wwPDB X-ray Structure Validation Summary Report (i)

Nov 13, 2023 – 11:07 AM JST

PDB ID	:	5XA7
Title	:	Complete structure factors and an atomic model of the calcium pump (SERCA1A) and associated phospholipids in the E1-2CA2+ crystals
Authors	:	Norimatsu, Y.; Hasegawa, K.; Shimizu, N.; Toyoshima, C.
Deposited on	:	2017-03-11
Resolution	:	3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

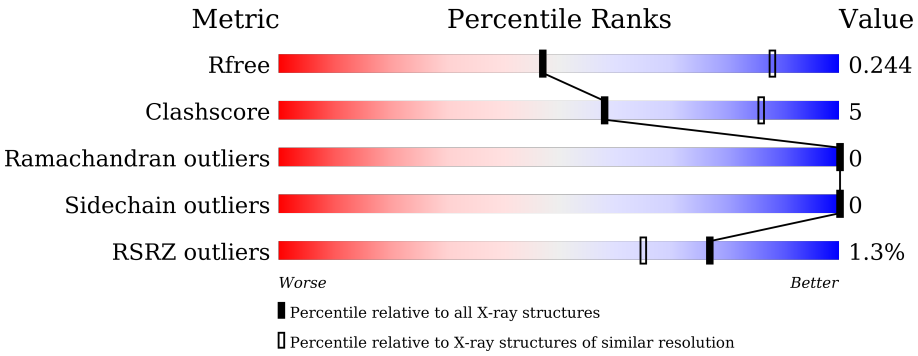
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	995	% 86% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PCW	A	1004	-	-	-	X
4	PCW	A	1005	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PCW	A	1006	-	-	-	X
4	PCW	A	1008	-	-	-	X
4	PCW	A	1009	-	-	-	X
4	PCW	A	1010	-	-	-	X
4	PCW	A	1012	-	-	-	X
4	PCW	A	1013	-	-	-	X
4	PCW	A	1014	-	-	-	X
4	PCW	A	1015	-	-	-	X
4	PCW	A	1016	-	-	-	X
4	PCW	A	1017	-	-	-	X
4	PCW	A	1018	-	-	-	X
4	PCW	A	1019	-	-	-	X
4	PCW	A	1020	-	-	-	X
4	PCW	A	1021	-	-	-	X
4	PCW	A	1022	-	-	-	X
4	PCW	A	1023	-	-	-	X
4	PCW	A	1024	-	-	-	X
4	PCW	A	1025	-	-	-	X
4	PCW	A	1026	-	-	-	X
4	PCW	A	1027	-	-	-	X
4	PCW	A	1028	-	-	-	X
4	PCW	A	1029	-	-	-	X
4	PCW	A	1030	-	-	-	X
4	PCW	A	1031	-	-	-	X
4	PCW	A	1032	-	-	-	X
4	PCW	A	1033	-	-	-	X
4	PCW	A	1034	-	-	-	X
4	PCW	A	1035	-	-	-	X
4	PCW	A	1037	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8542 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	0	0	0
			7674	4878	1287	1452	57			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP P04191

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

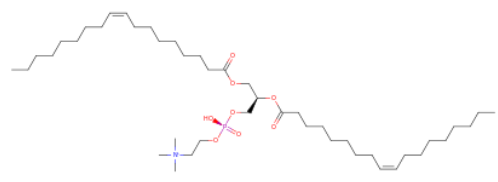
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).

PCW



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

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

- Molecule 5 is water.

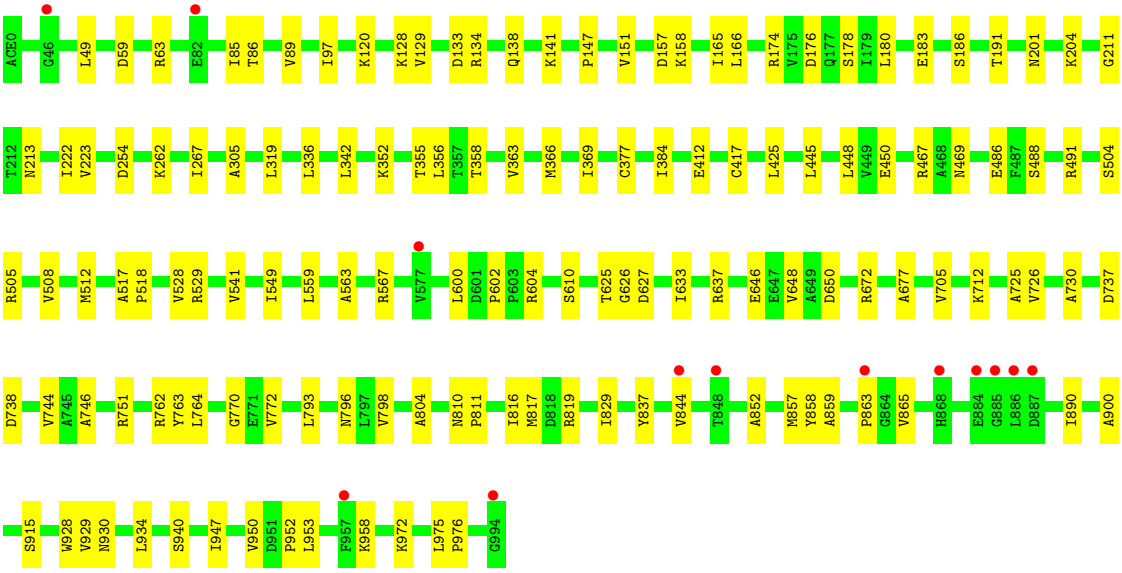
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	117	Total 117	O 117	0	0

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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.20Å 64.55Å 146.22Å 90.00° 98.12° 90.00°	Depositor
Resolution (Å)	82.27 – 3.20 144.75 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (82.27-3.20) 100.0 (144.75-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	19.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.225 , 0.244 0.226 , 0.244	Depositor DCC
R_{free} test set	1231 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8542	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PCW, ACE, CA, NA

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	0.20	0/7813	0.39	4/10594 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	857	MET	CB-CA-C	-7.12	96.16	110.40
1	A	133	ASP	CB-CA-C	-5.98	98.45	110.40
1	A	857	MET	N-CA-C	5.75	126.53	111.00
1	A	858	TYR	N-CA-CB	5.25	120.04	110.60

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	7674	0	7764	79	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	748	0	612	4	0
5	A	117	0	0	0	0
All	All	8542	0	8376	80	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 5.

The worst 5 of 80 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:120:LYS:O	1:A:141:LYS:HE2	1.89	0.71
1:A:600:LEU:HD12	1:A:602:PRO:N	2.07	0.68
1:A:158:LYS:HE3	1:A:211:GLY:HA2	1.76	0.67
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.95	0.66
1:A:559:LEU:CD2	1:A:600:LEU:HD23	2.26	0.66

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	993/995 (100%)	950 (96%)	43 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	840/840 (100%)	840 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 3 are monoatomic - leaving 34 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	$\#\|Z\| > 2$
4	PCW	A	1010	-	21,21,53	0.85	0	27,29,61	1.07	1 (3%)
4	PCW	A	1021	-	21,21,53	0.74	0	27,29,61	0.99	0
4	PCW	A	1037	-	21,21,53	0.72	0	27,29,61	1.02	1 (3%)
4	PCW	A	1011	-	21,21,53	0.72	0	27,29,61	2.52	4 (14%)
4	PCW	A	1004	-	21,21,53	0.76	0	27,29,61	1.02	1 (3%)
4	PCW	A	1008	-	21,21,53	0.70	0	27,29,61	1.25	2 (7%)
4	PCW	A	1019	-	21,21,53	0.78	0	27,29,61	1.25	2 (7%)
4	PCW	A	1029	-	21,21,53	0.90	0	27,29,61	1.04	1 (3%)
4	PCW	A	1027	-	21,21,53	0.83	0	27,29,61	1.04	1 (3%)
4	PCW	A	1024	-	21,21,53	0.74	0	27,29,61	1.02	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PCW	A	1016	-	21,21,53	0.69	0	27,29,61	1.24	2 (7%)
4	PCW	A	1023	-	21,21,53	0.70	0	27,29,61	1.01	1 (3%)
4	PCW	A	1022	-	21,21,53	1.00	1 (4%)	27,29,61	1.03	1 (3%)
4	PCW	A	1033	-	21,21,53	0.81	0	27,29,61	1.06	1 (3%)
4	PCW	A	1032	-	21,21,53	0.73	0	27,29,61	1.05	1 (3%)
4	PCW	A	1034	-	21,21,53	0.75	0	27,29,61	1.01	1 (3%)
4	PCW	A	1012	-	21,21,53	0.61	0	27,29,61	1.08	1 (3%)
4	PCW	A	1035	-	21,21,53	0.83	0	27,29,61	1.04	1 (3%)
4	PCW	A	1025	-	21,21,53	0.75	0	27,29,61	1.25	2 (7%)
4	PCW	A	1030	-	21,21,53	0.81	0	27,29,61	1.04	1 (3%)
4	PCW	A	1007	-	21,21,53	0.67	1 (4%)	27,29,61	1.26	2 (7%)
4	PCW	A	1006	-	21,21,53	0.81	1 (4%)	27,29,61	1.27	2 (7%)
4	PCW	A	1018	-	21,21,53	0.88	0	27,29,61	1.02	1 (3%)
4	PCW	A	1028	-	21,21,53	0.79	0	27,29,61	1.09	2 (7%)
4	PCW	A	1036	-	21,21,53	0.68	0	27,29,61	1.06	1 (3%)
4	PCW	A	1013	-	21,21,53	0.67	0	27,29,61	1.24	2 (7%)
4	PCW	A	1020	-	21,21,53	0.73	0	27,29,61	1.07	1 (3%)
4	PCW	A	1009	-	21,21,53	0.70	0	27,29,61	1.03	1 (3%)
4	PCW	A	1031	-	21,21,53	0.67	0	27,29,61	1.02	1 (3%)
4	PCW	A	1014	-	21,21,53	0.75	0	27,29,61	1.01	1 (3%)
4	PCW	A	1026	-	21,21,53	0.65	0	27,29,61	1.06	1 (3%)
4	PCW	A	1005	-	21,21,53	0.70	0	27,29,61	1.08	2 (7%)
4	PCW	A	1015	-	21,21,53	0.91	0	27,29,61	1.05	2 (7%)
4	PCW	A	1017	-	21,21,53	0.90	0	27,29,61	1.02	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
4	PCW	A	1010	-	-	10/23/23/57	-
4	PCW	A	1021	-	-	8/23/23/57	-
4	PCW	A	1037	-	-	10/23/23/57	-
4	PCW	A	1011	-	-	10/23/23/57	-
4	PCW	A	1004	-	-	8/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	A	1008	-	-	7/23/23/57	-
4	PCW	A	1019	-	-	6/23/23/57	-
4	PCW	A	1029	-	-	4/23/23/57	-
4	PCW	A	1027	-	-	10/23/23/57	-
4	PCW	A	1024	-	-	7/23/23/57	-
4	PCW	A	1016	-	-	9/23/23/57	-
4	PCW	A	1023	-	-	7/23/23/57	-
4	PCW	A	1022	-	-	5/23/23/57	-
4	PCW	A	1033	-	-	6/23/23/57	-
4	PCW	A	1032	-	-	10/23/23/57	-
4	PCW	A	1034	-	-	12/23/23/57	-
4	PCW	A	1012	-	-	6/23/23/57	-
4	PCW	A	1035	-	-	8/23/23/57	-
4	PCW	A	1025	-	-	8/23/23/57	-
4	PCW	A	1030	-	-	6/23/23/57	-
4	PCW	A	1007	-	-	11/23/23/57	-
4	PCW	A	1006	-	-	7/23/23/57	-
4	PCW	A	1018	-	-	6/23/23/57	-
4	PCW	A	1028	-	-	4/23/23/57	-
4	PCW	A	1036	-	-	6/23/23/57	-
4	PCW	A	1013	-	-	11/23/23/57	-
4	PCW	A	1020	-	-	3/23/23/57	-
4	PCW	A	1009	-	-	4/23/23/57	-
4	PCW	A	1031	-	-	7/23/23/57	-
4	PCW	A	1014	-	-	13/23/23/57	-
4	PCW	A	1026	-	-	4/23/23/57	-
4	PCW	A	1005	-	-	9/23/23/57	-
4	PCW	A	1015	-	-	7/23/23/57	-
4	PCW	A	1017	-	-	11/23/23/57	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1007	PCW	C5-C4	2.04	1.57	1.51
4	A	1006	PCW	P-O2P	2.03	1.58	1.50
4	A	1022	PCW	C3-C2	2.03	1.56	1.50

