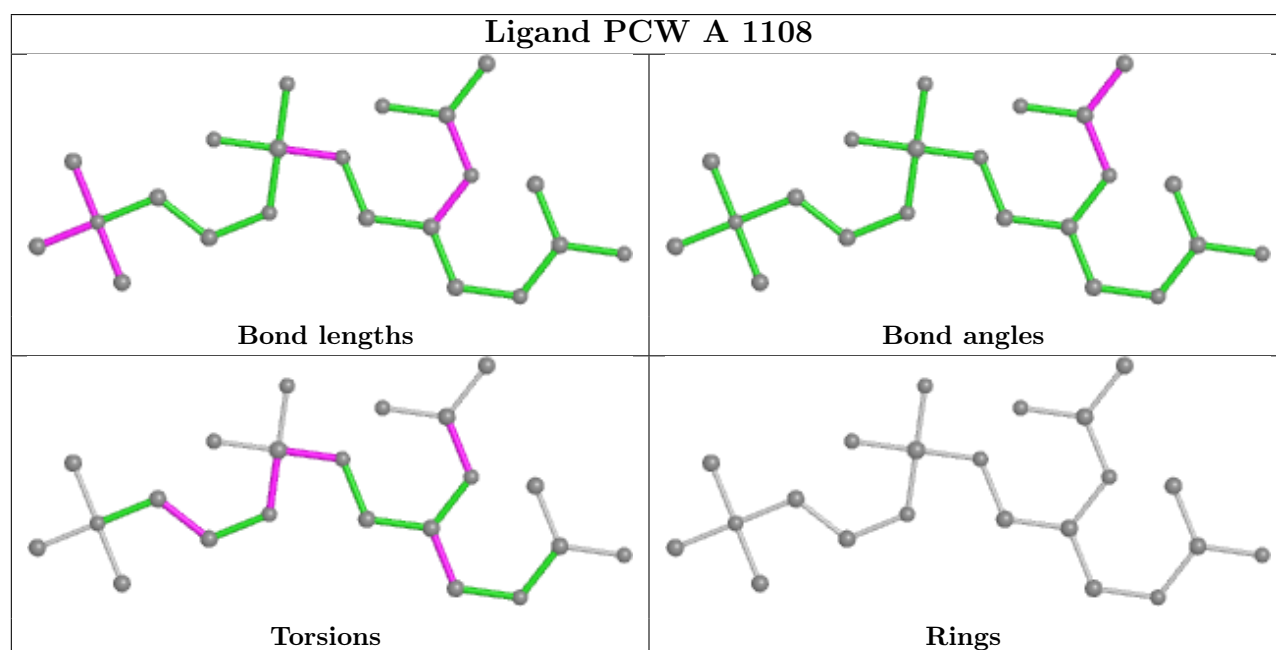




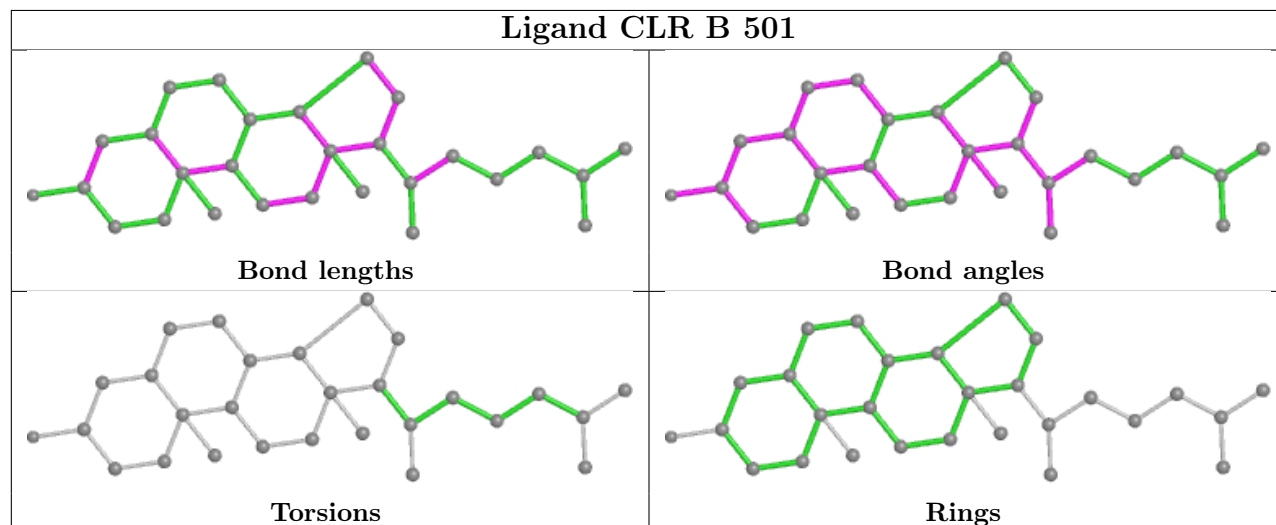
## Ligand CLR G 101

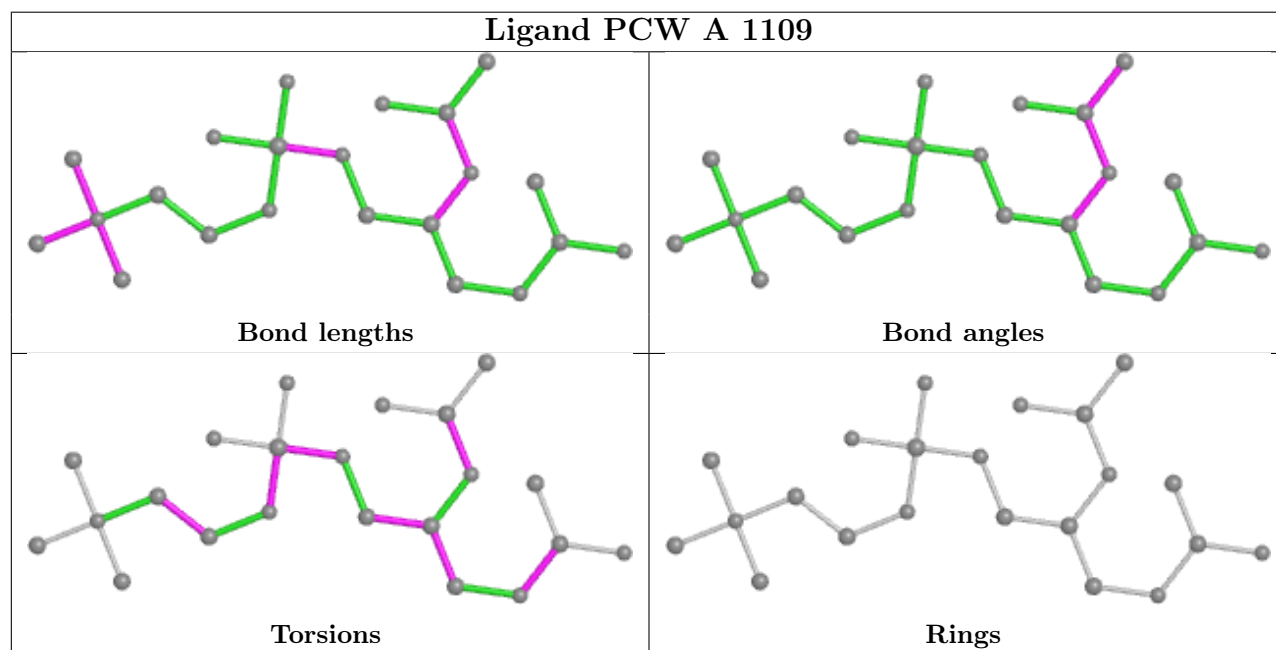
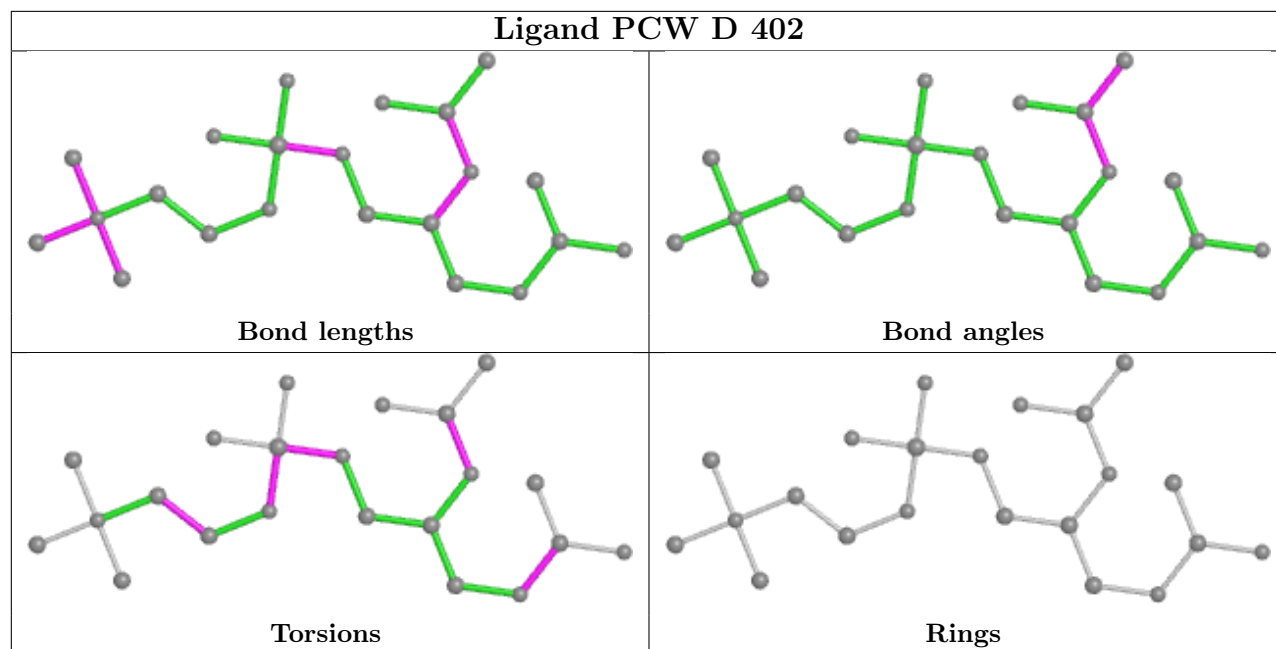


