



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 18, 2021 – 12:13 PM JST

PDB ID : 7D93  
Title : Crystal Structure of the Na<sup>+</sup>,K<sup>+</sup>-ATPase in the E2P state with bound Mg<sup>2+</sup> and anthrolyouabain (P2(1)2(1)2(1) symmetry)  
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Deposited on : 2020-10-12  
Resolution : 3.65 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

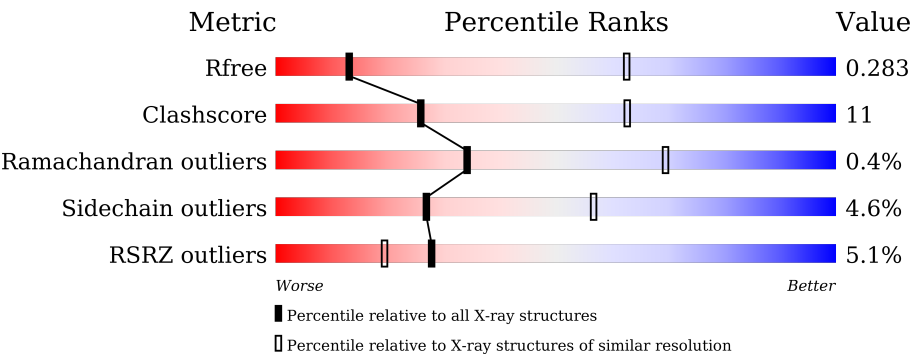
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 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	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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>6%</div><div><div></div><div>73%</div><div>24%</div><div>..</div></div></div>
1	C	1016	<div><div>4%</div><div><div></div><div>72%</div><div>25%</div><div>..</div></div></div>
2	B	303	<div><div>4%</div><div><div></div><div>64%</div><div>29%</div><div>..</div></div></div>
2	D	303	<div><div>7%</div><div><div></div><div>60%</div><div>33%</div><div>..</div></div></div>
3	E	65	<div><div></div><div><div></div><div>48%</div><div>51%</div><div>.</div></div></div>
3	G	65	<div><div></div><div><div></div><div>42%</div><div>8%</div><div>51%</div></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	2	-	-	-	X
4	NAG	J	2	-	-	-	X
8	PCW	A	1106	-	-	-	X
8	PCW	A	1107	-	-	-	X
8	PCW	C	1105	-	-	-	X
8	PCW	C	1109	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21396 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	291	Total	C	N	O	S	0	0	0
			2386	1546	390	437	13			

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

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

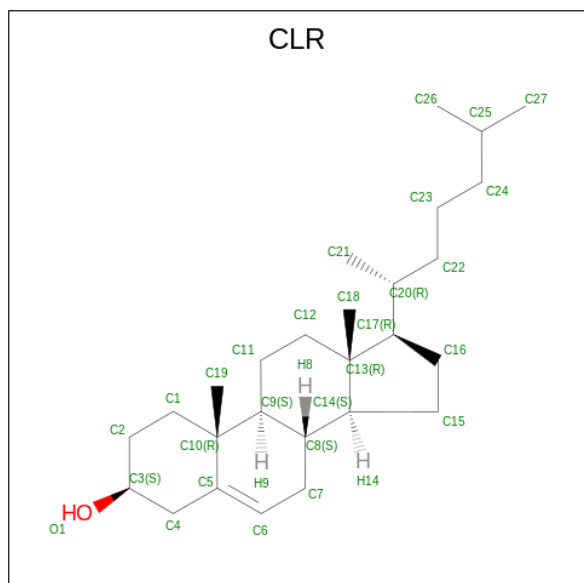
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

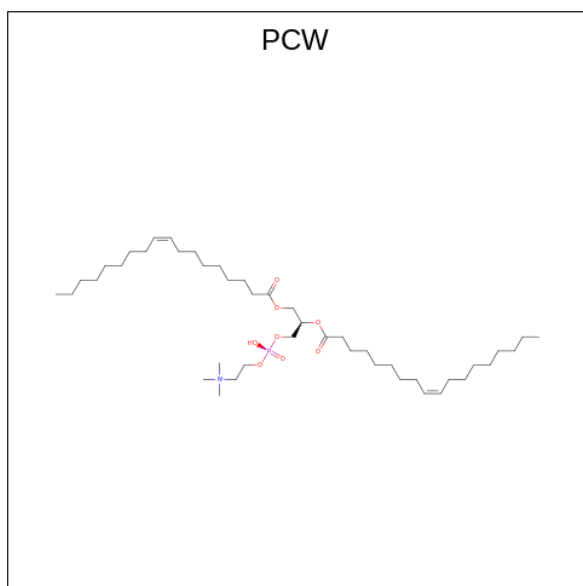
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



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

- Molecule 8 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula:  $C_{44}H_{85}NO_8P$ ).



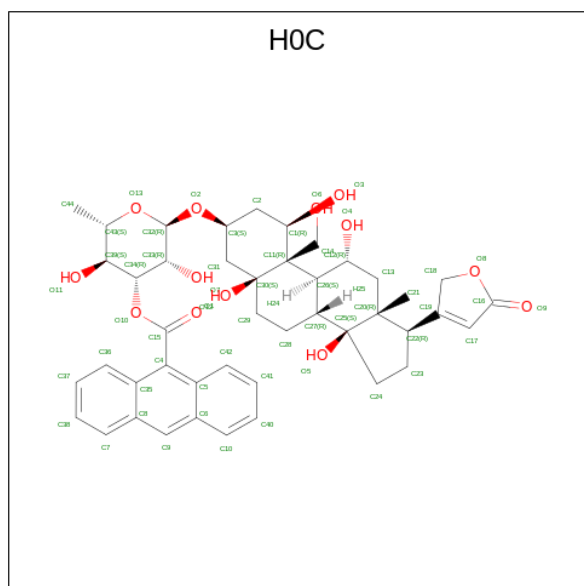
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

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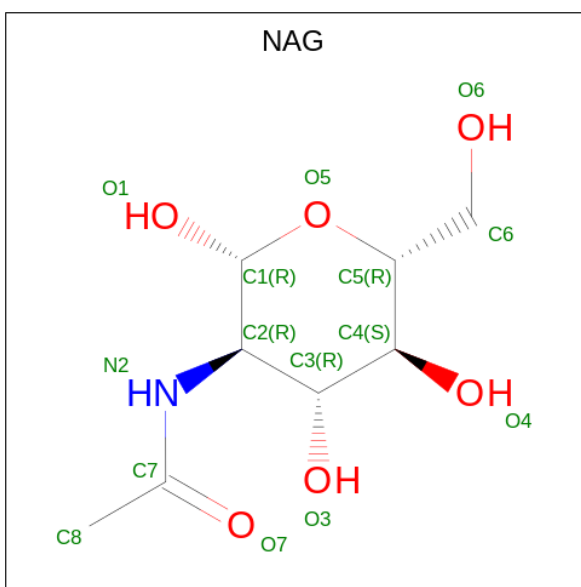
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	D	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

- Molecule 9 is [(2 {R},3 {R},4 {R},5 {S},6 {S})-2-[(1 {R},3 {S},5 {S},8 {R},9 {S},10 {R},11 {R},13 {R},14 {S},17 {R})-10-(hydroxymethyl)-13-methyl-1,5,11,14-tetrakis(oxidanyl)-17-(5-oxidanylidene-2 {H}-furan-3-yl)-2,3,4,6,7,8,9,11,12,15,16,17-dodecahydro-1 {H}-cyclopenta[a]phenanthren-3-yl]oxy]-6-methyl-3,5-bis(oxidanyl)oxan-4-yl] anthracene-9-carboxylate (three-letter code: HOC) (formula: C<sub>44</sub>H<sub>52</sub>O<sub>13</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			57	44	13		
9	C	1	Total	C	O	0	0
			57	44	13		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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.

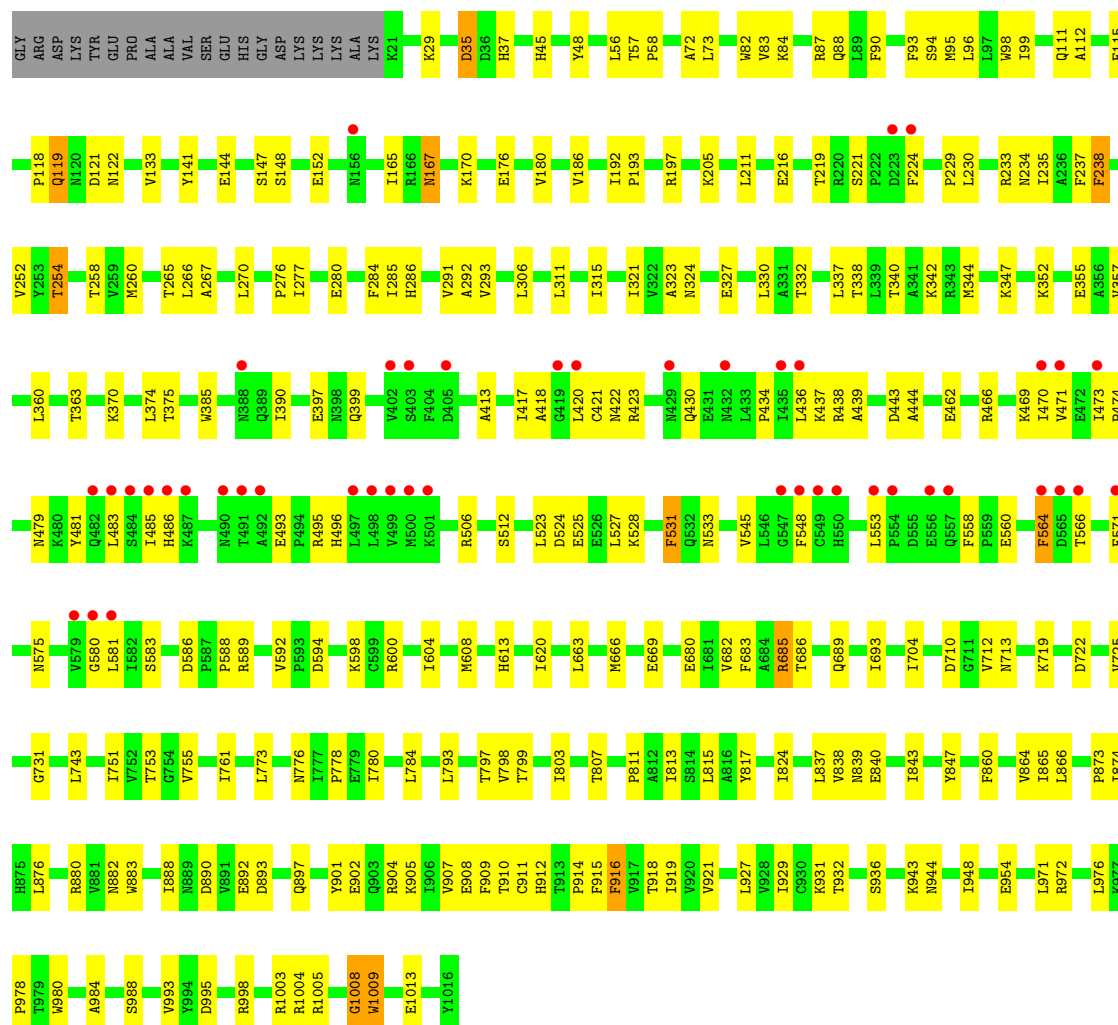
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	6	Total	O	0	0
			6	6		
11	C	6	Total	O	0	0
			6	6		



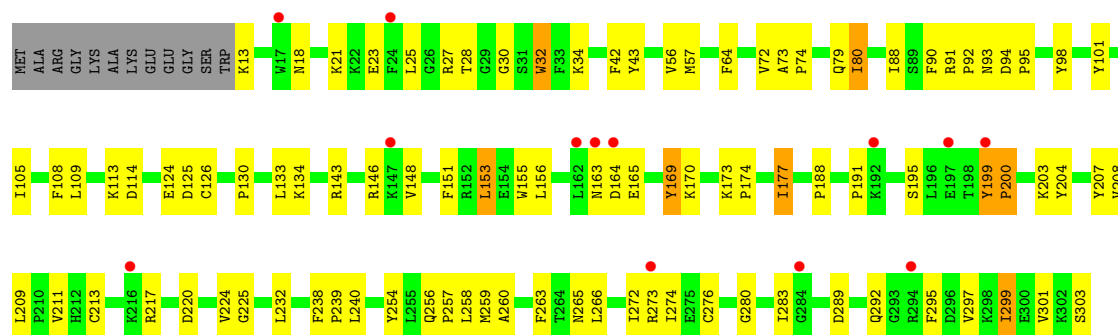


- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1



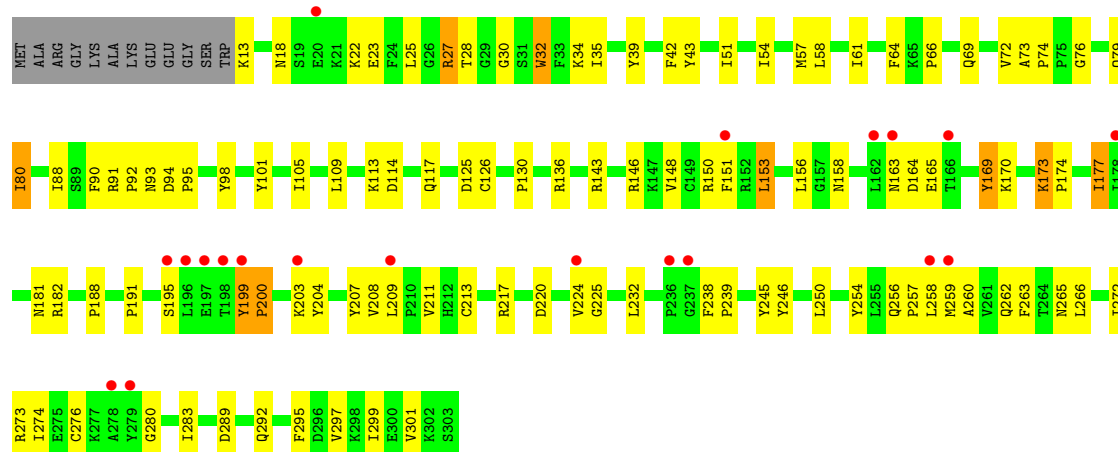


• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



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





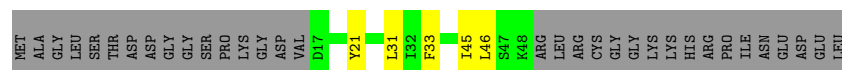
- Molecule 3: FXYD domain-containing ion transport regulator

Chain E: 48% 51%



- Molecule 3: FXYD domain-containing ion transport regulator

Chain G: 42% 8% 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: 

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.62Å 117.89Å 494.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.65 50.03 – 3.65	Depositor EDS
% Data completeness (in resolution range)	45.5 (15.00-3.65) 46.3 (50.03-3.65)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.233 , 0.274 0.249 , 0.283	Depositor DCC
$R_{free}$ test set	1758 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	131.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 64.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.084 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	21396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, H0C, 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	0.30	0/7867	0.52	0/10674
1	C	0.30	0/7867	0.53	1/10674 (0.0%)
2	B	0.31	0/2449	0.57	0/3301
2	D	0.31	0/2449	0.56	0/3301
3	E	0.33	0/261	0.54	0/354
3	G	0.33	0/261	0.49	0/354
All	All	0.30	0/21154	0.53	1/28658 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1008	GLY	N-CA-C	5.29	126.32	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	154	0
1	C	7730	0	7777	171	0
2	B	2386	0	2361	60	0
2	D	2386	0	2361	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	255	0	259	0	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	56	0	92	5	0
7	D	28	0	46	2	0
7	E	28	0	46	2	0
7	G	28	0	46	2	0
8	A	110	0	90	5	0
8	C	110	0	90	6	0
8	D	22	0	18	0	0
9	A	57	0	0	2	0
9	C	57	0	0	3	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	A	6	0	0	1	0
11	C	6	0	0	0	0
All	All	21396	0	21348	450	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 11.