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1011	PCW	O11-C11-C12	-11.17	84.13	124.81
4	A	1020	PCW	P-O3P-C1	-2.73	105.66	121.68
4	A	1012	PCW	P-O3P-C1	-2.58	106.54	121.68
4	A	1028	PCW	P-O3P-C1	-2.55	106.73	121.68
4	A	1013	PCW	P-O3P-C1	-2.47	107.18	121.68

There are no chirality outliers.

5 of 260 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1004	PCW	O4P-C4-C5-N
4	A	1005	PCW	C32-C31-O2-C2
4	A	1006	PCW	C32-C31-O2-C2
4	A	1008	PCW	O3P-C1-C2-O2
4	A	1009	PCW	O4P-C4-C5-N

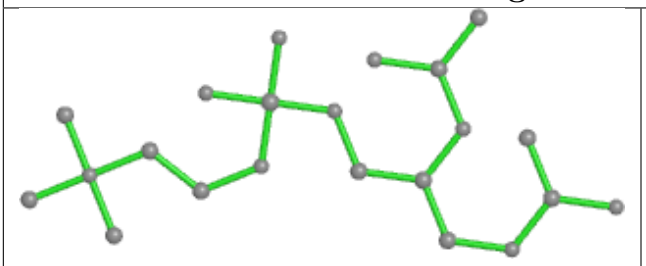
There are no ring outliers.

3 monomers are involved in 4 short contacts:

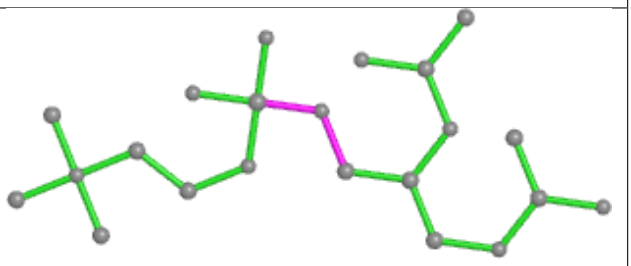
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1022	PCW	2	0
4	A	1013	PCW	1	0
4	A	1005	PCW	1	0

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

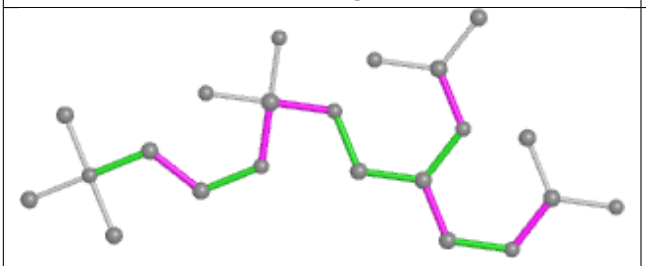
Ligand PCW A 1010



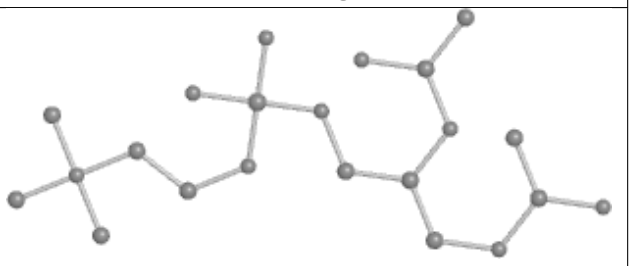
Bond lengths



Bond angles

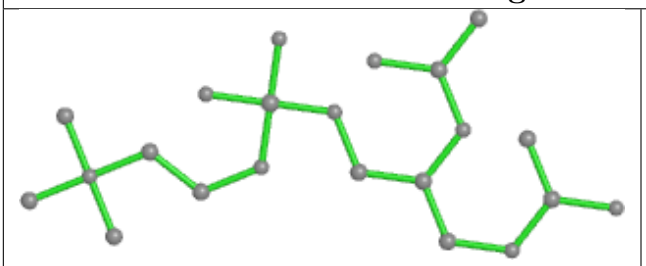


Torsions

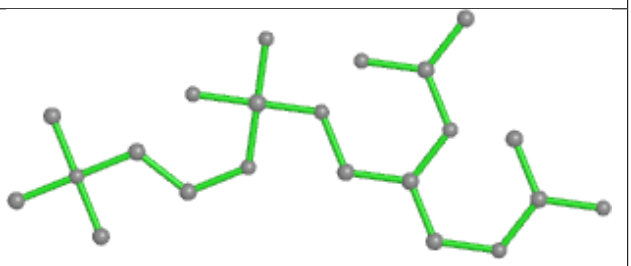


Rings

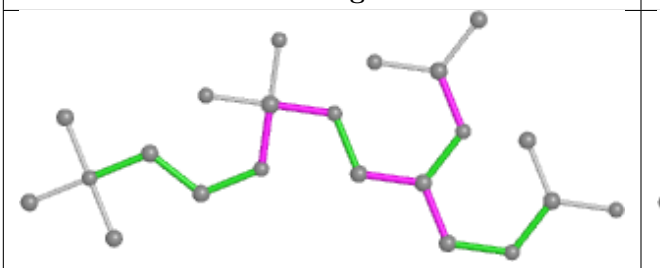
Ligand PCW A 1021



Bond lengths



Bond angles



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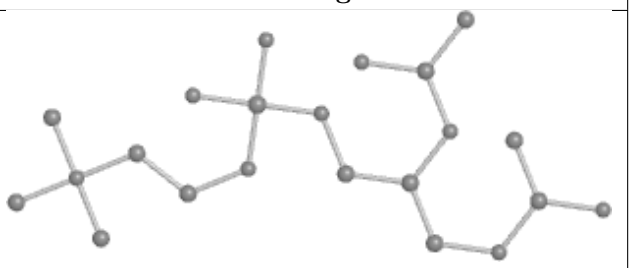
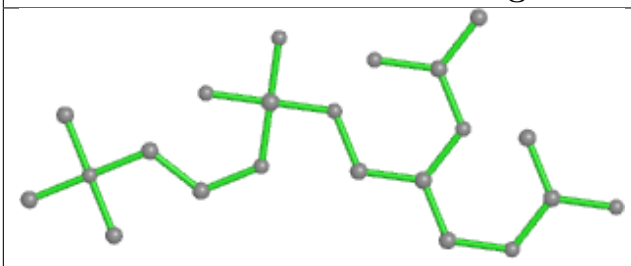
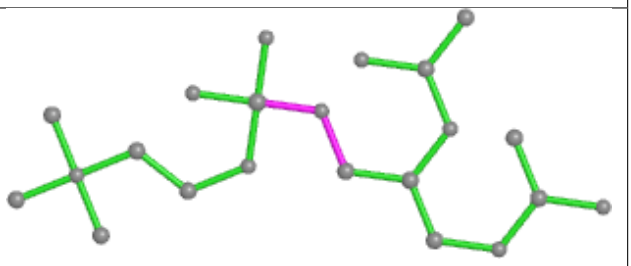


