



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2022 – 12:58 AM JST

PDB ID : 7WYT
Title : Crystal structures of Na⁺,K⁺-ATPase in complex with ouabain
Authors : Ogawa, H.; Cornelius, F.; Kanai, R.; Motoyama, K.; Vilsen, B.; Toyoshima, C.
Deposited on : 2022-02-16
Resolution : 2.90 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:

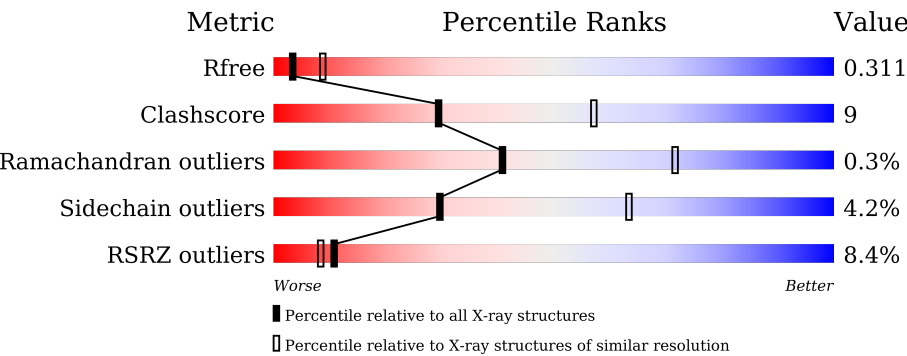
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & 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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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>10%</div><div><div>76%</div><div>21%</div><div>..</div></div></div>
1	C	1016	<div><div>6%</div><div><div>74%</div><div>23%</div><div>..</div></div></div>
2	B	303	<div><div>11%</div><div><div>67%</div><div>26%</div><div>..</div></div></div>
2	D	303	<div><div>8%</div><div><div>62%</div><div>30%</div><div>6%</div></div></div>
3	E	65	<div><div>2%</div><div><div>42%</div><div>8%</div><div>51%</div></div></div>
3	G	65	<div><div></div><div><div>43%</div><div>6%</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
10	NAG	D	401	-	-	-	X
4	NAG	F	2	-	-	-	X
4	NAG	H	1	-	-	-	X
4	NAG	H	2	-	-	-	X
8	PCW	A	1107	-	-	-	X
8	PCW	A	1109	-	-	-	X
8	PCW	A	1110	-	-	-	X
8	PCW	A	1111	-	-	-	X
8	PCW	C	1108	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 21354 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

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

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

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

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



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

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

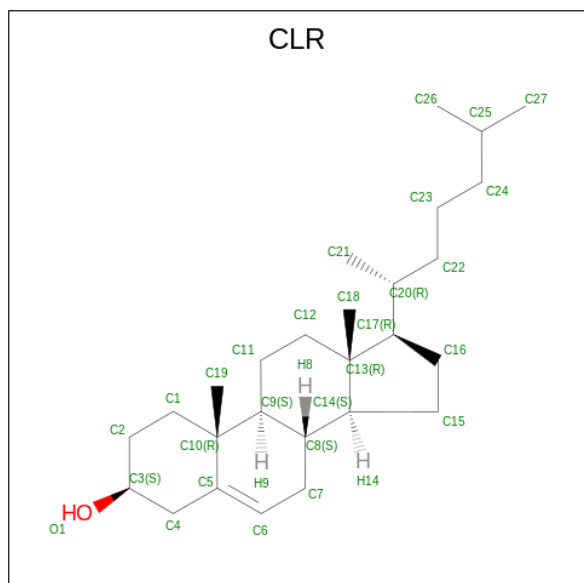
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

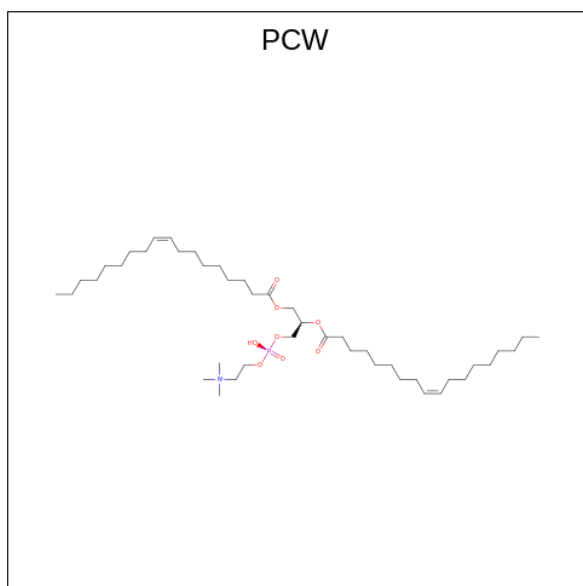
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



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

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



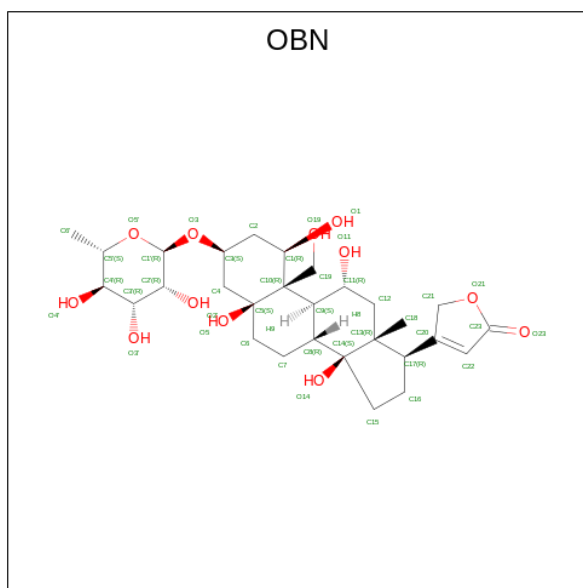
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

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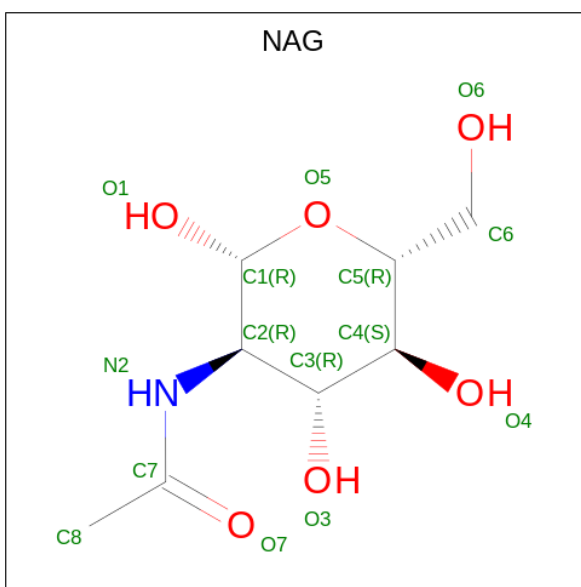
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

- Molecule 9 is OUABAIN (three-letter code: OBN) (formula: $C_{29}H_{44}O_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			41	29	12		
9	C	1	Total	C	O	0	0
			41	29	12		

- 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		

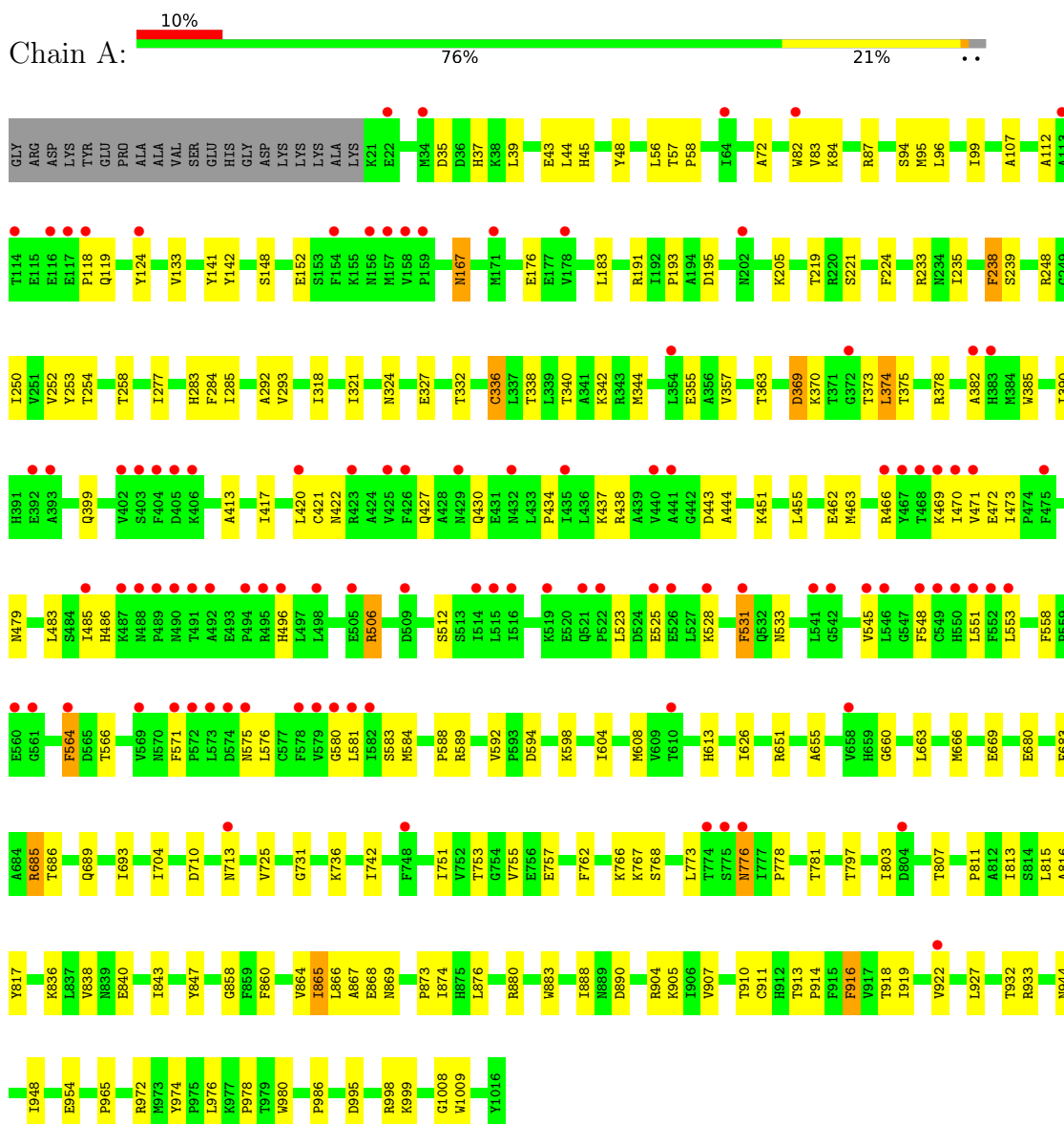
- Molecule 11 is water.

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

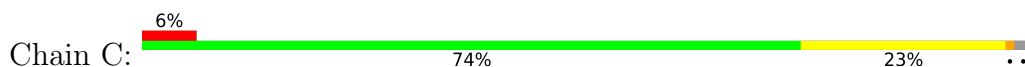
3 Residue-property plots [i](#)

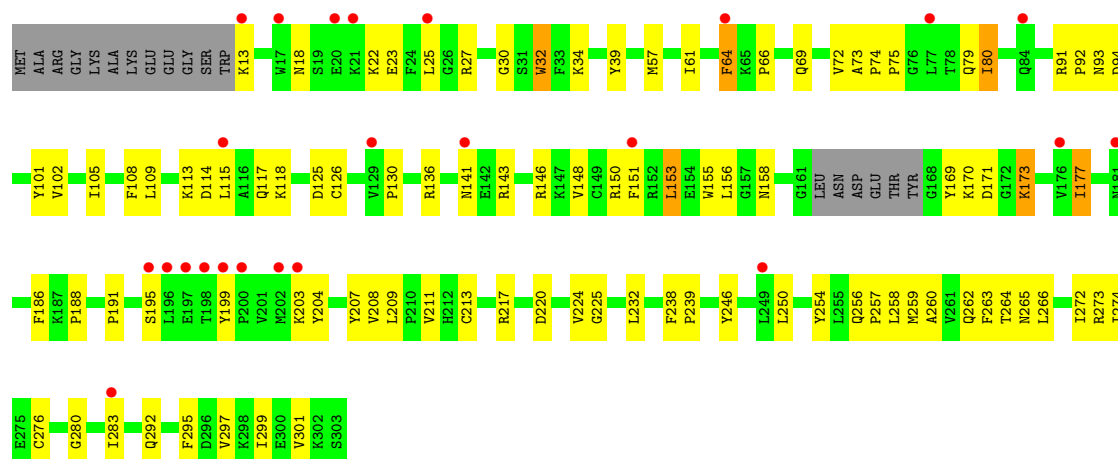
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