All (450) 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)
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.56	0.87
1:A:430:GLN:HG3	1:A:438:ARG:HB2	1.56	0.86
1:C:430:GLN:HG3	1:C:438:ARG:HB2	1.61	0.83
1:C:978:PRO:HB3	7:E:101:CLR:H192	1.61	0.82
2:D:80:ILE:HG12	2:D:177:ILE:HG12	1.62	0.82
2:B:80:ILE:HG12	2:B:177:ILE:HG12	1.65	0.79
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.64	0.78
1:C:685:ARG:HB3	1:C:685:ARG:HH11	1.47	0.78
1:A:84:LYS:HG3	1:A:141:TYR:HE1	1.51	0.75
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.71	0.71
1:A:978:PRO:HB3	7:G:101:CLR:H192	1.71	0.71
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.71	0.71
1:A:375:THR:HA	1:A:588:PRO:HA	1.74	0.69
1:C:84:LYS:HG3	1:C:141:TYR:HE1	1.57	0.69
1:C:807:THR:HB	1:C:954:GLU:HG3	1.75	0.68
1:A:807:THR:HB	1:A:954:GLU:HG3	1.75	0.68
1:A:96:LEU:HD22	1:A:285:ILE:HG23	1.76	0.67
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.77	0.67
1:C:221:SER:H	1:C:233:ARG:HB3	1.59	0.66
1:C:375:THR:HA	1:C:588:PRO:HA	1.78	0.66
1:A:512:SER:HB2	1:A:575:ASN:HA	1.80	0.64
2:B:204:TYR:HE1	2:B:207:TYR:HB2	1.63	0.64
1:C:901:TYR:HA	1:C:904:ARG:HE	1.63	0.64
2:D:204:TYR:HE1	2:D:207:TYR:HB2	1.63	0.63
1:A:385:TRP:HB3	1:A:581:LEU:H	1.64	0.63
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.80	0.63
1:C:907:VAL:HA	1:C:910:THR:HG22	1.80	0.63
1:C:434:PRO:HG2	1:C:437:LYS:HB2	1.81	0.62
1:C:883:TRP:HA	1:C:904:ARG:HH11	1.64	0.62
1:A:205:LYS:HA	1:A:219:THR:HA	1.80	0.62
2:D:177:ILE:HA	2:D:260:ALA:HA	1.82	0.62
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.81	0.61
1:A:763:ASP:OD2	1:A:933:ARG:NH1	2.34	0.61
1:A:385:TRP:HE3	1:A:580:GLY:HA2	1.64	0.61
1:C:558:PHE:HB3	1:C:564:PHE:HE2	1.66	0.61
1:A:558:PHE:HB3	1:A:564:PHE:HE2	1.66	0.60
1:C:470:ILE:HB	1:C:485:ILE:HG23	1.83	0.60
1:A:1009:TRP:HZ2	2:B:34:LYS:HB3	1.65	0.60
1:C:238:PHE:HD2	1:C:258:THR:HG21	1.66	0.60
2:D:276:CYS:HB2	2:D:295:PHE:HD2	1.66	0.60
2:B:80:ILE:HD11	2:B:177:ILE:H	1.66	0.60
1:C:843:ILE:HG23	1:C:847:TYR:HD2	1.67	0.60
1:C:96:LEU:HD22	1:C:285:ILE:HG23	1.84	0.59
1:C:512:SER:HB2	1:C:575:ASN:HA	1.85	0.59
1:A:363:THR:HA	1:A:704:ILE:HB	1.84	0.59
1:C:385:TRP:HD1	1:C:390:ILE:HD13	1.68	0.59
1:C:385:TRP:HB3	1:C:581:LEU:H	1.67	0.59
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.84	0.58
1:C:902:GLU:HB2	2:D:289:ASP:OD2	2.03	0.58
1:C:943:LYS:NZ	8:C:1108:PCW:H82	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:ASP:O	1:C:598:LYS:HG2	2.04	0.58
2:B:217:ARG:HH12	2:B:273:ARG:HD2	1.69	0.58
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.85	0.58
1:C:864:VAL:HG12	1:C:980:TRP:HZ3	1.68	0.58
2:D:225:GLY:HA3	2:D:265:ASN:HB3	1.86	0.58
2:D:280:GLY:HA3	2:D:283:ILE:HD13	1.85	0.57
1:A:221:SER:H	1:A:233:ARG:HB3	1.68	0.57
1:C:874:ILE:H	1:C:874:ILE:HD12	1.68	0.57
2:D:80:ILE:HD11	2:D:177:ILE:H	1.68	0.57
2:B:280:GLY:HA3	2:B:283:ILE:HD13	1.87	0.57
1:C:291:VAL:HG23	1:C:324:ASN:HD21	1.70	0.57
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.85	0.57
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.87	0.57
1:A:434:PRO:HG2	1:A:437:LYS:HB2	1.86	0.57
8:A:1109:PCW:H31	1:C:978:PRO:HB2	1.87	0.57
1:A:864:VAL:HG12	1:A:980:TRP:HZ3	1.69	0.57
2:B:191:PRO:HD3	2:B:280:GLY:HA2	1.87	0.57
1:C:385:TRP:HE3	1:C:580:GLY:HA2	1.70	0.57
1:C:284:PHE:CD1	1:C:838:VAL:HG21	2.39	0.56
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.87	0.56
2:D:191:PRO:HD3	2:D:280:GLY:HA2	1.85	0.56
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.87	0.56
2:D:217:ARG:HH12	2:D:273:ARG:HD2	1.70	0.56
1:A:84:LYS:HG3	1:A:141:TYR:CE1	2.39	0.56
1:C:284:PHE:HD1	1:C:838:VAL:HG21	1.71	0.56
1:A:370:LYS:HA	1:A:374:LEU:HB2	1.87	0.55
2:B:276:CYS:HB2	2:B:295:PHE:HD2	1.71	0.55
1:C:332:THR:HA	1:C:813:ILE:HD11	1.87	0.55
1:C:418:ALA:O	1:C:422:ASN:ND2	2.39	0.55
1:C:663:LEU:HA	1:C:666:MET:HG3	1.89	0.55
1:C:493:GLU:OE1	1:C:495:ARG:NH2	2.39	0.55
1:C:873:PRO:HA	1:C:876:LEU:HD12	1.87	0.55
1:A:965:PRO:HD3	3:G:31:LEU:HD11	1.88	0.55
1:C:469:LYS:HA	1:C:486:HIS:HD2	1.72	0.55
1:C:48:TYR:HE2	1:C:252:VAL:HG22	1.72	0.55
1:C:84:LYS:HG3	1:C:141:TYR:CE1	2.40	0.55
1:A:883:TRP:O	1:A:904:ARG:NH1	2.40	0.55
1:A:479:ASN:HA	1:A:506:ARG:HD3	1.89	0.55
1:A:902:GLU:HB2	2:B:289:ASP:OD2	2.06	0.55
1:A:836:LYS:HE3	8:A:1106:PCW:H72	1.89	0.54
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:266:LEU:HD22	2:D:272:ILE:HD11	1.89	0.54
1:C:72:ALA:HB2	1:C:176:GLU:HG2	1.90	0.54
1:A:594:ASP:O	1:A:598:LYS:HG2	2.07	0.54
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.90	0.54
2:D:143:ARG:HD2	2:D:146:ARG:NH1	2.23	0.54
1:A:928:VAL:HG22	1:A:942:MET:HE3	1.90	0.54
1:A:983:CYS:SG	7:A:1104:CLR:H21	2.48	0.54
1:C:399:GLN:HE21	1:C:436:LEU:HD11	1.72	0.54
2:D:18:ASN:HA	2:D:23:GLU:O	2.08	0.54
1:A:663:LEU:HA	1:A:666:MET:HG3	1.89	0.54
1:A:907:VAL:HA	1:A:910:THR:HG22	1.90	0.54
7:A:1104:CLR:H25	1:C:993:VAL:HG11	1.89	0.54
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.90	0.54
1:C:888:ILE:O	1:C:904:ARG:NH2	2.41	0.54
2:D:213:CYS:HA	2:D:276:CYS:HA	1.90	0.54
2:B:177:ILE:HA	2:B:260:ALA:HA	1.89	0.53
1:C:1009:TRP:HZ2	2:D:34:LYS:HB3	1.73	0.53
1:A:238:PHE:HD2	1:A:258:THR:HG21	1.73	0.53
1:A:762:PHE:CE1	1:A:766:LYS:HE3	2.43	0.53
1:A:344:MET:HG3	1:A:357:VAL:HG23	1.91	0.53
1:A:776:ASN:ND2	11:A:1201:HOH:O	2.42	0.53
1:C:553:LEU:HD11	1:C:571:PHE:HD1	1.73	0.53
2:D:224:VAL:HG21	2:D:274:ILE:HD11	1.91	0.53
2:B:225:GLY:HA3	2:B:265:ASN:HB3	1.91	0.52
2:B:27:ARG:HG3	2:B:32:TRP:CD1	2.45	0.52
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.90	0.52
2:D:151:PHE:HE2	2:D:258:LEU:HB2	1.74	0.52
2:D:173:LYS:HB3	2:D:262:GLN:HE21	1.75	0.52
1:A:338:THR:O	1:A:342:LYS:HG2	2.09	0.52
1:A:736:LYS:HG3	1:A:742:ILE:HD12	1.91	0.52
2:D:169:TYR:O	2:D:174:PRO:HA	2.10	0.52
1:A:385:TRP:HD1	1:A:390:ILE:HD13	1.74	0.52
1:A:976:LEU:HB3	1:A:980:TRP:HD1	1.74	0.52
1:C:798:VAL:HG11	1:C:971:LEU:HD22	1.92	0.52
2:B:156:LEU:HD13	2:B:260:ALA:HB2	1.92	0.52
9:C:1121:H0C:O6	9:C:1121:H0C:O3	2.27	0.52
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.92	0.51
2:B:18:ASN:HA	2:B:23:GLU:O	2.10	0.51
1:C:1004:ARG:HH21	1:C:1005:ARG:NH1	2.09	0.51
1:C:589:ARG:HB2	1:C:592:VAL:HG23	1.93	0.51
1:A:907:VAL:O	1:A:911:CYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:THR:O	1:C:344:MET:HG2	2.11	0.51
2:B:213:CYS:HA	2:B:276:CYS:HA	1.93	0.51
1:A:883:TRP:HA	1:A:904:ARG:HH11	1.76	0.51
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.93	0.50
2:B:92:PRO:HG3	2:B:301:VAL:HG12	1.92	0.50
1:C:525:GLU:HA	1:C:528:LYS:HB3	1.93	0.50
2:D:130:PRO:HB3	2:D:239:PRO:HB3	1.92	0.50
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.46	0.50
2:D:91:ARG:HG2	2:D:93:ASN:H	1.77	0.50
1:C:929:ILE:HD12	1:C:995:ASP:OD2	2.12	0.50
1:A:93:PHE:HB3	1:A:330:LEU:HD13	1.94	0.50
1:A:929:ILE:HD12	1:A:995:ASP:OD2	2.12	0.50
1:C:111:GLN:O	1:C:115:GLU:HG2	2.11	0.50
2:B:151:PHE:HE2	2:B:258:LEU:HB2	1.77	0.50
1:C:803:ILE:HG12	1:C:916:PHE:HD2	1.77	0.50
9:A:1121:H0C:O6	9:A:1121:H0C:O3	2.30	0.49
1:A:473:ILE:HB	1:A:483:LEU:HG	1.94	0.49
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.93	0.49
2:D:130:PRO:HD3	2:D:232:LEU:HD12	1.93	0.49
1:A:300:PHE:HD2	1:A:301:ILE:HD12	1.77	0.49
2:B:91:ARG:HG2	2:B:93:ASN:H	1.76	0.49
1:C:397:GLU:OE2	1:C:589:ARG:HB3	2.12	0.49
1:C:793:LEU:HB3	1:C:908:GLU:OE2	2.12	0.49
1:C:976:LEU:HB3	1:C:980:TRP:HD1	1.77	0.49
2:B:80:ILE:HB	2:B:105:ILE:HD12	1.94	0.49
1:C:337:LEU:HA	1:C:761:ILE:HD11	1.93	0.49
1:C:613:HIS:CE1	1:C:685:ARG:HH21	2.30	0.49
1:A:277:ILE:HG21	1:A:355:GLU:HB2	1.94	0.49
2:B:101:TYR:O	2:B:105:ILE:HG12	2.13	0.49
1:C:473:ILE:HB	1:C:483:LEU:HG	1.93	0.49
1:A:893:ASP:OD2	1:A:897:GLN:HB2	2.11	0.49
1:A:888:ILE:O	1:A:904:ARG:NH2	2.46	0.49
1:C:148:SER:O	1:C:152:GLU:HG2	2.13	0.49
1:A:83:VAL:O	1:A:87:ARG:HG2	2.12	0.49
1:C:363:THR:HA	1:C:704:ILE:HB	1.93	0.49
1:A:986:PRO:HG3	7:A:1104:CLR:H122	1.95	0.49
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.94	0.49
1:A:112:ALA:HA	1:A:118:PRO:HG2	1.94	0.48
1:C:839:ASN:HB3	8:C:1105:PCW:H82	1.95	0.48
1:A:683:PHE:HB3	1:A:686:THR:HG21	1.94	0.48
1:C:29:LYS:NZ	1:C:265:THR:HB	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:GLU:N	1:C:669:GLU:OE1	2.37	0.48
1:C:93:PHE:HB3	1:C:330:LEU:HD13	1.95	0.48
1:A:669:GLU:N	1:A:669:GLU:OE1	2.39	0.48
2:B:217:ARG:NH1	2:B:220:ASP:OD2	2.45	0.48
2:D:66:PRO:HG2	2:D:69:GLN:HG2	1.95	0.48
2:D:92:PRO:HG3	2:D:301:VAL:HG12	1.94	0.48
3:G:33:PHE:CZ	7:G:101:CLR:H151	2.48	0.48
1:C:112:ALA:HA	1:C:118:PRO:HG2	1.96	0.48
2:D:101:TYR:O	2:D:105:ILE:HG12	2.13	0.48
2:D:90:PHE:CZ	2:D:170:LYS:HG2	2.48	0.48
1:A:284:PHE:HD1	1:A:838:VAL:HG21	1.79	0.48
1:A:913:THR:HB	1:A:976:LEU:HD21	1.95	0.48
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.94	0.48
2:B:224:VAL:HG21	2:B:274:ILE:HD11	1.94	0.48
1:C:385:TRP:CH2	1:C:531:PHE:HB2	2.48	0.48
1:A:936:SER:OG	1:A:1003:ARG:NH2	2.47	0.48
1:A:470:ILE:HG22	1:A:471:VAL:HG23	1.96	0.48
1:A:710:ASP:HB2	1:A:731:GLY:HA2	1.95	0.48
1:C:211:LEU:HA	1:C:712:VAL:HG22	1.95	0.48
1:A:421:CYS:O	1:A:422:ASN:ND2	2.46	0.47
1:A:211:LEU:HA	1:A:712:VAL:HG22	1.96	0.47
2:D:217:ARG:NH1	2:D:220:ASP:OD2	2.46	0.47
2:D:80:ILE:HB	2:D:105:ILE:HD12	1.96	0.47
1:A:470:ILE:HB	1:A:485:ILE:HG23	1.96	0.47
1:C:90:PHE:O	1:C:94:SER:HB2	2.14	0.47
1:C:338:THR:O	1:C:342:LYS:HG2	2.14	0.47
1:C:883:TRP:HA	1:C:904:ARG:NH1	2.29	0.47
1:A:600:ARG:NH2	1:A:680:GLU:HG2	2.30	0.47
1:C:840:GLU:OE2	2:D:27:ARG:NH1	2.34	0.47
2:D:224:VAL:HG22	2:D:272:ILE:HD12	1.97	0.47
1:A:525:GLU:HA	1:A:528:LYS:HB3	1.95	0.47
1:A:1005:ARG:NE	8:A:1108:PCW:O1P	2.48	0.47
1:A:111:GLN:NE2	1:A:122:ASN:OD1	2.46	0.47
1:C:347:LYS:HD2	1:C:753:THR:HG21	1.96	0.47
1:C:421:CYS:O	1:C:422:ASN:ND2	2.48	0.47
1:A:768:SER:HA	1:A:815:LEU:HD23	1.97	0.47
1:C:943:LYS:HZ2	8:C:1108:PCW:H82	1.79	0.47
1:C:931:LYS:HG2	1:C:932:THR:HG23	1.95	0.47
1:A:284:PHE:CD1	1:A:838:VAL:HG21	2.50	0.47
1:A:399:GLN:CD	1:A:455:LEU:HD21	2.35	0.46
1:A:883:TRP:HA	1:A:904:ARG:NH1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:GLU:O	1:C:466:ARG:HB2	2.15	0.46
1:C:815:LEU:HA	1:C:815:LEU:HD12	1.82	0.46
2:D:27:ARG:HG3	2:D:32:TRP:CD1	2.50	0.46
1:A:469:LYS:HA	1:A:486:HIS:HD2	1.81	0.46
1:A:972:ARG:NH2	1:A:974:TYR:OH	2.48	0.46
2:D:156:LEU:HD13	2:D:260:ALA:HB2	1.97	0.46
1:A:111:GLN:O	1:A:115:GLU:HG2	2.15	0.46
1:C:784:LEU:HD13	7:D:501:CLR:H263	1.97	0.46
1:A:413:ALA:O	1:A:417:ILE:HG13	2.16	0.46
1:A:58:PRO:HD3	1:A:167:ASN:HB2	1.96	0.46
2:B:263:PHE:HB3	2:B:266:LEU:HD21	1.97	0.46
1:C:423:ARG:NH1	1:C:474:PRO:HB3	2.30	0.46
2:D:211:VAL:HG11	2:D:259:MET:HE1	1.97	0.46
2:D:39:TYR:CZ	7:D:501:CLR:H191	2.50	0.46
1:A:1009:TRP:CZ3	1:A:1013:GLU:HG3	2.51	0.46
1:A:713:ASN:N	1:A:713:ASN:OD1	2.49	0.46
2:B:143:ARG:HD2	2:B:146:ARG:NH1	2.29	0.46
2:B:266:LEU:HD22	2:B:272:ILE:HD11	1.97	0.46
1:C:186:VAL:HG11	1:C:192:ILE:HD13	1.97	0.46
1:C:211:LEU:HD13	1:C:237:PHE:HB3	1.96	0.46
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.80	0.46
1:A:39:LEU:HD22	1:A:43:GLU:HG2	1.96	0.46
1:C:119:GLN:HE22	9:C:1121:H0C:C14	2.27	0.46
2:B:90:PHE:CZ	2:B:170:LYS:HG2	2.51	0.46
1:A:369:PHD:OP1	1:A:371:THR:N	2.41	0.46
1:A:883:TRP:CH2	1:A:904:ARG:HB2	2.51	0.46
1:A:553:LEU:HD11	1:A:571:PHE:HD1	1.80	0.46
1:A:918:THR:O	1:A:922:VAL:HG22	2.16	0.46
1:C:710:ASP:HB2	1:C:731:GLY:HA2	1.97	0.46
1:A:944:ASN:O	1:A:948:ILE:HG12	2.16	0.46
2:B:80:ILE:HD12	2:B:105:ILE:HD12	1.98	0.46
1:C:915:PHE:O	1:C:919:ILE:HG12	2.15	0.46
2:B:92:PRO:HD2	2:B:303:SER:HA	1.98	0.45
1:C:205:LYS:HA	1:C:219:THR:HA	1.97	0.45
1:C:704:ILE:HA	1:C:722:ASP:OD2	2.16	0.45
2:B:204:TYR:O	2:B:208:VAL:HG12	2.16	0.45
2:B:91:ARG:HD2	2:B:94:ASP:HB2	1.97	0.45
2:B:130:PRO:HB3	2:B:239:PRO:HB3	1.98	0.45
1:C:874:ILE:HG12	8:C:1109:PCW:O1P	2.16	0.45
1:C:470:ILE:HG22	1:C:471:VAL:HG23	1.97	0.45
2:D:239:PRO:HD2	2:D:257:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:TRP:CE2	1:C:133:VAL:HG11	2.51	0.45
1:C:909:PHE:HB3	1:C:972:ARG:O	2.17	0.45
1:A:187:LYS:HB3	1:A:190:ASP:OD2	2.16	0.45
2:B:211:VAL:HG11	2:B:259:MET:HE1	1.99	0.45
1:A:890:ASP:N	1:A:890:ASP:OD1	2.50	0.45
2:B:27:ARG:HG3	2:B:32:TRP:HD1	1.80	0.45
1:C:893:ASP:OD2	1:C:897:GLN:HB2	2.16	0.45
1:C:944:ASN:O	1:C:948:ILE:HG12	2.16	0.45
1:A:197:ARG:CZ	1:A:234:ASN:HD22	2.30	0.45
2:D:91:ARG:HD2	2:D:94:ASP:HB2	1.99	0.45
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.98	0.45
1:A:93:PHE:HZ	1:A:329:LEU:HB3	1.81	0.45
1:C:413:ALA:O	1:C:417:ILE:HG13	2.16	0.45
1:C:890:ASP:OD1	1:C:890:ASP:N	2.48	0.45
1:C:799:THR:HG21	1:C:912:HIS:HB3	1.98	0.45
2:D:246:TYR:O	2:D:250:LEU:HB2	2.16	0.45
1:C:1009:TRP:CZ2	2:D:34:LYS:HB3	2.51	0.45
1:A:858:GLY:HA2	1:A:918:THR:HG21	1.99	0.45
1:C:479:ASN:O	1:C:481:TYR:HD1	2.00	0.45
2:D:158:ASN:OD1	4:I:1:NAG:N2	2.50	0.45
1:C:496:HIS:HB2	1:C:553:LEU:HB2	1.98	0.44
1:C:713:ASN:OD1	1:C:713:ASN:N	2.48	0.44
2:D:109:LEU:HD23	2:D:153:LEU:HD23	1.98	0.44
1:A:183:LEU:HD21	1:A:248:ARG:NH2	2.33	0.44
1:A:385:TRP:CH2	1:A:531:PHE:HB2	2.52	0.44
1:C:443:ASP:OD1	1:C:444:ALA:N	2.51	0.44
2:D:74:PRO:HG2	2:D:292:GLN:OE1	2.17	0.44
1:A:417:ILE:HG22	1:A:548:PHE:HD2	1.82	0.44
1:A:867:ALA:HB2	1:A:873:PRO:HD3	2.00	0.44
1:A:803:ILE:HG12	1:A:916:PHE:HD2	1.82	0.44
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.52	0.44
1:C:58:PRO:HD3	1:C:167:ASN:HB2	1.99	0.44
1:C:936:SER:HB2	1:C:1003:ARG:CZ	2.47	0.44
2:D:76:GLY:H	2:D:181:ASN:HB2	1.81	0.44
2:D:95:PRO:HA	2:D:98:TYR:CZ	2.52	0.44
1:A:655:ALA:HA	1:A:680:GLU:O	2.18	0.44
1:A:197:ARG:NH2	1:A:234:ASN:HD22	2.16	0.44
7:A:1104:CLR:H72	2:B:56:VAL:CG1	2.48	0.44
1:C:230:LEU:HA	1:C:237:PHE:HZ	1.81	0.44
1:C:291:VAL:HG23	1:C:324:ASN:ND2	2.31	0.44
8:A:1109:PCW:H31	1:C:978:PRO:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:THR:HG23	1:A:312:GLU:H	1.82	0.44
1:C:743:LEU:HD11	1:C:751:ILE:HD13	2.00	0.44
1:C:35:ASP:HB2	1:C:229:PRO:HG3	2.00	0.43
1:C:284:PHE:HE1	1:C:773:LEU:HD11	1.83	0.43
2:D:263:PHE:HB3	2:D:266:LEU:HD21	2.00	0.43
2:D:88:ILE:HB	2:D:299:ILE:HG22	2.00	0.43
2:D:91:ARG:HD2	2:D:94:ASP:H	1.83	0.43
1:A:119:GLN:NE2	9:A:1121:H0C:O12	2.49	0.43
1:A:196:LEU:HB2	1:A:236:ALA:HB3	2.00	0.43
1:A:340:THR:O	1:A:344:MET:HG2	2.18	0.43
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.53	0.43
1:A:1009:TRP:CZ2	2:B:34:LYS:HB3	2.49	0.43
1:C:197:ARG:CZ	1:C:234:ASN:HD22	2.32	0.43
1:C:918:THR:HG23	1:C:984:ALA:HB2	2.01	0.43
1:A:292:ALA:HB2	1:A:324:ASN:HD22	1.83	0.43
1:C:524:ASP:OD2	1:C:527:LEU:HD13	2.18	0.43
2:D:117:GLN:O	2:D:150:ARG:NH1	2.50	0.43
1:A:672:ASP:OD1	1:A:701:GLN:NE2	2.50	0.43
1:C:323:ALA:HB1	1:C:780:ILE:HG12	2.00	0.43
1:C:860:PHE:O	1:C:864:VAL:HG23	2.19	0.43
1:C:892:GLU:HA	1:C:897:GLN:O	2.18	0.43
1:C:95:MET:O	1:C:99:ILE:HG23	2.18	0.43
1:A:860:PHE:O	1:A:864:VAL:HG23	2.19	0.43
1:C:277:ILE:CG2	1:C:355:GLU:HB2	2.49	0.43
1:C:837:LEU:HG	1:C:838:VAL:HG23	2.01	0.43
1:C:866:LEU:HA	1:C:866:LEU:HD23	1.84	0.43
1:C:921:VAL:HG12	1:C:988:SER:OG	2.18	0.43
1:C:98:TRP:NE1	1:C:133:VAL:HG11	2.34	0.43
2:D:199:TYR:O	2:D:200:PRO:C	2.57	0.43
1:A:304:LEU:HD23	1:A:308:TYR:O	2.18	0.43
1:A:815:LEU:HD12	1:A:815:LEU:HA	1.83	0.43
2:B:108:PHE:HD1	2:B:109:LEU:HD12	1.83	0.43
1:C:111:GLN:NE2	1:C:122:ASN:OD1	2.43	0.43
1:C:608:MET:HB3	1:C:682:VAL:HG22	1.99	0.43
2:D:54:ILE:O	2:D:58:LEU:HG	2.18	0.43
1:A:72:ALA:HB2	1:A:176:GLU:HG2	2.01	0.43
1:A:818:GLU:CD	1:A:931:LYS:HG3	2.39	0.43
1:A:95:MET:O	1:A:99:ILE:HG23	2.19	0.43
2:B:124:GLU:OE2	2:B:134:LYS:NZ	2.47	0.43
1:A:98:TRP:CE2	1:A:133:VAL:HG11	2.53	0.43
1:A:347:LYS:HD2	1:A:753:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:VAL:HA	1:A:583:SER:HA	2.01	0.43
1:A:689:GLN:O	1:A:693:ILE:HG12	2.19	0.43
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.54	0.43
1:A:866:LEU:HA	1:A:866:LEU:HD23	1.90	0.43
1:C:266:LEU:O	1:C:270:LEU:HG	2.19	0.43
1:C:360:LEU:O	1:C:755:VAL:HG23	2.19	0.43
1:C:817:TYR:HB2	1:C:944:ASN:HD21	1.84	0.43
2:D:27:ARG:HG3	2:D:32:TRP:HD1	1.84	0.43
1:A:585:ILE:HA	1:A:585:ILE:HD12	1.94	0.42
7:A:1104:CLR:H152	2:B:56:VAL:HG11	2.00	0.42
1:A:462:GLU:O	1:A:466:ARG:HB2	2.20	0.42
2:B:169:TYR:O	2:B:174:PRO:HA	2.19	0.42
2:B:42:PHE:HD2	2:B:43:TYR:CD1	2.37	0.42
1:C:883:TRP:CH2	1:C:904:ARG:HB2	2.54	0.42
1:A:551:LEU:HD22	1:A:576:LEU:HD23	2.01	0.42
1:C:1013:GLU:OE2	2:D:35:ILE:HD11	2.19	0.42
1:C:88:GLN:NE2	1:C:144:GLU:OE2	2.52	0.42
1:C:267:ALA:O	1:C:719:LYS:NZ	2.52	0.42
1:A:148:SER:O	1:A:152:GLU:HG2	2.19	0.42
1:A:471:VAL:HG21	1:A:564:PHE:O	2.19	0.42
2:B:74:PRO:HG2	2:B:292:GLN:OE1	2.19	0.42
2:B:133:LEU:H	2:B:133:LEU:HD12	1.84	0.42
1:C:797:THR:OG1	9:C:1121:H0C:O5	2.36	0.42
1:C:292:ALA:O	1:C:321:ILE:HG12	2.19	0.42
1:C:417:ILE:HG22	1:C:548:PHE:HD2	1.84	0.42
1:A:186:VAL:HG11	1:A:192:ILE:HD13	2.01	0.42
1:A:911:CYS:C	1:A:914:PRO:HD2	2.40	0.42
2:B:21:LYS:HA	2:B:21:LYS:HD2	1.83	0.42
2:B:95:PRO:HA	2:B:98:TYR:CZ	2.55	0.42
2:D:136:ARG:O	2:D:146:ARG:NH1	2.52	0.42
1:C:73:LEU:HD11	1:C:260:MET:SD	2.60	0.42
1:C:293:VAL:HG12	1:C:321:ILE:HD13	2.01	0.42
1:C:83:VAL:O	1:C:87:ARG:HG2	2.20	0.42
1:A:799:THR:HG21	1:A:912:HIS:HB3	2.02	0.42
2:B:199:TYR:O	2:B:200:PRO:C	2.58	0.42
1:C:864:VAL:HG12	1:C:980:TRP:CZ3	2.52	0.42
1:A:293:VAL:HG12	1:A:321:ILE:HD13	2.01	0.42
2:B:130:PRO:HB2	2:B:207:TYR:O	2.20	0.42
1:C:370:LYS:HZ2	1:C:620:ILE:HG13	1.85	0.42
2:D:80:ILE:HD12	2:D:105:ILE:HD12	2.01	0.42
2:D:204:TYR:O	2:D:208:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ILE:HD11	1:A:550:HIS:ND1	2.35	0.42
1:A:921:VAL:HG12	1:A:988:SER:OG	2.20	0.42
1:A:139:PHE:CZ	8:A:1105:PCW:H11	2.55	0.41
1:A:918:THR:HG23	1:A:984:ALA:HB2	2.01	0.41
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.85	0.41
2:B:30:GLY:O	2:B:34:LYS:HG3	2.20	0.41
1:C:905:LYS:HA	1:C:905:LYS:HD3	1.85	0.41
2:D:276:CYS:HB2	2:D:295:PHE:CD2	2.51	0.41
1:A:369:PHD:OD2	1:A:371:THR:O	2.38	0.41
1:C:843:ILE:HG23	1:C:847:TYR:CD2	2.52	0.41
1:C:911:CYS:C	1:C:914:PRO:HD2	2.40	0.41
2:D:30:GLY:O	2:D:34:LYS:HG3	2.20	0.41
2:D:80:ILE:HG13	2:D:80:ILE:H	1.50	0.41
1:A:496:HIS:HB2	1:A:553:LEU:HB2	2.02	0.41
1:A:778:PRO:HB2	1:A:919:ILE:HD11	2.03	0.41
1:A:93:PHE:CD1	1:A:330:LEU:HB2	2.54	0.41
1:C:180:VAL:HG22	1:C:254:THR:HB	2.02	0.41
1:C:344:MET:HG3	1:C:357:VAL:HG23	2.02	0.41
1:C:683:PHE:HB3	1:C:686:THR:HG21	2.02	0.41
1:C:882:ASN:O	1:C:904:ARG:NH1	2.46	0.41
1:C:907:VAL:O	1:C:911:CYS:HB2	2.20	0.41
1:C:995:ASP:OD1	1:C:998:ARG:NH1	2.53	0.41
1:A:309:THR:OG1	1:A:310:TRP:N	2.53	0.41
2:D:146:ARG:HG2	2:D:146:ARG:H	1.67	0.41
1:A:1011:GLU:O	1:A:1015:TYR:HB3	2.21	0.41
1:A:443:ASP:OD1	1:A:444:ALA:N	2.54	0.41
1:A:423:ARG:NH1	1:A:474:PRO:HB3	2.35	0.41
1:A:660:GLY:HA3	1:A:685:ARG:O	2.20	0.41
1:A:905:LYS:HA	1:A:905:LYS:HD3	1.91	0.41
1:C:230:LEU:HA	1:C:237:PHE:CZ	2.56	0.41
1:C:280:GLU:HB3	1:C:837:LEU:CB	2.51	0.41
1:C:165:ILE:HG12	1:C:170:LYS:HG2	2.01	0.41
1:C:560:GLU:OE1	1:C:560:GLU:N	2.53	0.41
1:C:813:ILE:HD13	1:C:813:ILE:HA	1.81	0.41
1:A:493:GLU:OE1	1:A:495:ARG:NH2	2.52	0.41
1:A:753:THR:O	1:A:757:GLU:HG2	2.20	0.41
1:A:803:ILE:HD13	1:A:803:ILE:HA	1.78	0.41
1:C:803:ILE:HA	1:C:803:ILE:HD13	1.82	0.41
2:D:51:ILE:O	2:D:54:ILE:HG22	2.21	0.41
7:E:101:CLR:H231	7:E:101:CLR:H211	1.75	0.41
2:D:182:ARG:HD2	2:D:245:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:PHE:CE2	2:D:170:LYS:HG2	2.56	0.41
1:A:915:PHE:O	1:A:919:ILE:HG12	2.20	0.41
2:B:88:ILE:HB	2:B:299:ILE:HG22	2.02	0.41
1:C:600:ARG:NH2	1:C:680:GLU:HG2	2.36	0.41
1:C:839:ASN:CB	8:C:1105:PCW:H82	2.50	0.41
1:A:277:ILE:HG22	1:A:277:ILE:H	1.66	0.41
1:A:277:ILE:CG2	1:A:355:GLU:HB2	2.50	0.41
2:B:155:TRP:CD2	2:B:232:LEU:HD22	2.56	0.41
1:C:94:SER:HB3	1:C:133:VAL:HG13	2.03	0.41
1:C:370:LYS:NZ	1:C:620:ILE:HG13	2.35	0.41
1:C:545:VAL:HG22	1:C:583:SER:HB3	2.01	0.41
3:G:45:ILE:HD12	3:G:46:LEU:HG	2.02	0.41
2:B:133:LEU:HA	2:B:240:LEU:O	2.20	0.40
1:C:311:LEU:O	1:C:315:ILE:HG12	2.21	0.40
1:C:1009:TRP:HB2	8:C:1107:PCW:O2P	2.21	0.40
1:C:277:ILE:HG22	1:C:277:ILE:H	1.62	0.40
1:C:604:ILE:HD11	1:C:755:VAL:HG21	2.03	0.40
2:D:42:PHE:HD2	2:D:43:TYR:CD1	2.39	0.40
1:A:993:VAL:O	1:A:997:VAL:HG13	2.22	0.40
2:B:91:ARG:HD2	2:B:94:ASP:H	1.86	0.40
1:C:147:SER:OG	1:C:352:LYS:HA	2.21	0.40
1:A:48:TYR:HE2	1:A:252:VAL:HG22	1.87	0.40
1:A:423:ARG:HG3	1:A:482:GLN:NE2	2.36	0.40
1:C:778:PRO:HB2	1:C:919:ILE:HD11	2.04	0.40
1:A:332:THR:HA	1:A:813:ILE:HD11	2.03	0.40
1:A:817:TYR:HB2	1:A:944:ASN:HD21	1.85	0.40
2:B:224:VAL:HG22	2:B:272:ILE:HD12	2.03	0.40
1:C:276:PRO:O	1:C:280:GLU:HG2	2.22	0.40
1:C:430:GLN:HG2	1:C:439:ALA:O	2.21	0.40
1:C:689:GLN:O	1:C:693:ILE:HG12	2.21	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	78
1	C	993/1016 (98%)	923 (93%)	67 (7%)	3 (0%)	41	74
2	B	289/303 (95%)	261 (90%)	26 (9%)	2 (1%)	22	59
2	D	289/303 (95%)	257 (89%)	29 (10%)	3 (1%)	15	52
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
3	G	30/65 (46%)	27 (90%)	3 (10%)	0	100	100
All	All	2624/2768 (95%)	2419 (92%)	195 (7%)	10 (0%)	34	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	PRO
2	D	200	PRO
2	B	199	TYR
1	C	193	PRO
2	D	199	TYR
1	A	193	PRO
1	C	306	LEU
2	D	22	LYS
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%)	816 (96%)	30 (4%)	36	63
1	C	846/861 (98%)	818 (97%)	28 (3%)	38	64
2	B	261/269 (97%)	239 (92%)	22 (8%)	11	40
2	D	261/269 (97%)	238 (91%)	23 (9%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	26/52 (50%)	25 (96%)	1 (4%)	33	61
3	G	26/52 (50%)	25 (96%)	1 (4%)	33	61
All	All	2266/2364 (96%)	2161 (95%)	105 (5%)	27	57

