



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2025 – 04:39 PM JST

PDB ID : 7DDK
Title : Crystal structures of Na⁺,K⁺-ATPase in complex with rostafuroxin
Authors : Ogawa, H.; Cornelius, F.; Kanai, R.; Motoyama, K.; Vilsen, B.; Toyoshima, C.
Deposited on : 2020-10-29
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

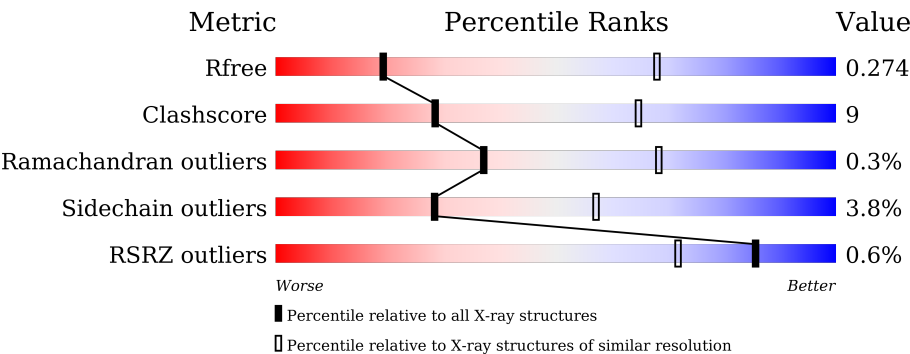
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 3.50 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}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>75%22%..</div></div>
1	C	1016	<div><div></div><div></div><div></div><div></div><div></div></div> <div>77%21%..</div>
2	B	303	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>70%24%. .</div></div>
2	D	303	<div><div></div><div></div><div></div><div></div><div></div></div> <div>65%27%. 6%</div>
3	E	65	<div><div></div><div></div><div></div><div></div><div></div></div> <div>45%. .51%</div>
3	G	65	<div><div></div><div></div><div></div><div></div><div></div></div> <div>35%14%51%</div>

Continued on next page...

Continued from previous page...

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%

2 Entry composition

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 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			

Continued on next page...

Continued from previous page...

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			

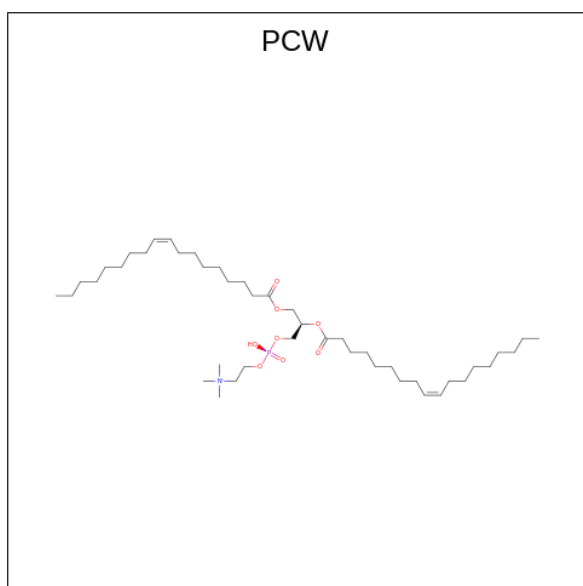
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

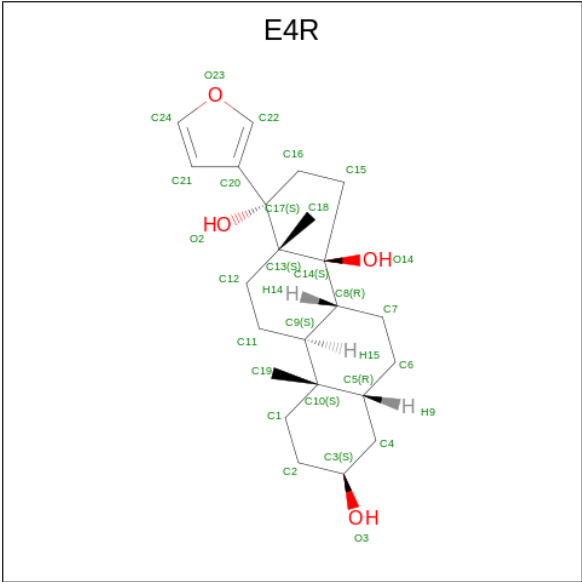
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

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



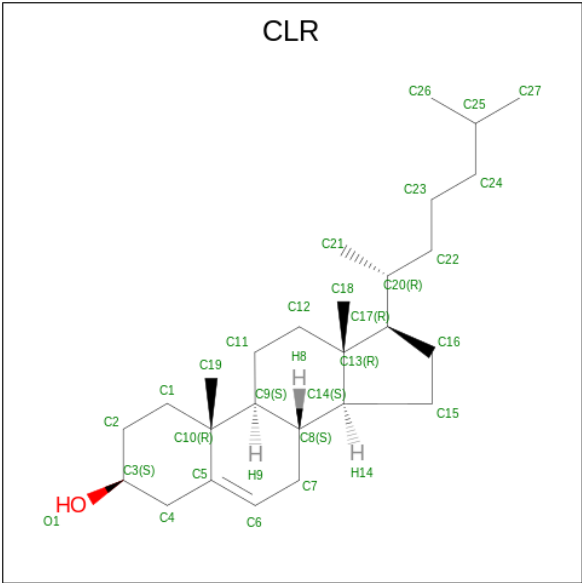
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	C	1	Total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

- Molecule 8 is (3S,5R,8R,9S,10S,13S,14S,17S)-17-(furan-3-yl)-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,15,16-dodecahydro-1H-cyclopenta[a]phenanthrene-3,14,17-triol (three-letter code: E4R) (formula: C₂₃H₃₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			27	23	4		
8	C	1	Total	C	O	0	0
			27	23	4		

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



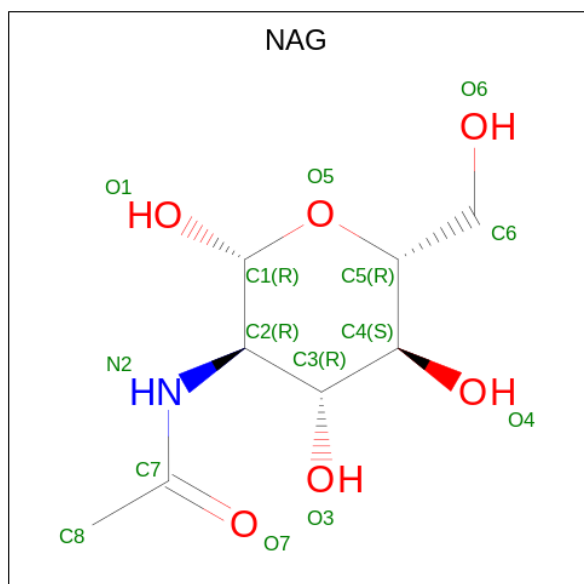
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			28	27	1		
9	B	1	Total	C	O	0	0
			28	27	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

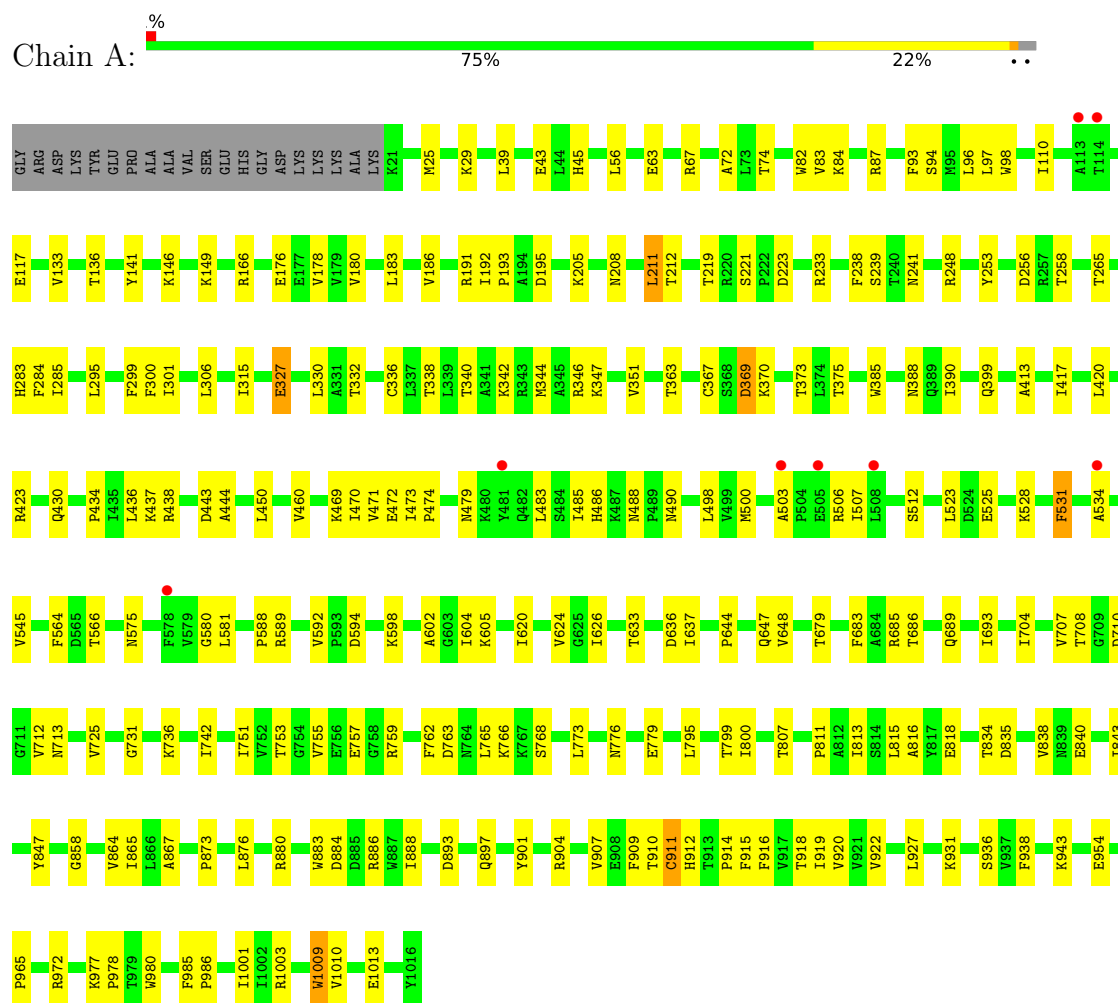
- Molecule 11 is water.

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

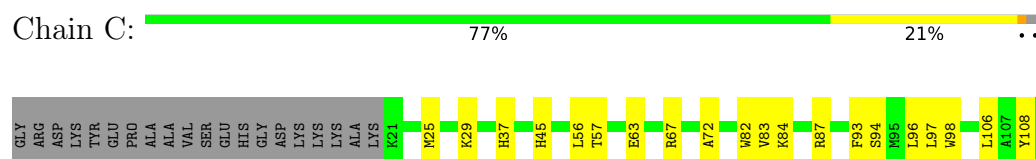
3 Residue-property plots

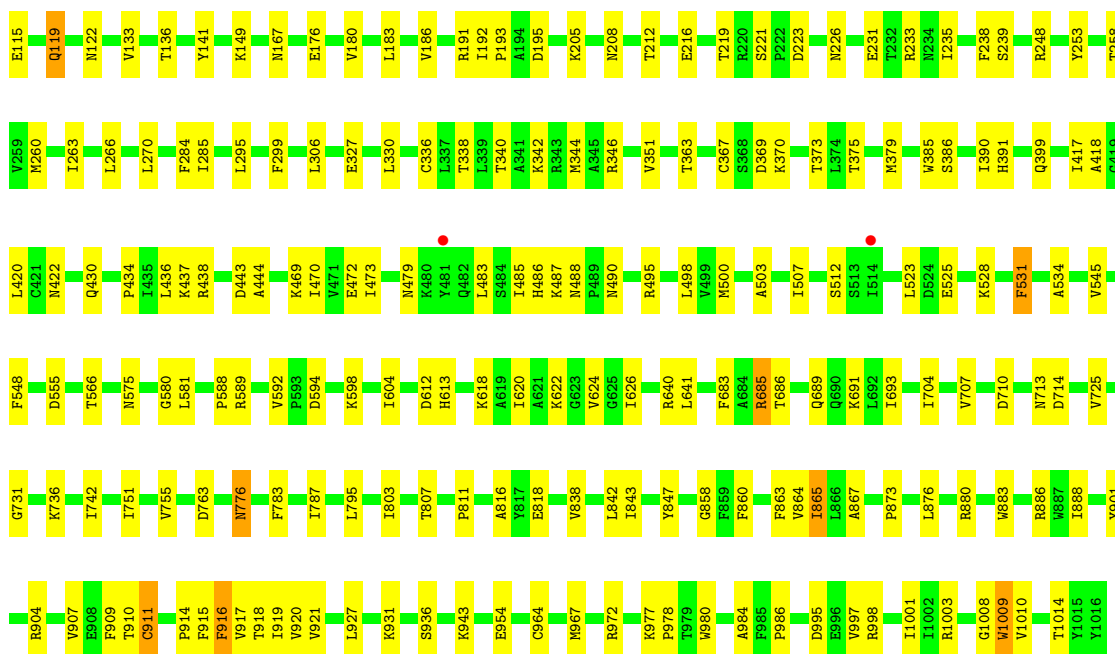
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

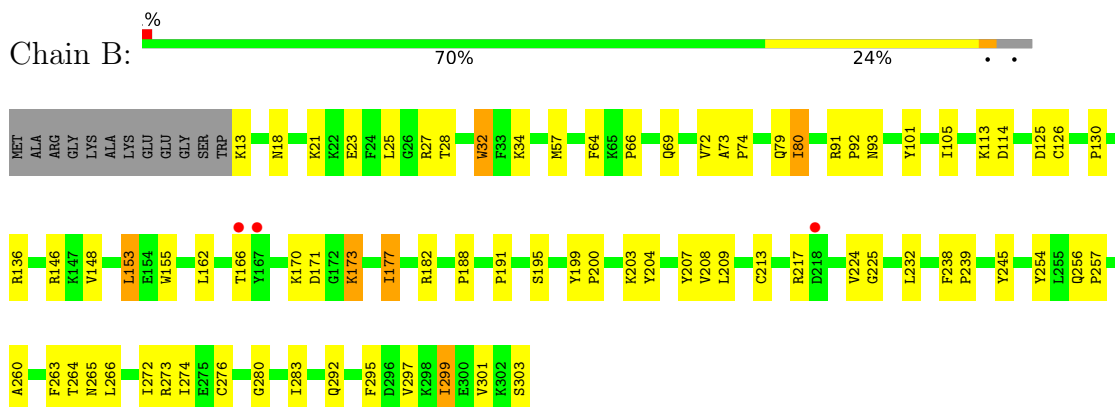


- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

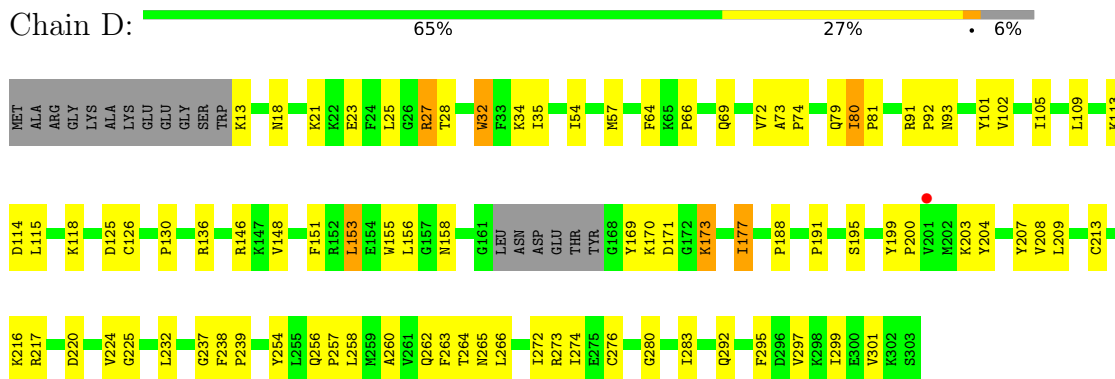




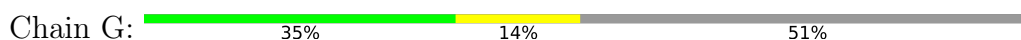
- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



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

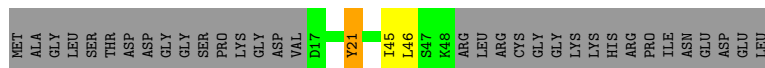


- Molecule 3: FXYP domain-containing ion transport regulator





- 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.36Å 118.18Å 494.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.00 – 3.50 16.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	57.9 (16.00-3.50) 57.2 (16.00-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.220 , 0.269 0.233 , 0.274	Depositor DCC
R_{free} test set	4178 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 77.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.049 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21354	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PCW, E4R, PHD, CLR, NA, MG