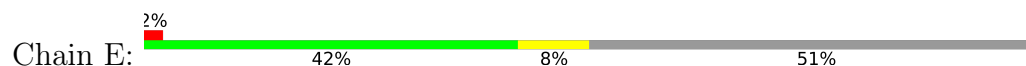




- Molecule 3: FXYD domain-containing ion transport regulator



- Molecule 3: FXYD 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:  50%  50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.62Å 117.81Å 493.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.99 – 2.90 36.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	48.8 (15.99-2.90) 49.0 (36.79-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.270 , 0.307 0.277 , 0.311	Depositor DCC
R_{free} test set	7301 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.126 for k,h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	21354	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: NA, MG, CLR, PHD, PCW, OBN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/7867	0.56	0/10674
1	C	0.29	0/7867	0.57	0/10674
2	B	0.29	0/2449	0.58	0/3301
2	D	0.30	0/2395	0.59	0/3225
3	E	0.31	0/261	0.57	0/354
3	G	0.32	0/261	0.53	0/354
All	All	0.29	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	135	0
1	C	7730	0	7777	147	0
2	B	2386	0	2361	55	0
2	D	2334	0	2317	61	0
3	E	255	0	259	3	0
3	G	255	0	259	2	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	28	0	46	1	0
7	C	56	0	92	4	0
7	D	28	0	46	2	0
7	G	28	0	46	1	0
8	A	198	0	162	10	0
8	C	88	0	72	9	0
9	A	41	0	44	3	0
9	C	41	0	44	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	0	0
All	All	21354	0	21428	404	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (404) 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:A:430:GLN:HG3	1:A:438:ARG:HB2	1.59	0.84
1:C:839:ASN:HB3	8:C:1106:PCW:H82	1.57	0.84
2:D:80:ILE:HG12	2:D:177:ILE:HG12	1.60	0.83
2:B:80:ILE:HG12	2:B:177:ILE:HG12	1.63	0.81
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.64	0.79
1:C:430:GLN:HG3	1:C:438:ARG:HB2	1.64	0.79
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.66	0.78
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.69	0.74
1:C:901:TYR:HA	1:C:904:ARG:HE	1.53	0.73
1:A:375:THR:HA	1:A:588:PRO:HA	1.71	0.73
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.70	0.72
1:C:981:TRP:CD2	7:C:1104:CLR:H72	2.26	0.71
1:A:978:PRO:HB3	7:G:101:CLR:H192	1.71	0.71
1:C:221:SER:H	1:C:233:ARG:HB3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:THR:HA	1:C:588:PRO:HA	1.74	0.69
2:D:177:ILE:HA	2:D:260:ALA:HA	1.76	0.68
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.76	0.68
1:C:283:HIS:HD2	8:C:1108:PCW:H62	1.60	0.67
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.77	0.66
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.77	0.66
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.78	0.66
1:A:807:THR:HB	1:A:954:GLU:HG3	1.78	0.64
1:C:238:PHE:HD2	1:C:258:THR:HG21	1.62	0.64
2:D:204:TYR:HE1	2:D:207:TYR:HB2	1.62	0.64
1:C:907:VAL:HA	1:C:910:THR:HG22	1.80	0.64
2:D:80:ILE:HD11	2:D:177:ILE:H	1.62	0.64
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.79	0.63
1:A:96:LEU:HD22	1:A:285:ILE:HG23	1.82	0.62
1:A:205:LYS:HA	1:A:219:THR:HA	1.81	0.62
1:A:864:VAL:HG12	1:A:980:TRP:HZ3	1.64	0.62
1:A:558:PHE:HB3	1:A:564:PHE:HE2	1.66	0.61
1:C:613:HIS:CE1	1:C:685:ARG:HH21	2.19	0.60
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.83	0.60
1:A:385:TRP:HB3	1:A:581:LEU:H	1.67	0.60
1:C:96:LEU:HD22	1:C:285:ILE:HG23	1.82	0.60
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.84	0.60
1:C:512:SER:HB2	1:C:575:ASN:HA	1.84	0.60
2:B:80:ILE:HD11	2:B:177:ILE:H	1.66	0.59
2:D:102:VAL:HG13	2:D:169:TYR:HD2	1.67	0.59
1:C:1004:ARG:HD2	8:C:1107:PCW:H52	1.85	0.59
2:D:191:PRO:HD3	2:D:280:GLY:HA2	1.83	0.59
1:A:363:THR:HA	1:A:704:ILE:HB	1.85	0.58
1:C:558:PHE:HB3	1:C:564:PHE:HE2	1.67	0.58
1:A:221:SER:H	1:A:233:ARG:HB3	1.68	0.58
1:C:663:LEU:HA	1:C:666:MET:HG3	1.86	0.58
1:C:807:THR:HB	1:C:954:GLU:HG3	1.85	0.58
1:A:84:LYS:HG3	1:A:141:TYR:HE1	1.69	0.58
1:C:385:TRP:HD1	1:C:390:ILE:HD13	1.68	0.58
1:C:385:TRP:HB3	1:C:581:LEU:H	1.67	0.58
1:C:594:ASP:O	1:C:598:LYS:HG2	2.04	0.58
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.86	0.57
1:A:907:VAL:HA	1:A:910:THR:HG22	1.86	0.57
2:B:177:ILE:HA	2:B:260:ALA:HA	1.85	0.57
1:A:385:TRP:HE3	1:A:580:GLY:HA2	1.68	0.57
1:C:843:ILE:HG23	1:C:847:TYR:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:LEU:HA	1:C:237:PHE:HZ	1.69	0.57
2:D:66:PRO:HG2	2:D:69:GLN:HG2	1.87	0.57
1:C:434:PRO:HG2	1:C:437:LYS:HB2	1.87	0.56
1:C:284:PHE:HD1	1:C:838:VAL:HG21	1.69	0.56
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.88	0.56
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.88	0.56
1:A:83:VAL:O	1:A:87:ARG:HG2	2.05	0.56
2:D:217:ARG:HH12	2:D:273:ARG:HD2	1.70	0.55
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.87	0.55
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.89	0.55
2:D:225:GLY:HA3	2:D:265:ASN:HB3	1.88	0.55
1:A:512:SER:HB2	1:A:575:ASN:HA	1.88	0.55
1:C:469:LYS:HA	1:C:486:HIS:HD2	1.71	0.55
1:A:434:PRO:HG2	1:A:437:LYS:HB2	1.89	0.55
2:D:130:PRO:HB3	2:D:239:PRO:HB3	1.87	0.55
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.72	0.55
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.89	0.55
2:B:225:GLY:HA3	2:B:265:ASN:HB3	1.89	0.55
1:A:238:PHE:HD2	1:A:258:THR:HG21	1.72	0.55
1:A:473:ILE:HB	1:A:483:LEU:HG	1.89	0.55
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.88	0.55
1:C:995:ASP:OD1	1:C:998:ARG:NH1	2.40	0.54
8:A:1113:PCW:H31	1:C:978:PRO:HB2	1.90	0.54
1:C:470:ILE:HB	1:C:485:ILE:HG23	1.89	0.54
1:C:685:ARG:HH11	1:C:685:ARG:HB3	1.71	0.54
1:A:94:SER:HB3	1:A:133:VAL:HG13	1.89	0.54
1:C:332:THR:HA	1:C:813:ILE:HD11	1.89	0.54
2:D:27:ARG:HG3	2:D:32:TRP:CD1	2.42	0.54
2:D:39:TYR:CE1	7:D:402:CLR:H191	2.42	0.54
1:A:370:LYS:HA	1:A:374:LEU:HB2	1.89	0.54
1:C:72:ALA:HB2	1:C:176:GLU:HG2	1.89	0.54
1:C:284:PHE:CD1	1:C:838:VAL:HG21	2.43	0.54
1:A:913:THR:HB	1:A:976:LEU:HD21	1.90	0.54
2:B:217:ARG:HH12	2:B:273:ARG:HD2	1.74	0.53
1:A:762:PHE:CE1	1:A:766:LYS:HE3	2.44	0.53
1:A:594:ASP:O	1:A:598:LYS:HG2	2.09	0.53
1:A:976:LEU:HB3	1:A:980:TRP:HD1	1.73	0.53
2:B:280:GLY:HA3	2:B:283:ILE:HD13	1.91	0.53
1:C:385:TRP:HE3	1:C:580:GLY:HA2	1.74	0.53
2:D:27:ARG:HG3	2:D:32:TRP:HD1	1.74	0.53
1:A:736:LYS:HG3	1:A:742:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:CYS:HB2	2:B:295:PHE:HD2	1.74	0.53
1:A:58:PRO:HD3	1:A:167:ASN:HB2	1.90	0.53
2:B:27:ARG:HG3	2:B:32:TRP:CD1	2.44	0.53
1:C:88:GLN:NE2	1:C:144:GLU:OE2	2.42	0.53
2:D:91:ARG:HG2	2:D:93:ASN:H	1.74	0.53
1:A:284:PHE:CD1	1:A:838:VAL:HG21	2.44	0.52
1:A:479:ASN:HA	1:A:506:ARG:HD3	1.91	0.52
1:A:663:LEU:HA	1:A:666:MET:HG3	1.90	0.52
2:B:80:ILE:HB	2:B:105:ILE:HD12	1.92	0.52
2:B:191:PRO:HD3	2:B:280:GLY:HA2	1.91	0.52
2:D:39:TYR:CZ	7:D:402:CLR:H191	2.44	0.52
2:B:66:PRO:HG2	2:B:69:GLN:HG2	1.91	0.52
1:C:363:THR:HA	1:C:704:ILE:HB	1.90	0.52
2:B:92:PRO:HG3	2:B:301:VAL:HG12	1.92	0.52
1:C:710:ASP:HB2	1:C:731:GLY:HA2	1.90	0.52
2:D:213:CYS:HA	2:D:276:CYS:HA	1.92	0.52
1:C:340:THR:O	1:C:344:MET:HG2	2.10	0.52
2:B:156:LEU:HD13	2:B:260:ALA:HB2	1.92	0.52
1:C:48:TYR:HE2	1:C:252:VAL:HG22	1.75	0.52
1:C:421:CYS:O	1:C:422:ASN:ND2	2.43	0.52
1:C:931:LYS:HG2	1:C:932:THR:HG23	1.91	0.52
1:C:589:ARG:HB2	1:C:592:VAL:HG23	1.92	0.52
1:A:776:ASN:ND2	11:A:1201:HOH:O	2.41	0.52
1:C:981:TRP:CE3	7:C:1104:CLR:H72	2.45	0.52
2:B:101:TYR:O	2:B:105:ILE:HG12	2.10	0.51
2:D:276:CYS:HB2	2:D:295:PHE:HD2	1.75	0.51
2:B:173:LYS:HG3	2:B:264:THR:O	2.11	0.51
8:A:1106:PCW:H72	2:B:13:LYS:NZ	2.25	0.51
1:A:986:PRO:HB3	7:A:1104:CLR:H221	1.92	0.51
8:A:1106:PCW:H83	2:B:13:LYS:NZ	2.26	0.51
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.75	0.51
1:A:338:THR:O	1:A:342:LYS:HG2	2.10	0.51
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.92	0.51
8:A:1106:PCW:H72	2:B:13:LYS:HZ3	1.76	0.51
2:B:266:LEU:HD22	2:B:272:ILE:HD11	1.93	0.51
1:A:142:TYR:CZ	8:A:1112:PCW:H83	2.45	0.51
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.92	0.50
1:A:112:ALA:HA	1:A:118:PRO:HG2	1.92	0.50
1:A:683:PHE:HB3	1:A:686:THR:HG21	1.92	0.50
1:A:883:TRP:CH2	1:A:904:ARG:HB2	2.46	0.50
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LYS:HA	1:A:486:HIS:HD2	1.76	0.50
1:C:473:ILE:HB	1:C:483:LEU:HG	1.93	0.50
1:C:776:ASN:HB3	1:C:847:TYR:HE1	1.76	0.50
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.92	0.50
2:B:213:CYS:HA	2:B:276:CYS:HA	1.94	0.50
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.47	0.50
1:C:496:HIS:HB2	1:C:553:LEU:HB2	1.93	0.50
1:C:798:VAL:HG11	1:C:971:LEU:HD22	1.94	0.50
1:A:284:PHE:HE1	1:A:773:LEU:HD11	1.76	0.50
1:C:111:GLN:O	1:C:115:GLU:HG2	2.12	0.50
1:A:344:MET:HG3	1:A:357:VAL:HG23	1.94	0.49
2:D:266:LEU:HD22	2:D:272:ILE:HD11	1.93	0.49
1:A:283:HIS:CE1	8:A:1106:PCW:H51	2.47	0.49
2:B:224:VAL:HG21	2:B:274:ILE:HD11	1.93	0.49
1:A:890:ASP:OD1	1:A:890:ASP:N	2.46	0.49
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.95	0.49
2:B:91:ARG:HG2	2:B:93:ASN:H	1.76	0.49
1:A:385:TRP:HD1	1:A:390:ILE:HD13	1.77	0.49
2:D:280:GLY:HA3	2:D:283:ILE:HD13	1.93	0.49
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.48	0.48
1:C:148:SER:O	1:C:152:GLU:HG2	2.13	0.48
2:D:224:VAL:HG21	2:D:274:ILE:HD11	1.95	0.48
1:C:689:GLN:O	1:C:693:ILE:HG12	2.13	0.48
1:A:84:LYS:HG3	1:A:141:TYR:CE1	2.48	0.48
1:C:277:ILE:HG21	1:C:355:GLU:HB2	1.95	0.48
2:D:18:ASN:HA	2:D:23:GLU:O	2.13	0.48
1:A:469:LYS:HD3	1:A:472:GLU:HB3	1.95	0.48
1:C:338:THR:O	1:C:342:LYS:HG2	2.13	0.48
1:A:293:VAL:HG12	1:A:321:ILE:HD13	1.94	0.48
1:A:710:ASP:HB2	1:A:731:GLY:HA2	1.95	0.48
1:C:73:LEU:HD11	1:C:260:MET:SD	2.54	0.48
2:D:92:PRO:HG3	2:D:301:VAL:HG12	1.95	0.48
1:C:1004:ARG:HG3	8:C:1107:PCW:H83	1.94	0.48
2:D:151:PHE:HE2	2:D:258:LEU:HB2	1.79	0.48
1:C:890:ASP:N	1:C:890:ASP:OD1	2.44	0.48
1:C:230:LEU:HA	1:C:237:PHE:CZ	2.47	0.48
1:A:613:HIS:CE1	1:A:685:ARG:HH21	2.32	0.47
1:C:553:LEU:HD11	1:C:571:PHE:HD1	1.78	0.47
1:A:292:ALA:HB2	1:A:324:ASN:HD22	1.79	0.47
1:C:119:GLN:HE21	1:C:119:GLN:HB2	1.49	0.47
2:D:101:TYR:O	2:D:105:ILE:HG12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:THR:O	1:A:757:GLU:HG2	2.15	0.47
1:A:867:ALA:HB2	1:A:873:PRO:HD3	1.97	0.47
2:B:204:TYR:HE1	2:B:207:TYR:HB2	1.80	0.47
1:C:834:THR:O	8:C:1106:PCW:H81	2.13	0.47
2:D:80:ILE:HD12	2:D:105:ILE:HD12	1.97	0.47
1:A:944:ASN:O	1:A:948:ILE:HG12	2.14	0.47
1:A:470:ILE:HG22	1:A:471:VAL:HG23	1.97	0.47
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.95	0.47
1:A:421:CYS:O	1:A:422:ASN:ND2	2.48	0.47
1:A:768:SER:HA	1:A:815:LEU:HD23	1.97	0.47
1:C:493:GLU:OE1	1:C:495:ARG:NH2	2.45	0.47
1:C:901:TYR:HA	1:C:904:ARG:NE	2.27	0.47
1:C:462:GLU:O	1:C:466:ARG:HB2	2.15	0.47
1:C:470:ILE:HG22	1:C:471:VAL:HG23	1.96	0.47
1:C:525:GLU:HA	1:C:528:LYS:HB3	1.95	0.47
1:C:873:PRO:HA	1:C:876:LEU:HD12	1.96	0.47
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.50	0.47
1:A:470:ILE:HB	1:A:485:ILE:HG23	1.97	0.46
1:C:205:LYS:HA	1:C:219:THR:HA	1.97	0.46
1:A:888:ILE:O	1:A:904:ARG:NH2	2.48	0.46
1:C:385:TRP:CH2	1:C:531:PHE:HB2	2.49	0.46
1:A:284:PHE:HD1	1:A:838:VAL:HG21	1.79	0.46
1:A:883:TRP:O	1:A:904:ARG:NH1	2.48	0.46
1:C:107:ALA:HB2	1:C:318:ILE:HG21	1.95	0.46
1:A:39:LEU:HD22	1:A:43:GLU:HG2	1.96	0.46
1:C:95:MET:O	1:C:99:ILE:HG23	2.16	0.46
1:C:277:ILE:CG2	1:C:355:GLU:HB2	2.45	0.46
1:C:976:LEU:HB3	1:C:980:TRP:HD1	1.81	0.46
8:C:1107:PCW:H73	8:C:1107:PCW:H42	1.73	0.46
2:B:151:PHE:HE2	2:B:258:LEU:HB2	1.80	0.46
1:C:165:ILE:HG12	1:C:170:LYS:HG2	1.97	0.46
1:C:944:ASN:O	1:C:948:ILE:HG12	2.15	0.46
1:A:918:THR:O	1:A:922:VAL:HG22	2.16	0.46
1:C:58:PRO:HD3	1:C:167:ASN:HB2	1.97	0.46
2:D:80:ILE:HB	2:D:105:ILE:HD12	1.97	0.46
2:D:130:PRO:HG2	2:D:204:TYR:CZ	2.51	0.46
2:D:153:LEU:H	2:D:153:LEU:HD12	1.81	0.46
1:A:72:ALA:HB2	1:A:176:GLU:HG2	1.98	0.46
1:A:336:CYS:SG	1:A:816:ALA:HB2	2.56	0.46
1:C:369:PHD:OP1	1:C:371:THR:N	2.44	0.46
1:C:83:VAL:O	1:C:87:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:PHE:O	1:C:94:SER:HB2	2.17	0.45
1:C:669:GLU:OE1	1:C:669:GLU:N	2.44	0.45
1:C:921:VAL:HG12	1:C:988:SER:OG	2.16	0.45
2:D:224:VAL:HG22	2:D:272:ILE:HD12	1.98	0.45
3:E:39:ILE:O	3:E:43:ILE:HG12	2.16	0.45
2:D:173:LYS:HG3	2:D:264:THR:O	2.17	0.45
1:A:107:ALA:HB2	1:A:318:ILE:HG21	1.99	0.45
1:C:883:TRP:CH2	1:C:904:ARG:HB2	2.52	0.45
2:D:211:VAL:HG11	2:D:259:MET:HE1	1.98	0.45
2:D:217:ARG:NH1	2:D:220:ASP:OD2	2.49	0.45
2:D:263:PHE:HB3	2:D:266:LEU:HD21	1.98	0.45
1:A:525:GLU:HA	1:A:528:LYS:HB3	1.98	0.45
1:A:713:ASN:OD1	1:A:713:ASN:N	2.50	0.45
1:C:604:ILE:HD11	1:C:755:VAL:HG21	1.99	0.45
1:A:183:LEU:HD21	1:A:248:ARG:NH2	2.32	0.45
1:A:866:LEU:HD23	1:A:866:LEU:HA	1.84	0.45
1:A:332:THR:HA	1:A:813:ILE:HD11	1.99	0.45
1:A:767:LYS:HE2	1:A:933:ARG:HG3	1.97	0.45
1:C:977:LYS:HD2	1:C:980:TRP:CZ2	2.51	0.45
1:A:778:PRO:HB2	1:A:919:ILE:HD11	1.98	0.45
1:A:965:PRO:HD3	3:G:31:LEU:HD11	1.99	0.45
2:D:136:ARG:O	2:D:146:ARG:NH1	2.50	0.45
1:A:399:GLN:CD	1:A:455:LEU:HD21	2.37	0.44
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.53	0.44
2:B:24:PHE:N	2:B:27:ARG:O	2.35	0.44
2:B:27:ARG:HG3	2:B:32:TRP:HD1	1.81	0.44
1:C:918:THR:HG23	1:C:984:ALA:HB2	2.00	0.44
1:A:907:VAL:O	1:A:911:CYS:HB2	2.18	0.44
1:A:972:ARG:NH2	1:A:974:TYR:OH	2.50	0.44
1:C:778:PRO:HB2	1:C:919:ILE:HD11	1.99	0.44
2:D:115:LEU:HD13	2:D:118:LYS:HD2	1.99	0.44
1:A:142:TYR:HE1	8:A:1112:PCW:H72	1.82	0.44
1:A:413:ALA:O	1:A:417:ILE:HG13	2.18	0.44
1:A:815:LEU:HA	1:A:815:LEU:HD12	1.79	0.44
2:B:74:PRO:HG2	2:B:292:GLN:OE1	2.17	0.44
1:C:488:ASN:ND2	1:C:493:GLU:O	2.51	0.44
1:A:932:THR:HG1	1:A:999:LYS:HZ2	1.59	0.44
1:C:803:ILE:HG12	1:C:916:PHE:HD2	1.82	0.44
1:A:382:ALA:H	1:A:584:MET:HA	1.82	0.44
1:C:399:GLN:HE21	1:C:436:LEU:HD11	1.83	0.44
1:A:385:TRP:CH2	1:A:531:PHE:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:915:PHE:O	1:C:919:ILE:HG12	2.17	0.44
9:C:1110:OBN:O1	9:C:1110:OBN:O5	2.30	0.44
2:D:156:LEU:HD13	2:D:260:ALA:HB2	2.00	0.44
1:C:660:GLY:HA3	1:C:685:ARG:O	2.17	0.44
1:A:689:GLN:O	1:A:693:ILE:HG12	2.18	0.44
2:B:211:VAL:HG11	2:B:259:MET:HE1	1.99	0.44
1:C:291:VAL:HG23	1:C:324:ASN:HD21	1.83	0.44
2:B:238:PHE:CD1	2:B:257:PRO:HB2	2.53	0.43
2:D:130:PRO:HD3	2:D:232:LEU:HD12	1.99	0.43
2:D:158:ASN:OD1	4:I:1:NAG:N2	2.51	0.43
1:C:211:LEU:HD13	1:C:237:PHE:HB3	1.99	0.43
1:C:883:TRP:HA	1:C:904:ARG:HH11	1.83	0.43
2:D:130:PRO:HG2	2:D:204:TYR:CE1	2.54	0.43
2:D:204:TYR:O	2:D:208:VAL:HG12	2.18	0.43
1:A:608:MET:HB2	1:A:626:ILE:HD13	2.00	0.43
1:C:93:PHE:HB3	1:C:330:LEU:HD13	1.99	0.43
1:A:462:GLU:O	1:A:466:ARG:HB2	2.19	0.43
1:A:865:ILE:O	1:A:869:ASN:ND2	2.40	0.43
2:B:263:PHE:HB3	2:B:266:LEU:HD21	2.01	0.43
1:C:663:LEU:HD11	1:C:694:ILE:HD11	1.98	0.43
2:D:30:GLY:O	2:D:34:LYS:HG3	2.18	0.43
2:D:246:TYR:O	2:D:250:LEU:HB2	2.18	0.43
1:A:669:GLU:OE1	1:A:669:GLU:N	2.45	0.43
1:C:831:ASN:HB3	1:C:834:THR:HB	2.00	0.43
1:A:496:HIS:HB2	1:A:553:LEU:HB2	2.01	0.43
2:B:92:PRO:HD2	2:B:303:SER:HA	1.99	0.43
2:B:156:LEU:HD22	2:B:260:ALA:H	1.84	0.43
1:C:771:TYR:OH	1:C:923:GLN:HB3	2.19	0.43
1:A:911:CYS:C	1:A:914:PRO:HD2	2.40	0.43
1:C:905:LYS:HD3	1:C:905:LYS:HA	1.90	0.43
1:C:949:PHE:HB2	3:E:45:ILE:HG23	2.01	0.43
1:A:340:THR:O	1:A:344:MET:HG2	2.19	0.42
1:A:553:LEU:HD11	1:A:571:PHE:HD1	1.83	0.42
1:A:655:ALA:HA	1:A:680:GLU:O	2.19	0.42
1:C:197:ARG:CZ	1:C:234:ASN:HD22	2.32	0.42
1:C:238:PHE:HD1	1:C:239:SER:N	2.16	0.42
1:C:479:ASN:O	1:C:481:TYR:HD1	2.02	0.42
1:A:443:ASP:OD1	1:A:444:ALA:N	2.52	0.42
1:A:660:GLY:HA3	1:A:685:ARG:O	2.19	0.42
1:C:998:ARG:HE	1:C:1014:THR:HB	1.84	0.42
1:A:817:TYR:HB2	1:A:944:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:ASP:OD1	1:A:998:ARG:NH1	2.52	0.42
1:C:191:ARG:NE	1:C:239:SER:HA	2.35	0.42
1:C:803:ILE:HA	1:C:803:ILE:HD13	1.81	0.42
1:A:797:THR:HG1	9:A:1114:OBN:HOF	1.58	0.42
1:C:815:LEU:HD11	1:C:931:LYS:HA	2.00	0.42
1:A:191:ARG:NE	1:A:239:SER:HA	2.35	0.42
1:C:196:LEU:HB2	1:C:236:ALA:HB3	2.00	0.42
1:C:287:ILE:HD12	8:C:1106:PCW:H2	2.00	0.42
1:A:277:ILE:HG21	1:A:355:GLU:HB2	2.01	0.42
2:B:80:ILE:HD12	2:B:105:ILE:HD12	2.01	0.42
1:C:683:PHE:HB3	1:C:686:THR:HG21	2.01	0.42
1:C:909:PHE:HB3	1:C:972:ARG:O	2.20	0.42
2:B:91:ARG:HD2	2:B:94:ASP:HB2	2.02	0.42
1:C:743:LEU:HD11	1:C:751:ILE:HD13	2.02	0.42
1:C:48:TYR:CE2	1:C:252:VAL:HG22	2.55	0.42
1:C:560:GLU:N	1:C:560:GLU:OE1	2.52	0.42
1:C:632:GLU:HB3	1:C:636:ASP:HB2	2.01	0.42
1:C:793:LEU:HB3	1:C:908:GLU:OE2	2.19	0.42
2:D:91:ARG:HD2	2:D:94:ASP:H	1.85	0.42
1:A:119:GLN:NE2	9:A:1114:OBN:H192	2.35	0.42
1:C:136:THR:HG21	1:C:330:LEU:HG	2.01	0.42
1:C:443:ASP:OD1	1:C:444:ALA:N	2.53	0.42
1:C:1001:ILE:HG22	1:C:1010:VAL:HG21	2.02	0.42
1:A:868:GLU:OE2	2:B:68:TYR:HE2	2.02	0.42
8:A:1106:PCW:H83	2:B:13:LYS:HZ1	1.85	0.42
2:B:130:PRO:HG2	2:B:204:TYR:CE1	2.55	0.42
1:C:815:LEU:HD12	1:C:815:LEU:HA	1.84	0.41
2:D:108:PHE:HD1	2:D:109:LEU:HD12	1.84	0.41
1:A:48:TYR:HE2	1:A:252:VAL:HG22	1.85	0.41
1:A:369:PHD:O	1:A:373:THR:HB	2.20	0.41
1:A:545:VAL:HA	1:A:583:SER:HA	2.02	0.41
1:A:836:LYS:HE3	8:A:1106:PCW:H82	2.02	0.41
1:A:858:GLY:HA2	1:A:918:THR:HG21	2.02	0.41
2:B:108:PHE:HD1	2:B:109:LEU:HD12	1.84	0.41
1:C:545:VAL:HA	1:C:583:SER:HA	2.03	0.41
7:C:1104:CLR:H211	7:C:1104:CLR:H231	1.77	0.41
2:D:238:PHE:CD1	2:D:257:PRO:HB2	2.55	0.41
1:A:374:LEU:HD21	1:A:626:ILE:HD11	2.02	0.41
1:A:378:ARG:HD2	1:A:451:LYS:HZ2	1.85	0.41
2:B:204:TYR:O	2:B:208:VAL:HG12	2.20	0.41
1:C:94:SER:HB3	1:C:133:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HD12	1:A:374:LEU:HA	1.89	0.41
1:A:471:VAL:HG21	1:A:564:PHE:O	2.20	0.41
8:A:1110:PCW:H62	8:A:1110:PCW:H41	1.86	0.41
2:D:74:PRO:HG2	2:D:292:GLN:OE1	2.20	0.41
1:A:651:ARG:HA	1:A:651:ARG:HD3	1.92	0.41
1:A:803:ILE:HG12	1:A:916:PHE:HD2	1.85	0.41
1:A:860:PHE:O	1:A:864:VAL:HG23	2.20	0.41
2:B:143:ARG:HD2	2:B:146:ARG:NH1	2.35	0.41
1:C:337:LEU:HA	1:C:761:ILE:HD11	2.02	0.41
1:C:427:GLN:HB2	1:C:430:GLN:OE1	2.21	0.41
1:A:874:ILE:HD12	1:A:874:ILE:H	1.86	0.41
2:B:130:PRO:HB3	2:B:239:PRO:HB3	2.02	0.41
3:G:36:LEU:HD23	3:G:39:ILE:HD11	2.02	0.41
1:C:784:LEU:O	1:C:788:ILE:HG12	2.21	0.41
1:C:799:THR:HG21	1:C:912:HIS:HB3	2.02	0.41
2:D:75:PRO:HG2	2:D:186:PHE:CE2	2.55	0.41
1:A:417:ILE:HG22	1:A:548:PHE:HD2	1.86	0.41
1:A:551:LEU:HD22	1:A:576:LEU:HD23	2.03	0.41
2:B:51:ILE:O	2:B:54:ILE:HG22	2.20	0.41
2:B:155:TRP:CD2	2:B:232:LEU:HD22	2.56	0.41
2:B:162:LEU:HD22	2:B:162:LEU:HA	1.92	0.41
2:B:209:LEU:HD12	2:B:209:LEU:HA	1.85	0.41
1:C:323:ALA:HB1	1:C:780:ILE:HG12	2.02	0.41
1:C:374:LEU:HD12	1:C:374:LEU:HA	1.92	0.41
1:C:880:ARG:NH2	9:C:1110:OBN:H6'3	2.35	0.41
1:C:913:THR:HB	1:C:976:LEU:HD21	2.02	0.41
2:D:173:LYS:HB3	2:D:262:GLN:HE21	1.85	0.41
2:D:265:ASN:HD22	4:J:1:NAG:C7	2.34	0.41
1:A:463:MET:HG2	1:A:466:ARG:NH2	2.36	0.41
1:C:309:THR:HG23	1:C:312:GLU:H	1.86	0.41
1:C:600:ARG:NH2	1:C:680:GLU:HG2	2.36	0.41
1:C:608:MET:HB3	1:C:682:VAL:HG22	2.02	0.41
2:D:155:TRP:CD2	2:D:232:LEU:HD22	2.56	0.41
1:A:148:SER:O	1:A:152:GLU:HG2	2.21	0.40
1:A:813:ILE:HD13	1:A:813:ILE:HA	1.89	0.40
1:A:905:LYS:HD3	1:A:905:LYS:HA	1.91	0.40
1:C:69:GLY:HA2	1:C:70:PRO:HD3	1.98	0.40
1:C:286:HIS:ND1	8:C:1108:PCW:H51	2.37	0.40
1:C:918:THR:O	1:C:922:VAL:HG22	2.21	0.40
1:A:95:MET:O	1:A:99:ILE:HG23	2.20	0.40
2:B:95:PRO:HA	2:B:98:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ASP:HB2	1:C:253:TYR:HB2	2.03	0.40
1:C:817:TYR:HB2	1:C:944:ASN:HD21	1.87	0.40
2:D:64:PHE:CZ	2:D:141:ASN:HB2	2.55	0.40
2:D:117:GLN:O	2:D:150:ARG:NH1	2.54	0.40
1:A:427:GLN:HB2	1:A:430:GLN:OE1	2.20	0.40
1:A:883:TRP:HA	1:A:904:ARG:HH11	1.87	0.40
2:B:18:ASN:HA	2:B:23:GLU:O	2.21	0.40
1:C:29:LYS:NZ	1:C:265:THR:HB	2.37	0.40
1:C:709:GLY:O	1:C:727:MET:HG2	2.22	0.40
7:C:1104:CLR:H182	7:C:1104:CLR:H8	1.95	0.40
8:C:1106:PCW:H41	8:C:1106:PCW:H62	1.76	0.40
3:E:32:ILE:HD13	3:E:32:ILE:HA	1.85	0.40
1:A:44:LEU:HD23	1:A:250:ILE:HD12	2.02	0.40
1:C:453:ILE:HG22	1:C:460:VAL:HG22	2.03	0.40
1:C:713:ASN:N	1:C:713:ASN:OD1	2.53	0.40
1:C:997:VAL:O	1:C:1001:ILE:HG12	2.22	0.40
1:A:119:GLN:NE2	9:A:1114:OBN:O5	2.39	0.40
1:A:843:ILE:HG23	1:A:847:TYR:HD2	1.86	0.40
1:C:287:ILE:HG21	1:C:843:ILE:HG13	2.04	0.40
1:C:329:LEU:HD21	1:C:769:ILE:HG12	2.02	0.40
2:D:143:ARG:HD2	2:D:146:ARG:NH1	2.37	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%)	924 (93%)	67 (7%)	2 (0%)	47	78
1	C	993/1016 (98%)	927 (93%)	64 (6%)	2 (0%)	47	78
2	B	289/303 (95%)	263 (91%)	24 (8%)	2 (1%)	22	54
2	D	281/303 (93%)	253 (90%)	26 (9%)	2 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
3	G	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
All	All	2616/2768 (94%)	2423 (93%)	185 (7%)	8 (0%)	41	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	22	LYS
2	D	22	LYS
1	C	193	PRO
1	A	193	PRO
2	B	199	TYR
2	D	199	TYR
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%)	820 (97%)	26 (3%)	40	74
1	C	846/861 (98%)	820 (97%)	26 (3%)	40	74
2	B	261/269 (97%)	240 (92%)	21 (8%)	12	33
2	D	255/269 (95%)	235 (92%)	20 (8%)	12	34
3	E	26/52 (50%)	25 (96%)	1 (4%)	33	67
3	G	26/52 (50%)	25 (96%)	1 (4%)	33	67
All	All	2260/2364 (96%)	2165 (96%)	95 (4%)	30	63

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	45	HIS

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Mol	Chain	Res	Type
1	A	56	LEU
1	A	57	THR
1	A	82	TRP
1	A	124	TYR
1	A	167	ASN
1	A	224	PHE
1	A	238	PHE
1	A	254	THR
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	781	THR
1	A	840	GLU
1	A	865	ILE
1	A	916	PHE
1	A	1009	TRP
2	B	13	LYS
2	B	25	LEU
2	B	32	TRP
2	B	64	PHE
2	B	72	VAL
2	B	80	ILE
2	B	114	ASP
2	B	125	ASP
2	B	126	CYS
2	B	153	LEU
2	B	162	LEU
2	B	166	THR
2	B	170	LYS
2	B	171	ASP
2	B	173	LYS
2	B	177	ILE
2	B	195	SER
2	B	203	LYS

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Mol	Chain	Res	Type
2	B	256	GLN
2	B	297	VAL
2	B	299	ILE
3	G	21	TYR
1	C	35	ASP
1	C	45	HIS
1	C	56	LEU
1	C	57	THR
1	C	82	TRP
1	C	119	GLN
1	C	121	ASP
1	C	167	ASN
1	C	224	PHE
1	C	238	PHE
1	C	254	THR
1	C	327	GLU
1	C	374	LEU
1	C	506	ARG
1	C	523	LEU
1	C	531	PHE
1	C	533	ASN
1	C	564	PHE
1	C	566	THR
1	C	586	ASP
1	C	685	ARG
1	C	776	ASN
1	C	824	ILE
1	C	865	ILE
1	C	916	PHE
1	C	1009	TRP
2	D	13	LYS
2	D	25	LEU
2	D	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	170	LYS

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Mol	Chain	Res	Type
2	D	171	ASP
2	D	173	LYS
2	D	177	ILE
2	D	195	SER
2	D	203	LYS
2	D	256	GLN
2	D	297	VAL
2	D	299	ILE
3	E	21	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	122	ASN
1	A	324	ASN
1	A	427	GLN
1	A	613	HIS
1	A	631	ASN
1	A	776	ASN
1	A	897	GLN
1	A	898	GLN
1	C	111	GLN
1	C	119	GLN
1	C	122	ASN
1	C	283	HIS
1	C	324	ASN
1	C	399	GLN
1	C	747	ASN
1	C	776	ASN
1	C	897	GLN
1	C	912	HIS
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	5,1	9,11,12	2.01	1 (11%)	10,15,17	1.03	1 (10%)
1	PHD	A	369	5,1	9,11,12	1.96	1 (11%)	10,15,17	1.15	1 (10%)