All (105) 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	124	TYR
1	A	138	CYS
1	A	139	PHE
1	A	167	ASN
1	A	224	PHE
1	A	238	PHE
1	A	286	HIS
1	A	327	GLU
1	A	336	CYS
1	A	374	LEU
1	A	506	ARG
1	A	523	LEU
1	A	531	PHE
1	A	533	ASN
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	884	ASP
1	A	916	PHE
1	A	936	SER
1	A	938	PHE
1	A	1009	TRP
2	B	13	LYS
2	B	25	LEU
2	B	28	THR
2	B	32	TRP

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Mol	Chain	Res	Type
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	163	ASN
2	B	164	ASP
2	B	165	GLU
2	B	169	TYR
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
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	121	ASP
1	C	167	ASN
1	C	216	GLU
1	C	224	PHE
1	C	238	PHE
1	C	254	THR
1	C	286	HIS
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

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Mol	Chain	Res	Type
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	27	ARG
2	D	28	THR
2	D	32	TRP
2	D	61	ILE
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	163	ASN
2	D	164	ASP
2	D	165	GLU
2	D	169	TYR
2	D	173	LYS
2	D	177	ILE
2	D	195	SER
2	D	203	LYS
2	D	256	GLN
2	D	297	VAL
3	E	21	TYR
3	G	21	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	ASN
1	A	427	GLN
1	A	488	ASN
1	A	613	HIS
1	A	898	GLN
1	C	119	GLN
1	C	324	ASN
1	C	399	GLN
1	C	631	ASN

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Mol	Chain	Res	Type
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	1.08	1 (10%)
1	PHD	C	369	1,5	9,11,12	0.93	0	10,15,17	1.01	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	-	2/8/11/13	-
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	2.01	116.63	111.11

There are no chirality outliers.

All (4) 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
1	A	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	0.38	0	17,19,21	0.43	0
4	NAG	F	2	4	14,14,15	0.32	0	17,19,21	0.50	0
4	NAG	H	1	2,4	14,14,15	0.70	1 (7%)	17,19,21	0.75	1 (5%)
4	NAG	H	2	4	14,14,15	0.30	0	17,19,21	0.35	0
4	NAG	I	1	2,4	14,14,15	0.37	0	17,19,21	0.47	0
4	NAG	I	2	4	14,14,15	0.28	0	17,19,21	0.49	0
4	NAG	J	1	2,4	14,14,15	0.75	1 (7%)	17,19,21	0.69	0
4	NAG	J	2	4	14,14,15	0.25	0	17,19,21	0.34	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	J	1	NAG	O5-C1	-2.72	1.39	1.43
4	H	1	NAG	O5-C1	-2.51	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	O4-C4-C3	-2.04	105.64	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

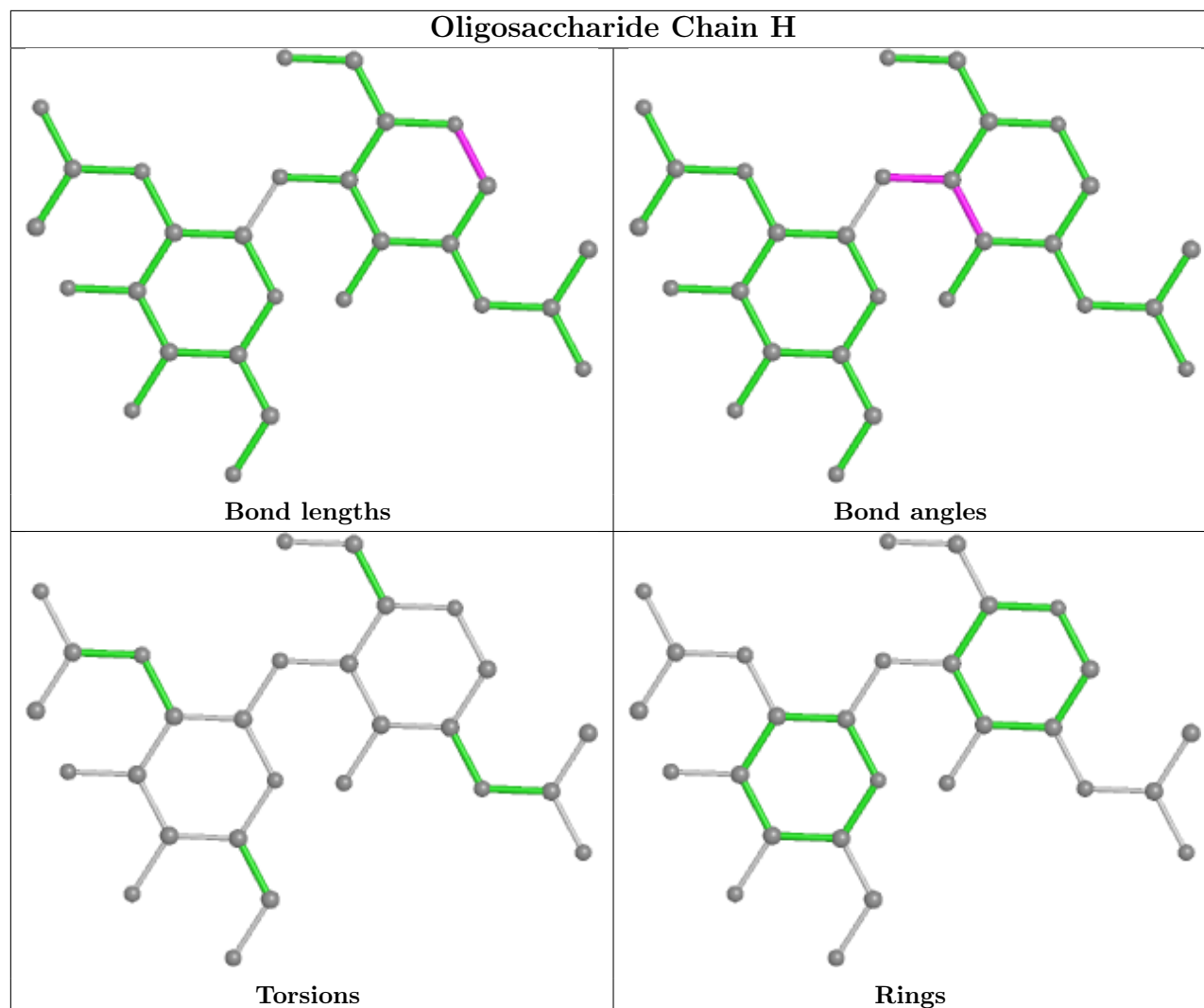
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6

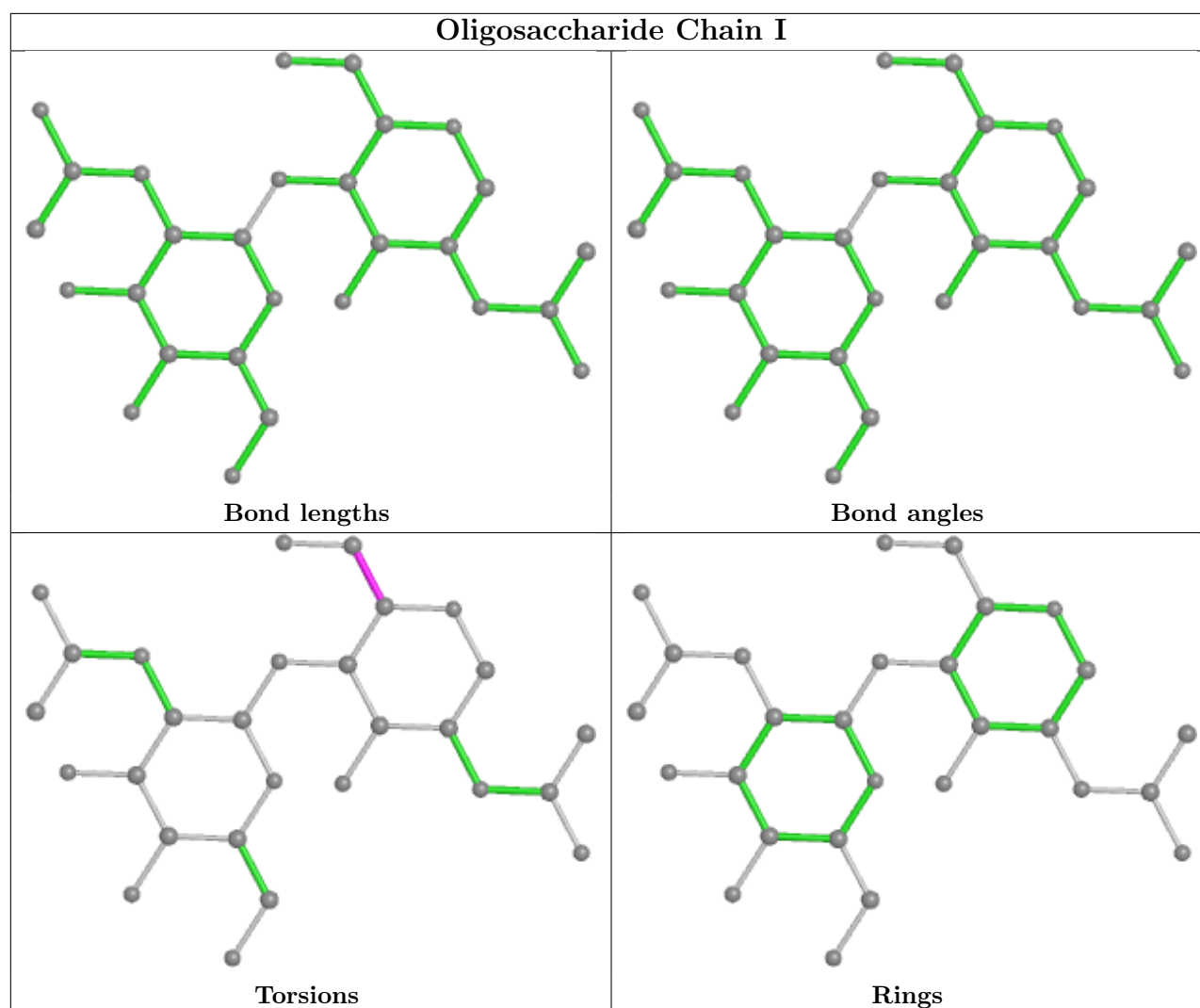
There are no ring outliers.

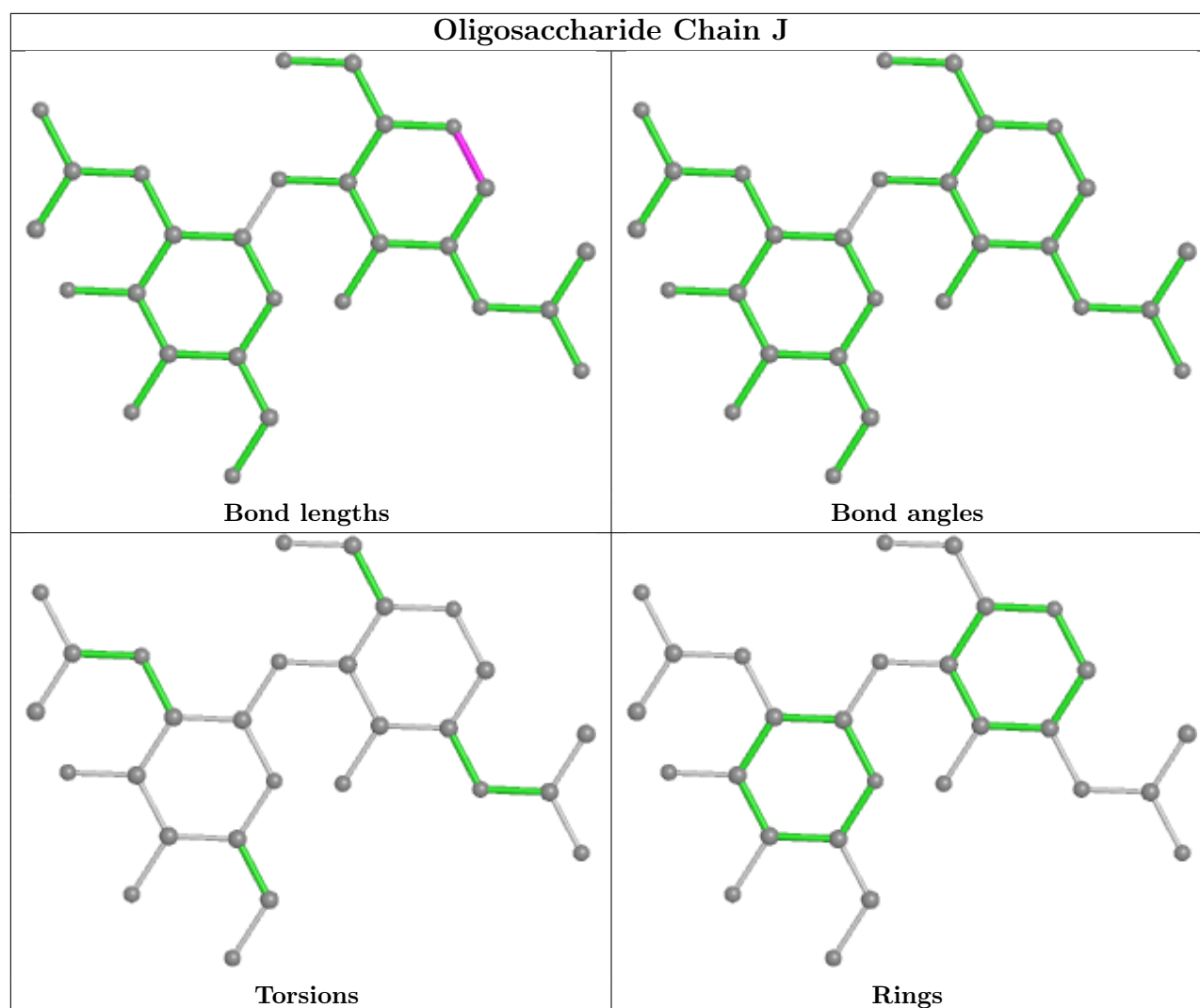
1 monomer is involved in 1 short contact:

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 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	PCW	C	1106	-	21,21,53	0.85	0	27,29,61	1.16	3 (11%)
8	PCW	C	1107	-	21,21,53	0.84	0	27,29,61	1.25	3 (11%)
10	NAG	B	411	2	14,14,15	0.26	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PCW	C	1109	-	21,21,53	0.85	0	27,29,61	1.28	3 (11%)
8	PCW	D	402	-	21,21,53	0.84	0	27,29,61	1.18	3 (11%)
8	PCW	A	1106	-	21,21,53	0.85	0	27,29,61	1.27	3 (11%)
8	PCW	A	1107	-	21,21,53	0.84	0	27,29,61	0.92	2 (7%)
7	CLR	A	1104	-	31,31,31	1.92	11 (35%)	48,48,48	1.50	8 (16%)
9	H0C	A	1121	-	63,65,65	1.15	3 (4%)	93,104,104	1.22	6 (6%)
7	CLR	D	501	-	31,31,31	1.85	7 (22%)	48,48,48	1.59	12 (25%)
8	PCW	A	1105	-	21,21,53	0.86	0	27,29,61	1.25	3 (11%)
9	H0C	C	1121	-	63,65,65	1.16	4 (6%)	93,104,104	1.23	7 (7%)
7	CLR	A	1111	-	31,31,31	2.04	13 (41%)	48,48,48	1.46	7 (14%)
7	CLR	E	101	-	31,31,31	2.04	9 (29%)	48,48,48	1.50	7 (14%)
8	PCW	C	1105	-	21,21,53	0.85	0	27,29,61	1.39	4 (14%)
7	CLR	G	101	-	31,31,31	2.08	9 (29%)	48,48,48	1.62	9 (18%)
8	PCW	A	1108	-	21,21,53	0.85	0	27,29,61	1.03	1 (3%)
8	PCW	C	1108	-	21,21,53	0.85	0	27,29,61	1.13	3 (11%)
10	NAG	D	411	2	14,14,15	0.24	0	17,19,21	0.49	0
8	PCW	A	1109	-	21,21,53	0.84	0	27,29,61	1.39	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PCW	C	1106	-	-	8/23/23/57	-
8	PCW	C	1107	-	-	8/23/23/57	-
10	NAG	B	411	2	-	1/6/23/26	0/1/1/1
8	PCW	C	1109	-	-	9/23/23/57	-
8	PCW	D	402	-	-	8/23/23/57	-
8	PCW	A	1106	-	-	9/23/23/57	-
8	PCW	A	1107	-	-	5/23/23/57	-
7	CLR	A	1104	-	-	1/10/68/68	0/4/4/4
9	H0C	A	1121	-	-	4/19/124/124	0/9/9/9
7	CLR	D	501	-	-	1/10/68/68	0/4/4/4
8	PCW	A	1105	-	-	10/23/23/57	-
9	H0C	C	1121	-	-	5/19/124/124	0/9/9/9
7	CLR	A	1111	-	-	3/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLR	E	101	-	-	2/10/68/68	0/4/4/4
8	PCW	C	1105	-	-	10/23/23/57	-
7	CLR	G	101	-	-	2/10/68/68	0/4/4/4
8	PCW	A	1108	-	-	9/23/23/57	-
8	PCW	C	1108	-	-	9/23/23/57	-
10	NAG	D	411	2	-	4/6/23/26	0/1/1/1
8	PCW	A	1109	-	-	7/23/23/57	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	101	CLR	C10-C9	5.74	1.65	1.56
7	E	101	CLR	C10-C9	5.40	1.65	1.56
7	D	501	CLR	C10-C9	5.12	1.64	1.56
7	E	101	CLR	C13-C14	4.34	1.63	1.55
7	G	101	CLR	C13-C14	4.20	1.63	1.55
7	E	101	CLR	C16-C17	4.09	1.62	1.54
7	A	1111	CLR	C10-C9	4.03	1.62	1.56
7	A	1104	CLR	C4-C3	3.88	1.58	1.52
7	A	1111	CLR	C13-C14	3.82	1.62	1.55
7	A	1111	CLR	C4-C3	3.82	1.58	1.52
7	G	101	CLR	C16-C17	3.79	1.62	1.54
7	D	501	CLR	C13-C14	3.62	1.61	1.55
7	A	1104	CLR	C10-C9	3.59	1.62	1.56
9	C	1121	H0C	C31-C30	3.49	1.57	1.53
7	A	1104	CLR	C13-C14	3.39	1.61	1.55
7	A	1104	CLR	C16-C17	3.34	1.61	1.54
7	D	501	CLR	C12-C11	3.22	1.60	1.53
7	A	1111	CLR	C16-C17	3.22	1.61	1.54
7	D	501	CLR	C16-C17	3.18	1.61	1.54
7	G	101	CLR	C12-C11	3.10	1.60	1.53
7	D	501	CLR	C12-C13	3.01	1.59	1.54
7	A	1111	CLR	C16-C15	2.89	1.61	1.54
7	G	101	CLR	C19-C10	2.87	1.59	1.54
7	G	101	CLR	C10-C5	2.79	1.58	1.52
9	A	1121	H0C	C31-C30	2.76	1.56	1.53
7	E	101	CLR	C19-C10	2.72	1.59	1.54
7	A	1111	CLR	C12-C11	2.72	1.59	1.53
7	E	101	CLR	C10-C5	2.68	1.58	1.52
7	A	1111	CLR	C11-C9	2.67	1.58	1.53
7	G	101	CLR	C12-C13	2.65	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	101	CLR	C12-C11	2.58	1.58	1.53
7	A	1104	CLR	C12-C11	2.58	1.58	1.53
9	A	1121	H0C	C26-C27	2.58	1.57	1.54
7	E	101	CLR	C4-C3	2.57	1.56	1.52
7	D	501	CLR	C10-C5	2.55	1.57	1.52
9	C	1121	H0C	C26-C27	2.50	1.57	1.54
9	A	1121	H0C	C25-C27	2.49	1.57	1.54
7	A	1104	CLR	C6-C5	2.49	1.38	1.33
7	A	1104	CLR	C16-C15	2.47	1.60	1.54
7	A	1104	CLR	C13-C17	2.40	1.59	1.55
7	E	101	CLR	C13-C17	2.39	1.59	1.55
7	A	1104	CLR	C11-C9	2.38	1.57	1.53
7	A	1111	CLR	C6-C5	2.30	1.38	1.33
7	A	1111	CLR	C20-C17	2.28	1.58	1.54
7	G	101	CLR	C13-C17	2.23	1.59	1.55
9	C	1121	H0C	C31-C3	2.21	1.55	1.51
7	D	501	CLR	C16-C15	2.18	1.60	1.54
7	G	101	CLR	C4-C3	2.17	1.55	1.52
7	A	1104	CLR	C19-C10	2.17	1.58	1.54
7	A	1104	CLR	C4-C5	2.15	1.56	1.51
9	C	1121	H0C	C25-C27	2.14	1.57	1.54
7	E	101	CLR	C12-C13	2.14	1.58	1.54
7	A	1111	CLR	C1-C10	-2.14	1.50	1.54
7	A	1111	CLR	C4-C5	2.11	1.56	1.51
7	A	1111	CLR	C22-C20	2.09	1.59	1.54
7	A	1111	CLR	C13-C17	2.02	1.58	1.55

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1121	H0C	O8-C16-C17	5.56	115.93	108.67
9	A	1121	H0C	O8-C16-C17	5.53	115.89	108.67
8	A	1109	PCW	C2-O2-C31	-5.35	107.92	117.90
8	D	402	PCW	C2-O2-C31	-4.40	109.69	117.90
7	G	101	CLR	C17-C13-C14	-4.38	94.88	100.07
7	G	101	CLR	C2-C3-C4	-4.29	104.43	110.31
9	A	1121	H0C	O9-C16-C17	-4.22	122.27	130.81
9	C	1121	H0C	O9-C16-C17	-4.21	122.29	130.81
8	C	1109	PCW	C2-O2-C31	-4.18	110.11	117.90
8	A	1105	PCW	C3-O3-C11	-4.16	106.65	117.10
7	D	501	CLR	C2-C3-C4	-4.14	104.63	110.31
8	C	1107	PCW	C2-O2-C31	-4.04	110.36	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1106	PCW	C2-O2-C31	-3.94	110.55	117.90
7	E	101	CLR	C2-C3-C4	-3.93	104.91	110.31
8	A	1106	PCW	C3-O3-C11	-3.91	107.28	117.10
8	C	1105	PCW	C3-O3-C11	-3.74	107.70	117.10
8	C	1108	PCW	C2-O2-C31	-3.63	111.13	117.90
8	A	1106	PCW	C2-O2-C31	-3.60	111.18	117.90
8	C	1105	PCW	O2-C31-C32	3.53	117.59	111.09
8	A	1105	PCW	C2-O2-C31	-3.30	111.74	117.90
8	A	1108	PCW	C3-O3-C11	-3.30	108.81	117.10
8	C	1109	PCW	C3-O3-C11	-3.29	108.84	117.10
8	C	1107	PCW	C3-O3-C11	-3.21	109.03	117.10
7	A	1104	CLR	C8-C7-C6	-3.19	108.15	112.73
7	A	1111	CLR	C8-C7-C6	-3.18	108.16	112.73
9	C	1121	H0C	C19-C17-C16	-3.05	102.50	108.84
9	A	1121	H0C	C19-C17-C16	-3.04	102.52	108.84
8	C	1106	PCW	C3-O3-C11	-3.04	109.47	117.10
7	D	501	CLR	C4-C5-C6	-3.03	116.23	120.61
7	E	101	CLR	C17-C13-C14	-3.03	96.48	100.07
8	C	1108	PCW	C3-O3-C11	-3.02	109.52	117.10
7	A	1104	CLR	C13-C17-C20	-3.02	114.76	119.49
7	A	1104	CLR	C3-C4-C5	2.93	117.00	112.03
7	G	101	CLR	C22-C20-C17	-2.86	104.38	110.28
8	A	1106	PCW	O2-C31-C32	2.86	116.35	111.09
7	A	1111	CLR	C13-C17-C20	-2.78	115.12	119.49
7	D	501	CLR	C8-C7-C6	-2.78	108.73	112.73
8	A	1109	PCW	C3-O3-C11	-2.57	110.65	117.10
7	A	1111	CLR	C3-C4-C5	2.57	116.38	112.03
7	A	1111	CLR	C2-C3-C4	-2.56	106.80	110.31
9	C	1121	H0C	C18-O8-C16	-2.55	105.76	108.85
9	A	1121	H0C	C18-O8-C16	-2.51	105.81	108.85
7	G	101	CLR	C7-C8-C14	-2.48	107.32	110.91
8	C	1105	PCW	C2-O2-C31	-2.44	113.34	117.90
7	E	101	CLR	C22-C20-C17	-2.43	105.26	110.28
8	D	402	PCW	C3-O3-C11	-2.41	111.03	117.10
8	A	1109	PCW	O2-C31-C32	2.39	115.48	111.09
9	A	1121	H0C	O2-C3-C31	2.37	114.82	107.83
8	A	1107	PCW	C3-O3-C11	-2.35	111.21	117.10
7	D	501	CLR	O1-C3-C2	2.34	116.13	110.16
7	E	101	CLR	C16-C17-C20	-2.33	108.53	112.15
7	A	1104	CLR	C2-C3-C4	-2.33	107.11	110.31
7	D	501	CLR	C17-C13-C14	-2.33	97.31	100.07
7	G	101	CLR	C16-C17-C20	-2.33	108.54	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1121	H0C	C30-C31-C3	-2.32	111.50	114.14
7	D	501	CLR	C16-C17-C20	-2.30	108.58	112.15
7	E	101	CLR	C4-C5-C6	-2.30	117.29	120.61
7	D	501	CLR	O1-C3-C4	2.30	114.60	109.68
7	A	1104	CLR	C4-C5-C10	-2.28	113.38	116.42
7	G	101	CLR	C4-C5-C6	-2.27	117.33	120.61
8	D	402	PCW	O2-C31-C32	2.27	115.27	111.09
8	C	1107	PCW	O2-C31-C32	2.26	115.25	111.09
7	D	501	CLR	C4-C5-C10	-2.26	113.42	116.42
8	A	1107	PCW	C2-O2-C31	-2.22	113.75	117.90
8	C	1105	PCW	C4-C5-N	-2.20	108.45	115.78
7	D	501	CLR	C18-C13-C12	2.18	114.03	110.59
7	D	501	CLR	C22-C20-C17	-2.17	105.80	110.28
8	C	1106	PCW	O2-C31-C32	2.16	115.06	111.09
8	C	1109	PCW	O2-C31-C32	2.15	115.04	111.09
9	C	1121	H0C	O2-C3-C31	2.14	114.16	107.83
7	E	101	CLR	O1-C3-C4	2.12	114.21	109.68
7	A	1111	CLR	C19-C10-C5	2.10	111.74	108.34
7	D	501	CLR	C19-C10-C5	2.09	111.73	108.34
7	A	1104	CLR	C23-C22-C20	-2.08	109.07	115.03
7	A	1104	CLR	C15-C14-C8	-2.07	115.67	119.08
7	E	101	CLR	O1-C3-C2	2.07	115.44	110.16
7	D	501	CLR	C11-C9-C10	2.07	115.80	113.08
8	C	1108	PCW	O2-C31-C32	2.06	114.89	111.09
7	A	1111	CLR	C13-C14-C8	-2.04	111.36	114.38
7	A	1111	CLR	C15-C14-C8	-2.04	115.72	119.08
7	G	101	CLR	O1-C3-C2	2.04	115.35	110.16
9	C	1121	H0C	C23-C24-C25	-2.03	101.74	105.19
7	A	1104	CLR	C21-C20-C22	-2.02	107.19	110.36
9	A	1121	H0C	C23-C24-C25	-2.02	101.76	105.19
8	A	1105	PCW	O3-C3-C2	2.02	114.31	108.43
7	G	101	CLR	O1-C3-C4	2.02	114.00	109.68
7	G	101	CLR	C19-C10-C5	2.01	111.59	108.34

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1106	PCW	C32-C31-O2-C2
8	C	1106	PCW	O31-C31-O2-C2
9	C	1121	H0C	C30-C11-C14-O6
8	A	1108	PCW	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
8	A	1108	PCW	C1-O3P-P-O2P
8	A	1108	PCW	C4-O4P-P-O1P
8	A	1108	PCW	C4-O4P-P-O2P
8	A	1108	PCW	C4-O4P-P-O3P
8	A	1106	PCW	C4-O4P-P-O1P
8	A	1106	PCW	C4-O4P-P-O2P
8	A	1106	PCW	C4-O4P-P-O3P
8	A	1109	PCW	C4-O4P-P-O1P
8	C	1107	PCW	C32-C31-O2-C2
8	C	1107	PCW	O31-C31-O2-C2
8	C	1107	PCW	C1-O3P-P-O1P
8	C	1107	PCW	C1-O3P-P-O2P
8	D	402	PCW	C32-C31-O2-C2
8	D	402	PCW	O31-C31-O2-C2
8	D	402	PCW	C1-O3P-P-O1P
8	D	402	PCW	C1-O3P-P-O2P
8	D	402	PCW	C1-O3P-P-O4P
8	C	1109	PCW	C32-C31-O2-C2
8	C	1109	PCW	O31-C31-O2-C2
8	C	1109	PCW	C1-O3P-P-O1P
8	C	1109	PCW	C1-O3P-P-O2P
8	C	1109	PCW	C1-O3P-P-O4P
8	A	1105	PCW	C1-O3P-P-O1P
8	A	1105	PCW	C1-O3P-P-O2P
8	A	1105	PCW	C4-O4P-P-O2P
8	A	1105	PCW	C4-O4P-P-O3P
8	C	1105	PCW	C32-C31-O2-C2
8	C	1105	PCW	C1-O3P-P-O2P
8	C	1105	PCW	C4-O4P-P-O1P
8	C	1105	PCW	C4-O4P-P-O2P
8	C	1105	PCW	C4-O4P-P-O3P
8	C	1108	PCW	C1-O3P-P-O1P
8	C	1108	PCW	C1-O3P-P-O2P
8	C	1108	PCW	C4-O4P-P-O1P
8	C	1108	PCW	C4-O4P-P-O3P
9	A	1121	H0C	C30-C11-C14-O6
8	A	1106	PCW	C32-C31-O2-C2
8	C	1105	PCW	O31-C31-O2-C2
8	A	1106	PCW	O31-C31-O2-C2
8	A	1105	PCW	O11-C11-O3-C3
8	C	1109	PCW	O11-C11-O3-C3
8	C	1108	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
8	A	1109	PCW	C12-C11-O3-C3
8	A	1105	PCW	C12-C11-O3-C3
8	A	1106	PCW	O11-C11-O3-C3
8	A	1109	PCW	O11-C11-O3-C3
8	C	1105	PCW	O11-C11-O3-C3
8	C	1109	PCW	C12-C11-O3-C3
8	C	1108	PCW	C12-C11-O3-C3
8	C	1105	PCW	C12-C11-O3-C3
8	A	1106	PCW	C12-C11-O3-C3
10	D	411	NAG	O5-C5-C6-O6
10	D	411	NAG	C4-C5-C6-O6
10	D	411	NAG	C8-C7-N2-C2
10	D	411	NAG	O7-C7-N2-C2
7	A	1111	CLR	C21-C20-C22-C23
8	A	1109	PCW	O31-C31-O2-C2
8	A	1108	PCW	C1-O3P-P-O4P
8	C	1107	PCW	C1-O3P-P-O4P
8	A	1107	PCW	C4-O4P-P-O3P
8	A	1105	PCW	C1-O3P-P-O4P
8	C	1108	PCW	C1-O3P-P-O4P
7	D	501	CLR	C21-C20-C22-C23
9	A	1121	H0C	O13-C32-O2-C3
7	E	101	CLR	C21-C20-C22-C23
8	A	1105	PCW	O31-C31-O2-C2
8	A	1109	PCW	C4-O4P-P-O3P
7	G	101	CLR	C21-C20-C22-C23
9	C	1121	H0C	C1-C11-C14-O6
9	A	1121	H0C	C1-C11-C14-O6
7	A	1104	CLR	C21-C20-C22-C23
10	B	411	NAG	O5-C5-C6-O6
7	E	101	CLR	C20-C22-C23-C24
8	C	1106	PCW	O11-C11-O3-C3
9	C	1121	H0C	C26-C11-C14-O6
9	A	1121	H0C	C26-C11-C14-O6
7	A	1111	CLR	C23-C24-C25-C27
8	C	1107	PCW	O11-C11-O3-C3
8	C	1105	PCW	C1-O3P-P-O4P
8	C	1106	PCW	C1-O3P-P-O2P
8	A	1109	PCW	C4-O4P-P-O2P
8	A	1107	PCW	C4-O4P-P-O1P
8	C	1108	PCW	C4-O4P-P-O2P
8	C	1106	PCW	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
8	A	1108	PCW	O4P-C4-C5-N
8	A	1106	PCW	O4P-C4-C5-N
8	A	1109	PCW	O4P-C4-C5-N
8	C	1107	PCW	O4P-C4-C5-N
8	D	402	PCW	O4P-C4-C5-N
8	C	1109	PCW	O4P-C4-C5-N
8	A	1107	PCW	O4P-C4-C5-N
8	A	1105	PCW	O4P-C4-C5-N
8	C	1105	PCW	O4P-C4-C5-N
8	C	1108	PCW	O4P-C4-C5-N
8	C	1106	PCW	C4-O4P-P-O3P
8	C	1107	PCW	C4-O4P-P-O3P
8	D	402	PCW	C4-O4P-P-O3P
8	C	1109	PCW	C4-O4P-P-O3P
8	A	1107	PCW	O31-C31-O2-C2
9	C	1121	H0C	O13-C32-O2-C3
7	G	101	CLR	C20-C22-C23-C24
8	C	1106	PCW	C12-C11-O3-C3
8	C	1106	PCW	C4-O4P-P-O2P
8	A	1106	PCW	C1-O3P-P-O2P
8	A	1107	PCW	C1-O3P-P-O2P
8	A	1108	PCW	C1-C2-O2-C31
8	A	1108	PCW	C3-C2-O2-C31
8	D	402	PCW	C3-C2-O2-C31
8	A	1105	PCW	C3-C2-O2-C31
9	C	1121	H0C	C33-C32-O2-C3
7	A	1111	CLR	C20-C22-C23-C24

There are no ring outliers.

