



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2022 – 01:02 AM JST

PDB ID : 7WYS
Title : Crystal structures of Na⁺,K⁺-ATPase in complex with istaroxime
Authors : Ogawa, H.; Cornelius, F.; Kanai, R.; Motoyama, K.; Vilsen, B.; Toyoshima, C.
Deposited on : 2022-02-16
Resolution : 3.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

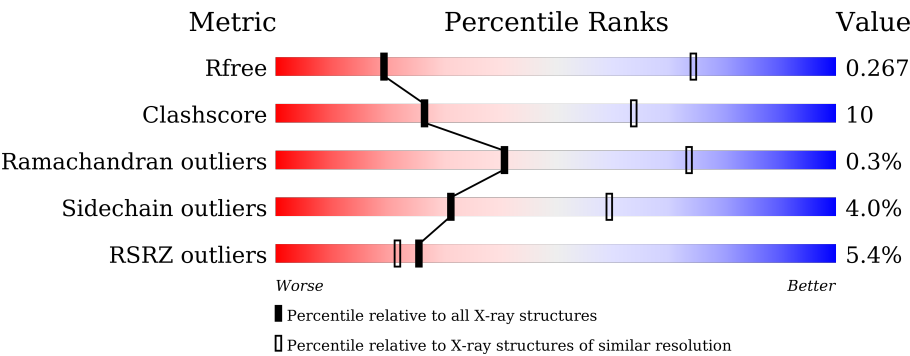
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1016	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>73%24%..</div></div>
1	C	1016	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>72%25%..</div></div>
2	B	303	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>67%27%. .</div></div>
2	D	303	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>63%29%. 6%</div></div>
3	E	65	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>40%9%51%</div></div>
3	G	65	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>38%11%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	H	2	-	-	-	X
4	NAG	J	2	-	-	-	X
7	PCW	A	1106	-	-	-	X
7	PCW	C	1107	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 21286 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 FXYD 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			

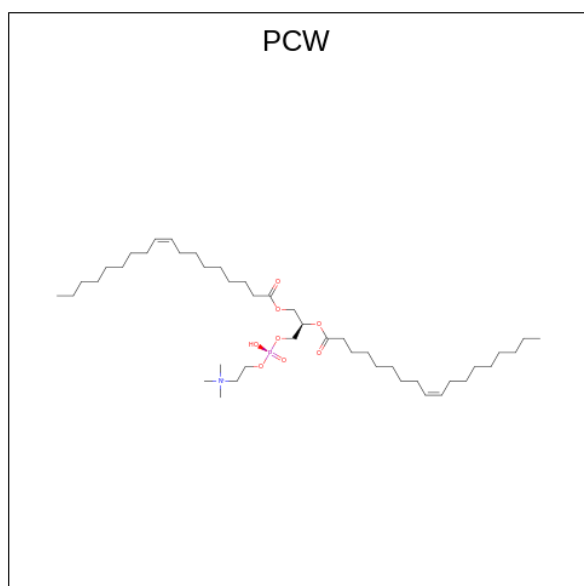
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

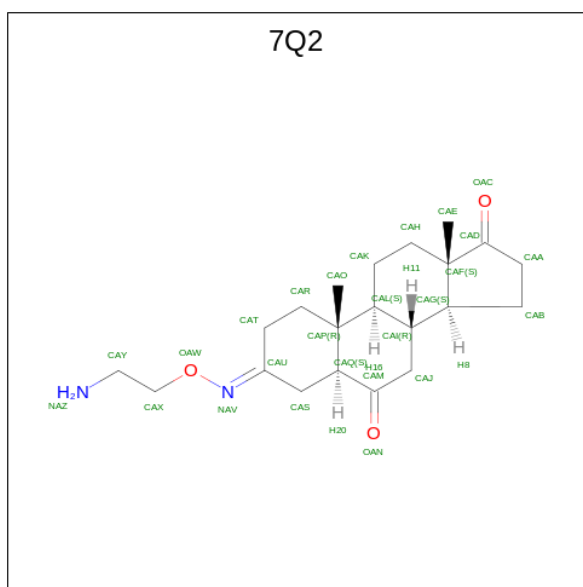
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



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	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 (3E,5S,8R,9S,10R,13S,14S)-3-(2-azanylethoxyimino)-10,13-dimethyl-1,2,4,5,7,8,9,11,12,14,15,16-dodecahydrocyclopenta[a]phenanthrene-6,17-dione (three-letter code: 7Q2) (formula: C₂₁H₃₂N₂O₃) (labeled as "Ligand of Interest" by depositor).



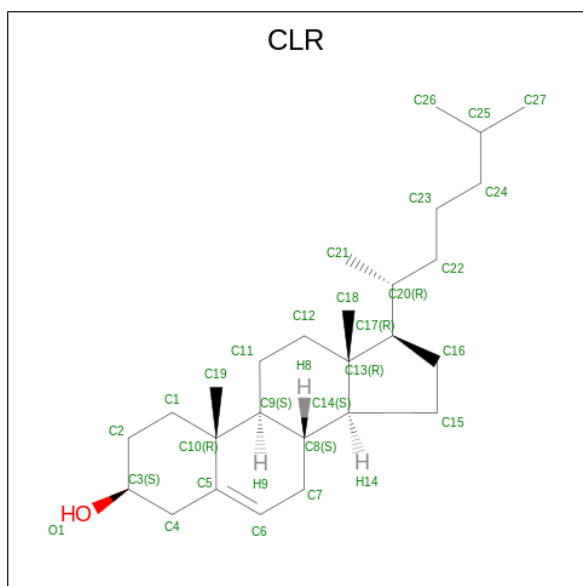
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			26	21	2	3		

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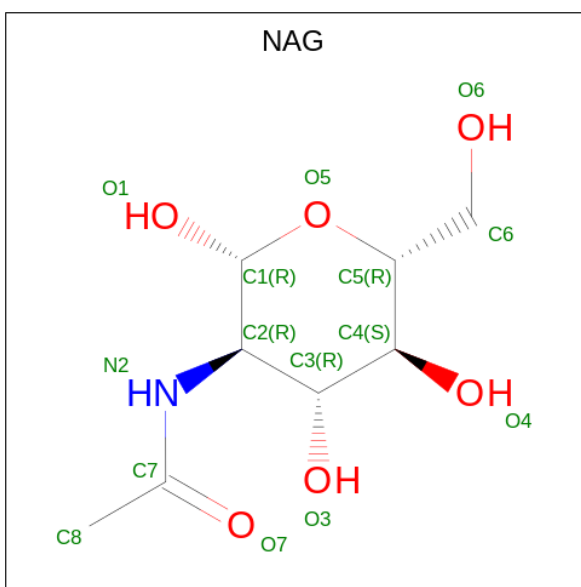
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			26	21	2	3		

- 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		

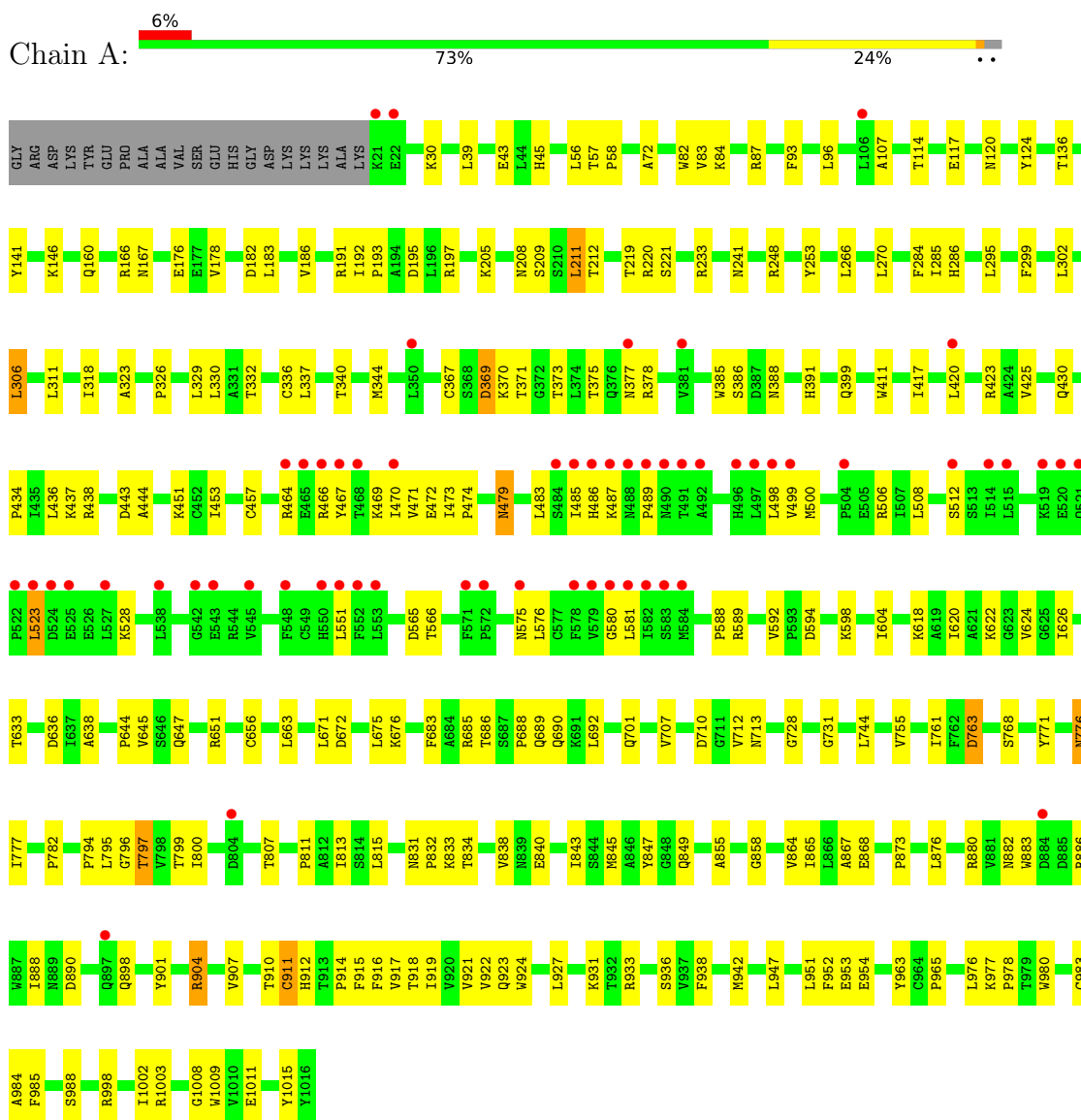
- Molecule 11 is water.

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

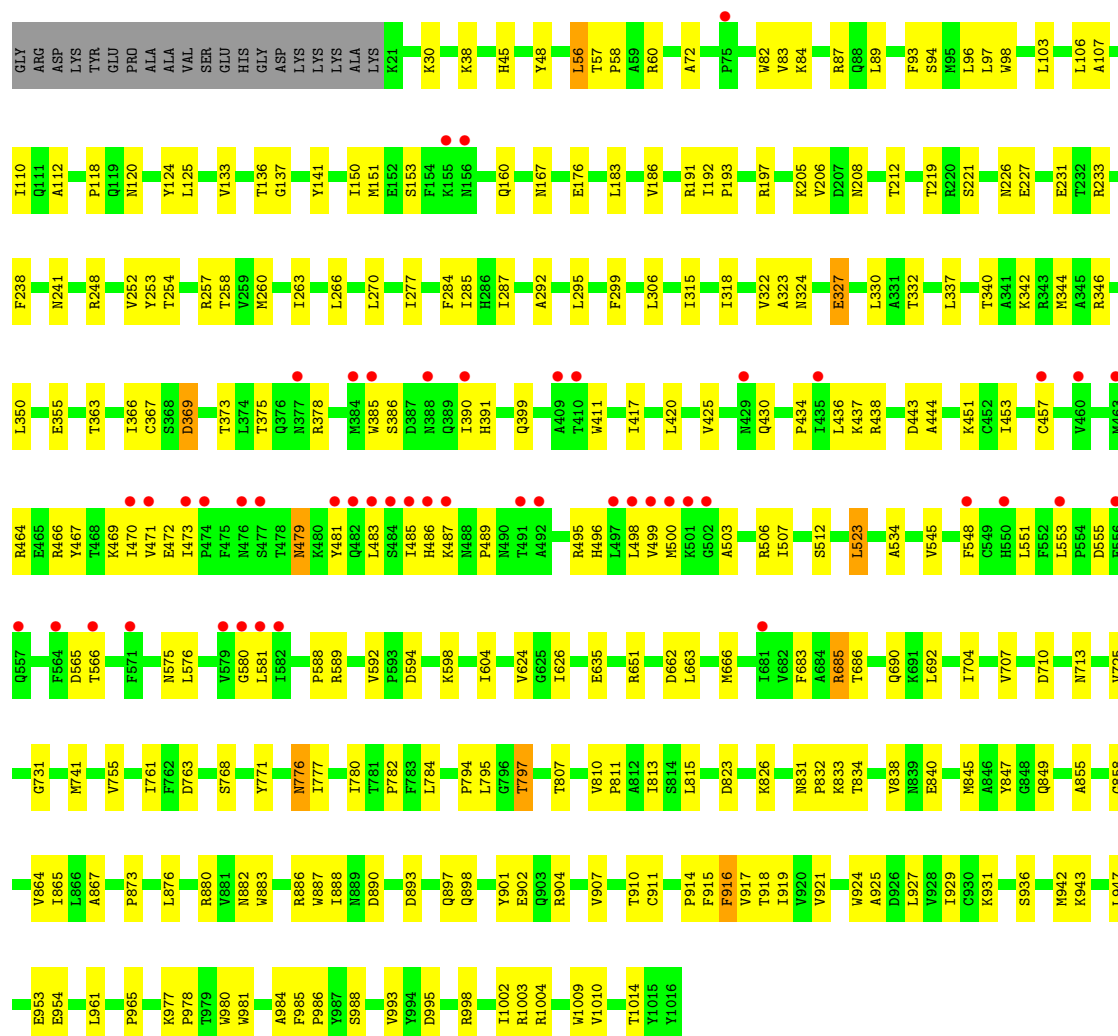
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

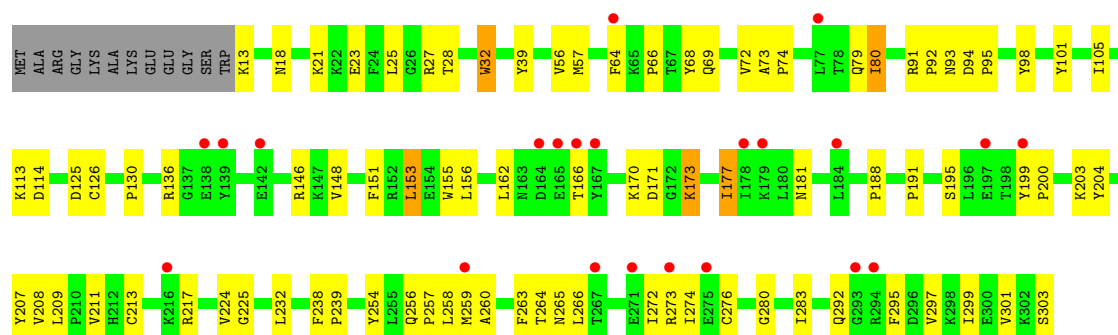


- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1



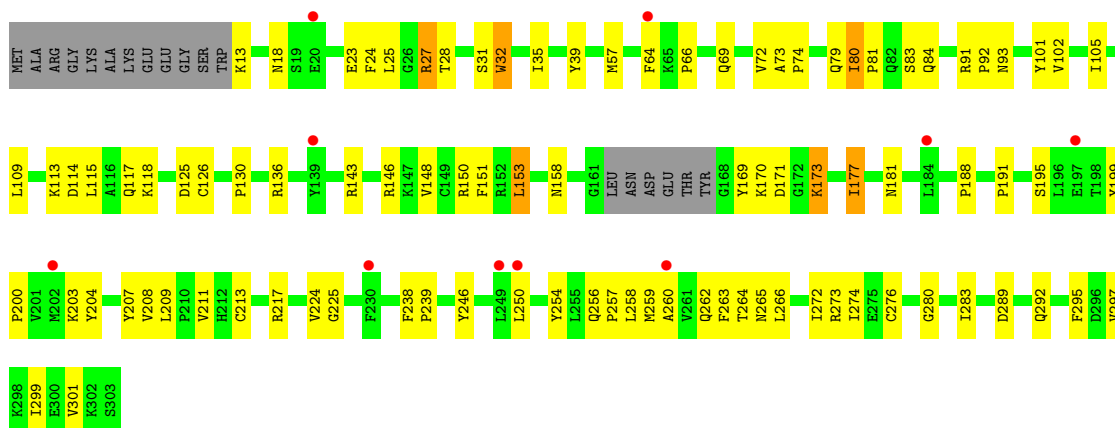


- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

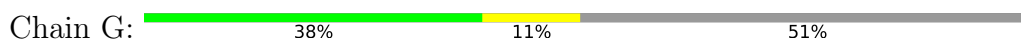


- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

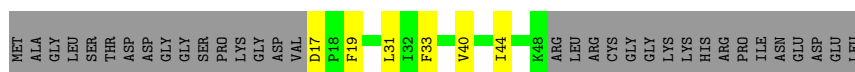




- Molecule 3: FXYP domain-containing ion transport regulator



- Molecule 3: FXYP domain-containing ion transport regulator



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



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



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



- 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, α , β , γ	115.11Å 117.47Å 491.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.98 – 3.71 49.84 – 3.71	Depositor EDS
% Data completeness (in resolution range)	35.4 (15.98-3.71) 36.3 (49.84-3.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.193 , 0.238 0.216 , 0.267	Depositor DCC
R_{free} test set	1325 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	122.0	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 107.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.062 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	21286	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, 7Q2, NAG, MG, NA, PHD, PCW

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	0.33	0/7867	0.57	0/10674
1	C	0.34	0/7867	0.57	0/10674
2	B	0.32	0/2449	0.59	0/3301
2	D	0.32	0/2395	0.60	0/3225
3	E	0.35	0/261	0.54	0/354
3	G	0.33	0/261	0.50	0/354
All	All	0.33	0/21100	0.57	0/28582

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7730	0	7777	153	0
1	C	7730	0	7777	176	0
2	B	2386	0	2361	51	0
2	D	2334	0	2317	60	0
3	E	255	0	259	4	0
3	G	255	0	259	6	0
4	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	0	0
4	I	28	0	25	1	0
4	J	28	0	25	1	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	110	0	90	4	0
7	C	88	0	72	7	0
7	D	22	0	18	0	0
8	A	26	0	0	2	0
8	C	26	0	0	2	0
9	A	28	0	46	2	0
9	B	28	0	46	2	0
9	C	28	0	46	5	0
9	D	28	0	46	2	0
9	E	28	0	46	5	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	1	0
11	C	5	0	0	1	0
All	All	21286	0	21332	440	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 10.