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	5,1	-	2/8/11/13	-
1	PHD	A	369	5,1	-	2/8/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	PHD	P-OD1	-5.37	1.51	1.59
1	A	369	PHD	P-OD1	-5.19	1.51	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	PHD	OD1-CG-CB	2.31	117.47	111.11
1	C	369	PHD	OD1-CG-CB	2.07	116.81	111.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	369	PHD	1	0
1	A	369	PHD	1	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	0.33	0	17,19,21	0.44	0
4	NAG	F	2	4	14,14,15	0.33	0	17,19,21	0.50	0
4	NAG	H	1	2,4	14,14,15	0.69	1 (7%)	17,19,21	0.74	0
4	NAG	H	2	4	14,14,15	0.25	0	17,19,21	0.34	0
4	NAG	I	1	2,4	14,14,15	0.36	0	17,19,21	0.46	0
4	NAG	I	2	4	14,14,15	0.36	0	17,19,21	0.48	0
4	NAG	J	1	2,4	14,14,15	0.74	1 (7%)	17,19,21	0.68	0
4	NAG	J	2	4	14,14,15	0.21	0	17,19,21	0.33	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

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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	-2.65	1.39	1.43
4	H	1	NAG	O5-C1	-2.47	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

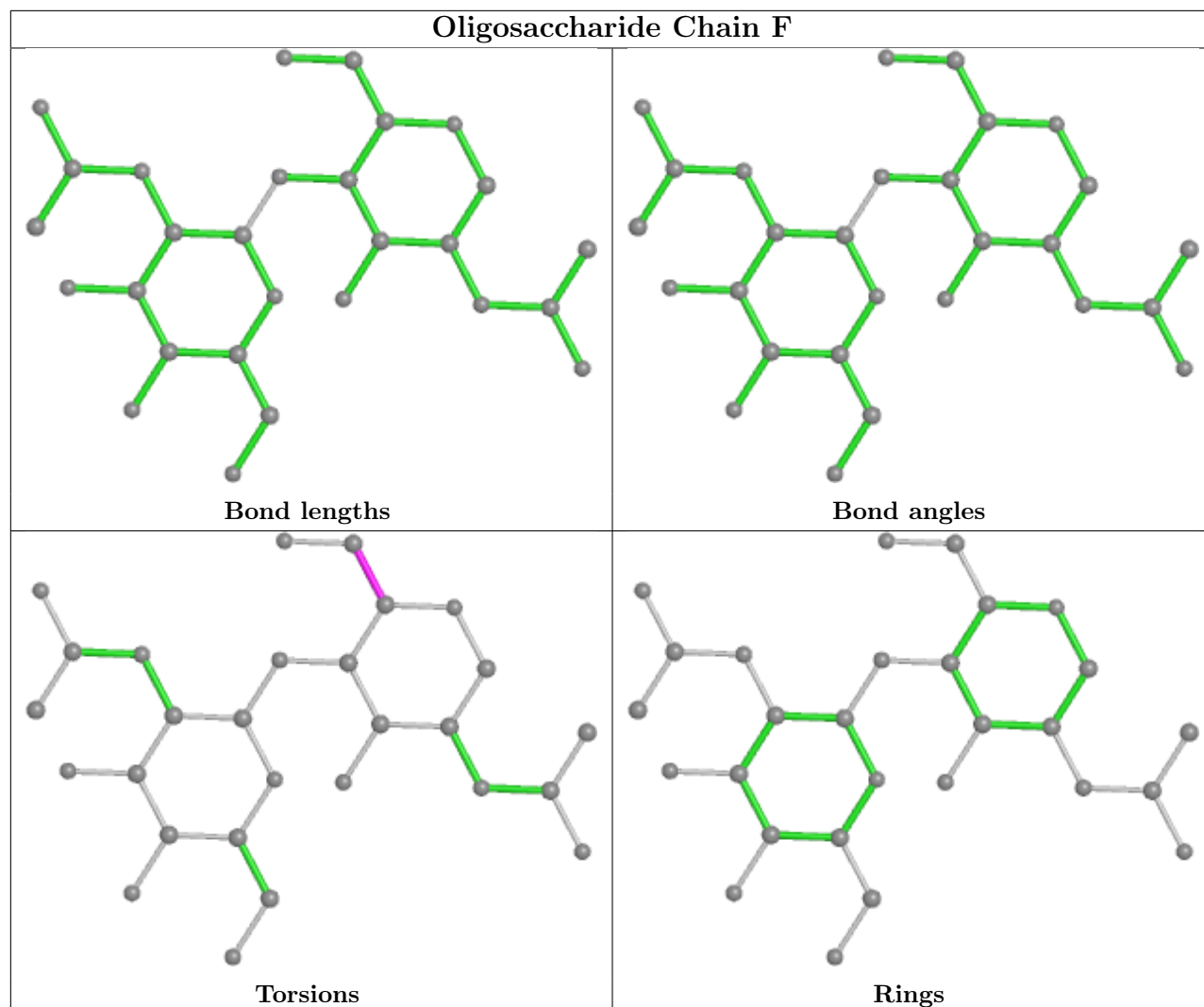
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6

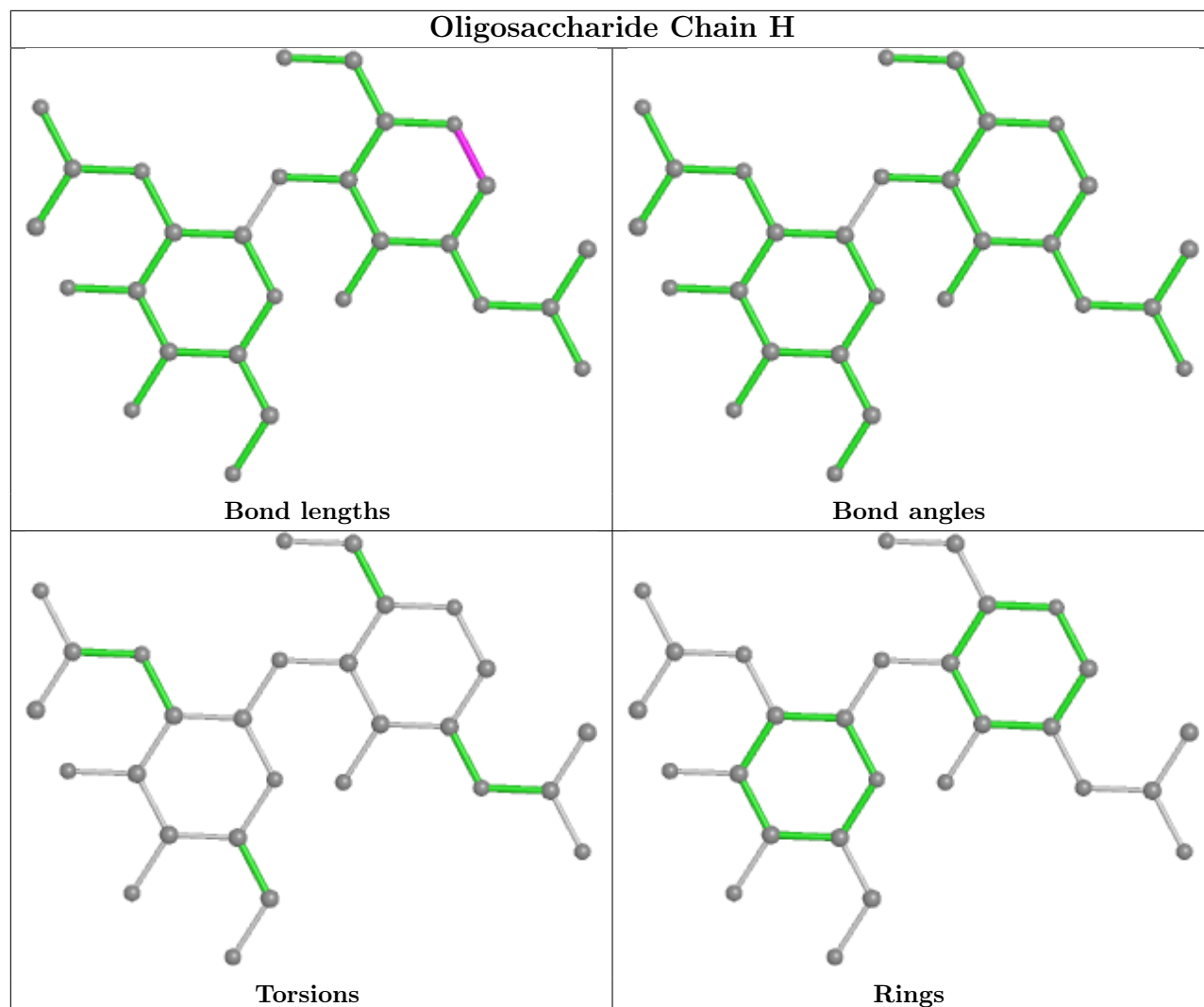
There are no ring outliers.

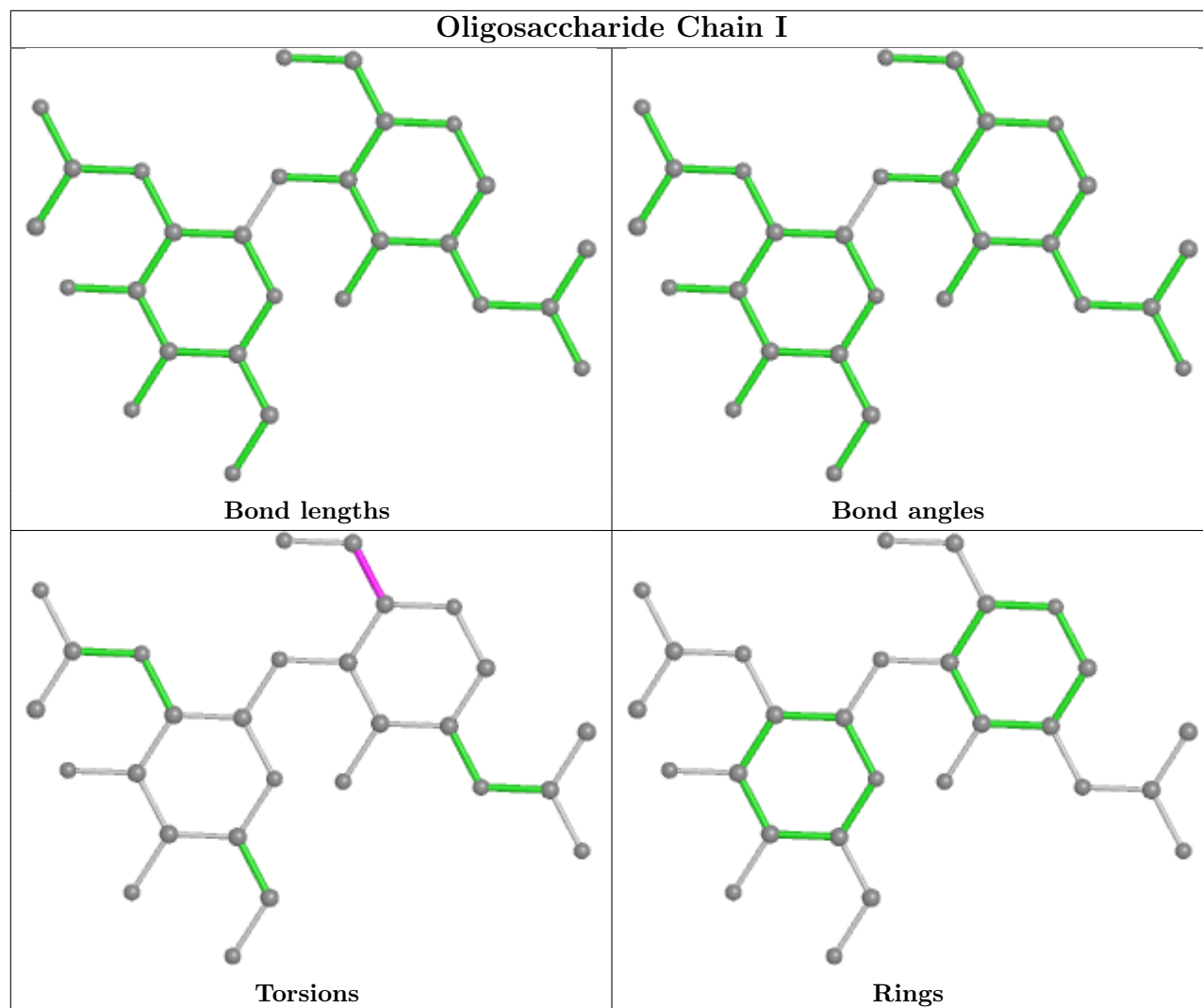
2 monomers are involved in 2 short contacts:

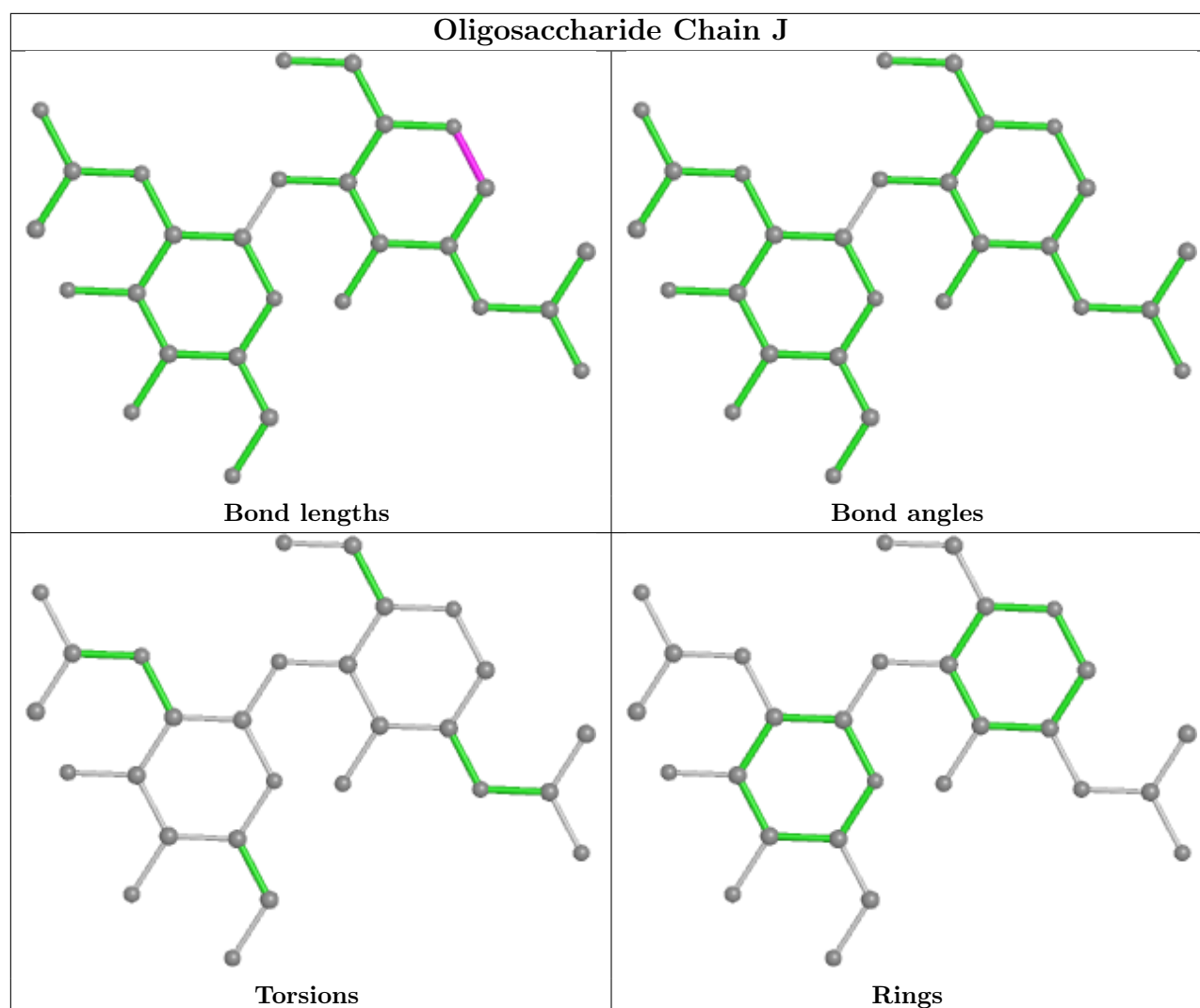
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
4	J	1	NAG	1	0

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 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 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	0.91	0	27,29,61	1.32	4 (14%)
8	PCW	C	1108	-	21,21,53	0.94	0	27,29,61	0.95	1 (3%)
8	PCW	A	1110	-	21,21,53	0.91	0	27,29,61	1.11	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	OBN	A	1114	-	44,46,46	1.27	4 (9%)	66,76,76	1.38	9 (13%)
7	CLR	D	402	-	31,31,31	1.80	9 (29%)	48,48,48	1.72	13 (27%)
8	PCW	A	1105	-	21,21,53	0.89	0	27,29,61	1.11	3 (11%)
8	PCW	C	1109	-	21,21,53	0.85	0	27,29,61	1.23	3 (11%)
8	PCW	A	1109	-	21,21,53	0.91	0	27,29,61	0.95	1 (3%)
10	NAG	D	401	2	14,14,15	0.27	0	17,19,21	0.52	0
8	PCW	A	1111	-	21,21,53	0.86	0	27,29,61	1.10	1 (3%)
7	CLR	C	1105	-	31,31,31	1.84	8 (25%)	48,48,48	1.61	12 (25%)
8	PCW	A	1108	-	21,21,53	0.89	0	27,29,61	1.02	3 (11%)
8	PCW	A	1106	-	21,21,53	0.91	0	27,29,61	1.09	3 (11%)
8	PCW	C	1107	-	21,21,53	0.86	0	27,29,61	0.97	3 (11%)
8	PCW	A	1112	-	21,21,53	0.92	0	27,29,61	1.11	3 (11%)
10	NAG	B	401	2	14,14,15	0.33	0	17,19,21	0.46	0
8	PCW	A	1113	-	21,21,53	0.89	0	27,29,61	1.30	3 (11%)
7	CLR	C	1104	-	31,31,31	2.33	11 (35%)	48,48,48	1.78	10 (20%)
7	CLR	A	1104	-	31,31,31	1.75	7 (22%)	48,48,48	1.59	11 (22%)
8	PCW	A	1107	-	21,21,53	0.88	0	27,29,61	0.97	3 (11%)
7	CLR	G	101	-	31,31,31	1.68	7 (22%)	48,48,48	1.61	12 (25%)
9	OBN	C	1110	-	44,46,46	1.25	3 (6%)	66,76,76	1.40	9 (13%)

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	1108	-	-	12/23/23/57	-
8	PCW	A	1110	-	-	12/23/23/57	-
9	OBN	A	1114	-	-	3/11/116/116	0/6/6/6
7	CLR	D	402	-	-	0/10/68/68	0/4/4/4
8	PCW	A	1105	-	-	10/23/23/57	-
8	PCW	C	1109	-	-	9/23/23/57	-
8	PCW	A	1109	-	-	12/23/23/57	-
10	NAG	D	401	2	-	4/6/23/26	0/1/1/1
8	PCW	A	1111	-	-	11/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLR	C	1105	-	-	2/10/68/68	0/4/4/4
8	PCW	A	1108	-	-	10/23/23/57	-
8	PCW	A	1106	-	-	12/23/23/57	-
8	PCW	C	1107	-	-	16/23/23/57	-
8	PCW	A	1112	-	-	9/23/23/57	-
10	NAG	B	401	2	-	1/6/23/26	0/1/1/1
8	PCW	A	1113	-	-	10/23/23/57	-
7	CLR	C	1104	-	-	3/10/68/68	0/4/4/4
7	CLR	A	1104	-	-	1/10/68/68	0/4/4/4
8	PCW	A	1107	-	-	7/23/23/57	-
7	CLR	G	101	-	-	2/10/68/68	0/4/4/4
9	OBN	C	1110	-	-	5/11/116/116	0/6/6/6

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1104	CLR	C12-C13	5.66	1.64	1.54
7	C	1104	CLR	C7-C8	4.73	1.61	1.53
7	C	1104	CLR	C12-C11	4.61	1.63	1.53
7	C	1104	CLR	C4-C5	4.36	1.61	1.51
7	A	1104	CLR	C10-C5	3.97	1.60	1.52
7	C	1105	CLR	C10-C9	3.91	1.62	1.56
7	D	402	CLR	C12-C13	3.74	1.60	1.54
7	G	101	CLR	C16-C17	3.73	1.62	1.54
7	D	402	CLR	C10-C5	3.73	1.60	1.52
7	G	101	CLR	C10-C5	3.62	1.60	1.52
7	C	1105	CLR	C10-C5	3.53	1.59	1.52
7	C	1104	CLR	C11-C9	3.52	1.59	1.53
7	A	1104	CLR	C16-C17	3.45	1.61	1.54
7	C	1105	CLR	C16-C17	3.42	1.61	1.54
7	A	1104	CLR	C13-C14	3.36	1.61	1.55
9	A	1114	OBN	C4-C5	3.29	1.57	1.53
9	C	1110	OBN	C4-C5	3.04	1.56	1.53
7	C	1105	CLR	C13-C14	2.96	1.60	1.55
7	C	1104	CLR	C16-C17	2.95	1.60	1.54
7	G	101	CLR	C10-C9	2.94	1.61	1.56
7	D	402	CLR	C16-C17	2.91	1.60	1.54
7	C	1105	CLR	C12-C13	2.90	1.59	1.54
7	C	1104	CLR	C7-C6	2.89	1.56	1.50
7	C	1104	CLR	C13-C17	2.89	1.60	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1105	CLR	C13-C17	2.87	1.60	1.55
7	G	101	CLR	C13-C14	2.87	1.60	1.55
7	C	1105	CLR	C12-C11	2.85	1.59	1.53
7	D	402	CLR	C12-C11	2.84	1.59	1.53
7	C	1104	CLR	C4-C3	2.78	1.57	1.52
9	A	1114	OBN	C9-C8	2.66	1.58	1.54
7	A	1104	CLR	C10-C9	2.62	1.60	1.56
7	A	1104	CLR	C16-C15	2.59	1.61	1.54
9	C	1110	OBN	C14-C8	2.57	1.57	1.54
9	A	1114	OBN	C14-C8	2.53	1.57	1.54
9	C	1110	OBN	C9-C8	2.51	1.57	1.54
7	A	1104	CLR	C13-C17	2.47	1.59	1.55
7	D	402	CLR	C16-C15	2.45	1.60	1.54
7	D	402	CLR	C10-C9	2.35	1.60	1.56
7	D	402	CLR	C13-C17	2.34	1.59	1.55
7	G	101	CLR	C16-C15	2.28	1.60	1.54
7	G	101	CLR	C13-C17	2.22	1.59	1.55
7	C	1104	CLR	C10-C9	2.19	1.59	1.56
9	A	1114	OBN	C4-C3	2.18	1.55	1.51
7	C	1104	CLR	C16-C15	2.10	1.59	1.54
7	D	402	CLR	C4-C5	2.09	1.56	1.51
7	A	1104	CLR	C12-C11	2.07	1.57	1.53
7	D	402	CLR	C1-C10	2.06	1.58	1.54
7	G	101	CLR	C19-C10	2.06	1.58	1.54
7	C	1105	CLR	C11-C9	2.04	1.57	1.53