Rings

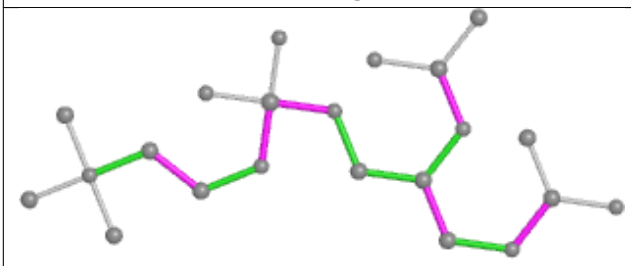
Ligand PCW A 1037



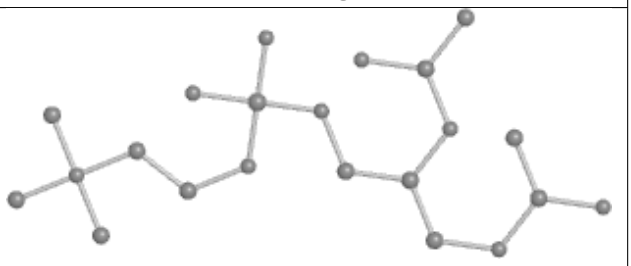
Bond lengths



Bond angles

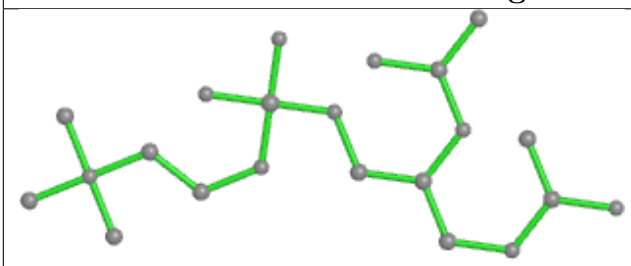


Torsions

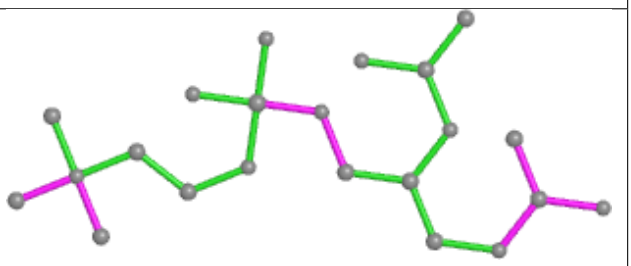


Rings

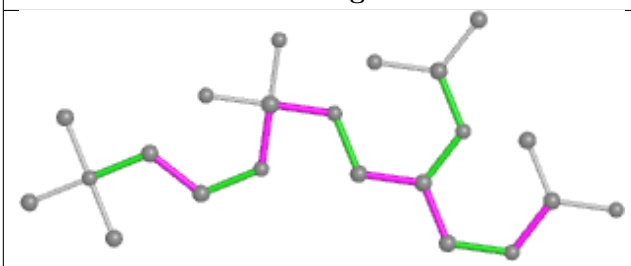
Ligand PCW A 1011



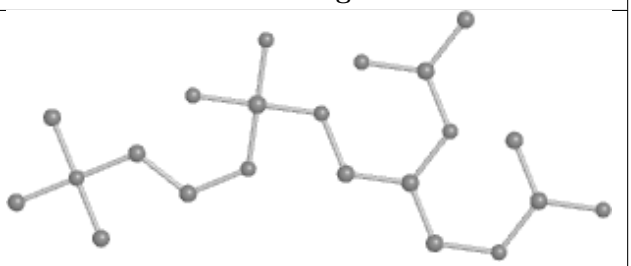
Bond lengths



Bond angles

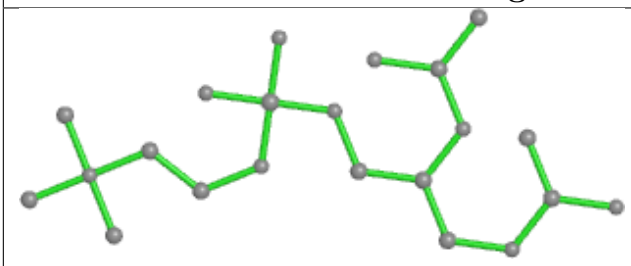


Torsions



Rings

Ligand PCW A 1004



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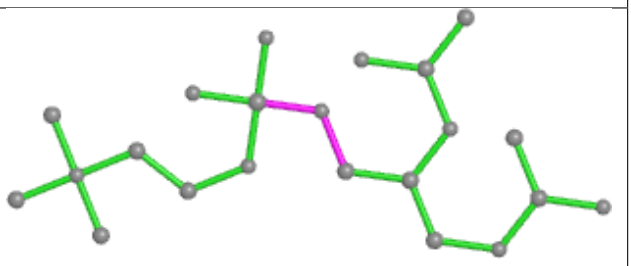
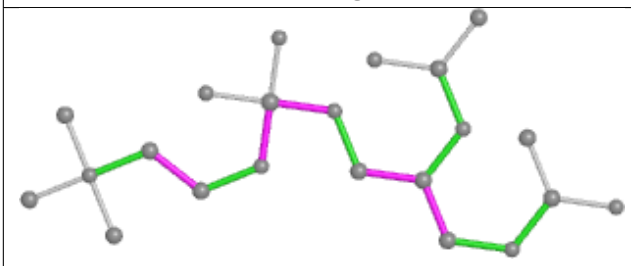


Bond angles



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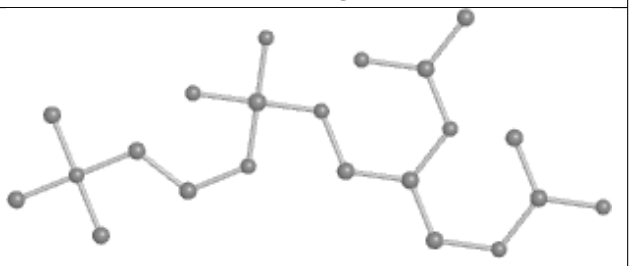
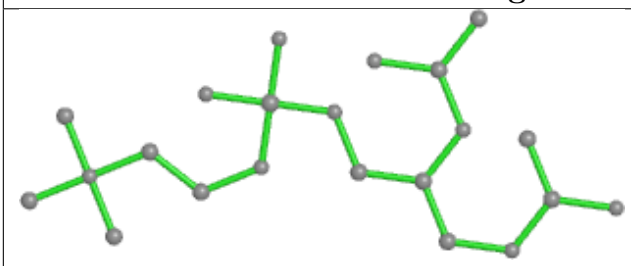


Rings

Ligand PCW A 1008



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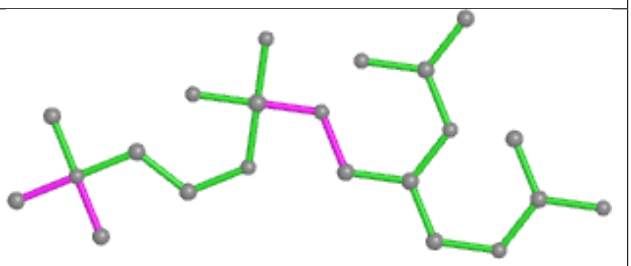

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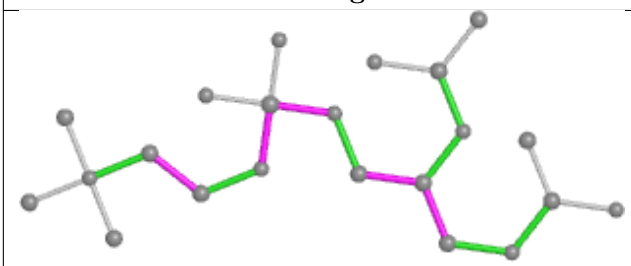

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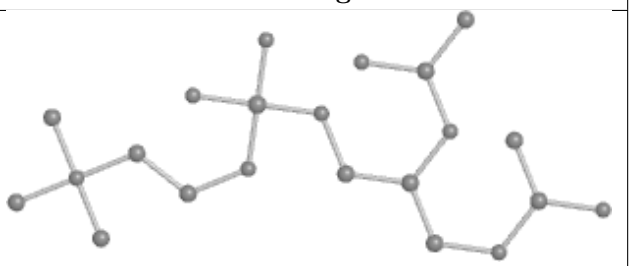
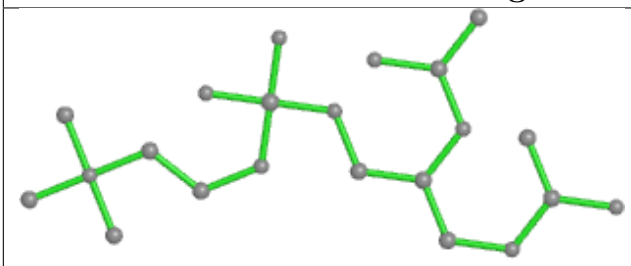


Rings

Ligand PCW A 1019



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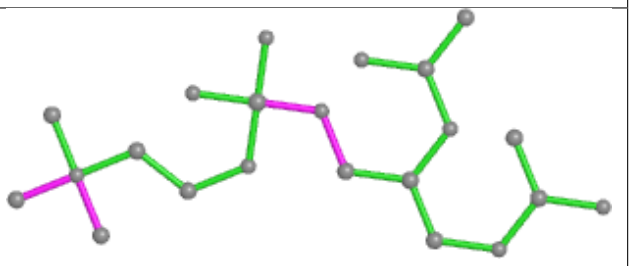

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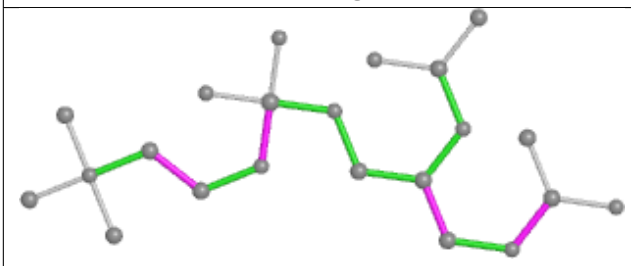