All (440) 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:807:THR:HB	1:C:954:GLU:HG3	1.61	0.82
2:D:80:ILE:HG12	2:D:177:ILE:HG12	1.61	0.82
2:B:80:ILE:HG12	2:B:177:ILE:HG12	1.65	0.79
1:C:84:LYS:HG3	1:C:141:TYR:HE1	1.46	0.79
9:A:1110:CLR:H213	1:C:986:PRO:HB3	1.67	0.77
1:A:807:THR:HB	1:A:954:GLU:HG3	1.69	0.73
1:A:84:LYS:HG3	1:A:141:TYR:HE1	1.52	0.73
1:A:120:ASN:O	1:A:124:TYR:HB2	1.89	0.73
1:C:84:LYS:HG3	1:C:141:TYR:CE1	2.23	0.72
1:C:470:ILE:HD11	1:C:487:LYS:HE2	1.71	0.72
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:C:845:MET:SD	1:C:849:GLN:NE2	2.62	0.71
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.74	0.70
2:D:177:ILE:HA	2:D:260:ALA:HA	1.74	0.70
1:A:845:MET:SD	1:A:849:GLN:NE2	2.64	0.70
1:A:375:THR:HA	1:A:588:PRO:HA	1.74	0.69
2:D:204:TYR:HE1	2:D:207:TYR:HB2	1.56	0.69
2:D:35:ILE:HG21	9:D:403:CLR:H22	1.74	0.69
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.74	0.68
1:A:983:CYS:SG	9:C:1104:CLR:H21	2.34	0.68
1:C:124:TYR:CE2	7:C:1107:PCW:H2	2.29	0.68
1:A:385:TRP:HB3	1:A:581:LEU:H	1.59	0.67
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.76	0.67
1:C:112:ALA:HA	1:C:118:PRO:HG2	1.77	0.67
1:C:901:TYR:HA	1:C:904:ARG:HE	1.59	0.66
1:C:385:TRP:HB3	1:C:581:LEU:H	1.61	0.66
1:C:375:THR:HA	1:C:588:PRO:HA	1.78	0.66
2:D:80:ILE:HD11	2:D:177:ILE:H	1.61	0.66
1:C:120:ASN:O	1:C:124:TYR:HB2	1.96	0.65
2:D:191:PRO:HD3	2:D:280:GLY:HA2	1.77	0.65
1:C:978:PRO:HB3	9:E:101:CLR:H192	1.78	0.64
1:C:183:LEU:HD11	1:C:248:ARG:HB3	1.79	0.64
1:C:160:GLN:HE22	1:C:191:ARG:HD3	1.60	0.64
1:A:512:SER:HA	1:A:523:LEU:HD23	1.79	0.64
1:A:160:GLN:HE22	1:A:191:ARG:HD3	1.63	0.64
1:C:907:VAL:HA	1:C:910:THR:HG22	1.80	0.63
1:C:120:ASN:HB2	1:C:124:TYR:HD1	1.61	0.63
1:A:901:TYR:HA	1:A:904:ARG:HE	1.63	0.63
1:A:183:LEU:HD11	1:A:248:ARG:HB3	1.79	0.62
1:A:96:LEU:HD22	1:A:285:ILE:HG23	1.81	0.62
1:C:434:PRO:HG2	1:C:437:LYS:HB2	1.80	0.62
1:A:907:VAL:HA	1:A:910:THR:HG22	1.82	0.62
1:A:385:TRP:HE3	1:A:580:GLY:HA2	1.65	0.61
1:A:399:GLN:HE21	1:A:436:LEU:HD11	1.65	0.61
1:C:685:ARG:HH11	1:C:685:ARG:HB3	1.65	0.61
1:C:323:ALA:HB1	1:C:780:ILE:HG12	1.82	0.61
2:D:27:ARG:NH1	2:D:31:SER:OG	2.33	0.61
1:A:479:ASN:HA	1:A:506:ARG:HD3	1.83	0.61
1:C:83:VAL:O	1:C:87:ARG:HG2	2.01	0.60
1:C:120:ASN:HB2	1:C:124:TYR:CD1	2.35	0.60
1:C:512:SER:HB3	1:C:575:ASN:HA	1.84	0.60
2:D:102:VAL:HG13	2:D:169:TYR:HD2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:867:ALA:HB2	1:C:873:PRO:HD3	1.84	0.59
1:A:470:ILE:HD11	1:A:487:LYS:HE2	1.85	0.59
1:A:205:LYS:HA	1:A:219:THR:HA	1.84	0.59
2:B:80:ILE:HD11	2:B:177:ILE:H	1.67	0.59
2:D:66:PRO:HG2	2:D:69:GLN:HG2	1.85	0.58
2:B:204:TYR:HE1	2:B:207:TYR:HB2	1.69	0.58
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.85	0.58
1:A:434:PRO:HG2	1:A:437:LYS:HB2	1.85	0.58
1:A:83:VAL:O	1:A:87:ARG:HG2	2.04	0.58
1:A:868:GLU:OE1	9:C:1104:CLR:O1	2.21	0.58
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.86	0.58
1:C:399:GLN:HE21	1:C:436:LEU:HD11	1.69	0.58
1:C:663:LEU:HD22	1:C:690:GLN:HG2	1.86	0.58
1:A:858:GLY:HA2	1:A:918:THR:HG21	1.84	0.57
2:B:136:ARG:O	2:B:146:ARG:NH1	2.38	0.57
2:B:177:ILE:HA	2:B:260:ALA:HA	1.85	0.57
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.70	0.57
1:A:470:ILE:HG22	1:A:471:VAL:HG23	1.87	0.57
1:C:186:VAL:HG11	1:C:192:ILE:HD13	1.88	0.56
1:C:873:PRO:HA	1:C:876:LEU:HD12	1.88	0.56
1:C:858:GLY:HA2	1:C:918:THR:HG21	1.85	0.56
1:A:843:ILE:HG23	1:A:847:TYR:HD2	1.71	0.56
1:C:238:PHE:HD2	1:C:258:THR:HG21	1.70	0.56
1:C:385:TRP:HE3	1:C:580:GLY:HA2	1.71	0.56
2:B:225:GLY:HA3	2:B:265:ASN:HB3	1.87	0.56
1:A:72:ALA:HB2	1:A:176:GLU:HG2	1.88	0.56
1:C:981:TRP:HB3	9:E:101:CLR:H182	1.87	0.55
1:C:124:TYR:HD2	7:C:1107:PCW:O31	1.88	0.55
1:C:683:PHE:HB3	1:C:686:THR:HG21	1.89	0.55
1:C:96:LEU:HD22	1:C:285:ILE:HG23	1.86	0.55
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.89	0.55
2:D:130:PRO:HB3	2:D:239:PRO:HB3	1.88	0.55
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.88	0.55
1:A:211:LEU:HA	1:A:712:VAL:HG22	1.87	0.55
1:A:84:LYS:HG3	1:A:141:TYR:CE1	2.37	0.55
1:A:867:ALA:HB2	1:A:873:PRO:HD3	1.89	0.55
1:C:292:ALA:HB2	1:C:324:ASN:ND2	2.22	0.55
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.89	0.55
1:A:782:PRO:HB3	1:A:794:PRO:HB2	1.89	0.54
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.89	0.54
2:B:56:VAL:HG11	9:C:1104:CLR:H152	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ILE:HB	2:B:105:ILE:HD12	1.89	0.54
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.90	0.54
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.89	0.54
2:D:225:GLY:HA3	2:D:265:ASN:HB3	1.90	0.54
1:A:483:LEU:HB3	1:A:500:MET:HG3	1.89	0.54
1:C:72:ALA:HB2	1:C:176:GLU:HG2	1.90	0.54
1:C:284:PHE:HD1	1:C:838:VAL:HG21	1.72	0.54
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.90	0.54
1:C:337:LEU:HA	1:C:761:ILE:HD11	1.89	0.54
1:A:39:LEU:HD22	1:A:43:GLU:HG2	1.89	0.53
1:A:467:TYR:HB3	1:A:486:HIS:HB3	1.90	0.53
2:B:217:ARG:HH12	2:B:273:ARG:HD2	1.72	0.53
2:D:217:ARG:HH12	2:D:273:ARG:HD2	1.73	0.53
1:C:208:ASN:HB3	1:C:212:THR:HG22	1.90	0.53
1:C:479:ASN:HA	1:C:506:ARG:HD3	1.90	0.53
1:A:332:THR:HA	1:A:813:ILE:HD11	1.91	0.53
1:A:512:SER:HB3	1:A:575:ASN:HA	1.90	0.53
1:A:907:VAL:O	1:A:911:CYS:HB2	2.08	0.53
2:B:66:PRO:HG2	2:B:69:GLN:HG2	1.91	0.53
1:C:136:THR:HG21	1:C:330:LEU:HG	1.89	0.53
1:A:663:LEU:HD22	1:A:690:GLN:HG2	1.91	0.53
1:C:469:LYS:HD3	1:C:472:GLU:HB3	1.90	0.53
1:A:186:VAL:HG11	1:A:192:ILE:HD13	1.90	0.53
2:B:27:ARG:HG3	2:B:32:TRP:CD1	2.44	0.53
1:C:103:LEU:HB3	1:C:318:ILE:HG23	1.91	0.53
1:C:594:ASP:O	1:C:598:LYS:HG2	2.08	0.53
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.44	0.53
1:A:965:PRO:HD3	3:G:31:LEU:HD11	1.91	0.53
2:B:92:PRO:HG3	2:B:301:VAL:HG12	1.91	0.53
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.43	0.52
1:C:58:PRO:HD3	1:C:167:ASN:HB2	1.91	0.52
1:C:292:ALA:HB2	1:C:324:ASN:HD22	1.73	0.52
1:C:512:SER:HA	1:C:523:LEU:HD23	1.90	0.52
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.90	0.52
2:B:156:LEU:HD13	2:B:260:ALA:HB2	1.92	0.52
2:B:276:CYS:HB2	2:B:295:PHE:HD2	1.74	0.52
1:C:470:ILE:HB	1:C:485:ILE:HG23	1.90	0.52
1:C:840:GLU:OE2	2:D:27:ARG:NH2	2.37	0.52
1:C:221:SER:H	1:C:233:ARG:HB3	1.75	0.52
2:D:91:ARG:HG2	2:D:93:ASN:H	1.75	0.52
2:D:276:CYS:HB2	2:D:295:PHE:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:LYS:HE2	1:A:622:LYS:HE3	1.92	0.52
1:C:378:ARG:HD2	1:C:451:LYS:HZ2	1.75	0.52
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.45	0.52
2:D:224:VAL:HG22	2:D:272:ILE:HD12	1.92	0.52
1:A:284:PHE:HD1	1:A:838:VAL:HG21	1.74	0.51
1:A:594:ASP:O	1:A:598:LYS:HG2	2.09	0.51
1:C:483:LEU:HD13	1:C:498:LEU:HD11	1.93	0.51
1:C:589:ARG:HB2	1:C:592:VAL:HG23	1.92	0.51
2:D:213:CYS:HA	2:D:276:CYS:HA	1.92	0.51
2:D:266:LEU:HD22	2:D:272:ILE:HD11	1.91	0.51
2:B:39:TYR:CG	9:B:402:CLR:H191	2.44	0.51
1:C:323:ALA:HB2	8:C:1109:7Q2:OAC	2.10	0.51
1:C:710:ASP:HB2	1:C:731:GLY:HA2	1.93	0.51
1:A:865:ILE:HD12	1:A:914:PRO:HG3	1.92	0.51
1:A:453:ILE:HG23	1:A:457:CYS:HB3	1.92	0.51
2:D:18:ASN:HA	2:D:23:GLU:O	2.11	0.51
1:C:782:PRO:HB3	1:C:794:PRO:HB2	1.92	0.51
1:C:470:ILE:HG22	1:C:471:VAL:HG23	1.93	0.50
2:B:91:ARG:HG2	2:B:93:ASN:H	1.75	0.50
2:B:173:LYS:HG3	2:B:264:THR:O	2.12	0.50
1:A:980:TRP:HA	1:A:983:CYS:SG	2.52	0.50
1:C:385:TRP:O	1:C:580:GLY:HA3	2.12	0.50
2:D:27:ARG:HG3	2:D:32:TRP:CD1	2.46	0.50
1:A:93:PHE:HA	1:A:285:ILE:HD11	1.94	0.50
1:C:887:TRP:NE1	2:D:84:GLN:O	2.45	0.50
2:D:80:ILE:HB	2:D:105:ILE:HD12	1.92	0.50
2:B:224:VAL:HG21	2:B:274:ILE:HD11	1.93	0.50
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.47	0.50
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.76	0.50
1:A:370:LYS:HZ2	1:A:620:ILE:HG13	1.77	0.49
1:C:977:LYS:HD2	1:C:980:TRP:CZ2	2.47	0.49
1:C:993:VAL:HG21	9:C:1104:CLR:H272	1.93	0.49
1:A:430:GLN:HG3	1:A:438:ARG:HB2	1.94	0.49
2:B:101:TYR:O	2:B:105:ILE:HG12	2.12	0.49
2:B:280:GLY:HA3	2:B:283:ILE:HD13	1.94	0.49
1:A:469:LYS:HD3	1:A:472:GLU:HB3	1.93	0.49
1:C:205:LYS:HA	1:C:219:THR:HA	1.93	0.49
1:C:420:LEU:HD23	1:C:464:ARG:HA	1.95	0.49
1:A:683:PHE:HB3	1:A:686:THR:HG21	1.94	0.49
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.94	0.49
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.95	0.49
3:E:40:VAL:O	3:E:44:ILE:HG12	2.12	0.49
2:B:266:LEU:HD22	2:B:272:ILE:HD11	1.94	0.49
1:C:936:SER:HB2	1:C:1003:ARG:NH2	2.28	0.49
1:A:888:ILE:O	1:A:904:ARG:NH2	2.45	0.49
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.94	0.49
1:A:84:LYS:HA	1:A:87:ARG:CG	2.43	0.48
1:C:890:ASP:N	1:C:890:ASP:OD1	2.46	0.48
1:C:918:THR:HG23	1:C:984:ALA:HB2	1.95	0.48
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.94	0.48
2:D:151:PHE:HE2	2:D:258:LEU:HB2	1.78	0.48
2:B:213:CYS:HA	2:B:276:CYS:HA	1.94	0.48
2:D:101:TYR:O	2:D:105:ILE:HG12	2.12	0.48
1:A:978:PRO:HB3	9:G:101:CLR:H192	1.95	0.48
2:B:191:PRO:HD3	2:B:280:GLY:HA2	1.95	0.48
1:A:385:TRP:O	1:A:580:GLY:HA3	2.14	0.48
1:C:942:MET:HE1	1:C:947:LEU:HD22	1.96	0.48
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.48	0.48
1:A:831:ASN:HB3	1:A:834:THR:HB	1.95	0.48
1:C:430:GLN:HG3	1:C:438:ARG:HB2	1.95	0.48
1:C:831:ASN:HB3	1:C:834:THR:HB	1.96	0.48
2:B:92:PRO:HD2	2:B:303:SER:HA	1.95	0.48
1:C:287:ILE:HD12	7:C:1105:PCW:O31	2.13	0.48
1:C:332:THR:HA	1:C:813:ILE:HD11	1.94	0.48
1:C:473:ILE:HB	1:C:483:LEU:HG	1.95	0.48
1:C:965:PRO:HD3	3:E:31:LEU:HD11	1.95	0.48
1:A:417:ILE:HG12	1:A:499:VAL:HG12	1.95	0.48
1:A:977:LYS:HD2	1:A:980:TRP:CZ2	2.49	0.48
1:A:420:LEU:HD23	1:A:464:ARG:HA	1.94	0.48
2:B:39:TYR:CD2	9:B:402:CLR:H191	2.49	0.48
3:G:33:PHE:CZ	9:G:101:CLR:H151	2.49	0.47
2:D:136:ARG:O	2:D:146:ARG:NH1	2.47	0.47
1:C:385:TRP:HD1	1:C:390:ILE:HD13	1.79	0.47
1:A:378:ARG:HD2	1:A:451:LYS:HZ2	1.79	0.47
3:G:45:ILE:H	3:G:45:ILE:HG13	1.54	0.47
2:D:39:TYR:CZ	9:D:403:CLR:H191	2.49	0.47
1:A:942:MET:HE1	1:A:947:LEU:HD22	1.96	0.47
1:C:106:LEU:O	1:C:110:ILE:HG12	2.14	0.47
1:C:367:CYS:HB2	1:C:707:VAL:HG22	1.97	0.47
1:A:323:ALA:HB2	8:A:1109:7Q2:OAC	2.14	0.47
2:D:92:PRO:HG3	2:D:301:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:SER:OG	1:A:377:ASN:ND2	2.48	0.47
1:A:367:CYS:HB2	1:A:707:VAL:HG22	1.97	0.47
1:A:473:ILE:HB	1:A:483:LEU:HG	1.96	0.47
1:A:777:ILE:HG22	1:A:855:ALA:HB2	1.96	0.47
1:A:890:ASP:OD1	1:A:890:ASP:N	2.48	0.47
1:A:998:ARG:O	1:A:1002:ILE:HG13	2.15	0.47
7:A:1108:PCW:H31	1:C:978:PRO:HB2	1.95	0.47
2:D:153:LEU:H	2:D:153:LEU:HD12	1.80	0.47
2:D:263:PHE:HB3	2:D:266:LEU:HD21	1.96	0.47
1:A:332:THR:O	1:A:336:CYS:HB2	2.15	0.47
2:D:280:GLY:HA3	2:D:283:ILE:HD13	1.95	0.47
1:A:633:THR:H	1:A:636:ASP:HB2	1.80	0.47
1:A:795:LEU:HD13	1:A:915:PHE:HB3	1.96	0.47
1:A:936:SER:HB2	1:A:1003:ARG:NH2	2.28	0.47
2:B:263:PHE:HB3	2:B:266:LEU:HD21	1.97	0.47
1:C:93:PHE:HA	1:C:285:ILE:HD11	1.95	0.47
1:C:124:TYR:CD2	7:C:1107:PCW:O31	2.67	0.46
1:C:915:PHE:O	1:C:919:ILE:HG12	2.16	0.46
2:D:224:VAL:HG21	2:D:274:ILE:HD11	1.96	0.46
1:A:136:THR:HG21	1:A:330:LEU:HG	1.97	0.46
1:A:483:LEU:HD13	1:A:498:LEU:HD11	1.97	0.46
3:G:39:ILE:O	3:G:43:ILE:HG12	2.16	0.46
1:C:832:PRO:HG2	1:C:833:LYS:HD2	1.97	0.46
1:C:888:ILE:O	1:C:904:ARG:NH2	2.47	0.46
1:C:998:ARG:O	1:C:1002:ILE:HG13	2.15	0.46
1:A:221:SER:H	1:A:233:ARG:HB3	1.81	0.46
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.97	0.46
1:A:370:LYS:NZ	1:A:620:ILE:HG13	2.30	0.46
2:B:18:ASN:HA	2:B:23:GLU:O	2.16	0.46
1:C:883:TRP:HA	1:C:904:ARG:HH11	1.81	0.46
1:C:898:GLN:NE2	2:D:181:ASN:HA	2.31	0.46
1:C:917:VAL:O	1:C:921:VAL:HG23	2.16	0.46
1:A:183:LEU:HD21	1:A:248:ARG:HH21	1.80	0.46
1:C:390:ILE:HD11	1:C:534:ALA:HB1	1.98	0.46
1:C:776:ASN:HB3	1:C:847:TYR:HE1	1.80	0.46
1:A:286:HIS:ND1	7:A:1107:PCW:O2P	2.45	0.46
2:B:130:PRO:HB3	2:B:239:PRO:HB3	1.97	0.46
1:C:254:THR:HG23	1:C:257:ARG:HH21	1.80	0.45
1:C:453:ILE:HG23	1:C:457:CYS:HB3	1.97	0.45
2:D:204:TYR:O	2:D:208:VAL:HG12	2.16	0.45
1:A:191:ARG:HA	1:A:241:ASN:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ARG:HG2	1:A:489:PRO:HG3	1.98	0.45
1:C:110:ILE:HB	1:C:315:ILE:HD11	1.97	0.45
1:C:725:VAL:HG13	1:C:741:MET:HE3	1.98	0.45
1:A:369:PHD:O	1:A:373:THR:HB	2.16	0.45
2:D:24:PHE:N	2:D:27:ARG:O	2.27	0.45
2:D:80:ILE:HD12	2:D:105:ILE:HD12	1.99	0.45
1:A:146:LYS:NZ	7:A:1104:PCW:H42	2.32	0.45
1:C:479:ASN:O	1:C:481:TYR:HD1	2.00	0.45
1:C:797:THR:HG23	8:C:1109:7Q2:CAB	2.46	0.45
2:D:115:LEU:HD13	2:D:118:LYS:HD2	1.97	0.45
1:A:927:LEU:HG	1:A:947:LEU:HD21	1.98	0.45
1:A:938:PHE:CE2	9:A:1110:CLR:H191	2.52	0.45
1:C:886:ARG:HG3	1:C:901:TYR:CE2	2.52	0.45
2:D:173:LYS:HG3	2:D:264:THR:O	2.17	0.45
1:A:30:LYS:HE2	1:A:692:LEU:HD21	1.98	0.45
1:C:1004:ARG:HD2	7:C:1106:PCW:O2P	2.17	0.45
1:A:166:ARG:HH22	1:A:178:VAL:HA	1.82	0.45
1:A:883:TRP:HA	1:A:904:ARG:HH11	1.82	0.45
1:C:503:ALA:O	1:C:507:ILE:HG12	2.15	0.45
1:C:882:ASN:O	1:C:904:ARG:NH1	2.50	0.45
1:A:763:ASP:OD2	1:A:933:ARG:NH1	2.50	0.44
1:C:97:LEU:HD21	1:C:327:GLU:HA	2.00	0.44
1:A:977:LYS:HD2	1:A:980:TRP:HZ2	1.81	0.44
1:C:776:ASN:ND2	11:C:1202:HOH:O	2.47	0.44
1:A:918:THR:HG23	1:A:984:ALA:HB2	1.99	0.44
2:B:130:PRO:HD3	2:B:232:LEU:HD12	2.00	0.44
2:B:151:PHE:HE2	2:B:258:LEU:HB2	1.82	0.44
1:C:466:ARG:HG2	1:C:489:PRO:HG3	2.00	0.44
1:C:467:TYR:HB3	1:C:486:HIS:HB3	1.99	0.44
1:C:483:LEU:HB3	1:C:500:MET:HG3	1.99	0.44
1:A:220:ARG:HA	1:A:233:ARG:HB3	2.00	0.44
1:C:363:THR:HA	1:C:704:ILE:HB	2.00	0.44
2:D:211:VAL:HG11	2:D:259:MET:HE1	2.00	0.44
1:A:963:TYR:CD2	3:G:30:GLY:HA3	2.52	0.44
1:C:929:ILE:HB	1:C:995:ASP:OD2	2.18	0.44
1:C:977:LYS:HD2	1:C:980:TRP:HZ2	1.83	0.44
1:A:710:ASP:HB2	1:A:731:GLY:HA2	1.98	0.44
1:C:125:LEU:HD21	1:C:322:VAL:HG11	1.99	0.44
1:C:369:PHD:O	1:C:373:THR:HB	2.17	0.44
2:D:143:ARG:HD2	2:D:146:ARG:NH1	2.33	0.44
1:A:58:PRO:HD3	1:A:167:ASN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:O	1:A:299:PHE:HB2	2.18	0.44
1:A:302:LEU:O	1:A:306:LEU:HG	2.18	0.44
1:A:638:ALA:HB2	1:A:645:VAL:HA	2.00	0.44
2:B:204:TYR:O	2:B:208:VAL:HG12	2.17	0.44
1:C:150:ILE:HG23	1:C:151:MET:HE2	1.99	0.44
2:D:27:ARG:HG3	2:D:32:TRP:HD1	1.83	0.44
1:A:672:ASP:HB3	1:A:676:LYS:HE3	2.00	0.43
1:A:832:PRO:HG2	1:A:833:LYS:HD2	1.98	0.43
1:A:898:GLN:NE2	2:B:181:ASN:HA	2.33	0.43
1:C:94:SER:HB3	1:C:133:VAL:HG13	1.99	0.43
2:D:74:PRO:HG2	2:D:292:GLN:OE1	2.18	0.43
1:A:470:ILE:HB	1:A:485:ILE:HG23	2.00	0.43
1:A:369:PHD:OP1	1:A:371:THR:N	2.50	0.43
1:A:644:PRO:HD2	1:A:647:GLN:NE2	2.33	0.43
1:C:902:GLU:HB2	2:D:289:ASP:OD2	2.19	0.43
2:B:211:VAL:HG11	2:B:259:MET:HE1	2.01	0.43
1:C:252:VAL:HG12	1:C:253:TYR:CD1	2.54	0.43
1:A:84:LYS:HA	1:A:87:ARG:HG3	2.00	0.43
1:A:195:ASP:HB2	1:A:253:TYR:HB2	2.00	0.43
1:A:917:VAL:O	1:A:921:VAL:HG23	2.19	0.43
1:C:780:ILE:HG22	1:C:784:LEU:HG	2.00	0.43
1:C:815:LEU:HD12	1:C:815:LEU:HA	1.82	0.43
1:C:927:LEU:HG	1:C:947:LEU:HD21	2.00	0.43
1:A:976:LEU:HB3	1:A:980:TRP:HD1	1.84	0.43
2:B:80:ILE:HD12	2:B:105:ILE:HD12	2.00	0.43
1:C:89:LEU:HD12	1:C:137:GLY:HA3	2.00	0.43
1:C:417:ILE:HG22	1:C:548:PHE:HD2	1.84	0.43
1:A:443:ASP:OD1	1:A:444:ALA:N	2.52	0.43
1:A:924:TRP:CD1	1:A:951:LEU:HD22	2.54	0.43
1:A:1011:GLU:O	1:A:1015:TYR:HB3	2.19	0.43
2:B:74:PRO:HG2	2:B:292:GLN:OE1	2.19	0.43
1:C:150:ILE:O	1:C:153:SER:OG	2.35	0.43
1:C:998:ARG:HH11	1:C:998:ARG:HB3	1.83	0.43
1:C:1010:VAL:O	1:C:1014:THR:OG1	2.35	0.43
1:A:915:PHE:O	1:A:919:ILE:HG12	2.19	0.42
1:C:545:VAL:HG11	1:C:581:LEU:HD13	2.00	0.42
1:C:823:ASP:CG	1:C:826:LYS:HD3	2.40	0.42
1:C:907:VAL:O	1:C:911:CYS:HB2	2.19	0.42
1:A:728:GLY:HA3	1:A:744:LEU:HA	1.99	0.42
2:B:91:ARG:HD2	2:B:94:ASP:HB2	2.01	0.42
1:C:924:TRP:HH2	9:E:101:CLR:H162	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:33:PHE:CE2	9:E:101:CLR:H151	2.55	0.42
1:C:434:PRO:HG3	1:C:437:LYS:HE2	2.01	0.42
1:C:624:VAL:HG23	1:C:626:ILE:HG13	2.00	0.42
1:A:473:ILE:HD12	1:A:483:LEU:HD11	2.00	0.42
1:A:768:SER:HA	1:A:815:LEU:HD23	2.01	0.42
7:A:1108:PCW:H72	7:A:1108:PCW:H41	1.84	0.42
1:C:226:ASN:ND2	1:C:231:GLU:OE2	2.52	0.42
1:C:604:ILE:HD11	1:C:755:VAL:HG21	2.02	0.42
1:C:635:GLU:OE1	1:C:635:GLU:N	2.51	0.42
1:C:865:ILE:HD12	1:C:914:PRO:HG3	2.00	0.42
1:C:260:MET:HA	1:C:263:ILE:HD12	2.00	0.42
1:C:993:VAL:HG11	9:C:1104:CLR:H25	2.01	0.42
1:A:411:TRP:CZ2	1:A:457:CYS:HB2	2.54	0.42
1:A:771:TYR:OH	1:A:923:GLN:HB3	2.20	0.42
1:A:921:VAL:HG12	1:A:988:SER:HG	1.83	0.42
1:A:977:LYS:HD3	2:B:68:TYR:CE1	2.55	0.42
3:G:21:TYR:OH	7:C:1108:PCW:O2P	2.28	0.42
1:C:266:LEU:O	1:C:270:LEU:HG	2.19	0.42
1:C:921:VAL:HG12	1:C:988:SER:OG	2.20	0.42
1:A:776:ASN:HB3	1:A:847:TYR:HE1	1.85	0.42
1:C:38:LYS:NZ	1:C:227:GLU:OE1	2.46	0.42
1:C:771:TYR:CE2	1:C:811:PRO:HB2	2.54	0.42
1:C:777:ILE:HG22	1:C:855:ALA:HB2	2.02	0.42
1:C:916:PHE:CZ	1:C:961:LEU:HD12	2.55	0.42
1:A:386:SER:HB2	1:A:391:HIS:NE2	2.35	0.42
1:C:277:ILE:HG21	1:C:355:GLU:HB2	2.01	0.42
1:C:495:ARG:HA	1:C:555:ASP:HB3	2.02	0.42
2:D:158:ASN:OD1	4:I:1:NAG:N2	2.53	0.42
2:B:224:VAL:HG22	2:B:272:ILE:HD12	2.01	0.42
1:C:420:LEU:HD13	1:C:486:HIS:HD1	1.84	0.42
2:D:109:LEU:HD23	2:D:153:LEU:HD23	2.01	0.42
2:D:246:TYR:O	2:D:250:LEU:HB2	2.20	0.42
1:A:688:PRO:HG3	1:A:713:ASN:HB3	2.02	0.41
2:B:156:LEU:HD22	2:B:260:ALA:H	1.85	0.41
1:C:795:LEU:HD13	1:C:915:PHE:HB3	2.01	0.41
1:A:266:LEU:O	1:A:270:LEU:HG	2.19	0.41
1:A:423:ARG:NH1	1:A:474:PRO:HB3	2.35	0.41
1:A:624:VAL:HG23	1:A:626:ILE:HG13	2.03	0.41
2:D:173:LYS:HB3	2:D:262:GLN:HE21	1.85	0.41
3:E:17:ASP:HB2	3:E:19:PHE:HD2	1.85	0.41
1:A:117:GLU:CD	1:A:886:ARG:HE	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASP:OD1	1:A:182:ASP:N	2.52	0.41
1:A:385:TRP:CZ2	1:A:388:ASN:HA	2.54	0.41
1:C:30:LYS:HE2	1:C:692:LEU:HD21	2.03	0.41
1:C:56:LEU:HD22	1:C:60:ARG:HG3	2.01	0.41
1:C:238:PHE:CD2	1:C:258:THR:HG21	2.52	0.41
1:C:342:LYS:O	1:C:346:ARG:HG3	2.21	0.41
1:C:893:ASP:OD2	1:C:897:GLN:HB2	2.20	0.41
2:D:80:ILE:H	2:D:80:ILE:HG13	1.49	0.41
1:A:107:ALA:HB2	1:A:318:ILE:HG21	2.02	0.41
1:A:796:GLY:O	1:A:800:ILE:HG13	2.20	0.41
1:C:411:TRP:CZ2	1:C:457:CYS:HB2	2.56	0.41
1:C:662:ASP:O	1:C:666:MET:HG3	2.21	0.41
1:C:496:HIS:HB2	1:C:553:LEU:HB2	2.02	0.41
1:C:768:SER:HA	1:C:815:LEU:HD23	2.02	0.41
1:A:671:LEU:O	1:A:675:LEU:HG	2.20	0.41
1:C:107:ALA:HB2	1:C:318:ILE:HG21	2.02	0.41
1:C:943:LYS:HG2	7:C:1108:PCW:O11	2.21	0.41
1:A:337:LEU:HA	1:A:761:ILE:HD11	2.02	0.41
1:A:340:THR:O	1:A:344:MET:HG2	2.21	0.41
1:A:651:ARG:HA	1:A:651:ARG:HD3	1.85	0.41
1:A:931:LYS:HD2	1:A:947:LEU:HD13	2.02	0.41
1:C:378:ARG:HD2	1:C:451:LYS:NZ	2.36	0.41
1:A:208:ASN:HB3	1:A:212:THR:HG22	2.02	0.41
1:A:551:LEU:HD22	1:A:576:LEU:HD23	2.03	0.41
1:A:882:ASN:O	1:A:904:ARG:NH1	2.52	0.41
2:B:21:LYS:HA	2:B:21:LYS:HD2	1.80	0.41
1:C:924:TRP:CH2	9:E:101:CLR:H162	2.55	0.41
2:D:265:ASN:HD22	4:J:1:NAG:C7	2.34	0.41
1:A:326:PRO:HB2	1:A:329:LEU:HB2	2.03	0.41
2:B:155:TRP:CD2	2:B:232:LEU:HD22	2.55	0.41
1:C:98:TRP:NE1	1:C:133:VAL:HG11	2.36	0.41
1:C:411:TRP:HZ2	1:C:457:CYS:HB2	1.86	0.41
1:C:417:ILE:HG12	1:C:499:VAL:HG12	2.03	0.41
1:C:443:ASP:OD1	1:C:444:ALA:N	2.53	0.41
1:A:689:GLN:OE1	1:A:689:GLN:N	2.54	0.41
1:A:921:VAL:HG12	1:A:988:SER:OG	2.20	0.41
1:C:340:THR:O	1:C:344:MET:HG2	2.20	0.41
1:C:651:ARG:HA	1:C:651:ARG:HD3	1.92	0.41
1:A:776:ASN:ND2	11:A:1202:HOH:O	2.54	0.40
1:A:918:THR:O	1:A:922:VAL:HG22	2.22	0.40
2:B:95:PRO:HA	2:B:98:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:SER:HB2	1:C:391:HIS:NE2	2.37	0.40
2:D:81:PRO:O	2:D:83:SER:N	2.54	0.40
1:A:797:THR:HG23	8:A:1109:7Q2:CAB	2.51	0.40
1:A:815:LEU:HD12	1:A:815:LEU:HA	1.82	0.40
2:B:27:ARG:HG3	2:B:32:TRP:HD1	1.83	0.40
1:C:191:ARG:HA	1:C:241:ASN:HA	2.02	0.40
1:C:551:LEU:HD22	1:C:576:LEU:HD23	2.03	0.40
1:C:815:LEU:HD11	1:C:931:LYS:HA	2.03	0.40
2:D:117:GLN:O	2:D:150:ARG:NH1	2.55	0.40
1:C:48:TYR:OH	1:C:252:VAL:HG13	2.21	0.40
1:C:295:LEU:O	1:C:299:PHE:HB2	2.22	0.40
1:C:713:ASN:OD1	1:C:713:ASN:N	2.54	0.40
2:D:130:PRO:HG2	2:D:204:TYR:CE1	2.57	0.40
2:D:146:ARG:H	2:D:146:ARG:HG2	1.65	0.40
1:A:508:LEU:HD11	1:A:528:LYS:HE3	2.03	0.40
1:A:672:ASP:OD1	1:A:701:GLN:NE2	2.55	0.40
1:A:799:THR:HG21	1:A:912:HIS:HB3	2.04	0.40
1:C:366:ILE:HG13	1:C:604:ILE:HG21	2.03	0.40
1:C:925:ALA:O	1:C:929:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	993/1016 (98%)	921 (93%)	69 (7%)	3 (0%)	41 74
1	C	993/1016 (98%)	923 (93%)	68 (7%)	2 (0%)	47 78
2	B	289/303 (95%)	259 (90%)	28 (10%)	2 (1%)	22 59
2	D	281/303 (93%)	252 (90%)	27 (10%)	2 (1%)	22 59
3	E	30/65 (46%)	29 (97%)	1 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	30/65 (46%)	29 (97%)	1 (3%)	0	100	100
All	All	2616/2768 (94%)	2413 (92%)	194 (7%)	9 (0%)	41	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	PRO
2	B	200	PRO
1	C	193	PRO
1	A	306	LEU
1	C	306	LEU
2	D	200	PRO
2	B	199	TYR
2	D	199	TYR
1	A	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%)	820 (97%)	26 (3%)	40	65
1	C	846/861 (98%)	824 (97%)	22 (3%)	46	69
2	B	261/269 (97%)	239 (92%)	22 (8%)	11	40
2	D	255/269 (95%)	234 (92%)	21 (8%)	11	40
3	E	26/52 (50%)	26 (100%)	0	100	100
3	G	26/52 (50%)	26 (100%)	0	100	100
All	All	2260/2364 (96%)	2169 (96%)	91 (4%)	31	59