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	0.51	0/10674
1	C	0.29	0/7867	0.51	1/10674 (0.0%)
2	B	0.29	0/2449	0.54	0/3301
2	D	0.30	0/2395	0.56	0/3225
3	E	0.32	0/261	0.50	0/354
3	G	0.30	0/261	0.46	0/354
All	All	0.29	0/21100	0.52	1/28582 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1008	GLY	N-CA-C	5.04	125.70	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7730	0	7777	135	0
1	C	7730	0	7777	134	0
2	B	2386	0	2361	44	0
2	D	2334	0	2317	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	255	0	259	3	0
3	G	255	0	259	6	0
4	F	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	1	0
4	J	28	0	25	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	132	0	108	9	0
7	C	154	0	126	5	0
8	A	27	0	0	0	0
8	C	27	0	0	0	0
9	A	28	0	46	1	0
9	B	28	0	46	0	0
9	C	28	0	46	3	0
9	D	28	0	46	1	0
9	E	28	0	46	2	0
9	G	28	0	46	2	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	A	5	0	0	0	0
11	C	5	0	0	0	0
All	All	21354	0	21386	373	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 (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:ILE:HG12	2:D:177:ILE:HG12	1.63	0.81
1:A:978:PRO:HB3	9:G:101:CLR:H192	1.64	0.80
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.64	0.79
2:B:80:ILE:HG12	2:B:177:ILE:HG12	1.65	0.79
1:A:430:GLN:HG3	1:A:438:ARG:HB2	1.65	0.79
1:C:221:SER:H	1:C:233:ARG:HB3	1.49	0.78
1:C:807:THR:HB	1:C:954:GLU:HG3	1.64	0.77
1:C:430:GLN:HG3	1:C:438:ARG:HB2	1.66	0.77
1:A:221:SER:H	1:A:233:ARG:HB3	1.50	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:THR:HA	1:C:588:PRO:HA	1.67	0.75
1:A:807:THR:HB	1:A:954:GLU:HG3	1.68	0.74
2:D:204:TYR:HE1	2:D:207:TYR:HB2	1.52	0.74
1:A:375:THR:HA	1:A:588:PRO:HA	1.71	0.71
2:D:177:ILE:HA	2:D:260:ALA:HA	1.73	0.71
1:A:84:LYS:HG3	1:A:141:TYR:HE1	1.55	0.71
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.72	0.70
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.75	0.68
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.75	0.68
1:C:96:LEU:HD22	1:C:285:ILE:HG23	1.76	0.67
1:A:512:SER:HB3	1:A:575:ASN:HA	1.77	0.66
2:B:204:TYR:HE1	2:B:207:TYR:HB2	1.60	0.66
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.77	0.66
3:E:45:ILE:HD12	3:E:46:LEU:HG	1.78	0.66
1:C:978:PRO:HB3	9:E:101:CLR:H192	1.76	0.66
1:A:385:TRP:HB3	1:A:581:LEU:H	1.62	0.65
1:C:434:PRO:HG2	1:C:437:LYS:HB2	1.80	0.64
1:C:108:TYR:HA	1:C:111:GLN:HE21	1.62	0.64
2:D:102:VAL:HG13	2:D:169:TYR:HD2	1.63	0.63
1:A:367:CYS:HB2	1:A:707:VAL:HG22	1.81	0.63
2:D:66:PRO:HG2	2:D:69:GLN:HG2	1.81	0.63
1:A:96:LEU:HD22	1:A:285:ILE:HG23	1.81	0.62
1:A:385:TRP:HE3	1:A:580:GLY:HA2	1.61	0.62
1:C:238:PHE:HD2	1:C:258:THR:HG21	1.65	0.62
1:C:907:VAL:HA	1:C:910:THR:HG22	1.82	0.61
2:D:80:ILE:HD11	2:D:177:ILE:H	1.65	0.61
1:A:907:VAL:HA	1:A:910:THR:HG22	1.83	0.60
1:C:183:LEU:HD11	1:C:248:ARG:HB3	1.82	0.60
1:A:363:THR:HA	1:A:704:ILE:HB	1.83	0.60
1:C:216:GLU:HA	1:C:379:MET:HE1	1.84	0.60
2:D:276:CYS:HB2	2:D:295:PHE:HD2	1.65	0.60
2:B:177:ILE:HA	2:B:260:ALA:HA	1.83	0.59
1:A:399:GLN:HE21	1:A:436:LEU:HD11	1.67	0.59
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.84	0.59
2:D:130:PRO:HB3	2:D:239:PRO:HB3	1.85	0.59
1:A:183:LEU:HD11	1:A:248:ARG:HB3	1.85	0.58
2:B:80:ILE:HD11	2:B:177:ILE:H	1.68	0.58
2:D:191:PRO:HD3	2:D:280:GLY:HA2	1.86	0.58
1:A:72:ALA:HB2	1:A:176:GLU:HG2	1.85	0.57
1:C:385:TRP:HB3	1:C:581:LEU:H	1.69	0.57
1:C:469:LYS:HD3	1:C:472:GLU:HB3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:943:LYS:NZ	7:C:1112:PCW:H52	2.19	0.57
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.86	0.57
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.39	0.57
1:C:84:LYS:HG3	1:C:141:TYR:HE1	1.70	0.57
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.87	0.57
1:A:483:LEU:HB3	1:A:500:MET:HG3	1.87	0.56
1:C:111:GLN:O	1:C:115:GLU:HG2	2.05	0.56
1:A:385:TRP:O	1:A:580:GLY:HA3	2.06	0.56
2:D:173:LYS:HB3	2:D:262:GLN:HE21	1.71	0.56
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.41	0.56
1:C:72:ALA:HB2	1:C:176:GLU:HG2	1.88	0.56
1:C:683:PHE:HB3	1:C:686:THR:HG21	1.88	0.56
1:C:226:ASN:ND2	1:C:231:GLU:OE2	2.40	0.55
1:A:907:VAL:O	1:A:911:CYS:HB2	2.06	0.55
1:C:399:GLN:HE21	1:C:436:LEU:HD11	1.69	0.55
2:D:224:VAL:HG21	2:D:274:ILE:HD11	1.88	0.55
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.87	0.55
1:C:208:ASN:HB3	1:C:212:THR:HG22	1.87	0.55
1:C:795:LEU:HD13	1:C:915:PHE:HB3	1.88	0.55
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.89	0.54
1:C:385:TRP:HE3	1:C:580:GLY:HA2	1.73	0.54
1:C:512:SER:HB3	1:C:575:ASN:HA	1.89	0.54
2:B:225:GLY:HA3	2:B:265:ASN:HB3	1.89	0.54
1:A:332:THR:HA	1:A:813:ILE:HD11	1.89	0.54
1:A:768:SER:HA	1:A:815:LEU:HD23	1.89	0.54
1:C:25:MET:O	1:C:29:LYS:HG3	2.08	0.54
1:A:883:TRP:O	1:A:904:ARG:NH1	2.40	0.54
1:A:84:LYS:HG3	1:A:141:TYR:CE1	2.41	0.53
1:C:483:LEU:HB3	1:C:500:MET:HG3	1.91	0.53
1:A:965:PRO:HD3	3:G:31:LEU:HD11	1.91	0.53
2:B:80:ILE:HB	2:B:105:ILE:HD12	1.91	0.53
2:D:136:ARG:O	2:D:146:ARG:NH1	2.42	0.53
1:A:39:LEU:HD22	1:A:43:GLU:HG2	1.91	0.53
2:B:217:ARG:HH12	2:B:273:ARG:HD2	1.73	0.53
1:A:689:GLN:O	1:A:693:ILE:HG12	2.08	0.53
1:A:1009:TRP:HZ2	2:B:34:LYS:HB3	1.74	0.53
1:C:470:ILE:HB	1:C:485:ILE:HG23	1.91	0.52
1:A:117:GLU:OE1	1:A:886:ARG:NE	2.41	0.52
1:C:618:LYS:HE2	1:C:622:LYS:HE3	1.91	0.52
2:B:66:PRO:HG2	2:B:69:GLN:HG2	1.90	0.52
1:A:83:VAL:O	1:A:87:ARG:HG2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PHE:HD2	1:A:301:ILE:HD12	1.74	0.52
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.90	0.52
1:C:858:GLY:HA2	1:C:918:THR:HG21	1.92	0.52
2:D:266:LEU:HD22	2:D:272:ILE:HD11	1.91	0.52
2:B:136:ARG:O	2:B:146:ARG:NH1	2.43	0.52
1:A:683:PHE:HB3	1:A:686:THR:HG21	1.90	0.52
2:B:276:CYS:HB2	2:B:295:PHE:HD2	1.75	0.52
1:C:84:LYS:HG3	1:C:141:TYR:CE1	2.45	0.52
2:D:27:ARG:HG3	2:D:32:TRP:CD1	2.45	0.52
1:A:149:LYS:HG3	7:A:1108:PCW:H41	1.92	0.52
1:C:803:ILE:HG12	1:C:916:PHE:HD1	1.75	0.52
1:C:186:VAL:HG11	1:C:192:ILE:HD13	1.90	0.52
2:B:266:LEU:HD22	2:B:272:ILE:HD11	1.93	0.51
1:C:385:TRP:O	1:C:580:GLY:HA3	2.10	0.51
2:D:35:ILE:HG21	9:D:501:CLR:H22	1.92	0.51
2:D:153:LEU:H	2:D:153:LEU:HD12	1.74	0.51
1:A:1009:TRP:CZ2	2:B:34:LYS:HB3	2.45	0.51
1:A:434:PRO:HG2	1:A:437:LYS:HB2	1.91	0.51
2:B:224:VAL:HG21	2:B:274:ILE:HD11	1.92	0.51
1:C:367:CYS:HB2	1:C:707:VAL:HG22	1.93	0.51
1:C:640:ARG:HH21	1:C:641:LEU:HD11	1.74	0.51
2:D:225:GLY:HA3	2:D:265:ASN:HB3	1.93	0.51
1:C:736:LYS:HG3	1:C:742:ILE:HD12	1.93	0.51
1:A:191:ARG:HA	1:A:241:ASN:HA	1.92	0.51
1:A:205:LYS:HA	1:A:219:THR:HA	1.92	0.51
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.75	0.51
1:A:94:SER:HB3	1:A:133:VAL:HG13	1.92	0.51
1:A:795:LEU:HD13	1:A:915:PHE:HB3	1.93	0.51
1:A:858:GLY:HA2	1:A:918:THR:HG21	1.93	0.51
2:D:91:ARG:HG2	2:D:93:ASN:H	1.76	0.51
1:A:867:ALA:HB2	1:A:873:PRO:HD3	1.92	0.50
3:G:45:ILE:HD12	3:G:46:LEU:HG	1.92	0.50
1:A:146:LYS:HZ3	7:A:1110:PCW:H42	1.75	0.50
2:D:213:CYS:HA	2:D:276:CYS:HA	1.94	0.50
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.93	0.50
1:C:986:PRO:HB3	9:C:1104:CLR:H213	1.94	0.50
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.76	0.50
1:C:385:TRP:CH2	1:C:531:PHE:HB2	2.47	0.50
1:A:470:ILE:HB	1:A:485:ILE:HG23	1.92	0.50
1:C:136:THR:HG21	1:C:330:LEU:HG	1.94	0.50
1:C:710:ASP:HB2	1:C:731:GLY:HA2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:783:PHE:O	1:C:787:ILE:HG13	2.12	0.50
2:D:18:ASN:HA	2:D:23:GLU:O	2.11	0.50
1:C:470:ILE:HD11	1:C:487:LYS:HE2	1.94	0.50
2:B:27:ARG:HG3	2:B:32:TRP:CD1	2.47	0.50
1:A:25:MET:O	1:A:29:LYS:HG3	2.12	0.50
1:A:283:HIS:HE1	7:A:1105:PCW:H42	1.76	0.50
1:A:938:PHE:CD2	9:C:1104:CLR:H192	2.47	0.50
1:C:685:ARG:HH11	1:C:685:ARG:HB3	1.76	0.50
1:C:838:VAL:HG13	1:C:842:LEU:HD22	1.92	0.50
1:A:920:VAL:HG13	1:A:954:GLU:HG2	1.94	0.49
2:B:101:TYR:O	2:B:105:ILE:HG12	2.12	0.49
1:C:907:VAL:O	1:C:911:CYS:HB2	2.12	0.49
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.94	0.49
1:C:589:ARG:HB2	1:C:592:VAL:HG23	1.95	0.49
1:C:83:VAL:O	1:C:87:ARG:HG2	2.12	0.49
1:A:191:ARG:HE	1:A:239:SER:HA	1.77	0.49
2:D:217:ARG:NH1	2:D:220:ASP:OD2	2.45	0.49
1:C:888:ILE:O	1:C:904:ARG:NH2	2.46	0.49
1:A:238:PHE:HD2	1:A:258:THR:HG21	1.76	0.49
2:B:130:PRO:HD3	2:B:232:LEU:HD12	1.95	0.49
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.77	0.49
1:A:336:CYS:SG	1:A:816:ALA:HB2	2.53	0.49
1:C:689:GLN:O	1:C:693:ILE:HG12	2.12	0.49
1:C:420:LEU:HB3	1:C:486:HIS:HE1	1.77	0.49
1:C:613:HIS:CE1	1:C:685:ARG:HH21	2.31	0.49
1:C:1009:TRP:HZ2	2:D:34:LYS:HB3	1.78	0.49
1:A:146:LYS:NZ	7:A:1110:PCW:H42	2.28	0.48
1:A:708:THR:HG22	1:A:725:VAL:HB	1.94	0.48
1:A:865:ILE:HD12	1:A:914:PRO:HG3	1.95	0.48
1:C:915:PHE:O	1:C:919:ILE:HG12	2.13	0.48
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.95	0.48
1:A:97:LEU:HD21	1:A:327:GLU:HA	1.95	0.48
1:A:633:THR:H	1:A:636:ASP:HB2	1.79	0.48
1:A:736:LYS:HG3	1:A:742:ILE:HD12	1.96	0.48
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.94	0.48
1:A:713:ASN:OD1	1:A:713:ASN:N	2.45	0.48
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.95	0.48
1:A:834:THR:O	7:A:1105:PCW:H81	2.13	0.48
1:A:843:ILE:HG23	1:A:847:TYR:HD2	1.78	0.48
1:C:977:LYS:HD2	1:C:980:TRP:CZ2	2.49	0.48
2:D:217:ARG:HH12	2:D:273:ARG:HD2	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LYS:HD3	1:A:472:GLU:HB3	1.94	0.48
1:A:525:GLU:HA	1:A:528:LYS:HB3	1.96	0.48
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.94	0.48
2:B:92:PRO:HG3	2:B:301:VAL:HG12	1.96	0.48
1:C:443:ASP:OD1	1:C:444:ALA:N	2.46	0.48
1:C:594:ASP:O	1:C:598:LYS:HG2	2.13	0.48
1:C:624:VAL:HG23	1:C:626:ILE:HG13	1.95	0.48
2:B:213:CYS:HA	2:B:276:CYS:HA	1.95	0.48
2:D:92:PRO:HG3	2:D:301:VAL:HG12	1.95	0.48
1:A:624:VAL:HG23	1:A:626:ILE:HG13	1.95	0.48
2:B:91:ARG:HG2	2:B:93:ASN:H	1.78	0.48
1:A:369:PHD:O	1:A:373:THR:HB	2.14	0.48
1:A:605:LYS:HE3	1:A:679:THR:O	2.14	0.48
1:A:985:PHE:HZ	9:G:101:CLR:H20	1.79	0.48
1:A:347:LYS:HD2	1:A:753:THR:HG21	1.96	0.47
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.96	0.47
1:C:363:THR:HA	1:C:704:ILE:HB	1.96	0.47
1:C:909:PHE:HB3	1:C:972:ARG:O	2.14	0.47
1:C:995:ASP:OD1	1:C:998:ARG:NH1	2.46	0.47
1:A:443:ASP:OD1	1:A:444:ALA:N	2.47	0.47
2:D:80:ILE:HD12	2:D:105:ILE:HD12	1.96	0.47
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.49	0.47
1:C:205:LYS:HA	1:C:219:THR:HA	1.96	0.47
1:C:336:CYS:SG	1:C:816:ALA:HB2	2.55	0.47
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.96	0.47
1:A:186:VAL:HG11	1:A:192:ILE:HD13	1.96	0.47
1:A:338:THR:O	1:A:342:LYS:HG2	2.15	0.47
2:B:204:TYR:O	2:B:208:VAL:HG12	2.15	0.47
1:C:266:LEU:O	1:C:270:LEU:HG	2.14	0.47
1:A:473:ILE:HB	1:A:483:LEU:HG	1.97	0.46
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.96	0.46
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.50	0.46
2:B:21:LYS:HD2	2:B:21:LYS:HA	1.72	0.46
2:D:109:LEU:HD23	2:D:153:LEU:HD23	1.98	0.46
2:D:224:VAL:HG22	2:D:272:ILE:HD12	1.98	0.46
1:A:208:ASN:HB3	1:A:212:THR:HG22	1.96	0.46
1:C:691:LYS:NZ	1:C:714:ASP:OD1	2.48	0.46
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.96	0.46
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.96	0.46
2:D:101:TYR:O	2:D:105:ILE:HG12	2.14	0.46
1:A:762:PHE:CE2	1:A:766:LYS:HE3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.96	0.46
1:C:97:LEU:HD12	1:C:330:LEU:HD22	1.97	0.46
1:C:943:LYS:HZ1	7:C:1112:PCW:H52	1.80	0.46
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.50	0.46
2:D:173:LYS:HG3	2:D:264:THR:O	2.16	0.46
1:C:295:LEU:O	1:C:299:PHE:HB2	2.16	0.45
2:B:274:ILE:HG13	2:B:299:ILE:HD11	1.98	0.45
1:C:260:MET:HA	1:C:263:ILE:HD12	1.97	0.45
1:C:340:THR:O	1:C:344:MET:HG2	2.16	0.45
1:C:1001:ILE:HG22	1:C:1010:VAL:HG21	1.97	0.45
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.99	0.45
1:C:418:ALA:O	1:C:422:ASN:ND2	2.49	0.45
1:A:488:ASN:HD21	1:A:490:ASN:HB2	1.82	0.45
1:A:644:PRO:HD2	1:A:647:GLN:NE2	2.31	0.45
7:A:1108:PCW:H42	7:A:1108:PCW:H73	1.76	0.45
2:B:263:PHE:HB3	2:B:266:LEU:HD21	1.99	0.45
2:D:239:PRO:HD2	2:D:257:PRO:HB3	1.99	0.45
1:A:818:GLU:CD	1:A:931:LYS:HG3	2.37	0.45
1:C:63:GLU:O	1:C:67:ARG:HB2	2.16	0.45
1:C:713:ASN:OD1	1:C:713:ASN:N	2.50	0.45
1:C:370:LYS:NZ	1:C:620:ILE:HG13	2.32	0.45
1:C:776:ASN:HB3	1:C:847:TYR:HE1	1.82	0.45
2:D:80:ILE:HD12	2:D:81:PRO:HD3	1.98	0.45
2:D:216:LYS:H	2:D:220:ASP:HB2	1.82	0.45
1:A:503:ALA:HB3	1:A:506:ARG:HG2	1.99	0.45
2:B:92:PRO:HD2	2:B:303:SER:HA	1.98	0.45
2:B:191:PRO:HD3	2:B:280:GLY:HA2	1.99	0.45
2:D:204:TYR:O	2:D:208:VAL:HG12	2.17	0.45
1:A:594:ASP:O	1:A:598:LYS:HG2	2.17	0.44
3:G:39:ILE:O	3:G:43:ILE:HG12	2.16	0.44
1:C:284:PHE:CD1	1:C:838:VAL:HG21	2.52	0.44
1:C:843:ILE:HG23	1:C:847:TYR:HD2	1.82	0.44
1:C:918:THR:HG23	1:C:984:ALA:HB2	1.98	0.44
1:C:964:CYS:HB3	1:C:967:MET:HG2	1.98	0.44
1:A:471:VAL:HG21	1:A:564:PHE:O	2.17	0.44
1:A:779:GLU:HG2	1:A:800:ILE:HG23	1.99	0.44
2:D:151:PHE:HE2	2:D:258:LEU:HB2	1.83	0.44
1:C:108:TYR:HB2	1:C:122:ASN:HB3	1.98	0.44
1:C:503:ALA:O	1:C:507:ILE:HG12	2.17	0.44
2:D:21:LYS:HD2	2:D:21:LYS:HA	1.81	0.44
2:D:130:PRO:HD3	2:D:232:LEU:HD12	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:O	1:A:344:MET:HG2	2.16	0.44
1:C:525:GLU:HA	1:C:528:LYS:HB3	1.98	0.44
1:C:342:LYS:O	1:C:346:ARG:HG3	2.18	0.44
2:D:263:PHE:HB3	2:D:266:LEU:HD21	1.99	0.44
1:A:390:ILE:HD11	1:A:534:ALA:HB1	2.00	0.44
1:A:370:LYS:HZ2	1:A:620:ILE:HG13	1.83	0.44
2:D:80:ILE:HB	2:D:105:ILE:HD12	1.98	0.44
1:A:545:VAL:HG11	1:A:581:LEU:HD13	2.00	0.44
1:A:986:PRO:HB3	9:A:1104:CLR:H213	2.00	0.44
1:C:473:ILE:HB	1:C:483:LEU:HG	2.00	0.44
1:C:488:ASN:HD21	1:C:490:ASN:HB2	1.83	0.44
1:A:295:LEU:O	1:A:299:PHE:HB2	2.18	0.43
2:B:173:LYS:HG3	2:B:264:THR:O	2.17	0.43
1:A:503:ALA:O	1:A:507:ILE:HG12	2.18	0.43
1:A:1001:ILE:HG22	1:A:1010:VAL:HG21	2.01	0.43
1:C:604:ILE:HD11	1:C:755:VAL:HG21	1.99	0.43
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.87	0.43
1:A:888:ILE:O	1:A:904:ARG:NH2	2.51	0.43
1:C:873:PRO:HA	1:C:876:LEU:HD12	2.00	0.43
1:C:998:ARG:HE	1:C:1014:THR:HB	1.84	0.43
1:C:106:LEU:O	1:C:110:ILE:HG12	2.17	0.43
1:C:883:TRP:HA	1:C:904:ARG:HH11	1.84	0.43
3:E:45:ILE:H	3:E:45:ILE:HG13	1.66	0.43
1:A:98:TRP:NE1	1:A:133:VAL:HG11	2.33	0.43
1:A:149:LYS:HD3	1:A:149:LYS:HA	1.86	0.43
1:A:483:LEU:HD13	1:A:498:LEU:HD11	2.00	0.43
1:C:98:TRP:CE2	1:C:133:VAL:HG11	2.54	0.43
1:C:936:SER:HB2	1:C:1003:ARG:CZ	2.49	0.43
1:A:93:PHE:HB3	1:A:330:LEU:HD13	2.00	0.43
1:A:342:LYS:O	1:A:346:ARG:HG3	2.18	0.43
1:C:191:ARG:HE	1:C:239:SER:HA	1.82	0.43
1:A:637:ILE:HG22	1:A:648:VAL:HG11	2.01	0.43
1:A:977:LYS:NZ	3:G:23:TYR:OH	2.45	0.43
1:C:986:PRO:HG3	9:C:1104:CLR:H122	1.99	0.43
1:C:865:ILE:HD12	1:C:914:PRO:HG3	2.01	0.43
1:C:1009:TRP:CZ2	2:D:34:LYS:HB3	2.54	0.42
1:A:915:PHE:O	1:A:919:ILE:HG12	2.18	0.42
1:A:936:SER:HB2	1:A:1003:ARG:CZ	2.48	0.42
2:B:130:PRO:HB3	2:B:239:PRO:HB3	2.00	0.42
1:C:998:ARG:HH11	1:C:998:ARG:HB3	1.83	0.42
2:D:146:ARG:H	2:D:146:ARG:HG2	1.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:45:ILE:H	3:G:45:ILE:HG13	1.65	0.42
2:B:155:TRP:CD2	2:B:232:LEU:HD22	2.54	0.42
2:D:74:PRO:HG2	2:D:292:GLN:OE1	2.19	0.42
2:D:155:TRP:CD2	2:D:232:LEU:HD22	2.54	0.42
1:A:166:ARG:HH22	1:A:178:VAL:HA	1.84	0.42
1:A:1009:TRP:CZ3	1:A:1013:GLU:HG3	2.55	0.42
1:C:93:PHE:HA	1:C:285:ILE:HD11	2.01	0.42
1:C:338:THR:O	1:C:342:LYS:HG2	2.20	0.42
1:C:863:PHE:HB2	2:D:54:ILE:HD11	2.00	0.42
2:D:158:ASN:OD1	4:I:1:NAG:N2	2.53	0.42
1:A:977:LYS:HD2	1:A:980:TRP:CZ2	2.55	0.42
2:B:18:ASN:HA	2:B:23:GLU:O	2.19	0.42
1:C:119:GLN:H	1:C:119:GLN:NE2	2.18	0.42
2:D:209:LEU:O	2:D:237:GLY:HA3	2.20	0.42
2:B:280:GLY:HA3	2:B:283:ILE:HD13	2.02	0.42
1:C:495:ARG:HA	1:C:555:ASP:HB3	2.02	0.42
1:A:29:LYS:HE2	1:A:265:THR:HB	2.02	0.42
1:A:284:PHE:HE1	1:A:773:LEU:HD11	1.84	0.42
2:B:74:PRO:HG2	2:B:292:GLN:OE1	2.20	0.42
1:C:860:PHE:O	1:C:864:VAL:HG23	2.20	0.42
1:C:94:SER:HB3	1:C:133:VAL:HG13	2.01	0.42
1:C:149:LYS:HG3	7:C:1111:PCW:H41	2.02	0.42
1:C:369:PHD:O	1:C:373:THR:HB	2.20	0.42
7:C:1111:PCW:H73	7:C:1111:PCW:H42	1.78	0.42
1:C:370:LYS:HZ2	1:C:620:ILE:HG13	1.85	0.42
1:C:920:VAL:HG13	1:C:954:GLU:HG2	2.02	0.42
1:A:283:HIS:CE1	7:A:1105:PCW:H42	2.53	0.41
2:B:80:ILE:HD12	2:B:105:ILE:HD12	2.01	0.41
2:B:182:ARG:HD2	2:B:245:TYR:CZ	2.55	0.41
1:C:149:LYS:HD3	1:C:149:LYS:HA	1.80	0.41
1:C:867:ALA:HB2	1:C:873:PRO:HD3	2.02	0.41
1:C:917:VAL:O	1:C:921:VAL:HG23	2.20	0.41
1:C:390:ILE:HD11	1:C:534:ALA:HB1	2.01	0.41
1:A:110:ILE:HB	1:A:315:ILE:HD11	2.03	0.41
1:C:420:LEU:HD13	1:C:486:HIS:HD1	1.85	0.41
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.54	0.41
1:C:911:CYS:C	1:C:914:PRO:HD2	2.40	0.41
7:C:1107:PCW:H62	7:C:1107:PCW:H41	1.84	0.41
1:A:385:TRP:CH2	1:A:531:PHE:HB2	2.55	0.41
1:A:413:ALA:O	1:A:417:ILE:HG13	2.20	0.41
1:A:918:THR:O	1:A:922:VAL:HG22	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ASP:HB2	1:C:253:TYR:HB2	2.01	0.41
1:A:63:GLU:O	1:A:67:ARG:HB2	2.20	0.41
2:B:224:VAL:HG22	2:B:272:ILE:HD12	2.02	0.41
1:C:612:ASP:OD1	1:C:613:HIS:N	2.54	0.41
1:A:602:ALA:HB1	1:A:759:ARG:HH12	1.85	0.41
1:C:417:ILE:HG22	1:C:548:PHE:HD2	1.85	0.41
1:C:483:LEU:HD13	1:C:498:LEU:HD11	2.01	0.41
2:D:156:LEU:HD13	2:D:260:ALA:HB2	2.01	0.41
2:B:238:PHE:CD1	2:B:257:PRO:HB2	2.56	0.41
1:C:818:GLU:CD	1:C:931:LYS:HG3	2.41	0.41
1:C:964:CYS:HB3	1:C:967:MET:CG	2.50	0.41
1:A:893:ASP:OD2	1:A:897:GLN:HB2	2.21	0.41
7:A:1109:PCW:H73	3:E:21:TYR:CE1	2.56	0.41
1:C:98:TRP:NE1	1:C:133:VAL:HG11	2.36	0.41
1:C:545:VAL:HG11	1:C:581:LEU:HD13	2.03	0.41
1:A:136:THR:HG21	1:A:330:LEU:HG	2.03	0.41
1:A:450:LEU:HD12	1:A:460:VAL:HG21	2.03	0.41
1:A:710:ASP:HB2	1:A:731:GLY:HA2	2.03	0.41
1:A:1009:TRP:CE3	1:A:1013:GLU:HG3	2.56	0.41
2:D:115:LEU:HD13	2:D:118:LYS:HD2	2.03	0.41
9:E:101:CLR:H211	9:E:101:CLR:H231	1.71	0.41
1:A:74:THR:HG23	1:A:256:ASP:OD1	2.21	0.40
1:A:211:LEU:HA	1:A:712:VAL:HG22	2.03	0.40
1:A:420:LEU:HD13	1:A:486:HIS:HD1	1.86	0.40
1:A:284:PHE:CD1	1:A:838:VAL:HG21	2.56	0.40
1:C:386:SER:HB2	1:C:391:HIS:CD2	2.56	0.40
1:C:469:LYS:HA	1:C:486:HIS:CD2	2.56	0.40
1:C:997:VAL:O	1:C:1001:ILE:HG12	2.22	0.40
1:A:385:TRP:CZ2	1:A:388:ASN:HA	2.56	0.40
1:A:753:THR:O	1:A:757:GLU:HG2	2.21	0.40
1:A:909:PHE:HB3	1:A:972:ARG:O	2.21	0.40
2:D:80:ILE:CD1	2:D:177:ILE:HG23	2.52	0.40
3:G:40:VAL:O	3:G:44:ILE:HG12	2.21	0.40
1:C:238:PHE:CD2	1:C:258:THR:HG21	2.51	0.40
1:A:423:ARG:NH1	1:A:474:PRO:HB3	2.37	0.40
1:A:943:LYS:NZ	7:A:1109:PCW:H82	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	993/1016 (98%)	927 (93%)	64 (6%)	2 (0%)	44	75
1	C	993/1016 (98%)	930 (94%)	61 (6%)	2 (0%)	44	75
2	B	289/303 (95%)	261 (90%)	26 (9%)	2 (1%)	19	53
2	D	281/303 (93%)	254 (90%)	25 (9%)	2 (1%)	19	53
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
3	G	30/65 (46%)	27 (90%)	3 (10%)	0	100	100
All	All	2616/2768 (94%)	2427 (93%)	181 (7%)	8 (0%)	37	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	PRO
1	A	193	PRO
1	C	193	PRO
1	C	306	LEU
2	D	200	PRO
1	A	306	LEU
2	B	199	TYR
2	D	199	TYR