## Ligand PCW A 1108

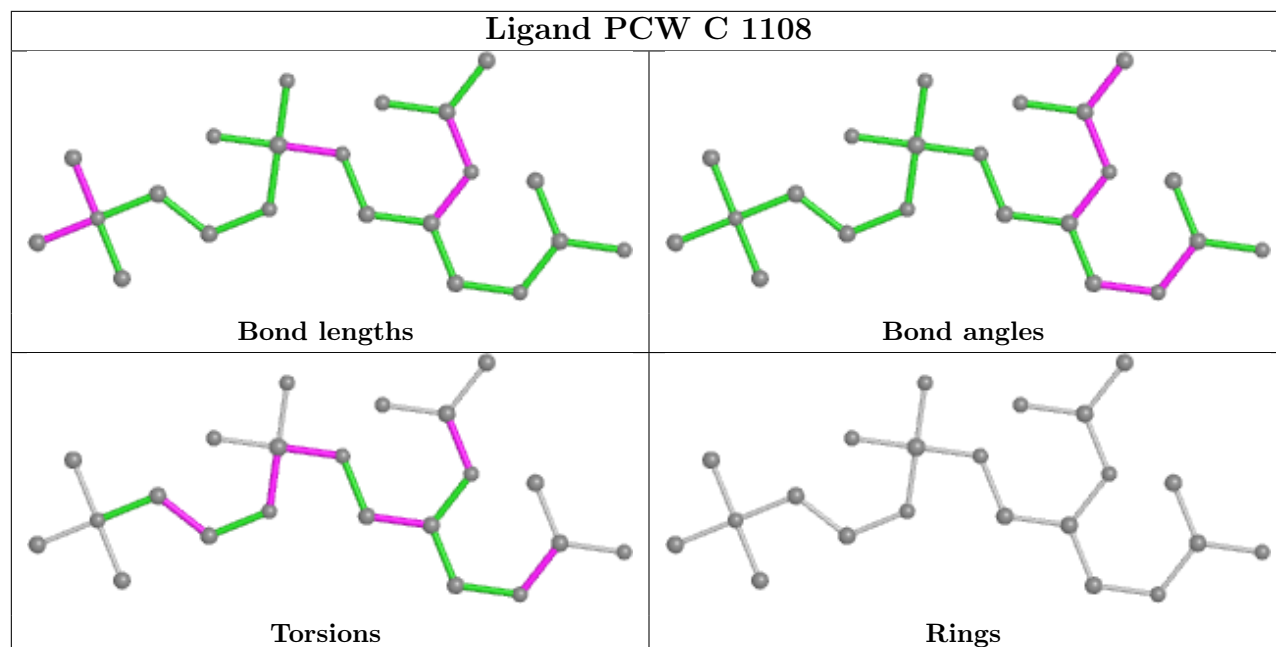


## Ligand CLR B 501

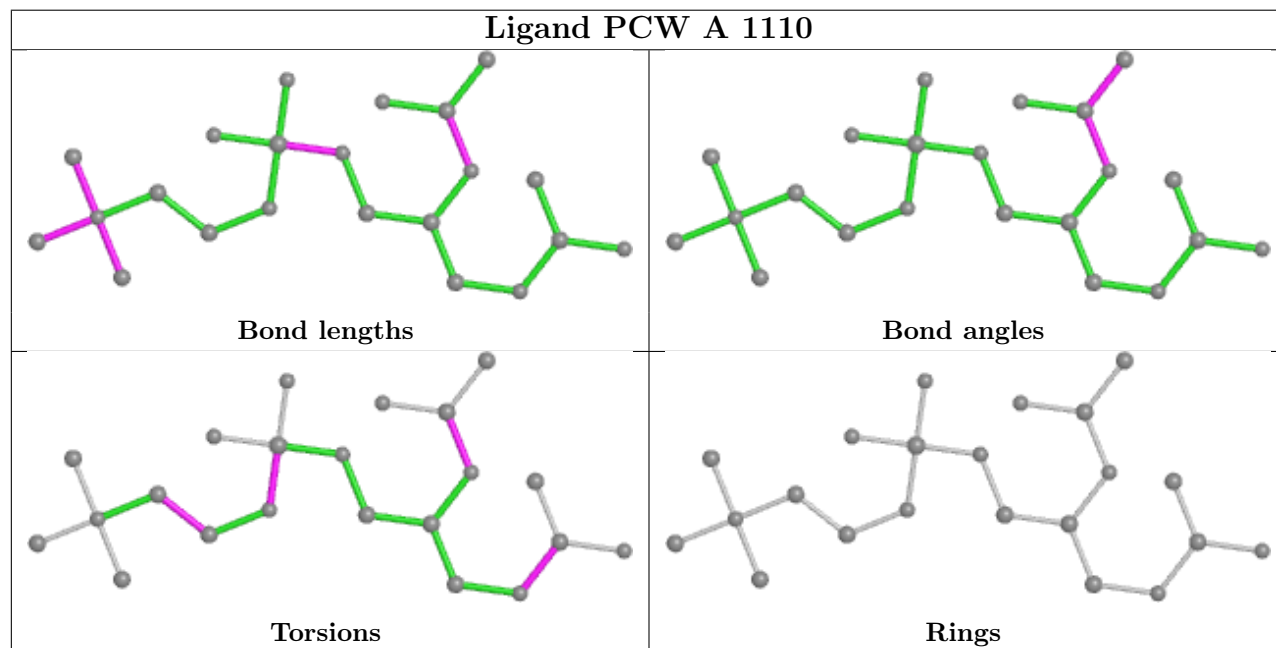




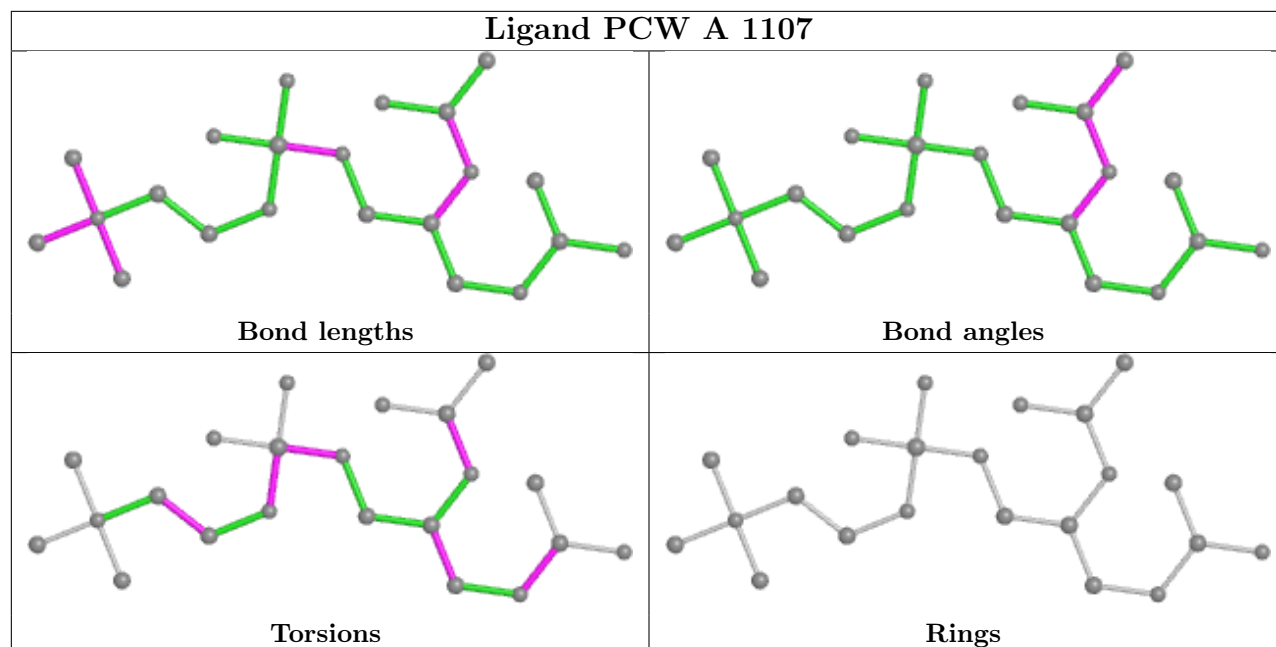
## Ligand PCW C 1108



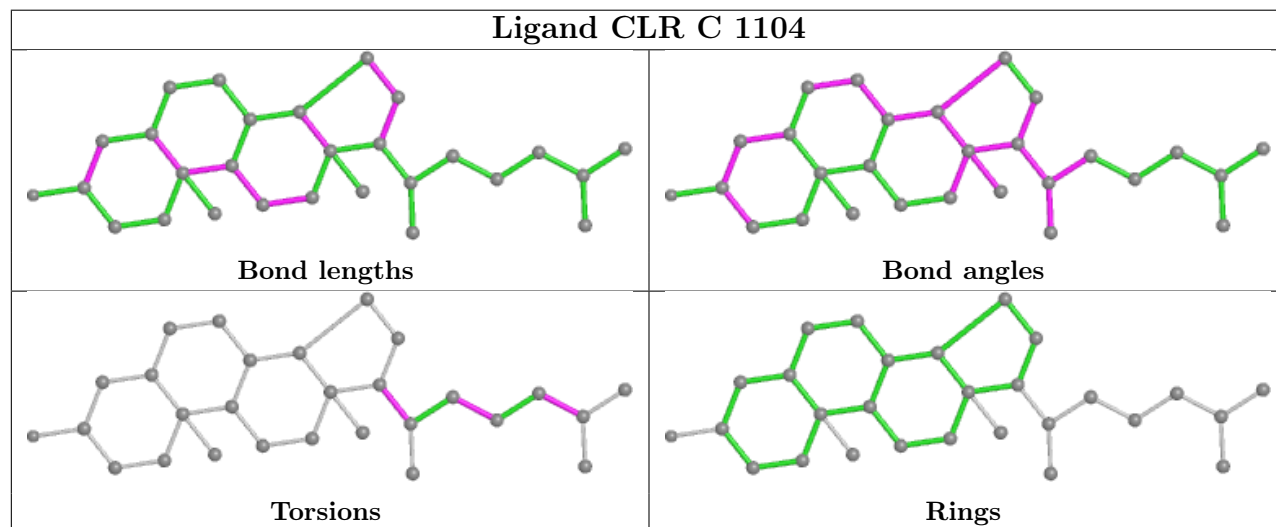
## Ligand PCW A 1110



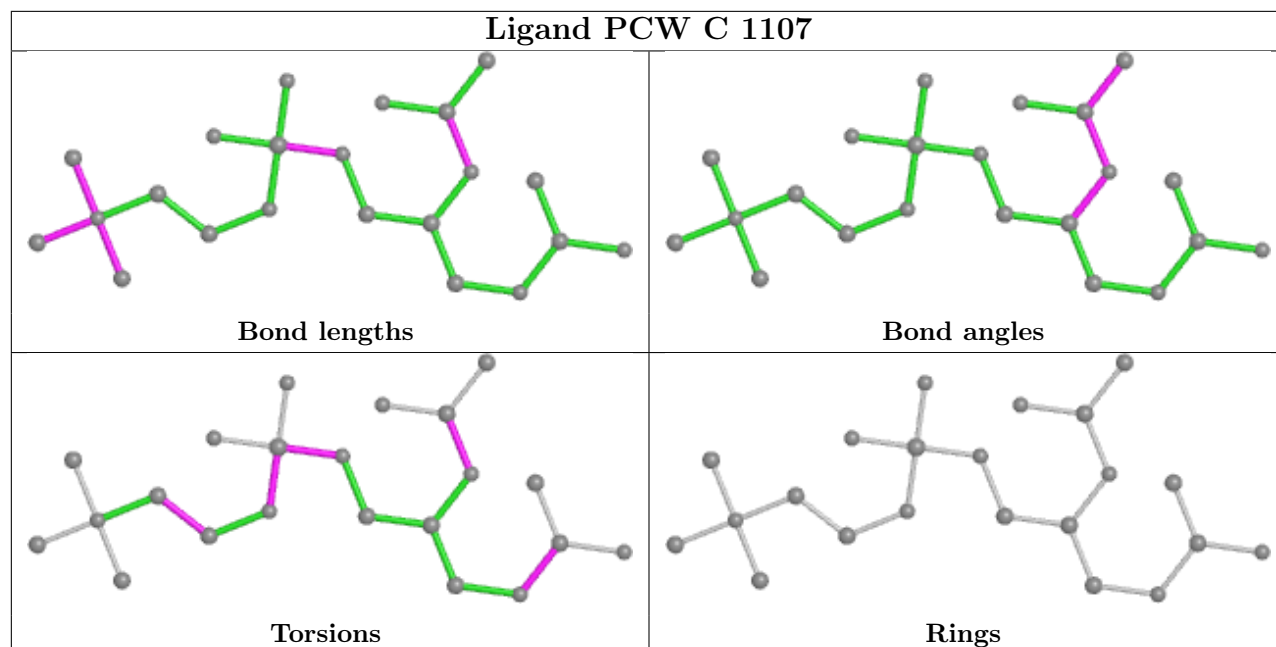
## Ligand PCW A 1107



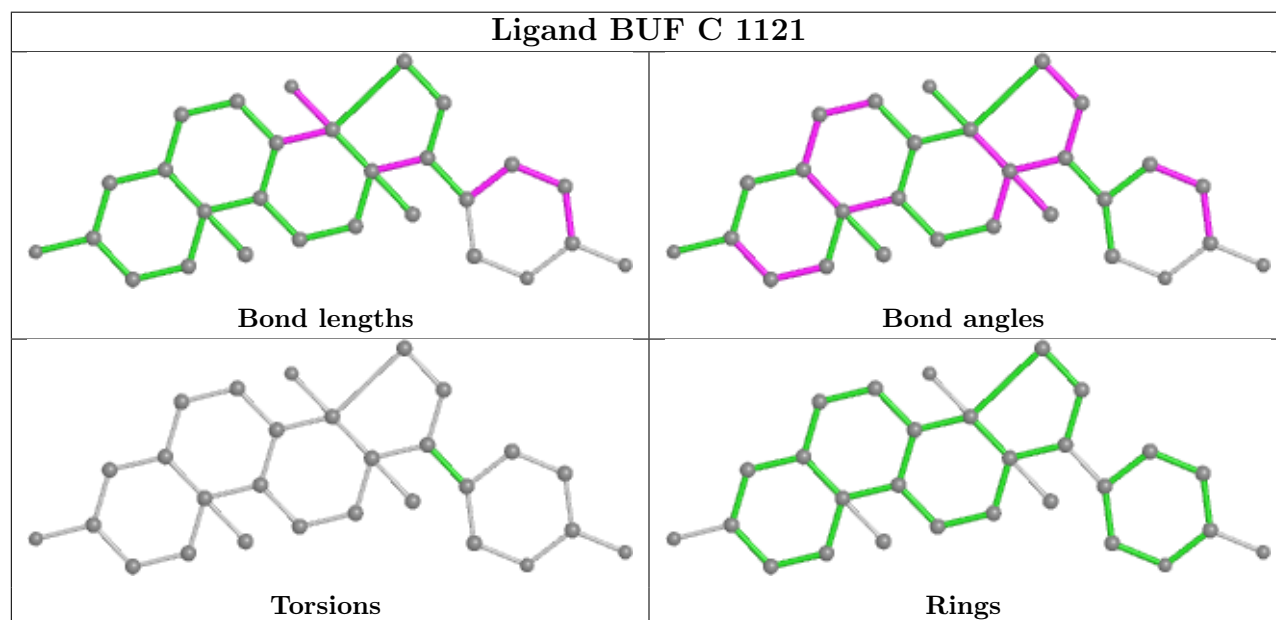
## Ligand CLR C 1104

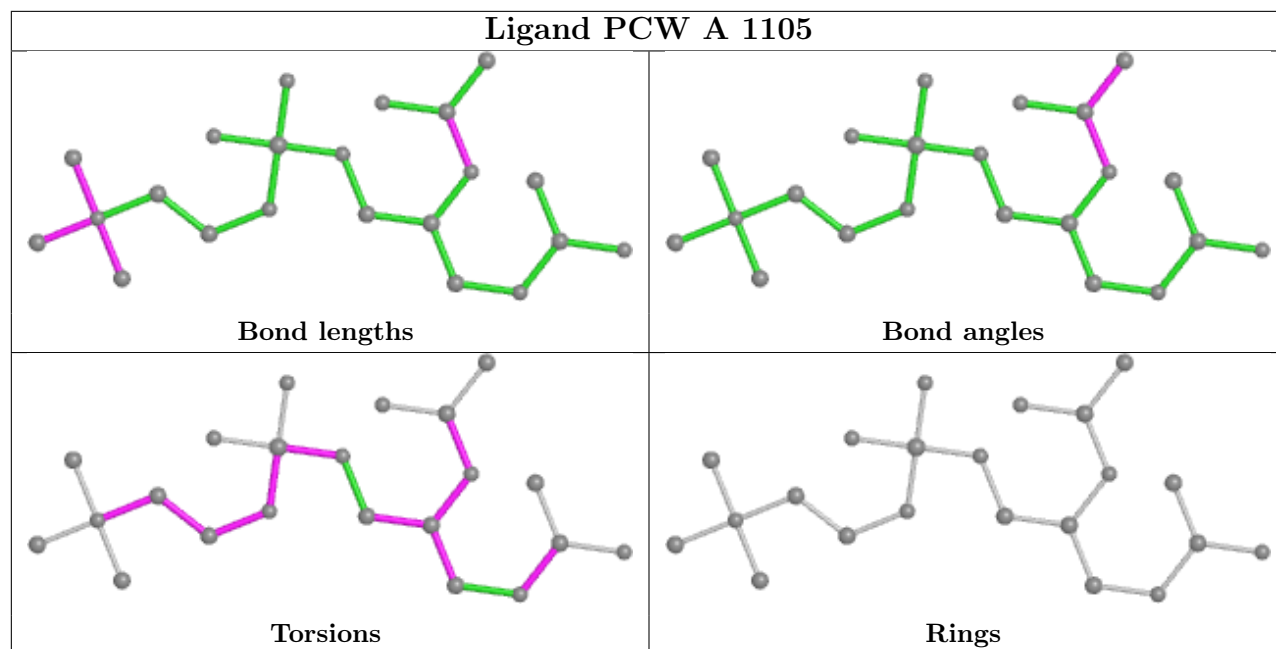


## Ligand PCW C 1107



## Ligand BUF C 1121





## 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	995/1016 (97%)	0.33	94 (9%) <b>8</b> <b>4</b>	41, 101, 230, 273	0
1	C	995/1016 (97%)	0.11	50 (5%) <b>28</b> <b>16</b>	36, 96, 187, 224	0
2	B	291/303 (96%)	0.33	24 (8%) <b>11</b> <b>6</b>	56, 125, 187, 236	0
2	D	285/303 (94%)	0.20	21 (7%) <b>14</b> <b>8</b>	38, 128, 177, 226	0
3	E	32/65 (49%)	-0.22	0 <b>100</b> <b>100</b>	34, 70, 123, 131	0
3	G	32/65 (49%)	-0.40	0 <b>100</b> <b>100</b>	43, 72, 118, 139	0
All	All	2630/2768 (95%)	0.22	189 (7%) <b>15</b> <b>9</b>	34, 104, 208, 273	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	LEU	11.7
1	A	489	PRO	11.5
1	A	578	PHE	9.8
1	A	550	HIS	9.7
2	B	166	THR	9.6
1	A	484	SER	9.4
2	B	165	GLU	8.2
1	A	571	PHE	8.1
1	A	470	ILE	7.9
1	A	552	PHE	7.6
1	A	582	ILE	7.4
1	C	429	ASN	7.3
1	A	581	LEU	7.2
1	A	486	HIS	7.1
1	A	496	HIS	7.1
1	A	485	ILE	6.8
1	A	522	PRO	6.7
1	A	551	LEU	6.7
1	A	499	VAL	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	514	ILE	6.5
1	A	403	SER	6.1
1	A	497	LEU	6.0
1	C	471	VAL	6.0
1	C	470	ILE	5.9
1	A	420	LEU	5.8
1	C	435	ILE	5.7
1	A	469	LYS	5.6
1	A	548	PHE	5.5
1	C	499	VAL	5.5
1	A	515	LEU	5.4
1	A	419	GLY	5.4
1	C	472	GLU	5.3
1	A	488	ASN	5.3
1	A	467	TYR	5.3
2	B	212	HIS	5.0
1	A	494	PRO	5.0
1	A	468	THR	4.9
1	A	382	ALA	4.8
1	A	580	GLY	4.8