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1110	OBN	O21-C23-C22	5.48	115.83	108.67
9	A	1114	OBN	O21-C23-C22	5.38	115.69	108.67
7	C	1104	CLR	C7-C8-C9	5.30	116.14	109.71
8	A	1113	PCW	C2-O2-C31	-5.05	108.48	117.90
7	C	1104	CLR	C3-C4-C5	4.38	119.46	112.03
7	D	402	CLR	C8-C7-C6	-4.21	106.68	112.73
8	A	1110	PCW	C2-O2-C31	-4.17	110.12	117.90
9	A	1114	OBN	O23-C23-C22	-4.11	122.48	130.81
8	C	1109	PCW	C2-O2-C31	-4.10	110.26	117.90
7	C	1104	CLR	C11-C9-C10	4.08	118.46	113.08
9	C	1110	OBN	O23-C23-C22	-4.05	122.60	130.81
8	A	1111	PCW	C3-O3-C11	-3.94	107.20	117.10
9	C	1110	OBN	C9-C10-C1	3.53	118.40	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1106	PCW	C3-O3-C11	-3.46	108.41	117.10
8	C	1109	PCW	C3-O3-C11	-3.34	108.70	117.10
9	C	1110	OBN	C5-C4-C3	-3.31	110.38	114.14
8	A	1105	PCW	C2-O2-C31	-3.29	111.76	117.90
7	C	1105	CLR	C2-C3-C4	-3.13	106.01	110.31
7	G	101	CLR	C17-C13-C14	-3.12	96.38	100.07
8	A	1108	PCW	C2-O2-C31	-3.10	112.12	117.90
7	G	101	CLR	C8-C7-C6	-3.10	108.28	112.73
7	A	1104	CLR	C2-C3-C4	-3.08	106.08	110.31
7	A	1104	CLR	C8-C7-C6	-3.07	108.32	112.73
7	G	101	CLR	C2-C3-C4	-3.07	106.09	110.31
9	A	1114	OBN	C9-C10-C1	3.05	117.39	110.96
9	A	1114	OBN	C20-C22-C23	-2.98	102.65	108.84
8	C	1106	PCW	C2-O2-C31	-2.96	112.39	117.90
8	A	1112	PCW	C3-O3-C11	-2.94	109.73	117.10
7	C	1105	CLR	C22-C20-C17	-2.90	104.28	110.28
9	C	1110	OBN	C20-C22-C23	-2.89	102.85	108.84
8	A	1106	PCW	C2-O2-C31	-2.88	112.53	117.90
7	G	101	CLR	C22-C20-C17	-2.87	104.35	110.28
7	D	402	CLR	C2-C3-C4	-2.85	106.40	110.31
7	G	101	CLR	C7-C8-C14	-2.84	106.80	110.91
7	D	402	CLR	C16-C17-C20	-2.79	107.83	112.15
7	C	1105	CLR	C8-C7-C6	-2.78	108.74	112.73
7	A	1104	CLR	C22-C20-C17	-2.76	104.58	110.28
7	C	1105	CLR	C16-C17-C20	-2.74	107.91	112.15
7	D	402	CLR	C4-C5-C10	-2.72	112.80	116.42
7	C	1104	CLR	C16-C17-C20	-2.68	108.00	112.15
9	C	1110	OBN	C21-O21-C23	-2.66	105.62	108.85
8	A	1105	PCW	C3-O3-C11	-2.63	110.50	117.10
7	C	1105	CLR	C17-C13-C14	-2.61	96.98	100.07
8	A	1112	PCW	C2-O2-C31	-2.61	113.04	117.90
9	A	1114	OBN	O11-C11-C12	-2.61	103.84	109.91
7	C	1104	CLR	C15-C14-C13	2.58	106.95	103.84
9	C	1110	OBN	O11-C11-C12	-2.56	103.94	109.91
7	C	1104	CLR	C11-C9-C8	-2.56	108.07	111.75
7	D	402	CLR	C11-C9-C10	2.55	116.44	113.08
7	C	1105	CLR	C7-C8-C14	-2.54	107.22	110.91
8	A	1107	PCW	C3-O3-C11	-2.53	110.75	117.10
8	A	1106	PCW	O2-C31-C32	2.51	115.71	111.09
7	C	1105	CLR	C4-C5-C6	-2.50	117.00	120.61
7	A	1104	CLR	O1-C3-C2	2.49	116.51	110.16
7	A	1104	CLR	C16-C17-C20	-2.47	108.32	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1108	PCW	O2-C31-C32	2.47	115.64	111.09
7	G	101	CLR	C16-C17-C20	-2.45	108.35	112.15
8	C	1108	PCW	C3-O3-C11	-2.45	110.94	117.10
8	C	1106	PCW	O2-C31-C32	2.43	115.57	111.09
8	A	1109	PCW	O2-C31-C32	2.43	115.56	111.09
7	D	402	CLR	C19-C10-C1	-2.42	105.61	109.43
8	C	1107	PCW	O2-C31-C32	2.41	115.52	111.09
7	D	402	CLR	C15-C14-C13	2.40	106.74	103.84
8	C	1107	PCW	C3-O3-C11	-2.40	111.07	117.10
7	D	402	CLR	C22-C20-C17	-2.40	105.33	110.28
9	A	1114	OBN	C16-C15-C14	-2.40	101.11	105.19
9	A	1114	OBN	C21-O21-C23	-2.38	105.97	108.85
7	G	101	CLR	O1-C3-C2	2.37	116.21	110.16
7	C	1105	CLR	O1-C3-C2	2.37	116.20	110.16
7	D	402	CLR	O1-C3-C2	2.37	116.20	110.16
8	A	1105	PCW	O2-C31-C32	2.37	115.44	111.09
8	A	1113	PCW	C3-O3-C11	-2.34	111.22	117.10
7	A	1104	CLR	C17-C13-C14	-2.33	97.31	100.07
7	D	402	CLR	C18-C13-C12	2.33	114.27	110.59
7	C	1105	CLR	C21-C20-C17	2.32	116.48	112.92
7	A	1104	CLR	C7-C8-C14	-2.32	107.54	110.91
7	C	1104	CLR	C18-C13-C12	2.32	114.25	110.59
8	A	1110	PCW	O2-C31-C32	2.31	115.35	111.09
7	C	1105	CLR	C15-C14-C8	-2.29	115.31	119.08
7	D	402	CLR	C21-C20-C17	2.29	116.42	112.92
8	C	1107	PCW	C2-O2-C31	-2.28	113.65	117.90
7	D	402	CLR	C3-C4-C5	2.27	115.88	112.03
7	C	1105	CLR	C11-C9-C10	2.25	116.05	113.08
8	A	1108	PCW	C3-O3-C11	-2.21	111.54	117.10
7	C	1105	CLR	C18-C13-C12	2.20	114.06	110.59
9	A	1114	OBN	C5-C4-C3	-2.19	111.65	114.14
7	G	101	CLR	C21-C20-C17	2.19	116.28	112.92
8	A	1113	PCW	O2-C31-C32	2.19	115.12	111.09
7	A	1104	CLR	C4-C5-C6	-2.18	117.46	120.61
9	A	1114	OBN	O3-C3-C4	2.14	114.15	107.83
7	A	1104	CLR	C21-C20-C17	2.13	116.19	112.92
8	A	1112	PCW	O2-C31-C32	2.12	114.99	111.09
7	C	1104	CLR	C21-C20-C17	2.12	116.17	112.92
9	C	1110	OBN	C16-C15-C14	-2.11	101.60	105.19
7	G	101	CLR	C13-C14-C8	2.11	117.50	114.38
7	C	1104	CLR	C13-C17-C20	-2.09	116.22	119.49
8	A	1107	PCW	C2-O2-C31	-2.08	114.01	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	101	CLR	C15-C14-C8	-2.08	115.66	119.08
7	A	1104	CLR	C15-C14-C8	-2.07	115.67	119.08
8	C	1109	PCW	O2-C31-C32	2.07	114.89	111.09
8	A	1107	PCW	O2-C31-C32	2.06	114.88	111.09
9	C	1110	OBN	O14-C14-C13	-2.05	103.32	108.29
8	A	1106	PCW	C3-O3-C11	-2.05	111.96	117.10
7	D	402	CLR	C15-C14-C8	-2.04	115.73	119.08
7	G	101	CLR	C18-C13-C12	2.04	113.81	110.59
8	C	1106	PCW	P-O4P-C4	-2.03	111.61	121.59
7	G	101	CLR	C24-C23-C22	-2.01	103.99	113.24
7	A	1104	CLR	C11-C9-C10	2.01	115.72	113.08
7	C	1104	CLR	C15-C14-C8	-2.01	115.78	119.08

There are no chirality outliers.

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1105	PCW	C32-C31-O2-C2
8	A	1105	PCW	C1-O3P-P-O2P
8	A	1106	PCW	C1-O3P-P-O1P
8	A	1107	PCW	C32-C31-O2-C2
8	A	1107	PCW	C1-O3P-P-O2P
8	A	1108	PCW	C32-C31-O2-C2
8	A	1108	PCW	O31-C31-O2-C2
8	A	1109	PCW	C32-C31-O2-C2
8	A	1109	PCW	C1-O3P-P-O2P
8	A	1109	PCW	C4-O4P-P-O1P
8	A	1109	PCW	C4-O4P-P-O2P
8	A	1109	PCW	C4-O4P-P-O3P
8	A	1110	PCW	C1-O3P-P-O1P
8	A	1110	PCW	C1-O3P-P-O2P
8	A	1110	PCW	C1-O3P-P-O4P
8	A	1111	PCW	C1-O3P-P-O2P
8	A	1111	PCW	C4-O4P-P-O1P
8	A	1111	PCW	C4-O4P-P-O2P
8	A	1112	PCW	C1-O3P-P-O2P
8	A	1112	PCW	C4-O4P-P-O1P
8	A	1112	PCW	C4-O4P-P-O2P
8	A	1112	PCW	C4-O4P-P-O3P
8	A	1113	PCW	C32-C31-O2-C2
8	A	1113	PCW	C4-O4P-P-O2P
8	A	1113	PCW	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
8	C	1106	PCW	O4P-C4-C5-N
8	C	1106	PCW	C1-O3P-P-O2P
8	C	1107	PCW	O4P-C4-C5-N
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	C	1107	PCW	C1-O3P-P-O4P
8	C	1108	PCW	C1-O3P-P-O1P
8	C	1108	PCW	C1-O3P-P-O2P
8	C	1108	PCW	C4-O4P-P-O3P
8	C	1109	PCW	C4-O4P-P-O2P
9	C	1110	OBN	C1-C10-C19-O19
9	C	1110	OBN	C5-C10-C19-O19
9	C	1110	OBN	C9-C10-C19-O19
8	A	1106	PCW	C32-C31-O2-C2
8	C	1106	PCW	C32-C31-O2-C2
8	C	1109	PCW	C32-C31-O2-C2
8	A	1109	PCW	O31-C31-O2-C2
8	A	1110	PCW	C32-C31-O2-C2
8	A	1111	PCW	C32-C31-O2-C2
8	A	1106	PCW	O31-C31-O2-C2
8	C	1106	PCW	O31-C31-O2-C2
8	A	1105	PCW	O31-C31-O2-C2
8	A	1107	PCW	O31-C31-O2-C2
8	A	1112	PCW	C32-C31-O2-C2
8	A	1113	PCW	O31-C31-O2-C2
8	A	1105	PCW	O11-C11-O3-C3
8	C	1108	PCW	O11-C11-O3-C3
8	A	1110	PCW	C12-C11-O3-C3
8	C	1109	PCW	O31-C31-O2-C2
8	A	1111	PCW	O31-C31-O2-C2
8	C	1109	PCW	O11-C11-O3-C3
8	A	1105	PCW	C12-C11-O3-C3
8	C	1109	PCW	C12-C11-O3-C3
8	A	1109	PCW	O11-C11-O3-C3
8	C	1106	PCW	O11-C11-O3-C3
8	A	1109	PCW	C12-C11-O3-C3
8	C	1108	PCW	C12-C11-O3-C3
8	C	1106	PCW	C12-C11-O3-C3
8	A	1110	PCW	O31-C31-O2-C2
8	A	1106	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
8	A	1113	PCW	O11-C11-O3-C3
8	C	1107	PCW	C12-C11-O3-C3
10	D	401	NAG	O5-C5-C6-O6
8	A	1106	PCW	C12-C11-O3-C3
8	A	1113	PCW	C12-C11-O3-C3
10	D	401	NAG	C8-C7-N2-C2
10	D	401	NAG	O7-C7-N2-C2
8	A	1110	PCW	O11-C11-O3-C3
10	D	401	NAG	C4-C5-C6-O6
8	C	1107	PCW	O11-C11-O3-C3
8	A	1112	PCW	O31-C31-O2-C2
8	A	1105	PCW	C4-O4P-P-O3P
8	A	1106	PCW	C1-O3P-P-O4P
8	A	1106	PCW	C4-O4P-P-O3P
8	A	1107	PCW	C1-O3P-P-O4P
8	A	1109	PCW	C1-O3P-P-O4P
8	A	1110	PCW	C4-O4P-P-O3P
8	A	1111	PCW	C4-O4P-P-O3P
8	C	1108	PCW	C1-O3P-P-O4P
8	C	1108	PCW	C32-C31-O2-C2
8	A	1105	PCW	C1-O3P-P-O4P
8	C	1108	PCW	O31-C31-O2-C2
8	A	1111	PCW	O3P-C1-C2-C3
8	A	1113	PCW	O3P-C1-C2-C3
9	A	1114	OBN	C9-C10-C19-O19
8	A	1109	PCW	C3-C2-O2-C31
8	A	1108	PCW	O3P-C1-C2-O2
8	C	1109	PCW	O3P-C1-C2-C3
8	A	1110	PCW	C1-C2-C3-O3
8	A	1106	PCW	O3P-C1-C2-O2
7	C	1104	CLR	C21-C20-C22-C23
8	A	1108	PCW	O3P-C1-C2-C3
8	C	1108	PCW	C3-C2-O2-C31
9	C	1110	OBN	O5'-C1'-O3-C3
8	A	1113	PCW	O3P-C1-C2-O2
8	C	1109	PCW	O3P-C1-C2-O2
10	B	401	NAG	O5-C5-C6-O6
8	A	1110	PCW	O2-C2-C3-O3
8	C	1109	PCW	C4-O4P-P-O3P
8	A	1105	PCW	C1-O3P-P-O1P
8	A	1105	PCW	C4-O4P-P-O2P
8	A	1106	PCW	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
8	A	1106	PCW	C4-O4P-P-O2P
8	A	1109	PCW	C1-O3P-P-O1P
8	A	1110	PCW	C4-O4P-P-O2P
8	C	1108	PCW	C4-O4P-P-O2P
8	A	1106	PCW	O3P-C1-C2-C3
9	A	1114	OBN	C1-C10-C19-O19
8	A	1111	PCW	O3P-C1-C2-O2
8	C	1107	PCW	C4-C5-N-C7
8	A	1105	PCW	O4P-C4-C5-N
8	A	1106	PCW	O4P-C4-C5-N
8	A	1107	PCW	O4P-C4-C5-N
8	A	1108	PCW	O4P-C4-C5-N
8	A	1109	PCW	O4P-C4-C5-N
8	A	1110	PCW	O4P-C4-C5-N
8	A	1111	PCW	O4P-C4-C5-N
8	A	1112	PCW	O4P-C4-C5-N
8	A	1113	PCW	O4P-C4-C5-N
8	C	1108	PCW	O4P-C4-C5-N
8	C	1109	PCW	O4P-C4-C5-N
8	A	1108	PCW	O2-C2-C3-O3
7	C	1104	CLR	C20-C22-C23-C24
8	A	1111	PCW	C3-C2-O2-C31
8	C	1107	PCW	C4-C5-N-C8
8	A	1107	PCW	C4-O4P-P-O3P
8	A	1108	PCW	C1-O3P-P-O4P
8	A	1108	PCW	C4-O4P-P-O3P
8	A	1111	PCW	C1-O3P-P-O4P
8	A	1112	PCW	C1-O3P-P-O4P
8	C	1106	PCW	C1-O3P-P-O4P
8	C	1106	PCW	C4-O4P-P-O3P
8	C	1107	PCW	C4-O4P-P-O3P
9	C	1110	OBN	C2'-C1'-O3-C3
8	C	1108	PCW	O2-C2-C3-O3
8	A	1112	PCW	C1-C2-C3-O3
7	C	1105	CLR	C22-C23-C24-C25
8	C	1107	PCW	C1-C2-O2-C31
8	C	1107	PCW	C4-C5-N-C6
7	G	101	CLR	C21-C20-C22-C23
7	C	1104	CLR	C22-C23-C24-C25
7	A	1104	CLR	C20-C22-C23-C24
8	C	1107	PCW	O2-C2-C3-O3
7	G	101	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	C	1107	PCW	C3-C2-O2-C31
9	A	1114	OBN	O5'-C1'-O3-C3
8	A	1108	PCW	C1-C2-C3-O3
8	C	1107	PCW	C1-C2-C3-O3
8	A	1107	PCW	C4-O4P-P-O2P
8	A	1108	PCW	C1-O3P-P-O2P
7	C	1105	CLR	C20-C22-C23-C24
8	A	1113	PCW	C4-C5-N-C7

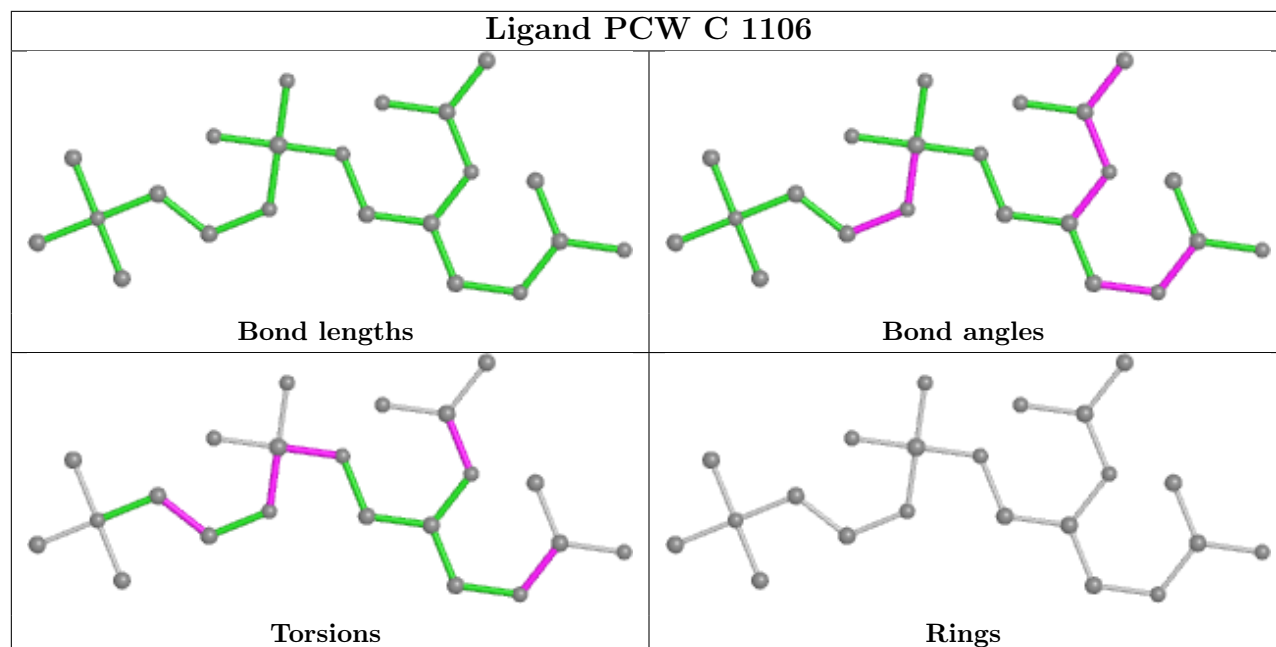
There are no ring outliers.

13 monomers are involved in 32 short contacts:

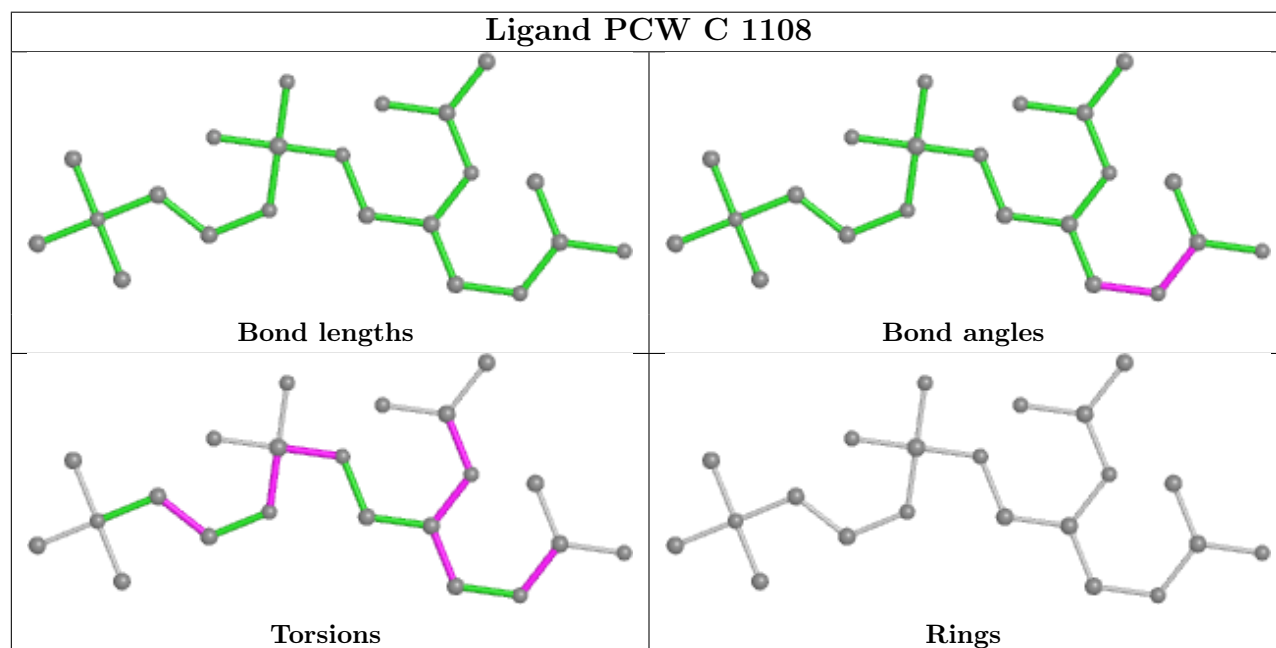
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1106	PCW	4	0
8	C	1108	PCW	2	0
8	A	1110	PCW	1	0
9	A	1114	OBN	3	0
7	D	402	CLR	2	0
8	A	1106	PCW	6	0
8	C	1107	PCW	3	0
8	A	1112	PCW	2	0
8	A	1113	PCW	1	0
7	C	1104	CLR	4	0
7	A	1104	CLR	1	0
7	G	101	CLR	1	0
9	C	1110	OBN	2	0

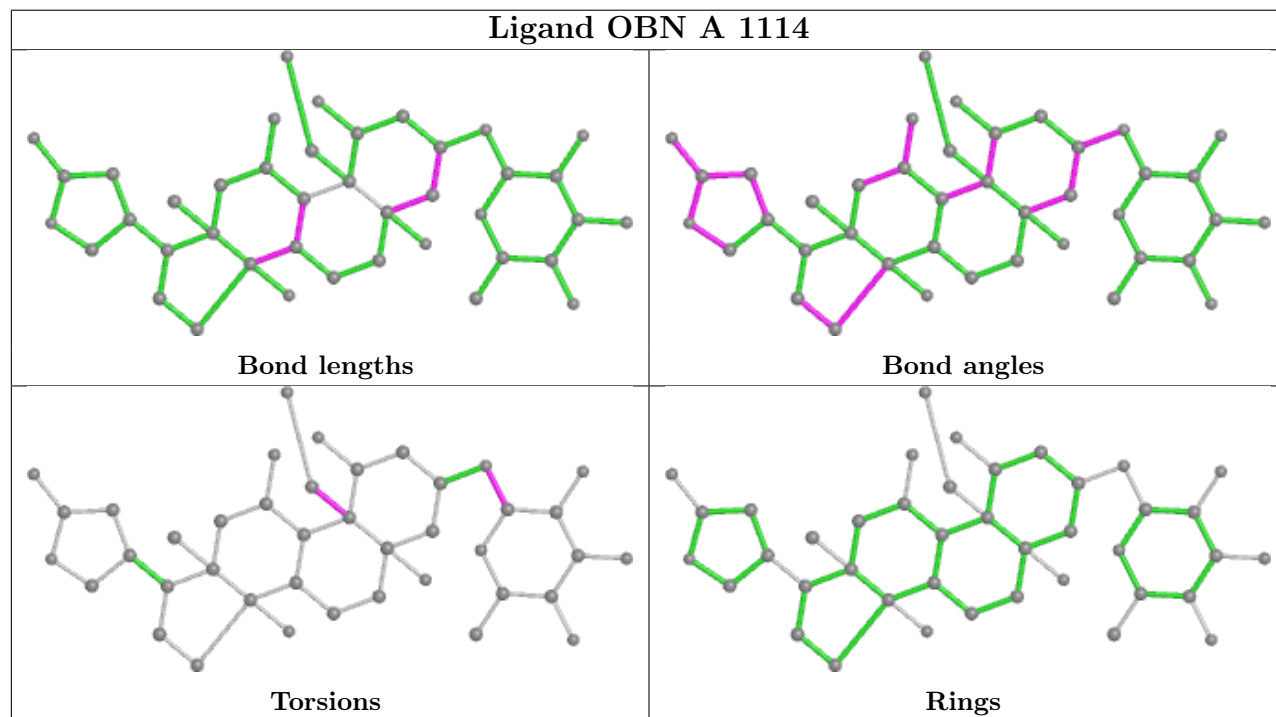
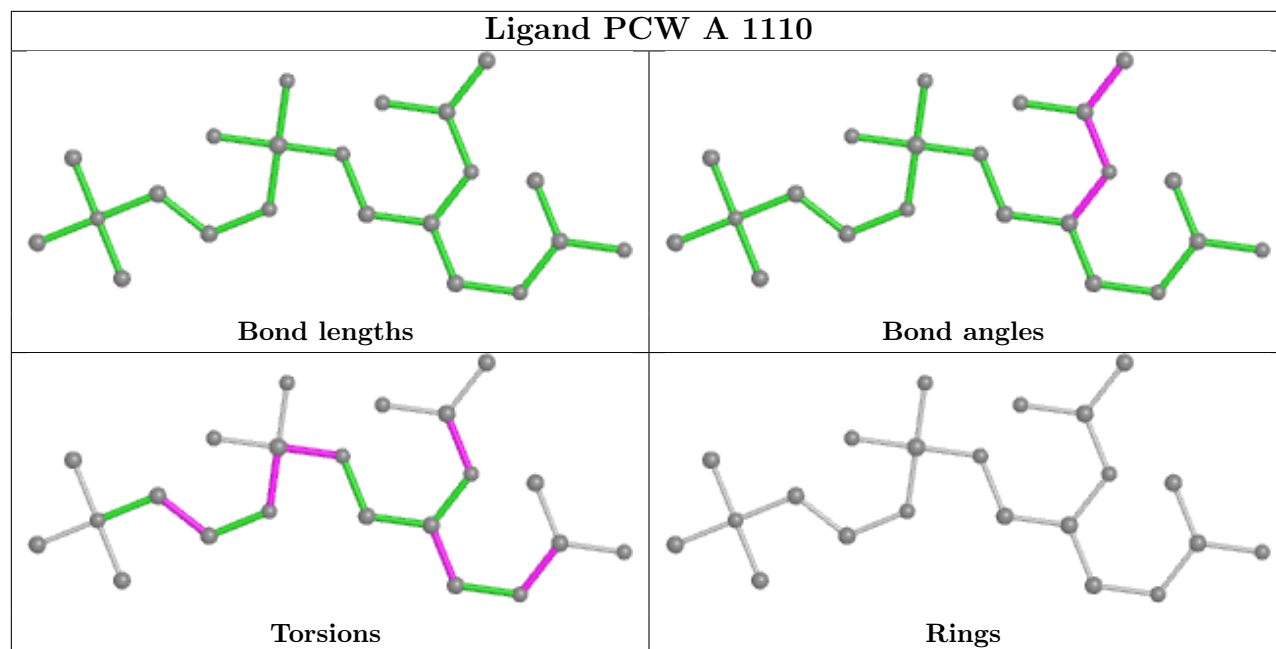
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 1106