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	846/861 (98%)	825 (98%)	21 (2%)	42 67
1	C	846/861 (98%)	825 (98%)	21 (2%)	42 67
2	B	261/269 (97%)	239 (92%)	22 (8%)	9 32
2	D	255/269 (95%)	234 (92%)	21 (8%)	9 33
3	E	26/52 (50%)	25 (96%)	1 (4%)	28 57
3	G	26/52 (50%)	25 (96%)	1 (4%)	28 57
All	All	2260/2364 (96%)	2173 (96%)	87 (4%)	28 57

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	56	LEU
1	A	82	TRP
1	A	180	VAL
1	A	211	LEU
1	A	223	ASP
1	A	327	GLU
1	A	351	VAL
1	A	479	ASN
1	A	523	LEU
1	A	531	PHE
1	A	566	THR
1	A	685	ARG
1	A	763	ASP
1	A	776	ASN
1	A	835	ASP
1	A	840	GLU
1	A	884	ASP
1	A	911	CYS
1	A	916	PHE
1	A	1009	TRP
2	B	13	LYS
2	B	25	LEU
2	B	28	THR
2	B	32	TRP
2	B	64	PHE
2	B	72	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	80	ILE
2	B	114	ASP
2	B	125	ASP
2	B	126	CYS
2	B	153	LEU
2	B	162	LEU
2	B	166	THR
2	B	170	LYS
2	B	171	ASP
2	B	173	LYS
2	B	177	ILE
2	B	195	SER
2	B	203	LYS
2	B	256	GLN
2	B	297	VAL
2	B	299	ILE
3	G	21	TYR
1	C	45	HIS
1	C	56	LEU
1	C	57	THR
1	C	82	TRP
1	C	119	GLN
1	C	167	ASN
1	C	180	VAL
1	C	223	ASP
1	C	327	GLU
1	C	351	VAL
1	C	479	ASN
1	C	523	LEU
1	C	531	PHE
1	C	566	THR
1	C	685	ARG
1	C	763	ASP
1	C	776	ASN
1	C	865	ILE
1	C	911	CYS
1	C	916	PHE
1	C	1009	TRP
2	D	13	LYS
2	D	25	LEU
2	D	27	ARG
2	D	28	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	32	TRP
2	D	64	PHE
2	D	72	VAL
2	D	80	ILE
2	D	114	ASP
2	D	125	ASP
2	D	126	CYS
2	D	153	LEU
2	D	170	LYS
2	D	171	ASP
2	D	173	LYS
2	D	177	ILE
2	D	195	SER
2	D	203	LYS
2	D	256	GLN
2	D	297	VAL
2	D	299	ILE
3	E	21	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	122	ASN
1	A	283	HIS
1	A	399	GLN
1	A	479	ASN
1	A	488	ASN
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	488	ASN
1	C	613	HIS
1	C	776	ASN
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	0.93	0	10,15,17	1.08	0
1	PHD	A	369	1,5	9,11,12	0.93	0	10,15,17	1.47	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	-	0/8/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	PHD	CA-CB-CG	2.99	119.12	112.86
1	A	369	PHD	OD1-CG-CB	2.64	118.38	111.11

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

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	4,2	14,14,15	0.34	0	17,19,21	0.46	0
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	H	1	4,2	14,14,15	0.63	1 (7%)	17,19,21	0.70	0
4	NAG	H	2	4	14,14,15	0.36	0	17,19,21	0.36	0
4	NAG	I	1	4,2	14,14,15	0.37	0	17,19,21	0.47	0
4	NAG	I	2	4	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	J	1	4,2	14,14,15	0.61	1 (7%)	17,19,21	0.67	0
4	NAG	J	2	4	14,14,15	0.33	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	4,2	-	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	4,2	-	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	4,2	-	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	4,2	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	-2.20	1.40	1.43
4	J	1	NAG	O5-C1	-2.11	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

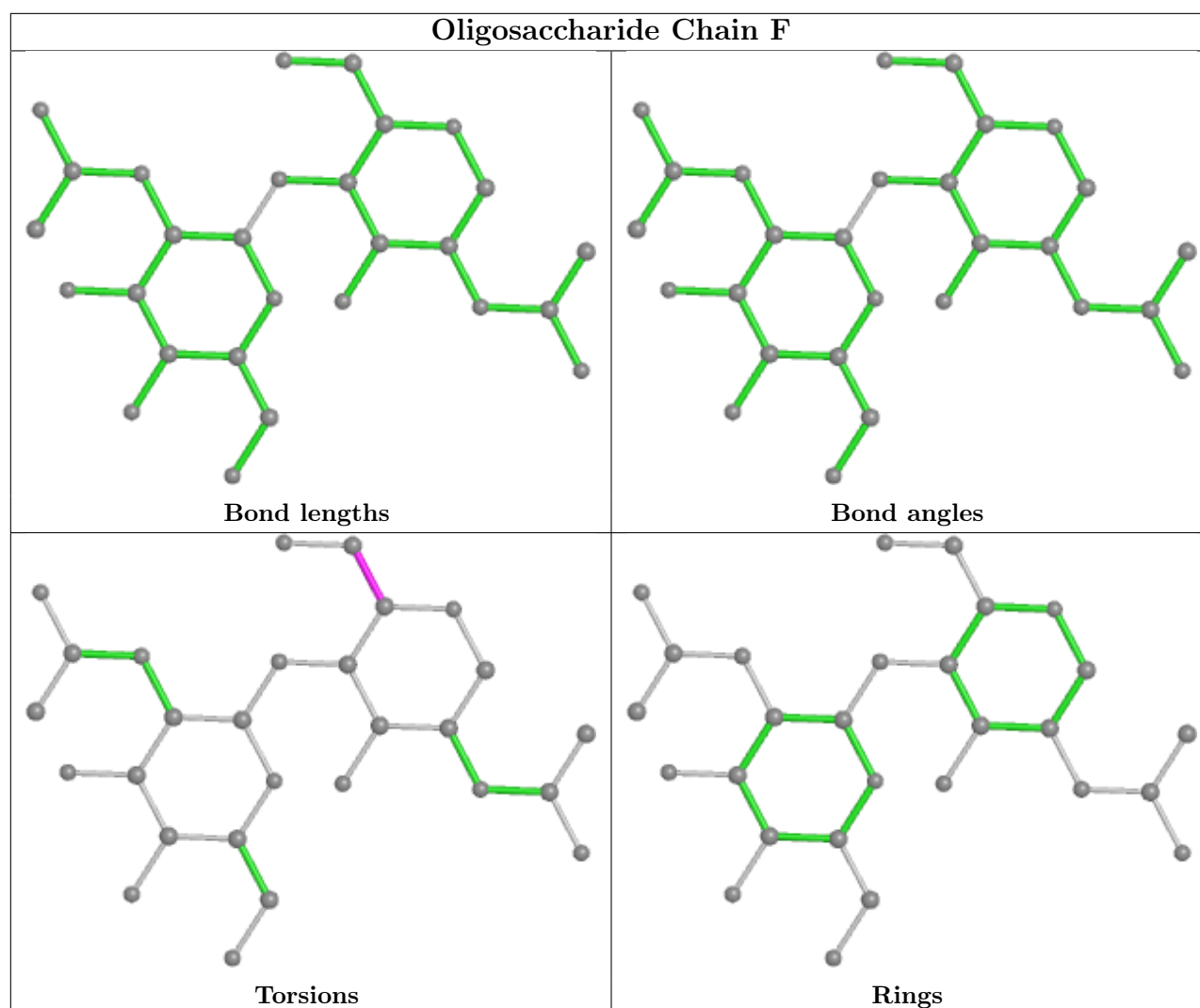
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6

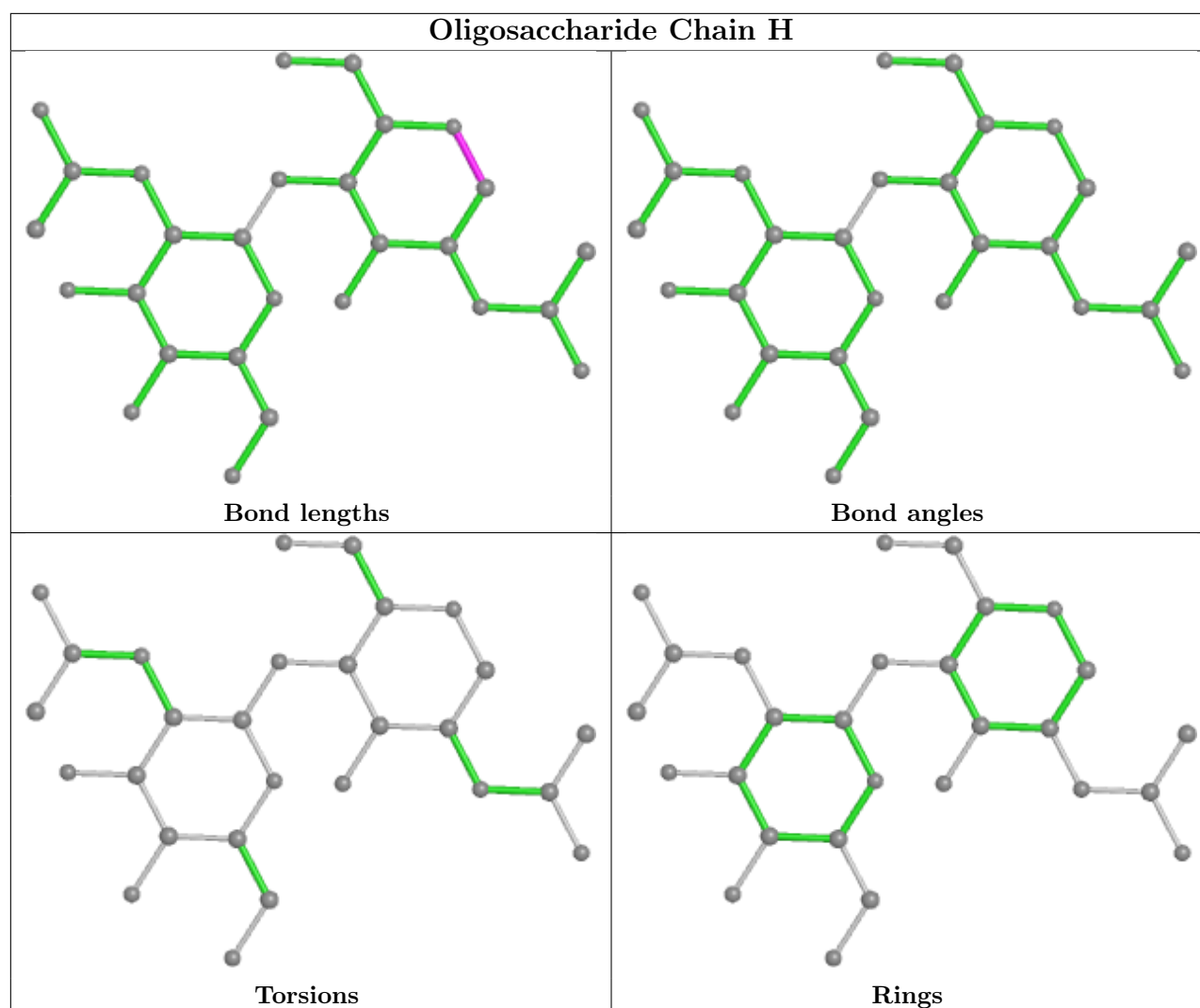
There are no ring outliers.

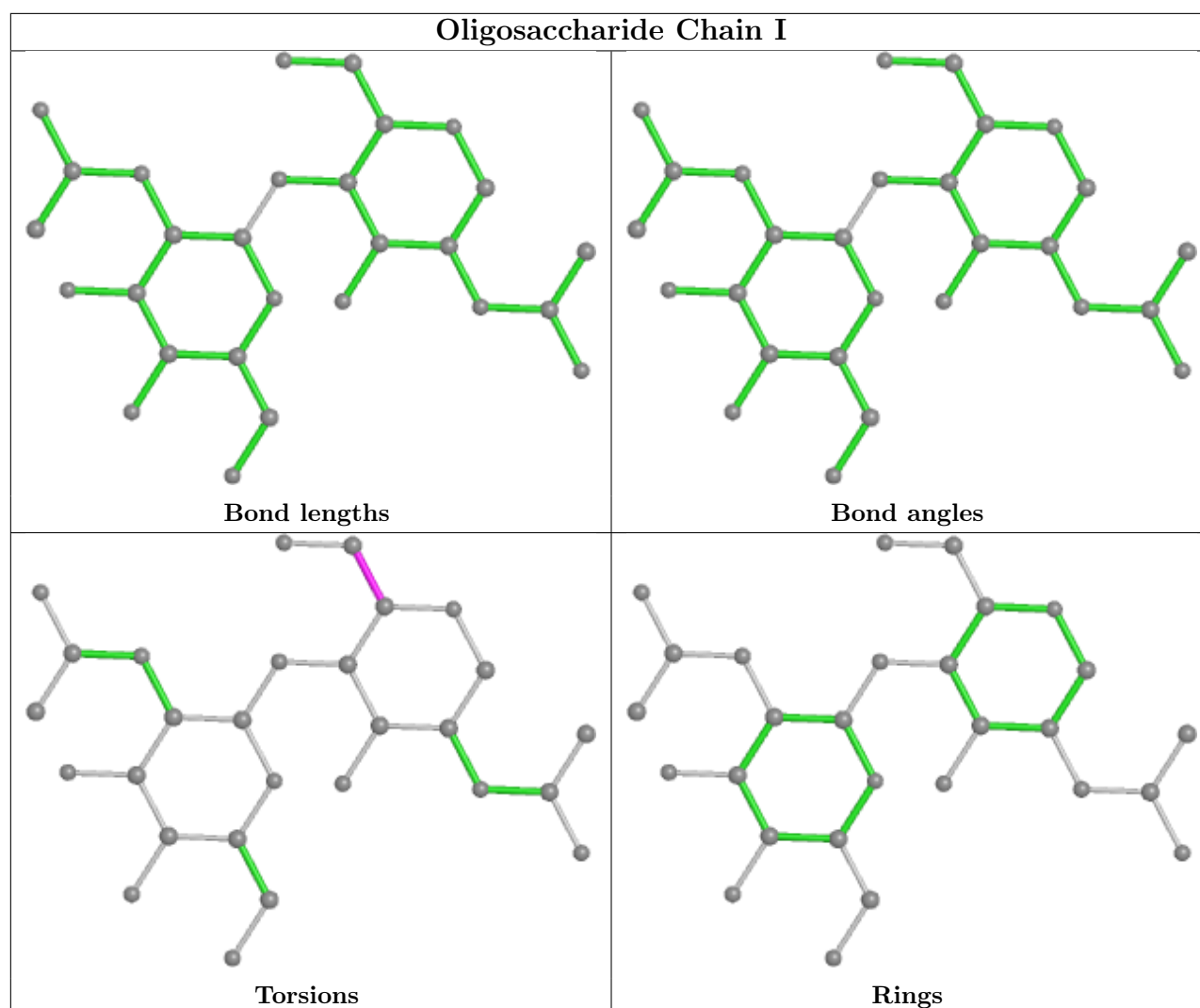
1 monomer is involved in 1 short contact:

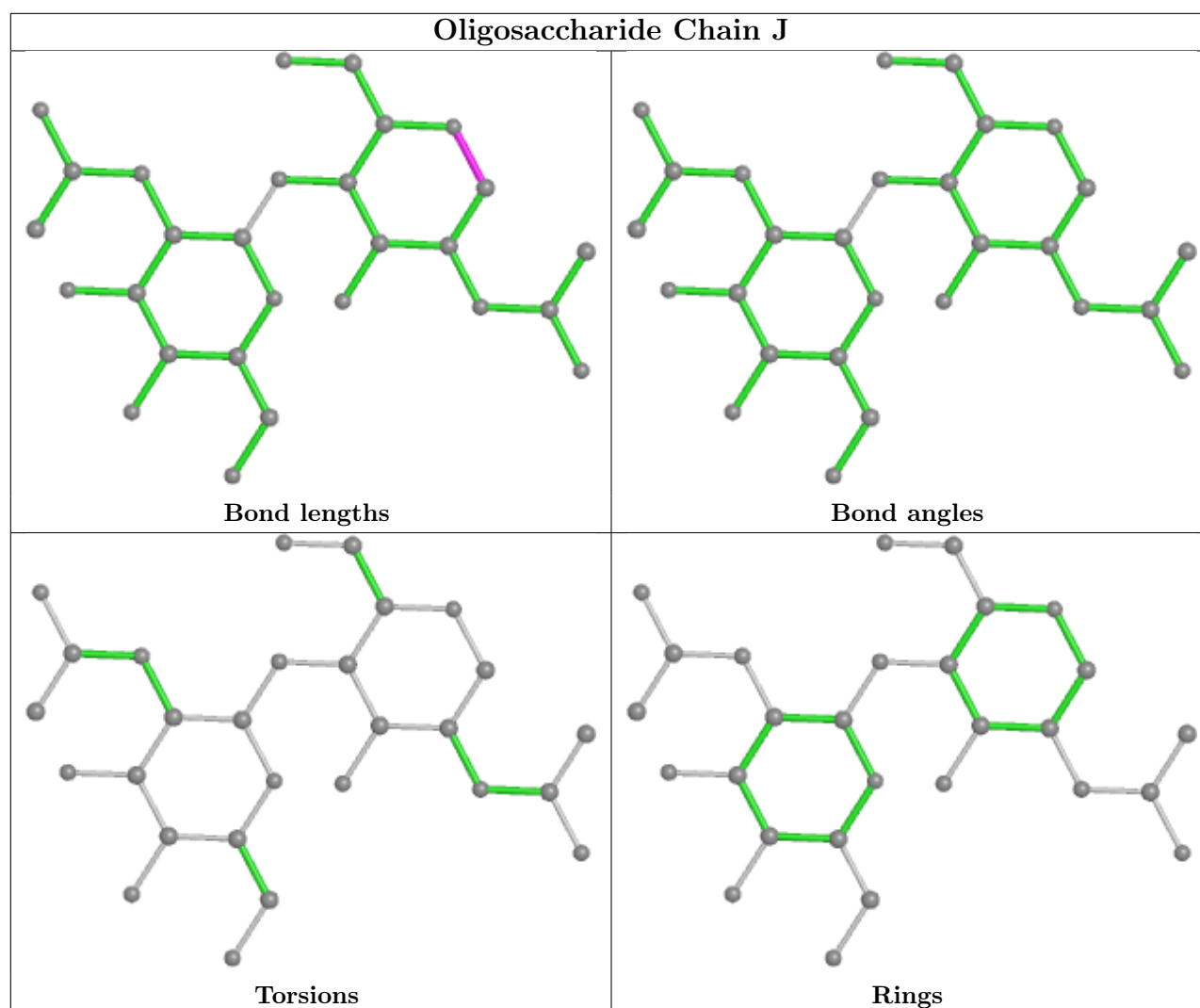
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 6 are monoatomic - leaving 23 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
10	NAG	D	401	2	14,14,15	0.34	0	17,19,21	0.56	0
7	PCW	A	1110	-	21,21,53	1.72	6 (28%)	27,29,61	1.26	1 (3%)
9	CLR	B	501	-	31,31,31	2.00	12 (38%)	48,48,48	1.61	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PCW	C	1111	-	21,21,53	1.72	5 (23%)	27,29,61	1.18	1 (3%)
8	E4R	C	1121	-	26,31,31	1.32	2 (7%)	41,52,52	1.84	5 (12%)
7	PCW	C	1107	-	21,21,53	1.69	6 (28%)	27,29,61	1.23	2 (7%)
7	PCW	A	1106	-	21,21,53	1.70	6 (28%)	27,29,61	1.19	1 (3%)
9	CLR	D	501	-	31,31,31	1.87	11 (35%)	48,48,48	1.49	12 (25%)
10	NAG	B	401	2	14,14,15	0.26	0	17,19,21	0.44	0
9	CLR	C	1104	-	31,31,31	1.71	9 (29%)	48,48,48	1.63	12 (25%)
7	PCW	C	1108	-	21,21,53	1.70	5 (23%)	27,29,61	1.18	1 (3%)
7	PCW	C	1109	-	21,21,53	1.75	4 (19%)	27,29,61	1.27	1 (3%)
7	PCW	A	1105	-	21,21,53	1.68	4 (19%)	27,29,61	1.16	1 (3%)
9	CLR	E	101	-	31,31,31	1.86	11 (35%)	48,48,48	1.63	12 (25%)
7	PCW	A	1108	-	21,21,53	1.69	6 (28%)	27,29,61	1.17	1 (3%)
8	E4R	A	1121	-	26,31,31	1.47	4 (15%)	41,52,52	1.81	6 (14%)
7	PCW	A	1107	-	21,21,53	1.67	6 (28%)	27,29,61	1.25	1 (3%)
7	PCW	C	1110	-	21,21,53	1.69	5 (23%)	27,29,61	1.21	1 (3%)
9	CLR	G	101	-	31,31,31	1.87	12 (38%)	48,48,48	1.70	14 (29%)
9	CLR	A	1104	-	31,31,31	1.80	12 (38%)	48,48,48	1.57	12 (25%)
7	PCW	C	1112	-	21,21,53	1.68	4 (19%)	27,29,61	1.40	3 (11%)
7	PCW	A	1109	-	21,21,53	1.70	6 (28%)	27,29,61	1.44	3 (11%)
7	PCW	C	1106	-	21,21,53	1.73	5 (23%)	27,29,61	1.26	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	D	401	2	-	4/6/23/26	0/1/1/1
7	PCW	A	1110	-	-	9/23/23/57	-
9	CLR	B	501	-	-	2/10/68/68	0/4/4/4
7	PCW	C	1111	-	-	10/23/23/57	-
8	E4R	C	1121	-	-	0/0/74/74	0/5/5/5
7	PCW	C	1107	-	-	12/23/23/57	-
7	PCW	A	1106	-	-	11/23/23/57	-
9	CLR	D	501	-	-	1/10/68/68	0/4/4/4
10	NAG	B	401	2	-	1/6/23/26	0/1/1/1
9	CLR	C	1104	-	-	5/10/68/68	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	C	1108	-	-	10/23/23/57	-
7	PCW	C	1109	-	-	9/23/23/57	-
7	PCW	A	1105	-	-	16/23/23/57	-
9	CLR	E	101	-	-	3/10/68/68	0/4/4/4
7	PCW	A	1108	-	-	10/23/23/57	-
8	E4R	A	1121	-	-	0/0/74/74	0/5/5/5
7	PCW	A	1107	-	-	7/23/23/57	-
7	PCW	C	1110	-	-	13/23/23/57	-
9	CLR	G	101	-	-	6/10/68/68	0/4/4/4
9	CLR	A	1104	-	-	4/10/68/68	0/4/4/4
7	PCW	C	1112	-	-	11/23/23/57	-
7	PCW	A	1109	-	-	11/23/23/57	-
7	PCW	C	1106	-	-	11/23/23/57	-