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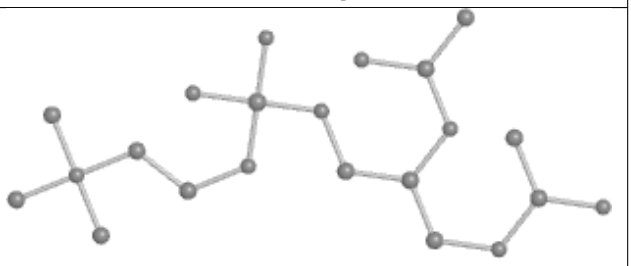
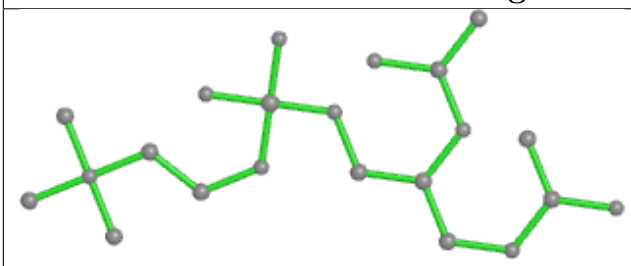


Rings

Ligand PCW A 1029



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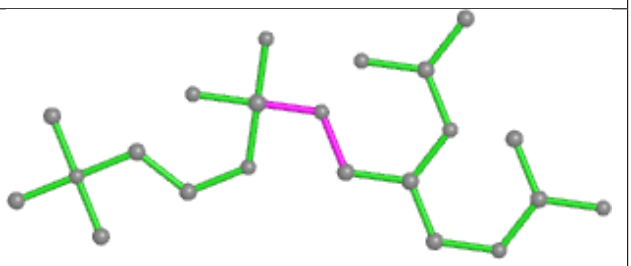
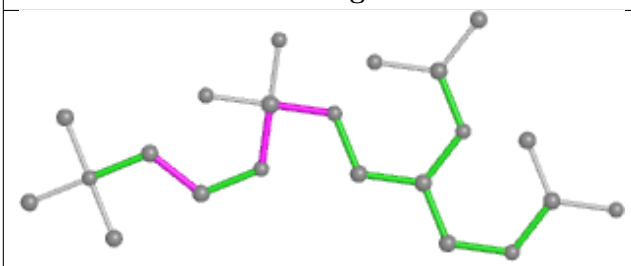


Bond angles



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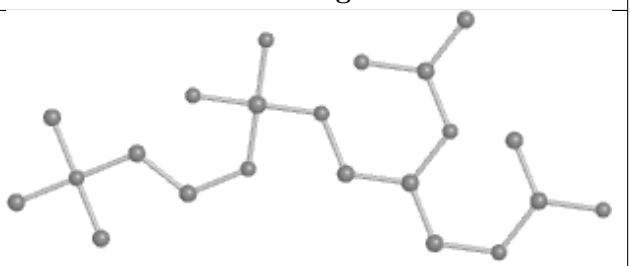
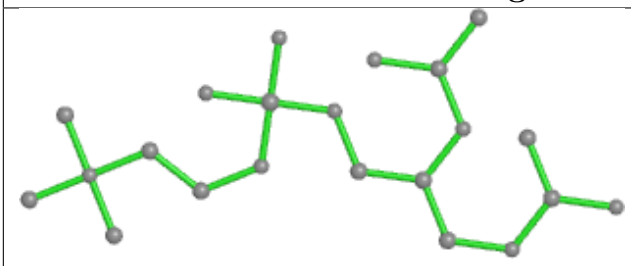


Rings

Ligand PCW A 1027



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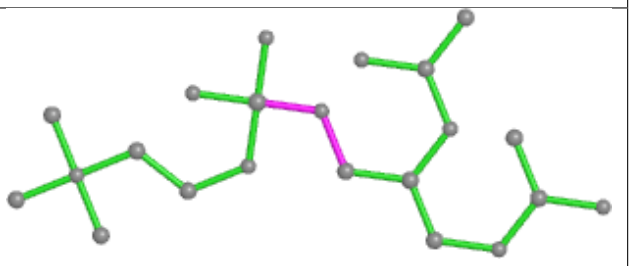
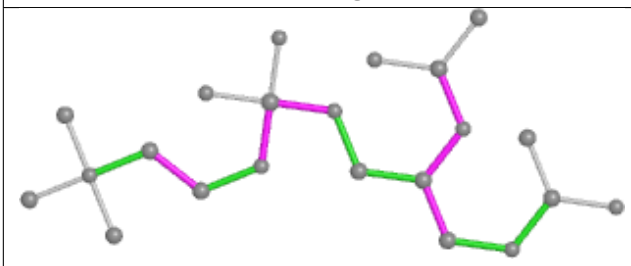


Bond angles



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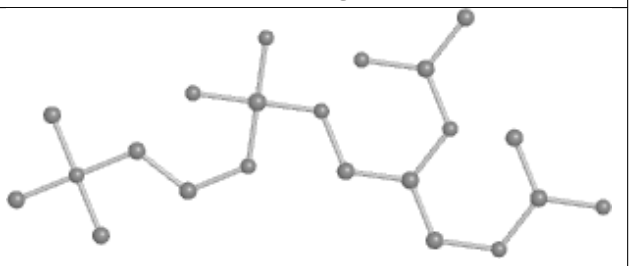
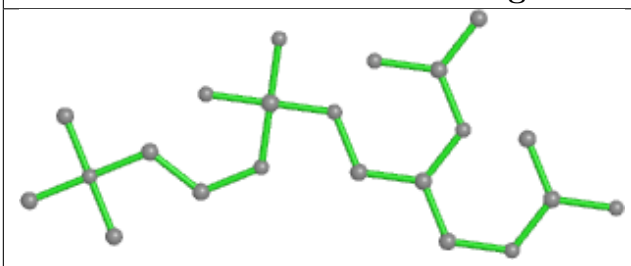


Rings

Ligand PCW A 1024



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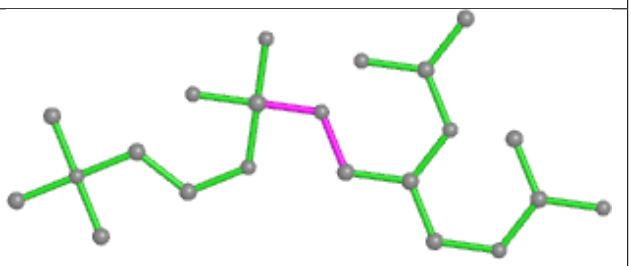
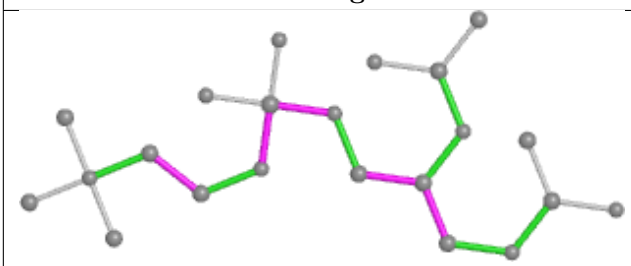


Bond angles



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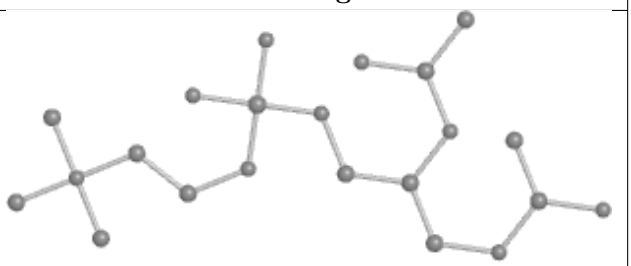
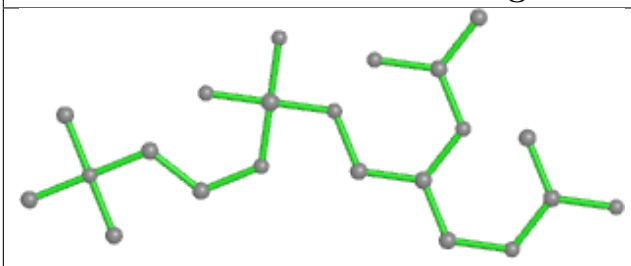


Rings

Ligand PCW A 1016



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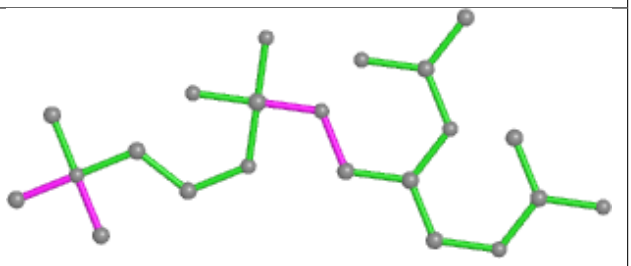

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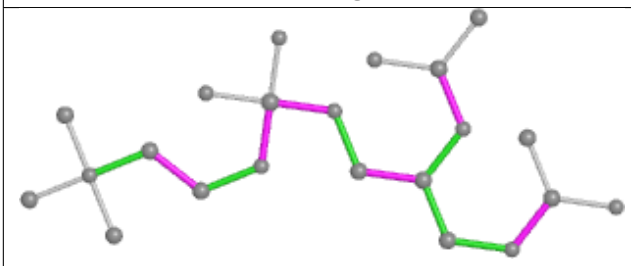