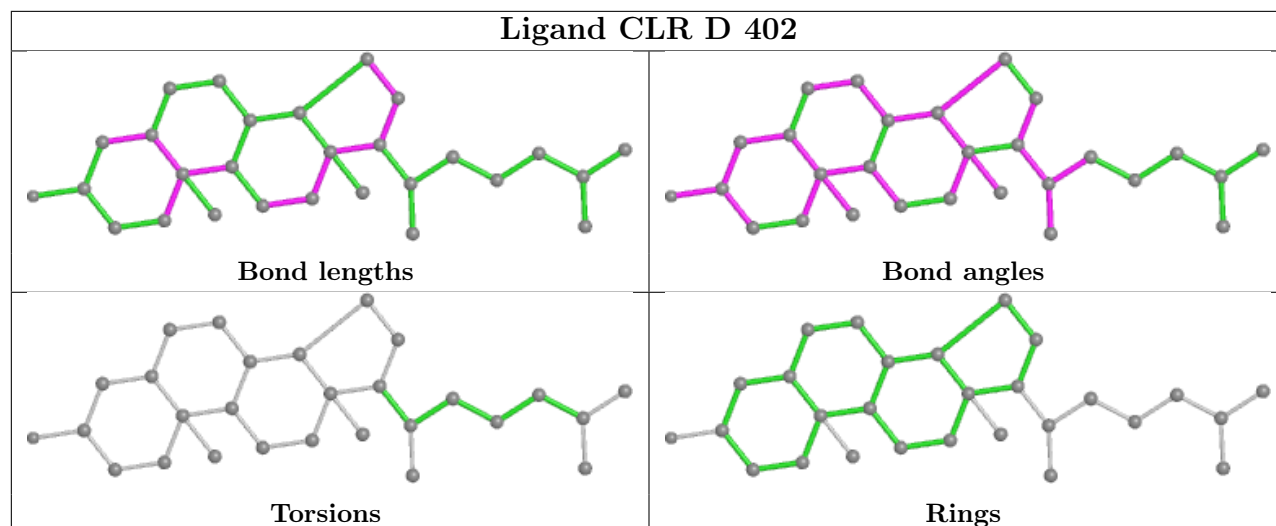


Ligand PCW C 1108

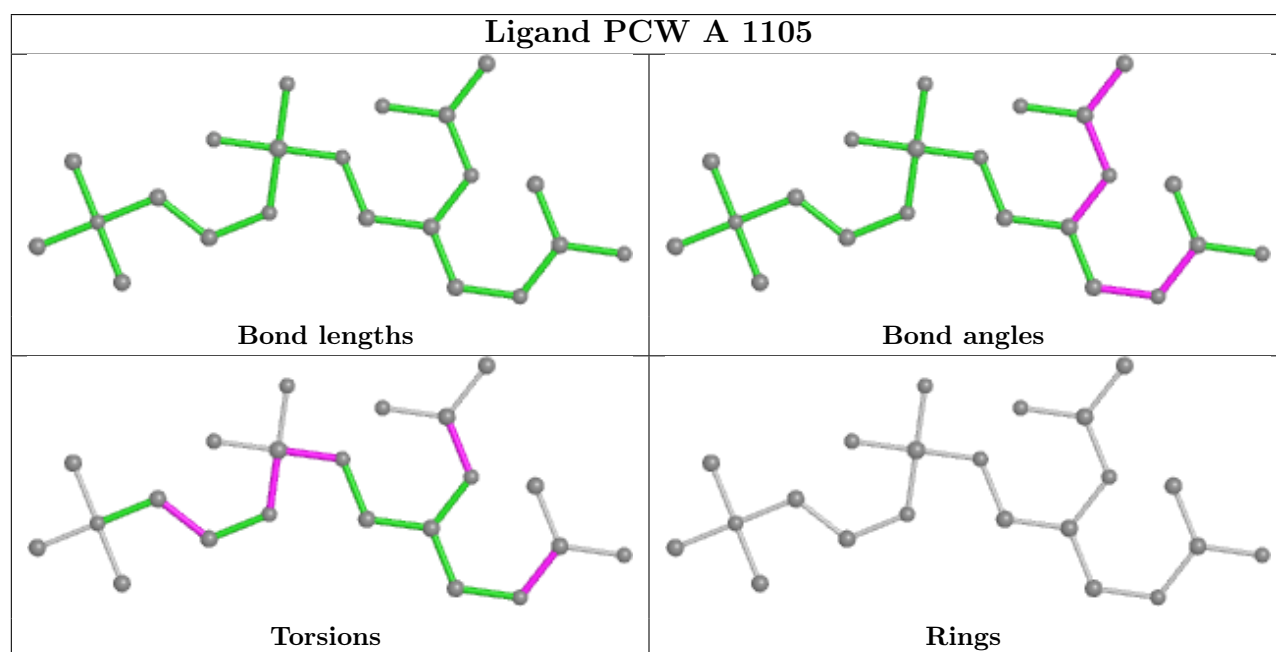




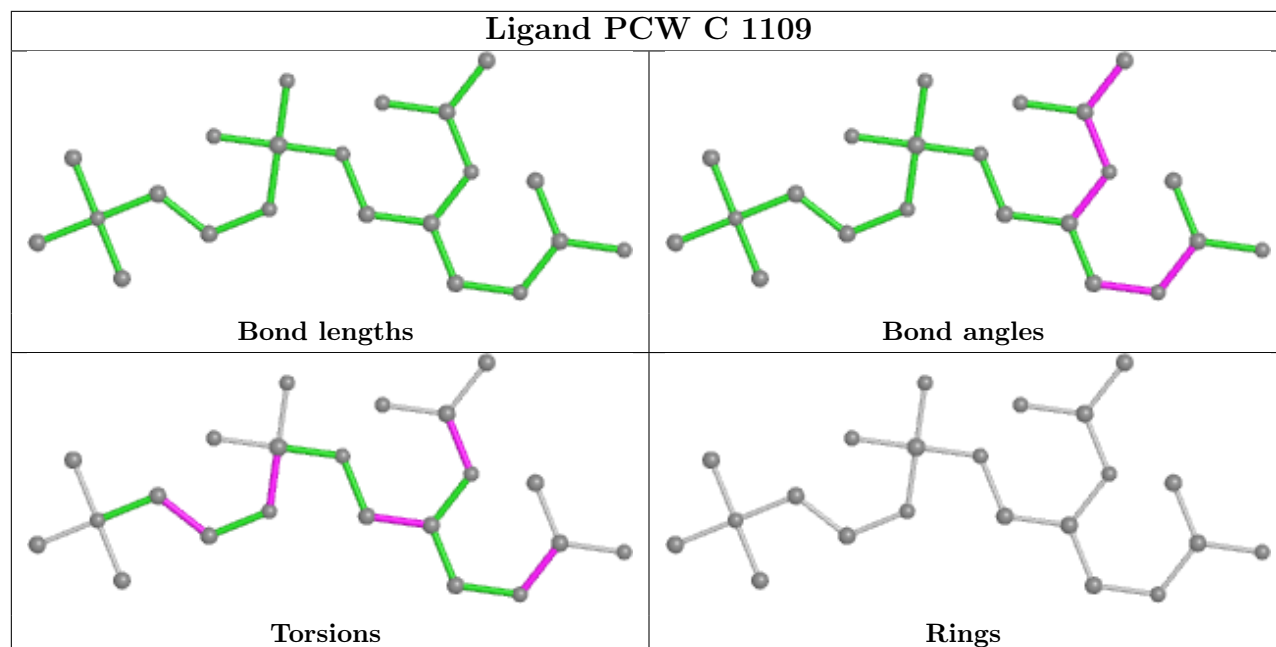
Ligand CLR D 402



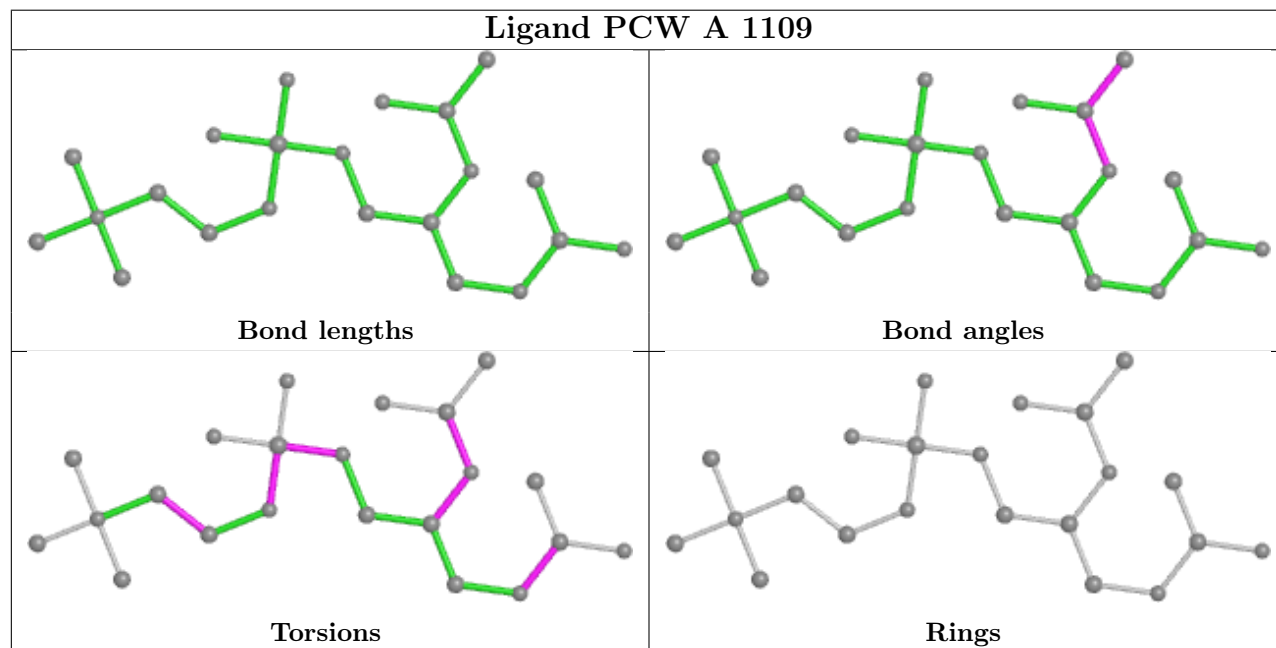
Ligand PCW A 1105



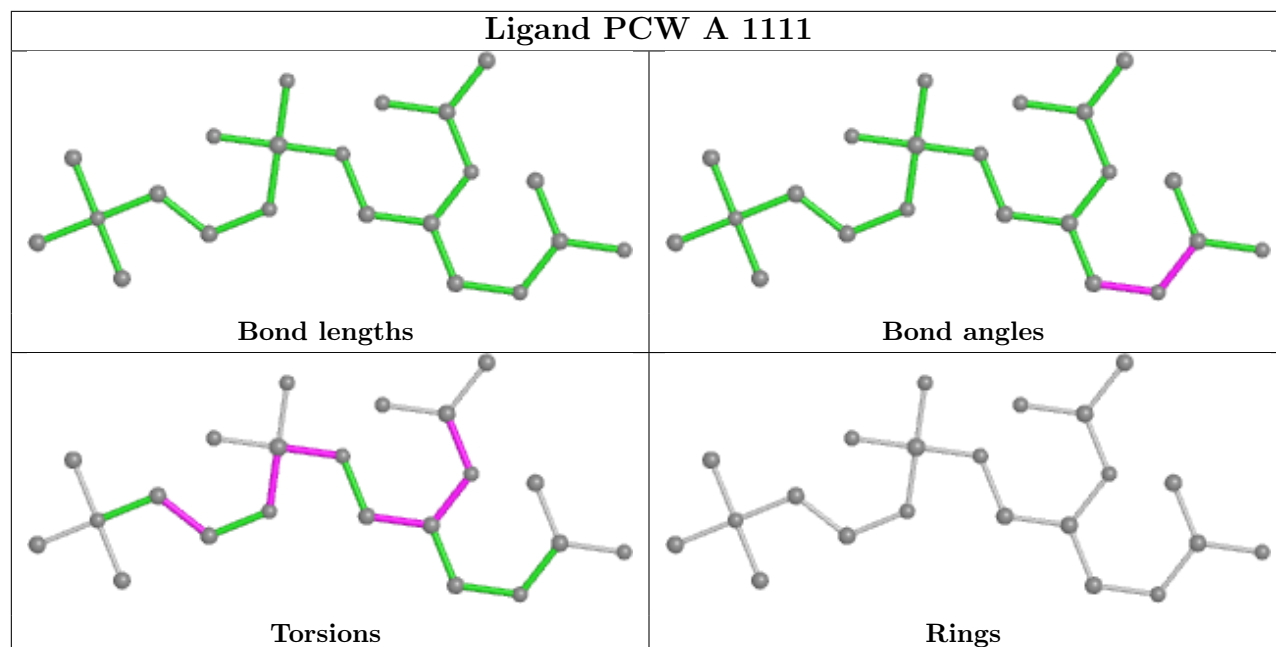
Ligand PCW C 1109



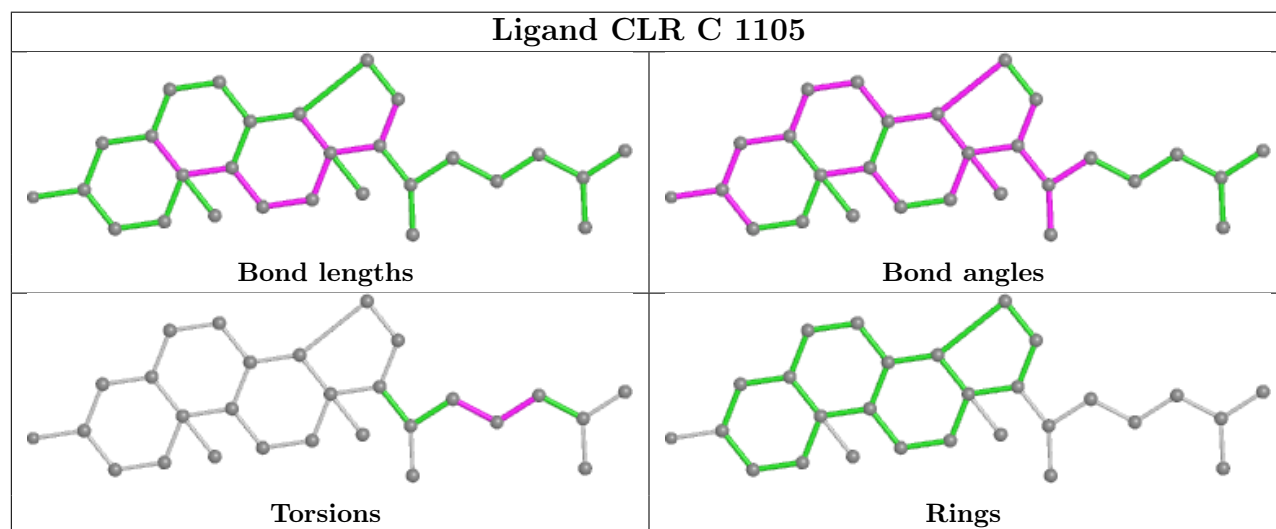
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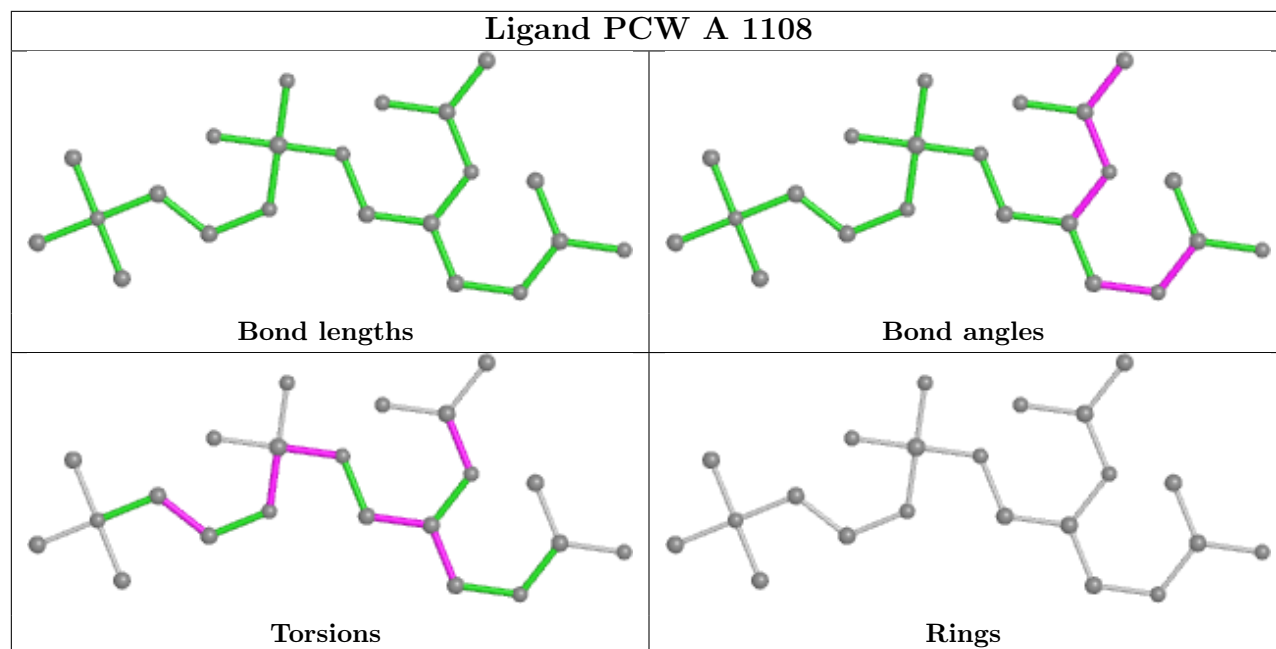
Ligand PCW A 1111