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	CLR	C10-C9	5.24	1.64	1.56
9	G	101	CLR	C10-C9	4.37	1.63	1.56
9	E	101	CLR	C10-C9	4.24	1.63	1.56
7	C	1109	PCW	O2-C31	4.21	1.44	1.35
9	A	1104	CLR	C10-C9	4.12	1.62	1.56
9	D	501	CLR	C10-C9	4.03	1.62	1.56
7	C	1106	PCW	O2-C31	3.99	1.44	1.35
7	C	1111	PCW	O2-C31	3.85	1.43	1.35
7	C	1110	PCW	O2-C31	3.81	1.43	1.35
7	A	1110	PCW	O2-C31	3.76	1.43	1.35
7	A	1105	PCW	O2-C31	3.71	1.43	1.35
7	C	1108	PCW	O2-C31	3.71	1.43	1.35
7	A	1108	PCW	O2-C31	3.67	1.43	1.35
9	E	101	CLR	C16-C17	3.66	1.62	1.54
7	C	1112	PCW	O2-C31	3.65	1.43	1.35
7	A	1106	PCW	O2-C31	3.64	1.43	1.35
9	C	1104	CLR	C10-C9	3.61	1.62	1.56
7	C	1107	PCW	O2-C31	3.58	1.43	1.35
7	A	1107	PCW	O2-C31	3.55	1.43	1.35
7	A	1109	PCW	O2-C31	3.51	1.43	1.35
9	G	101	CLR	C16-C17	3.45	1.61	1.54
9	B	501	CLR	C16-C17	3.37	1.61	1.54
9	D	501	CLR	C16-C17	3.37	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	501	CLR	C13-C14	3.36	1.61	1.55
9	G	101	CLR	C4-C5	3.31	1.58	1.51
9	E	101	CLR	C13-C14	3.27	1.61	1.55
9	C	1104	CLR	C11-C9	3.06	1.58	1.53
9	B	501	CLR	C13-C14	3.04	1.60	1.55
9	C	1104	CLR	C16-C17	3.03	1.60	1.54
9	B	501	CLR	C12-C11	2.99	1.59	1.53
9	A	1104	CLR	C12-C11	2.98	1.59	1.53
9	E	101	CLR	C10-C5	2.96	1.58	1.52
9	A	1104	CLR	C16-C17	2.95	1.60	1.54
9	B	501	CLR	C4-C5	2.94	1.58	1.51
9	B	501	CLR	C13-C17	2.90	1.60	1.55
9	B	501	CLR	C12-C13	2.89	1.59	1.54
9	D	501	CLR	C4-C3	2.88	1.57	1.52
9	D	501	CLR	C12-C13	2.82	1.59	1.54
9	E	101	CLR	C4-C5	2.79	1.57	1.51
9	A	1104	CLR	C12-C13	2.79	1.59	1.54
9	A	1104	CLR	C11-C9	2.78	1.58	1.53
9	B	501	CLR	C10-C5	2.77	1.58	1.52
9	G	101	CLR	C7-C8	2.77	1.57	1.53
9	D	501	CLR	C4-C5	2.72	1.57	1.51
9	G	101	CLR	C13-C14	2.69	1.60	1.55
9	G	101	CLR	C10-C5	2.64	1.58	1.52
9	C	1104	CLR	C4-C5	2.62	1.57	1.51
9	A	1104	CLR	C13-C14	2.56	1.59	1.55
7	A	1105	PCW	C6-N	-2.55	1.42	1.50
9	D	501	CLR	C13-C17	2.54	1.59	1.55
9	D	501	CLR	C12-C11	2.53	1.58	1.53
9	C	1104	CLR	C10-C5	2.53	1.57	1.52
7	A	1109	PCW	C6-N	-2.53	1.42	1.50
9	D	501	CLR	C16-C15	2.53	1.60	1.54
7	A	1109	PCW	C7-N	-2.52	1.42	1.50
9	C	1104	CLR	C12-C11	2.52	1.58	1.53
7	C	1106	PCW	C7-N	-2.52	1.42	1.50
8	A	1121	E4R	C14-C8	2.51	1.57	1.54
7	A	1110	PCW	C7-N	-2.50	1.42	1.50
7	A	1110	PCW	C6-N	-2.49	1.42	1.50
7	C	1112	PCW	C7-N	-2.48	1.42	1.50
7	C	1108	PCW	C6-N	-2.48	1.42	1.50
9	A	1104	CLR	C10-C5	2.47	1.57	1.52
7	C	1107	PCW	C6-N	-2.47	1.42	1.50
7	C	1106	PCW	C6-N	-2.46	1.42	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1104	CLR	C4-C3	2.46	1.56	1.52
7	C	1111	PCW	C6-N	-2.46	1.42	1.50
7	C	1111	PCW	C7-N	-2.46	1.42	1.50
7	C	1110	PCW	C6-N	-2.45	1.42	1.50
7	A	1107	PCW	C6-N	-2.45	1.42	1.50
7	A	1106	PCW	C6-N	-2.45	1.42	1.50
8	A	1121	E4R	C18-C13	2.44	1.57	1.53
7	C	1109	PCW	C6-N	-2.44	1.42	1.50
7	A	1106	PCW	C7-N	-2.44	1.42	1.50
7	C	1112	PCW	C6-N	-2.44	1.42	1.50
7	A	1108	PCW	C6-N	-2.44	1.42	1.50
7	C	1109	PCW	C7-N	-2.43	1.42	1.50
7	C	1107	PCW	C7-N	-2.42	1.42	1.50
7	A	1108	PCW	C7-N	-2.42	1.43	1.50
7	C	1108	PCW	C7-N	-2.41	1.43	1.50
7	C	1110	PCW	C7-N	-2.39	1.43	1.50
7	A	1107	PCW	C7-N	-2.38	1.43	1.50
9	C	1104	CLR	C13-C14	2.37	1.59	1.55
9	E	101	CLR	C12-C11	2.35	1.58	1.53
9	C	1104	CLR	C8-C14	-2.34	1.49	1.53
7	A	1105	PCW	C8-N	-2.34	1.43	1.50
9	E	101	CLR	C13-C17	2.34	1.59	1.55
7	A	1105	PCW	C7-N	-2.31	1.43	1.50
9	E	101	CLR	C12-C13	2.30	1.58	1.54
8	C	1121	E4R	C18-C13	2.29	1.57	1.53
9	C	1104	CLR	C4-C3	2.28	1.56	1.52
9	A	1104	CLR	C4-C5	2.27	1.56	1.51
9	B	501	CLR	C11-C9	2.27	1.57	1.53
7	C	1109	PCW	P-O3P	2.26	1.68	1.59
9	B	501	CLR	C4-C3	2.23	1.56	1.52
9	A	1104	CLR	C8-C14	-2.23	1.49	1.53
7	A	1109	PCW	O2-C2	-2.22	1.41	1.46
9	G	101	CLR	C16-C15	2.22	1.60	1.54
7	A	1110	PCW	P-O3P	2.21	1.68	1.59
7	C	1107	PCW	O2-C2	-2.20	1.41	1.46
7	C	1108	PCW	P-O3P	2.20	1.68	1.59
7	C	1111	PCW	P-O3P	2.20	1.68	1.59
7	C	1106	PCW	P-O3P	2.19	1.68	1.59
8	A	1121	E4R	C4-C3	2.18	1.55	1.51
9	E	101	CLR	C16-C15	2.18	1.60	1.54
8	C	1121	E4R	C4-C3	2.18	1.55	1.51
7	C	1112	PCW	O2-C2	-2.16	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	101	CLR	C12-C13	2.16	1.58	1.54
7	A	1109	PCW	P-O3P	2.14	1.68	1.59
9	D	501	CLR	C22-C20	2.14	1.59	1.54
7	A	1108	PCW	P-O3P	2.13	1.67	1.59
9	G	101	CLR	C19-C10	2.12	1.58	1.54
9	G	101	CLR	C11-C9	2.11	1.57	1.53
9	B	501	CLR	C22-C20	2.10	1.59	1.54
7	C	1110	PCW	P-O3P	2.10	1.67	1.59
7	C	1107	PCW	P-O3P	2.10	1.67	1.59
9	E	101	CLR	C19-C10	2.09	1.58	1.54
9	G	101	CLR	C13-C17	2.09	1.59	1.55
7	A	1106	PCW	P-O3P	2.08	1.67	1.59
7	A	1107	PCW	C8-N	-2.08	1.43	1.50
7	C	1107	PCW	C8-N	-2.07	1.44	1.50
7	A	1110	PCW	C8-N	-2.07	1.44	1.50
7	A	1109	PCW	C8-N	-2.06	1.44	1.50
8	A	1121	E4R	C15-C14	2.05	1.57	1.54
7	C	1110	PCW	C8-N	-2.05	1.44	1.50
9	D	501	CLR	C10-C5	2.05	1.56	1.52
9	E	101	CLR	C11-C9	2.05	1.57	1.53
7	A	1107	PCW	P-O3P	2.05	1.67	1.59
9	G	101	CLR	C22-C20	2.04	1.59	1.54
9	A	1104	CLR	C13-C17	2.04	1.58	1.55
7	A	1106	PCW	C8-N	-2.03	1.44	1.50
7	A	1108	PCW	C8-N	-2.03	1.44	1.50
9	B	501	CLR	C16-C15	2.03	1.59	1.54
9	A	1104	CLR	C16-C15	2.03	1.59	1.54
7	C	1108	PCW	C8-N	-2.03	1.44	1.50
7	A	1107	PCW	O2-C2	-2.03	1.41	1.46
7	C	1111	PCW	C8-N	-2.02	1.44	1.50
7	C	1106	PCW	C8-N	-2.02	1.44	1.50
7	A	1108	PCW	O2-C2	-2.01	1.41	1.46
7	A	1106	PCW	O2-C2	-2.01	1.41	1.46
7	A	1110	PCW	O2-C2	-2.01	1.41	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1121	E4R	C12-C13-C17	-7.98	106.49	116.87
8	A	1121	E4R	C12-C13-C17	-7.61	106.96	116.87
7	C	1112	PCW	O2-C31-C32	5.24	120.72	111.09
7	C	1106	PCW	O2-C31-C32	5.21	120.68	111.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1110	PCW	O2-C31-C32	5.14	120.54	111.09
7	A	1109	PCW	O2-C31-C32	5.13	120.53	111.09
8	A	1121	E4R	O2-C17-C20	-5.11	98.35	108.58
7	A	1107	PCW	O2-C31-C32	5.00	120.28	111.09
8	C	1121	E4R	O2-C17-C20	-4.90	98.76	108.58
7	C	1111	PCW	O2-C31-C32	4.86	120.03	111.09
7	C	1110	PCW	O2-C31-C32	4.85	120.01	111.09
7	C	1109	PCW	O2-C31-C32	4.82	119.96	111.09
7	C	1108	PCW	O2-C31-C32	4.82	119.95	111.09
7	A	1105	PCW	O2-C31-C32	4.75	119.83	111.09
7	C	1107	PCW	O2-C31-C32	4.71	119.76	111.09
7	A	1108	PCW	O2-C31-C32	4.59	119.53	111.09
7	A	1106	PCW	O2-C31-C32	4.56	119.48	111.09
9	C	1104	CLR	C8-C7-C6	-4.11	106.83	112.73
9	A	1104	CLR	C8-C7-C6	-3.89	107.15	112.73
9	E	101	CLR	C2-C3-C4	-3.26	105.84	110.31
9	B	501	CLR	C2-C3-C4	-3.16	105.97	110.31
9	B	501	CLR	C11-C9-C10	3.12	117.19	113.08
9	G	101	CLR	C8-C7-C6	-3.08	108.31	112.73
7	A	1109	PCW	C2-O2-C31	-3.06	112.19	117.90
9	G	101	CLR	C11-C9-C10	3.06	117.10	113.08
9	E	101	CLR	C17-C13-C14	-3.05	96.45	100.07
9	G	101	CLR	C2-C3-C4	-3.05	106.13	110.31
9	D	501	CLR	C8-C7-C6	-2.93	108.52	112.73
9	B	501	CLR	C8-C7-C6	-2.90	108.56	112.73
9	C	1104	CLR	C15-C14-C8	-2.87	114.36	119.08
9	G	101	CLR	C22-C20-C17	-2.86	104.37	110.28
9	B	501	CLR	C4-C5-C10	-2.78	112.73	116.42
9	E	101	CLR	C11-C9-C10	2.77	116.73	113.08
9	E	101	CLR	C22-C20-C17	-2.76	104.57	110.28
9	C	1104	CLR	C2-C3-C4	-2.69	106.61	110.31
9	D	501	CLR	C4-C5-C10	-2.68	112.85	116.42
9	E	101	CLR	C8-C7-C6	-2.64	108.94	112.73
8	A	1121	E4R	O2-C17-C16	2.61	114.78	108.76
9	G	101	CLR	C4-C5-C6	-2.58	116.88	120.61
9	E	101	CLR	C19-C10-C5	2.58	112.52	108.34
8	C	1121	E4R	O2-C17-C16	2.57	114.70	108.76
7	C	1112	PCW	C2-O2-C31	-2.56	113.12	117.90
9	B	501	CLR	C19-C10-C5	2.54	112.45	108.34
9	D	501	CLR	C2-C3-C4	-2.54	106.83	110.31
9	G	101	CLR	C19-C10-C5	2.52	112.42	108.34
9	A	1104	CLR	C22-C20-C17	-2.52	105.08	110.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	101	CLR	C17-C13-C14	-2.51	97.10	100.07
9	A	1104	CLR	C4-C5-C10	-2.47	113.13	116.42
9	A	1104	CLR	C2-C3-C4	-2.47	106.92	110.31
9	G	101	CLR	C4-C5-C10	-2.47	113.14	116.42
9	E	101	CLR	C4-C5-C6	-2.45	117.07	120.61
9	D	501	CLR	C19-C10-C5	2.45	112.31	108.34
9	B	501	CLR	C16-C17-C20	-2.44	108.37	112.15
9	B	501	CLR	C22-C20-C17	-2.44	105.25	110.28
8	C	1121	E4R	C21-C20-C17	-2.44	123.77	126.72
9	A	1104	CLR	C19-C10-C5	2.43	112.27	108.34
9	E	101	CLR	C4-C5-C10	-2.43	113.20	116.42
9	G	101	CLR	C7-C8-C14	-2.42	107.39	110.91
9	G	101	CLR	C16-C17-C20	-2.42	108.40	112.15
9	C	1104	CLR	C19-C10-C5	2.41	112.24	108.34
9	B	501	CLR	C4-C5-C6	-2.41	117.14	120.61
9	C	1104	CLR	C4-C5-C10	-2.40	113.22	116.42
9	C	1104	CLR	C16-C17-C20	-2.38	108.46	112.15
9	A	1104	CLR	C15-C14-C8	-2.36	115.19	119.08
8	A	1121	E4R	C21-C20-C17	-2.36	123.86	126.72
9	G	101	CLR	C15-C14-C8	-2.31	115.28	119.08
7	C	1112	PCW	C3-O3-C11	-2.28	111.38	117.10
9	C	1104	CLR	C22-C20-C17	-2.28	105.58	110.28
9	C	1104	CLR	C19-C10-C9	-2.27	108.97	111.68
9	A	1104	CLR	C16-C17-C20	-2.26	108.65	112.15
9	B	501	CLR	C17-C13-C14	-2.25	97.41	100.07
9	B	501	CLR	C21-C20-C17	2.23	116.34	112.92
9	C	1104	CLR	C10-C5-C6	2.23	126.32	122.90
9	G	101	CLR	O1-C3-C2	2.23	115.83	110.16
9	D	501	CLR	C18-C13-C12	2.23	114.11	110.59
9	D	501	CLR	C22-C20-C17	-2.23	105.68	110.28
9	D	501	CLR	C11-C9-C10	2.22	116.01	113.08
9	D	501	CLR	C21-C20-C17	2.20	116.29	112.92
9	A	1104	CLR	C18-C13-C12	2.20	114.06	110.59
9	E	101	CLR	C16-C17-C20	-2.18	108.77	112.15
8	C	1121	E4R	C11-C9-C10	-2.17	111.41	113.91
7	A	1109	PCW	C3-O3-C11	-2.17	111.65	117.10
9	C	1104	CLR	C21-C20-C17	2.16	116.23	112.92
9	E	101	CLR	C7-C8-C14	-2.16	107.78	110.91
8	A	1121	E4R	C19-C10-C1	-2.15	104.79	108.26
9	G	101	CLR	C19-C10-C9	-2.15	109.12	111.68
9	E	101	CLR	O1-C3-C2	2.10	115.50	110.16
9	B	501	CLR	C15-C14-C8	-2.09	115.63	119.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1104	CLR	C13-C17-C20	-2.09	116.21	119.49
9	G	101	CLR	C10-C5-C6	2.09	126.10	122.90
9	B	501	CLR	O1-C3-C2	2.09	115.47	110.16
9	D	501	CLR	C17-C13-C14	-2.07	97.62	100.07
9	B	501	CLR	C18-C13-C12	2.06	113.85	110.59
8	A	1121	E4R	C1-C10-C9	2.06	114.59	111.35
9	A	1104	CLR	O1-C3-C2	2.06	115.39	110.16
9	C	1104	CLR	C12-C13-C14	-2.05	104.08	107.27
9	A	1104	CLR	C4-C5-C6	-2.04	117.67	120.61
7	C	1107	PCW	C2-O2-C31	-2.03	114.12	117.90
9	A	1104	CLR	C21-C20-C17	2.02	116.02	112.92
9	D	501	CLR	O1-C3-C2	2.02	115.30	110.16
9	D	501	CLR	C4-C5-C6	-2.02	117.70	120.61
9	E	101	CLR	C21-C20-C17	2.01	116.01	112.92
9	D	501	CLR	C16-C17-C20	-2.01	109.04	112.15
9	A	1104	CLR	C15-C14-C13	2.00	106.26	103.84