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	56	LEU

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Mol	Chain	Res	Type
1	A	57	THR
1	A	82	TRP
1	A	114	THR
1	A	197	ARG
1	A	211	LEU
1	A	311	LEU
1	A	425	VAL
1	A	479	ASN
1	A	523	LEU
1	A	565	ASP
1	A	566	THR
1	A	656	CYS
1	A	685	ARG
1	A	763	ASP
1	A	776	ASN
1	A	797	THR
1	A	840	GLU
1	A	904	ARG
1	A	911	CYS
1	A	916	PHE
1	A	952	PHE
1	A	953	GLU
1	A	985	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

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Mol	Chain	Res	Type
2	B	203	LYS
2	B	256	GLN
2	B	297	VAL
2	B	299	ILE
1	C	45	HIS
1	C	56	LEU
1	C	57	THR
1	C	82	TRP
1	C	197	ARG
1	C	206	VAL
1	C	327	GLU
1	C	350	LEU
1	C	425	VAL
1	C	479	ASN
1	C	523	LEU
1	C	565	ASP
1	C	566	THR
1	C	685	ARG
1	C	763	ASP
1	C	776	ASN
1	C	797	THR
1	C	810	VAL
1	C	916	PHE
1	C	953	GLU
1	C	985	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	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

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Mol	Chain	Res	Type
2	D	195	SER
2	D	203	LYS
2	D	256	GLN
2	D	297	VAL
2	D	299	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	160	GLN
1	A	241	ASN
1	A	324	ASN
1	A	377	ASN
1	A	399	GLN
1	A	488	ASN
1	A	521	GLN
1	A	849	GLN
1	A	897	GLN
1	A	898	GLN
1	C	160	GLN
1	C	324	ASN
1	C	377	ASN
1	C	488	ASN
1	C	521	GLN
1	C	678	HIS
1	C	849	GLN
1	C	897	GLN
1	C	898	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	C	369	1,5	9,11,12	1.87	1 (11%)	10,15,17	1.37	2 (20%)
1	PHD	A	369	1,5	9,11,12	1.82	1 (11%)	10,15,17	1.61	2 (20%)

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	C	369	1,5	-	1/8/11/13	-
1	PHD	A	369	1,5	-	1/8/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	PHD	P-OD1	-4.92	1.51	1.59
1	A	369	PHD	P-OD1	-4.72	1.52	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	PHD	CA-CB-CG	3.35	119.88	112.86
1	C	369	PHD	CA-CB-CG	2.96	119.05	112.86
1	A	369	PHD	OD1-CG-CB	2.82	118.86	111.11
1	C	369	PHD	OD1-CG-CB	2.34	117.54	111.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	369	PHD	O-C-CA-CB
1	C	369	PHD	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	369	PHD	1	0
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	0.32	0	17,19,21	0.47	0
4	NAG	F	2	4	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	H	1	2,4	14,14,15	0.62	1 (7%)	17,19,21	0.71	0
4	NAG	H	2	4	14,14,15	0.37	0	17,19,21	0.37	0
4	NAG	I	1	2,4	14,14,15	0.34	0	17,19,21	0.47	0
4	NAG	I	2	4	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	J	1	2,4	14,14,15	0.68	1 (7%)	17,19,21	0.69	0
4	NAG	J	2	4	14,14,15	0.36	0	17,19,21	0.36	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	-	1/6/23/26	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	J	1	NAG	O5-C1	-2.42	1.39	1.43
4	H	1	NAG	O5-C1	-2.17	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

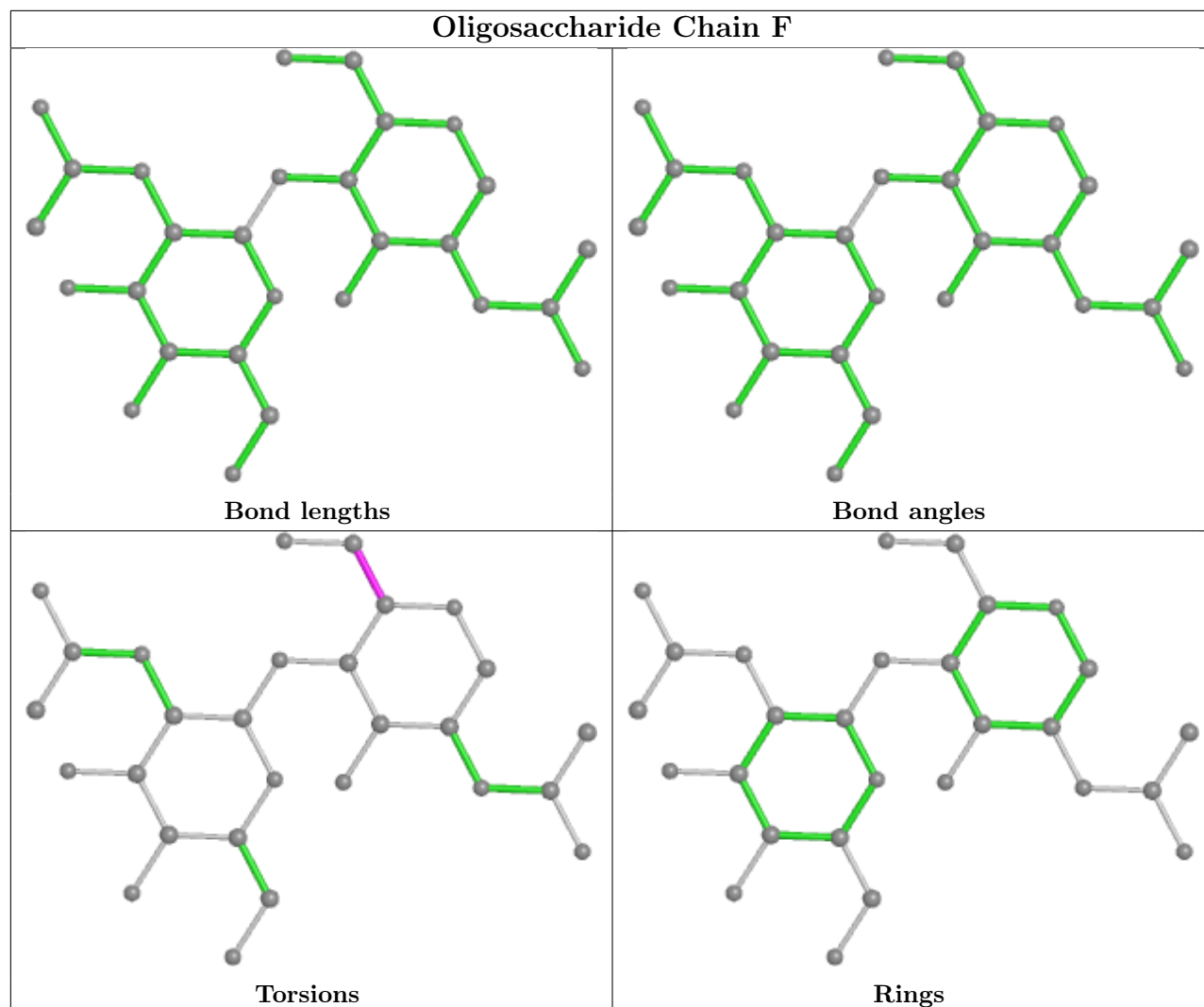
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6

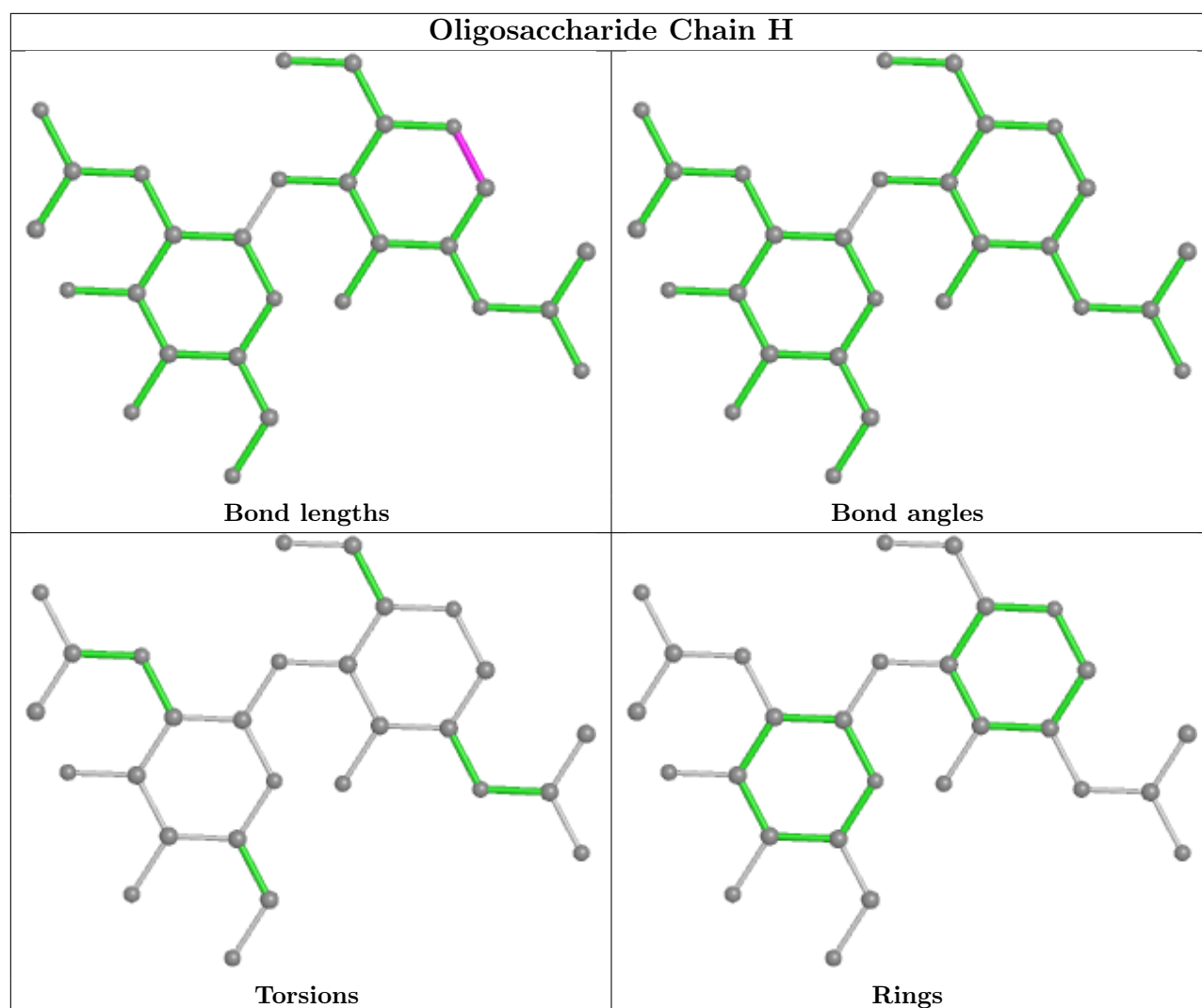
There are no ring outliers.

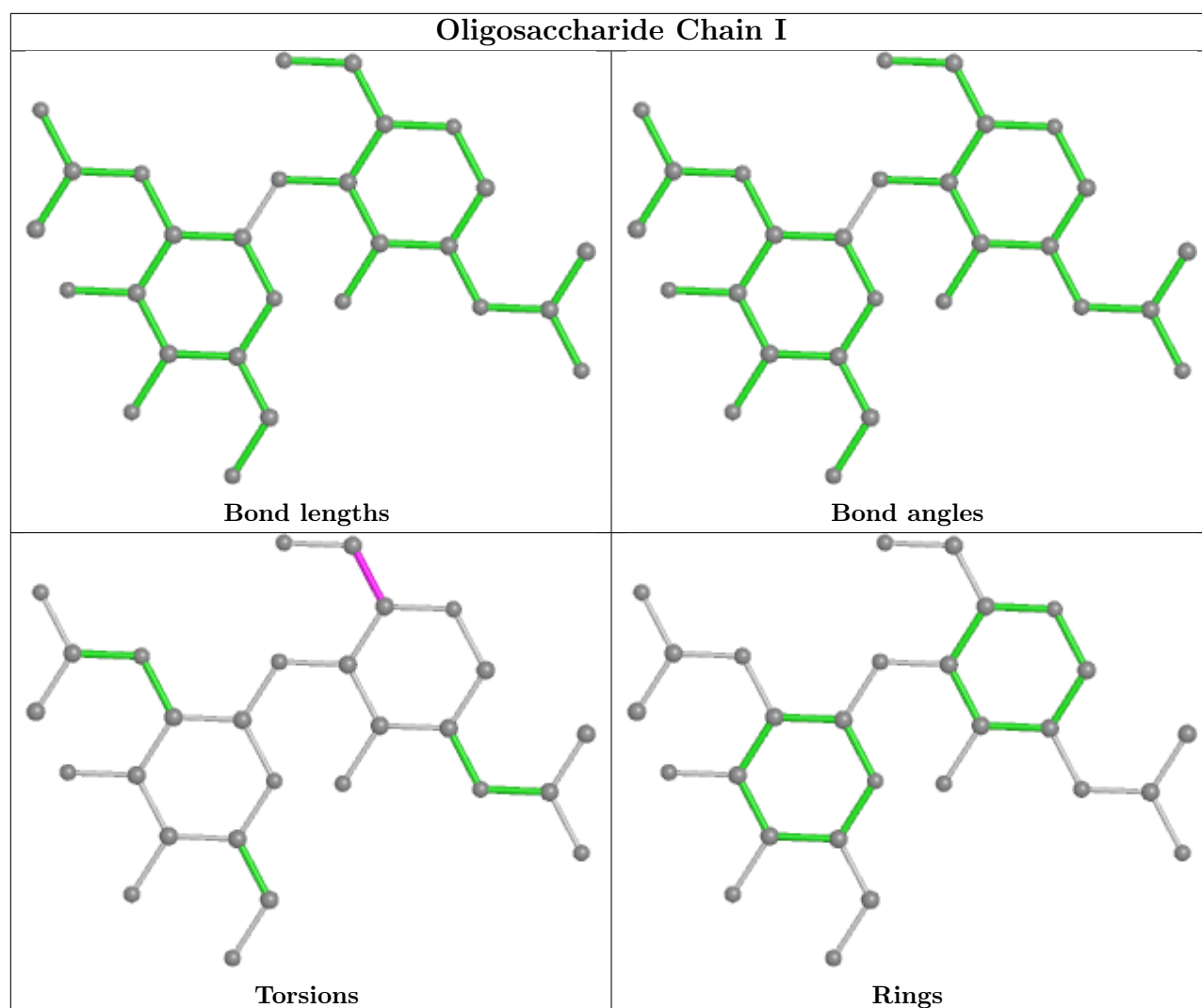
2 monomers are involved in 2 short contacts:

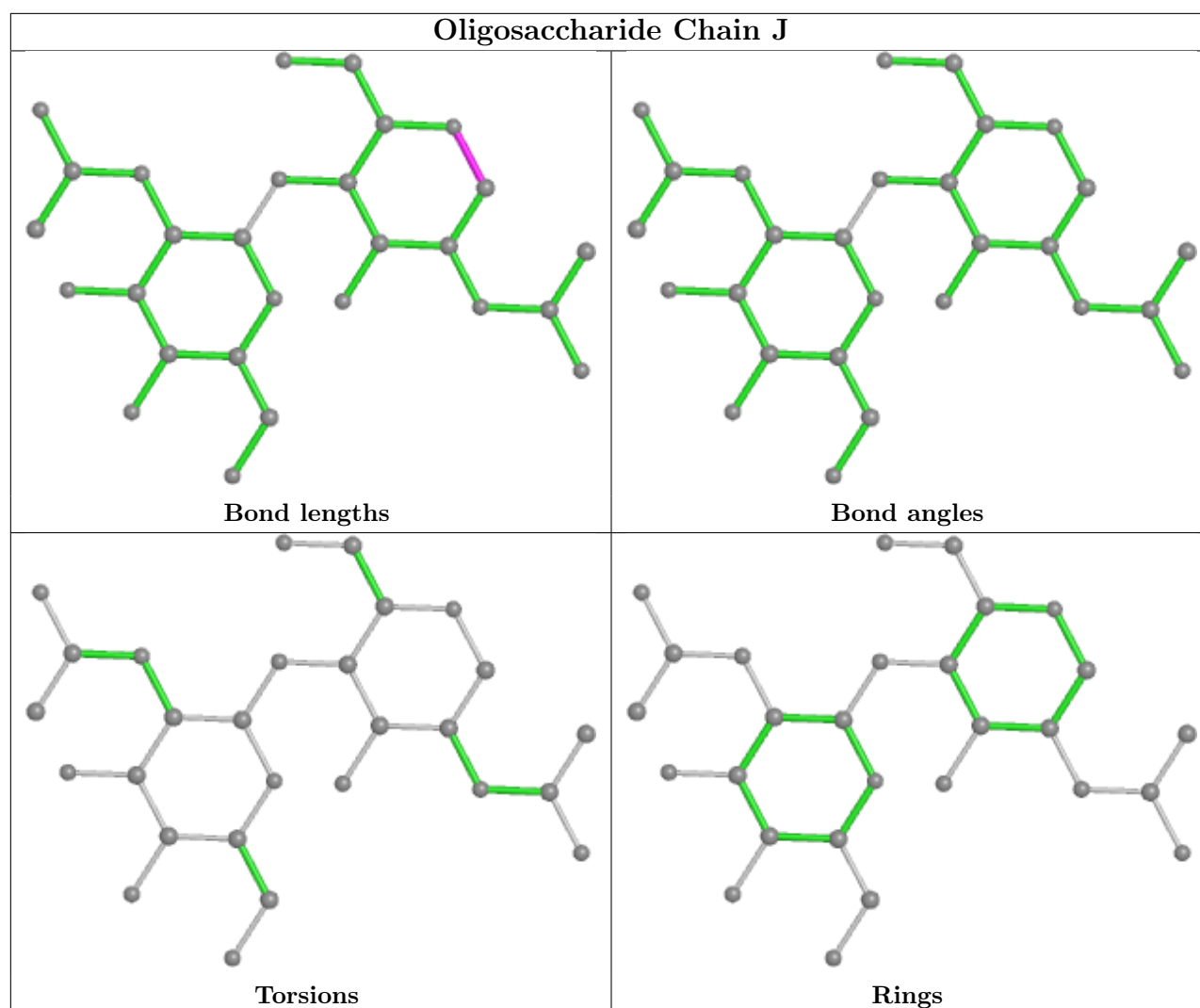
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
4	J	1	NAG	1	0