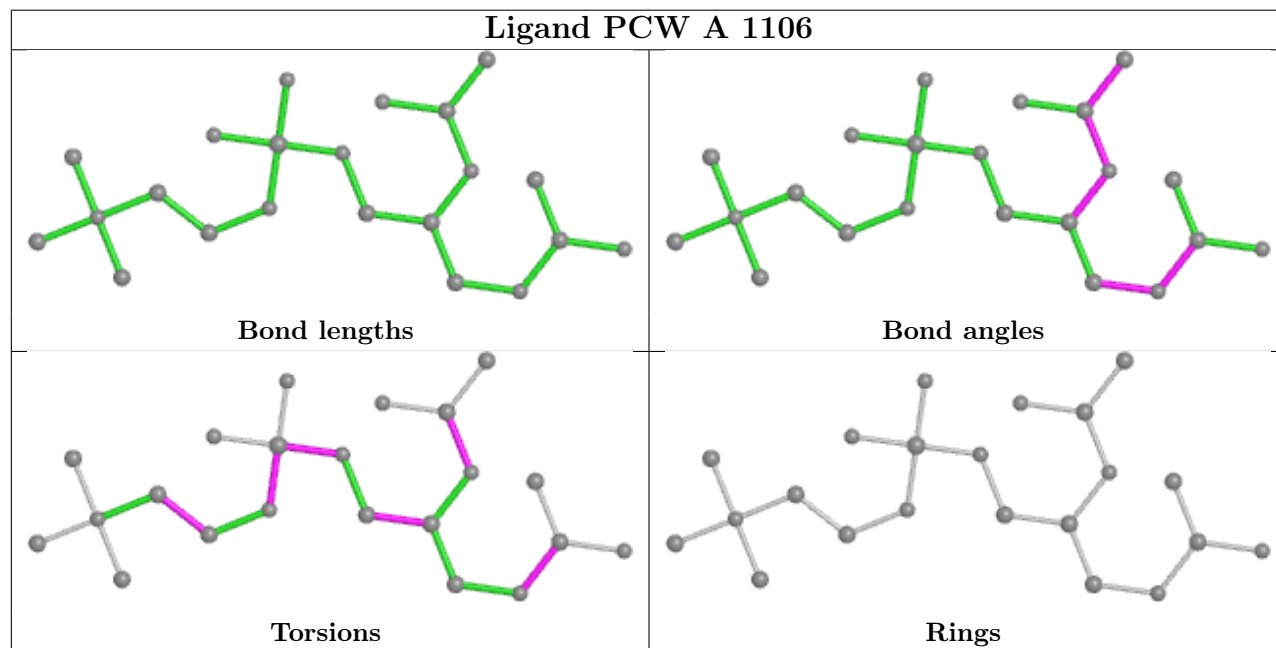
Ligand CLR C 1105



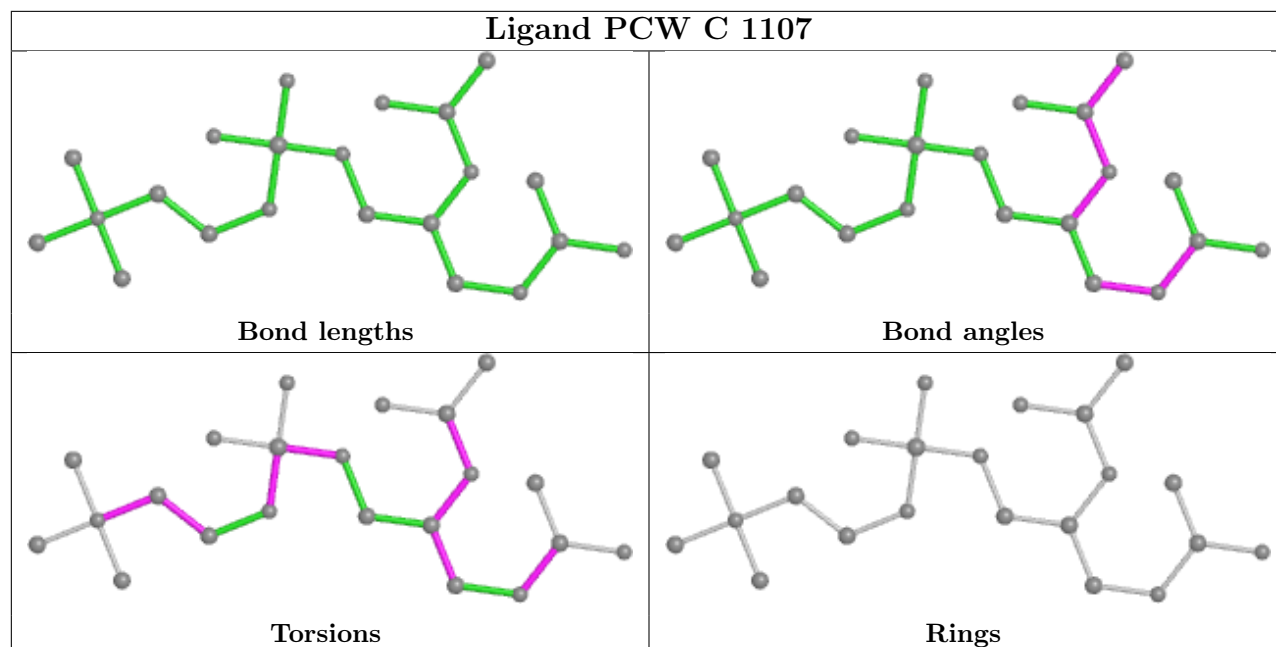
Ligand PCW A 1108



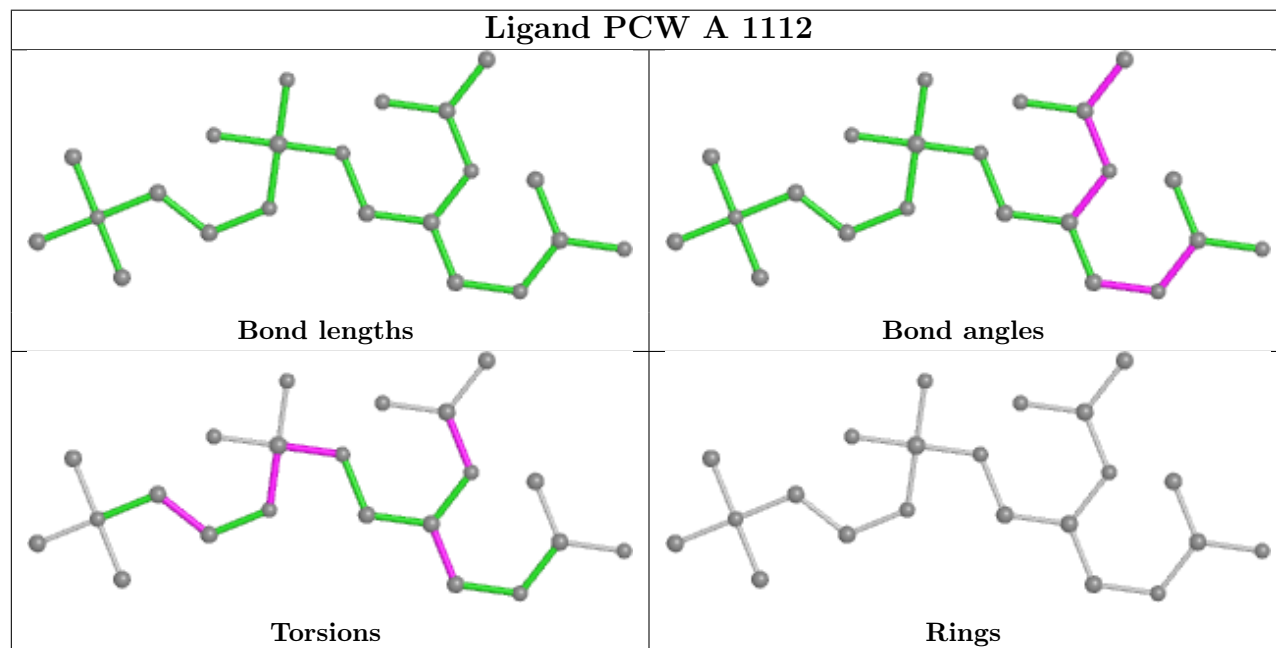
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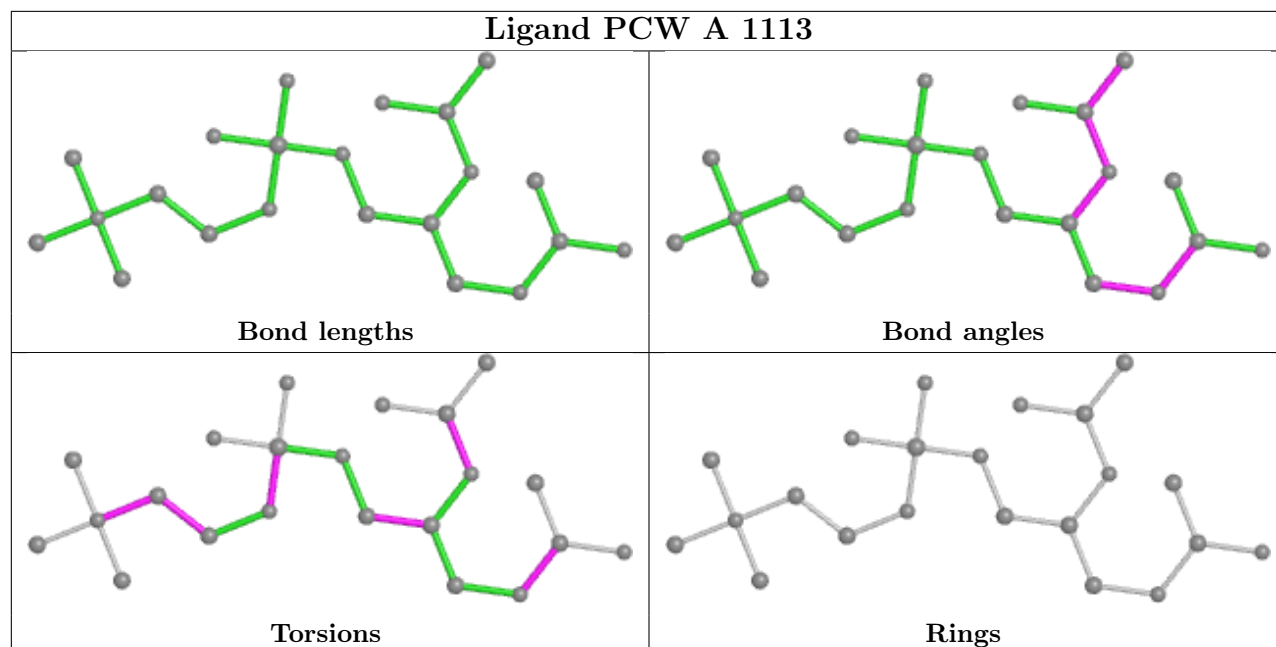
Ligand PCW C 1107



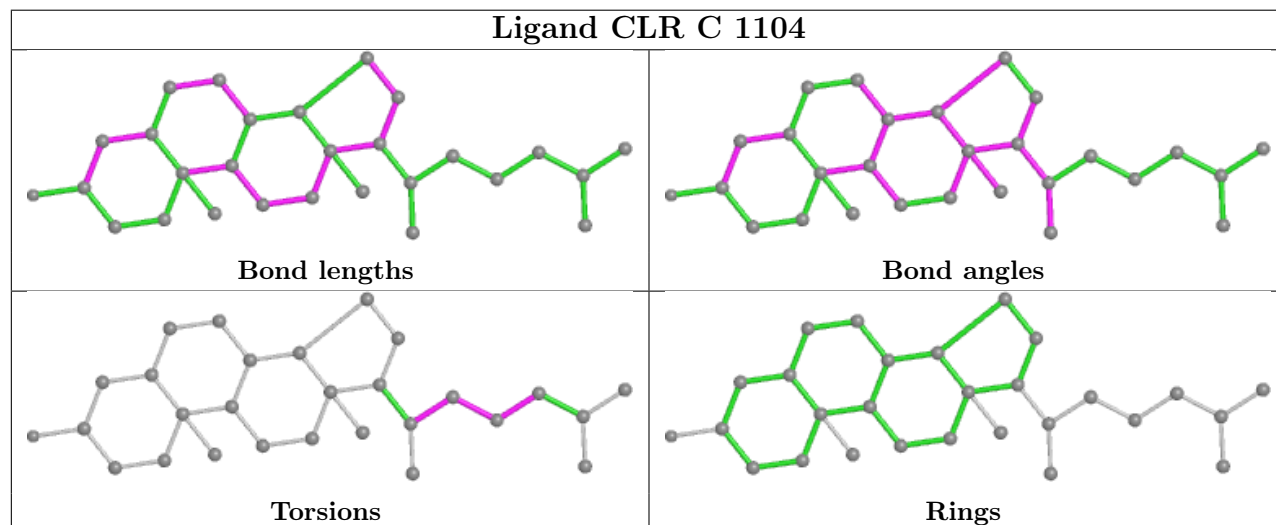
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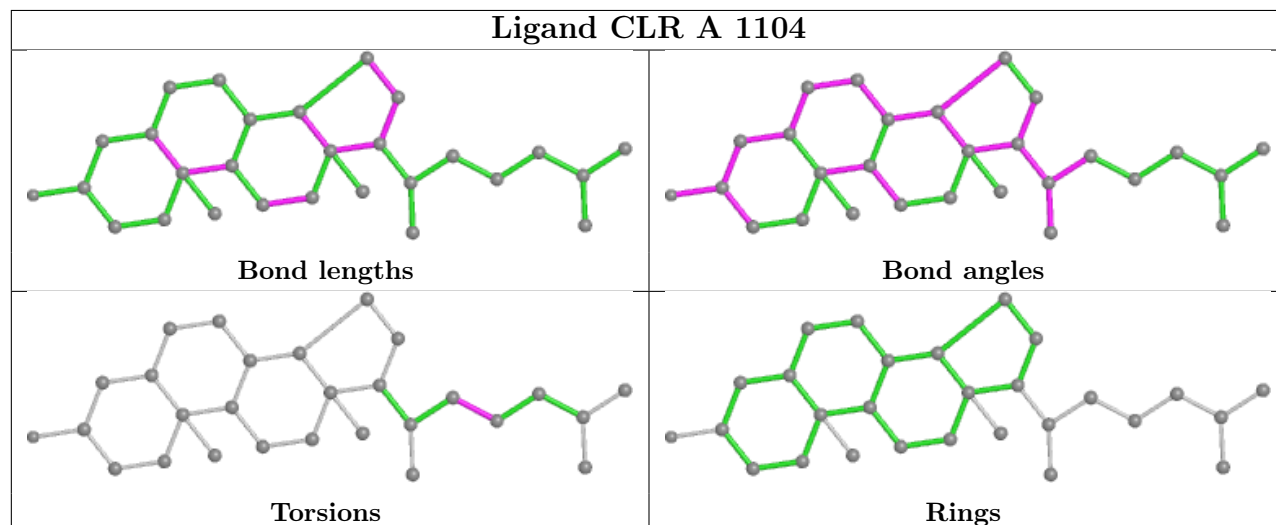
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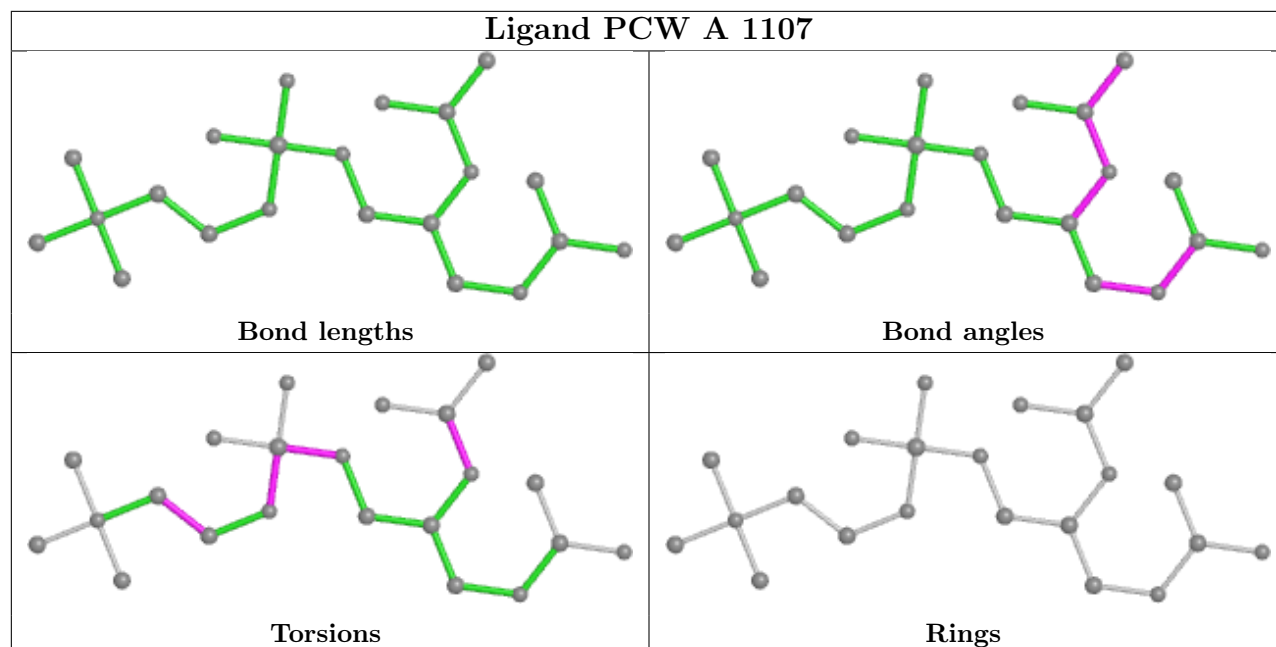
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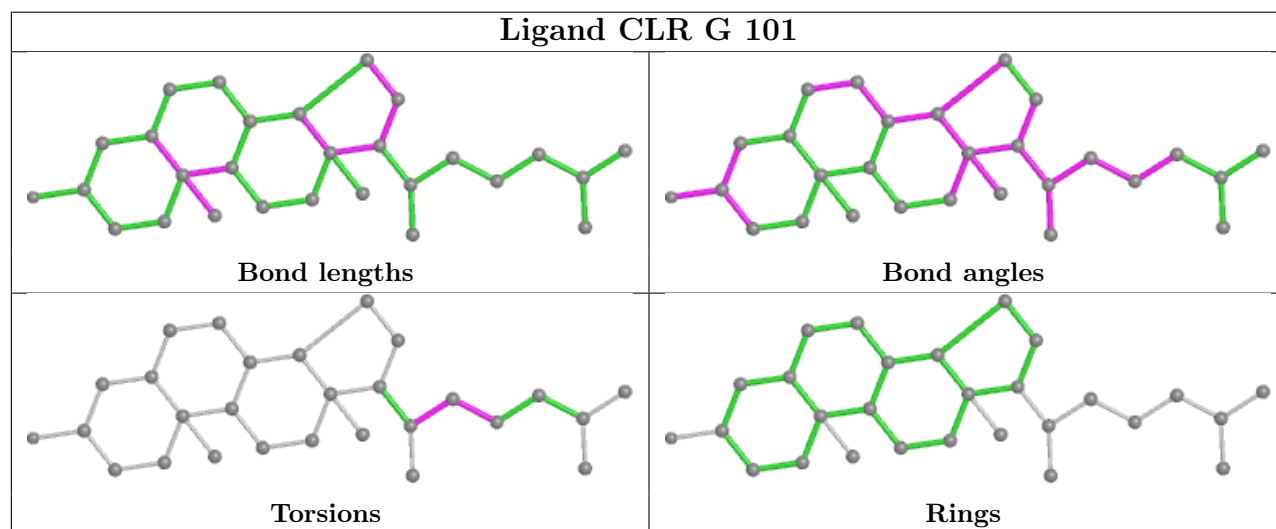
Ligand CLR A 1104

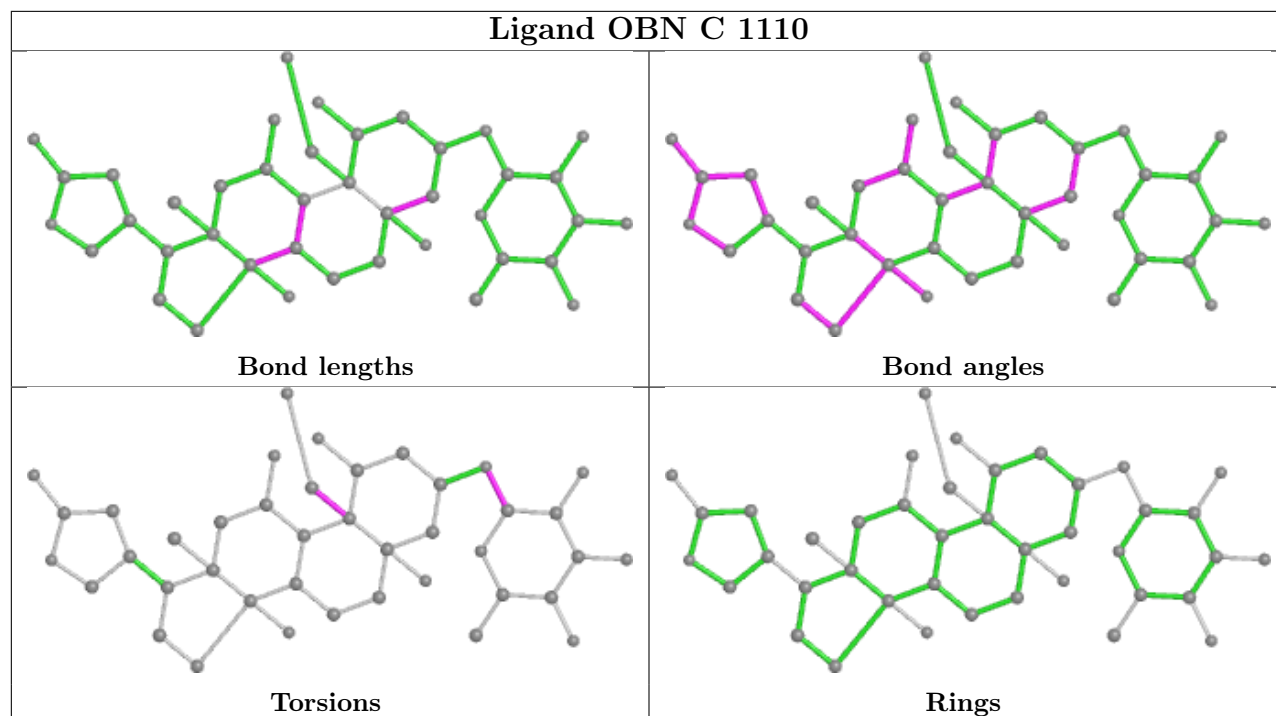


Ligand PCW A 1107



Ligand CLR G 101





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%)	0.47	101 (10%) 6 5	11, 53, 154, 182	0
1	C	995/1016 (97%)	0.24	63 (6%) 20 16	9, 47, 115, 141	0
2	B	291/303 (96%)	0.41	33 (11%) 5 4	25, 77, 120, 152	0
2	D	285/303 (94%)	0.30	24 (8%) 11 8	22, 72, 109, 126	0
3	E	32/65 (49%)	-0.08	1 (3%) 49 44	16, 33, 63, 67	0
3	G	32/65 (49%)	-0.46	0 100 100	18, 35, 63, 76	0
All	All	2630/2768 (95%)	0.34	222 (8%) 11 8	9, 55, 135, 182	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	LEU	11.1
1	A	571	PHE	10.8
1	A	491	THR	9.5
2	B	165	GLU	9.2
2	B	166	THR	9.1
1	A	467	TYR	8.9
1	A	578	PHE	8.1
1	A	579	VAL	8.0
1	A	489	PRO	7.2
1	A	496	HIS	6.8
1	C	571	PHE	6.7
1	A	552	PHE	6.6
1	C	553	LEU	6.6
1	A	492	ALA	6.3
1	C	564	PHE	6.1
1	C	491	THR	6.1
1	A	580	GLY	6.1
1	A	471	VAL	6.0
2	D	203	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
2	B	164	ASP	5.8
1	C	435	ILE	5.8
1	A	487	LYS	5.7
1	A	466	ARG	5.5
1	A	522	PRO	5.4
1	C	497	LEU	5.3
1	A	564	PHE	5.2
1	A	158	VAL	5.0
1	A	404	PHE	5.0
1	A	519	LYS	4.8
1	A	382	ALA	4.7
2	B	162	LEU	4.7
2	D	195	SER	4.7
2	B	202	MET	4.7
2	D	249	LEU	4.7
2	B	17	TRP	4.7
1	A	553	LEU	4.6
1	A	117	GLU	4.6
2	B	196	LEU	4.5
2	D	64	PHE	4.5
1	A	582	ILE	4.5
1	A	114	THR	4.5
1	A	560	GLU	4.5
2	D	196	LEU	4.5
2	B	197	GLU	4.5
1	A	403	SER	4.5
1	A	435	ILE	4.4
2	B	200	PRO	4.4
1	A	516	ILE	4.4
2	D	199	TYR	4.2
1	A	157	MET	4.1
1	A	573	LEU	4.1
1	A	392	GLU	4.1
1	A	178	VAL	4.0
1	C	579	VAL	4.0
1	A	551	LEU	4.0
2	B	203	LYS	4.0
1	C	402	VAL	4.0
1	A	440	VAL	4.0
1	C	429	ASN	4.0
1	A	405	ASP	4.0
1	A	514	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	545	VAL	3.9
1	A	423	ARG	3.8
1	A	488	ASN	3.8
1	C	480	LYS	3.7
1	A	82	TRP	3.7
1	C	116	GLU	3.7
2	B	198	THR	3.7
1	C	496	HIS	3.7
1	A	116	GLU	3.7
2	D	202	MET	3.7
1	C	581	LEU	3.6
2	B	22	LYS	3.6
1	A	406	LYS	3.6
1	C	578	PHE	3.6
1	A	561	GLY	3.6
1	A	470	ILE	3.5
1	C	582	ILE	3.5
1	C	471	VAL	3.5
1	A	485	ILE	3.5
2	B	25	LEU	3.5
2	B	167	TYR	3.5
1	C	158	VAL	3.4
1	A	494	PRO	3.4
1	C	440	VAL	3.4
2	B	199	TYR	3.4
1	C	545	VAL	3.4
1	A	541	LEU	3.3
1	A	550	HIS	3.3
1	C	157	MET	3.3
1	A	776	ASN	3.3
1	A	432	ASN	3.3
1	A	515	LEU	3.3
1	A	468	THR	3.3
1	A	575	ASN	3.2
1	A	113	ALA	3.2
1	A	525	GLU	3.2
1	C	481	TYR	3.2
1	A	542	GLY	3.2
2	D	13	LYS	3.2
1	C	514	ILE	3.2
1	A	156	ASN	3.2
1	C	487	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	34	MET	3.1
1	A	159	PRO	3.1
1	C	154	PHE	3.1
2	B	100	SER	3.1
1	A	498	LEU	3.1
2	D	200	PRO	3.1
1	C	500	MET	3.0
2	D	20	GLU	3.0
1	A	402	VAL	3.0
1	A	775	SER	3.0
1	A	509	ASP	3.0
2	B	121	MET	3.0
1	A	490	ASN	3.0
1	A	505	GLU	3.0
1	C	499	VAL	3.0
1	C	556	GLU	3.0
2	D	21	LYS	2.9
1	A	475	PHE	2.9
2	D	198	THR	2.9
1	C	851	GLY	2.9
2	B	122	ILE	2.9
2	D	197	GLU	2.9
1	C	426	PHE	2.9
1	A	528	LYS	2.8
2	B	273	ARG	2.8
1	C	124	TYR	2.8
1	C	498	LEU	2.8
1	A	393	ALA	2.8
2	B	192	LYS	2.8
1	C	548	PHE	2.8
1	C	1008	GLY	2.8
1	A	521	GLN	2.8
3	E	23	TYR	2.8
2	D	141	ASN	2.7
1	C	552	PHE	2.7
2	B	201	VAL	2.7
1	A	202	ASN	2.7
2	D	17	TRP	2.7
2	B	212	HIS	2.7
1	C	117	GLU	2.7
1	A	574	ASP	2.7
1	C	748	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	216	LYS	2.7
2	D	129	VAL	2.6
1	C	78	THR	2.6
1	A	469	LYS	2.6
1	A	546	LEU	2.6
1	A	34	MET	2.6
1	C	485	ILE	2.6
1	C	519	LYS	2.6
2	B	20	GLU	2.6
1	A	429	ASN	2.6
2	D	181	ASN	2.5
1	A	804	ASP	2.5
2	D	283	ILE	2.5
2	B	13	LYS	2.5
1	C	566	THR	2.5
1	A	118	PRO	2.5
1	C	385	TRP	2.5
1	C	550	HIS	2.5
1	A	774	THR	2.4
1	A	548	PHE	2.4
1	C	455	LEU	2.4
1	C	1012	LYS	2.4
1	A	526	GLU	2.4
1	A	383	HIS	2.4
1	C	774	THR	2.4
2	B	195	SER	2.4
1	A	372	GLY	2.3
1	A	748	PHE	2.3
1	C	209	SER	2.3
2	B	263	PHE	2.3
1	C	223	ASP	2.3
1	C	776	ASN	2.3
1	A	64	ILE	2.3
2	D	176	VAL	2.3
1	C	196	LEU	2.3
1	A	549	CYS	2.3
1	A	22	GLU	2.3
1	A	441	ALA	2.3
1	A	531	PHE	2.3
1	A	354	LEU	2.3
1	A	154	PHE	2.3
1	C	73	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	769	ILE	2.2
2	B	64	PHE	2.2
1	A	922	VAL	2.2
2	B	107	ARG	2.2
1	C	988	SER	2.2
2	D	25	LEU	2.2
1	C	547	GLY	2.2
2	D	151	PHE	2.2
1	A	572	PRO	2.2
1	A	495	ARG	2.2
1	C	854	GLN	2.2
1	C	504	PRO	2.1
1	A	713	ASN	2.1
2	B	163	ASN	2.1
1	A	658	VAL	2.1
1	C	773	LEU	2.1
1	C	495	ARG	2.1
1	C	546	LEU	2.1
2	D	115	LEU	2.1
1	A	425	VAL	2.1
1	A	610	THR	2.1
1	A	426	PHE	2.1
1	C	33	SER	2.1
1	C	427	GLN	2.1
2	B	176	VAL	2.1
1	A	420	LEU	2.0
1	A	124	TYR	2.0
1	C	775	SER	2.0
1	A	171	MET	2.0
1	A	569	VAL	2.0
1	C	159	PRO	2.0
2	B	24	PHE	2.0
2	B	115	LEU	2.0
2	D	84	GLN	2.0
2	D	77	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(\AA^2)	Q<0.9
1	PHD	C	369	12/13	0.92	0.32	29,44,59,71	0
1	PHD	A	369	12/13	0.95	0.31	34,40,47,48	0