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1106	PCW	O2-C2-C3-O3
7	A	1106	PCW	C4-O4P-P-O2P
7	A	1107	PCW	C32-C31-O2-C2
7	A	1107	PCW	O31-C31-O2-C2
7	A	1108	PCW	C4-O4P-P-O1P
7	C	1106	PCW	C32-C31-O2-C2
7	C	1107	PCW	C1-O3P-P-O1P
7	C	1107	PCW	C1-O3P-P-O2P
7	C	1107	PCW	C1-O3P-P-O4P
7	C	1108	PCW	C32-C31-O2-C2
7	C	1109	PCW	C4-O4P-P-O1P
7	C	1109	PCW	C4-O4P-P-O2P
7	C	1109	PCW	C4-O4P-P-O3P
7	C	1110	PCW	C32-C31-O2-C2
7	C	1110	PCW	C1-O3P-P-O2P
7	C	1110	PCW	C1-O3P-P-O4P
7	C	1111	PCW	C4-O4P-P-O1P
7	C	1112	PCW	C4-O4P-P-O2P
7	C	1112	PCW	C4-O4P-P-O3P
7	A	1110	PCW	C32-C31-O2-C2
7	A	1105	PCW	C32-C31-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	1109	PCW	C32-C31-O2-C2
7	C	1107	PCW	C32-C31-O2-C2
7	C	1112	PCW	C32-C31-O2-C2
7	A	1106	PCW	C32-C31-O2-C2
7	C	1109	PCW	C32-C31-O2-C2
7	A	1105	PCW	O31-C31-O2-C2
7	C	1106	PCW	O11-C11-O3-C3
7	C	1106	PCW	O31-C31-O2-C2
7	A	1110	PCW	O31-C31-O2-C2
7	C	1107	PCW	O31-C31-O2-C2
7	C	1110	PCW	O11-C11-O3-C3
7	C	1106	PCW	C12-C11-O3-C3
7	C	1108	PCW	O31-C31-O2-C2
7	C	1110	PCW	O31-C31-O2-C2
7	A	1110	PCW	O11-C11-O3-C3
7	C	1107	PCW	O11-C11-O3-C3
7	A	1109	PCW	O31-C31-O2-C2
7	C	1111	PCW	C32-C31-O2-C2
7	C	1112	PCW	O31-C31-O2-C2
7	A	1108	PCW	C32-C31-O2-C2
7	C	1109	PCW	O31-C31-O2-C2
7	A	1106	PCW	O31-C31-O2-C2
10	D	401	NAG	O5-C5-C6-O6
9	G	101	CLR	C21-C20-C22-C23
7	A	1110	PCW	C12-C11-O3-C3
7	C	1107	PCW	C12-C11-O3-C3
7	C	1110	PCW	C12-C11-O3-C3
7	C	1112	PCW	O11-C11-O3-C3
7	A	1109	PCW	O11-C11-O3-C3
10	D	401	NAG	C4-C5-C6-O6
7	C	1112	PCW	C12-C11-O3-C3
7	A	1109	PCW	C12-C11-O3-C3
7	A	1105	PCW	C4-C5-N-C7
10	D	401	NAG	C8-C7-N2-C2
10	D	401	NAG	O7-C7-N2-C2
9	G	101	CLR	C17-C20-C22-C23
9	C	1104	CLR	C20-C22-C23-C24
9	A	1104	CLR	C20-C22-C23-C24
9	G	101	CLR	C22-C23-C24-C25
9	G	101	CLR	C20-C22-C23-C24
9	E	101	CLR	C20-C22-C23-C24
7	A	1110	PCW	C4-O4P-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	1108	PCW	C4-O4P-P-O3P
7	A	1109	PCW	C4-O4P-P-O3P
7	C	1106	PCW	C4-O4P-P-O3P
7	C	1108	PCW	C4-O4P-P-O3P
7	C	1111	PCW	C4-O4P-P-O3P
9	E	101	CLR	C21-C20-C22-C23
7	A	1105	PCW	C4-C5-N-C8
7	C	1111	PCW	O31-C31-O2-C2
7	A	1108	PCW	O31-C31-O2-C2
7	A	1105	PCW	O11-C11-O3-C3
7	C	1108	PCW	C12-C11-O3-C3
7	A	1105	PCW	C12-C11-O3-C3
9	B	501	CLR	C21-C20-C22-C23
7	C	1108	PCW	O11-C11-O3-C3
7	C	1111	PCW	C1-C2-C3-O3
7	A	1106	PCW	C12-C11-O3-C3
7	A	1105	PCW	C4-C5-N-C6
7	C	1109	PCW	C12-C11-O3-C3
7	A	1107	PCW	C12-C11-O3-C3
9	A	1104	CLR	C23-C24-C25-C26
7	A	1105	PCW	O2-C2-C3-O3
7	A	1106	PCW	C4-O4P-P-O3P
7	A	1109	PCW	C1-O3P-P-O4P
7	C	1112	PCW	C1-O3P-P-O4P
7	A	1105	PCW	O3P-C1-C2-C3
7	C	1110	PCW	O3P-C1-C2-C3
7	A	1106	PCW	C1-C2-C3-O3
7	A	1108	PCW	C1-C2-C3-O3
9	C	1104	CLR	C23-C24-C25-C26
7	C	1106	PCW	O2-C2-C3-O3
7	A	1110	PCW	O3P-C1-C2-C3
7	A	1109	PCW	O3P-C1-C2-C3
7	C	1107	PCW	O3P-C1-C2-C3
7	C	1112	PCW	O3P-C1-C2-C3
7	A	1106	PCW	O11-C11-O3-C3
9	G	101	CLR	C23-C24-C25-C26
7	C	1112	PCW	O3P-C1-C2-O2
7	C	1109	PCW	O11-C11-O3-C3
7	C	1106	PCW	O3P-C1-C2-C3
9	A	1104	CLR	C23-C24-C25-C27
7	A	1110	PCW	O3P-C1-C2-O2
7	A	1109	PCW	O3P-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	1107	PCW	O3P-C1-C2-O2
7	C	1110	PCW	O3P-C1-C2-O2
7	A	1107	PCW	O11-C11-O3-C3
7	C	1109	PCW	C1-O3P-P-O4P
7	A	1110	PCW	C4-O4P-P-O2P
7	A	1108	PCW	C4-O4P-P-O2P
7	A	1109	PCW	C1-O3P-P-O1P
7	A	1109	PCW	C4-O4P-P-O2P
7	C	1106	PCW	C4-O4P-P-O2P
7	C	1108	PCW	C4-O4P-P-O2P
7	C	1110	PCW	C1-O3P-P-O1P
7	C	1111	PCW	C4-O4P-P-O2P
7	C	1112	PCW	C1-O3P-P-O1P
9	A	1104	CLR	C13-C17-C20-C21
7	C	1108	PCW	O3P-C1-C2-C3
7	A	1105	PCW	O3P-C1-C2-O2
7	C	1108	PCW	O3P-C1-C2-O2
7	A	1110	PCW	O4P-C4-C5-N
7	A	1105	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	A	1109	PCW	O4P-C4-C5-N
7	C	1106	PCW	C1-C2-C3-O3
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	C	1109	PCW	O4P-C4-C5-N
7	C	1110	PCW	O4P-C4-C5-N
7	C	1111	PCW	O4P-C4-C5-N
7	C	1112	PCW	O4P-C4-C5-N
7	A	1108	PCW	O2-C2-C3-O3
7	C	1111	PCW	O2-C2-C3-O3
9	E	101	CLR	C22-C23-C24-C25
7	A	1105	PCW	C3-C2-O2-C31
7	A	1105	PCW	C1-O3P-P-O4P
7	A	1105	PCW	C4-O4P-P-O3P
7	A	1106	PCW	C1-O3P-P-O4P
7	A	1107	PCW	C1-O3P-P-O4P
7	A	1107	PCW	C4-O4P-P-O3P
7	A	1108	PCW	C1-O3P-P-O4P
7	C	1107	PCW	C4-O4P-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	1108	PCW	C1-O3P-P-O4P
7	C	1110	PCW	C4-O4P-P-O3P
7	C	1111	PCW	C1-O3P-P-O4P
9	C	1104	CLR	C23-C24-C25-C27
10	B	401	NAG	O5-C5-C6-O6
9	G	101	CLR	C23-C24-C25-C27
9	C	1104	CLR	C13-C17-C20-C21
7	C	1106	PCW	O3P-C1-C2-O2
7	C	1110	PCW	O2-C2-C3-O3
9	B	501	CLR	C22-C23-C24-C25
7	A	1105	PCW	C1-C2-C3-O3
7	C	1110	PCW	C1-C2-C3-O3
7	A	1106	PCW	C1-O3P-P-O2P
7	A	1108	PCW	C1-O3P-P-O2P
7	C	1107	PCW	C4-O4P-P-O2P
7	C	1111	PCW	C1-O3P-P-O2P
9	C	1104	CLR	C22-C23-C24-C25
9	D	501	CLR	C23-C24-C25-C26
7	A	1105	PCW	C5-C4-O4P-P

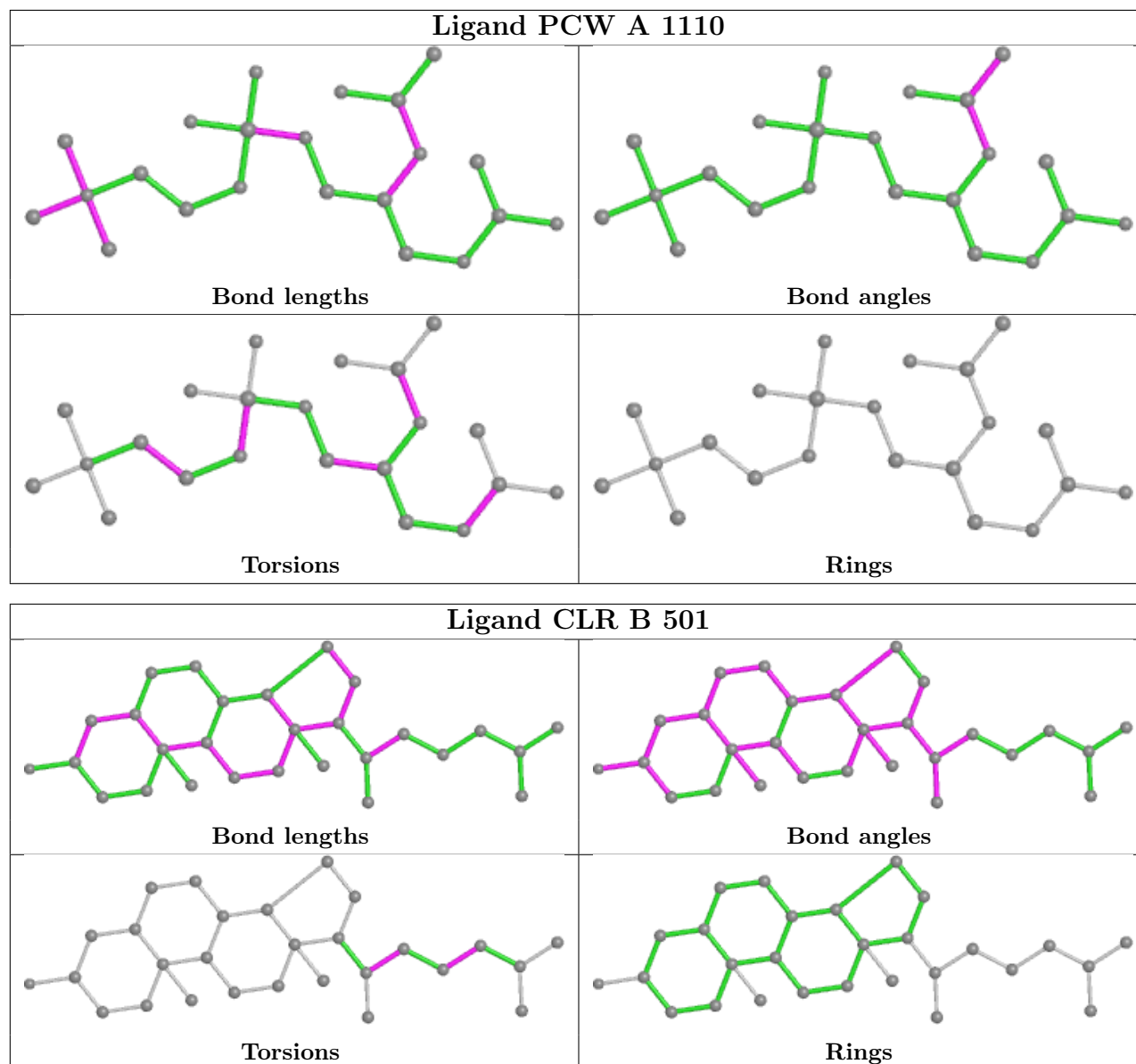
There are no ring outliers.

12 monomers are involved in 23 short contacts:

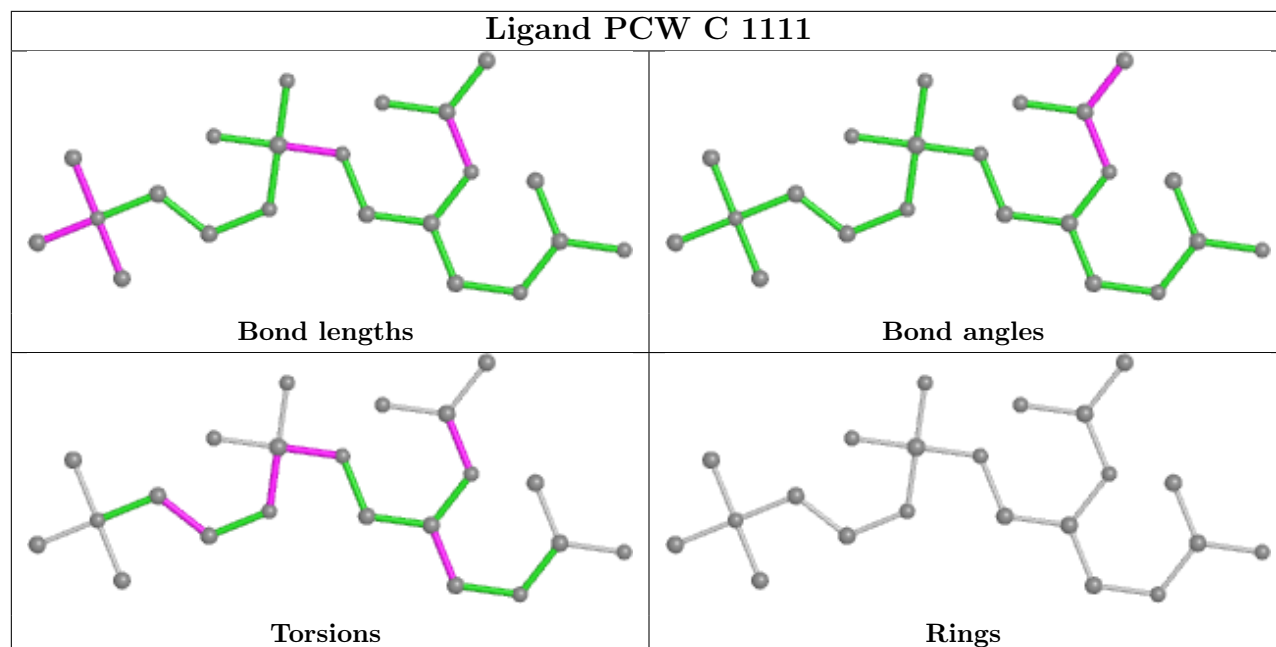
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1110	PCW	2	0
7	C	1111	PCW	2	0
7	C	1107	PCW	1	0
9	D	501	CLR	1	0
9	C	1104	CLR	3	0
7	A	1105	PCW	3	0
9	E	101	CLR	2	0
7	A	1108	PCW	2	0
9	G	101	CLR	2	0
9	A	1104	CLR	1	0
7	C	1112	PCW	2	0
7	A	1109	PCW	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

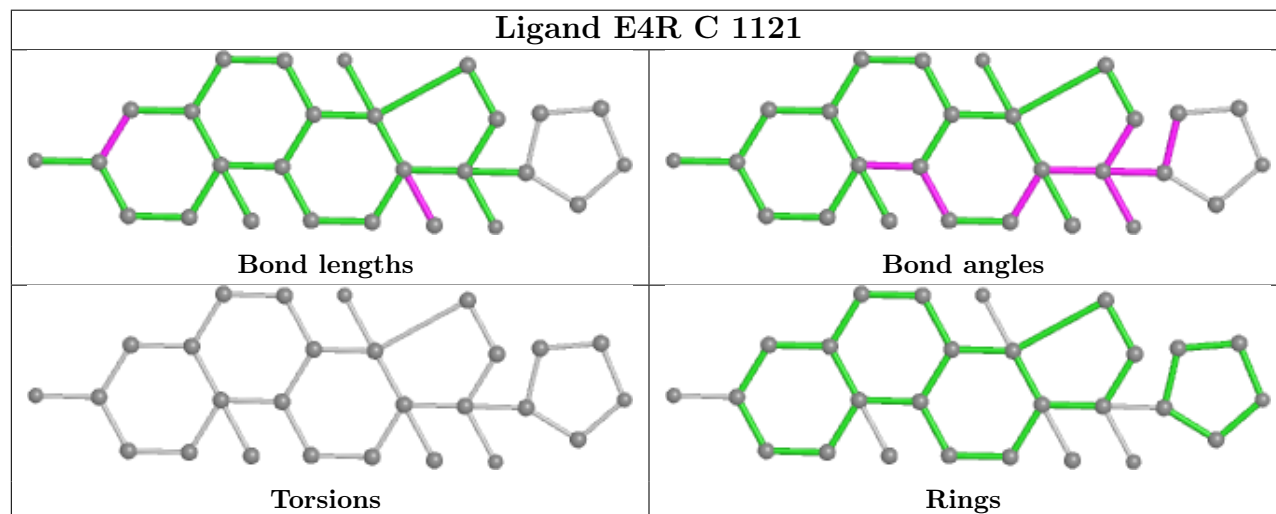
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