1	A	466	ARG	4.8
1	A	547	GLY	4.7
1	A	553	LEU	4.7
2	D	202	MET	4.7
1	A	545	VAL	4.7
1	C	500	MET	4.6
2	B	199	TYR	4.6
2	B	167	TYR	4.5
1	A	406	LYS	4.4
1	C	491	THR	4.4
1	A	549	CYS	4.3
1	C	571	PHE	4.2
1	C	550	HIS	4.1
1	C	548	PHE	4.0
1	A	471	VAL	3.9
1	A	490	ASN	3.9
1	C	473	ILE	3.8
1	C	428	ALA	3.8
1	A	418	ALA	3.8
1	C	556	GLU	3.7
1	A	527	LEU	3.7
2	B	176	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	504	PRO	3.6
2	D	230	PHE	3.6
1	A	381	VAL	3.6
2	D	25	LEU	3.6
1	A	524	ASP	3.5
2	B	164	ASP	3.5
1	C	440	VAL	3.5
1	A	404	PHE	3.5
1	A	516	ILE	3.5
2	B	236	PRO	3.4
1	C	403	SER	3.4
1	A	554	PRO	3.3
1	A	80	PRO	3.3
1	C	420	LEU	3.3
2	B	261	VAL	3.3
2	B	260	ALA	3.3
2	D	151	PHE	3.3
1	A	491	THR	3.2
1	A	521	GLN	3.2
2	B	200	PRO	3.1
2	D	195	SER	3.1
2	B	162	LEU	3.1
1	A	520	GLU	3.1
1	A	179	VAL	3.1
1	A	82	TRP	3.0
2	D	203	LYS	3.0
1	A	557	GLN	3.0
2	D	263	PHE	3.0
2	D	229	TYR	3.0
1	C	549	CYS	3.0
1	A	526	GLU	3.0
1	A	564	PHE	2.9
1	C	580	GLY	2.9
2	B	259	MET	2.9
1	C	33	SER	2.9
1	C	497	LEU	2.9
1	A	573	LEU	2.9
1	A	500	MET	2.9
1	C	402	VAL	2.9
1	A	577	CYS	2.9
1	C	485	ILE	2.9
2	B	202	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	198	THR	2.8
1	C	484	SER	2.8
1	A	507	ILE	2.8
1	A	463	MET	2.8
2	D	236	PRO	2.8
1	C	436	LEU	2.8
1	A	487	LYS	2.8
1	A	556	GLU	2.8
2	B	197	GLU	2.7
1	C	387	ASP	2.7
1	A	579	VAL	2.7
2	B	178	ILE	2.7
1	C	386	SER	2.6
1	C	564	PHE	2.6
1	A	519	LYS	2.6
1	C	426	PHE	2.6
1	A	505	GLU	2.6
1	A	416	ARG	2.6
2	B	13	LYS	2.6
1	A	405	ASP	2.6
1	A	440	VAL	2.6
2	D	176	VAL	2.6
1	A	566	THR	2.6
1	C	474	PRO	2.6
1	A	546	LEU	2.5
1	A	796	GLY	2.5
2	D	199	TYR	2.5
1	C	579	VAL	2.5
1	A	495	ARG	2.5
1	C	385	TRP	2.4
1	A	531	PHE	2.4
1	A	884	ASP	2.4
2	B	216	LYS	2.4
1	C	78	THR	2.4
1	A	501	LYS	2.4
2	B	210	PRO	2.4
1	C	236	ALA	2.4
2	D	197	GLU	2.4
2	D	178	ILE	2.4