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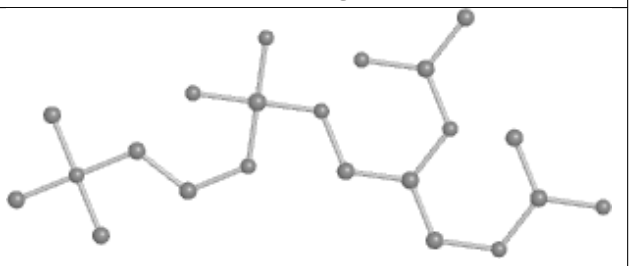
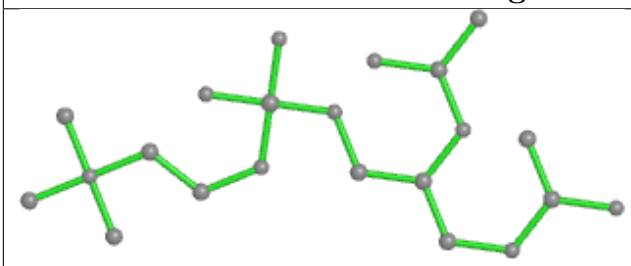


Rings

Ligand PCW A 1023



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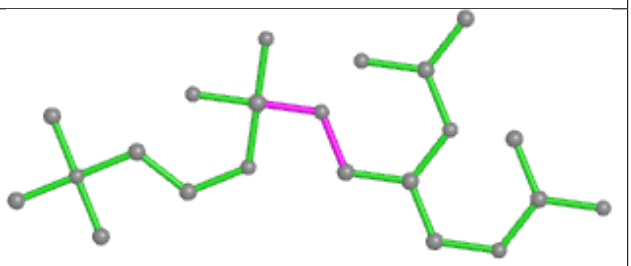
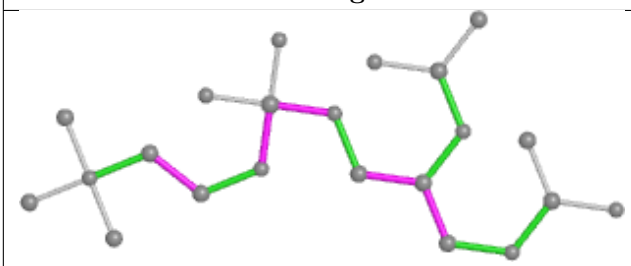
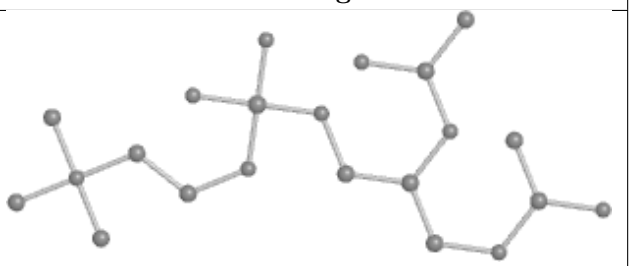


Bond angles

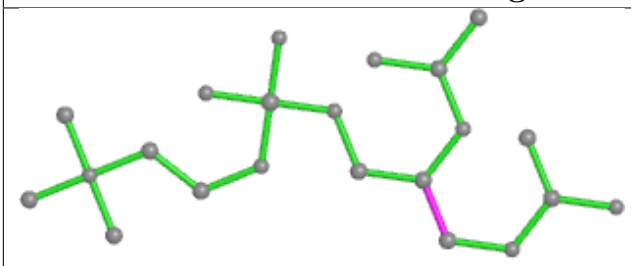


Torsions

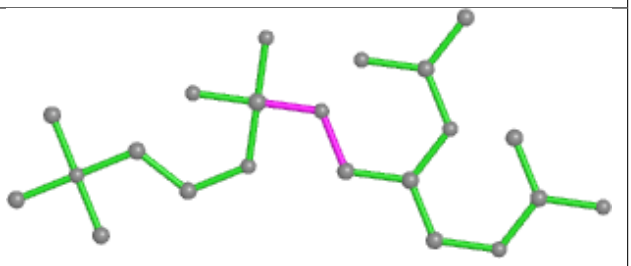


Rings

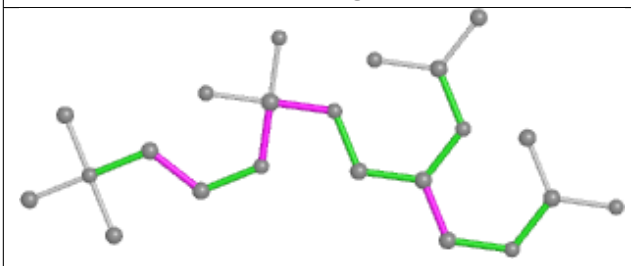
Ligand PCW A 1022



Bond lengths



Bond angles



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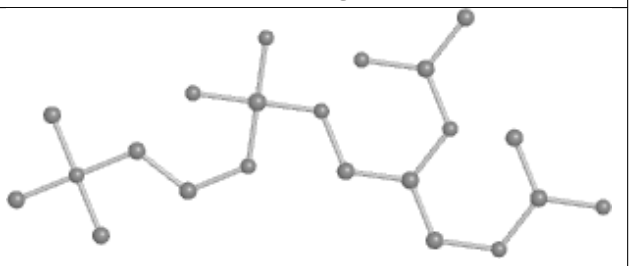
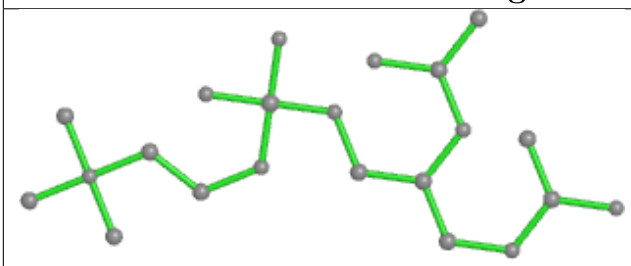
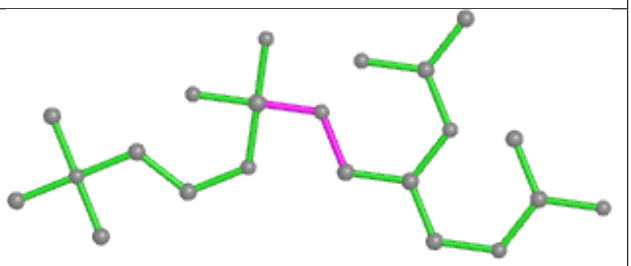


Rings

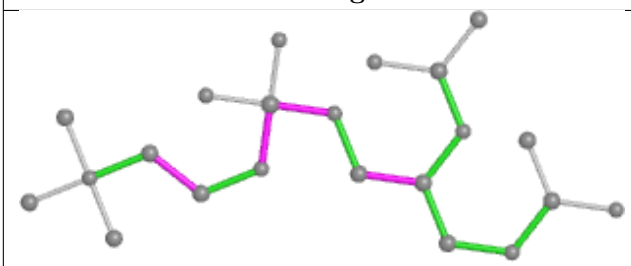
Ligand PCW A 1033



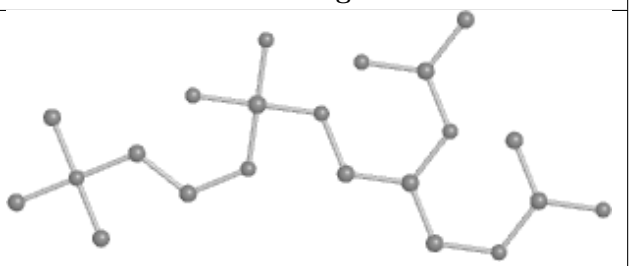
Bond lengths



Bond angles

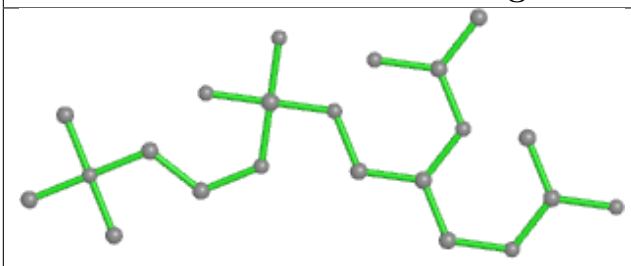


Torsions

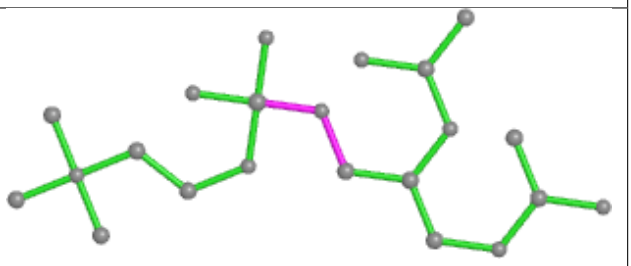


Rings

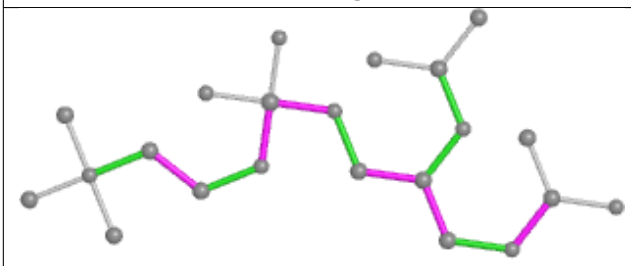
Ligand PCW A 1032



Bond lengths



Bond angles



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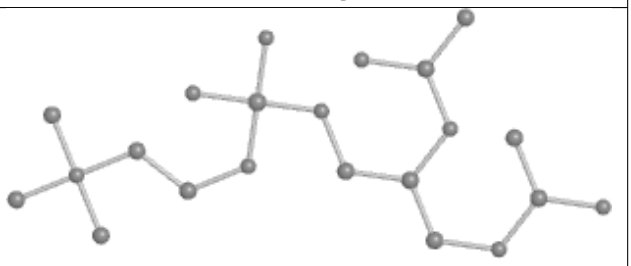
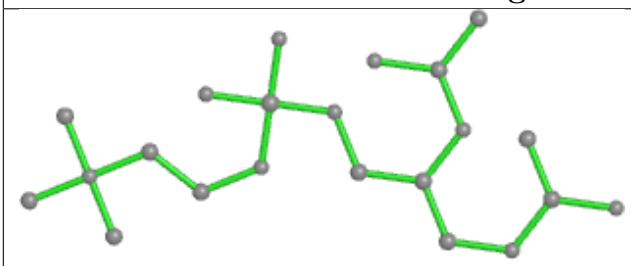
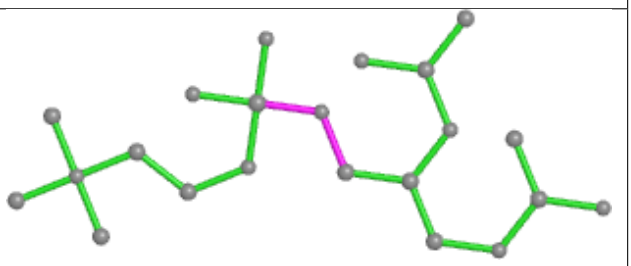