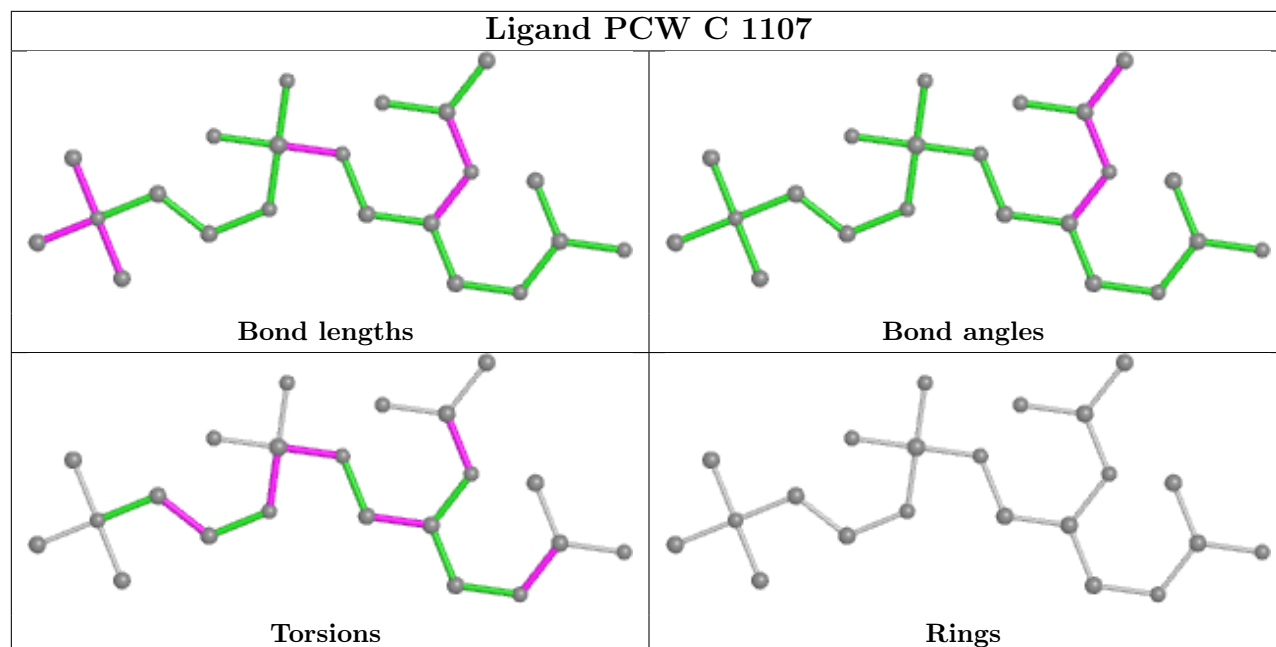
Ligand PCW C 1111



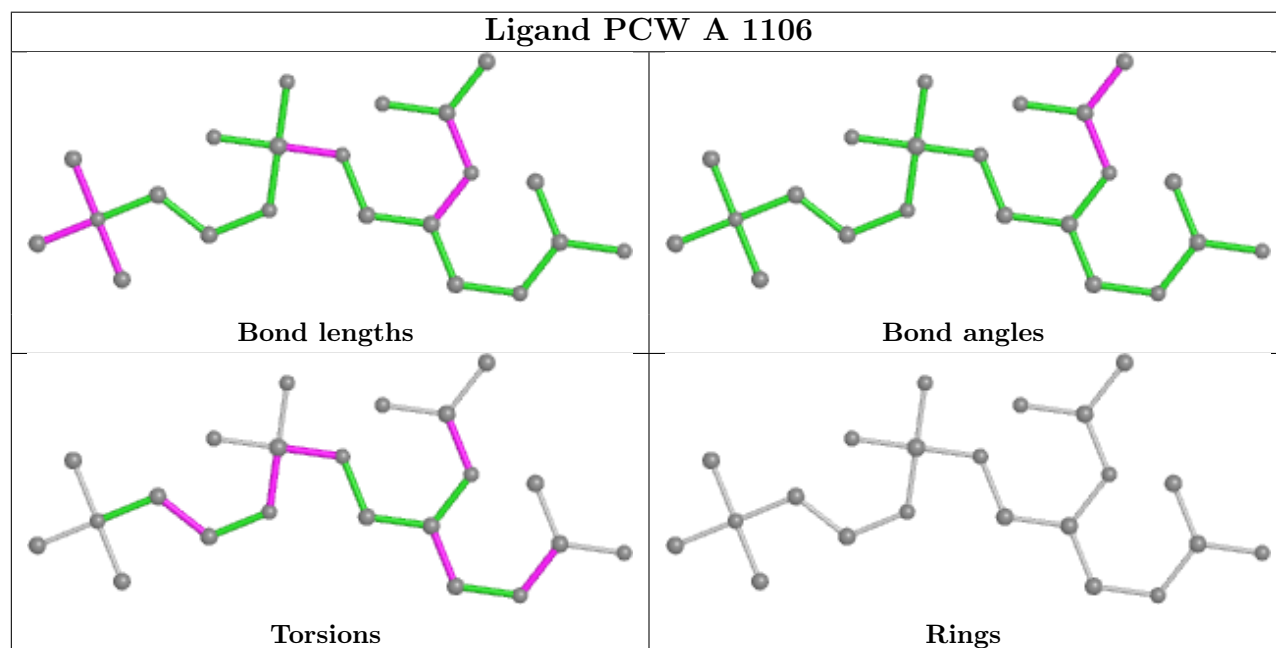
Ligand E4R C 1121



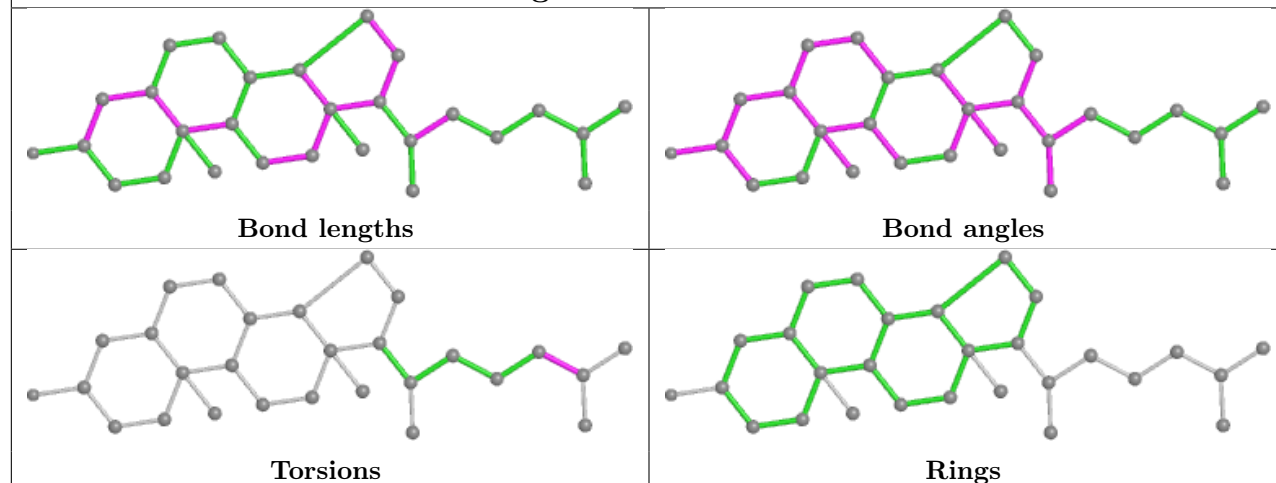
Ligand PCW C 1107



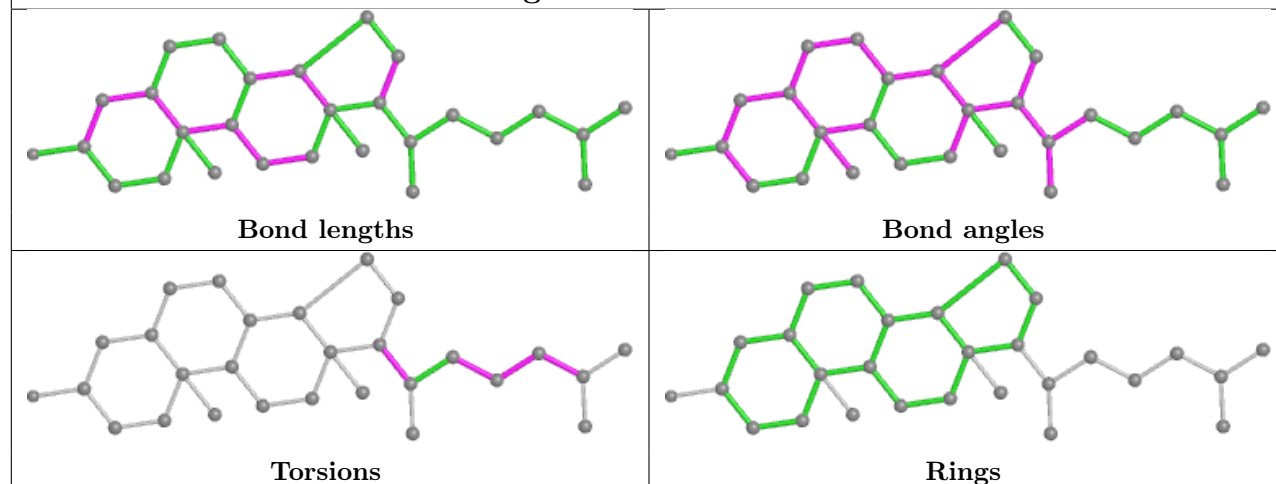
Ligand PCW A 1106



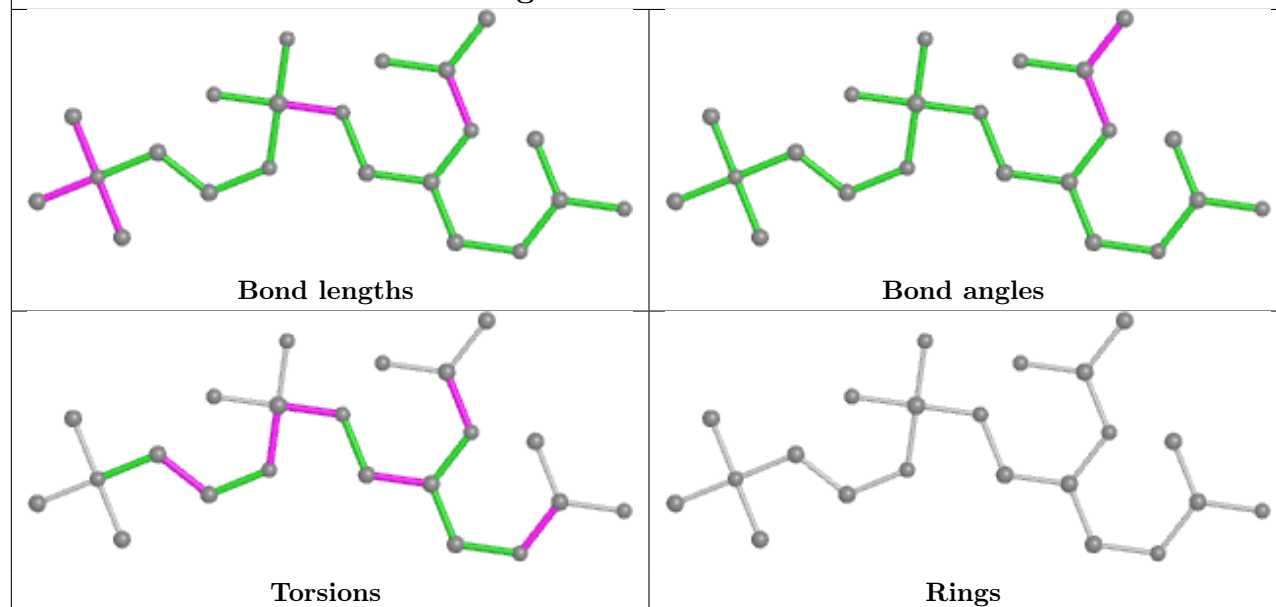
Ligand CLR D 501



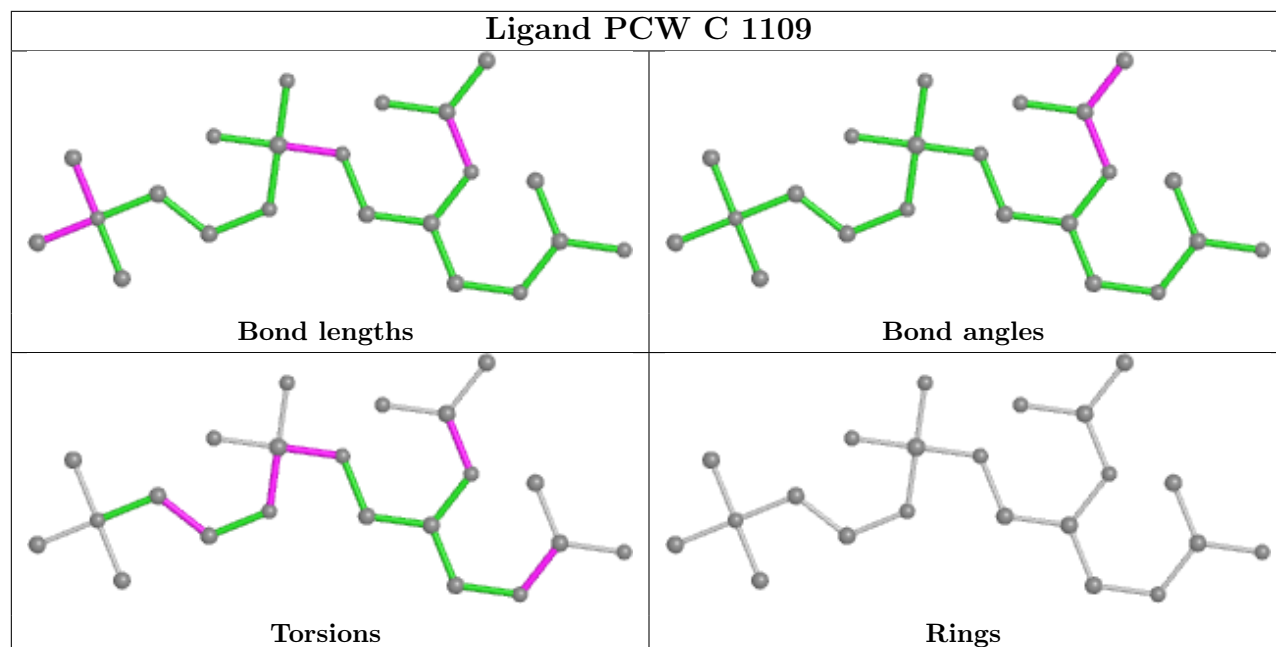
Ligand CLR C 1104



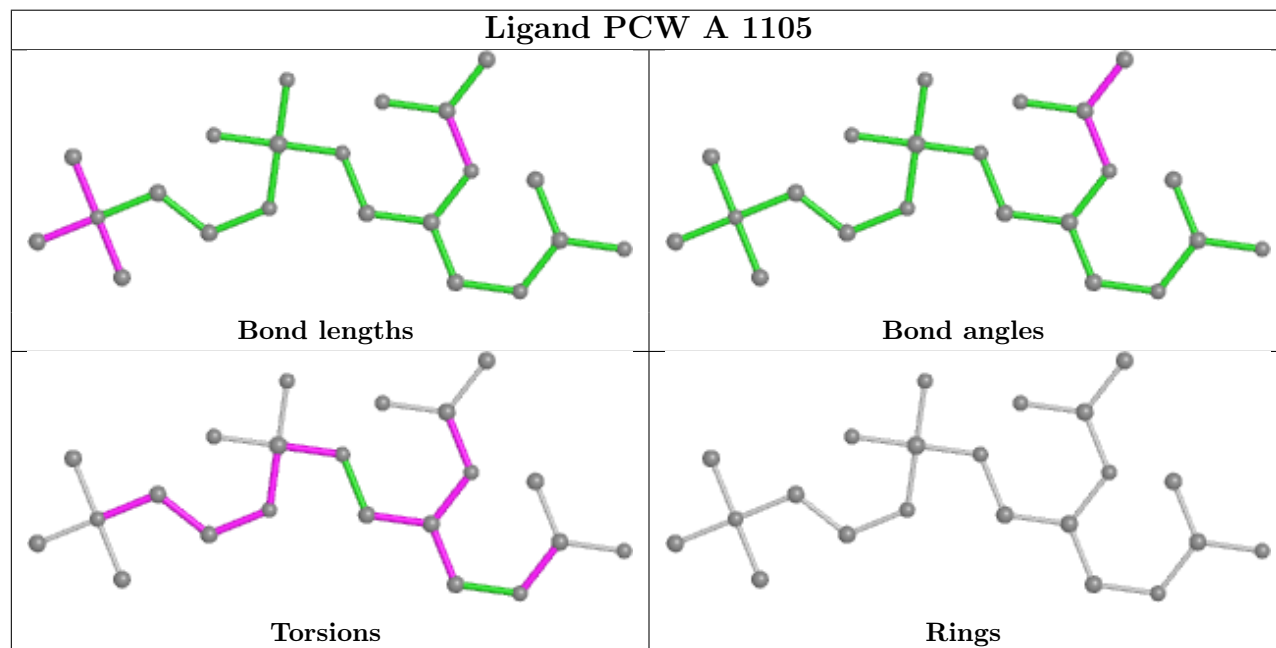
Ligand PCW C 1108



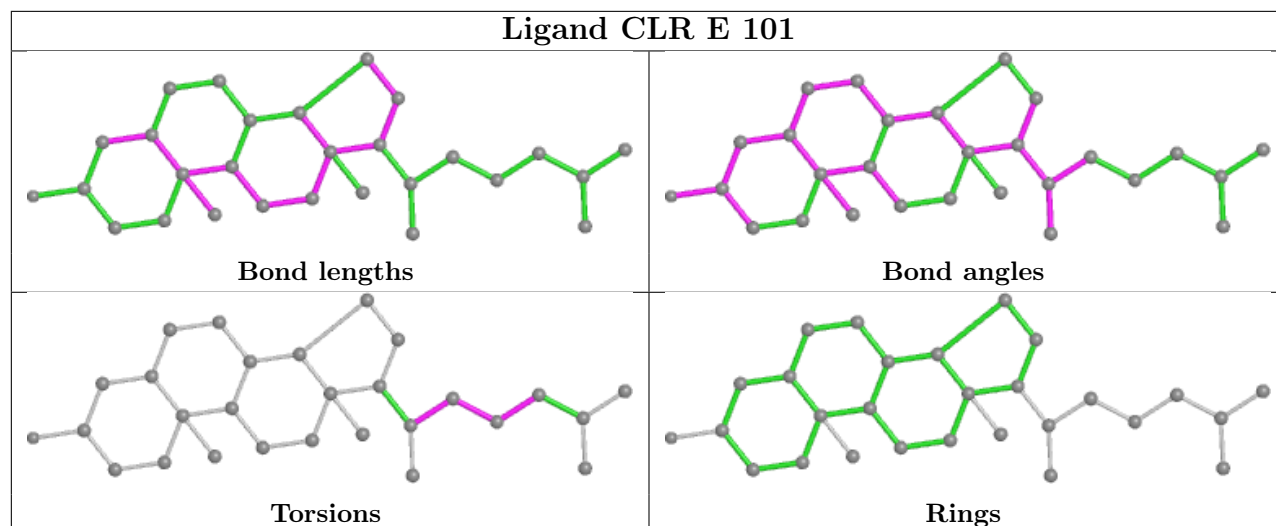
Ligand PCW C 1109



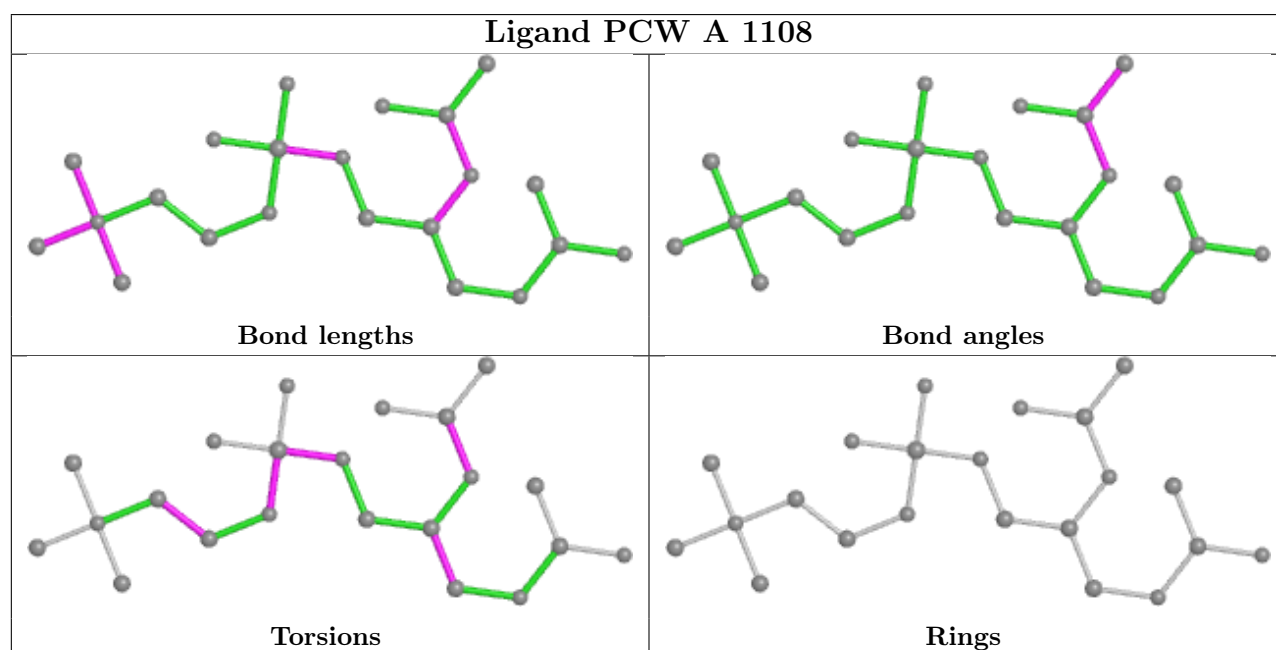
Ligand PCW A 1105



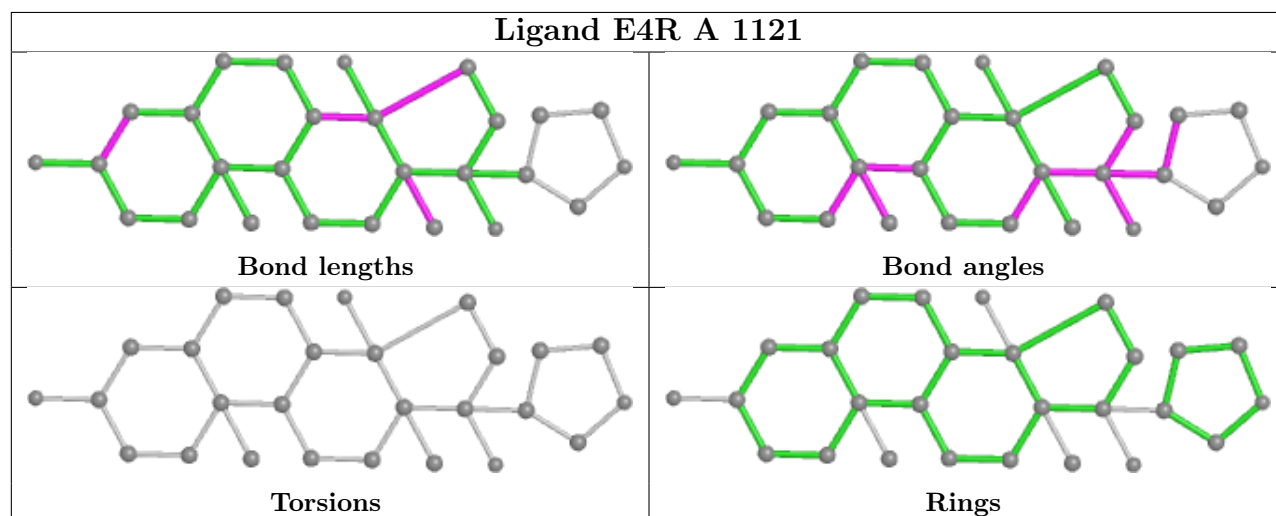
Ligand CLR E 101



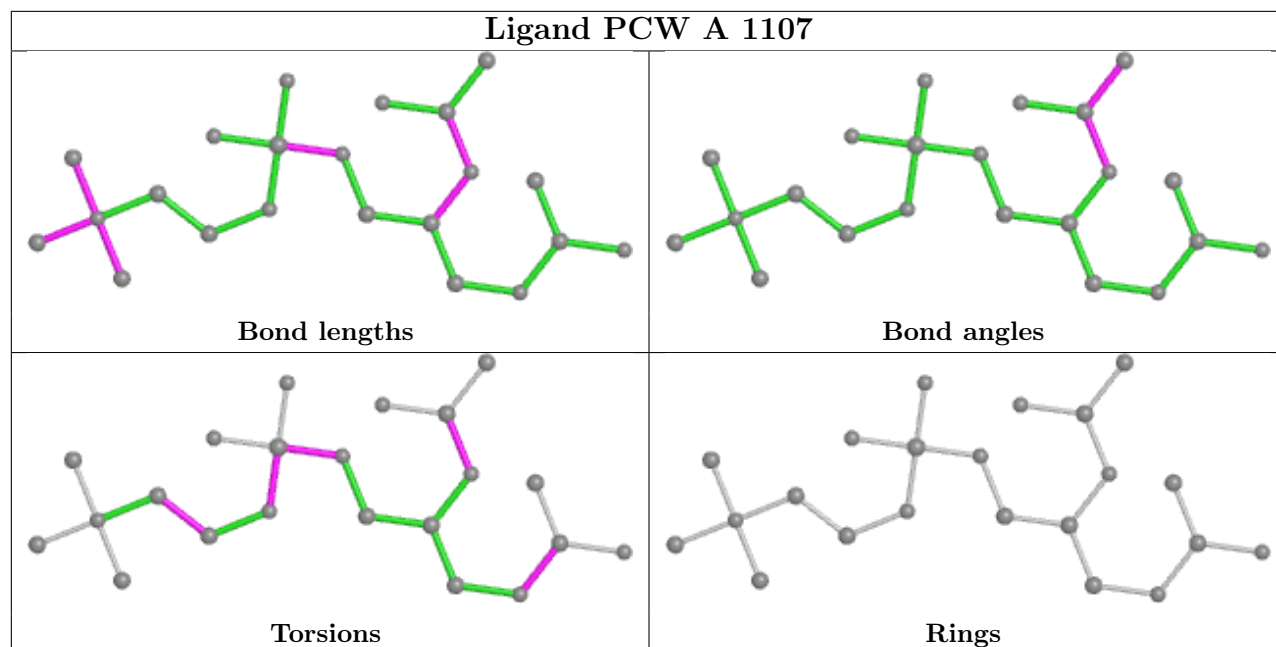
Ligand PCW A 1108



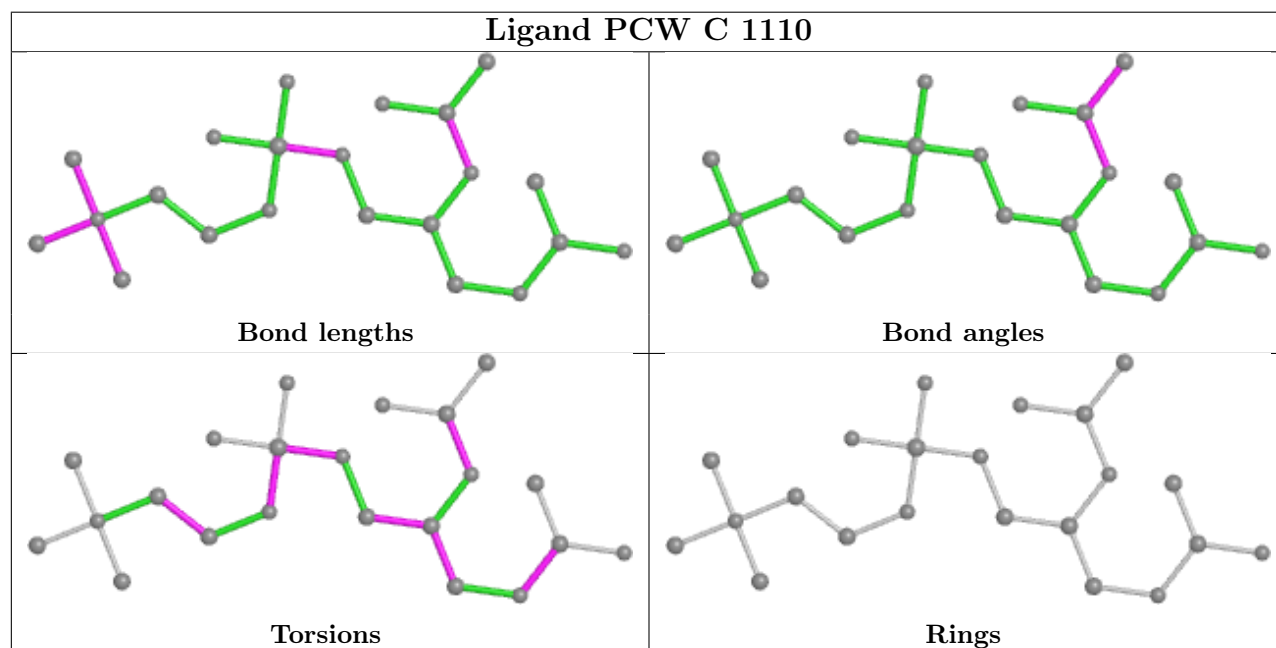
Ligand E4R A 1121



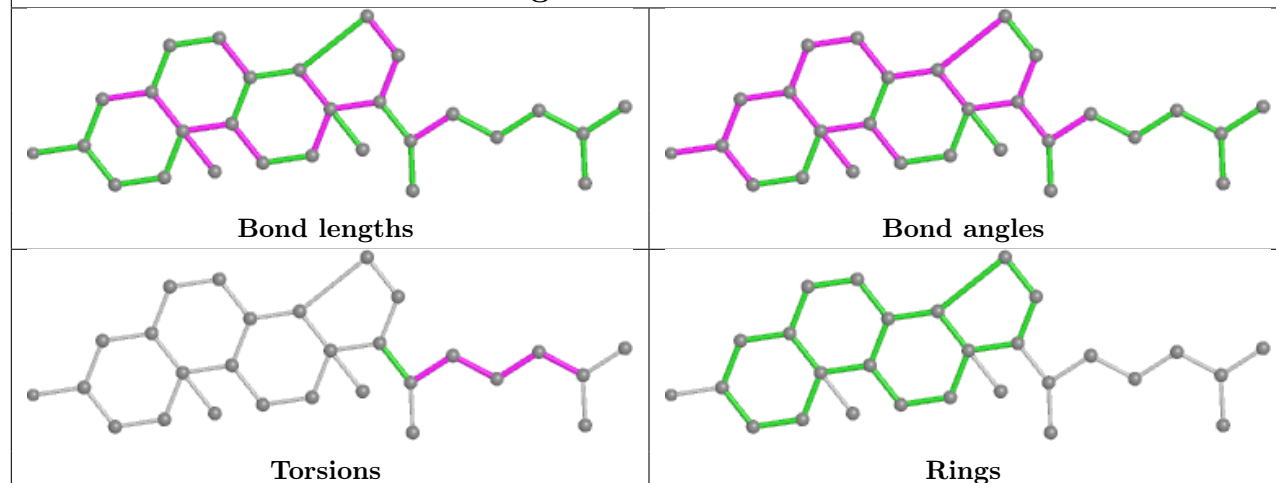
Ligand PCW A 1107



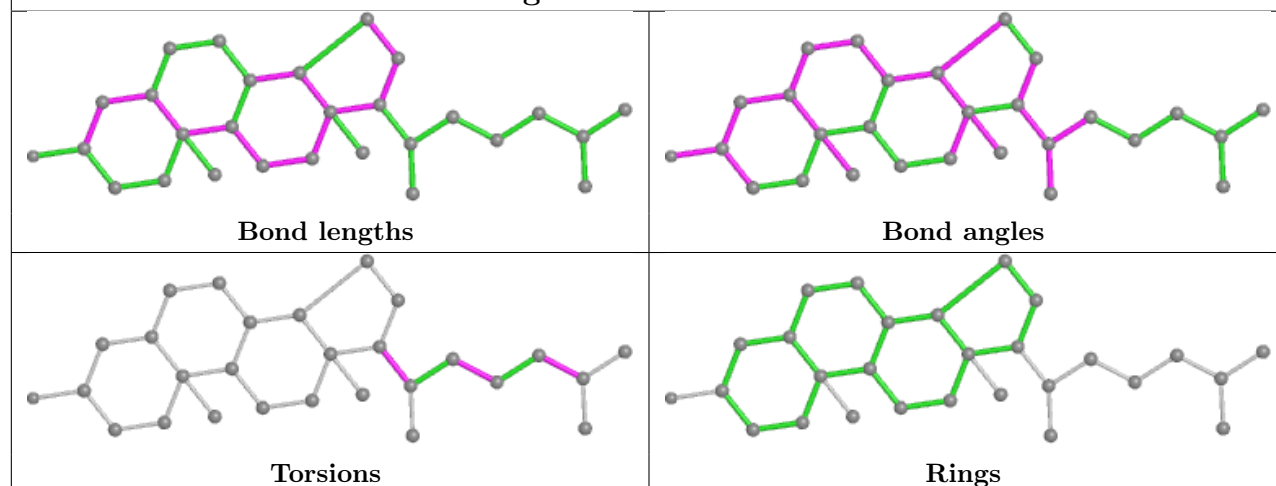
Ligand PCW C 1110



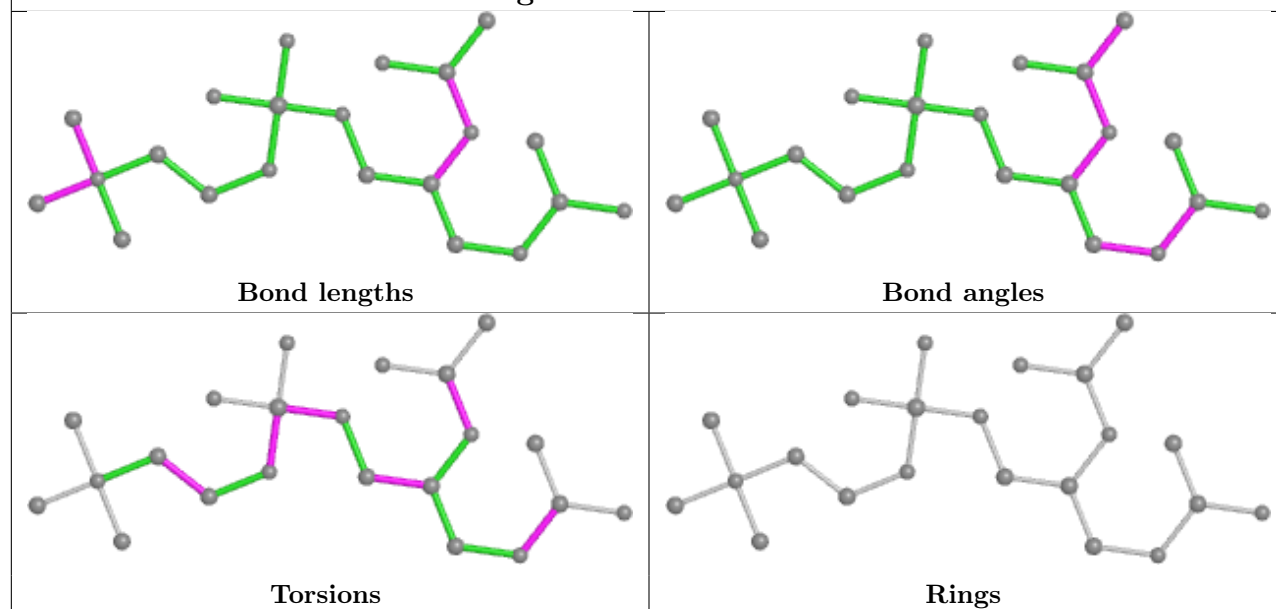
Ligand CLR G 101

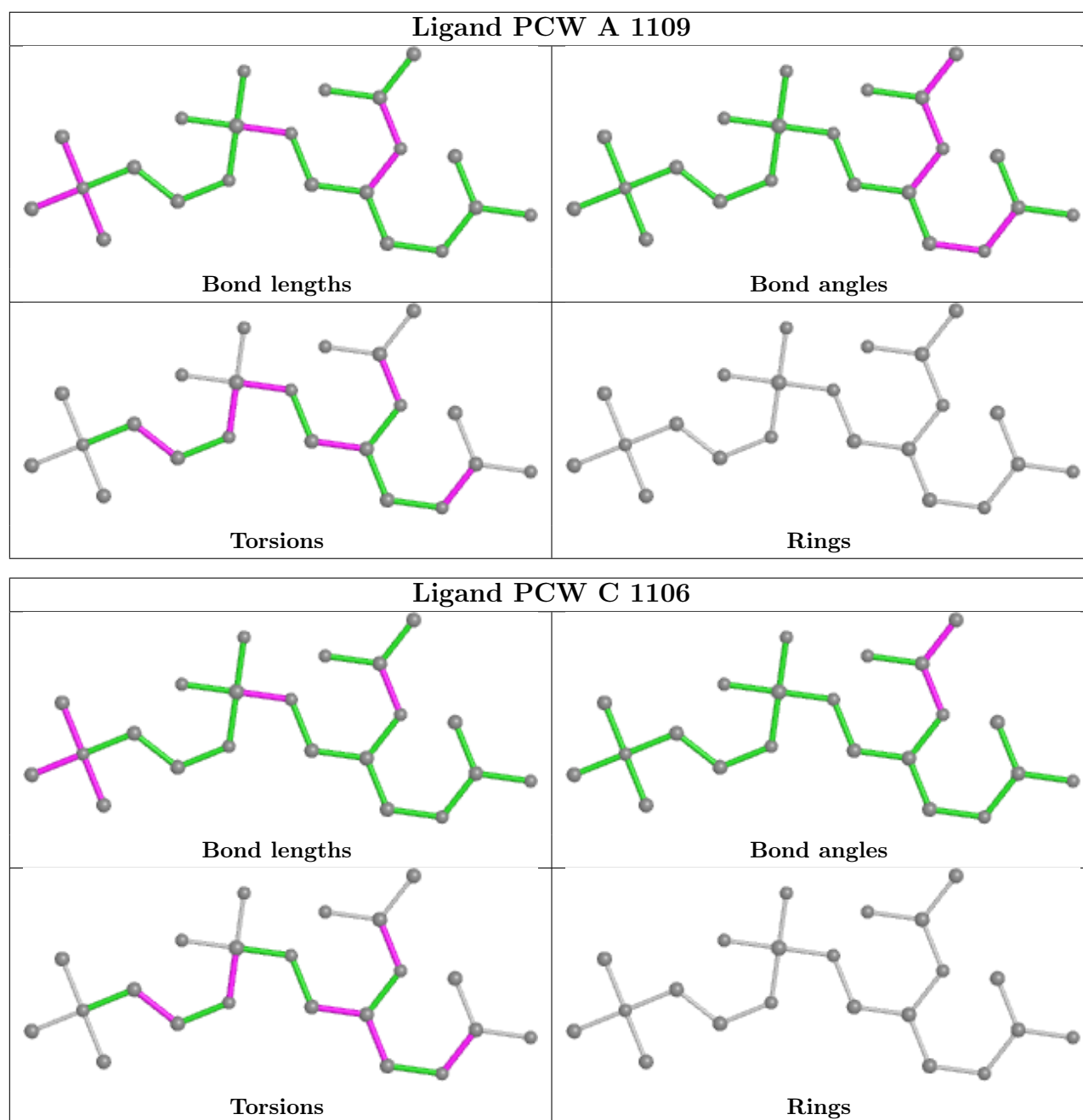


Ligand CLR A 1104



Ligand PCW C 1112





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%)	-0.58	8 (0%) 82 67	28, 89, 228, 316	0
1	C	995/1016 (97%)	-0.61	3 (0%) 90 82	25, 89, 197, 229	0
2	B	291/303 (96%)	-0.28	3 (1%) 79 61	50, 124, 205, 251	0
2	D	285/303 (94%)	-0.39	1 (0%) 89 79	27, 104, 179, 230	0
3	E	32/65 (49%)	-0.94	0 100 100	36, 68, 123, 127	0
3	G	32/65 (49%)	-0.95	0 100 100	24, 62, 121, 146	0
All	All	2630/2768 (95%)	-0.55	15 (0%) 85 72	24, 95, 210, 316	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	PHE	3.6
2	B	166	THR	3.1
1	A	534	ALA	3.0
1	A	508	LEU	2.9
1	A	503	ALA	2.9
1	A	113	ALA	2.8
1	A	114	THR	2.6
2	B	167	TYR	2.5
1	A	481	TYR	2.3
2	D	201	VAL	2.3
1	C	514	ILE	2.3
1	C	114	THR	2.2
1	C	481	TYR	2.1
1	A	505	GLU	2.1
2	B	218	ASP	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	C	369	12/13	0.97	0.06	40,59,80,83	0
1	PHD	A	369	12/13	0.98	0.05	32,62,76,80	0

6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

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
10	NAG	D	401	14/15	0.39	0.10	125,171,184,187	0
7	PCW	A	1108	22/54	0.51	0.23	135,172,205,211	0
7	PCW	C	1111	22/54	0.60	0.21	113,178,200,206	0
7	PCW	C	1108	22/54	0.60	0.15	138,183,205,208	0
7	PCW	A	1107	22/54	0.68	0.17	146,185,203,209	0
7	PCW	A	1105	22/54	0.71	0.18	155,173,197,214	0
7	PCW	C	1109	22/54	0.72	0.22	148,173,221,228	0
7	PCW	C	1110	22/54	0.74	0.20	155,186,192,193	0