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$
9	CLR	G	101	-	31,31,31	1.45	4 (12%)	48,48,48	1.53	10 (20%)
7	PCW	D	402	-	21,21,53	1.01	0	27,29,61	0.89	1 (3%)
9	CLR	B	402	-	31,31,31	1.57	7 (22%)	48,48,48	1.45	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLR	D	403	-	31,31,31	1.65	8 (25%)	48,48,48	1.41	8 (16%)
7	PCW	C	1107	-	21,21,53	1.48	3 (14%)	27,29,61	1.99	4 (14%)
7	PCW	A	1106	-	21,21,53	0.96	0	27,29,61	0.85	1 (3%)
7	PCW	C	1106	-	21,21,53	1.03	0	27,29,61	0.86	2 (7%)
9	CLR	A	1110	-	31,31,31	1.53	7 (22%)	48,48,48	1.52	9 (18%)
9	CLR	E	101	-	31,31,31	1.48	6 (19%)	48,48,48	1.47	11 (22%)
8	7Q2	A	1109	-	29,29,29	3.79	15 (51%)	43,45,45	2.03	14 (32%)
10	NAG	D	401	2	14,14,15	0.32	0	17,19,21	0.52	0
7	PCW	A	1108	-	21,21,53	0.99	0	27,29,61	1.12	2 (7%)
7	PCW	A	1104	-	21,21,53	1.07	0	27,29,61	1.00	2 (7%)
7	PCW	C	1108	-	21,21,53	0.95	0	27,29,61	1.16	3 (11%)
10	NAG	B	401	2	14,14,15	0.32	0	17,19,21	0.47	0
7	PCW	A	1107	-	21,21,53	0.98	0	27,29,61	1.09	3 (11%)
9	CLR	C	1104	-	31,31,31	1.55	8 (25%)	48,48,48	1.48	9 (18%)
7	PCW	A	1105	-	21,21,53	0.94	0	27,29,61	0.89	1 (3%)
7	PCW	C	1105	-	21,21,53	1.00	0	27,29,61	1.06	2 (7%)
8	7Q2	C	1109	-	29,29,29	3.76	16 (55%)	43,45,45	2.04	14 (32%)

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	G	101	-	-	3/10/68/68	0/4/4/4
7	PCW	D	402	-	-	9/23/23/57	-
9	CLR	B	402	-	-	0/10/68/68	0/4/4/4
9	CLR	D	403	-	-	0/10/68/68	0/4/4/4
7	PCW	C	1107	-	-	12/23/23/57	-
7	PCW	A	1106	-	-	10/23/23/57	-
7	PCW	C	1106	-	-	15/23/23/57	-
9	CLR	A	1110	-	-	4/10/68/68	0/4/4/4
9	CLR	E	101	-	-	3/10/68/68	0/4/4/4
8	7Q2	A	1109	-	-	0/5/66/66	0/4/4/4
10	NAG	D	401	2	-	4/6/23/26	0/1/1/1
7	PCW	A	1108	-	-	11/23/23/57	-
7	PCW	A	1104	-	-	8/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	C	1108	-	-	9/23/23/57	-
10	NAG	B	401	2	-	1/6/23/26	0/1/1/1
7	PCW	A	1107	-	-	11/23/23/57	-
9	CLR	C	1104	-	-	5/10/68/68	0/4/4/4
7	PCW	A	1105	-	-	16/23/23/57	-
7	PCW	C	1105	-	-	10/23/23/57	-
8	7Q2	C	1109	-	-	0/5/66/66	0/4/4/4

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1109	7Q2	CAF-CAD	-8.19	1.41	1.52
8	C	1109	7Q2	CAF-CAD	-8.05	1.41	1.52
8	A	1109	7Q2	CAS-CAU	-7.93	1.41	1.50
8	C	1109	7Q2	CAS-CAU	-7.75	1.41	1.50
8	A	1109	7Q2	CAT-CAU	-7.69	1.42	1.50
8	C	1109	7Q2	CAT-CAU	-7.22	1.42	1.50
8	C	1109	7Q2	CAU-NAV	6.83	1.33	1.28
8	A	1109	7Q2	CAU-NAV	6.66	1.33	1.28
8	C	1109	7Q2	CAF-CAG	-5.61	1.44	1.54
8	A	1109	7Q2	CAF-CAG	-5.46	1.44	1.54
8	C	1109	7Q2	CAB-CAG	-5.21	1.43	1.54
8	A	1109	7Q2	CAB-CAG	-5.15	1.43	1.54
8	A	1109	7Q2	CAQ-CAM	-4.72	1.42	1.51
8	C	1109	7Q2	CAQ-CAM	-4.60	1.43	1.51
8	C	1109	7Q2	CAJ-CAM	-4.50	1.42	1.50
8	A	1109	7Q2	CAJ-CAM	-4.45	1.42	1.50
8	C	1109	7Q2	CAI-CAG	-3.88	1.46	1.53
8	A	1109	7Q2	CAI-CAG	-3.76	1.46	1.53
8	A	1109	7Q2	CAP-CAL	-3.73	1.49	1.56
8	C	1109	7Q2	CAP-CAL	-3.55	1.49	1.56
9	D	403	CLR	C4-C3	3.49	1.58	1.52
7	C	1107	PCW	O2-C31	3.48	1.43	1.35
9	E	101	CLR	C16-C17	3.42	1.61	1.54
9	D	403	CLR	C16-C17	3.32	1.61	1.54
9	G	101	CLR	C16-C17	3.30	1.61	1.54
8	C	1109	7Q2	CAH-CAF	-3.27	1.48	1.54
8	A	1109	7Q2	CAH-CAF	-3.21	1.48	1.54
9	D	403	CLR	C13-C14	3.20	1.61	1.55
8	A	1109	7Q2	CAK-CAL	3.19	1.59	1.53
9	B	402	CLR	C16-C17	3.16	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1109	7Q2	CAK-CAL	3.12	1.59	1.53
9	A	1110	CLR	C16-C17	3.08	1.60	1.54
8	A	1109	7Q2	CAP-CAQ	-3.04	1.51	1.56
8	C	1109	7Q2	CAP-CAQ	-2.97	1.51	1.56
9	C	1104	CLR	C16-C17	2.96	1.60	1.54
9	G	101	CLR	C10-C5	2.95	1.58	1.52
9	A	1110	CLR	C4-C3	2.92	1.57	1.52
9	C	1104	CLR	C4-C3	2.86	1.57	1.52
9	B	402	CLR	C12-C13	2.81	1.59	1.54
9	E	101	CLR	C13-C14	2.79	1.60	1.55
9	B	402	CLR	C4-C3	2.73	1.56	1.52
7	C	1107	PCW	C1-C2	2.71	1.59	1.50
8	A	1109	7Q2	OAW-NAV	2.71	1.46	1.42
8	C	1109	7Q2	OAW-NAV	2.66	1.46	1.42
9	B	402	CLR	C13-C14	2.65	1.60	1.55
9	D	403	CLR	C13-C17	2.59	1.59	1.55
9	G	101	CLR	C13-C14	2.57	1.59	1.55
9	C	1104	CLR	C10-C9	2.55	1.60	1.56
9	C	1104	CLR	C10-C5	2.52	1.57	1.52
8	A	1109	7Q2	CAH-CAK	2.50	1.58	1.53
8	C	1109	7Q2	CAH-CAK	2.49	1.58	1.53
9	E	101	CLR	C10-C5	2.49	1.57	1.52
9	B	402	CLR	C10-C9	2.42	1.60	1.56
9	B	402	CLR	C13-C17	2.35	1.59	1.55
9	E	101	CLR	C4-C3	2.34	1.56	1.52
9	A	1110	CLR	C10-C9	2.34	1.60	1.56
9	E	101	CLR	C12-C13	2.31	1.58	1.54
9	D	403	CLR	C16-C15	2.28	1.60	1.54
9	D	403	CLR	C12-C13	2.27	1.58	1.54
9	D	403	CLR	C22-C20	2.26	1.60	1.54
9	A	1110	CLR	C13-C14	2.24	1.59	1.55
9	A	1110	CLR	C13-C17	2.21	1.59	1.55
9	G	101	CLR	C12-C13	2.18	1.58	1.54
9	B	402	CLR	C22-C20	2.18	1.60	1.54
9	C	1104	CLR	C11-C9	2.17	1.57	1.53
7	C	1107	PCW	O2-C2	2.17	1.52	1.46
9	C	1104	CLR	C13-C14	2.15	1.59	1.55
9	A	1110	CLR	C11-C9	2.09	1.57	1.53
8	C	1109	7Q2	CAJ-CAI	-2.07	1.50	1.53
9	D	403	CLR	C7-C8	2.07	1.56	1.53
9	E	101	CLR	C13-C17	2.06	1.58	1.55
9	C	1104	CLR	C12-C11	2.04	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1110	CLR	C10-C5	2.04	1.56	1.52
9	C	1104	CLR	C12-C13	2.01	1.57	1.54

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1107	PCW	C2-O2-C31	7.80	132.43	117.90
8	C	1109	7Q2	OAW-NAV-CAU	5.86	117.30	110.81
8	A	1109	7Q2	OAW-NAV-CAU	5.83	117.26	110.81
8	C	1109	7Q2	CAB-CAG-CAI	-4.02	112.46	119.08
8	A	1109	7Q2	CAB-CAG-CAI	-4.02	112.47	119.08
7	A	1108	PCW	C2-O2-C31	-3.76	110.89	117.90
9	A	1110	CLR	C8-C7-C6	-3.64	107.50	112.73
8	C	1109	7Q2	CAF-CAG-CAI	-3.53	109.34	113.12
8	A	1109	7Q2	CAF-CAG-CAI	-3.53	109.35	113.12
8	A	1109	7Q2	CAT-CAR-CAP	-3.49	109.00	113.47
7	C	1108	PCW	C2-O2-C31	-3.49	111.40	117.90
8	C	1109	7Q2	CAT-CAR-CAP	-3.48	109.01	113.47
9	G	101	CLR	C17-C13-C14	-3.46	95.97	100.07
8	C	1109	7Q2	CAB-CAA-CAD	-3.43	102.25	105.70
9	G	101	CLR	C22-C20-C17	-3.42	103.21	110.28
7	C	1107	PCW	O2-C31-C32	3.40	117.34	111.09
8	A	1109	7Q2	CAB-CAA-CAD	-3.37	102.31	105.70
7	C	1107	PCW	O31-C31-C32	-3.28	112.87	124.81
7	A	1107	PCW	C2-O2-C31	-3.23	111.87	117.90
9	C	1104	CLR	C8-C7-C6	-3.23	108.09	112.73
8	C	1109	7Q2	CAP-CAL-CAI	-3.19	109.07	112.42
8	A	1109	7Q2	CAP-CAL-CAI	-3.11	109.16	112.42
7	C	1105	PCW	O2-C31-C32	3.05	116.70	111.09
9	E	101	CLR	C17-C13-C14	-3.05	96.46	100.07
7	C	1107	PCW	O2-C31-O31	3.04	128.99	122.96
9	B	402	CLR	C8-C7-C6	-3.02	108.39	112.73
9	E	101	CLR	C22-C20-C17	-3.00	104.08	110.28
9	D	403	CLR	C4-C5-C10	-2.98	112.46	116.42
9	B	402	CLR	C4-C5-C10	-2.95	112.50	116.42
7	C	1108	PCW	O2-C31-C32	2.92	116.47	111.09
8	C	1109	7Q2	CAK-CAL-CAP	-2.85	110.63	113.91
8	A	1109	7Q2	CAK-CAL-CAP	-2.83	110.65	113.91
9	A	1110	CLR	C4-C5-C10	-2.74	112.78	116.42
9	D	403	CLR	C8-C7-C6	-2.74	108.80	112.73
8	C	1109	7Q2	CAE-CAF-CAD	2.73	110.21	105.18
8	A	1109	7Q2	CAE-CAF-CAD	2.73	110.20	105.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1104	PCW	O2-C31-C32	2.71	116.08	111.09
7	D	402	PCW	O2-C31-C32	2.69	116.04	111.09
9	G	101	CLR	C19-C10-C9	-2.69	108.48	111.68
9	C	1104	CLR	C19-C10-C9	-2.67	108.49	111.68
9	B	402	CLR	C22-C20-C17	-2.67	104.78	110.28
9	E	101	CLR	C19-C10-C9	-2.61	108.57	111.68
7	C	1105	PCW	C3-O3-C11	-2.61	110.55	117.10
8	C	1109	7Q2	CAJ-CAM-CAQ	2.60	119.27	115.35
9	C	1104	CLR	C22-C20-C17	-2.59	104.93	110.28
8	A	1109	7Q2	CAJ-CAM-CAQ	2.59	119.26	115.35
9	C	1104	CLR	C4-C5-C10	-2.56	113.01	116.42
9	B	402	CLR	C11-C9-C10	2.56	116.45	113.08
7	A	1104	PCW	C2-O2-C31	-2.56	113.13	117.90
9	A	1110	CLR	C19-C10-C9	-2.56	108.64	111.68
9	D	403	CLR	C22-C20-C17	-2.55	105.01	110.28
7	A	1108	PCW	O2-C31-C32	2.54	115.76	111.09
9	E	101	CLR	C4-C5-C10	-2.53	113.06	116.42
9	A	1110	CLR	C22-C20-C17	-2.52	105.08	110.28
9	G	101	CLR	C7-C8-C14	-2.49	107.29	110.91
8	C	1109	7Q2	CAH-CAF-CAD	-2.48	112.95	116.67
8	A	1109	7Q2	CAH-CAF-CAD	-2.47	112.96	116.67
8	A	1109	7Q2	CAG-CAF-CAD	2.44	103.38	100.59
8	C	1109	7Q2	CAG-CAF-CAD	2.40	103.34	100.59
9	G	101	CLR	C4-C5-C10	-2.37	113.27	116.42
9	D	403	CLR	C19-C10-C9	-2.33	108.90	111.68
7	C	1106	PCW	O2-C31-C32	2.32	115.37	111.09
9	G	101	CLR	C2-C3-C4	-2.32	107.12	110.31
7	A	1105	PCW	O2-C31-C32	2.32	115.35	111.09
9	B	402	CLR	C19-C10-C5	2.30	112.06	108.34
9	G	101	CLR	C16-C17-C20	-2.29	108.60	112.15
7	A	1106	PCW	O2-C31-C32	2.28	115.28	111.09
7	A	1107	PCW	O2-C31-C32	2.28	115.28	111.09
9	A	1110	CLR	C16-C17-C20	-2.24	108.67	112.15
9	D	403	CLR	C21-C20-C17	2.23	116.34	112.92
9	A	1110	CLR	C21-C20-C17	2.22	116.32	112.92
9	G	101	CLR	C18-C13-C12	2.19	114.05	110.59
9	G	101	CLR	C21-C20-C17	2.18	116.26	112.92
9	B	402	CLR	C19-C10-C9	-2.18	109.08	111.68
9	E	101	CLR	C18-C13-C12	2.17	114.02	110.59
8	A	1109	7Q2	CAK-CAH-CAF	-2.16	108.07	112.74
9	B	402	CLR	C21-C20-C17	2.15	116.21	112.92
8	C	1109	7Q2	CAK-CAH-CAF	-2.15	108.09	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1104	CLR	C15-C14-C13	2.14	106.43	103.84
9	B	402	CLR	C16-C17-C20	-2.14	108.84	112.15
9	D	403	CLR	C18-C13-C12	2.13	113.96	110.59
8	C	1109	7Q2	CAH-CAK-CAL	-2.13	109.42	113.11
9	A	1110	CLR	C1-C2-C3	2.13	113.20	110.47
9	A	1110	CLR	C19-C10-C5	2.13	111.79	108.34
7	C	1108	PCW	C3-O3-C11	-2.13	111.76	117.10
8	A	1109	7Q2	CAH-CAK-CAL	-2.12	109.44	113.11
7	A	1107	PCW	C3-O3-C11	-2.11	111.79	117.10
9	E	101	CLR	C21-C20-C17	2.11	116.16	112.92
9	D	403	CLR	C1-C2-C3	2.11	113.17	110.47
9	D	403	CLR	C17-C13-C14	-2.11	97.58	100.07
9	E	101	CLR	C2-C3-C4	-2.09	107.44	110.31
9	C	1104	CLR	C19-C10-C5	2.09	111.72	108.34
9	C	1104	CLR	C18-C13-C12	2.08	113.87	110.59
9	A	1110	CLR	C15-C14-C13	2.06	106.33	103.84
9	E	101	CLR	C19-C10-C5	2.06	111.68	108.34
9	G	101	CLR	C24-C23-C22	-2.05	103.80	113.24
7	C	1106	PCW	C2-O2-C31	-2.05	114.08	117.90
9	C	1104	CLR	C16-C17-C20	-2.04	108.98	112.15
9	E	101	CLR	C16-C17-C20	-2.04	108.99	112.15
8	A	1109	7Q2	CAE-CAF-CAG	-2.02	110.00	112.98
9	C	1104	CLR	C1-C2-C3	2.01	113.04	110.47
8	C	1109	7Q2	CAE-CAF-CAG	-2.01	110.02	112.98
9	B	402	CLR	C18-C13-C12	2.01	113.76	110.59
9	E	101	CLR	C7-C8-C14	-2.00	108.00	110.91
9	E	101	CLR	C8-C7-C6	-2.00	109.86	112.73

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1104	PCW	C32-C31-O2-C2
7	A	1105	PCW	O4P-C4-C5-N
7	A	1105	PCW	C4-O4P-P-O2P
7	A	1106	PCW	C1-O3P-P-O2P
7	A	1108	PCW	C32-C31-O2-C2
7	C	1105	PCW	O4P-C4-C5-N
7	C	1105	PCW	C4-O4P-P-O2P
7	C	1106	PCW	C32-C31-O2-C2
7	C	1106	PCW	C4-O4P-P-O2P
7	C	1107	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
7	C	1107	PCW	C1-O3P-P-O1P
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	D	402	PCW	C32-C31-O2-C2
7	D	402	PCW	O31-C31-O2-C2
7	A	1105	PCW	C32-C31-O2-C2
7	C	1105	PCW	C32-C31-O2-C2
7	C	1107	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	1104	PCW	O31-C31-O2-C2
7	C	1105	PCW	O31-C31-O2-C2
7	A	1106	PCW	C32-C31-O2-C2
7	A	1108	PCW	O31-C31-O2-C2
7	C	1106	PCW	O31-C31-O2-C2
7	A	1104	PCW	O11-C11-O3-C3
7	A	1104	PCW	C12-C11-O3-C3
7	A	1107	PCW	C12-C11-O3-C3
7	A	1105	PCW	C4-C5-N-C7
7	C	1105	PCW	O11-C11-O3-C3
7	C	1105	PCW	C12-C11-O3-C3
7	A	1107	PCW	O31-C31-O2-C2
7	A	1105	PCW	O11-C11-O3-C3
7	C	1108	PCW	O11-C11-O3-C3
7	A	1108	PCW	O11-C11-O3-C3
7	C	1107	PCW	C12-C11-O3-C3
10	D	401	NAG	O5-C5-C6-O6
7	C	1108	PCW	O31-C31-O2-C2
7	C	1108	PCW	C12-C11-O3-C3
9	E	101	CLR	C21-C20-C22-C23
7	A	1108	PCW	C12-C11-O3-C3
10	D	401	NAG	C4-C5-C6-O6
10	D	401	NAG	C8-C7-N2-C2
10	D	401	NAG	O7-C7-N2-C2
7	A	1106	PCW	O31-C31-O2-C2
9	A	1110	CLR	C20-C22-C23-C24
9	G	101	CLR	C21-C20-C22-C23
7	A	1105	PCW	C12-C11-O3-C3
7	C	1107	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
7	A	1107	PCW	O11-C11-O3-C3
9	E	101	CLR	C20-C22-C23-C24
7	A	1104	PCW	C4-O4P-P-O3P
7	A	1108	PCW	C4-O4P-P-O3P
7	C	1107	PCW	C1-O3P-P-O4P
7	A	1105	PCW	C4-C5-N-C8
7	C	1106	PCW	C12-C11-O3-C3
7	A	1105	PCW	C4-C5-N-C6
9	A	1110	CLR	C23-C24-C25-C26
9	A	1110	CLR	C23-C24-C25-C27
9	C	1104	CLR	C20-C22-C23-C24
9	E	101	CLR	C22-C23-C24-C25
7	C	1106	PCW	O11-C11-O3-C3
7	A	1106	PCW	C1-O3P-P-O4P
7	A	1108	PCW	C1-O3P-P-O4P
7	C	1105	PCW	C1-O3P-P-O4P
7	A	1105	PCW	O3P-C1-C2-C3
9	G	101	CLR	C22-C23-C24-C25
7	A	1108	PCW	O3P-C1-C2-O2
7	A	1106	PCW	O2-C2-C3-O3
9	G	101	CLR	C20-C22-C23-C24
7	A	1108	PCW	O3P-C1-C2-C3
7	C	1108	PCW	O3P-C1-C2-C3
7	A	1107	PCW	C1-C2-C3-O3
7	C	1106	PCW	C4-O4P-P-O3P
10	B	401	NAG	O5-C5-C6-O6
9	C	1104	CLR	C23-C24-C25-C26
7	D	402	PCW	C12-C11-O3-C3
9	C	1104	CLR	C13-C17-C20-C21
7	C	1107	PCW	C3-C2-O2-C31
7	C	1108	PCW	O3P-C1-C2-O2
7	A	1105	PCW	C4-O4P-P-O3P
7	C	1108	PCW	C4-O4P-P-O3P
7	A	1104	PCW	C4-O4P-P-O2P
7	A	1108	PCW	C1-O3P-P-O2P
7	A	1108	PCW	C4-O4P-P-O2P
7	C	1105	PCW	C1-O3P-P-O1P
7	C	1105	PCW	C1-O3P-P-O2P
7	A	1104	PCW	O3P-C1-C2-C3
7	C	1106	PCW	O3P-C1-C2-C3
7	A	1105	PCW	O3P-C1-C2-O2
7	C	1106	PCW	O3P-C1-C2-O2