Rings

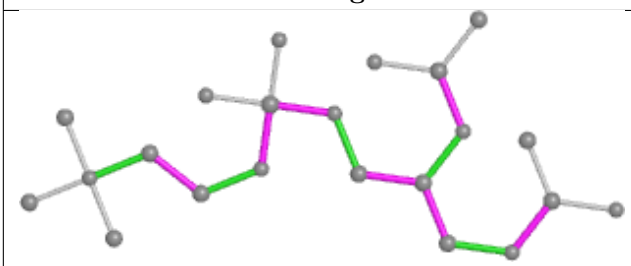
Ligand PCW A 1034



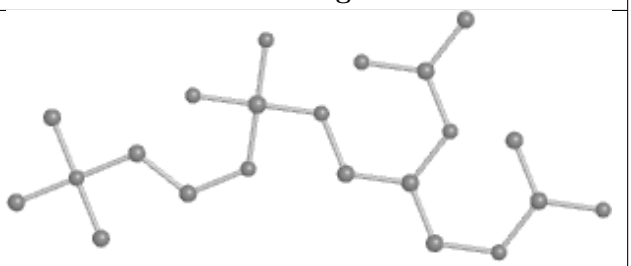
Bond lengths



Bond angles

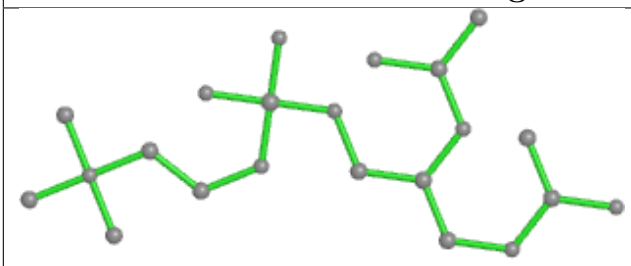


Torsions

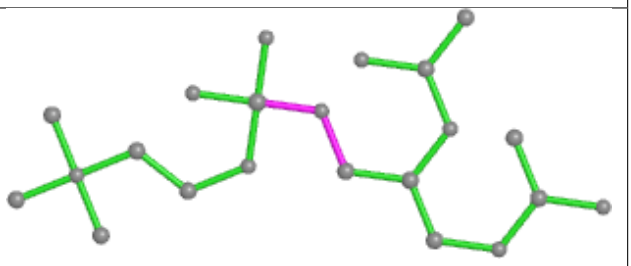


Rings

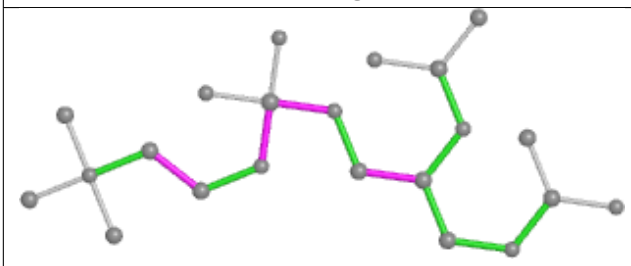
Ligand PCW A 1012



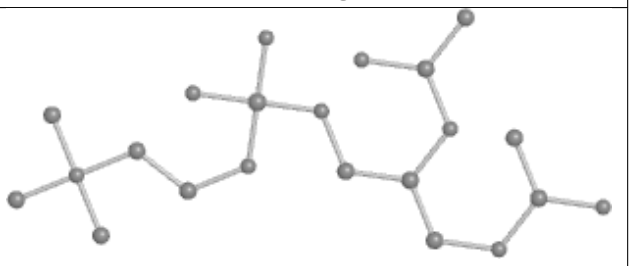
Bond lengths



Bond angles

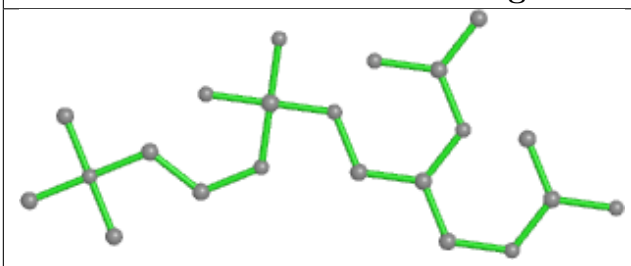


Torsions

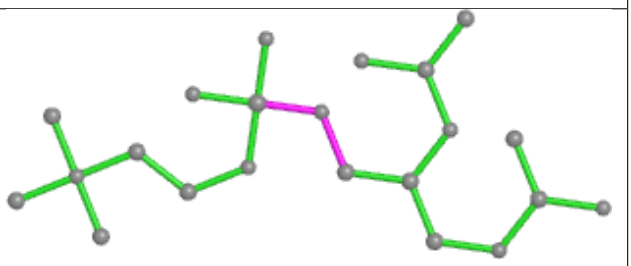


Rings

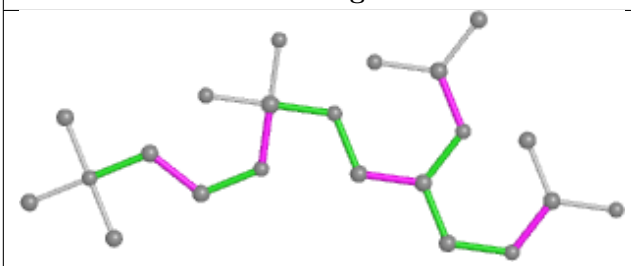
Ligand PCW A 1035



Bond lengths



Bond angles



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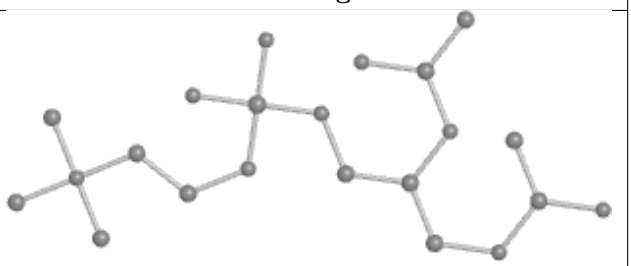
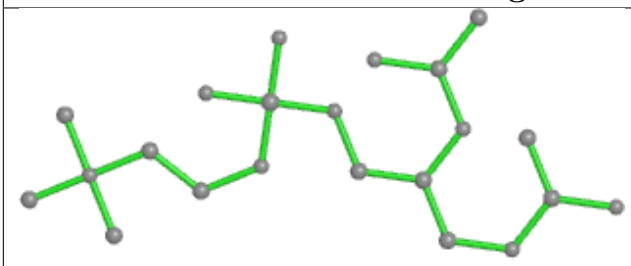


Rings

Ligand PCW A 1025



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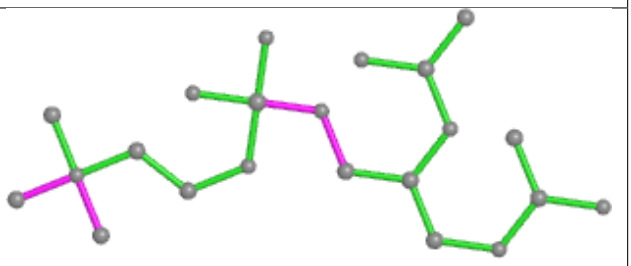

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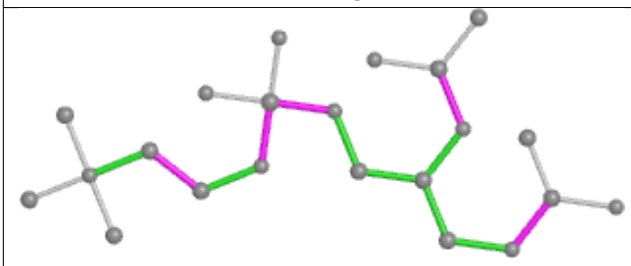

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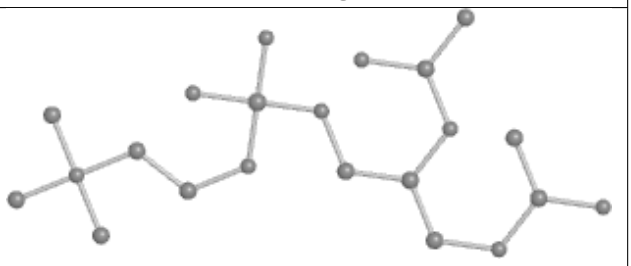
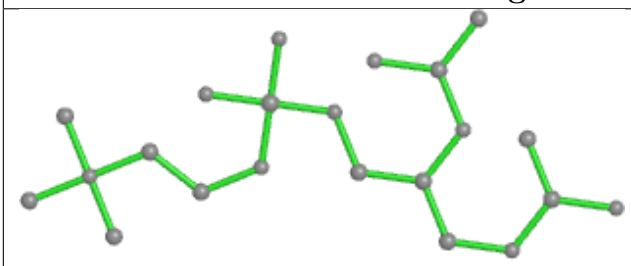
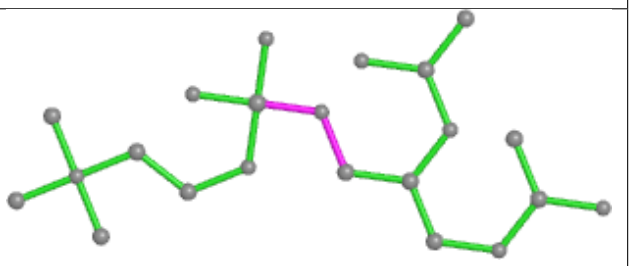