14 monomers are involved in 27 short contacts:

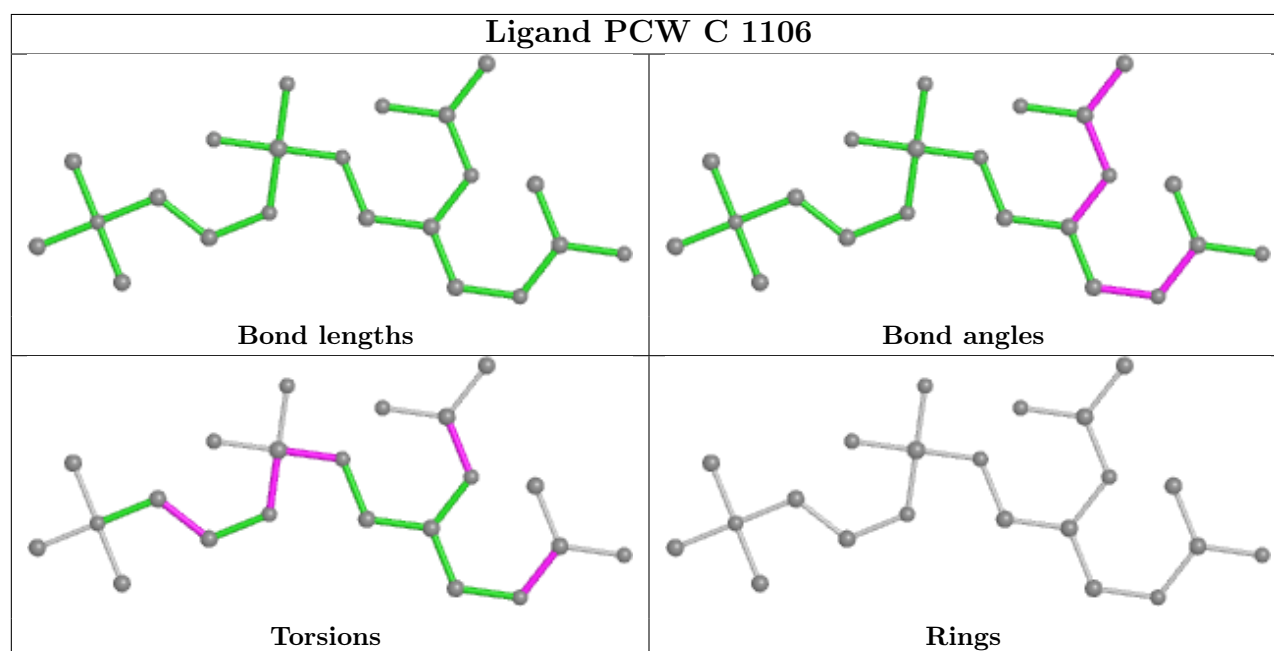
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1107	PCW	1	0
8	C	1109	PCW	1	0
8	A	1106	PCW	1	0
7	A	1104	CLR	5	0
9	A	1121	H0C	2	0
7	D	501	CLR	2	0
8	A	1105	PCW	1	0
9	C	1121	H0C	3	0
7	E	101	CLR	2	0
8	C	1105	PCW	2	0

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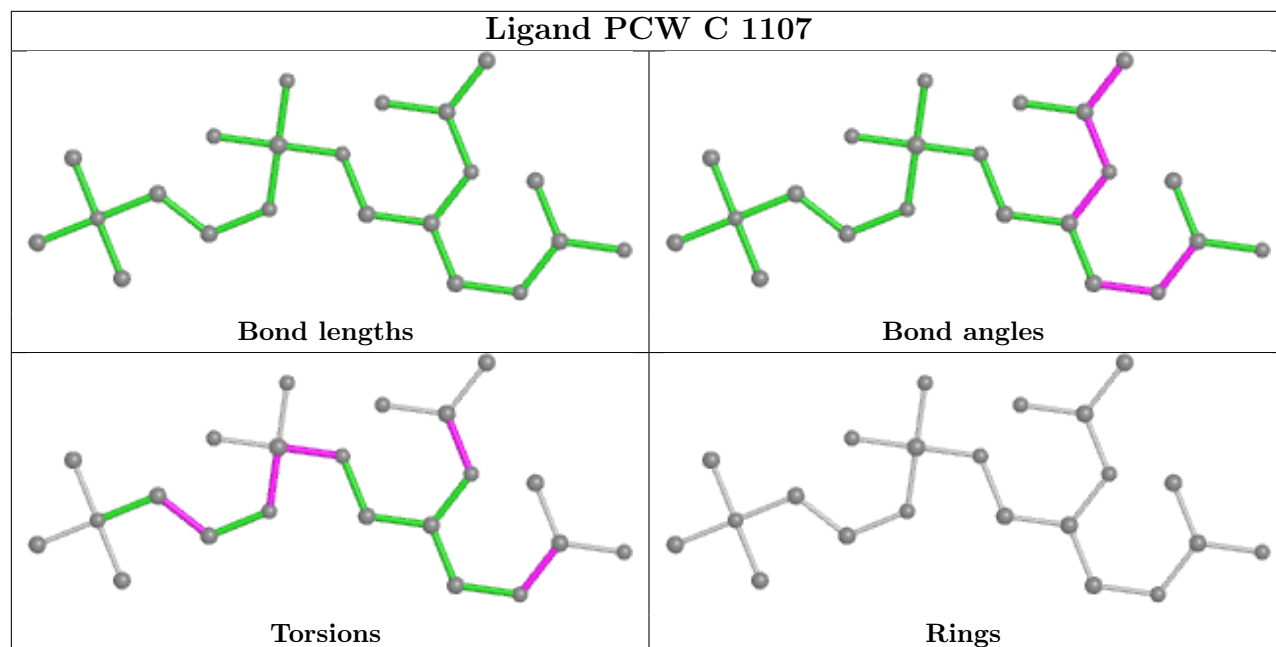
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	101	CLR	2	0
8	A	1108	PCW	1	0
8	C	1108	PCW	2	0
8	A	1109	PCW	2	0

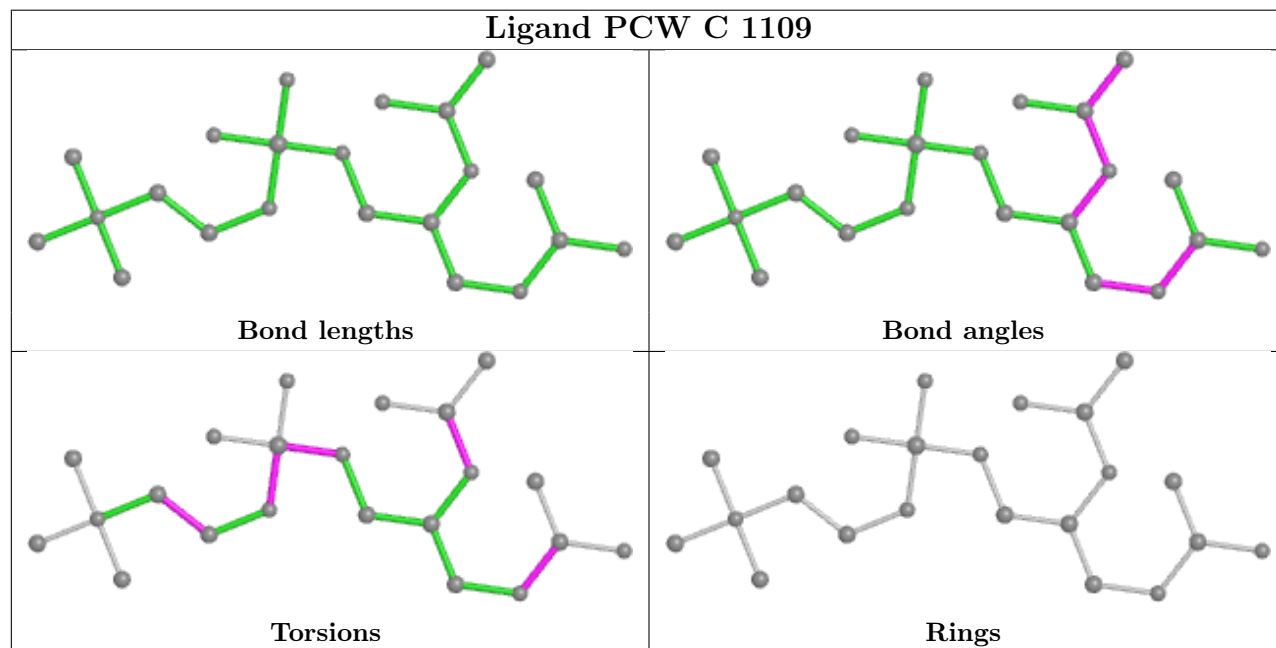
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

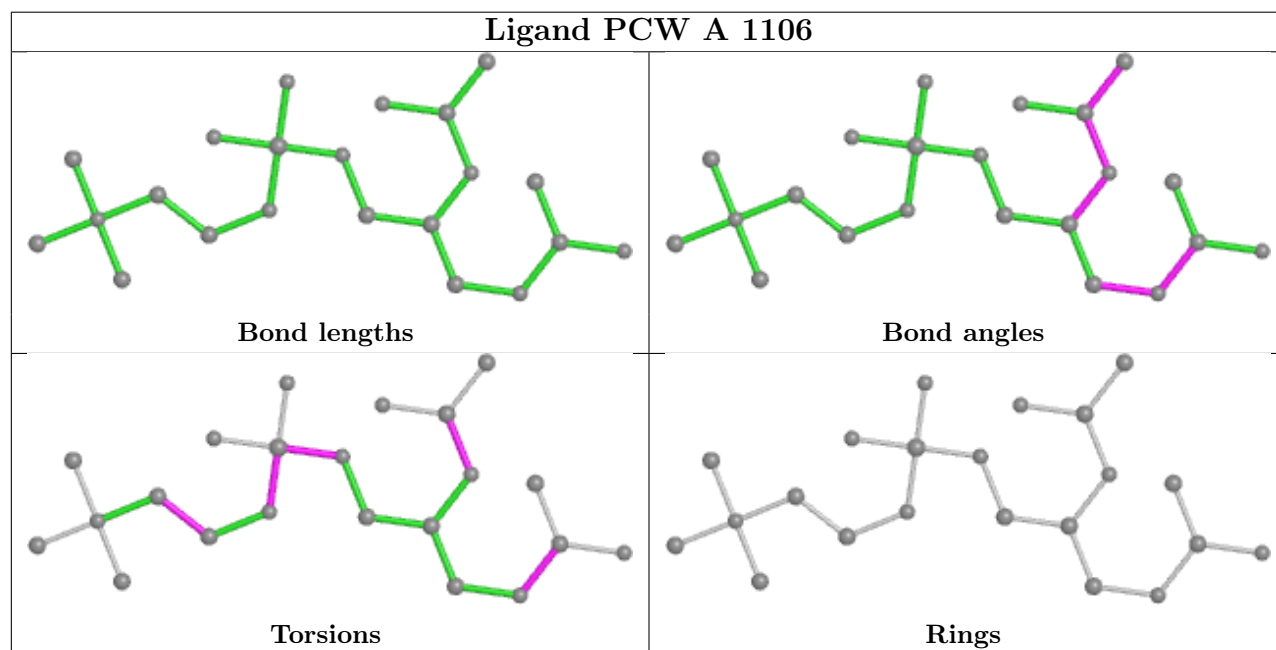
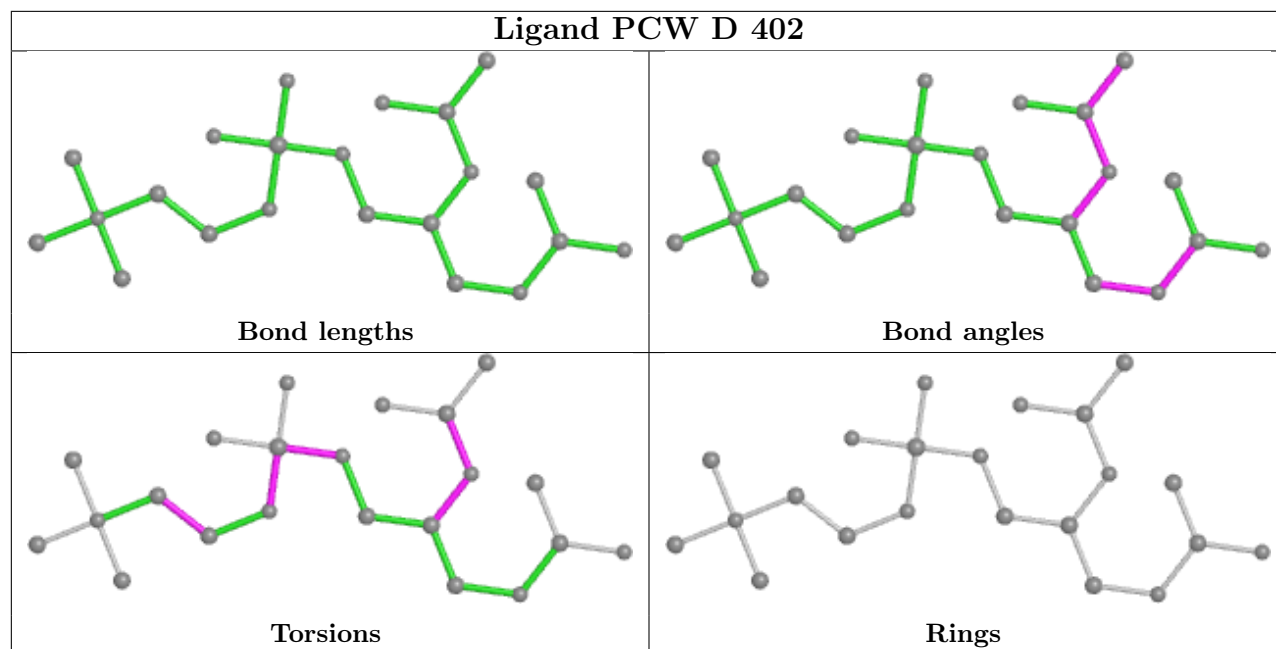