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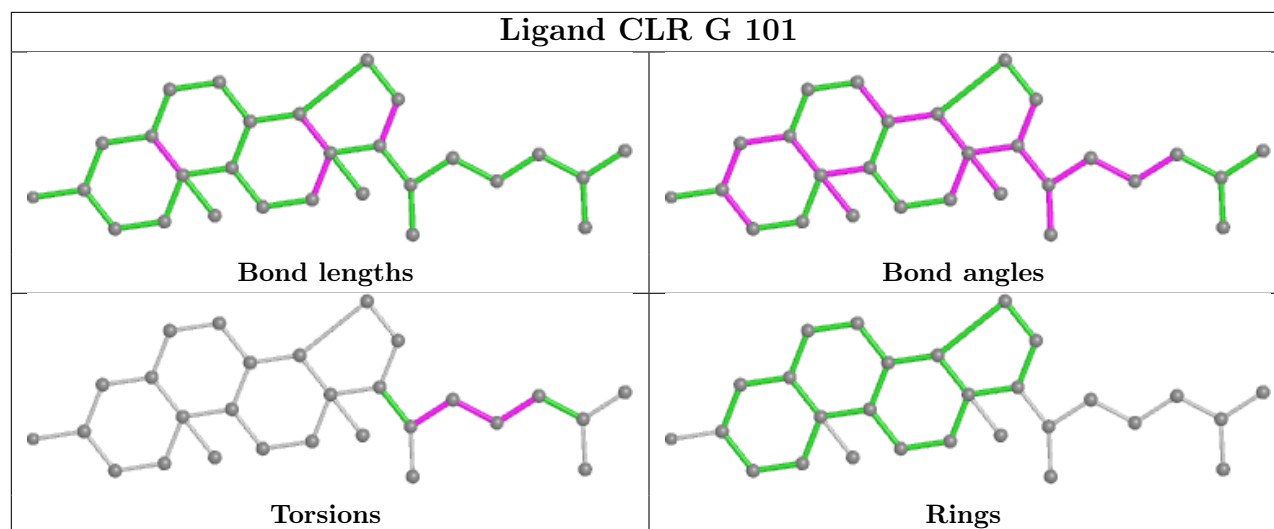
Mol	Chain	Res	Type	Atoms
7	C	1106	PCW	C4-C5-N-C6
7	A	1104	PCW	O4P-C4-C5-N
7	A	1106	PCW	O4P-C4-C5-N
7	A	1107	PCW	O4P-C4-C5-N
7	A	1108	PCW	O4P-C4-C5-N
7	C	1106	PCW	O4P-C4-C5-N
7	C	1107	PCW	O4P-C4-C5-N
7	C	1108	PCW	O4P-C4-C5-N
7	D	402	PCW	O4P-C4-C5-N
7	A	1105	PCW	O2-C2-C3-O3
7	A	1107	PCW	O2-C2-C3-O3
7	A	1105	PCW	C3-C2-O2-C31
7	A	1105	PCW	C1-O3P-P-O4P
7	A	1106	PCW	C4-O4P-P-O3P
7	A	1107	PCW	C1-O3P-P-O4P
7	A	1107	PCW	C4-O4P-P-O3P
7	C	1105	PCW	C4-O4P-P-O3P
7	C	1106	PCW	C1-O3P-P-O4P
7	D	402	PCW	C1-O3P-P-O4P
7	D	402	PCW	C4-O4P-P-O3P
7	A	1106	PCW	C1-C2-C3-O3
7	C	1106	PCW	C4-C5-N-C8
9	C	1104	CLR	C23-C24-C25-C27
7	C	1106	PCW	C4-C5-N-C7
9	A	1110	CLR	C13-C17-C20-C21
7	A	1106	PCW	C12-C11-O3-C3
7	D	402	PCW	O11-C11-O3-C3
7	C	1107	PCW	C1-C2-O2-C31
7	A	1105	PCW	C1-C2-C3-O3
9	C	1104	CLR	C13-C17-C20-C22
7	C	1106	PCW	C1-C2-C3-O3
7	A	1106	PCW	C4-O4P-P-O2P
7	A	1107	PCW	C1-O3P-P-O2P
7	A	1107	PCW	C4-O4P-P-O2P
7	C	1106	PCW	C1-O3P-P-O2P
7	D	402	PCW	C1-O3P-P-O2P
7	D	402	PCW	C3-C2-O2-C31

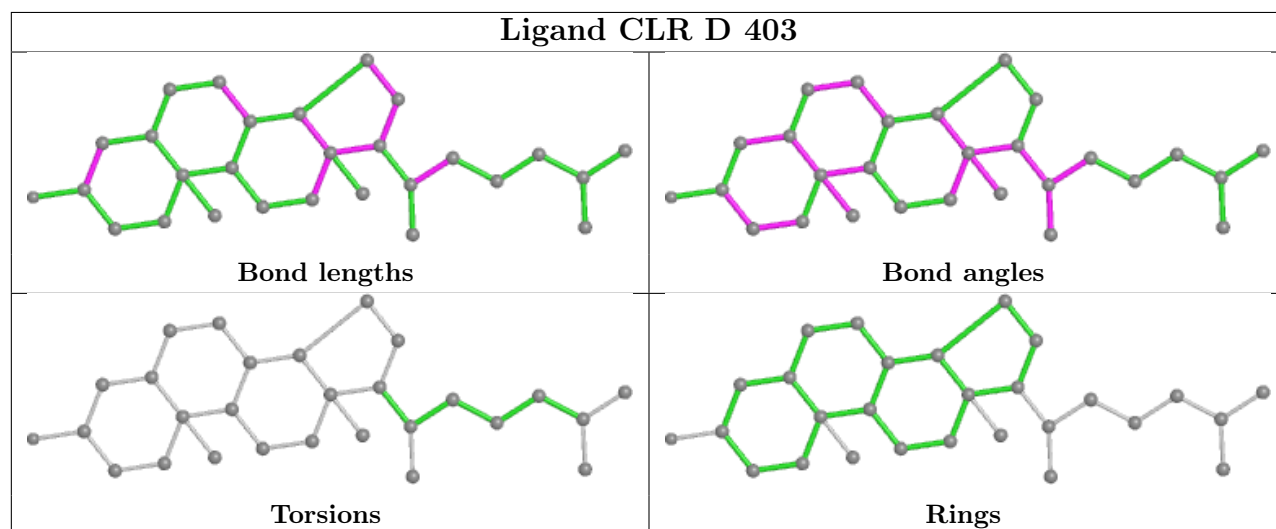
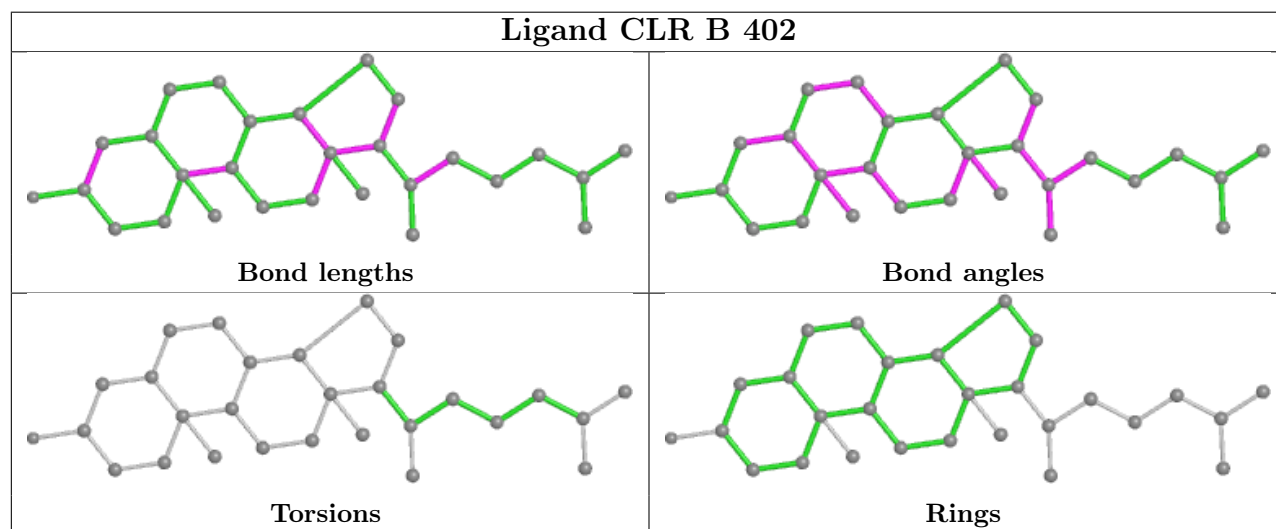
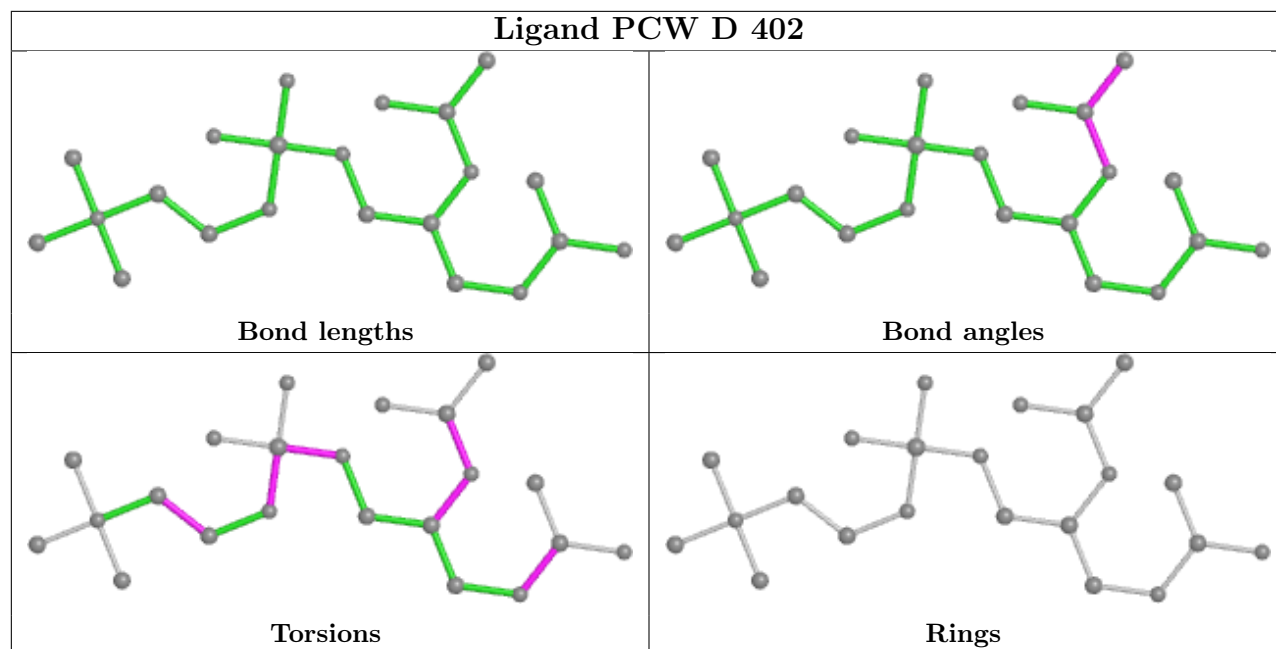
There are no ring outliers.

15 monomers are involved in 33 short contacts:

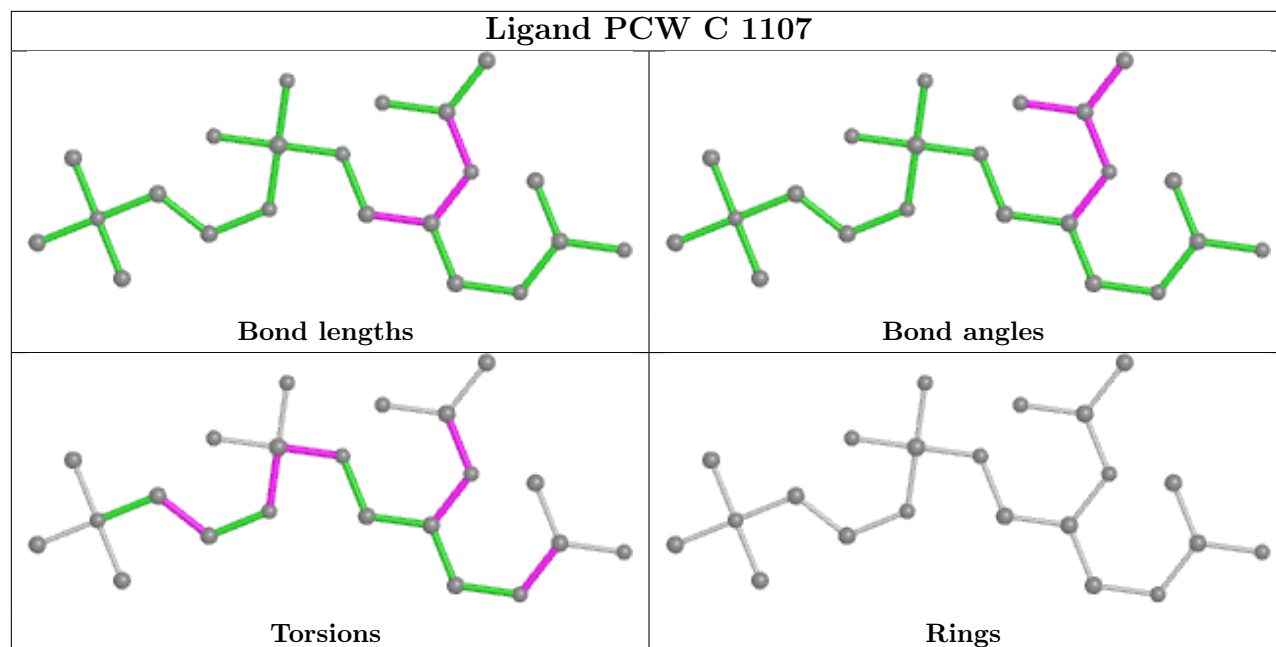
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	101	CLR	2	0
9	B	402	CLR	2	0
9	D	403	CLR	2	0
7	C	1107	PCW	3	0
7	C	1106	PCW	1	0
9	A	1110	CLR	2	0
9	E	101	CLR	5	0
8	A	1109	7Q2	2	0
7	A	1108	PCW	2	0
7	A	1104	PCW	1	0
7	C	1108	PCW	2	0
7	A	1107	PCW	1	0
9	C	1104	CLR	5	0
7	C	1105	PCW	1	0
8	C	1109	7Q2	2	0

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.