2	B	266	LEU	2.4
1	A	572	PRO	2.4
1	C	522	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	178	VAL	2.3
1	A	529	ASP	2.3
2	B	263	PHE	2.3
1	C	501	LYS	2.3
1	A	508	LEU	2.3
1	A	435	ILE	2.3
2	D	17	TRP	2.3
2	D	20	GLU	2.3
2	D	200	PRO	2.3
1	A	411	TRP	2.3
1	A	464	ARG	2.3
1	A	559	PRO	2.2
2	D	285	TYR	2.2
1	A	432	ASN	2.2
1	A	576	LEU	2.2
1	C	481	TYR	2.2
1	A	78	THR	2.2
2	B	211	VAL	2.2
1	C	566	THR	2.2
2	B	95	PRO	2.2
1	A	539	GLY	2.2
1	C	487	LYS	2.2
1	C	535	TYR	2.1
2	B	267	THR	2.1
1	A	384	MET	2.1
1	C	41	LEU	2.1
2	D	196	LEU	2.1
1	C	432	ASN	2.1
1	C	75	PRO	2.1
1	A	455	LEU	2.1
1	C	498	LEU	2.1
1	C	582	ILE	2.1
1	C	486	HIS	2.1
1	C	553	LEU	2.1
1	C	796	GLY	2.1
2	D	201	VAL	2.0
1	A	492	ALA	2.0
1	C	483	LEU	2.0
2	D	243	TYR	2.0
1	A	748	PHE	2.0
1	C	482	GLN	2.0
1	A	528	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	569	VAL	2.0
1	A	560	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	PHD	C	369	12/13	0.96	0.24	62,73,82,83	0
1	PHD	A	369	12/13	0.98	0.21	60,75,85,89	0

## 6.3 Carbohydrates [i](#)

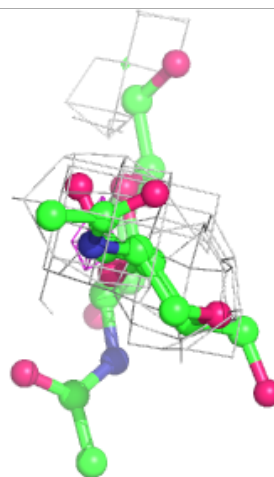
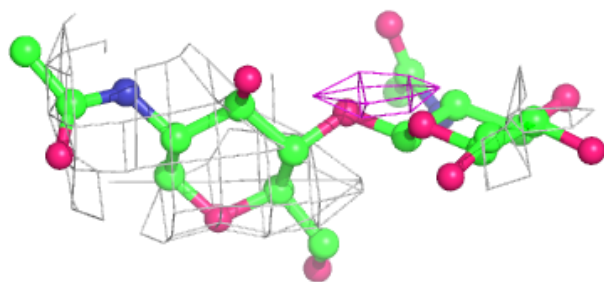
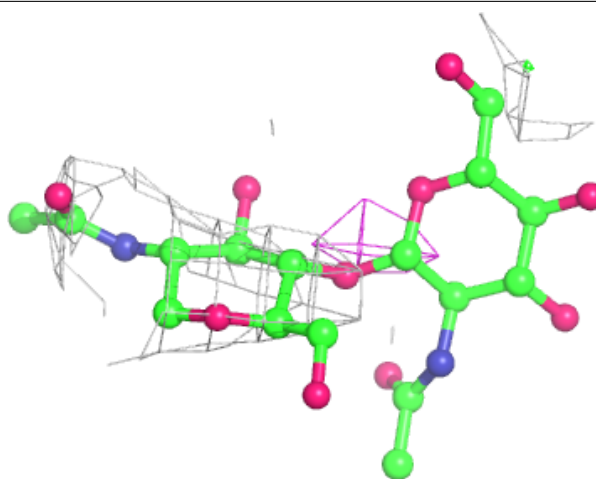
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	NAG	H	2	14/15	0.25	0.85	230,252,263,264	0
4	NAG	H	1	14/15	0.60	0.54	171,218,239,255	0
4	NAG	F	1	14/15	0.67	0.26	143,169,191,198	0
4	NAG	F	2	14/15	0.74	0.51	176,206,218,221	0
4	NAG	J	2	14/15	0.77	0.63	187,206,211,212	0
4	NAG	J	1	14/15	0.81	0.36	172,192,204,210	0
4	NAG	I	1	14/15	0.84	0.23	151,160,180,192	0
4	NAG	I	2	14/15	0.84	0.29	159,184,194,196	0

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

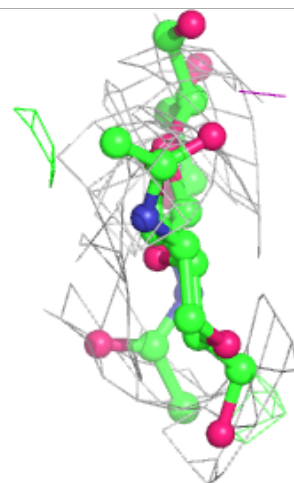
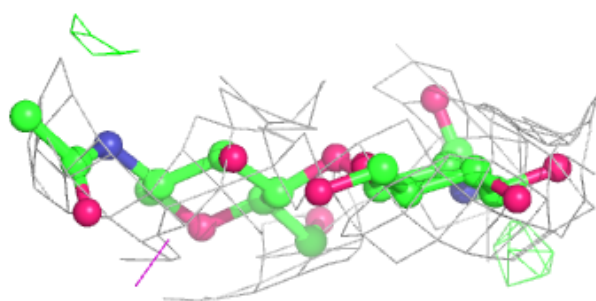
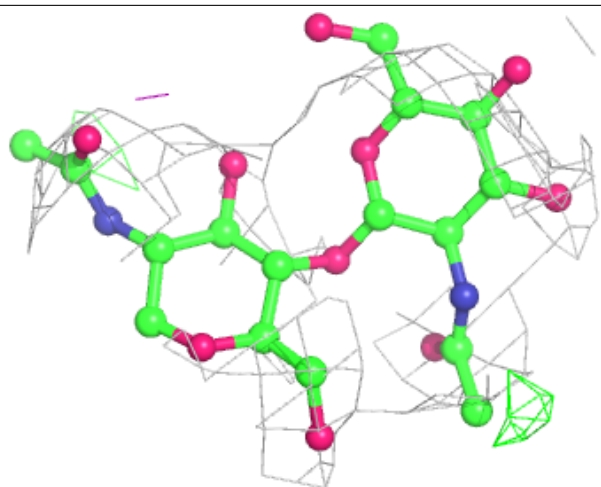
**Electron density around Chain H:**