9	CLR	D	501	28/28	0.75	0.14	129,147,159,161	0
7	PCW	A	1110	22/54	0.75	0.14	127,149,169,170	0
7	PCW	C	1106	22/54	0.76	0.15	129,161,166,173	0
10	NAG	B	401	14/15	0.78	0.10	129,183,195,196	0
9	CLR	B	501	28/28	0.78	0.14	116,148,158,161	0
9	CLR	A	1104	28/28	0.87	0.18	104,132,147,150	0
7	PCW	C	1107	22/54	0.88	0.11	103,130,147,154	0
7	PCW	A	1106	22/54	0.91	0.13	128,166,191,201	0
6	NA	A	1102	1/1	0.91	0.22	37,37,37,37	0
9	CLR	C	1104	28/28	0.92	0.12	66,102,130,139	0
7	PCW	C	1112	22/54	0.92	0.12	78,116,153,158	0
7	PCW	A	1109	22/54	0.94	0.12	73,107,124,132	0

Continued on next page...

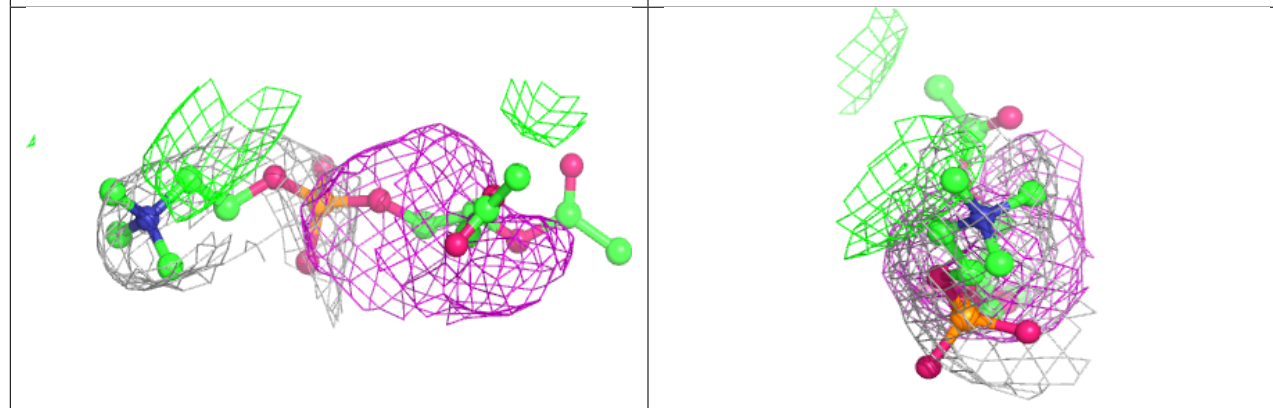
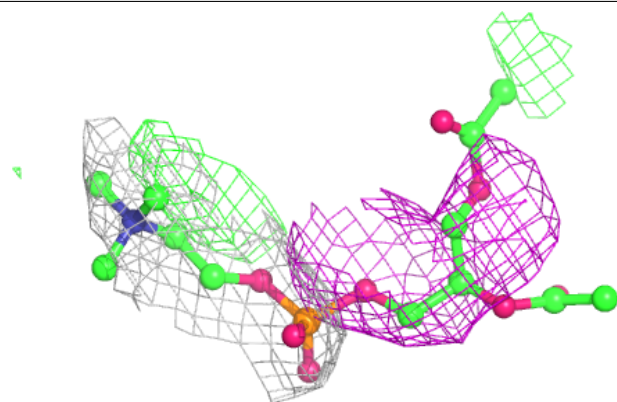
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	C	1101	1/1	0.94	0.06	61,61,61,61	0
8	E4R	A	1121	27/27	0.95	0.08	69,106,122,139	0
9	CLR	G	101	28/28	0.95	0.08	22,48,80,101	0
8	E4R	C	1121	27/27	0.96	0.08	40,77,101,108	0
9	CLR	E	101	28/28	0.96	0.07	20,46,76,85	0
6	NA	C	1102	1/1	0.99	0.15	13,13,13,13	0
5	MG	A	1101	1/1	0.99	0.03	84,84,84,84	0
5	MG	C	1103	1/1	1.00	0.03	26,26,26,26	0
5	MG	A	1103	1/1	1.00	0.02	78,78,78,78	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.

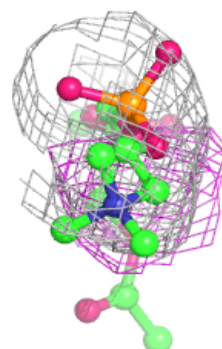
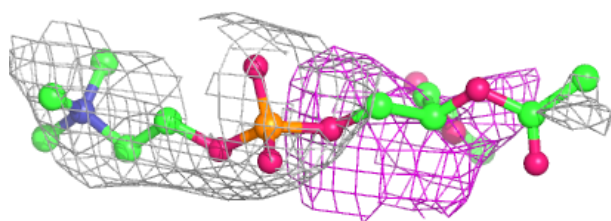
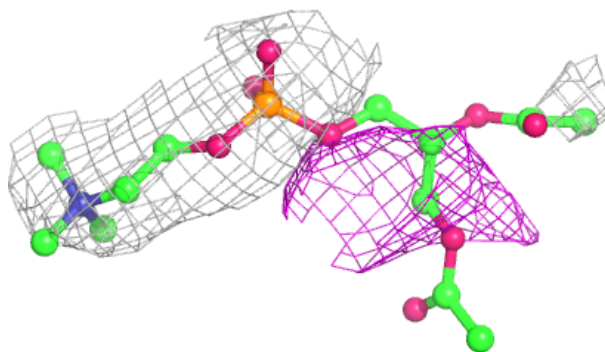
Electron density around PCW A 1108:

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

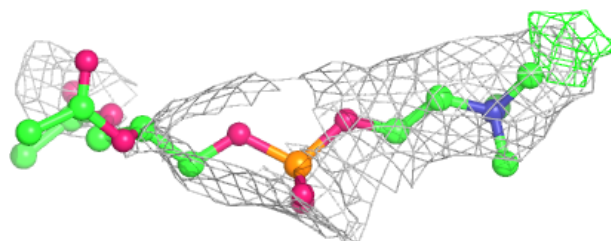
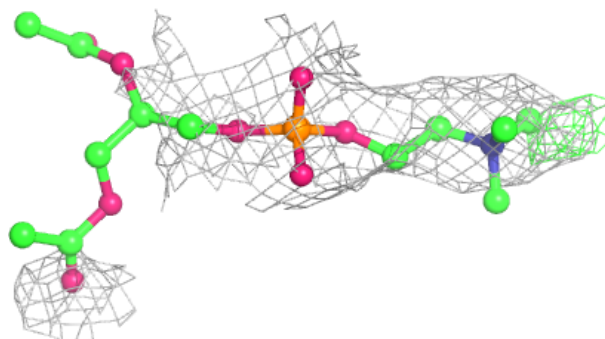


Electron density around PCW C 1111:

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

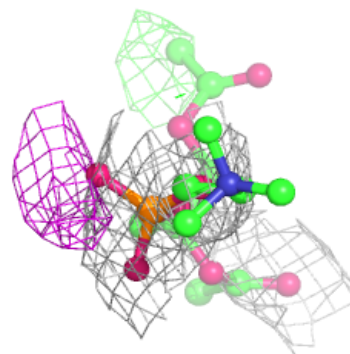
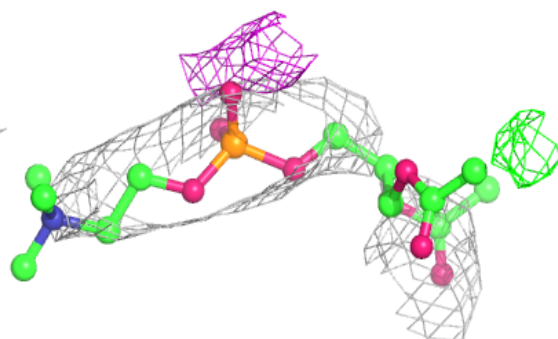
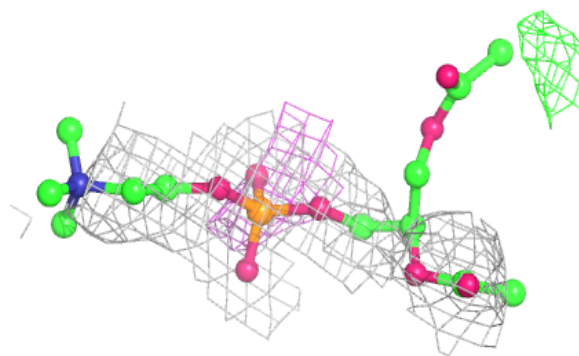
**Electron density around PCW C 1108:**

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

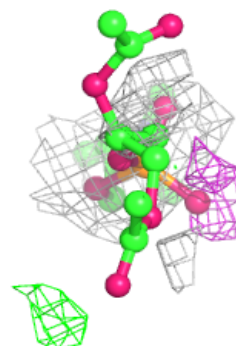
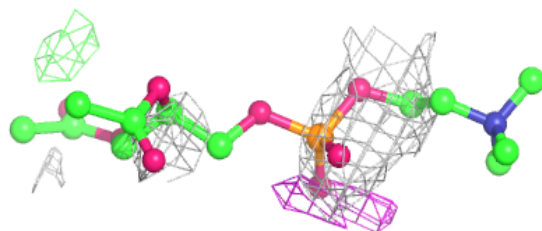
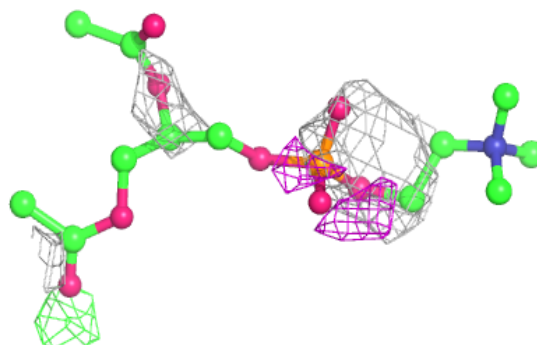


Electron density around PCW A 1107:

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

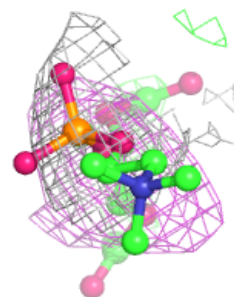
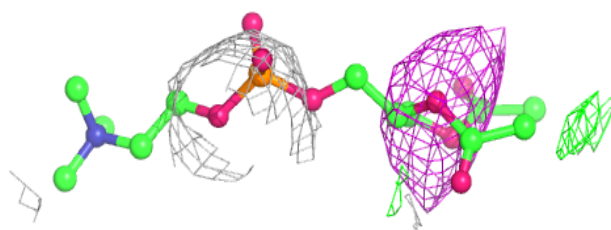
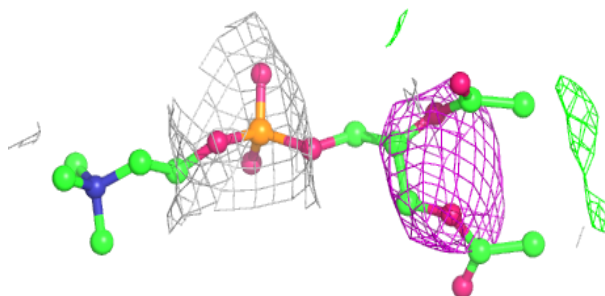
**Electron density around PCW A 1105:**

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

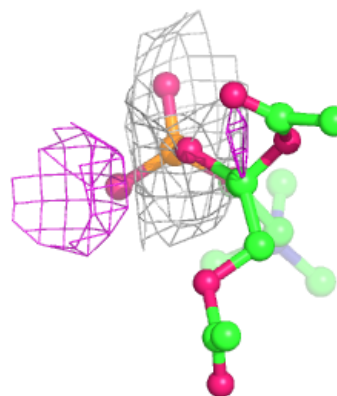
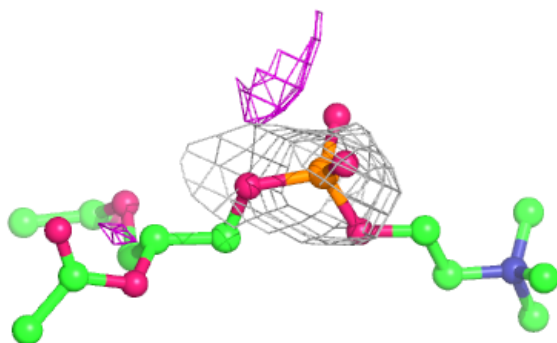
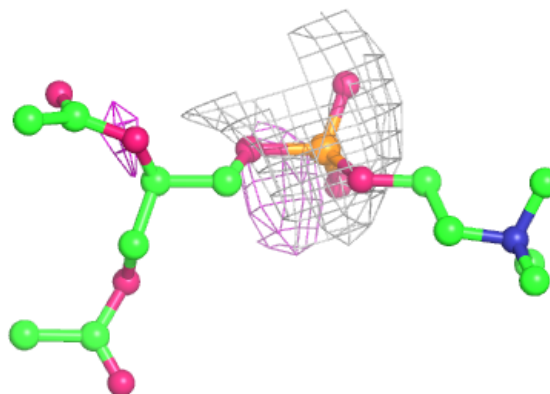