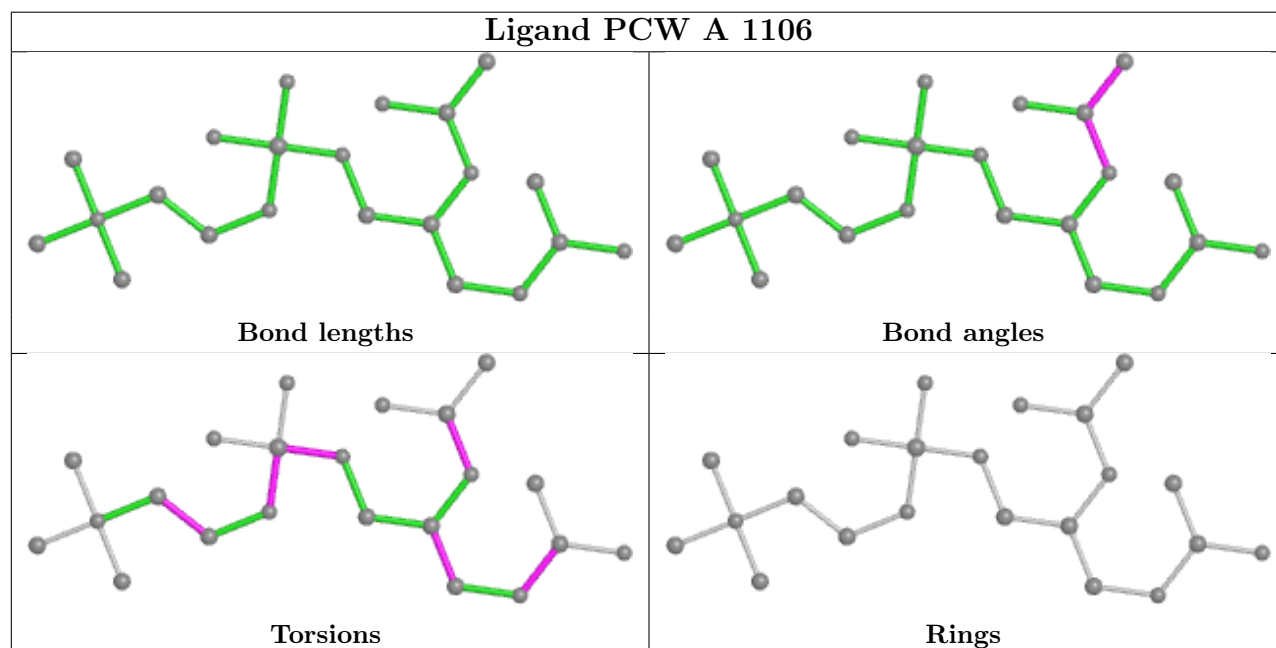




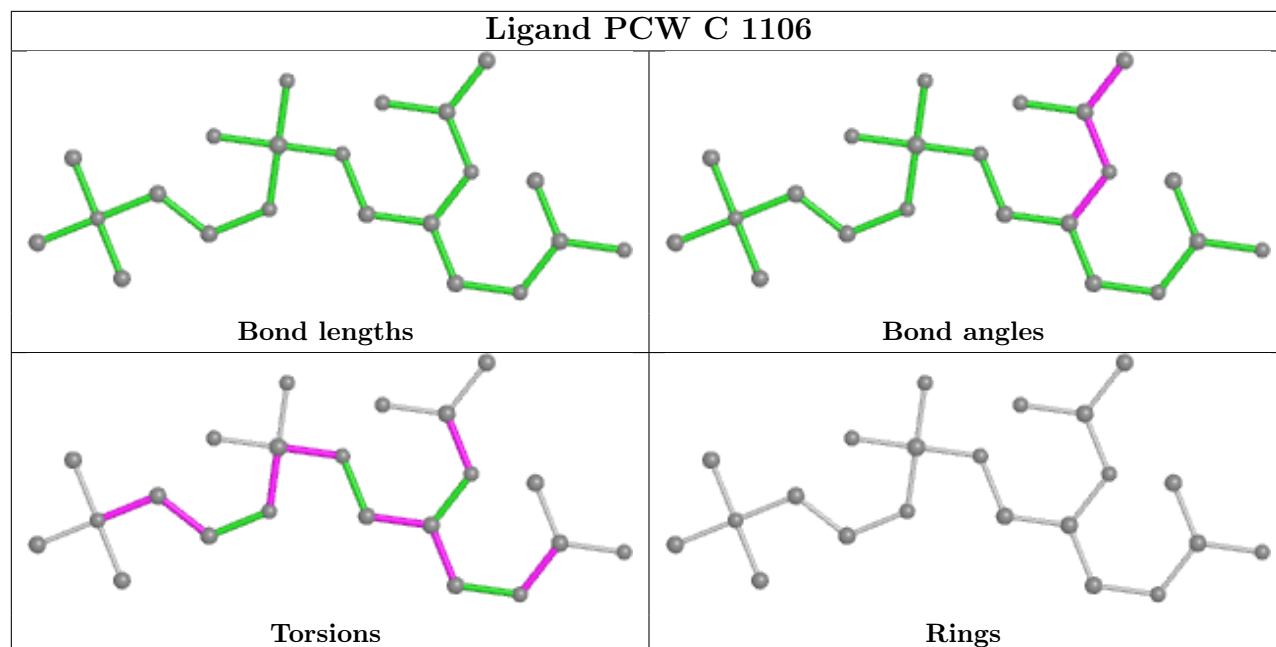
Ligand PCW C 1107



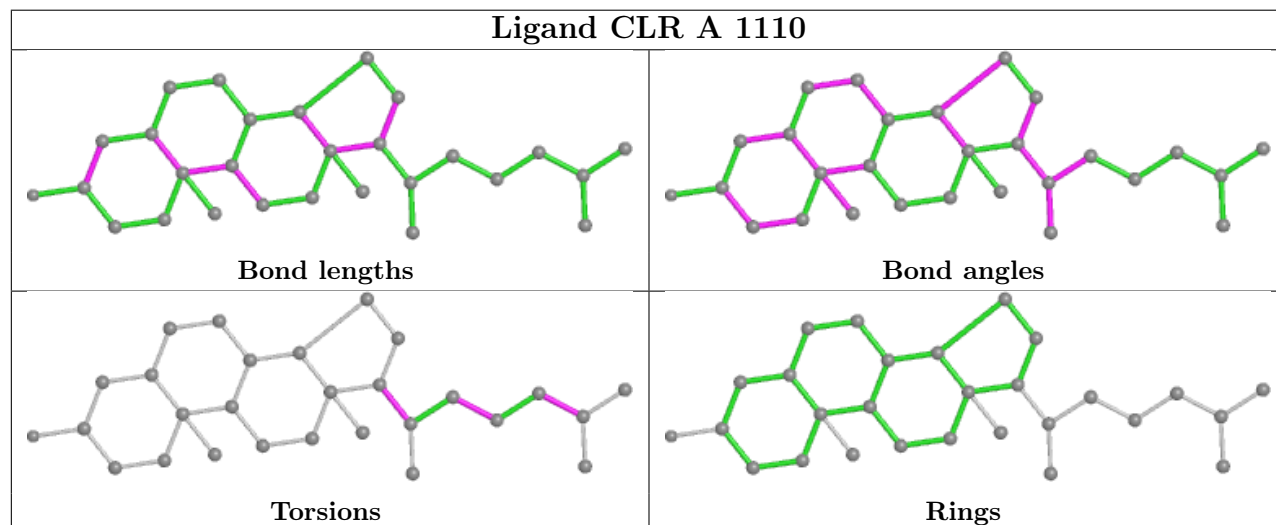
Ligand PCW A 1106



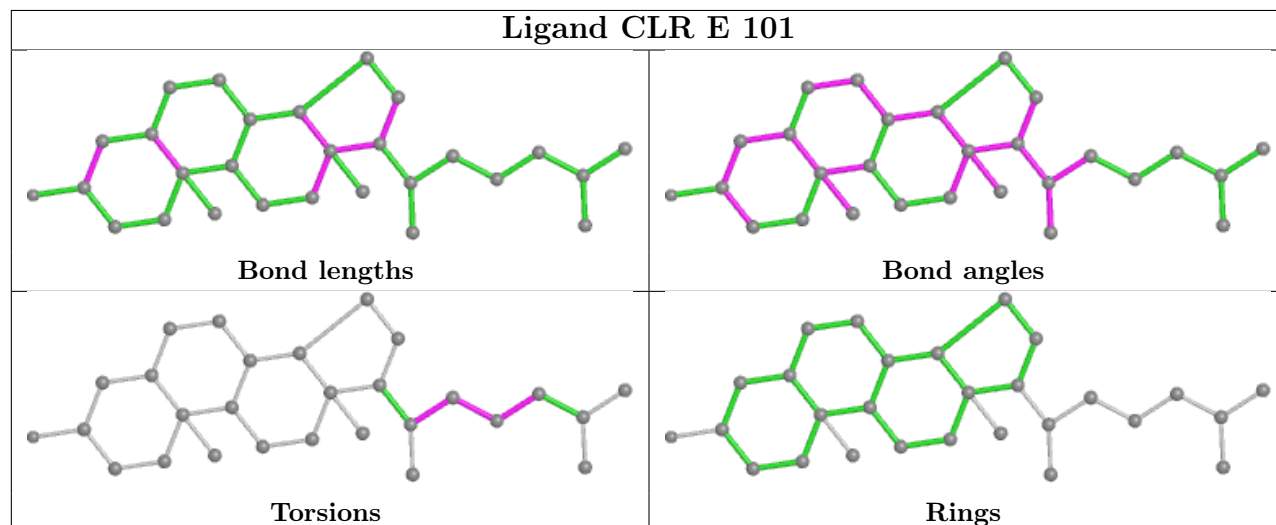
Ligand PCW C 1106

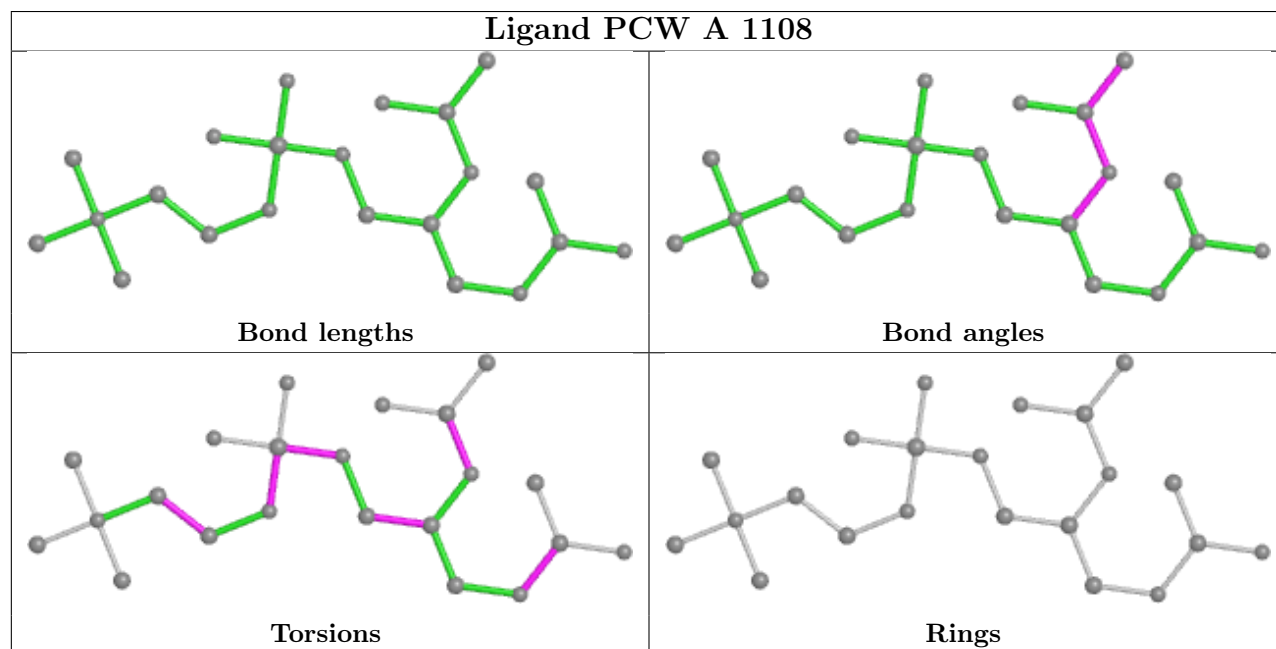
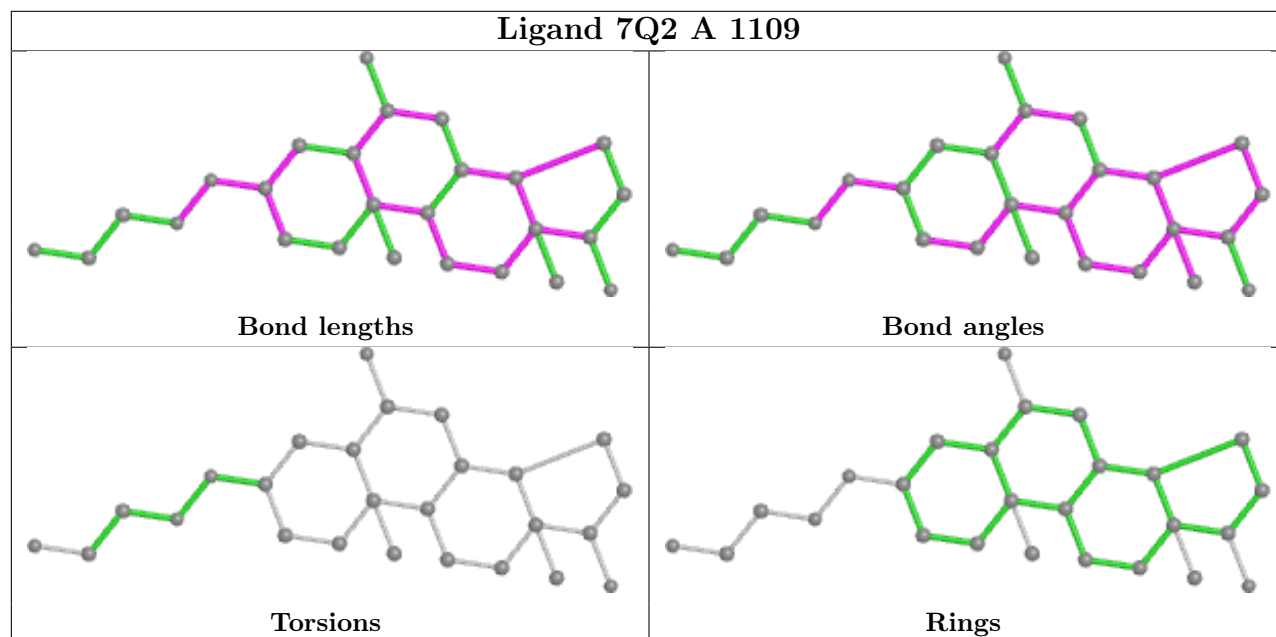


Ligand CLR A 1110

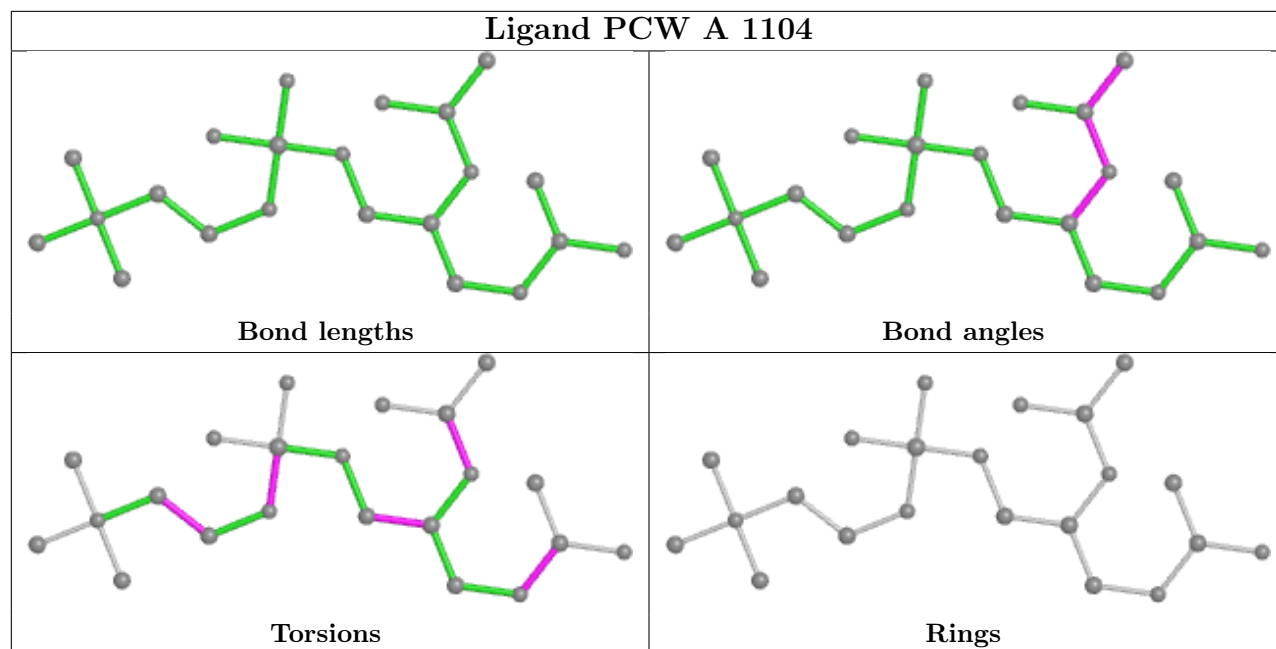


Ligand CLR E 101

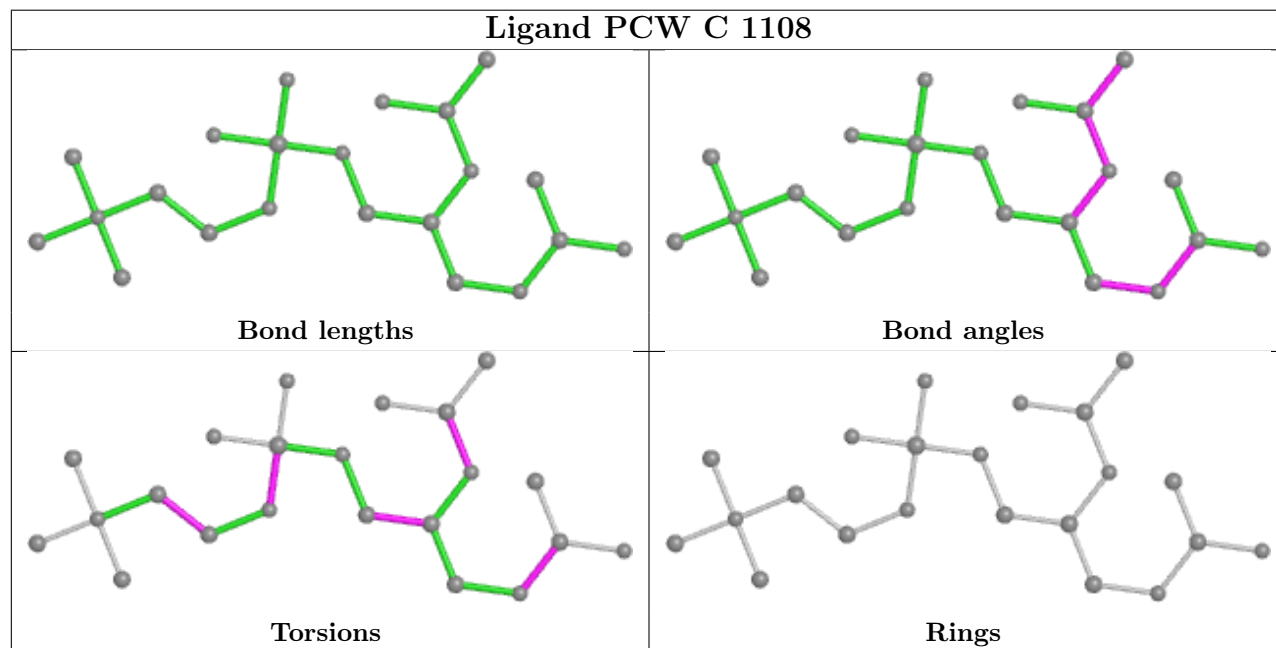




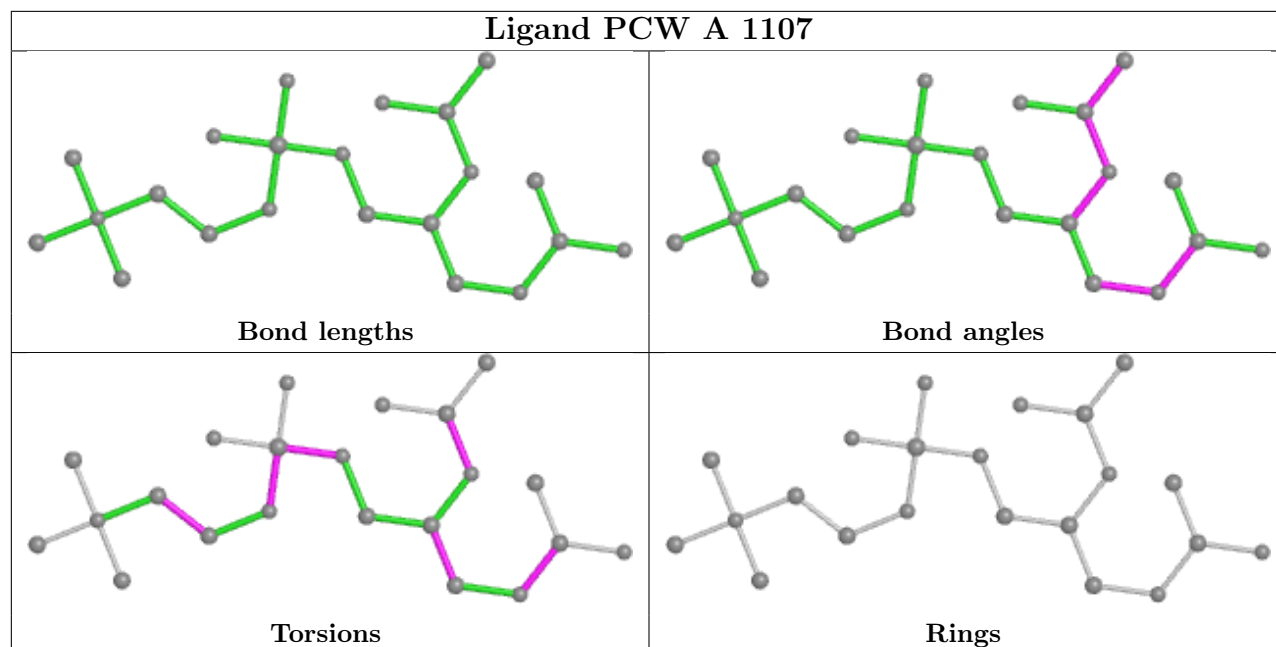
Ligand PCW A 1104



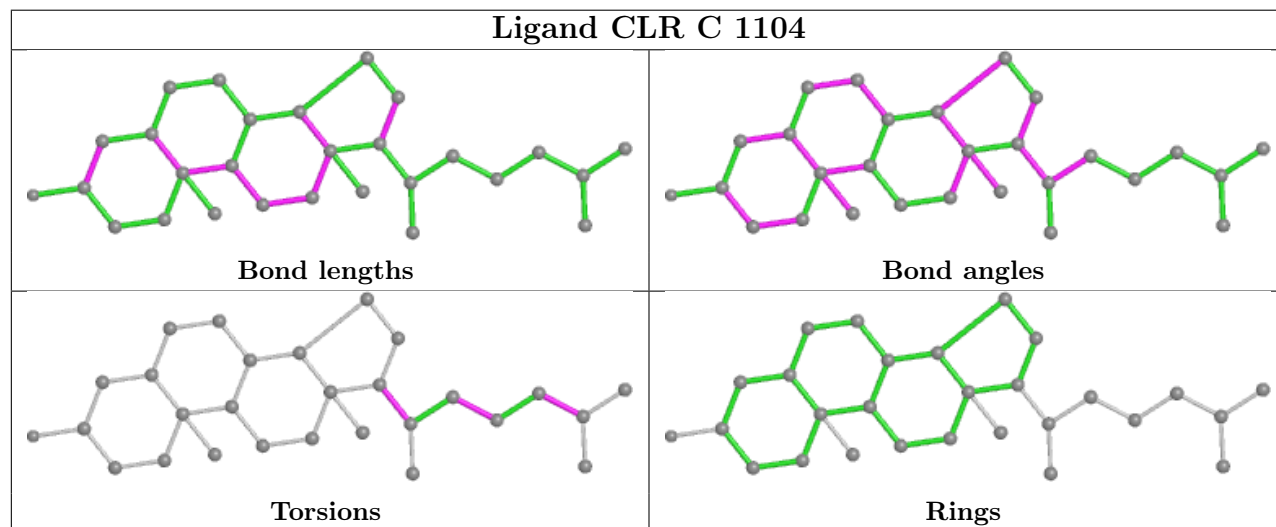
Ligand PCW C 1108



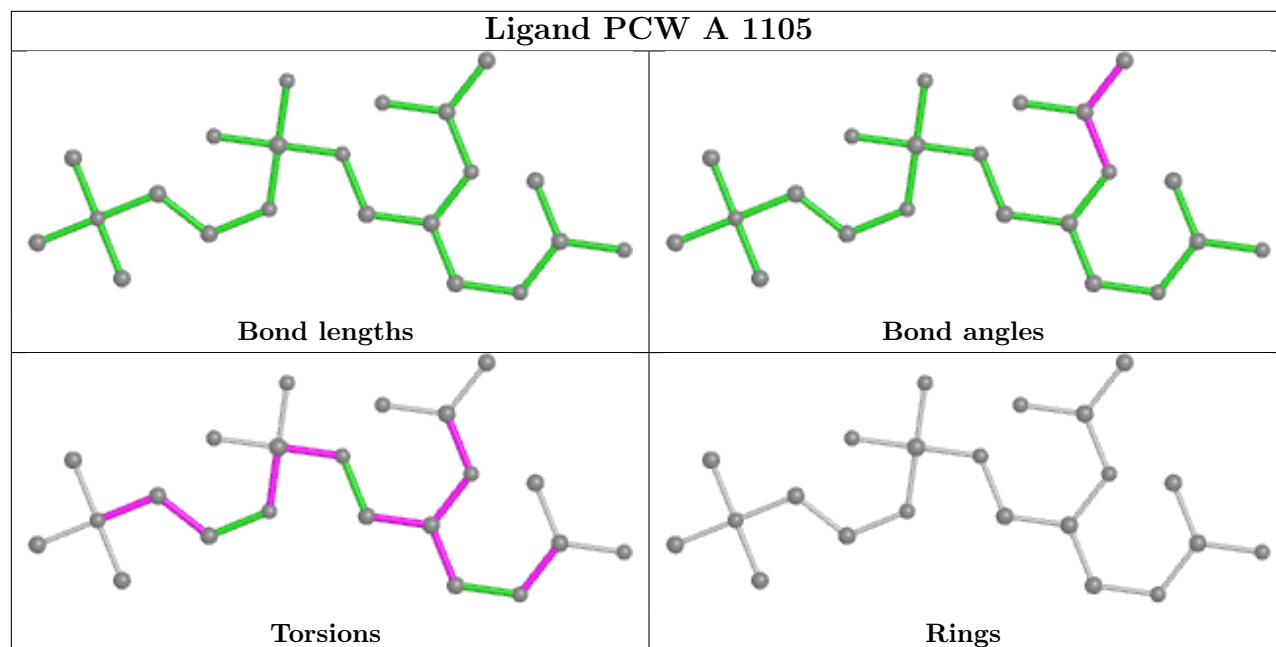
Ligand PCW A 1107



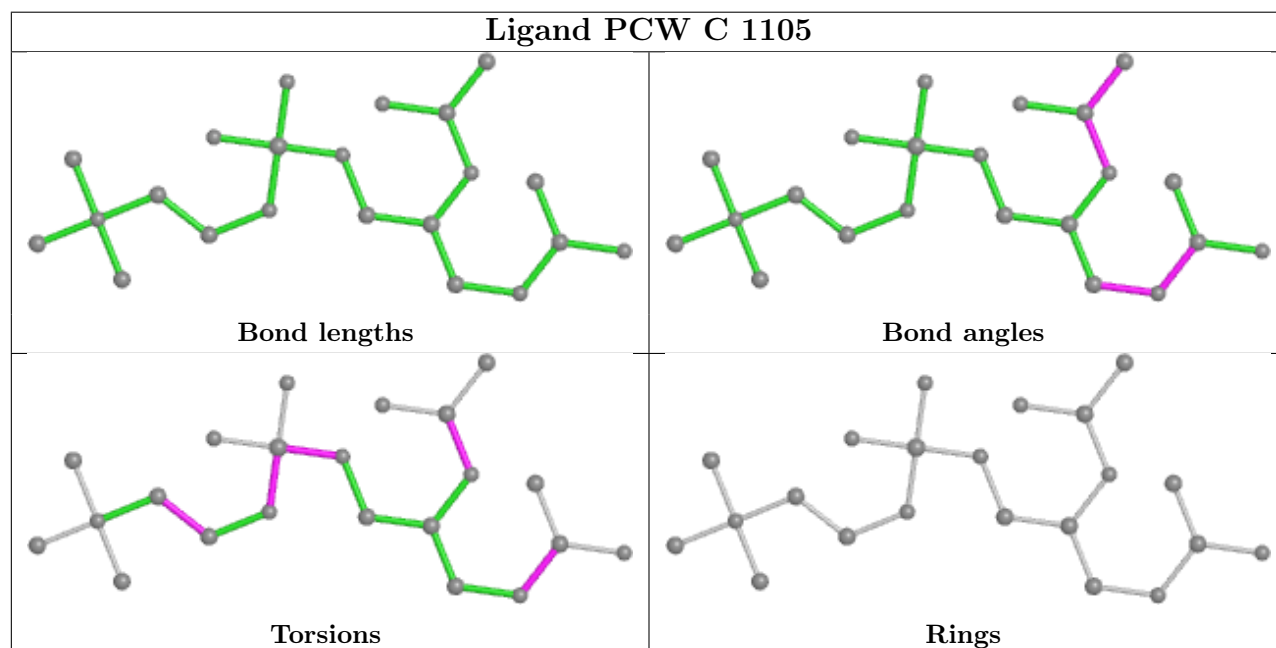
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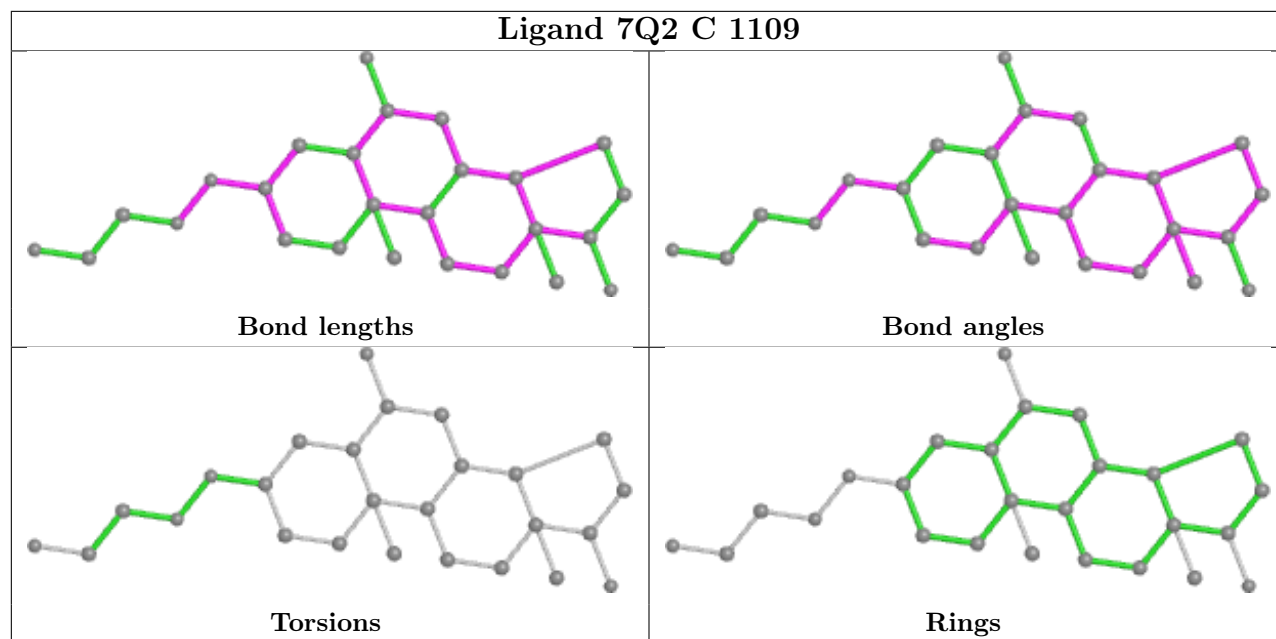