Rings

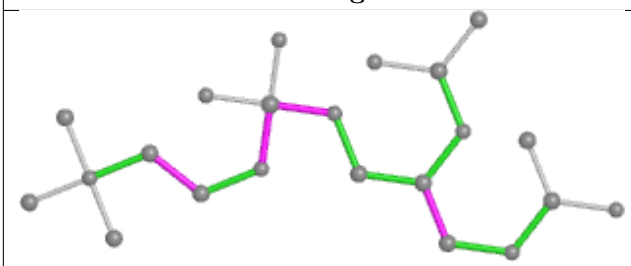
Ligand PCW A 1030



Bond lengths



Bond angles



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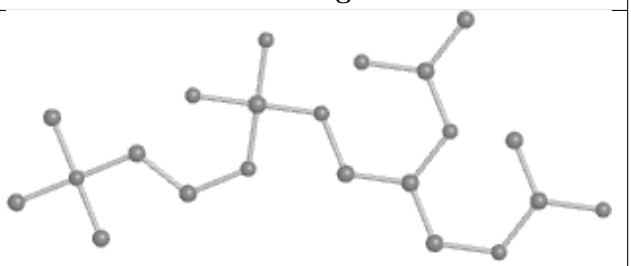
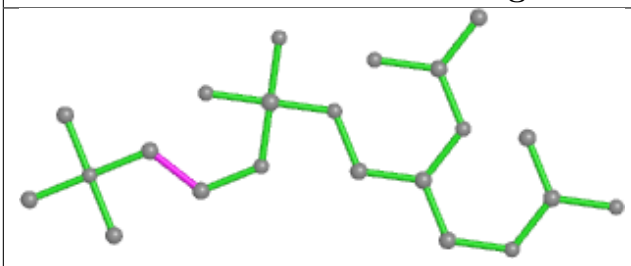


Rings

Ligand PCW A 1007



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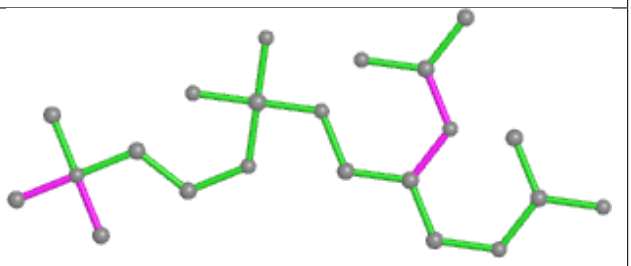
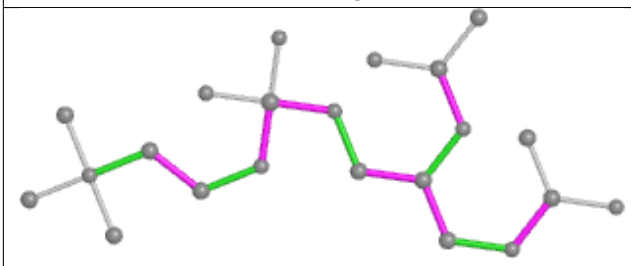
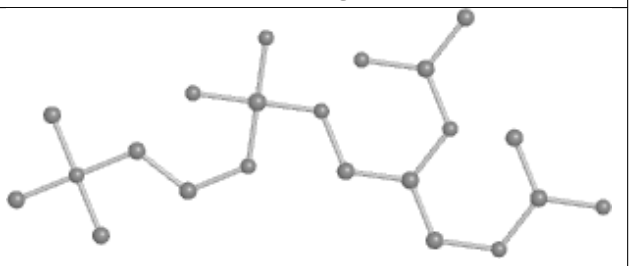


Bond angles

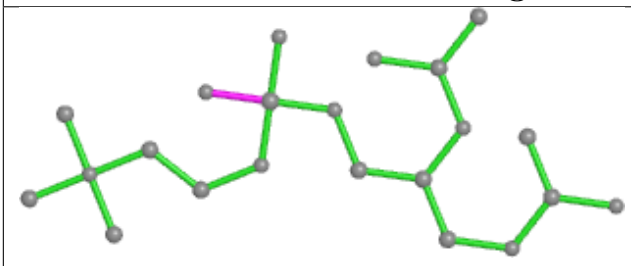


Torsions



Rings

Ligand PCW A 1006



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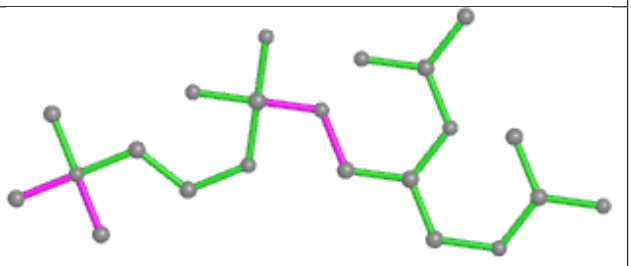
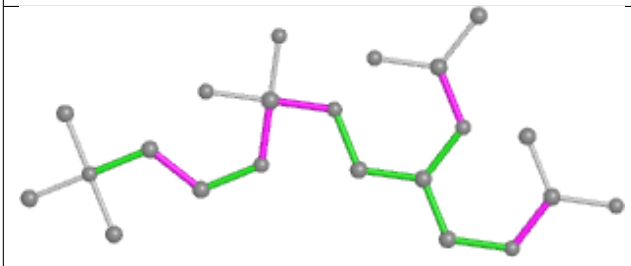
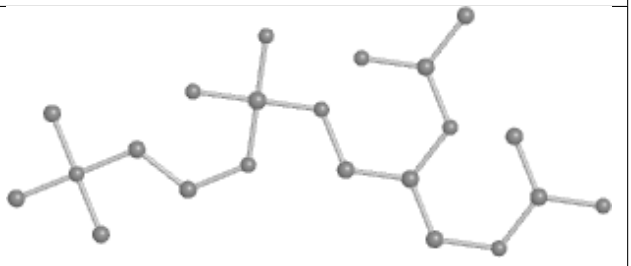