## Ligand PCW C 1107

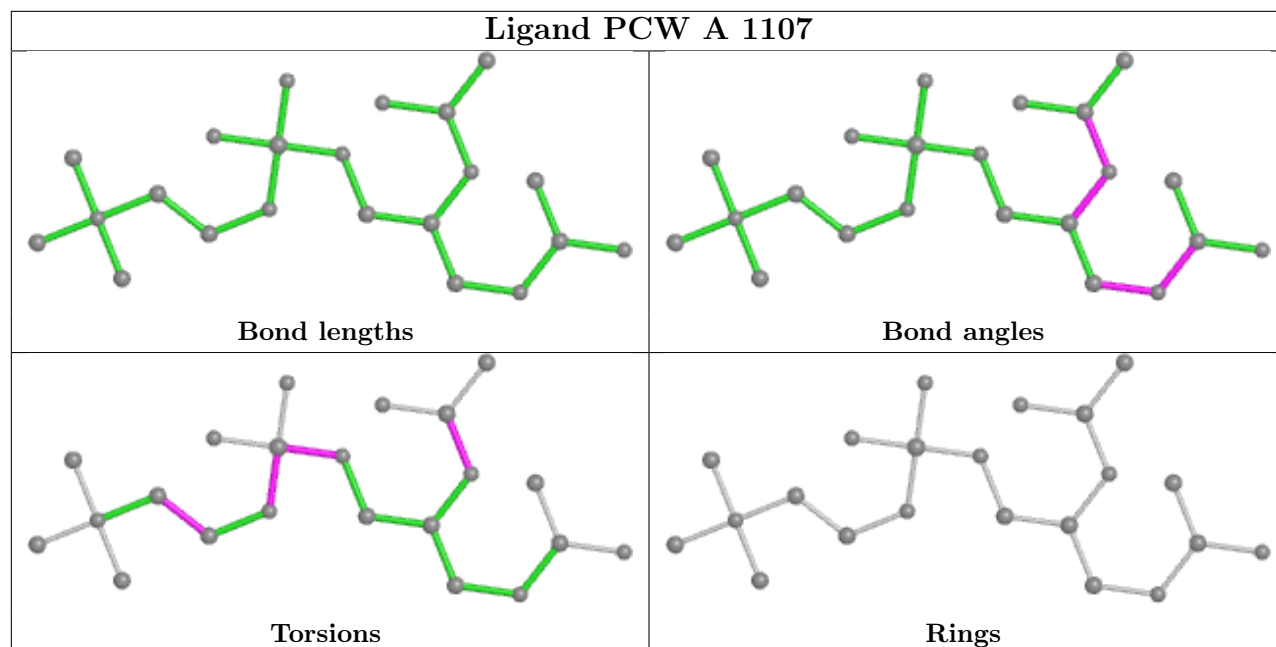


## Ligand PCW C 1109

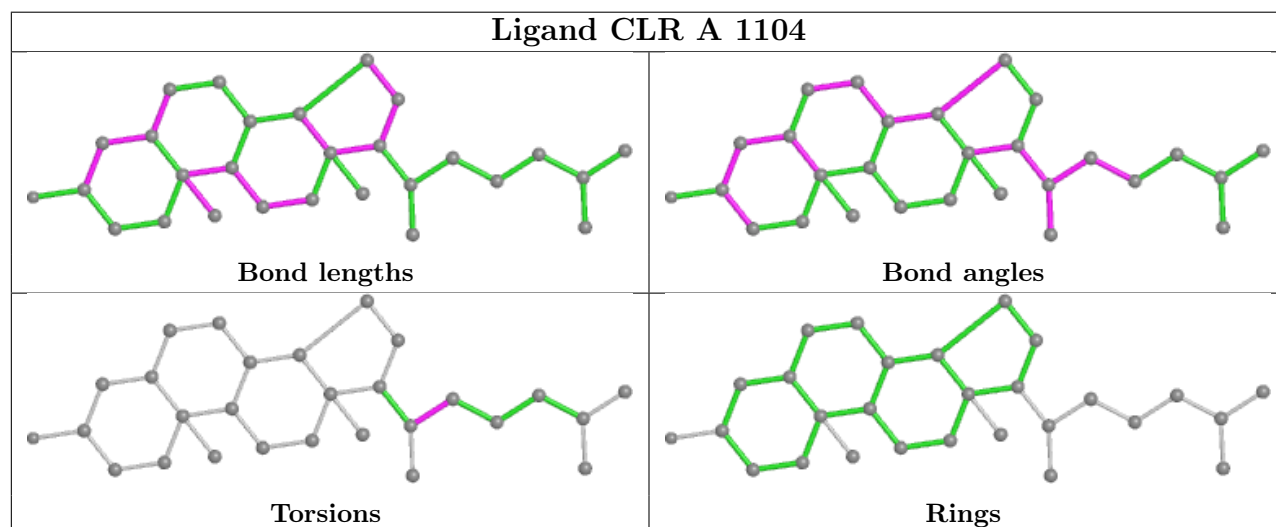




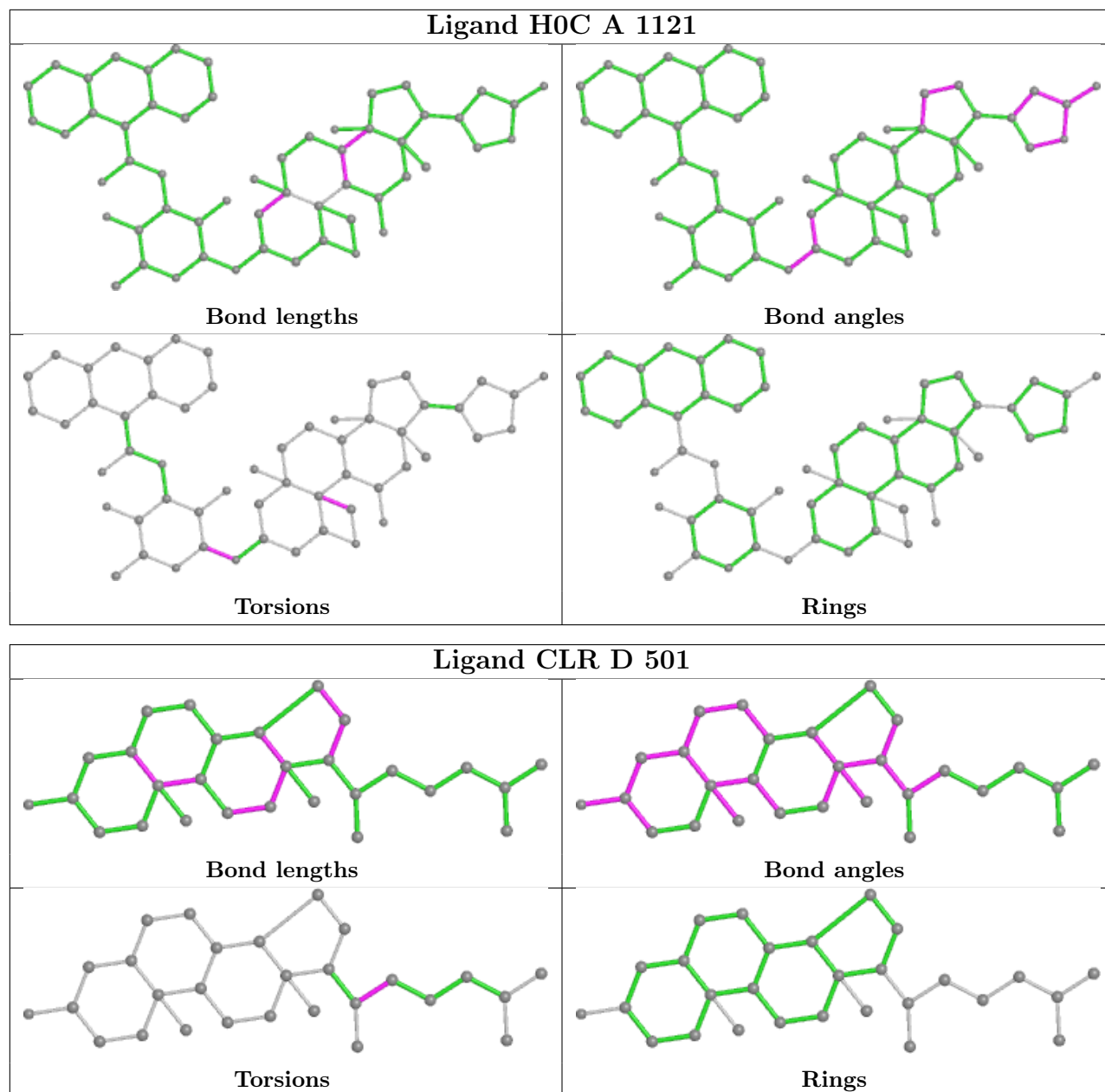
## Ligand PCW A 1107



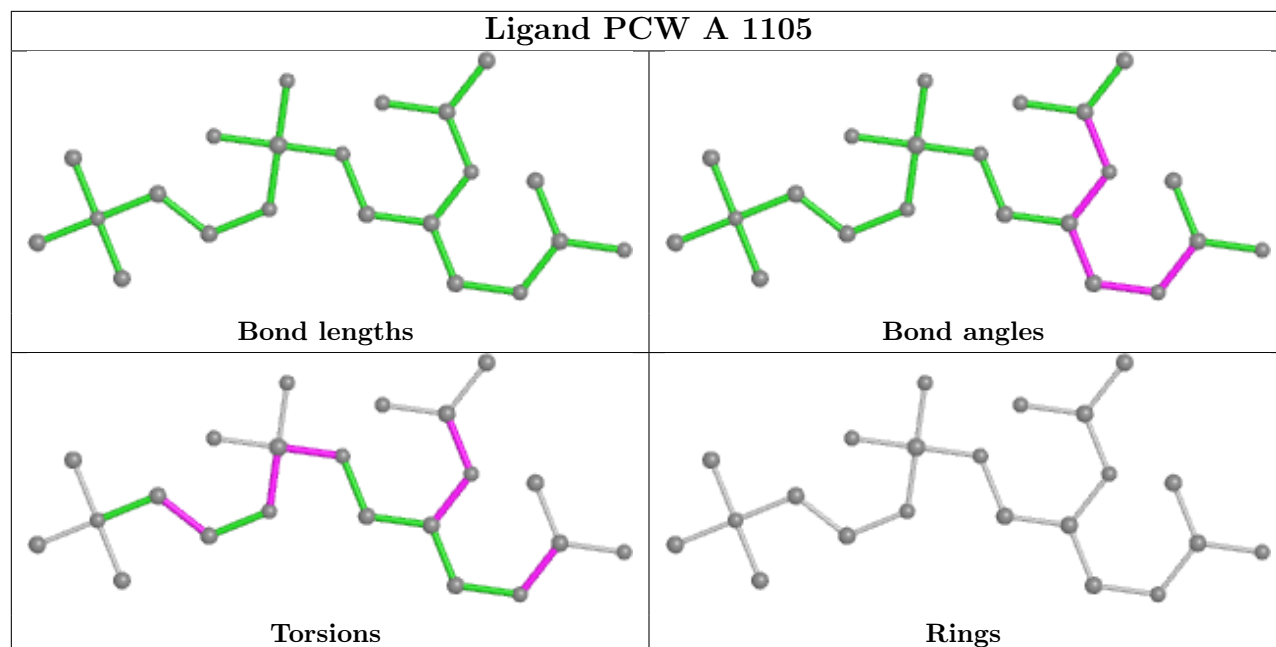
## Ligand CLR A 1104



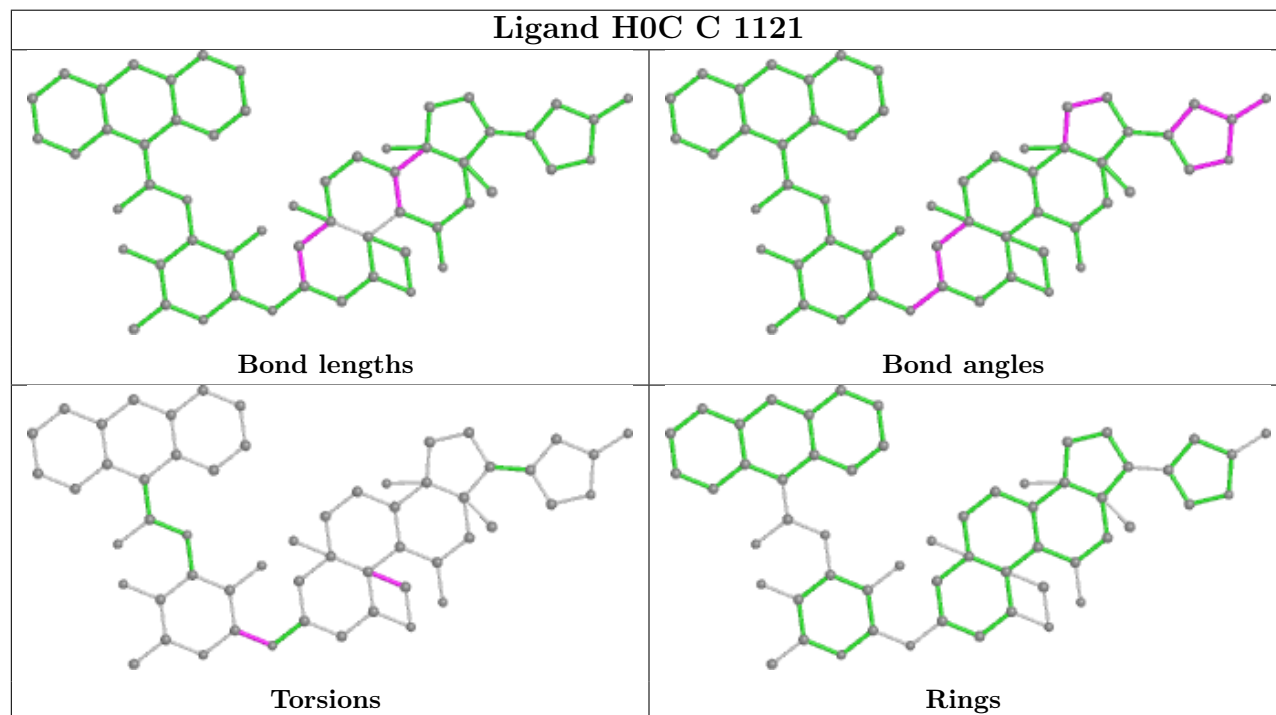




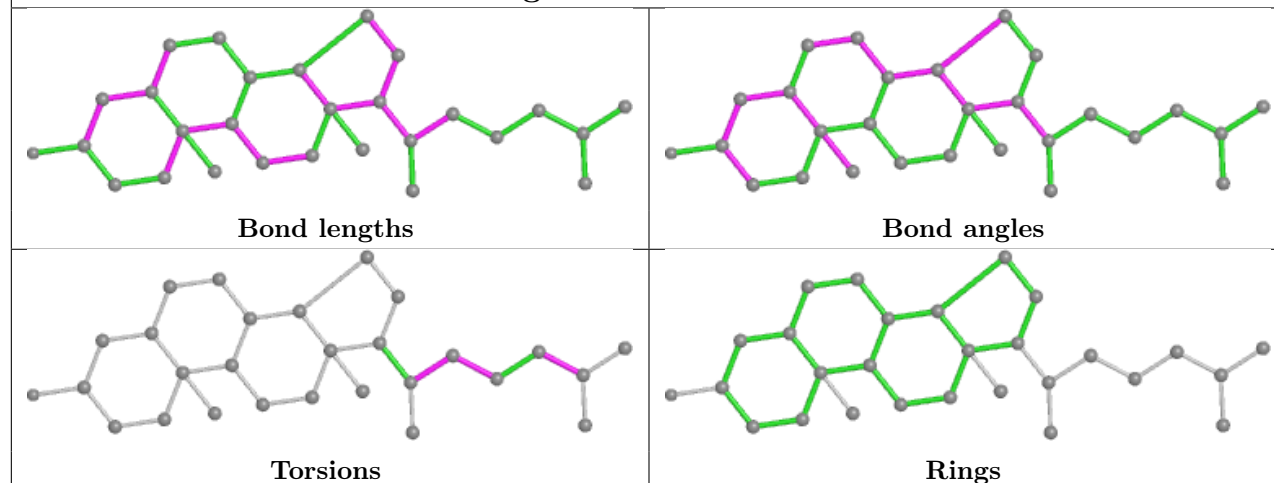
## Ligand PCW A 1105



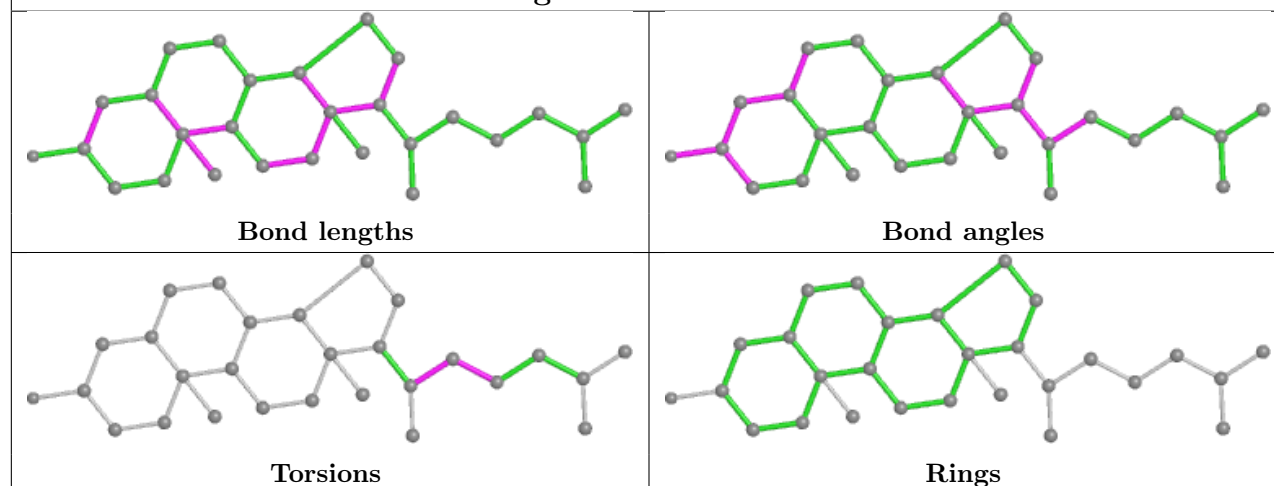
## Ligand H0C C 1121



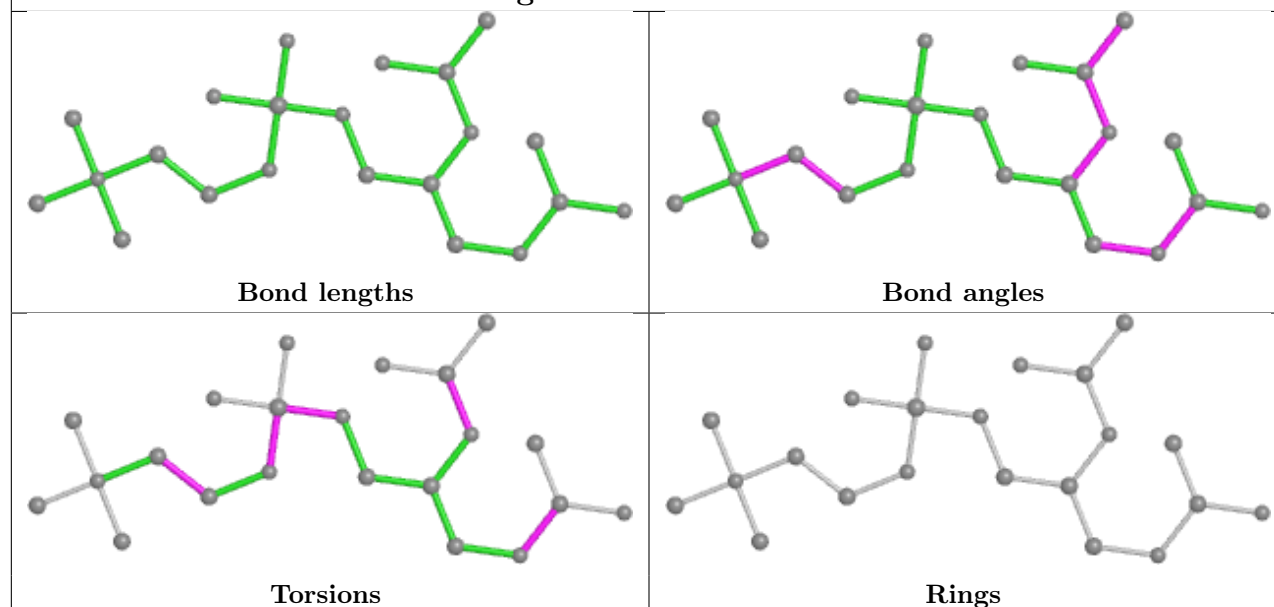
## Ligand CLR A 1111



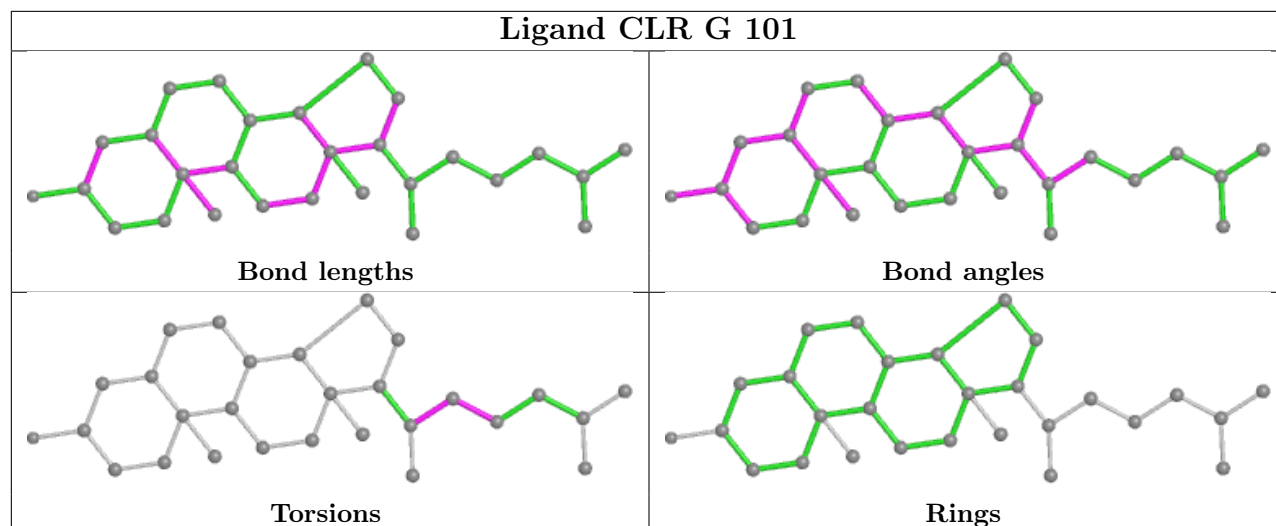
## Ligand CLR E 101



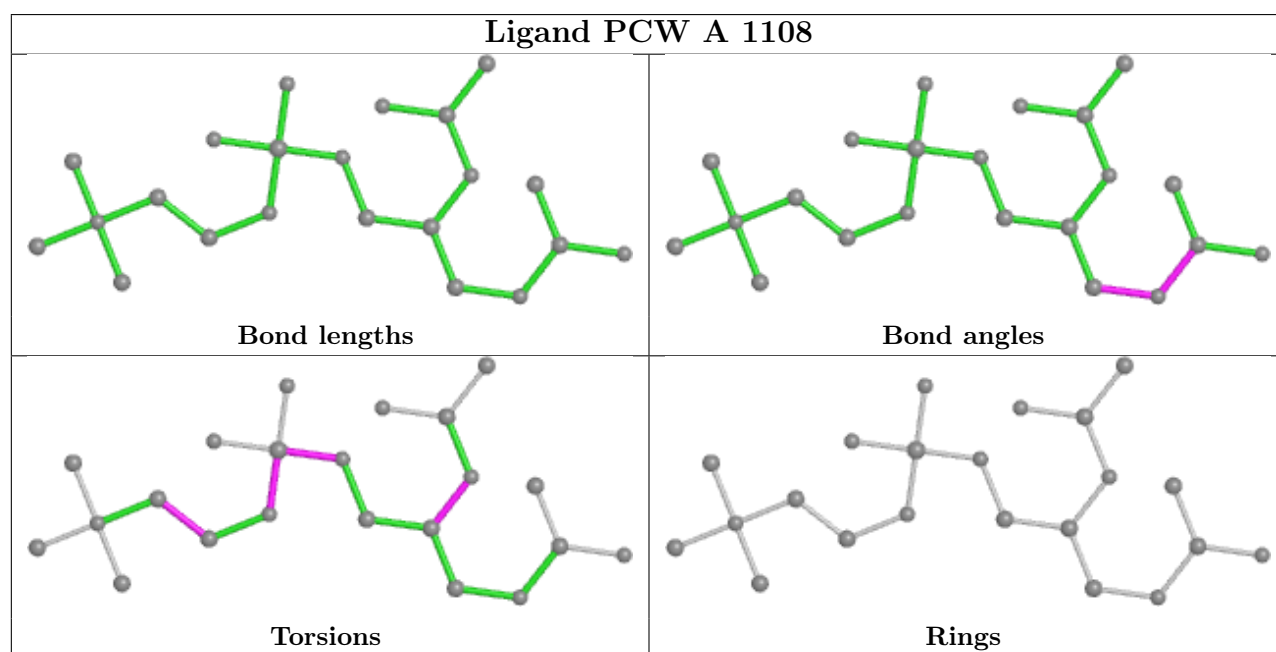
## Ligand PCW C 1105

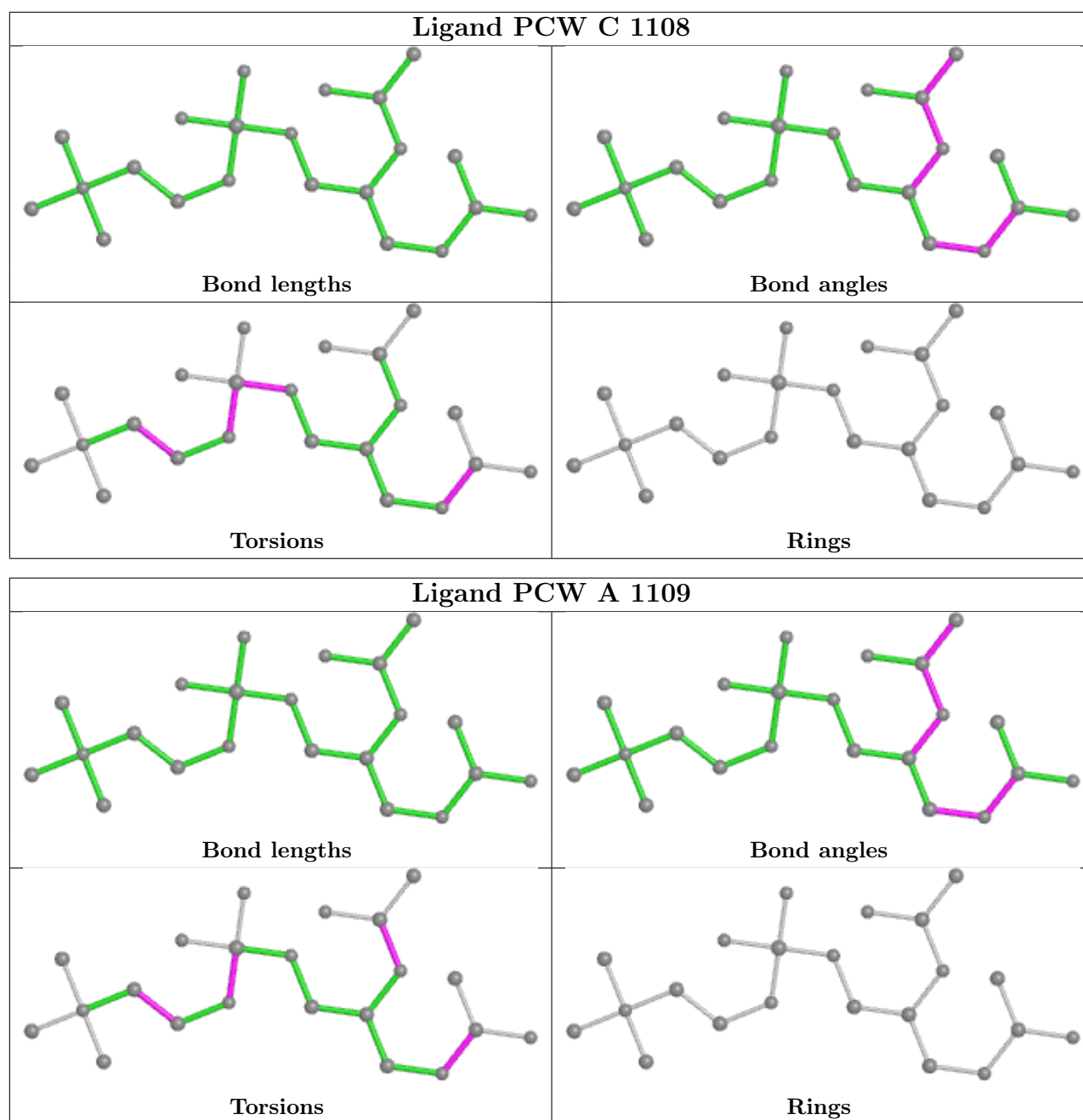


## Ligand CLR G 101



## Ligand PCW A 1108





## 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%)	0.06	57 (5%)	23	16	78, 126, 244, 271	0
1	C	995/1016 (97%)	-0.02	45 (4%)	33	23	66, 121, 202, 234	0
2	B	291/303 (96%)	0.08	13 (4%)	33	23	97, 148, 198, 220	0
2	D	291/303 (96%)	0.10	20 (6%)	16	11	93, 153, 193, 239	0
3	E	32/65 (49%)	-0.28	0	100	100	65, 95, 148, 151	0
3	G	32/65 (49%)	-0.70	0	100	100	77, 108, 141, 153	0
All	All	2636/2768 (95%)	0.02	135 (5%)	28	19	65, 130, 227, 271	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	PRO	10.7
1	A	581	LEU	6.7
1	A	467	TYR	6.6
1	A	466	ARG	6.6
1	C	499	VAL	6.2
1	A	419	GLY	5.9
1	A	486	HIS	5.8
1	C	548	PHE	5.6
1	A	578	PHE	5.4
1	A	488	ASN	5.3
1	C	484	SER	5.2
2	B	163	ASN	5.1
1	A	491	THR	5.1
1	C	500	MET	5.0
1	A	420	LEU	5.0
1	A	550	HIS	4.9
1	A	490	ASN	4.7
1	C	429	ASN	4.6
1	A	548	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	198	THR	4.5
2	B	162	LEU	4.4
1	A	497	LEU	4.4
2	D	166	THR	4.4
2	D	163	ASN	4.3
1	A	522	PRO	4.2
1	C	579	VAL	4.2
1	C	485	ILE	4.1
1	C	501	LYS	4.0
1	A	465	GLU	4.0
1	A	382	ALA	3.9
1	A	468	THR	3.9
1	C	497	LEU	3.8
1	C	547	GLY	3.8
1	A	582	ILE	3.7
2	D	162	LEU	3.6
1	A	432	ASN	3.6
1	C	403	SER	3.6
1	C	564	PHE	3.5
1	A	464	ARG	3.5
1	C	571	PHE	3.4
1	C	436	LEU	3.4
1	A	514	ILE	3.4
1	C	486	HIS	3.4
2	B	164	ASP	3.4
1	A	521	GLN	3.4
1	A	545	VAL	3.4
1	A	547	GLY	3.3
2	D	237	GLY	3.3
1	C	402	VAL	3.3
1	A	487	LYS	3.3
2	D	151	PHE	3.2
1	C	556	GLU	3.2
2	D	197	GLU	3.2
1	C	471	VAL	3.2
1	C	435	ILE	3.2
1	C	483	LEU	3.2
1	A	469	LYS	3.1
1	A	484	SER	3.1
1	A	580	GLY	3.1
1	C	473	ILE	3.1
1	C	419	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	566	THR	3.1
1	C	470	ILE	3.0
1	C	581	LEU	3.0
1	C	553	LEU	3.0
1	A	552	PHE	2.9
1	C	498	LEU	2.9
1	C	487	LYS	2.9
1	A	384	MET	2.8
1	A	496	HIS	2.8
1	A	508	LEU	2.8
2	B	24	PHE	2.8
2	D	258	LEU	2.8
2	D	224	VAL	2.8
1	C	565	ASP	2.8
1	A	504	PRO	2.8
2	D	195	SER	2.8
1	C	549	CYS	2.7
1	A	485	ILE	2.7
1	A	515	LEU	2.7
2	D	196	LEU	2.7
1	C	405	ASP	2.6
1	A	418	ALA	2.6
1	C	432	ASN	2.5
1	A	463	MET	2.5
2	B	273	ARG	2.5
2	B	216	LYS	2.5
2	D	199	TYR	2.5
1	A	381	VAL	2.5
1	C	580	GLY	2.5
2	B	294	ARG	2.5
1	C	482	GLN	2.4
2	B	199	TYR	2.4
1	A	499	VAL	2.4
1	A	494	PRO	2.4
2	D	236	PRO	2.4
1	C	420	LEU	2.4
1	C	388	ASN	2.4
1	A	416	ARG	2.4
2	D	278	ALA	2.4
1	A	404	PHE	2.3
2	B	192	LYS	2.3
2	D	279	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	575	ASN	2.3
2	B	17	TRP	2.3
1	A	429	ASN	2.3
1	A	571	PHE	2.3
1	A	527	LEU	2.3
1	C	550	HIS	2.3
1	C	491	THR	2.2
1	C	223	ASP	2.2
2	D	178	ILE	2.2
1	A	553	LEU	2.2
1	A	549	CYS	2.2
1	A	524	ASP	2.2
1	A	507	ILE	2.2
2	B	147	LYS	2.2
1	A	538	LEU	2.2
1	C	224	PHE	2.2
1	A	449	LEU	2.2
2	D	209	LEU	2.2
1	C	554	PRO	2.1
1	C	490	ASN	2.1
1	C	492	ALA	2.1
1	A	202	ASN	2.1
1	A	557	GLN	2.1
2	D	20	GLU	2.1
1	A	157	MET	2.0
2	D	259	MET	2.0
1	A	69	GLY	2.0
1	C	557	GLN	2.0
2	B	197	GLU	2.0
2	D	203	LYS	2.0
2	B	284	GLY	2.0
1	C	156	ASN	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	A	369	12/13	0.97	0.18	99,110,123,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PHD	C	369	12/13	0.97	0.19	91,94,108,122	0