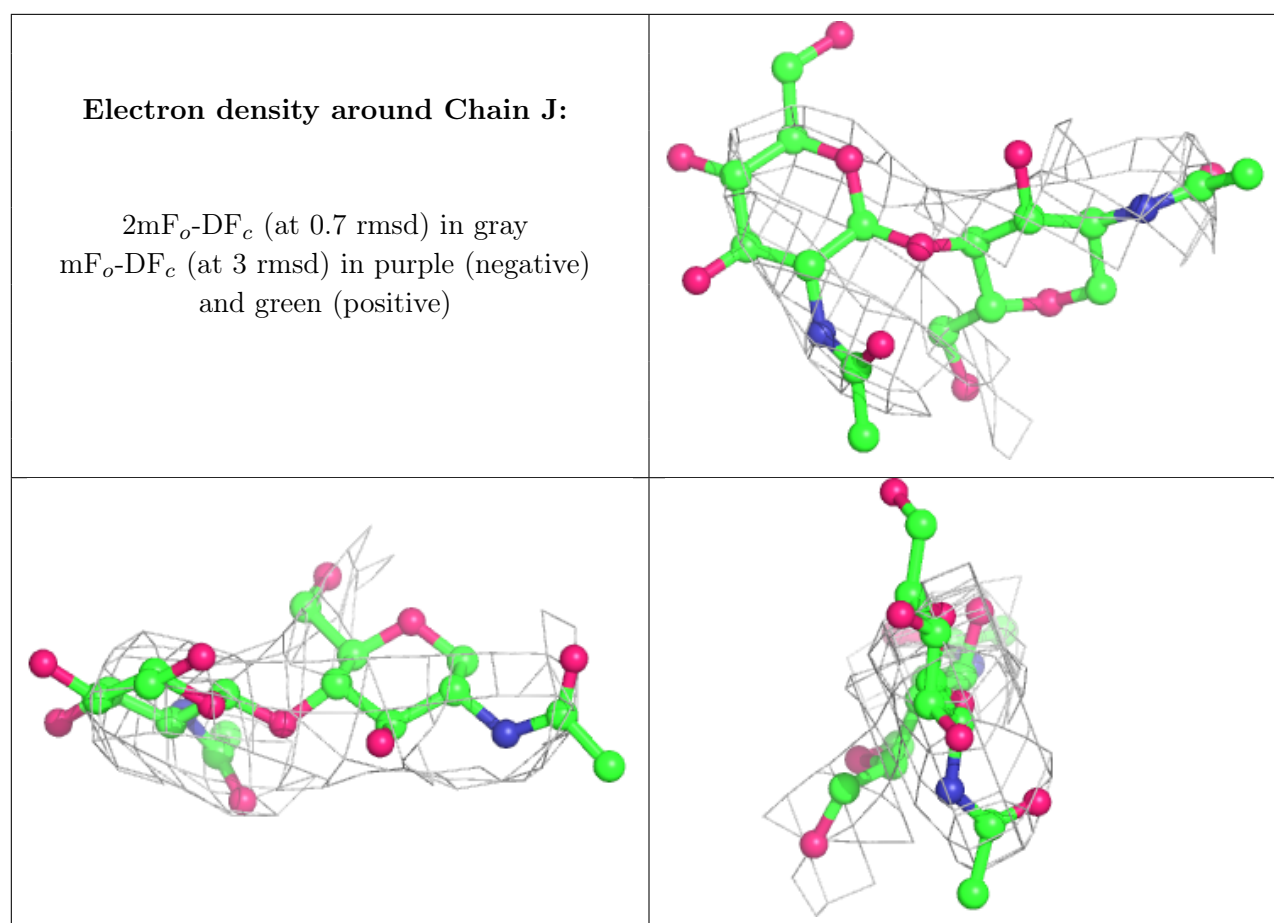
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain I:**

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





## 6.4 Ligands [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, 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( $\text{\AA}^2$ )	Q<0.9
7	PCW	C	1107	22/54	0.56	0.80	109,153,185,199	0
7	PCW	A	1108	22/54	0.69	0.83	116,167,194,200	0
7	PCW	A	1106	22/54	0.76	0.63	124,156,181,189	0
7	PCW	A	1105	22/54	0.77	0.39	164,177,204,214	0
10	NAG	B	401	14/15	0.83	0.21	125,162,175,179	0
7	PCW	C	1105	22/54	0.84	0.27	125,161,173,177	0
7	PCW	A	1110	22/54	0.84	0.30	117,138,157,169	0
7	PCW	A	1109	22/54	0.85	0.37	90,120,140,163	0
7	PCW	C	1106	22/54	0.85	0.36	116,163,187,192	0
10	NAG	D	401	14/15	0.85	0.29	130,169,178,180	0
7	PCW	D	402	22/54	0.86	0.48	142,173,195,199	0
7	PCW	A	1107	22/54	0.88	0.59	132,184,202,203	0

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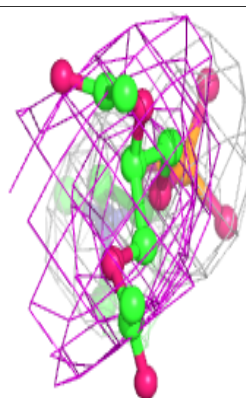
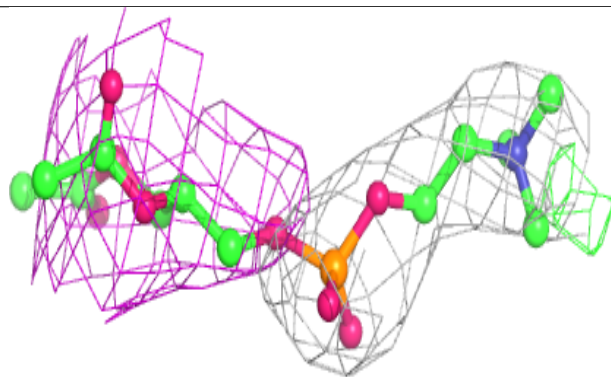
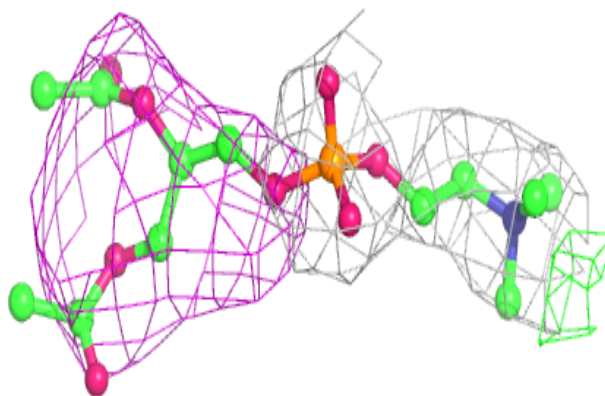
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PCW	C	1108	22/54	0.90	0.28	55,109,162,172	0
9	CLR	D	501	28/28	0.91	0.23	96,112,125,131	0
9	CLR	A	1104	28/28	0.92	0.43	67,95,117,121	0
9	CLR	C	1104	28/28	0.93	0.34	59,95,121,136	0
8	BUF	C	1121	28/28	0.94	0.26	48,75,94,116	0
8	BUF	A	1121	28/28	0.94	0.25	76,109,130,136	0
9	CLR	B	501	28/28	0.94	0.49	105,128,143,148	0
6	NA	A	1102	1/1	0.97	0.21	15,15,15,15	0
5	MG	C	1103	1/1	0.98	0.23	62,62,62,62	0
9	CLR	E	101	28/28	0.98	0.24	25,43,65,76	0
5	MG	A	1103	1/1	0.98	0.30	91,91,91,91	0
9	CLR	G	101	28/28	0.98	0.24	32,49,75,98	0
5	MG	C	1101	1/1	0.98	0.15	96,96,96,96	0
6	NA	C	1102	1/1	0.99	0.29	15,15,15,15	0
5	MG	A	1101	1/1	0.99	0.20	101,101,101,101	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 PCW C 1107:

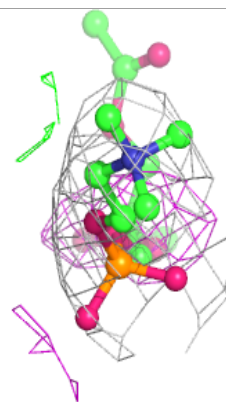
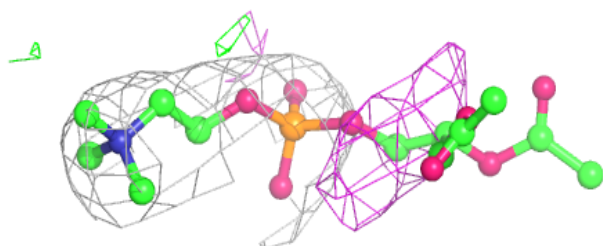
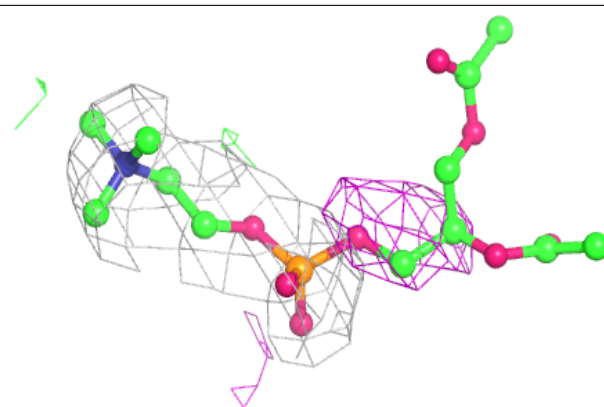
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