6.3 Carbohydrates [i](#)

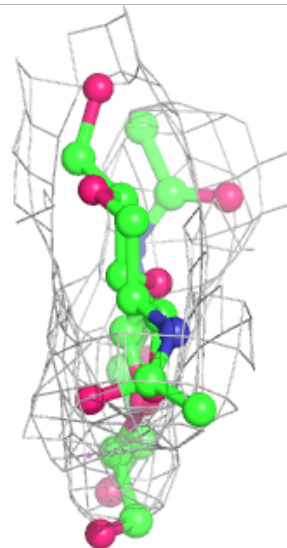
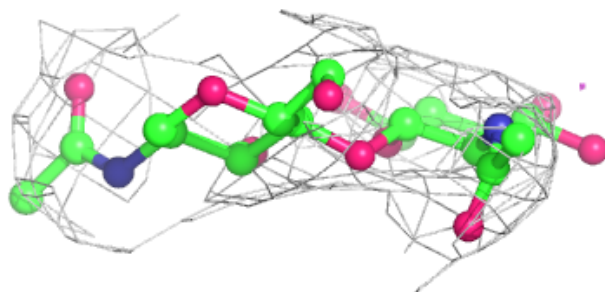
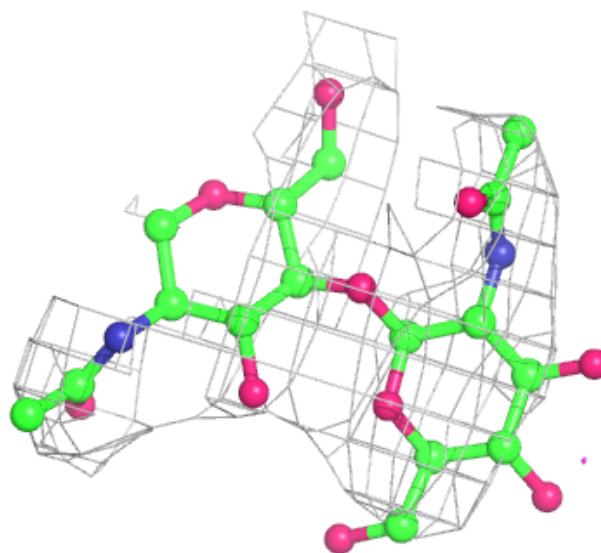
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	H	1	14/15	0.56	0.57	122,128,152,168	0
4	NAG	H	2	14/15	0.57	1.12	134,145,160,162	0
4	NAG	F	1	14/15	0.79	0.24	95,96,132,140	0
4	NAG	F	2	14/15	0.80	0.63	102,117,125,130	0
4	NAG	J	1	14/15	0.84	0.45	95,109,119,126	0
4	NAG	I	2	14/15	0.91	0.38	87,102,113,115	0
4	NAG	J	2	14/15	0.91	0.68	106,121,132,138	0
4	NAG	I	1	14/15	0.93	0.24	80,84,99,116	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.

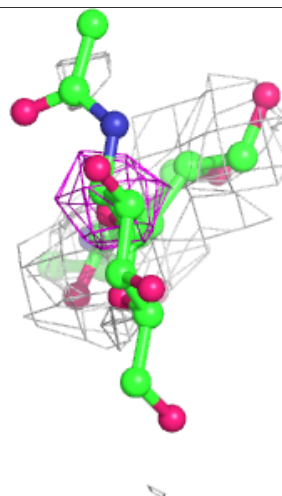
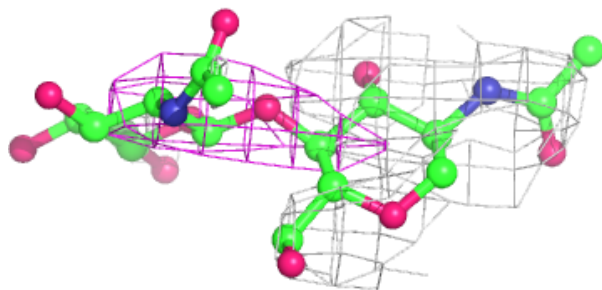
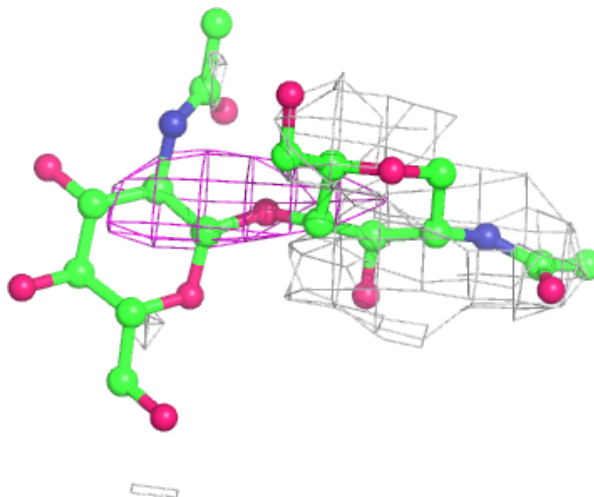
Electron density around Chain F:

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



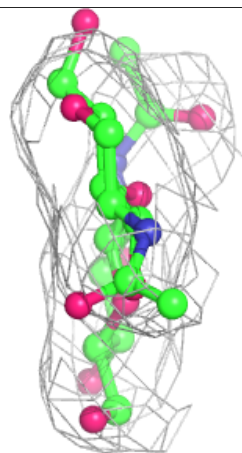
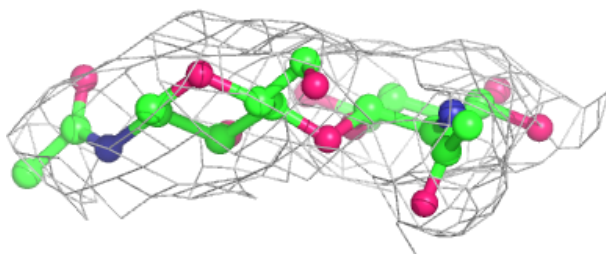
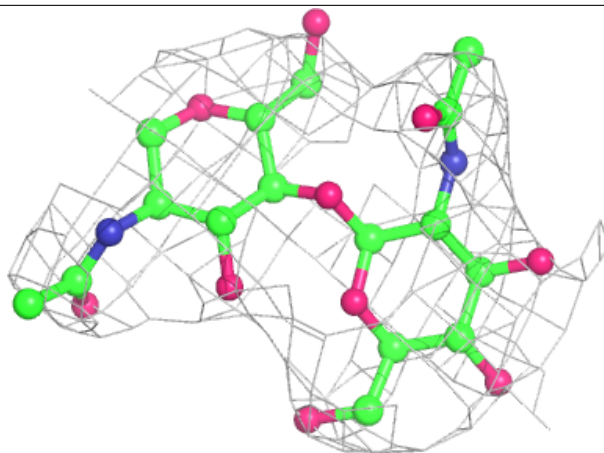
Electron density around Chain H:

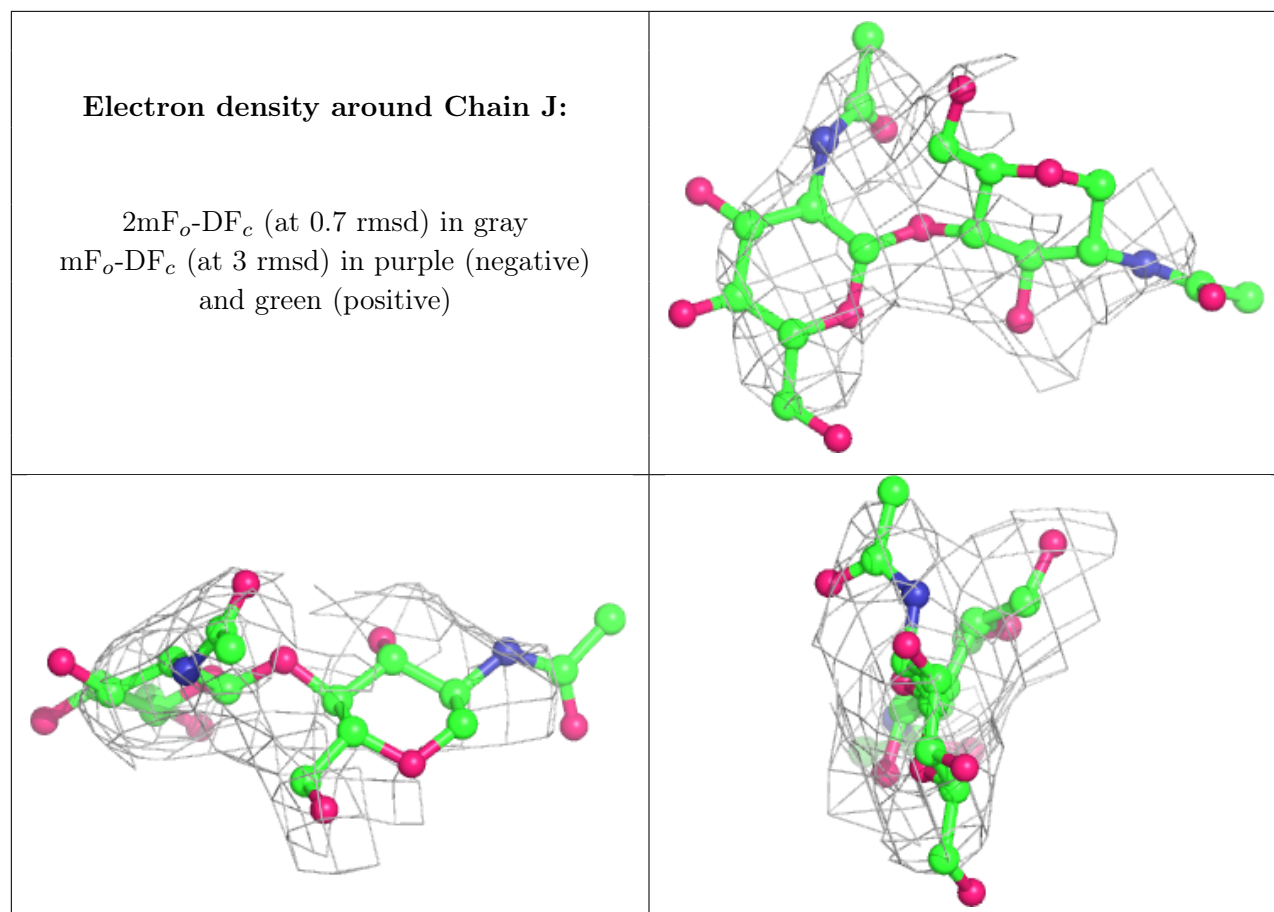
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(\AA^2)	Q<0.9
8	PCW	A	1109	22/54	0.65	0.76	62,78,123,124	0
8	PCW	C	1108	22/54	0.73	0.48	63,96,127,136	0
8	PCW	A	1107	22/54	0.77	0.61	88,100,123,137	0
10	NAG	B	401	14/15	0.77	0.28	101,116,127,129	0
8	PCW	A	1111	22/54	0.79	0.71	93,108,128,134	0
10	NAG	D	401	14/15	0.79	0.40	99,110,119,120	0
8	PCW	A	1112	22/54	0.80	0.68	57,114,131,139	0
8	PCW	A	1110	22/54	0.80	0.47	68,88,134,144	0
7	CLR	A	1104	28/28	0.82	0.67	42,62,73,81	0
7	CLR	C	1105	28/28	0.82	0.56	32,53,80,83	0
8	PCW	C	1106	22/54	0.84	0.36	46,75,98,127	0
8	PCW	A	1106	22/54	0.84	0.55	74,92,112,113	0

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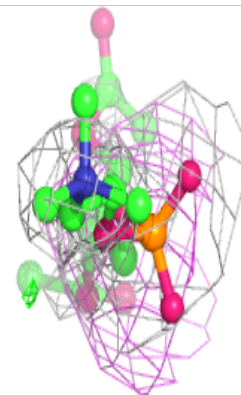
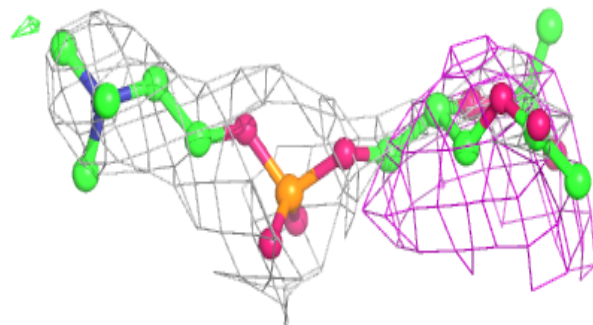
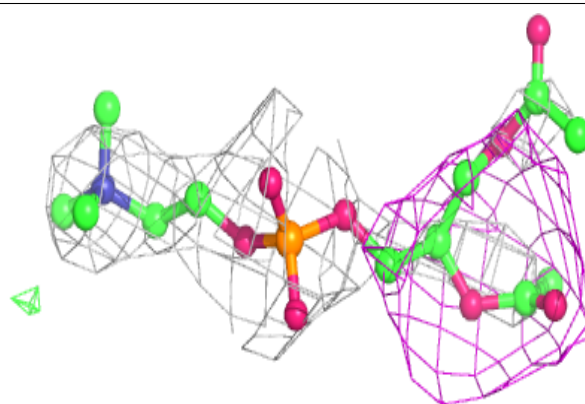
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PCW	A	1113	22/54	0.85	0.27	38,64,80,89	0
8	PCW	A	1105	22/54	0.86	0.33	71,95,114,129	0
7	CLR	D	402	28/28	0.88	0.48	59,75,88,115	0
8	PCW	A	1108	22/54	0.88	0.40	85,103,124,131	0
8	PCW	C	1107	22/54	0.88	0.44	69,100,109,124	0
5	MG	C	1103	1/1	0.92	0.22	25,25,25,25	0
5	MG	A	1103	1/1	0.92	0.27	40,40,40,40	0
9	OBN	A	1114	41/41	0.93	0.21	44,59,79,89	0
5	MG	A	1101	1/1	0.93	0.27	40,40,40,40	0
8	PCW	C	1109	22/54	0.93	0.20	30,44,81,86	0
9	OBN	C	1110	41/41	0.94	0.16	27,44,56,59	0
6	NA	A	1102	1/1	0.94	0.34	12,12,12,12	0
5	MG	C	1101	1/1	0.94	0.22	39,39,39,39	0
7	CLR	C	1104	28/28	0.95	0.25	11,22,43,51	0
6	NA	C	1102	1/1	0.96	0.39	9,9,9,9	0
7	CLR	G	101	28/28	0.96	0.22	16,17,45,53	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.

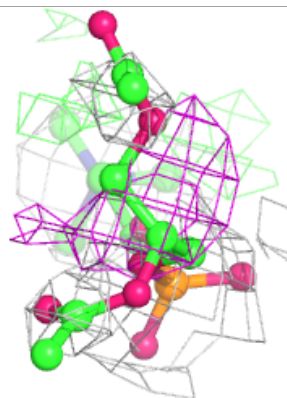
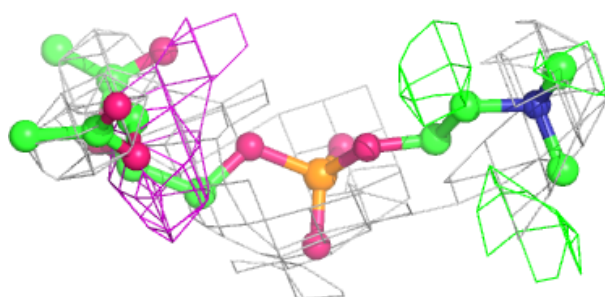
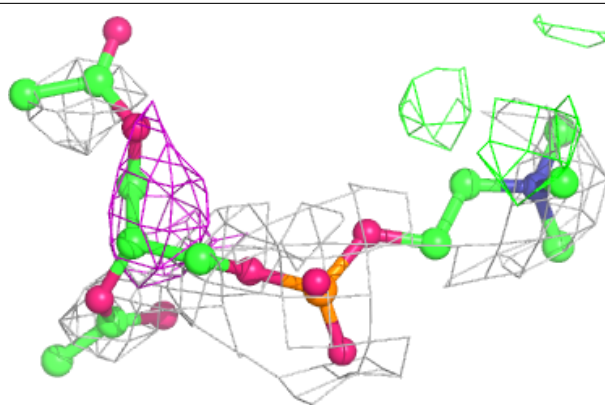
Electron density around PCW A 1109:

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

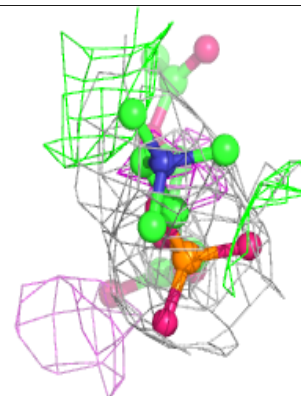
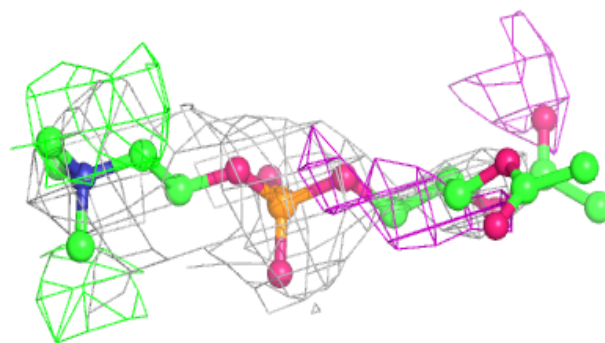
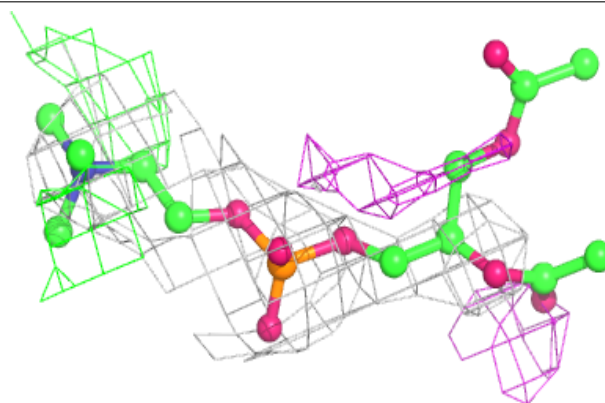


Electron density around PCW C 1108:

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

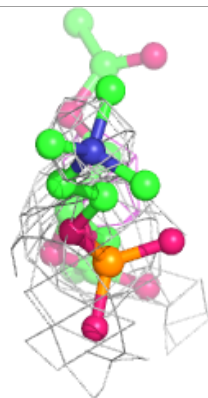
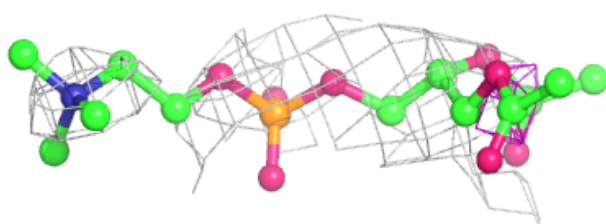
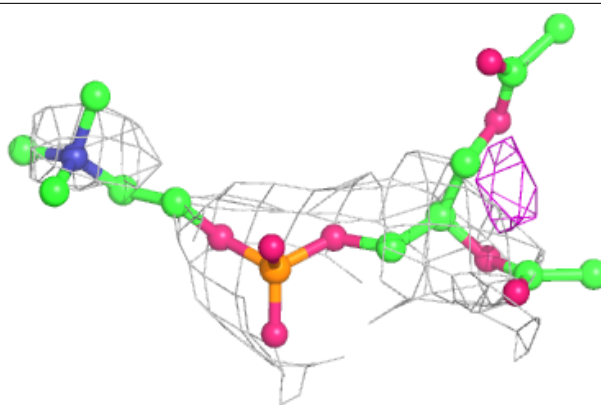
**Electron density around PCW A 1107:**

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

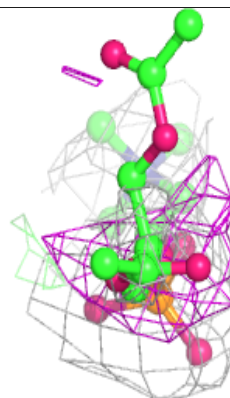
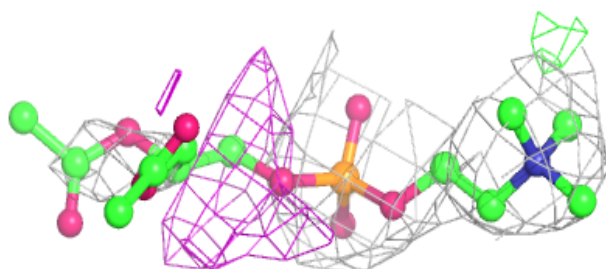
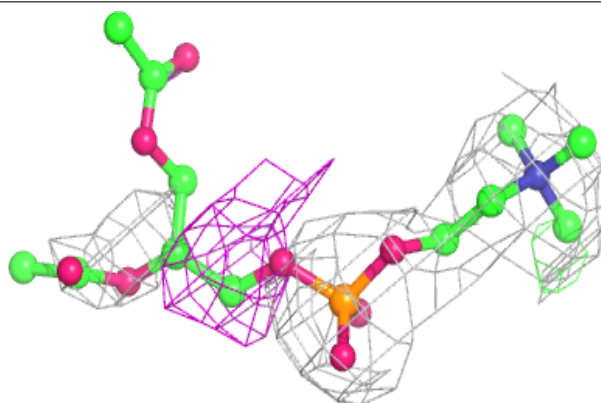


Electron density around PCW A 1111:

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

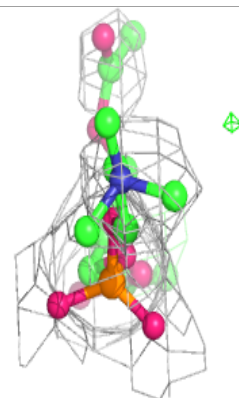
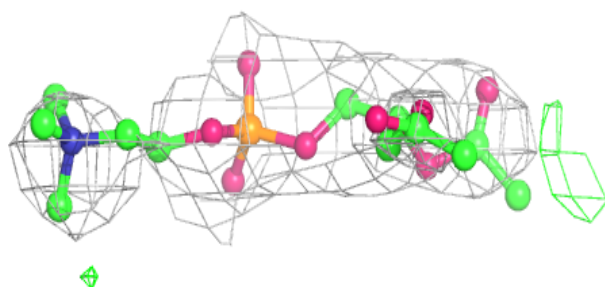
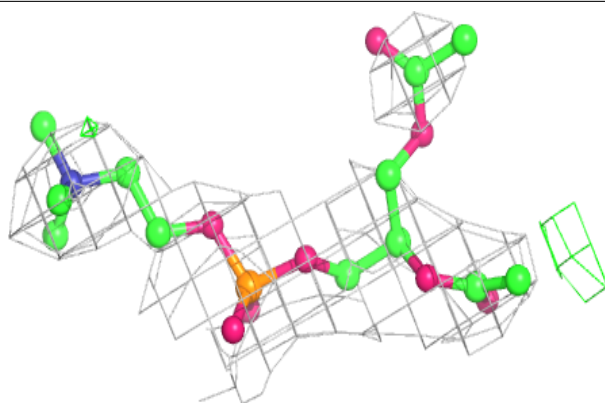
**Electron density around PCW A 1112:**