### 6.3 Carbohydrates

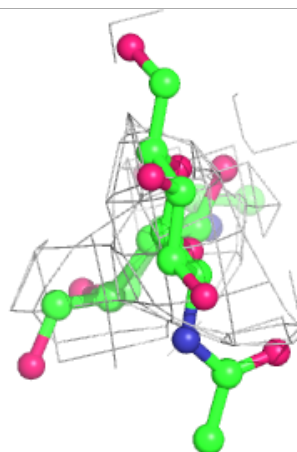
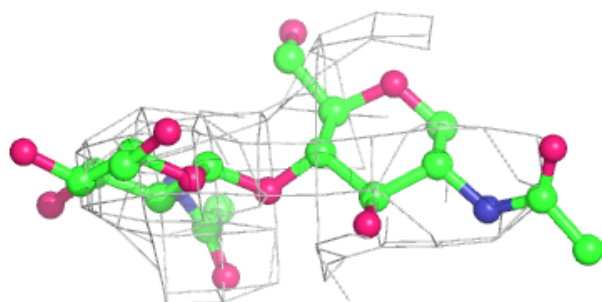
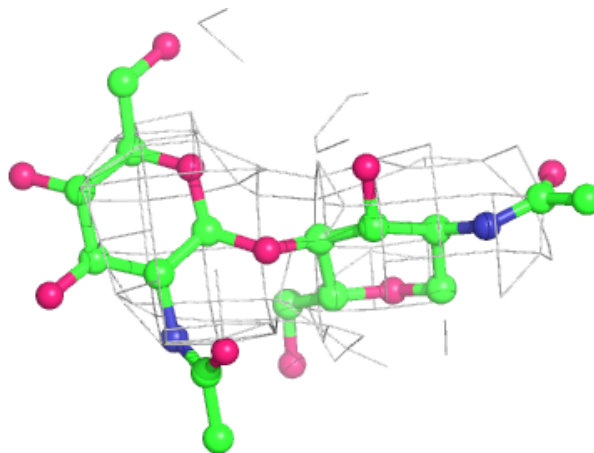
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	H	2	14/15	0.65	0.63	197,218,232,235	0
4	NAG	F	2	14/15	0.70	0.88	178,211,221,224	0
4	NAG	J	2	14/15	0.77	0.82	188,218,227,231	0
4	NAG	I	2	14/15	0.78	0.37	188,225,226,232	0
4	NAG	F	1	14/15	0.79	0.36	166,176,189,208	0
4	NAG	I	1	14/15	0.83	0.21	173,182,210,228	0
4	NAG	H	1	14/15	0.85	0.47	180,186,221,238	0
4	NAG	J	1	14/15	0.91	0.37	174,180,200,217	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.

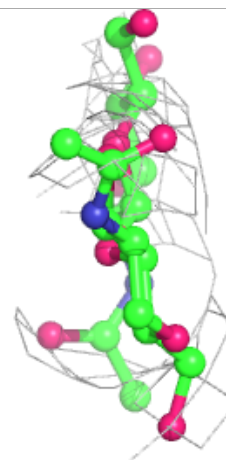
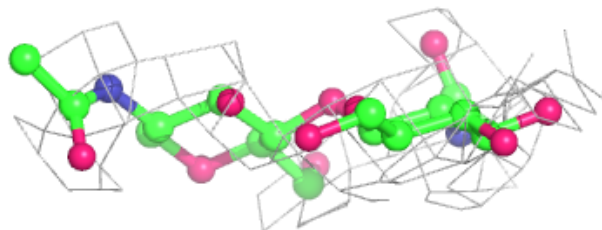
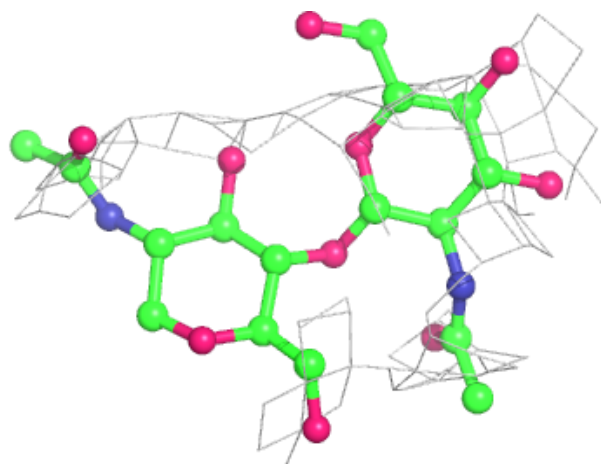
**Electron density around Chain H:**

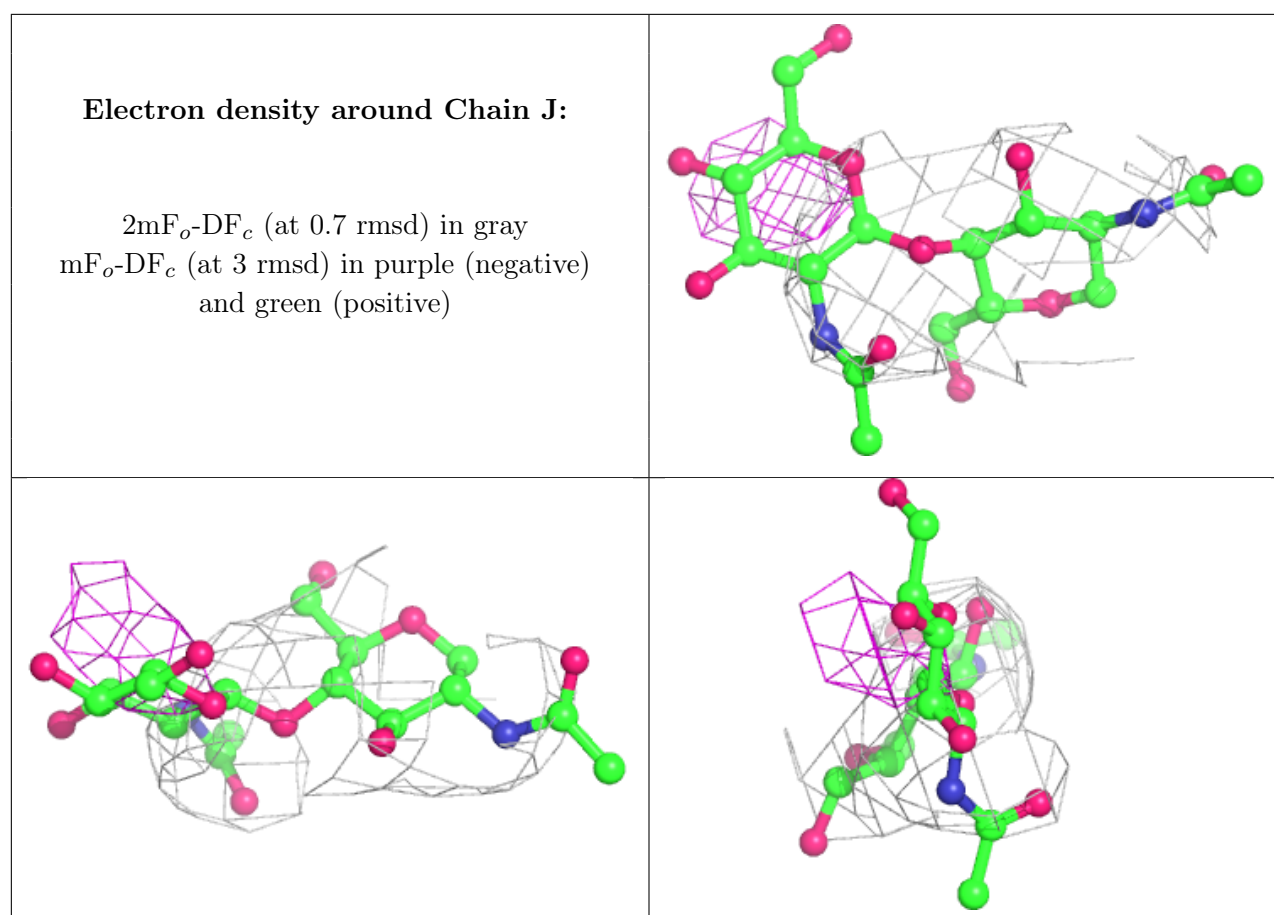
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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(Å <sup>2</sup> )	Q<0.9
8	PCW	A	1107	22/54	0.61	0.60	136,161,228,233	0
10	NAG	D	411	14/15	0.69	0.25	173,184,205,208	0
8	PCW	C	1105	22/54	0.73	0.43	151,168,190,201	0
8	PCW	A	1106	22/54	0.74	0.54	153,179,209,215	0
10	NAG	B	411	14/15	0.79	0.25	157,167,180,183	0
8	PCW	C	1109	22/54	0.79	0.45	121,177,189,206	0
8	PCW	A	1109	22/54	0.80	0.39	110,136,158,166	0
6	NA	A	1102	1/1	0.80	0.39	84,84,84,84	0
8	PCW	D	402	22/54	0.81	0.47	138,196,214,216	0
8	PCW	A	1108	22/54	0.82	0.29	139,178,187,192	0
8	PCW	C	1107	22/54	0.82	0.34	144,158,169,175	0
8	PCW	A	1105	22/54	0.84	0.33	144,172,200,201	0

*Continued on next page...*

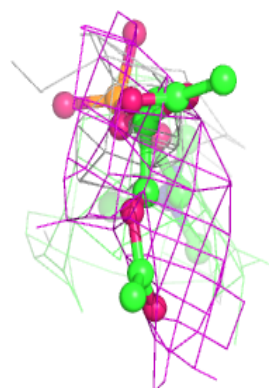
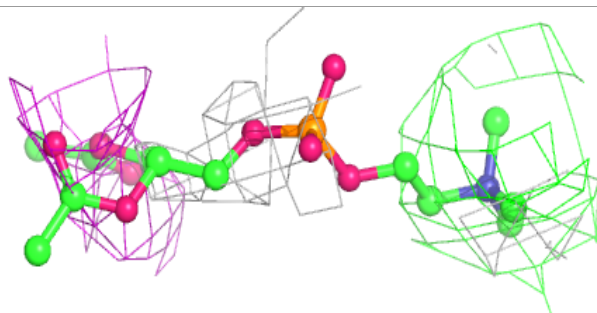
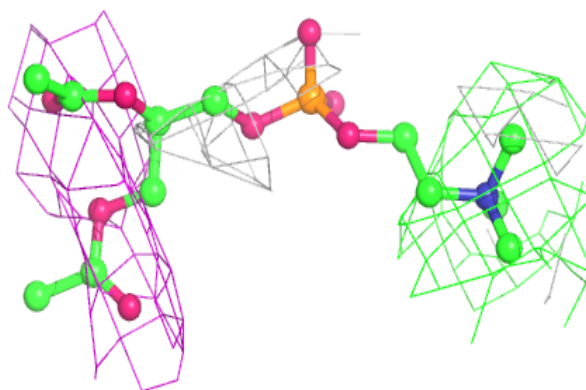
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CLR	A	1104	28/28	0.84	0.57	98,120,142,147	0
8	PCW	C	1106	22/54	0.84	0.38	161,176,204,218	0
7	CLR	A	1111	28/28	0.85	0.40	99,133,144,146	0
8	PCW	C	1108	22/54	0.86	0.27	89,129,169,179	0
7	CLR	D	501	28/28	0.88	0.36	111,140,159,177	0
9	H0C	C	1121	57/57	0.89	0.29	102,121,166,169	0
9	H0C	A	1121	57/57	0.89	0.31	122,141,182,207	0
7	CLR	G	101	28/28	0.91	0.26	77,78,117,130	0
7	CLR	E	101	28/28	0.94	0.25	72,73,98,100	0
6	NA	C	1102	1/1	0.94	0.48	75,75,75,75	0
5	MG	A	1101	1/1	0.97	0.15	136,136,136,136	0
5	MG	C	1103	1/1	0.98	0.32	112,112,112,112	0
5	MG	C	1101	1/1	0.99	0.17	114,114,114,114	0
5	MG	A	1103	1/1	0.99	0.37	136,136,136,136	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.

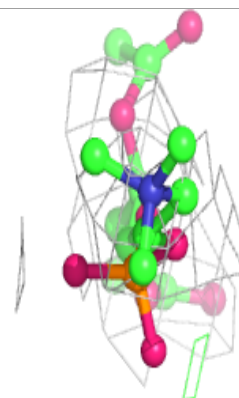
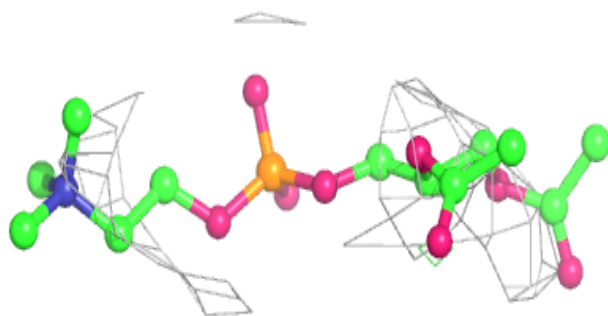
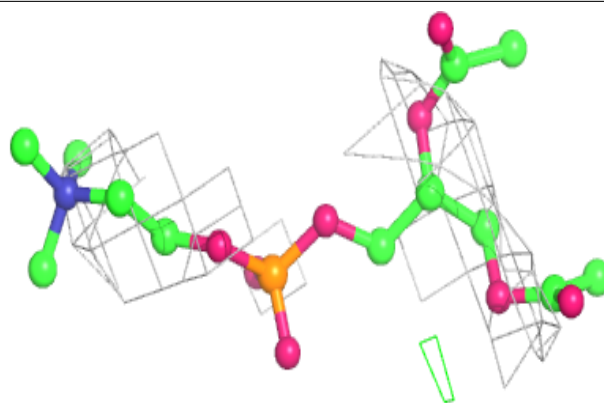
**Electron density around PCW A 1107:**

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)

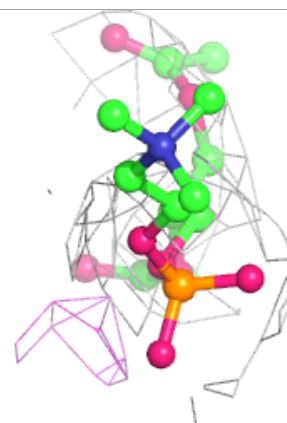
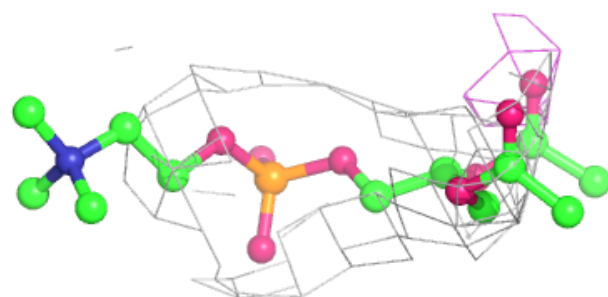
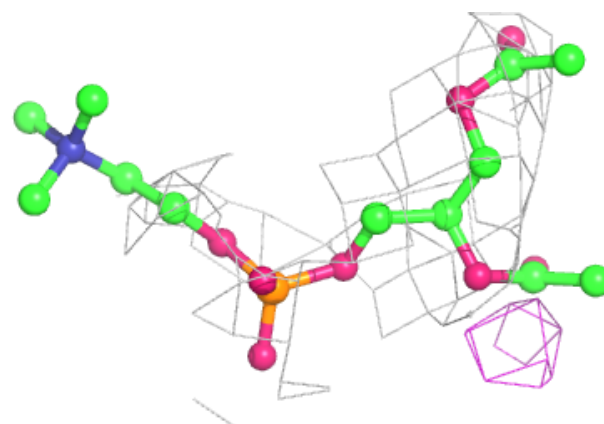


**Electron density around PCW C 1105:**

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

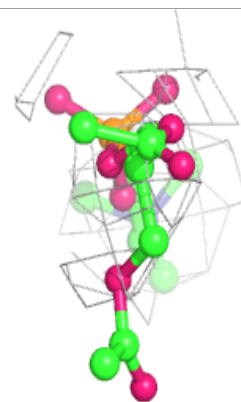
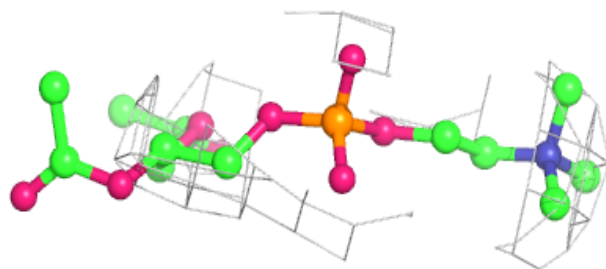
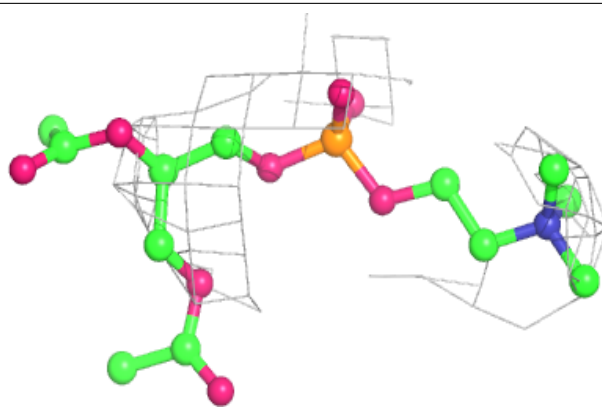
**Electron density around PCW A 1106:**

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

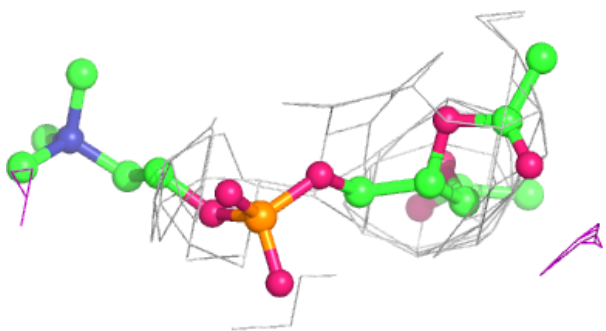
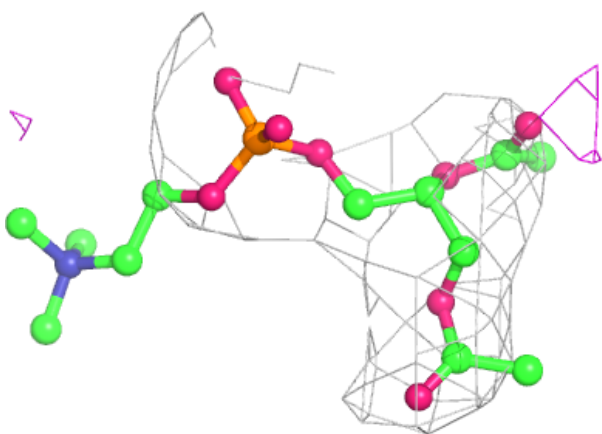


**Electron density around PCW C 1109:**

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

**Electron density around PCW A 1109:**

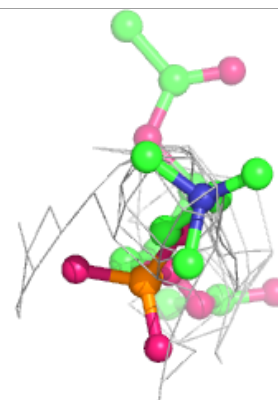
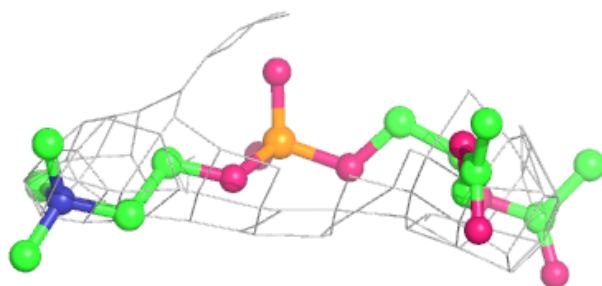
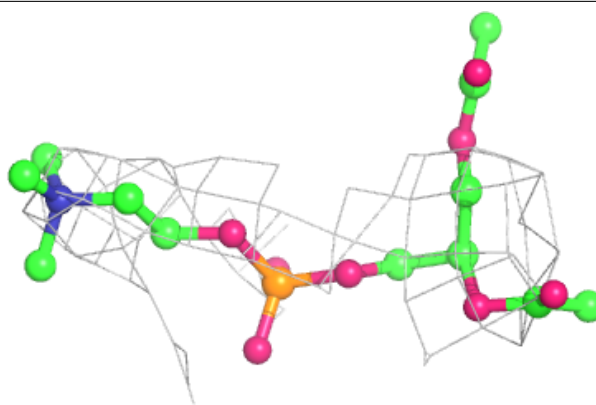
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