Electron density around PCW C 1109:

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

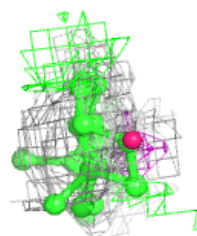
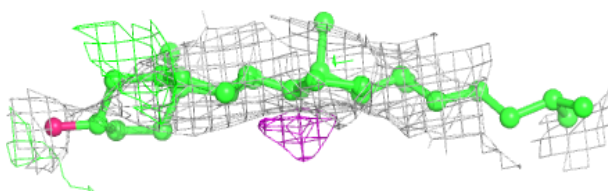
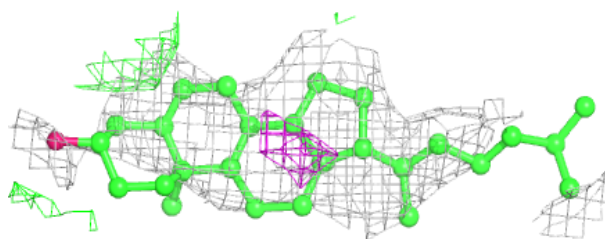
**Electron density around PCW C 1110:**

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

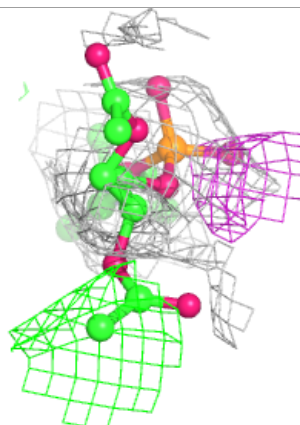
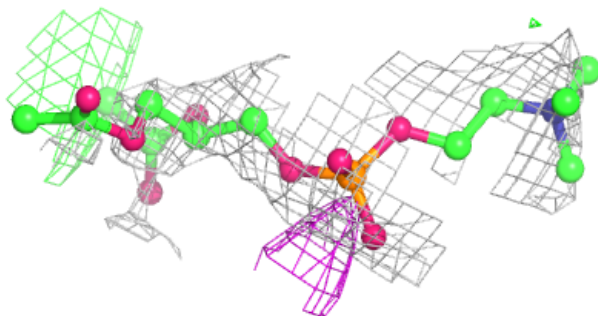
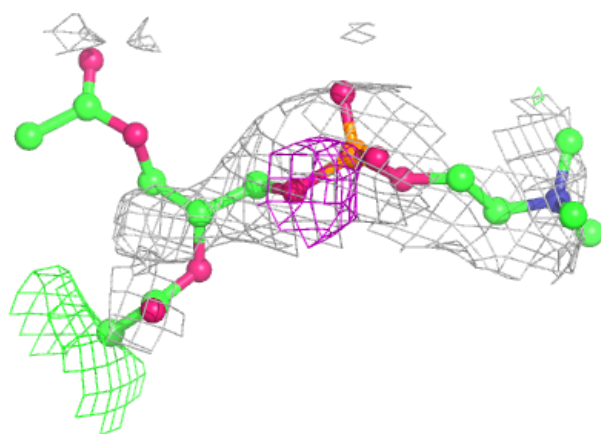


Electron density around CLR D 501:

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

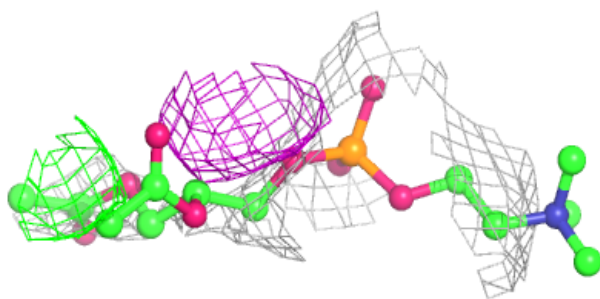
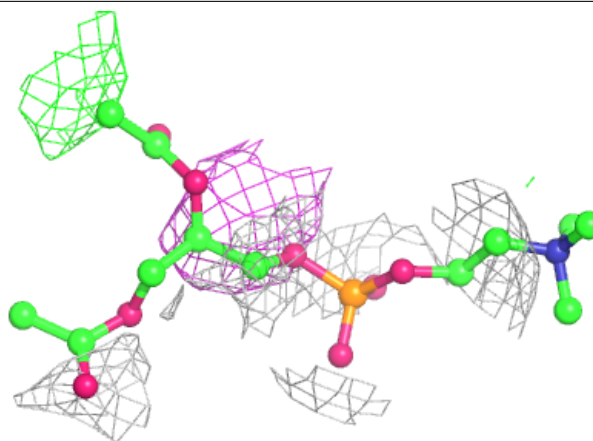
**Electron density around PCW A 1110:**

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

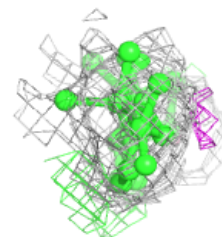
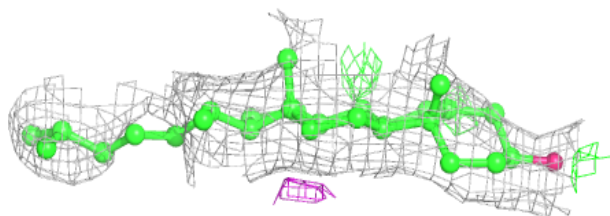
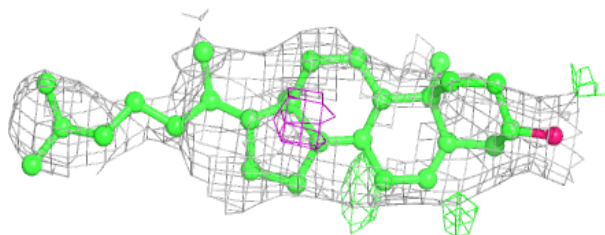


Electron density around PCW C 1106:

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

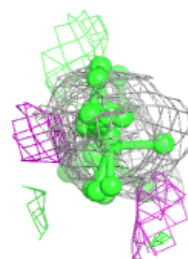
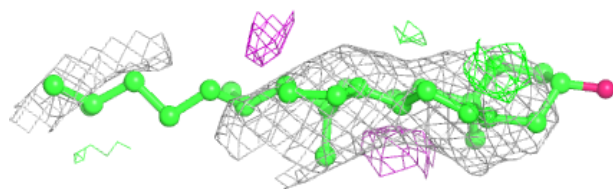
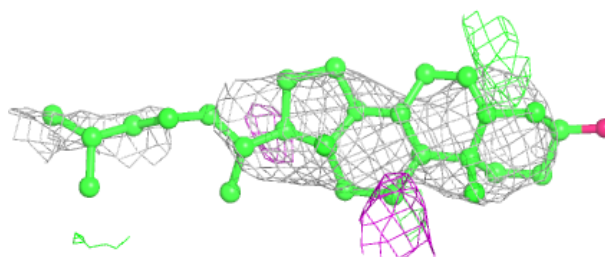
**Electron density around CLR B 501:**

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



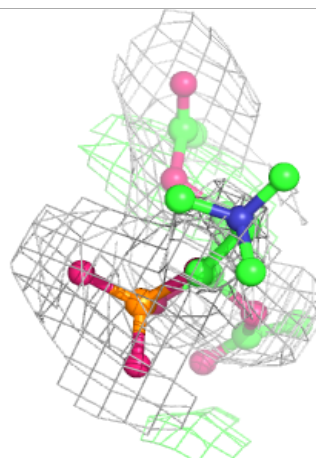
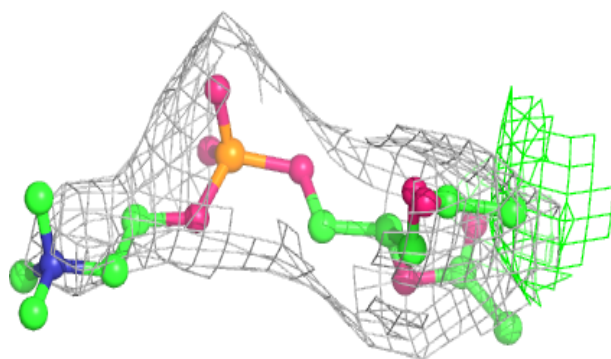
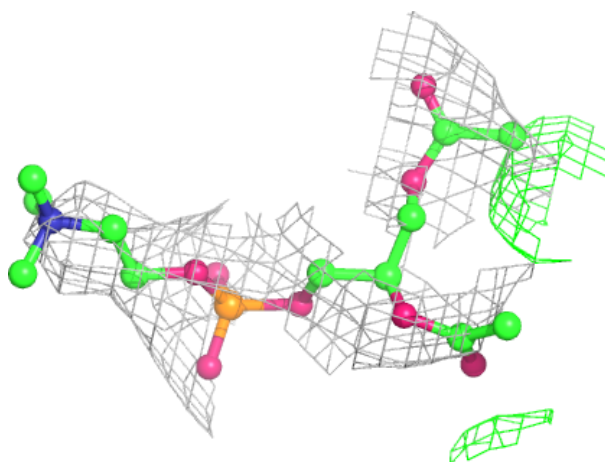
Electron density around CLR A 1104:

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



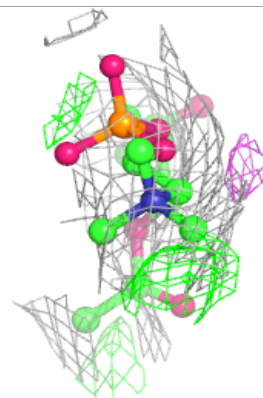
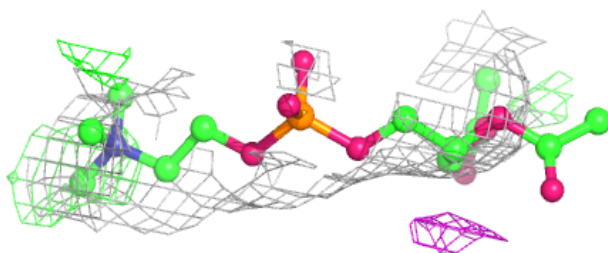
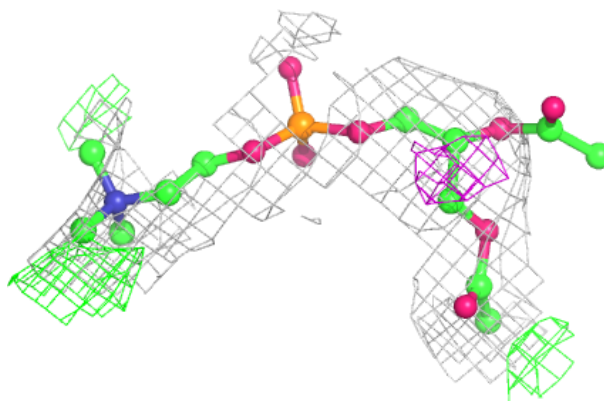
Electron density around PCW C 1107:

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

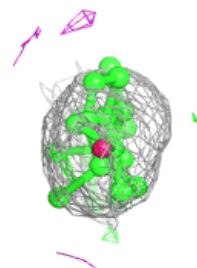
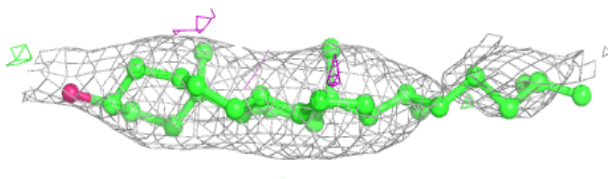
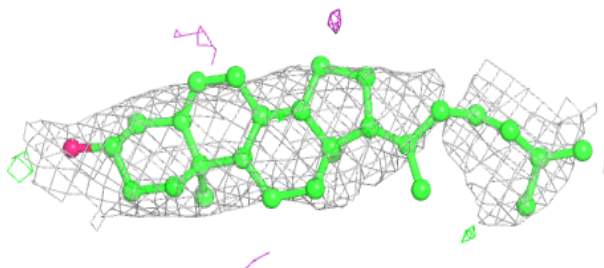


Electron density around PCW A 1106:

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

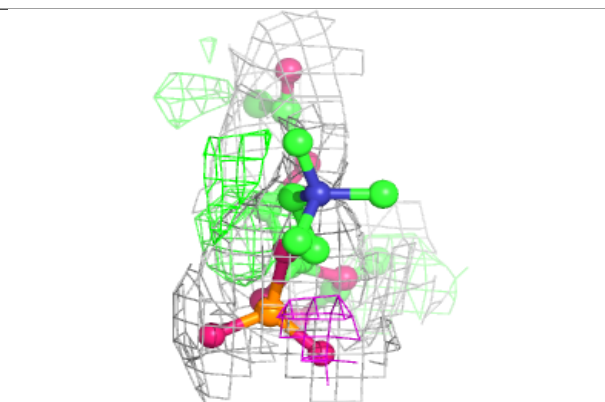
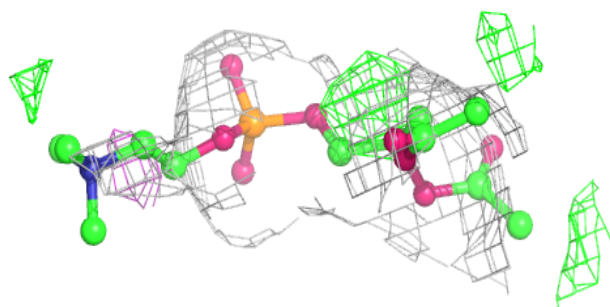
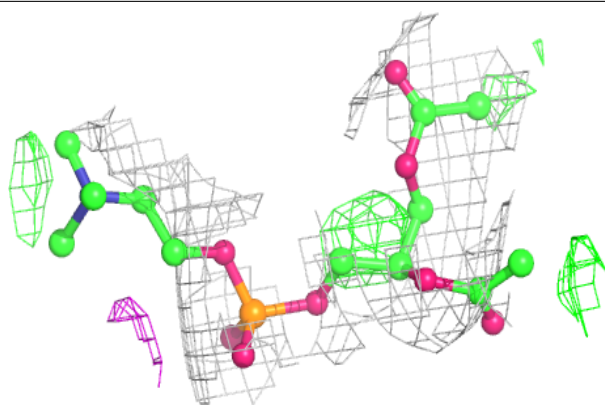
**Electron density around CLR C 1104:**

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

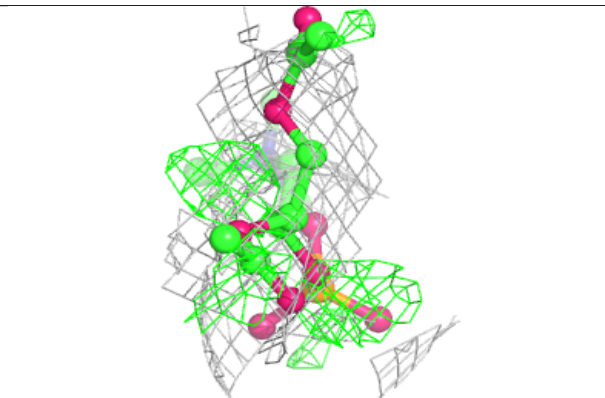
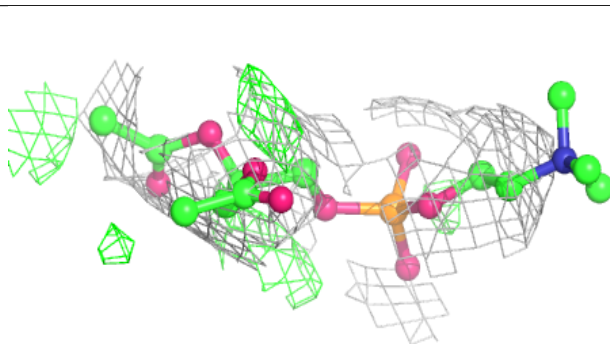
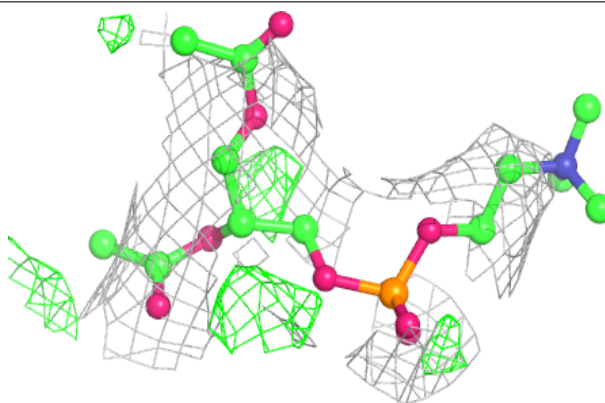


Electron density around PCW C 1112:

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

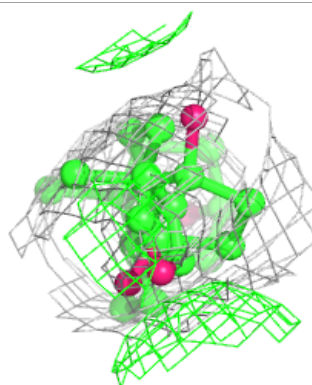
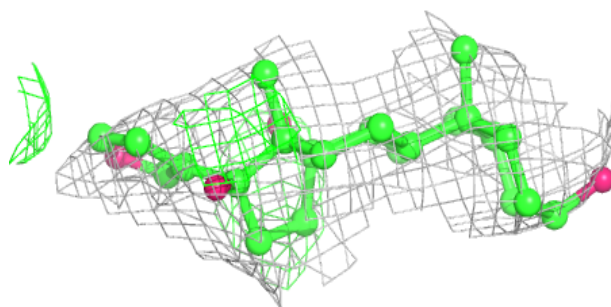
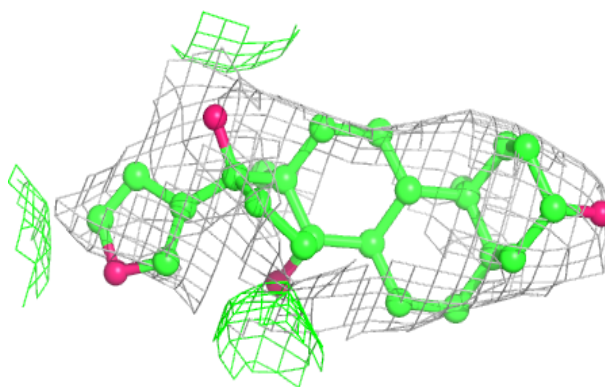
**Electron density around PCW A 1109:**

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

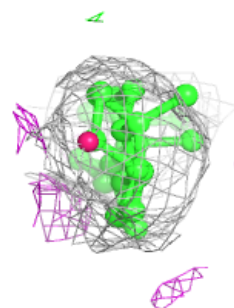
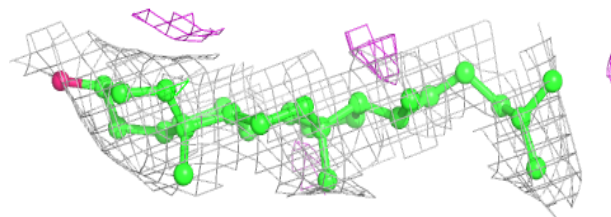
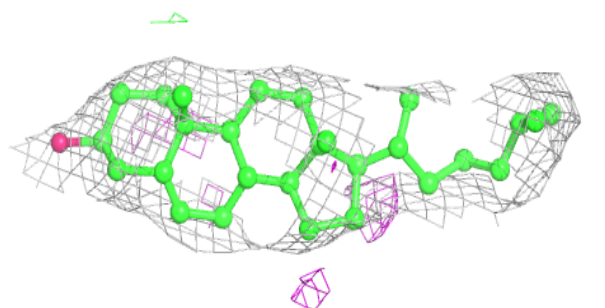


Electron density around E4R A 1121:

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

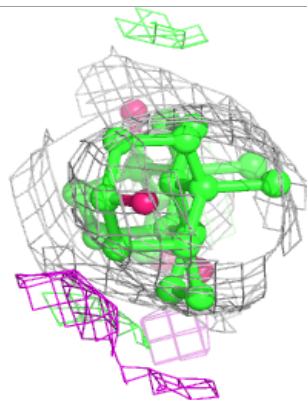
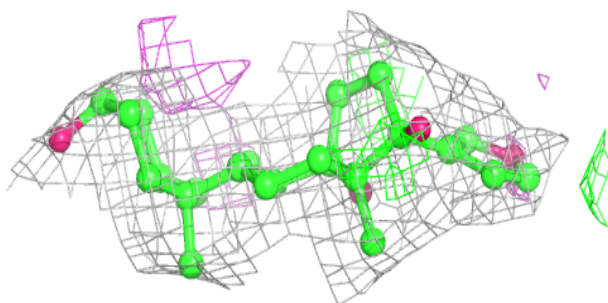
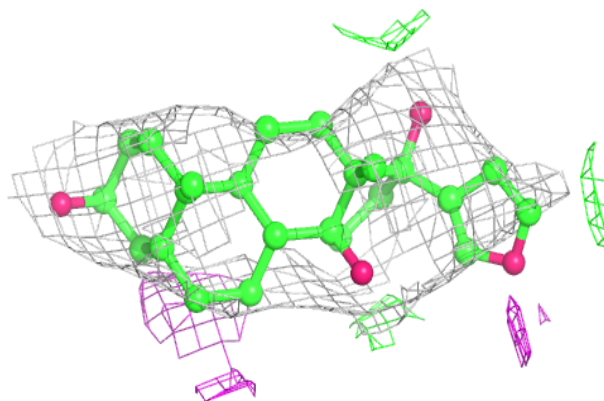
**Electron density around CLR G 101:**

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

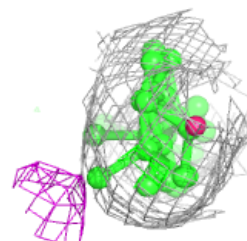
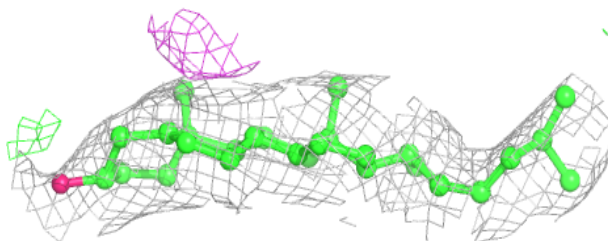
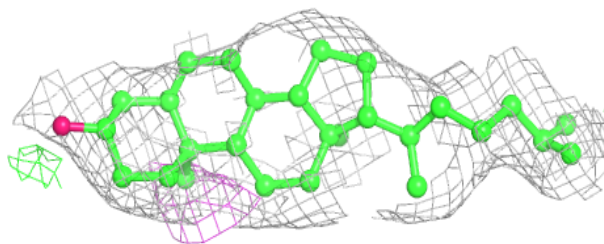


Electron density around E4R C 1121:

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

**Electron density around 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.