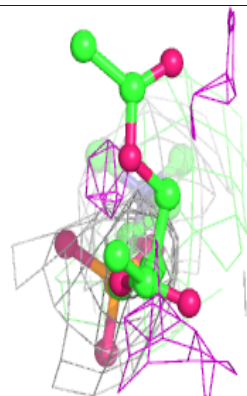
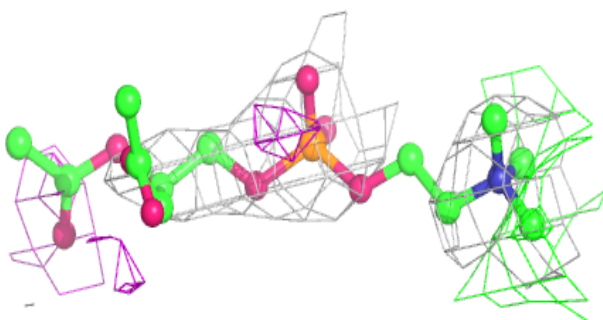
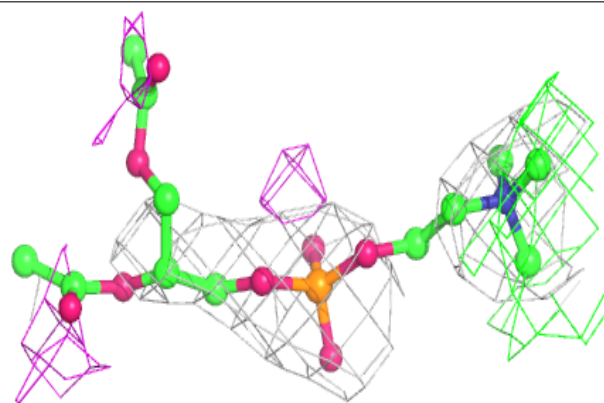


**Electron density around PCW A 1108:**

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

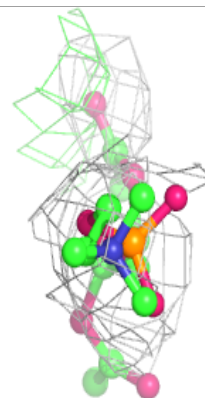
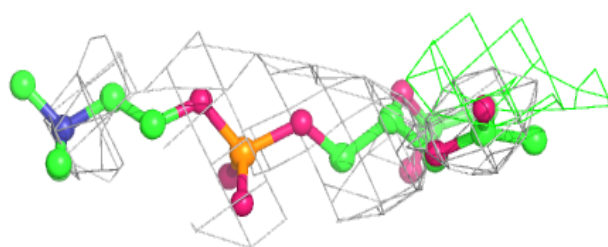
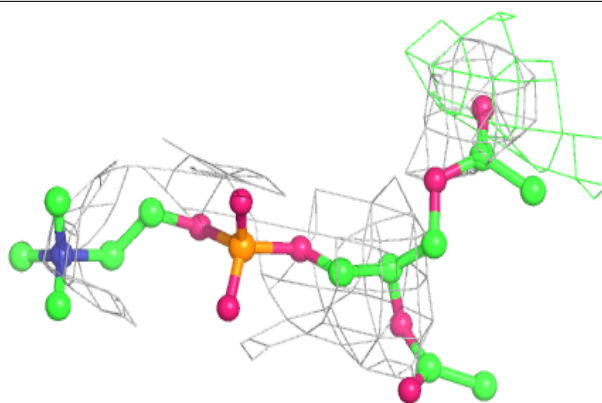
**Electron density around PCW A 1106:**

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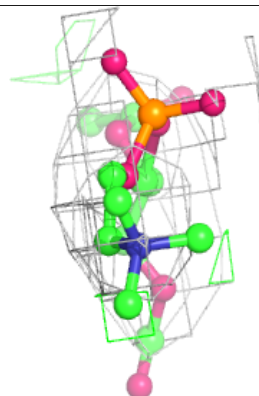
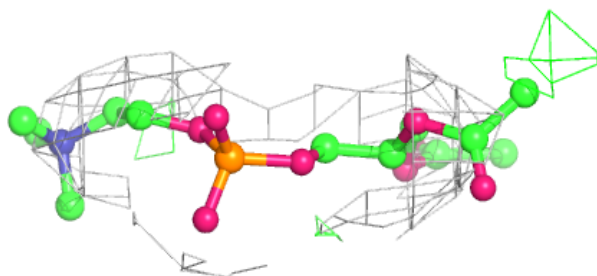
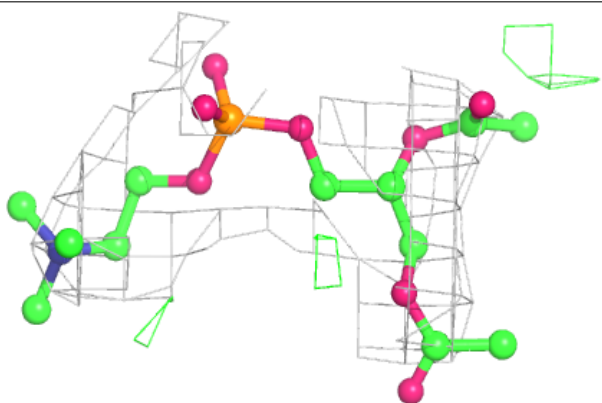


**Electron density around PCW A 1105:**

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and green (positive)

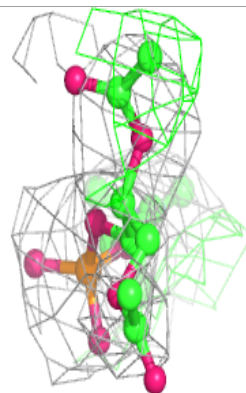
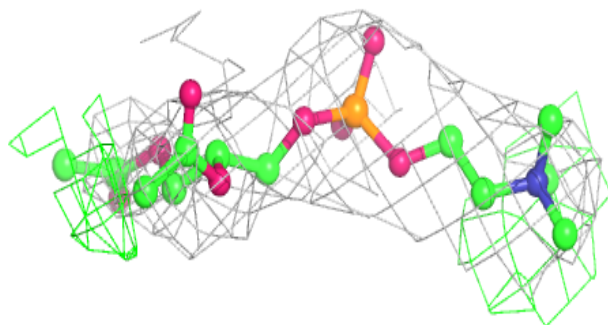
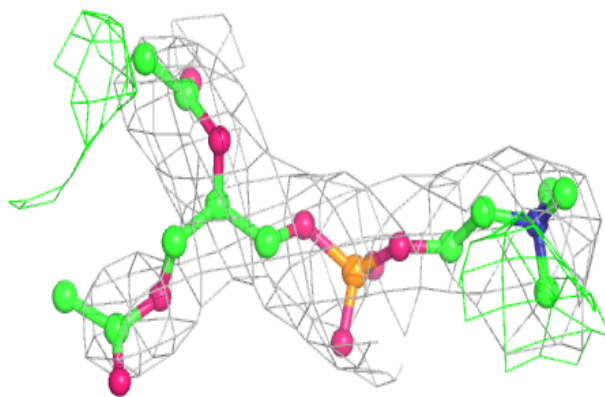
**Electron density around PCW C 1105:**

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and green (positive)



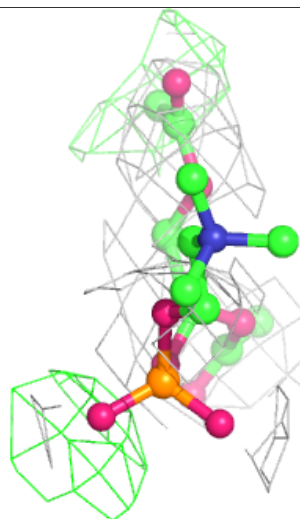
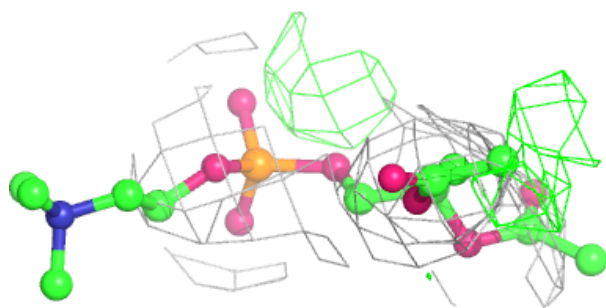
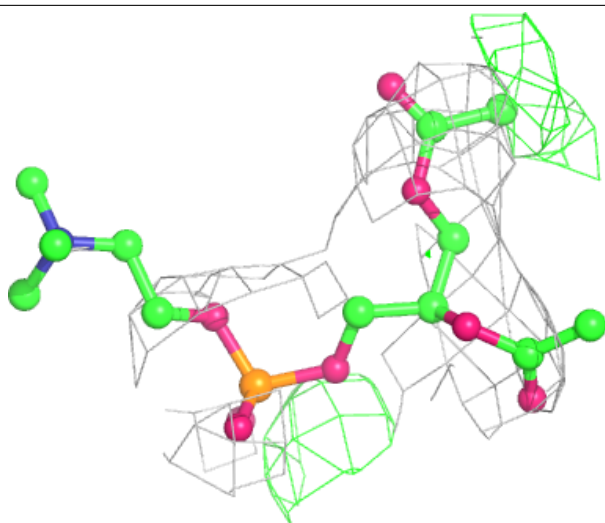
**Electron density around PCW A 1110:**