Ligand PCW A 1105



Ligand PCW C 1105





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	995/1016 (97%)	0.00	60 (6%)	21	16	60, 143, 261, 354	0
1	C	995/1016 (97%)	-0.06	49 (4%)	29	25	56, 136, 228, 281	0
2	B	291/303 (96%)	0.18	22 (7%)	13	11	93, 169, 234, 288	0
2	D	285/303 (94%)	-0.09	10 (3%)	44	36	70, 157, 217, 285	0
3	E	32/65 (49%)	-0.35	0	100	100	68, 110, 174, 191	0
3	G	32/65 (49%)	-0.65	0	100	100	62, 115, 166, 172	0
All	All	2630/2768 (95%)	-0.02	141 (5%)	25	22	56, 145, 243, 354	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	499	VAL	7.9
1	A	498	LEU	7.4
1	A	522	PRO	7.1
2	B	166	THR	6.0
1	A	489	PRO	6.0
1	C	571	PHE	5.4
1	A	553	LEU	5.4
1	A	467	TYR	5.3
1	A	491	THR	5.0
1	C	471	VAL	5.0
1	C	500	MET	5.0
1	C	485	ILE	4.9
1	C	498	LEU	4.8
1	A	490	ASN	4.7
1	A	550	HIS	4.7
1	C	548	PHE	4.5
1	A	485	ILE	4.5
1	C	483	LEU	4.4
1	C	484	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	551	LEU	4.4
1	C	491	THR	4.3
1	A	497	LEU	4.3
1	C	579	VAL	4.2
1	C	501	LYS	4.2
1	A	520	GLU	4.0
2	B	165	GLU	4.0
1	A	578	PHE	4.0
2	D	20	GLU	4.0
1	A	571	PHE	3.9
1	C	497	LEU	3.9
1	A	552	PHE	3.8
2	B	184	LEU	3.8
2	D	197	GLU	3.8
1	A	523	LEU	3.7
1	A	521	GLN	3.7
1	A	575	ASN	3.7
1	C	473	ILE	3.6
2	B	167	TYR	3.6
1	C	482	GLN	3.6
1	A	514	ILE	3.6
1	A	486	HIS	3.5
1	A	496	HIS	3.5
2	D	139	TYR	3.5
1	A	519	LYS	3.5
1	A	21	LYS	3.4
1	C	481	TYR	3.4
1	C	384	MET	3.4
1	C	550	HIS	3.4
1	C	556	GLU	3.4
1	A	465	GLU	3.3
1	C	470	ILE	3.3
2	B	216	LYS	3.3
1	A	466	ARG	3.2
2	B	275	GLU	3.2
1	A	499	VAL	3.2
1	A	22	GLU	3.2
2	B	178	ILE	3.1
1	C	486	HIS	3.1
1	C	435	ILE	3.1
1	C	582	ILE	3.1
2	B	139	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	557	GLN	3.1
1	A	488	ASN	3.1
2	B	271	GLU	3.0
1	A	420	LEU	2.9
1	A	381	VAL	2.9
1	C	474	PRO	2.9
1	A	524	ASP	2.9
1	A	580	GLY	2.9
2	D	64	PHE	2.9
1	A	106	LEU	2.8
1	A	542	GLY	2.8
1	A	582	ILE	2.8
1	A	583	SER	2.8
1	A	527	LEU	2.8
1	A	545	VAL	2.8
1	A	464	ARG	2.8
1	A	492	ALA	2.8
2	D	260	ALA	2.8
1	A	377	ASN	2.8
1	C	410	THR	2.8
1	A	581	LEU	2.7
2	D	184	LEU	2.7
2	D	230	PHE	2.7
1	C	553	LEU	2.6
2	B	267	THR	2.6
1	C	564	PHE	2.6
1	A	484	SER	2.6
1	A	468	THR	2.6
2	B	64	PHE	2.6
2	B	199	TYR	2.5
1	A	470	ILE	2.5
2	B	138	GLU	2.5
2	B	273	ARG	2.5
1	C	385	TRP	2.5
1	A	572	PRO	2.5
1	C	476	ASN	2.4
1	C	155	LYS	2.4
2	B	259	MET	2.4
1	A	584	MET	2.4
1	A	884	ASP	2.4
1	C	388	ASN	2.4
2	B	77	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	197	GLU	2.4
1	C	487	LYS	2.4
2	B	164	ASP	2.4
1	A	515	LEU	2.4
1	C	75	PRO	2.3
1	A	579	VAL	2.3
1	A	548	PHE	2.3
1	A	350	LEU	2.3
1	C	681	ILE	2.3
2	D	250	LEU	2.3
1	A	512	SER	2.3
2	B	294	ARG	2.3
1	A	538	LEU	2.2
1	C	390	ILE	2.2
1	A	525	GLU	2.2
2	D	249	LEU	2.2
1	A	897	GLN	2.2
1	C	581	LEU	2.2
2	B	142	GLU	2.2
2	D	202	MET	2.2
1	C	492	ALA	2.2
2	B	179	LYS	2.2
1	C	463	MET	2.2
1	C	477	SER	2.2
1	C	429	ASN	2.2
2	B	293	GLY	2.1
1	A	504	PRO	2.1
1	C	580	GLY	2.1
1	C	457	CYS	2.1
1	C	502	GLY	2.1
1	C	566	THR	2.1
1	A	543	GLU	2.1
1	C	377	ASN	2.1
1	A	804	ASP	2.1
1	C	409	ALA	2.0
1	A	487	LYS	2.0
1	C	156	ASN	2.0
1	C	460	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PHD	A	369	12/13	0.98	0.24	95,111,131,134	0
1	PHD	C	369	12/13	0.98	0.18	89,98,110,112	0

6.3 Carbohydrates [i](#)

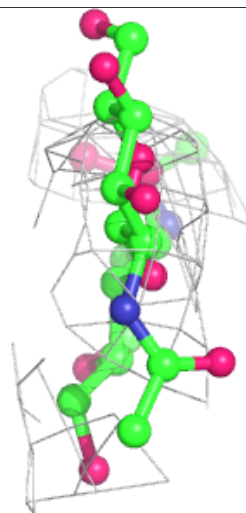
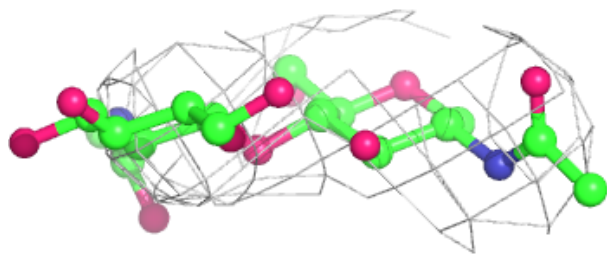
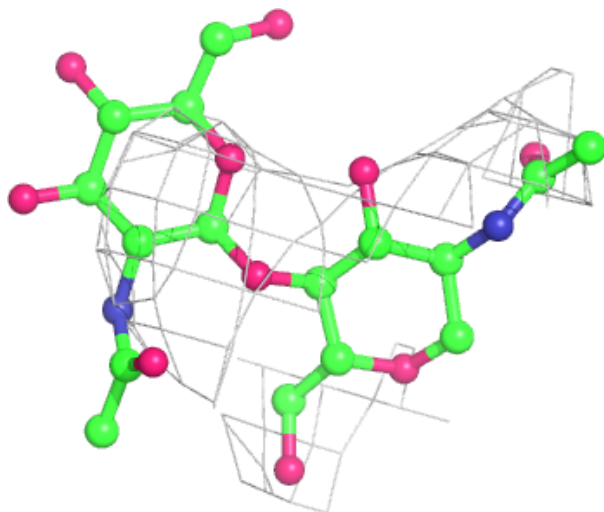
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	H	2	14/15	0.60	0.55	312,318,320,320	0
4	NAG	F	1	14/15	0.70	0.28	179,217,236,250	0
4	NAG	J	2	14/15	0.78	0.84	224,253,261,270	0
4	NAG	F	2	14/15	0.80	0.61	242,266,274,275	0
4	NAG	J	1	14/15	0.83	0.57	206,223,237,247	0
4	NAG	H	1	14/15	0.86	0.29	234,263,289,306	0
4	NAG	I	1	14/15	0.88	0.19	191,197,205,207	0
4	NAG	I	2	14/15	0.91	0.17	188,210,226,246	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.

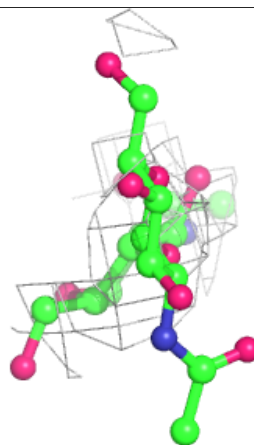
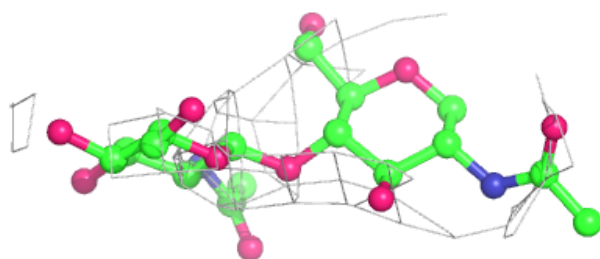
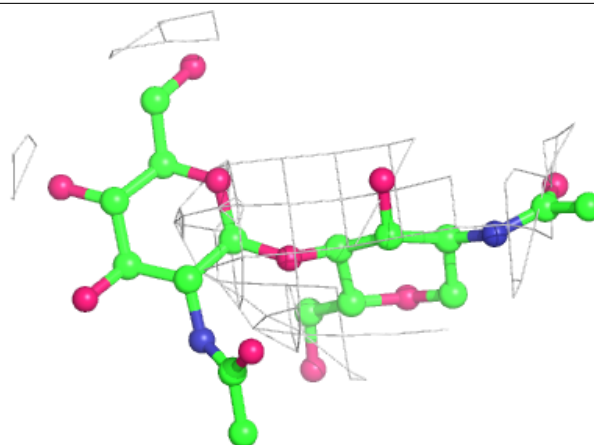
Electron density around Chain F:

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



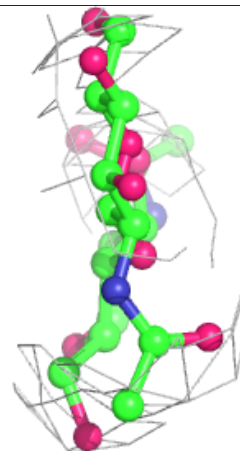
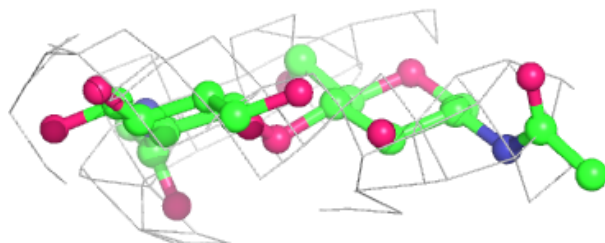
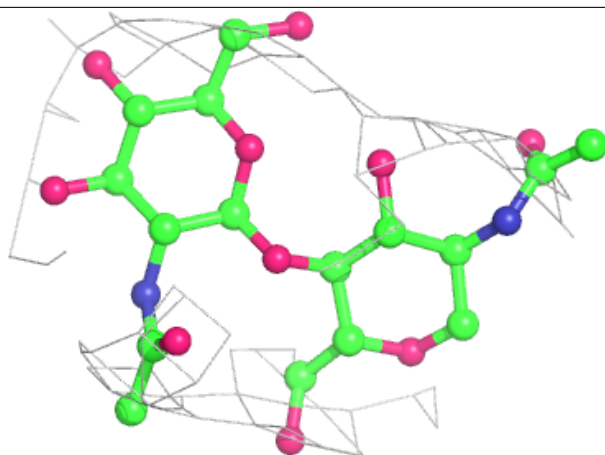
Electron density around Chain H:

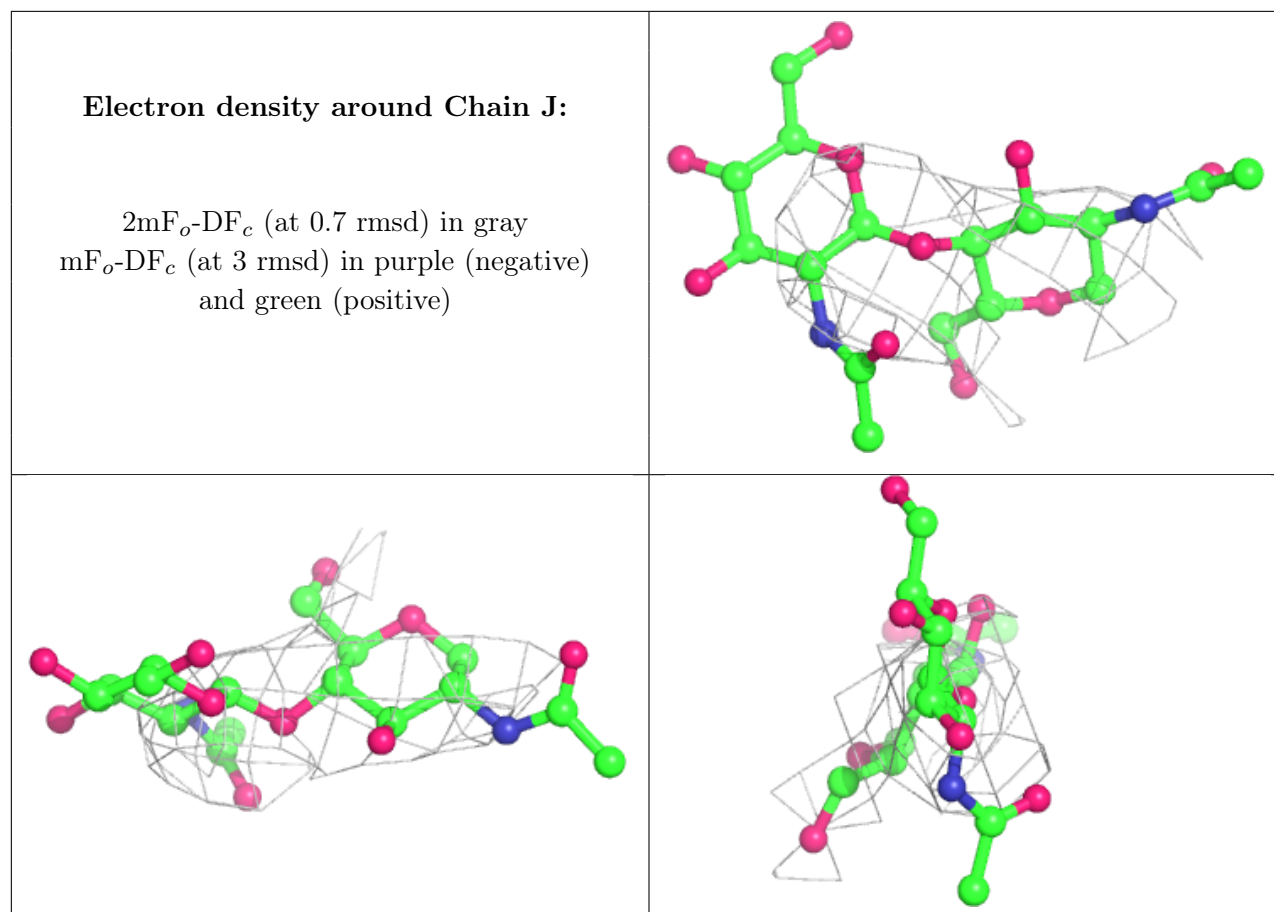
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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

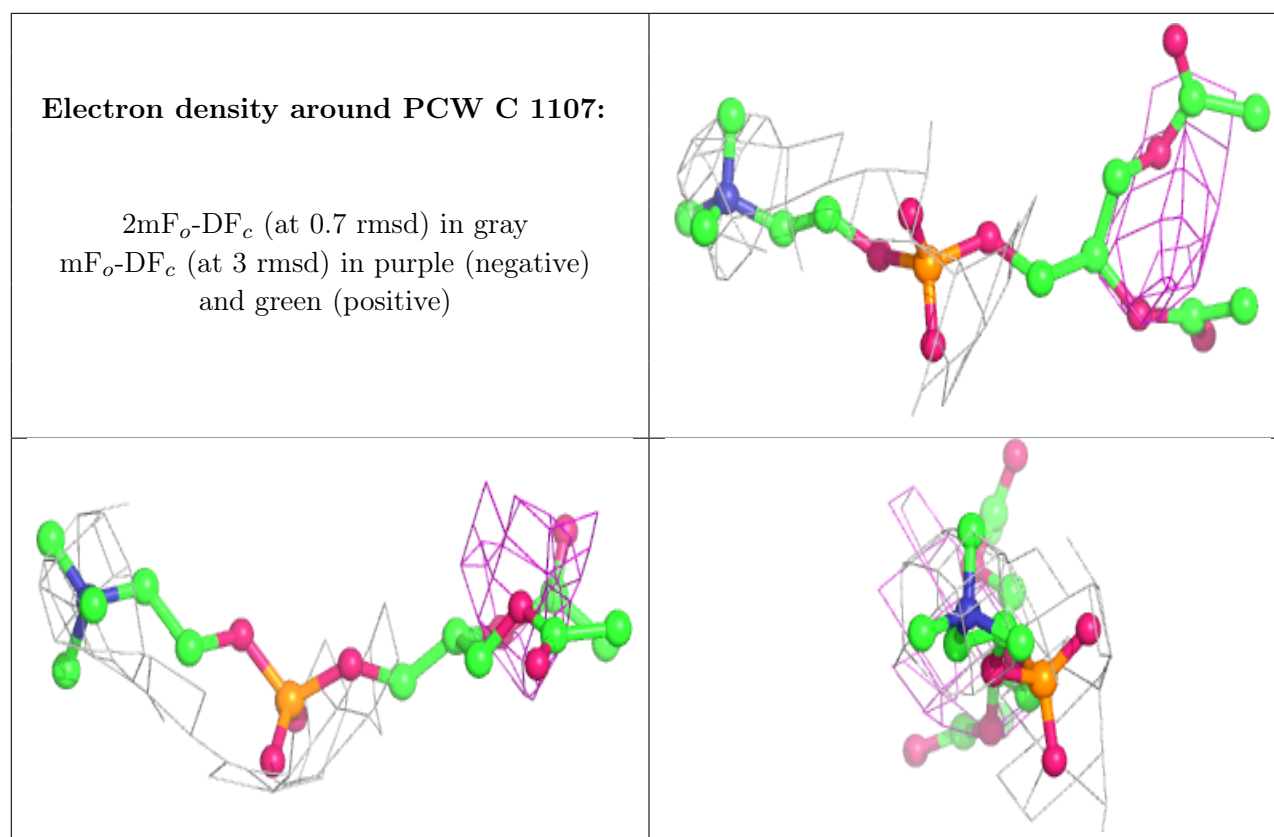
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PCW	C	1107	22/54	0.46	0.72	185,210,228,231	0
7	PCW	A	1106	22/54	0.68	0.42	153,206,219,220	0
7	PCW	A	1104	22/54	0.76	0.39	165,201,247,265	0
7	PCW	A	1105	22/54	0.79	0.32	175,215,243,250	0
7	PCW	D	402	22/54	0.79	0.30	177,227,246,247	0
7	PCW	C	1106	22/54	0.80	0.37	157,223,236,247	0
9	CLR	D	403	28/28	0.80	0.54	126,189,202,208	0
10	NAG	B	401	14/15	0.83	0.18	172,205,225,226	0
7	PCW	C	1105	22/54	0.85	0.36	173,194,231,232	0
9	CLR	B	402	28/28	0.88	0.70	163,176,193,209	0
9	CLR	C	1104	28/28	0.88	0.55	160,168,198,200	0
10	NAG	D	401	14/15	0.88	0.12	160,186,190,191	0

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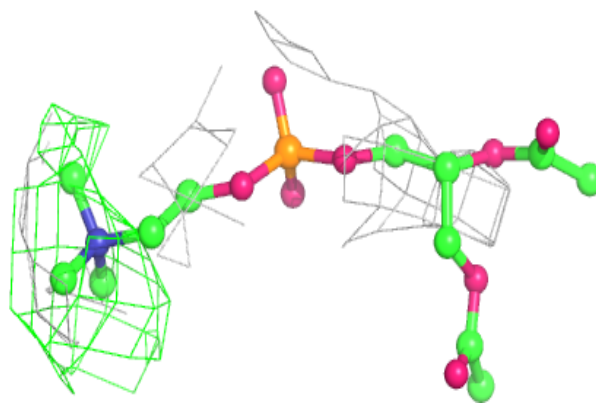
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PCW	A	1108	22/54	0.89	0.37	104,136,185,192	0
8	7Q2	C	1109	26/26	0.90	0.29	117,155,185,189	0
7	PCW	C	1108	22/54	0.90	0.24	128,143,165,170	0
8	7Q2	A	1109	26/26	0.90	0.32	124,171,184,204	0
7	PCW	A	1107	22/54	0.91	0.39	177,251,271,285	0
6	NA	A	1102	1/1	0.91	0.23	57,57,57,57	0
9	CLR	A	1110	28/28	0.92	0.34	132,145,154,163	0
9	CLR	E	101	28/28	0.92	0.32	71,99,109,114	0
6	NA	C	1102	1/1	0.94	0.31	27,27,27,27	0
9	CLR	G	101	28/28	0.96	0.31	61,74,110,120	0
5	MG	A	1101	1/1	0.96	0.23	160,160,160,160	0
5	MG	A	1103	1/1	0.96	0.28	176,176,176,176	0
5	MG	C	1103	1/1	0.97	0.18	168,168,168,168	0
5	MG	C	1101	1/1	0.99	0.13	126,126,126,126	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.

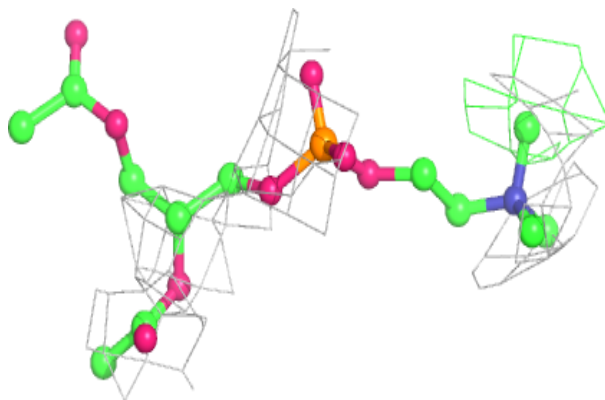


Electron density around PCW A 1106:

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

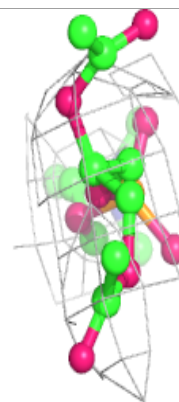
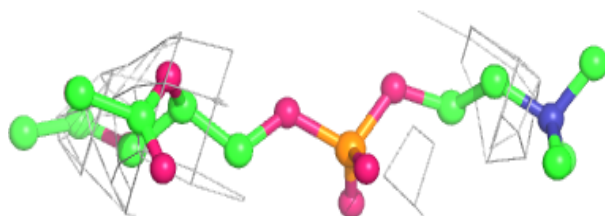
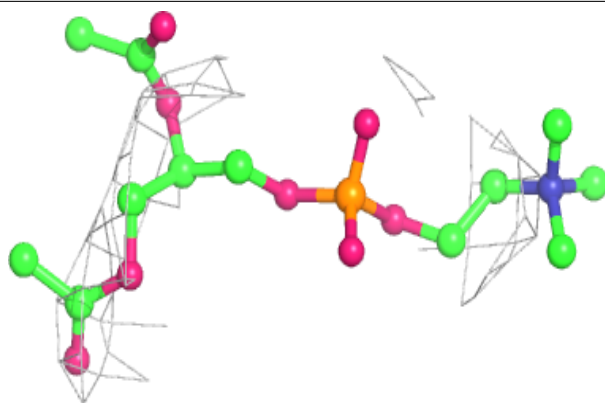
**Electron density around PCW A 1104:**

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

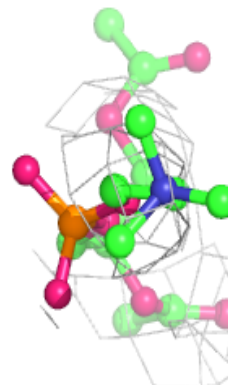
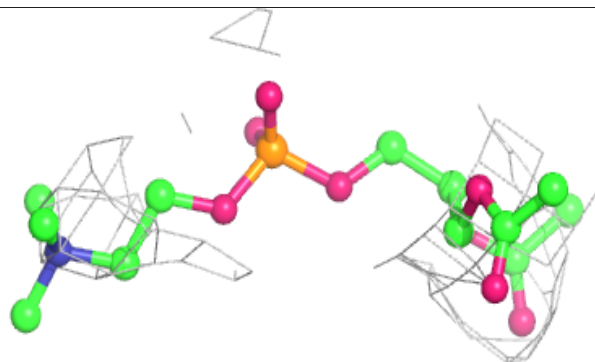
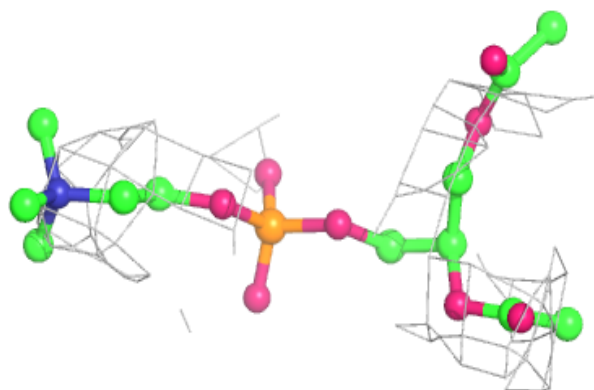


Electron density around PCW A 1105:

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

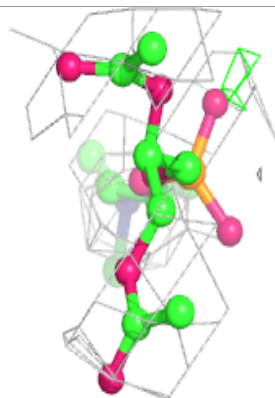
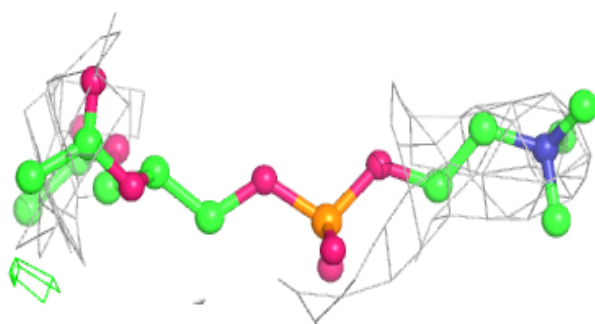
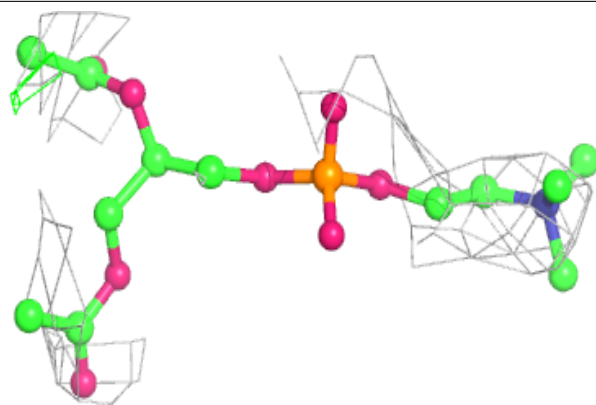
**Electron density around PCW D 402:**

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

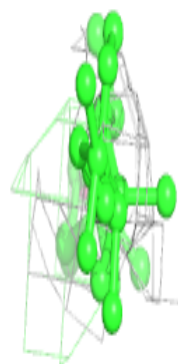
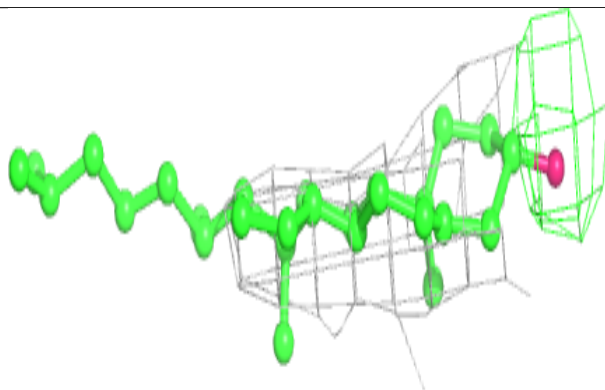
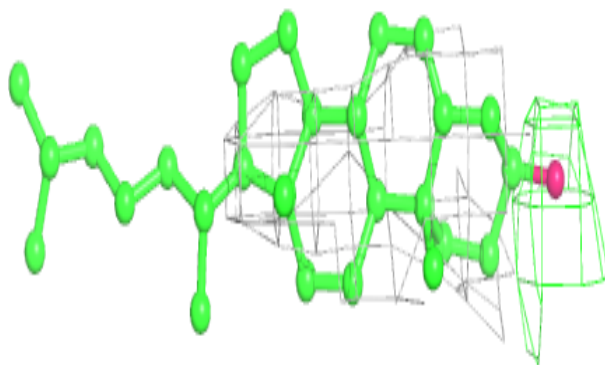


Electron density around PCW C 1106:

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

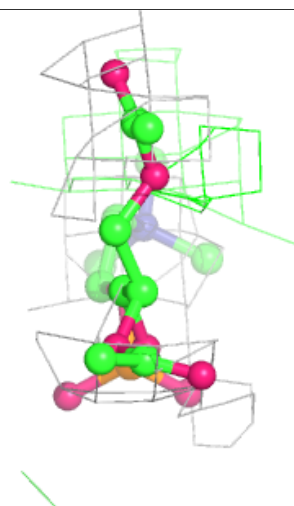
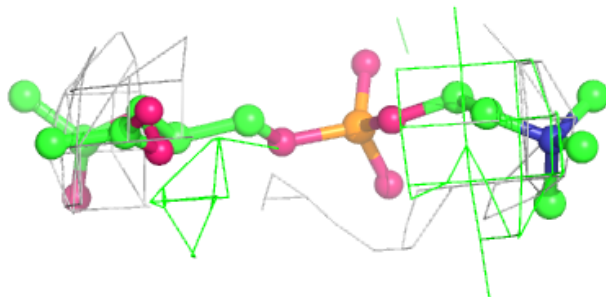
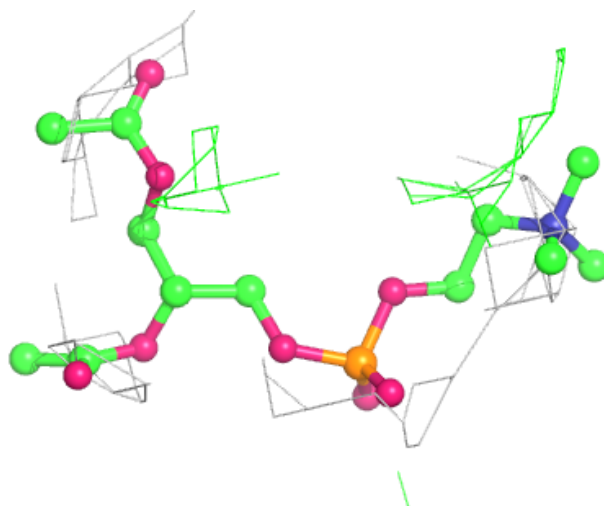
**Electron density around CLR D 403:**

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



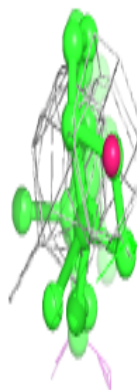
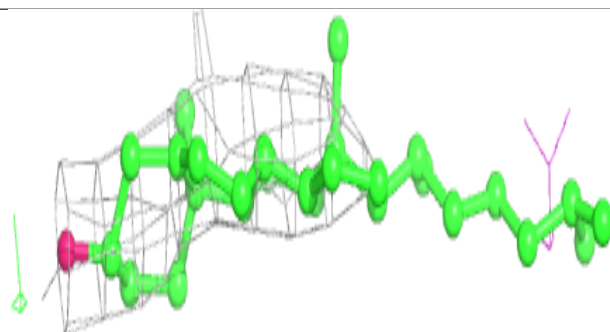
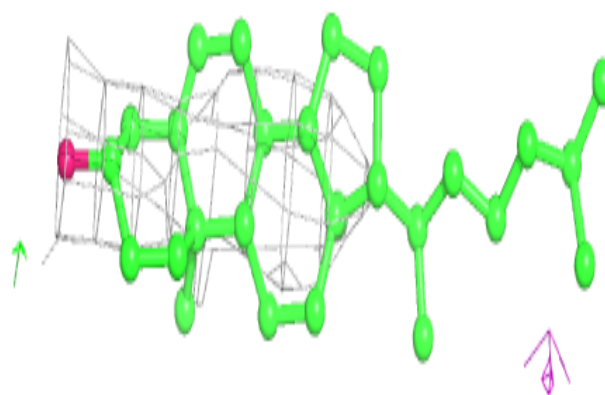
Electron density around PCW C 1105:

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

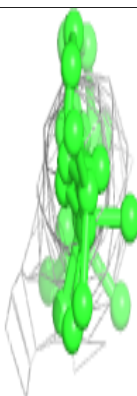
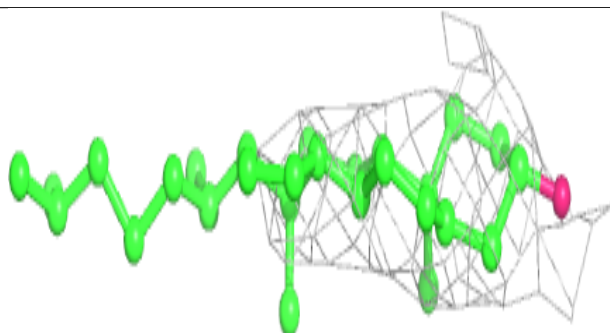
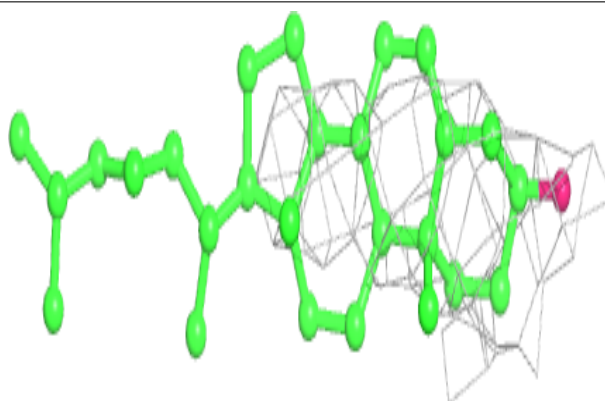


Electron density around CLR B 402:

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

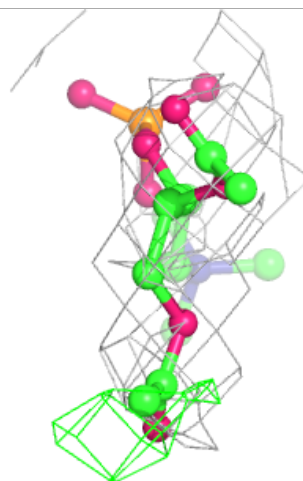
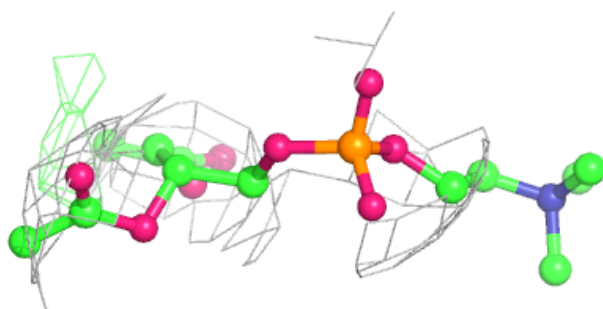
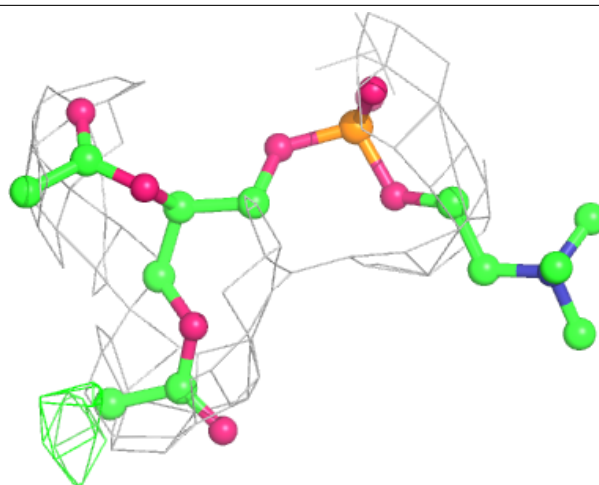
**Electron density around CLR C 1104:**

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



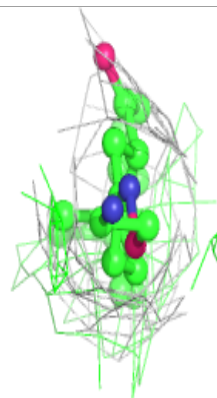
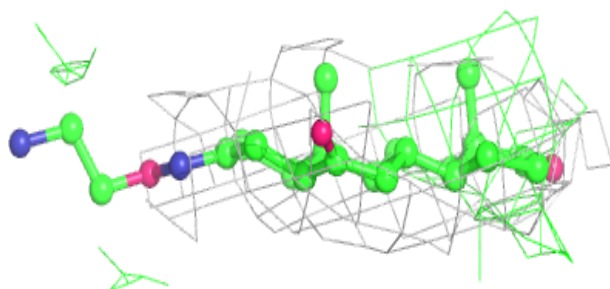
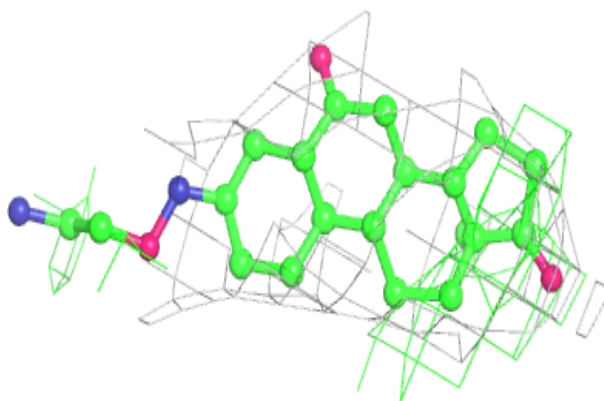
Electron density around PCW A 1108:

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

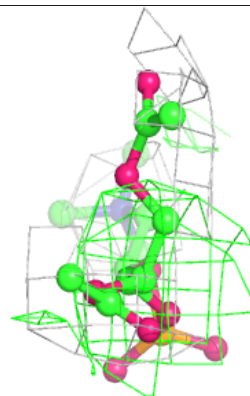
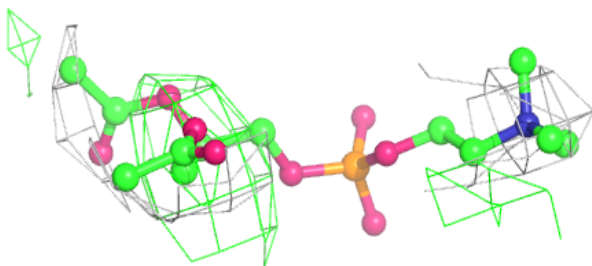
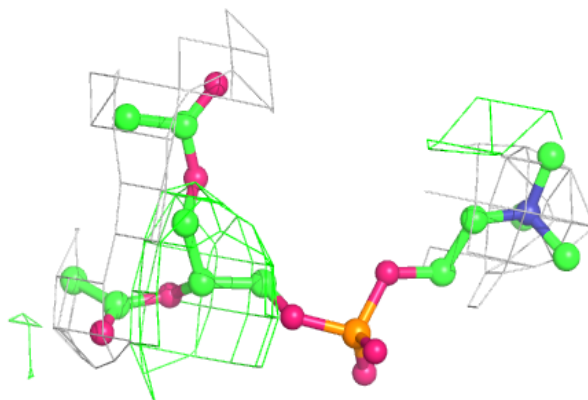


Electron density around 7Q2 C 1109:

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

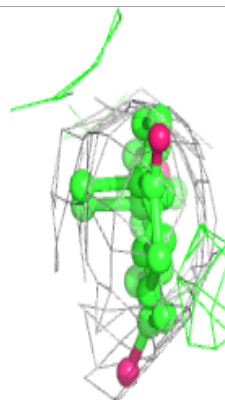
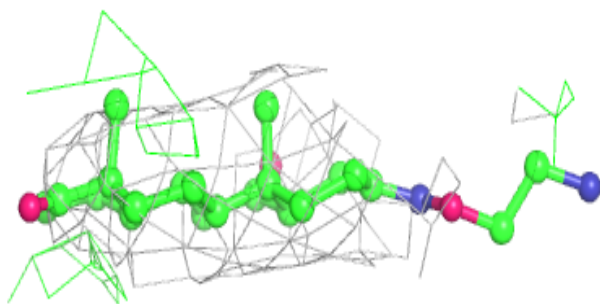
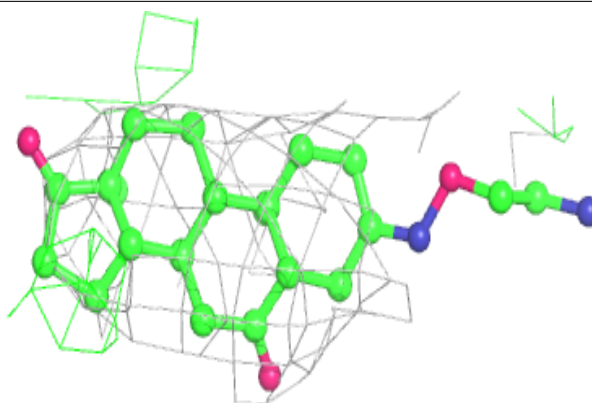
**Electron density around PCW C 1108:**

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

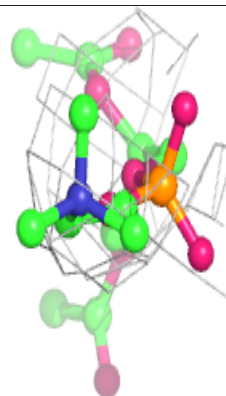
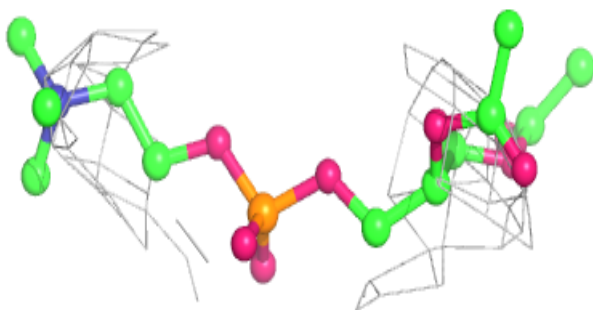
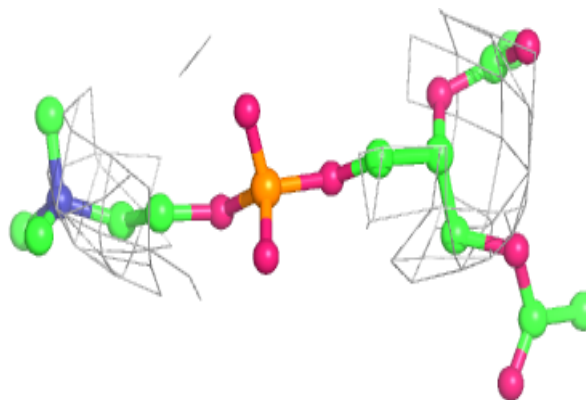


Electron density around 7Q2 A 1109:

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

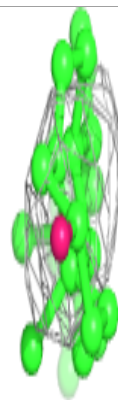
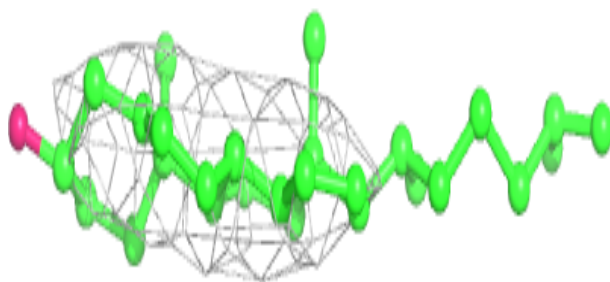
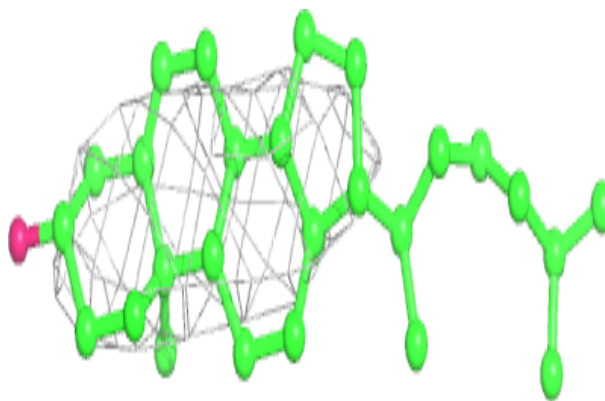
**Electron density around PCW A 1107:**

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

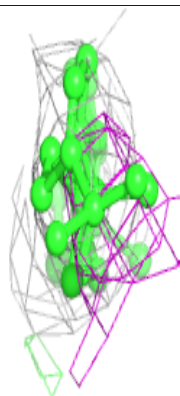
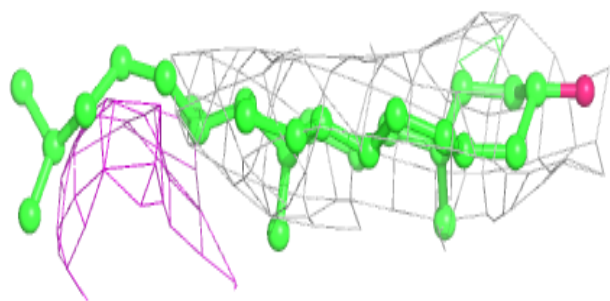
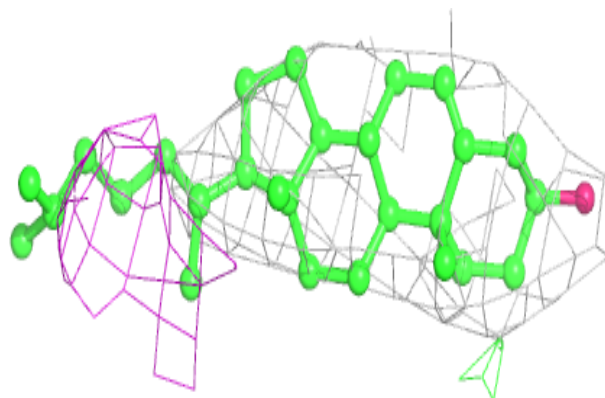


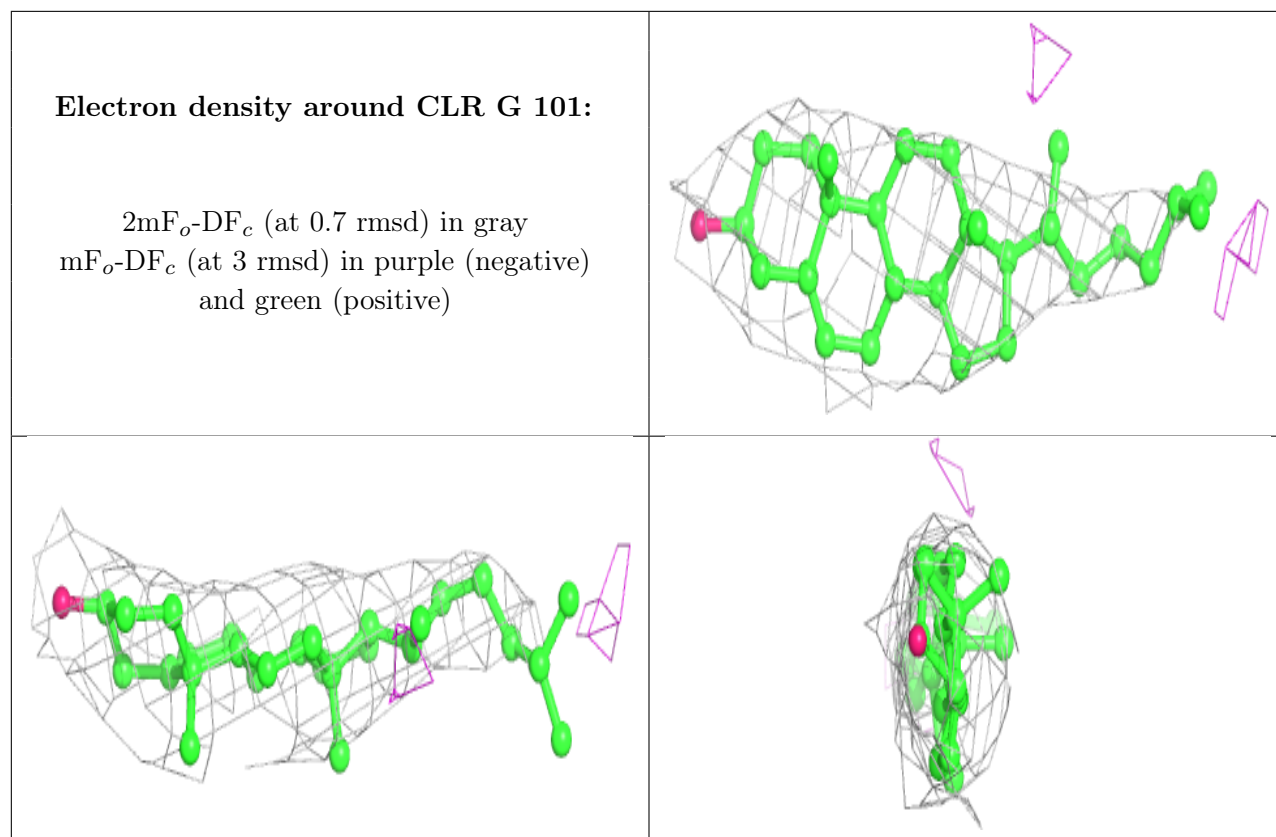
Electron density around CLR A 1110:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.