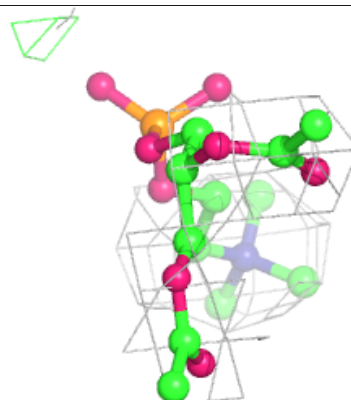
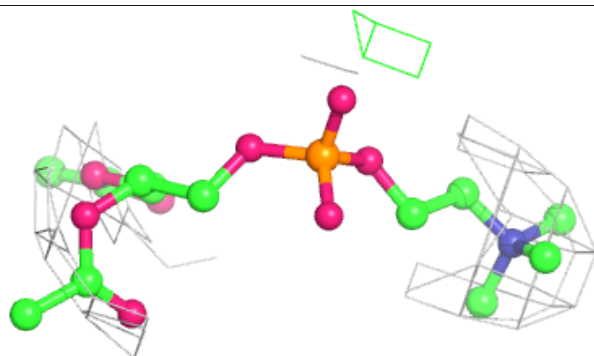
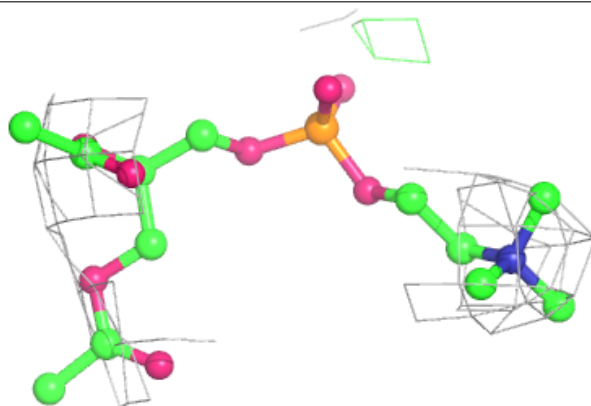


**Electron density around PCW D 402:**

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

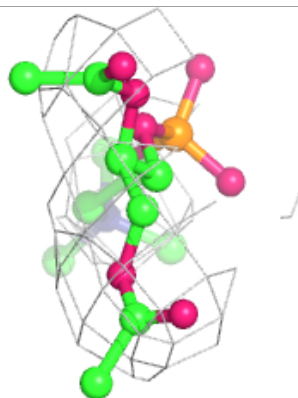
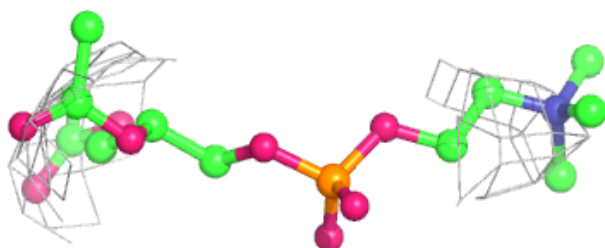
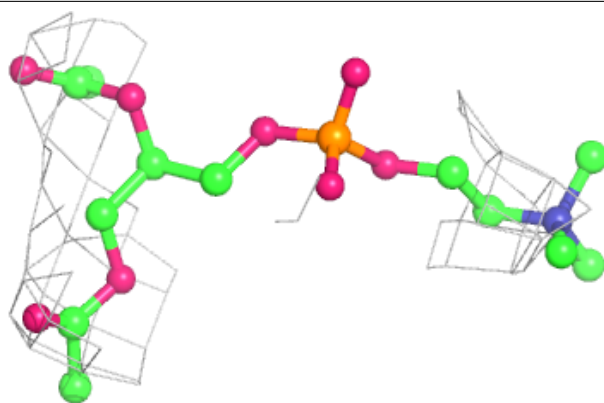
**Electron density around PCW A 1108:**

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

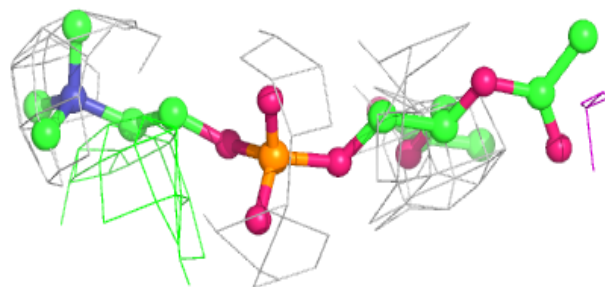
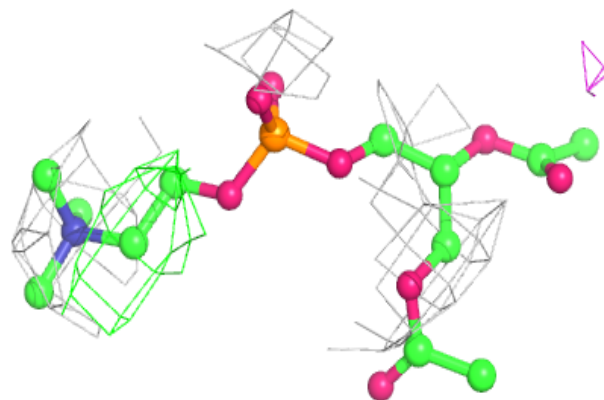


**Electron density around PCW C 1107:**

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

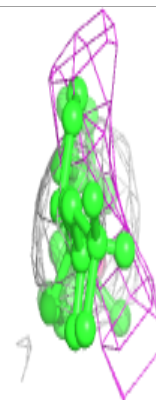
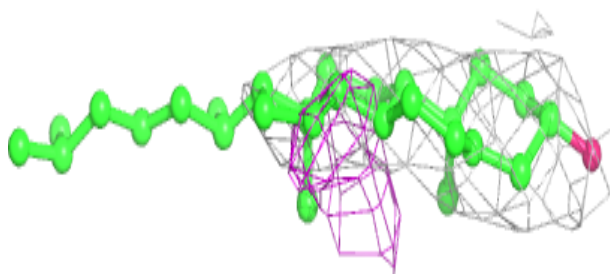
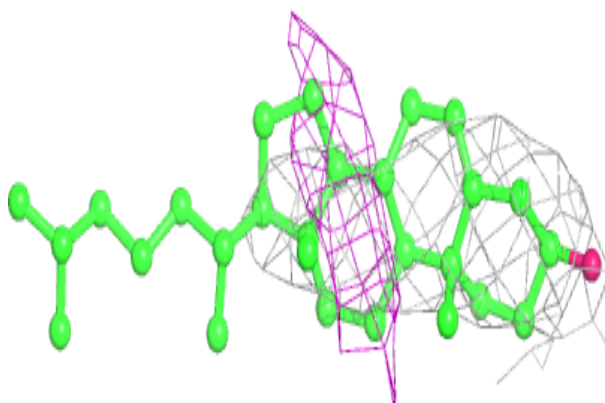
**Electron density around PCW A 1105:**

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

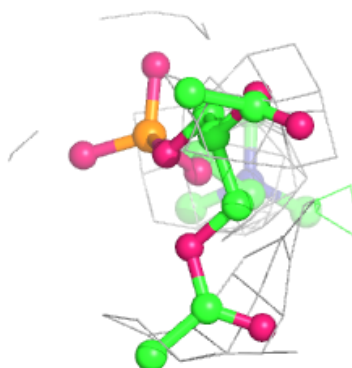
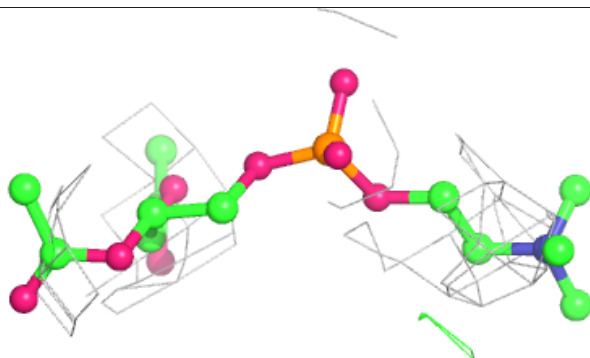
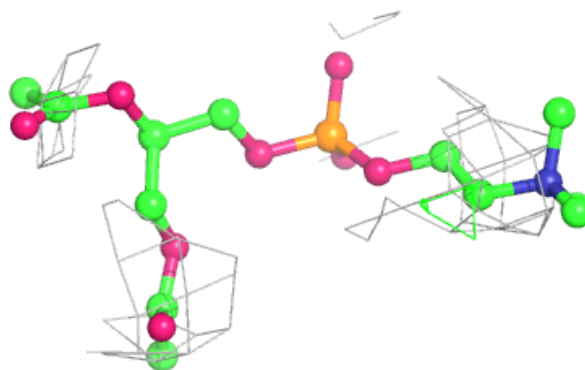


**Electron density around CLR A 1104:**

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

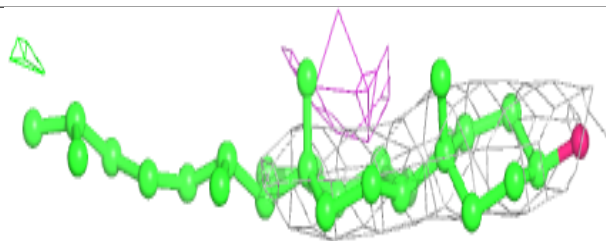
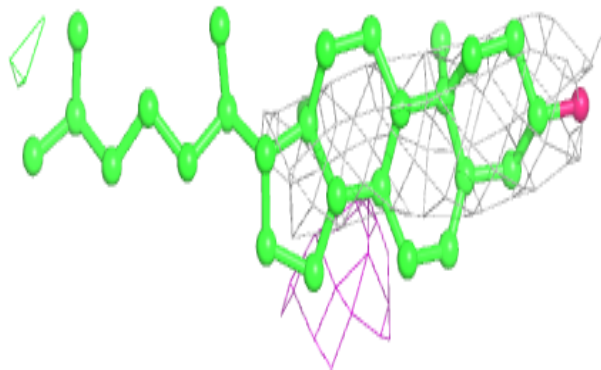
**Electron density around PCW C 1106:**

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

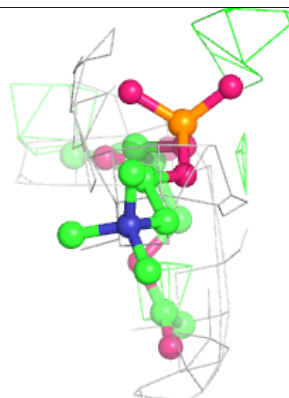
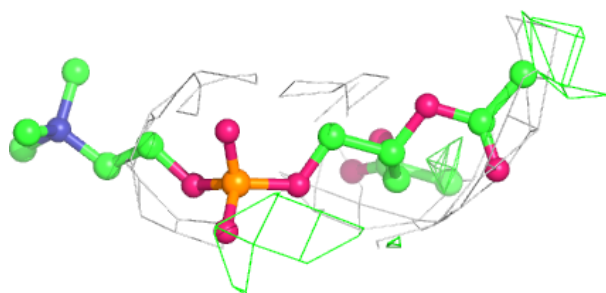
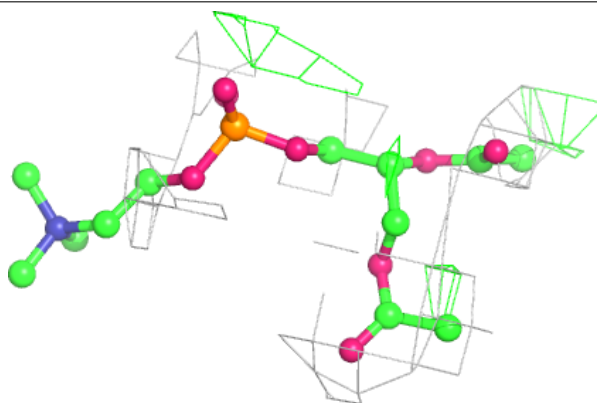


**Electron density around CLR A 1111:**

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

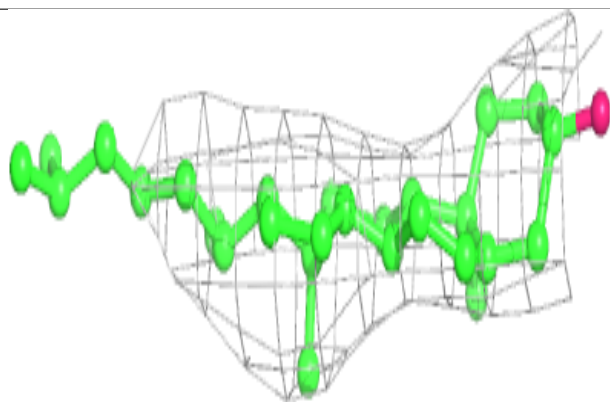
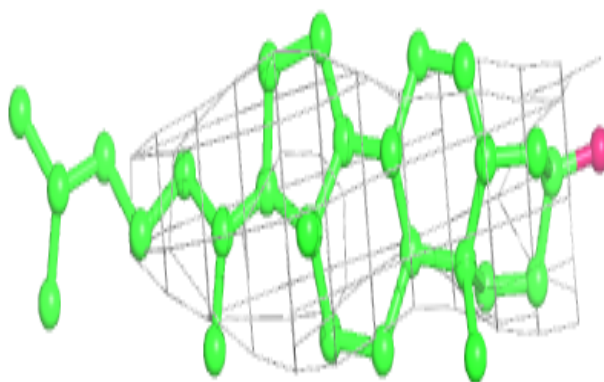
**Electron density around PCW C 1108:**

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

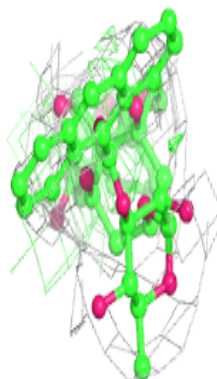
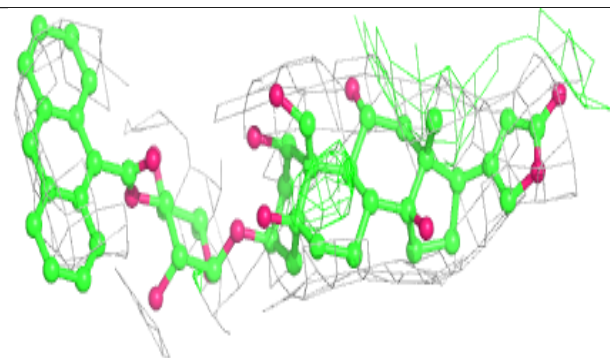
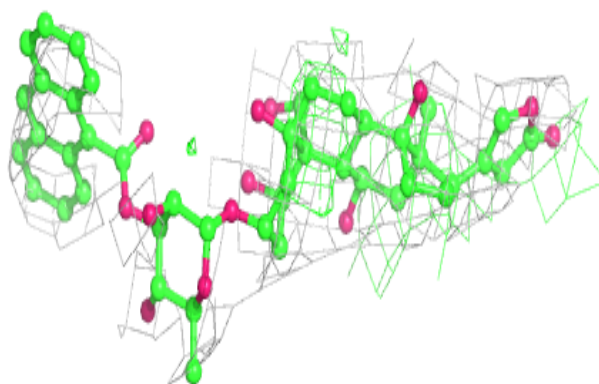


**Electron density around CLR D 501:**

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

**Electron density around H0C C 1121:**

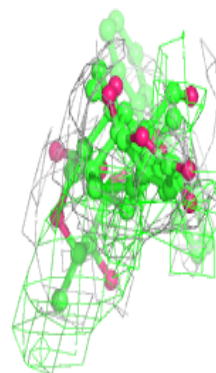
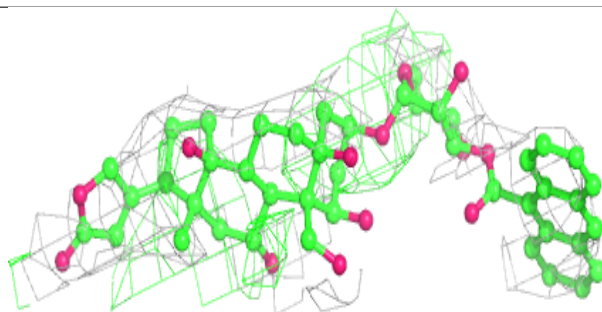
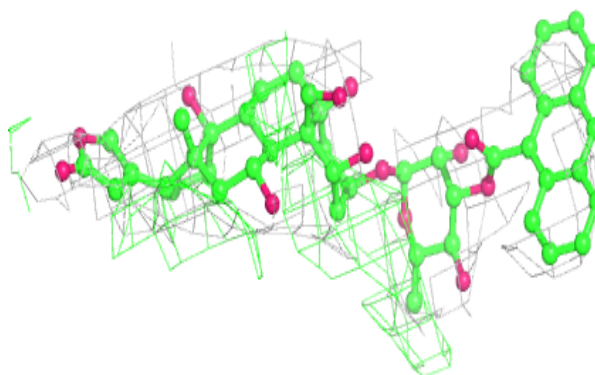
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



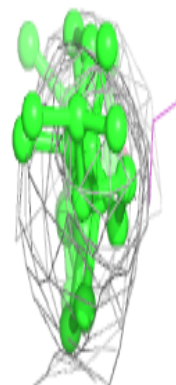
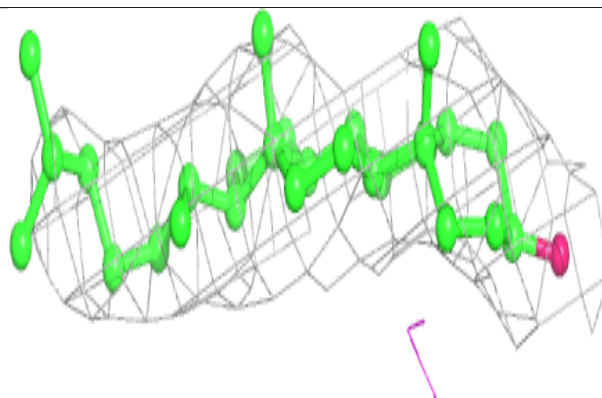
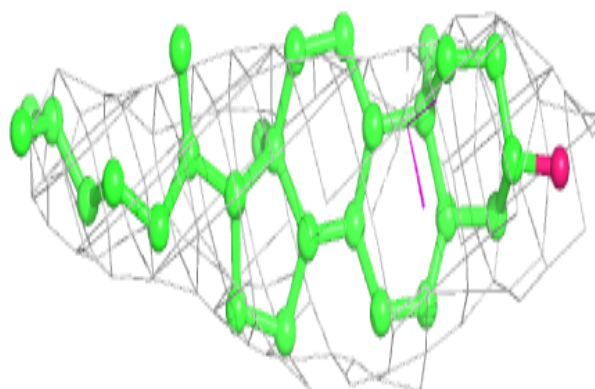


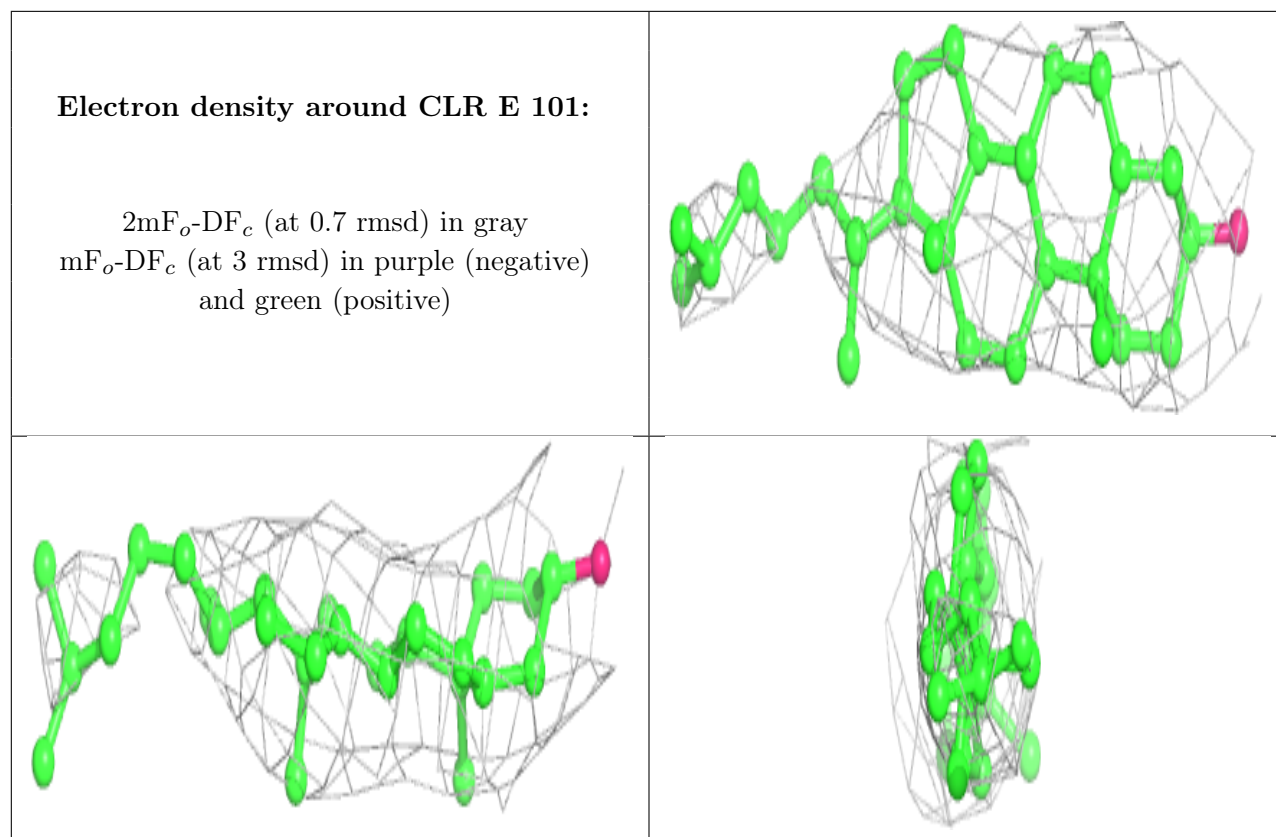
**Electron density around H0C A 1121:**

$2mF_o-DF_c$  (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.