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



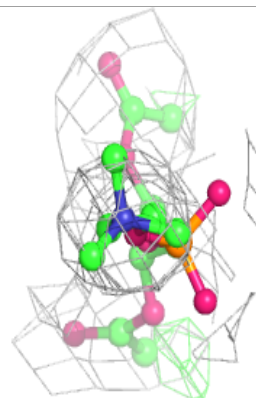
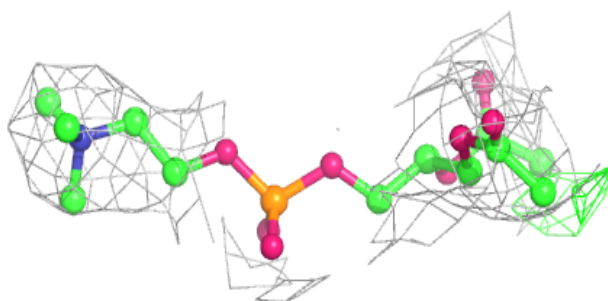
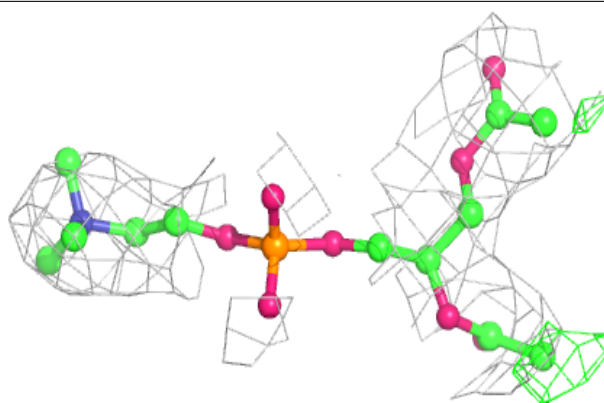
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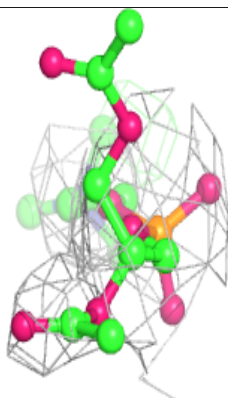
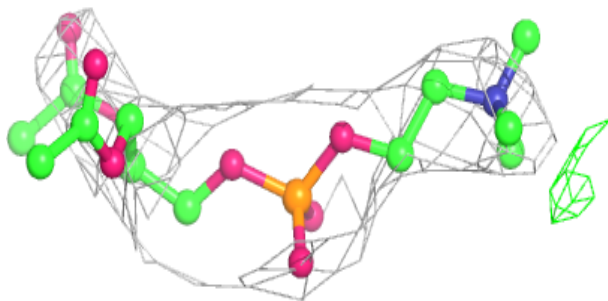
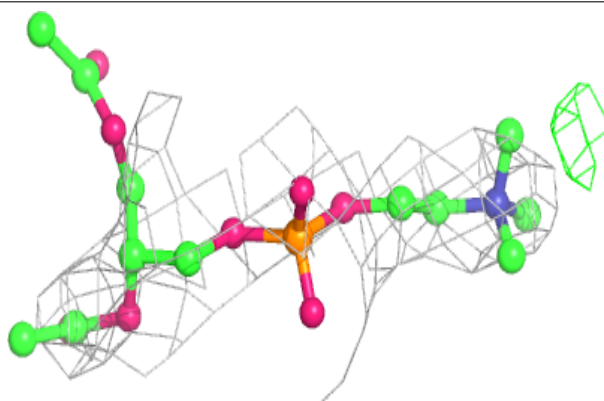


**Electron density around PCW C 1106:**

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and green (positive)

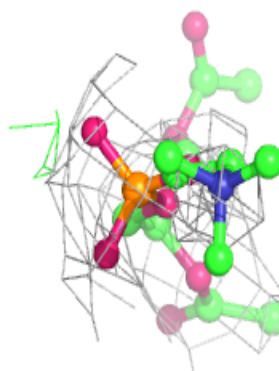
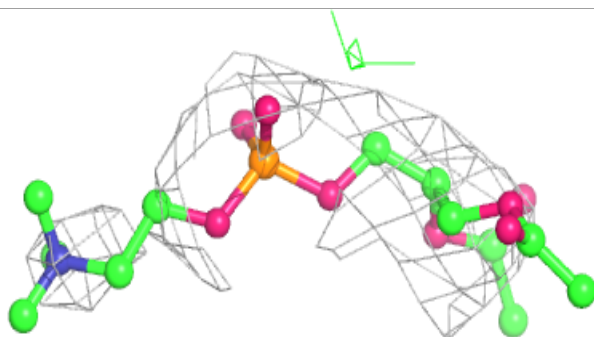
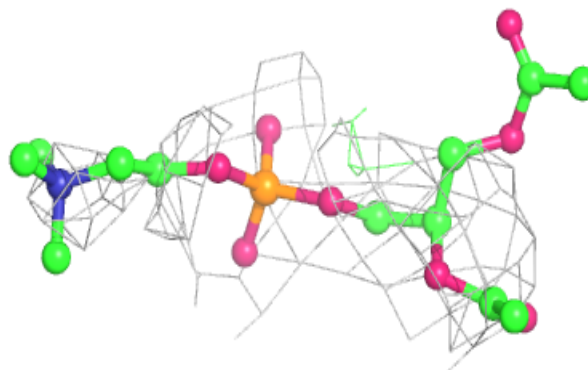
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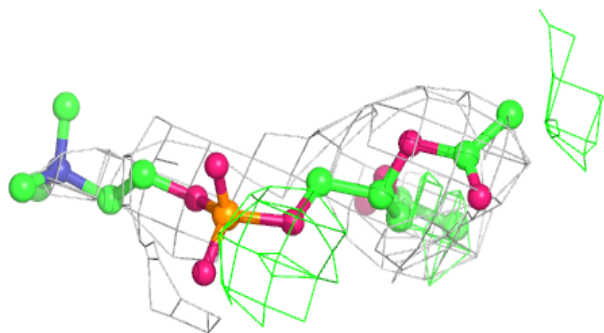
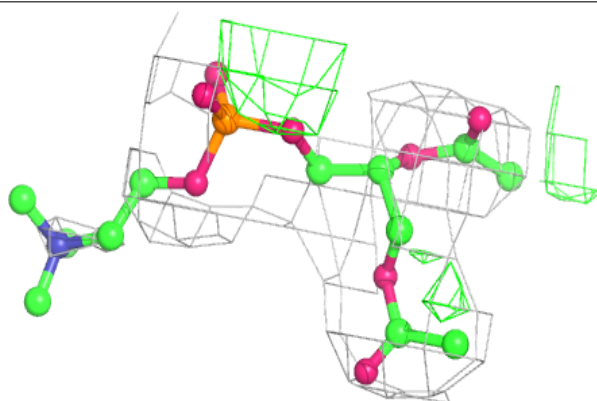


**Electron density around PCW A 1107:**

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and green (positive)

**Electron density around PCW C 1108:**

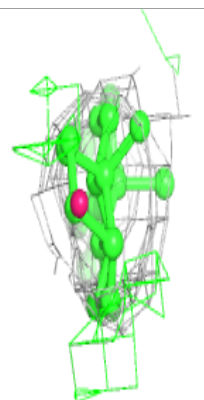
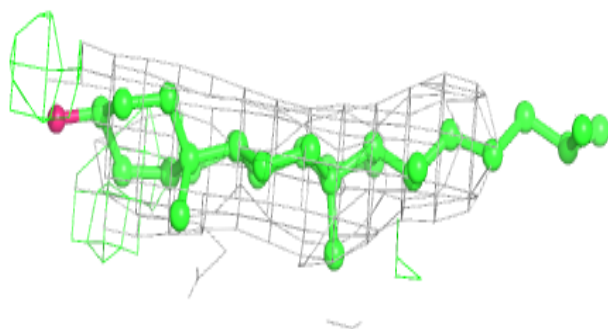
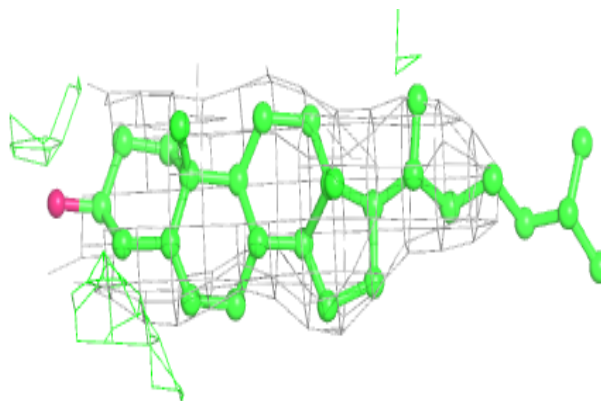
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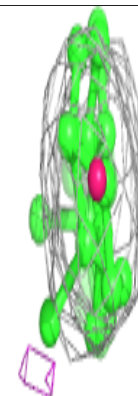
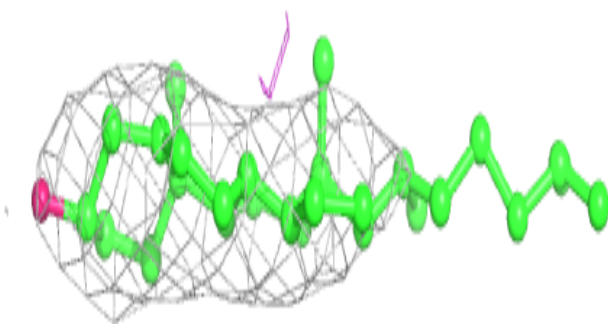
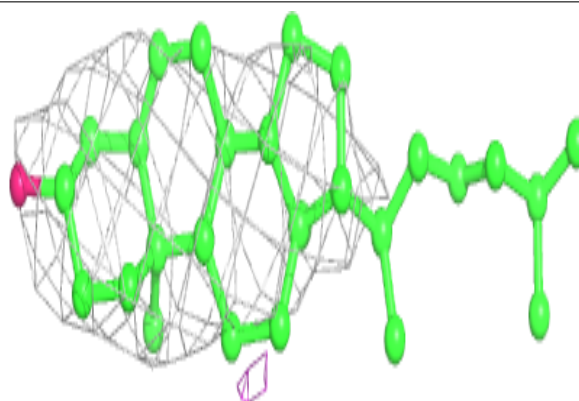