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

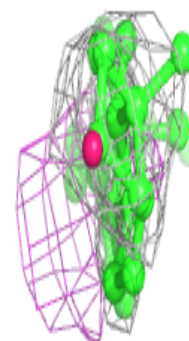
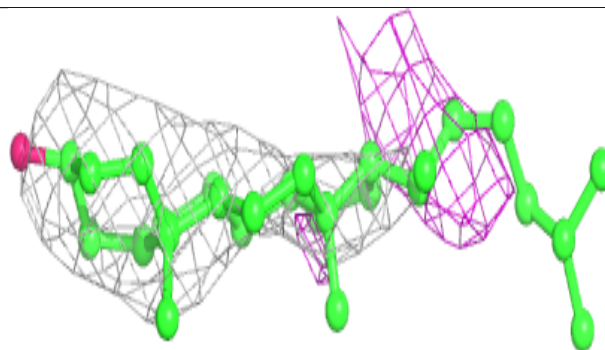
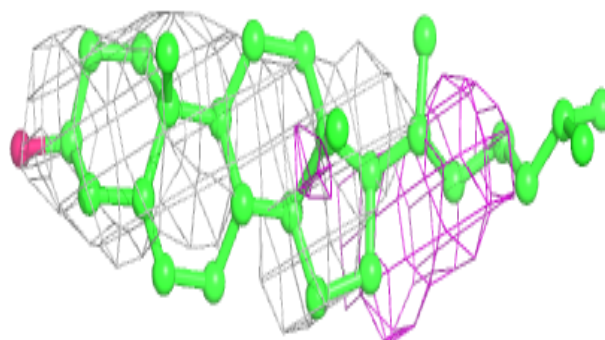


Electron density around PCW A 1110:

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

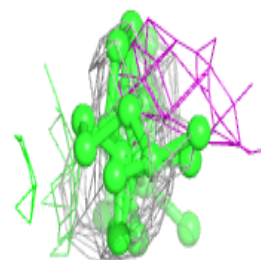
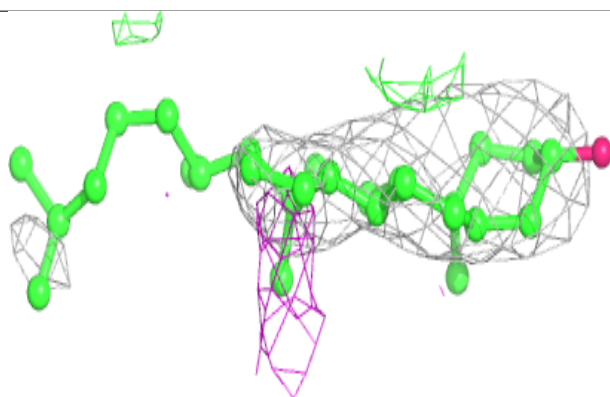
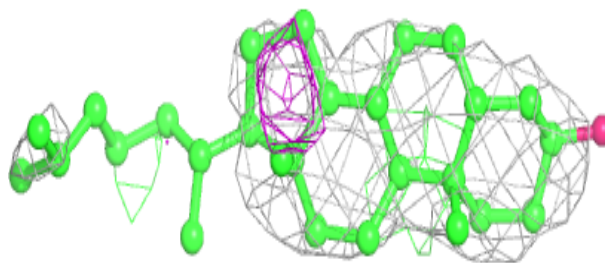
**Electron density around CLR A 1104:**

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

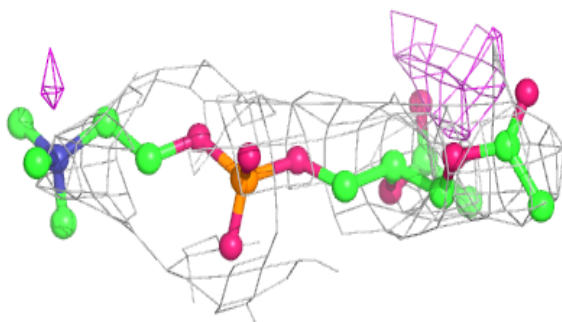
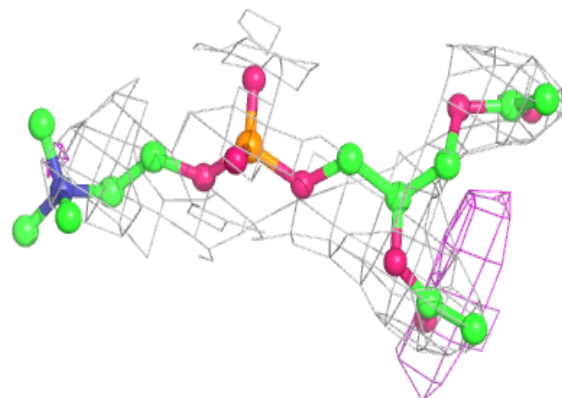


Electron density around CLR C 1105:

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and green (positive)

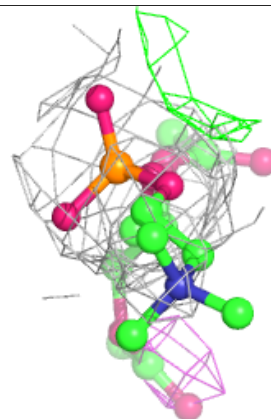
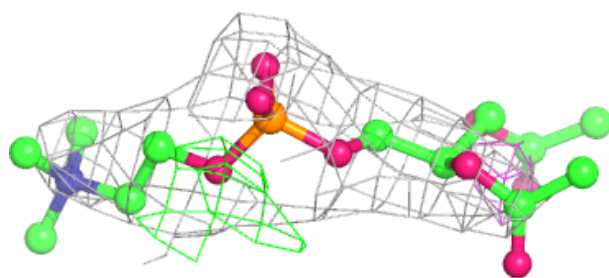
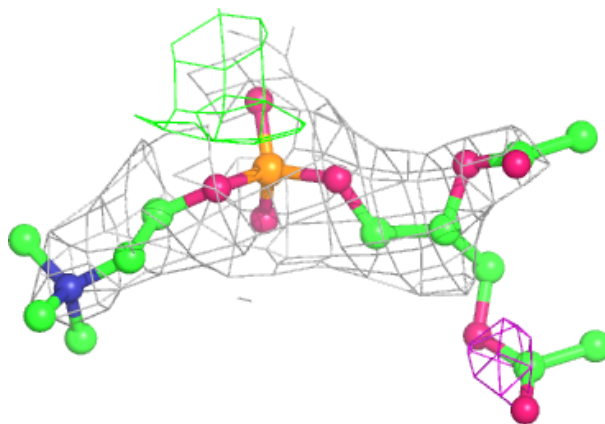
**Electron density around PCW C 1106:**

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



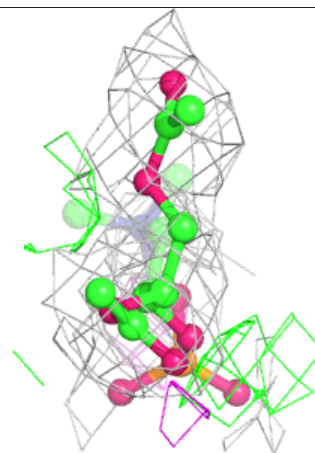
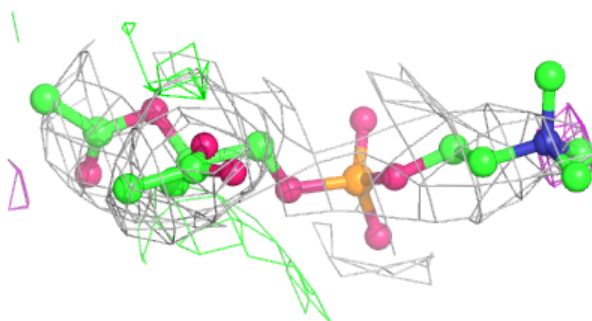
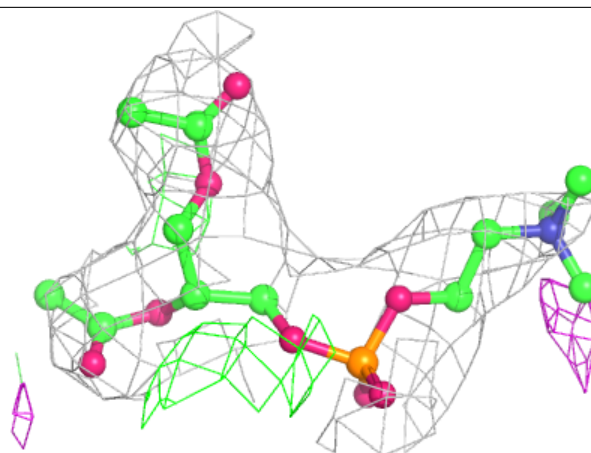
Electron density around PCW A 1106:

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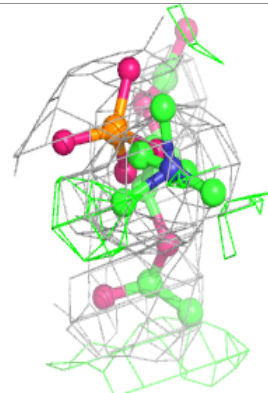
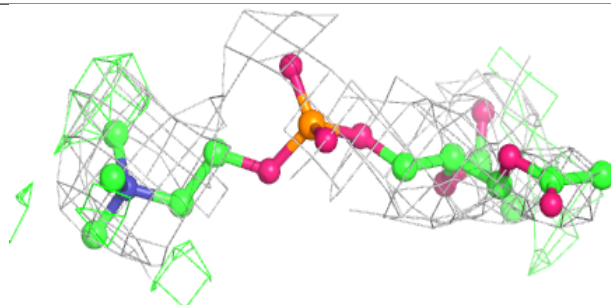
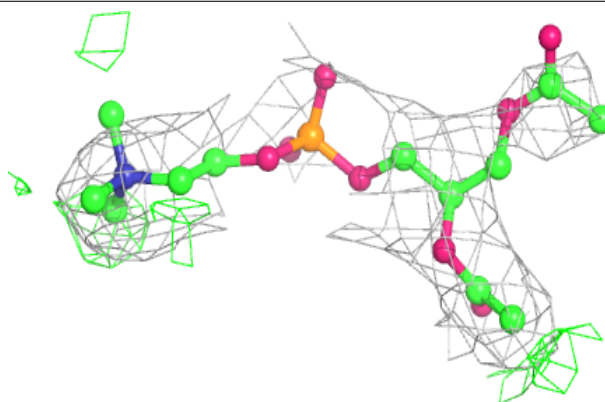


Electron density around PCW A 1113:

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

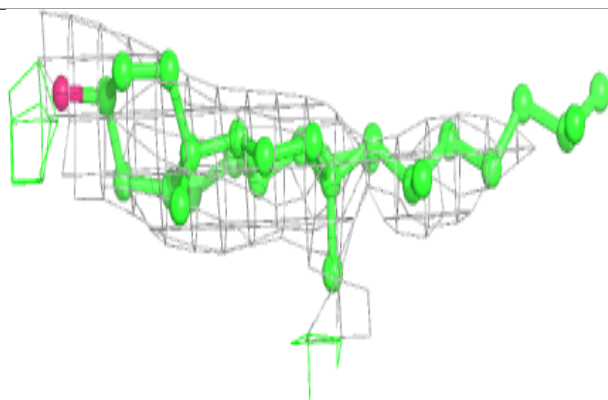
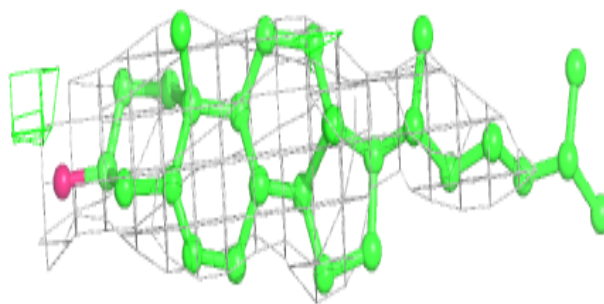
**Electron density around PCW A 1105:**

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and green (positive)

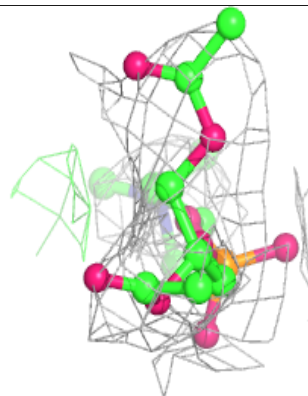
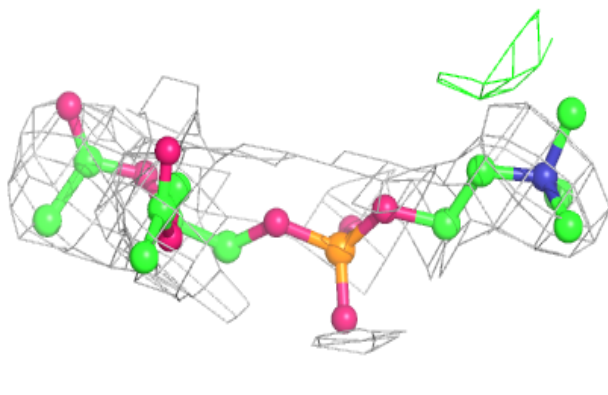
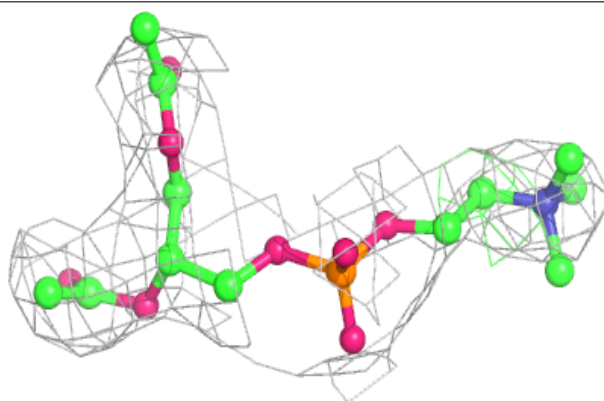


Electron density around CLR D 402:

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and green (positive)

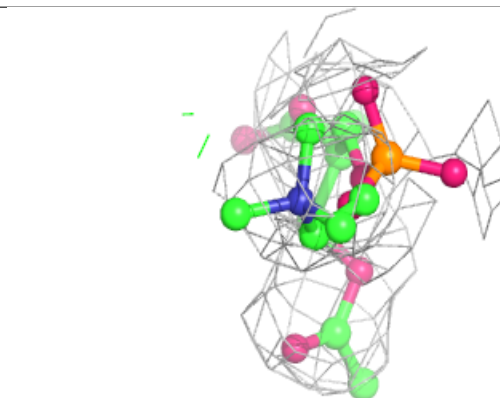
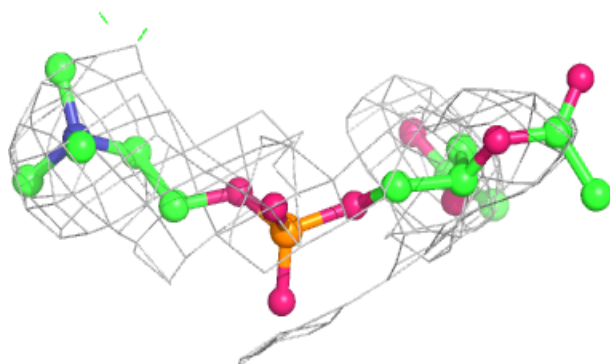
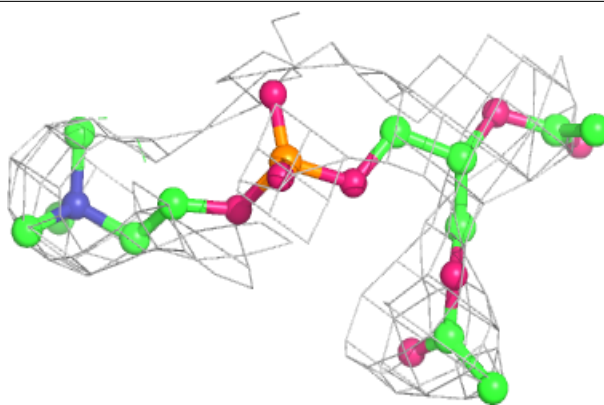
**Electron density around PCW A 1108:**

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and green (positive)

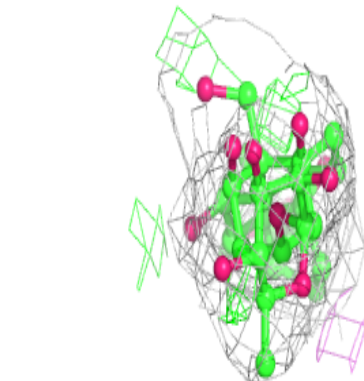
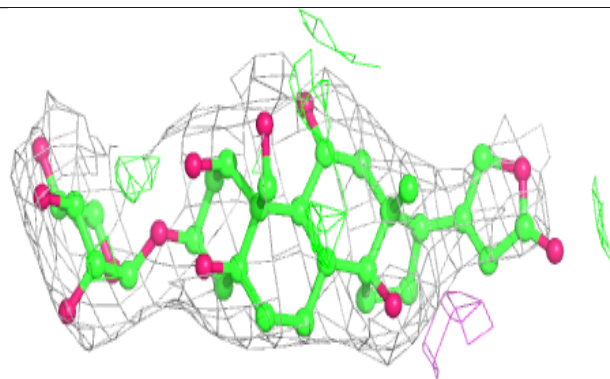
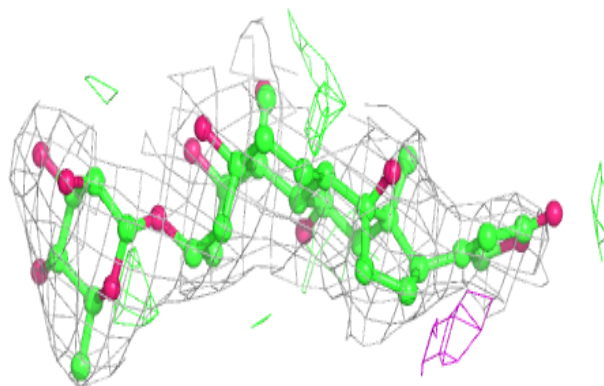


Electron density around PCW C 1107:

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

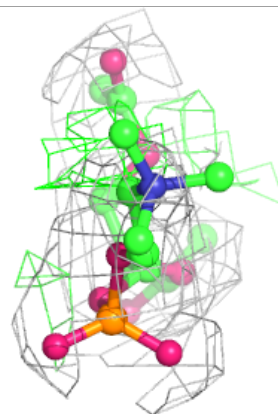
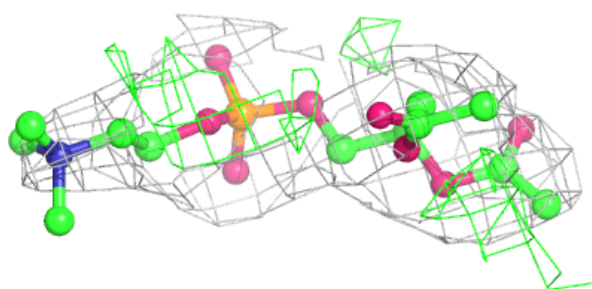
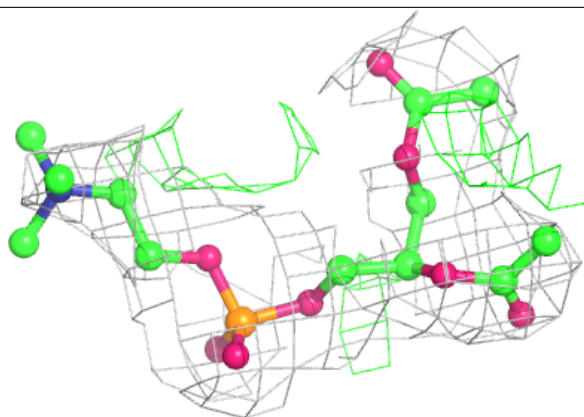
**Electron density around OBN A 1114:**

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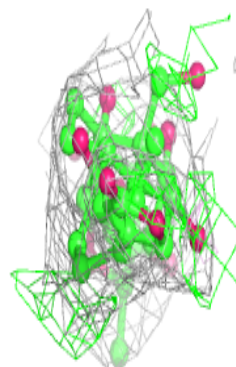
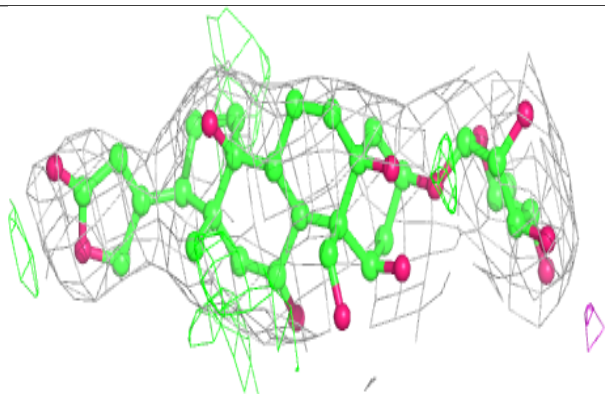
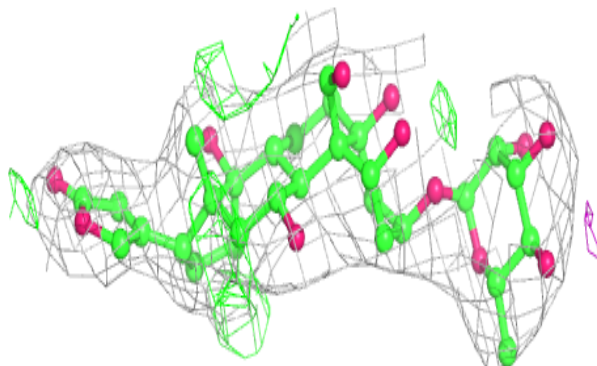


Electron density around PCW C 1109:

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

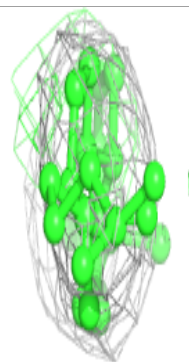
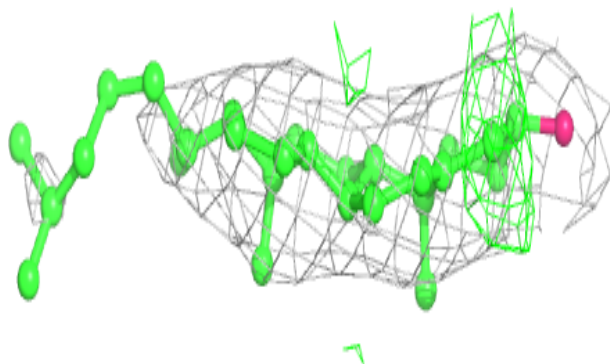
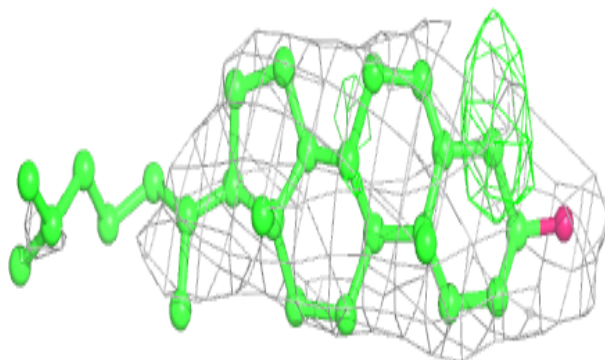
**Electron density around OBN C 1110:**

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

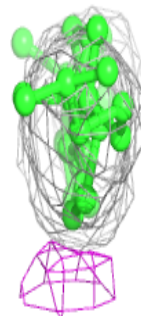
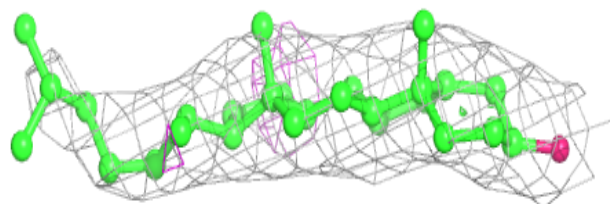
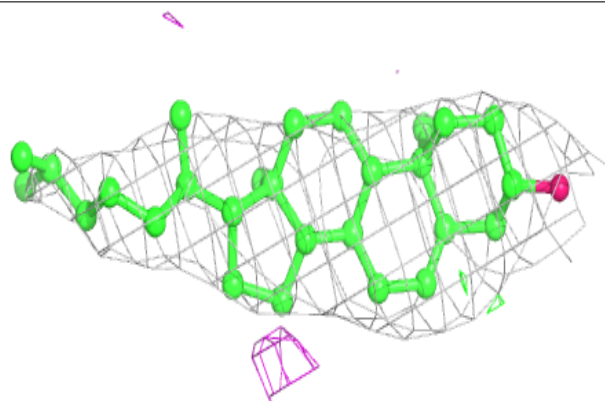


Electron density around CLR C 1104:

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

**Electron density around 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.