**Electron density around CLR D 501:**

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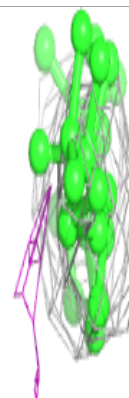
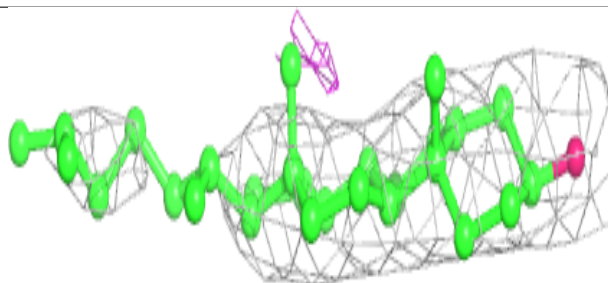
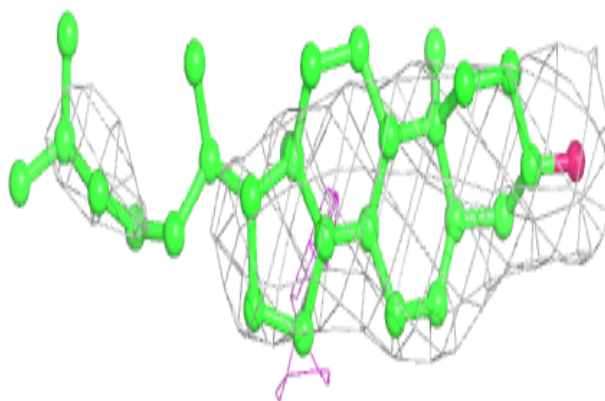
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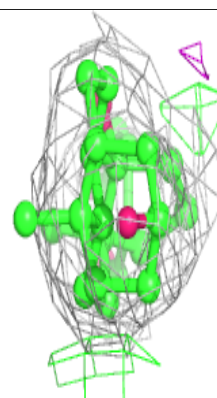
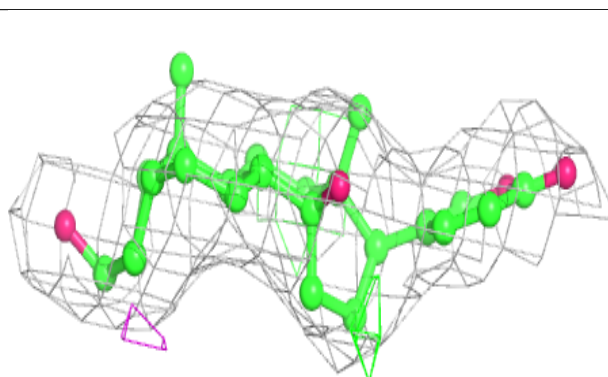
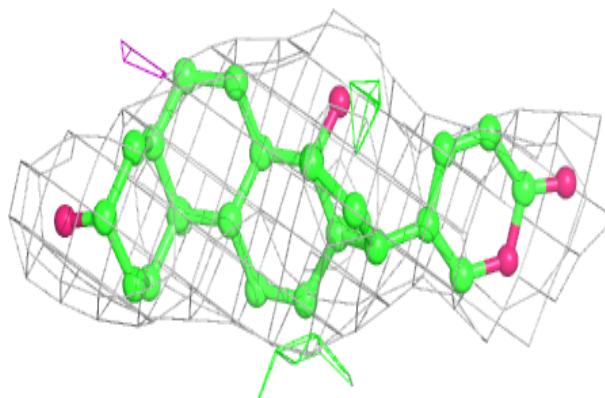


**Electron density around CLR C 1104:**

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**Electron density around BUF C 1121:**

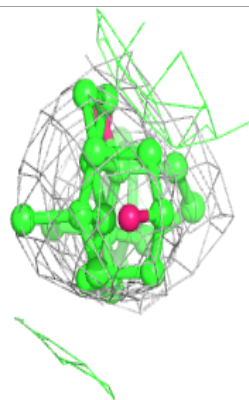
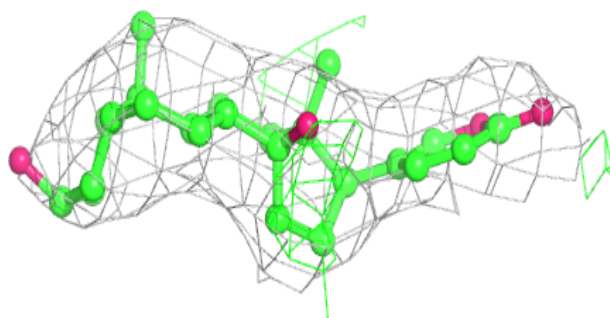
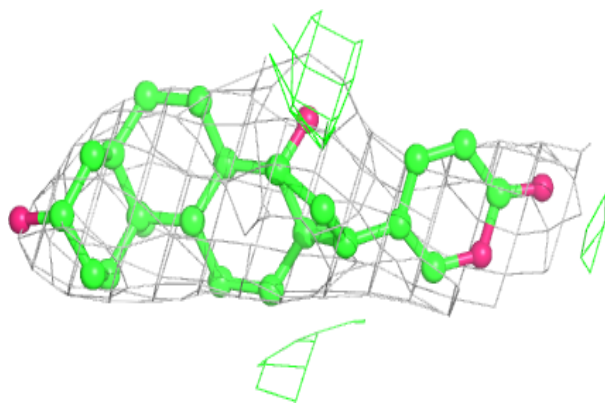
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and green (positive)



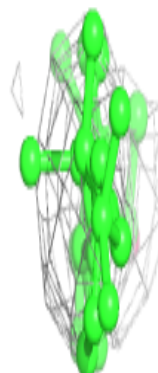
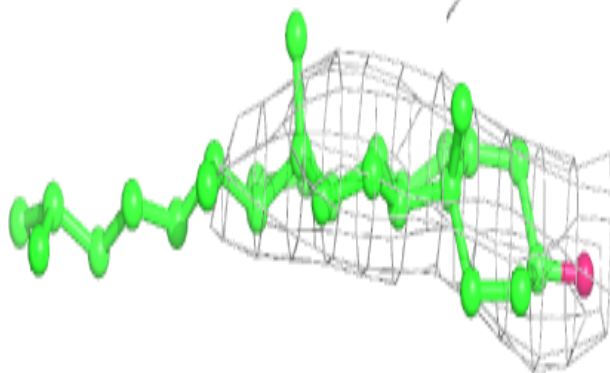
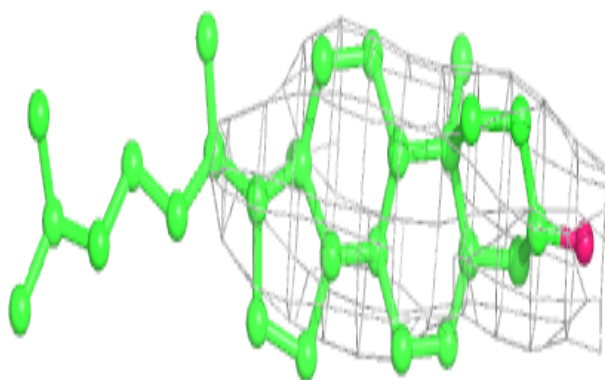


**Electron density around BUF A 1121:**

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

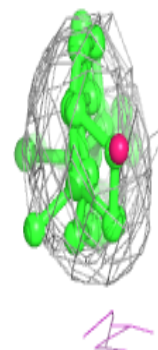
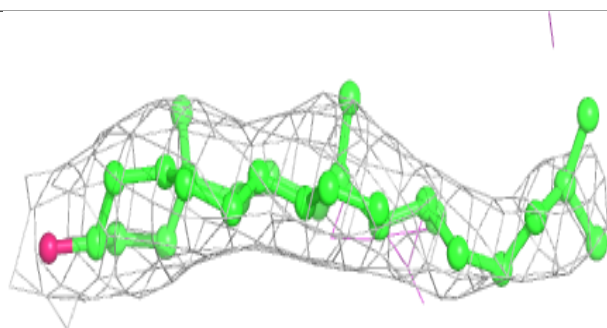
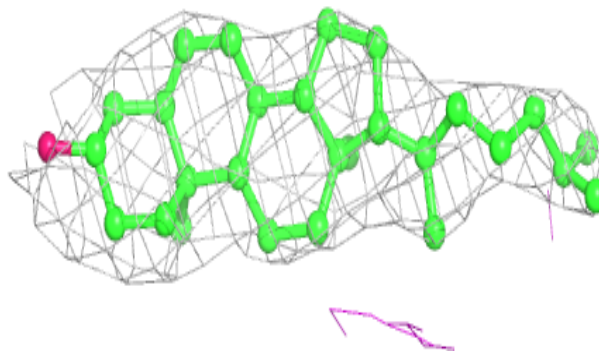
**Electron density around CLR B 501:**

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

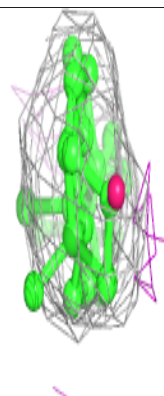
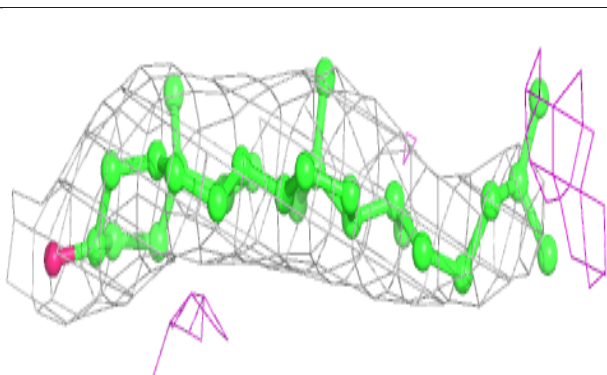
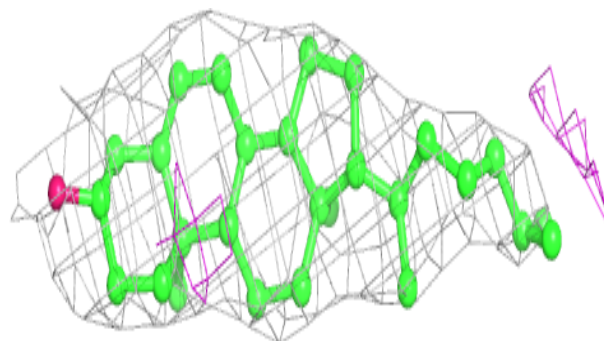


**Electron density around CLR E 101:**

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

**Electron density around CLR G 101:**

$2mF_o-DF_c$  (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.