Bond angles

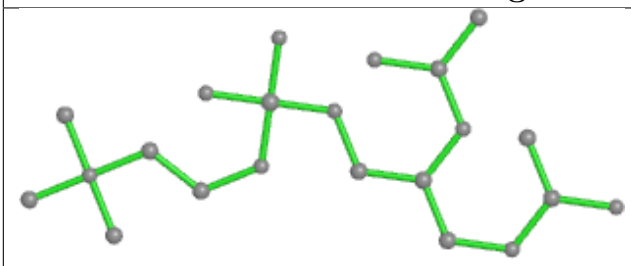


Torsions

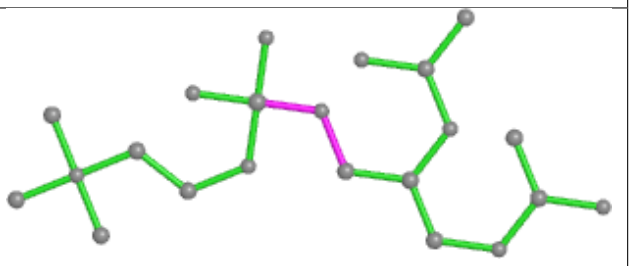


Rings

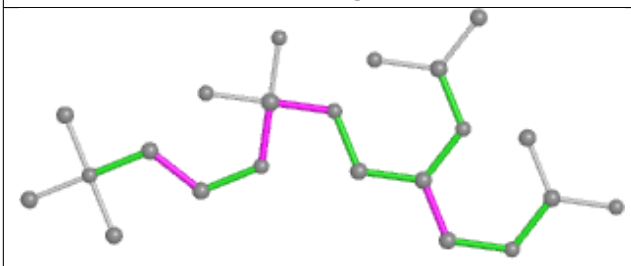
Ligand PCW A 1018



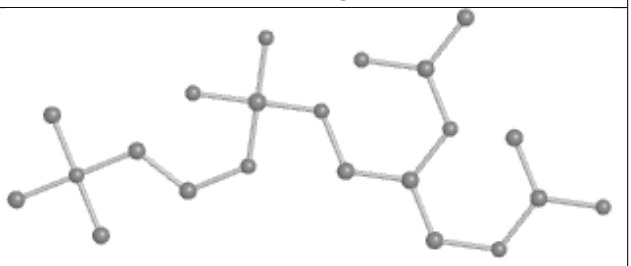
Bond lengths



Bond angles

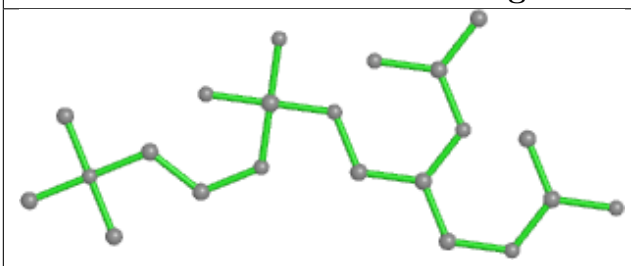


Torsions

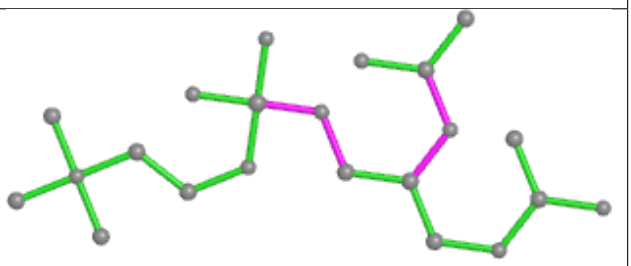


Rings

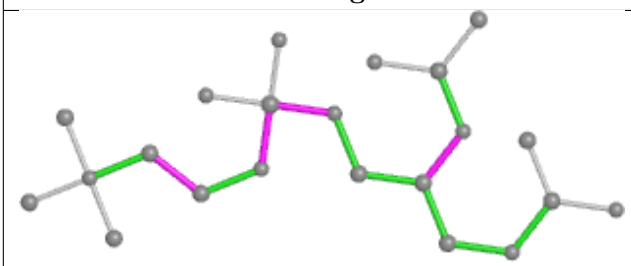
Ligand PCW A 1028



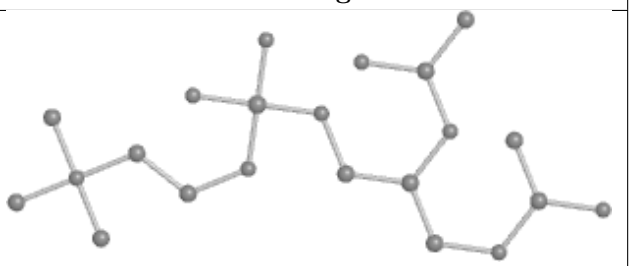
Bond lengths



Bond angles

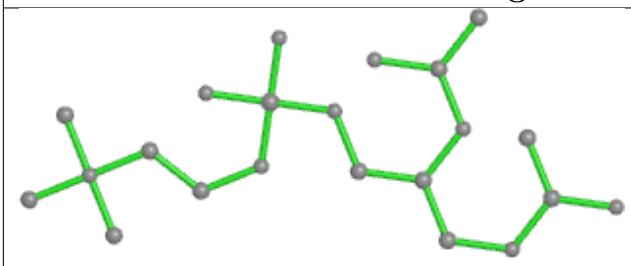


Torsions

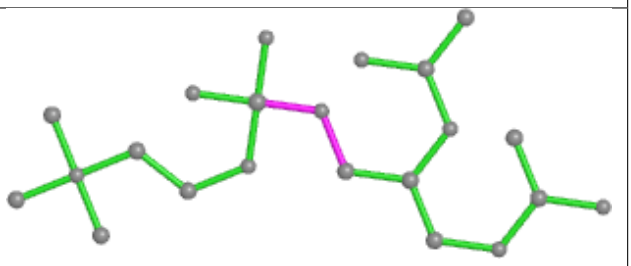


Rings

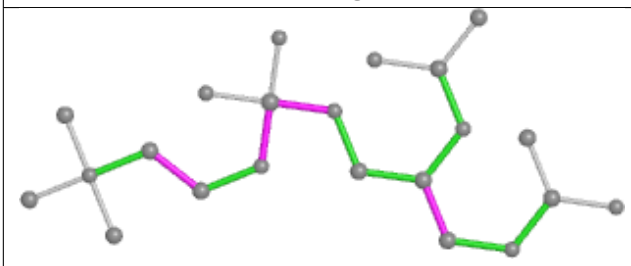
Ligand PCW A 1036



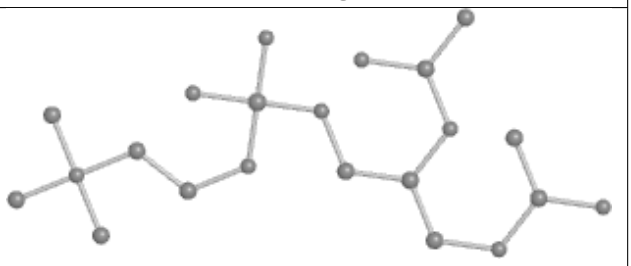
Bond lengths



Bond angles

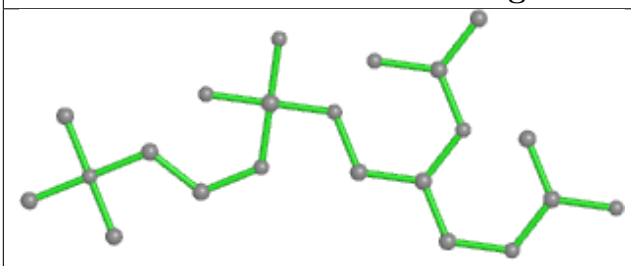


Torsions

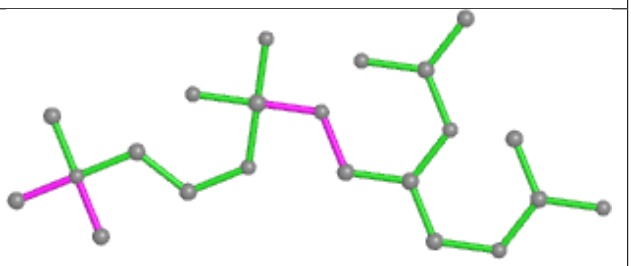


Rings

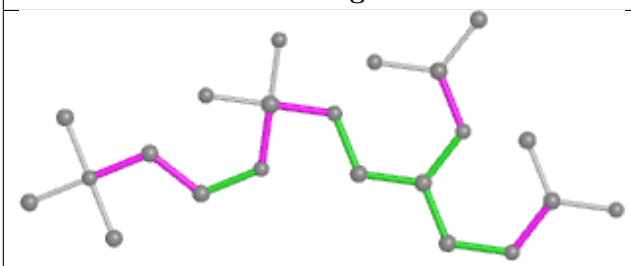
Ligand PCW A 1013



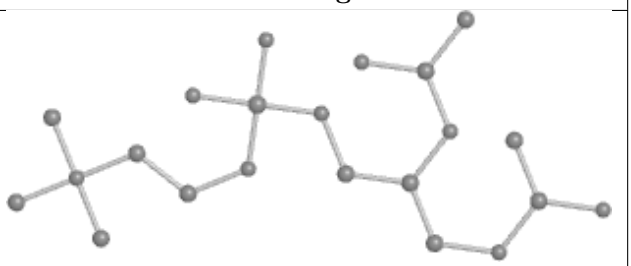
Bond lengths



Bond angles

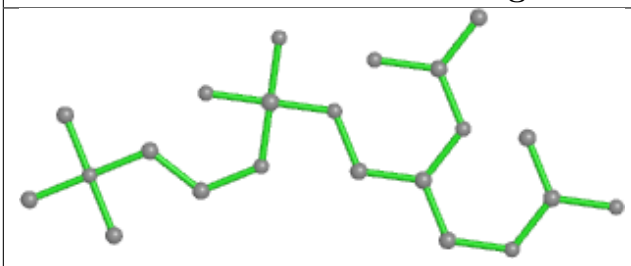


Torsions

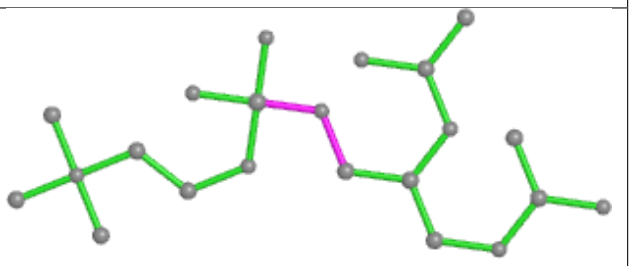


Rings

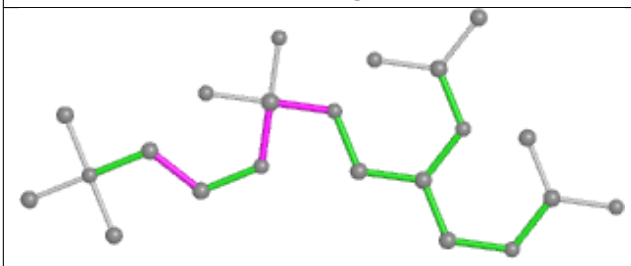
Ligand PCW A 1020



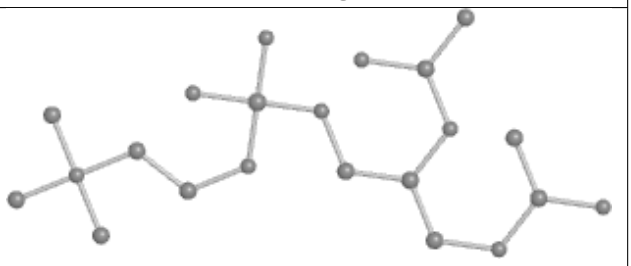
Bond lengths



Bond angles

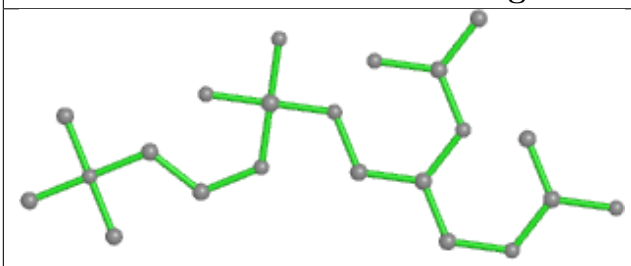


Torsions

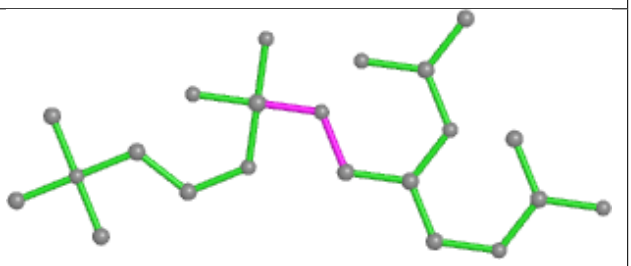


Rings

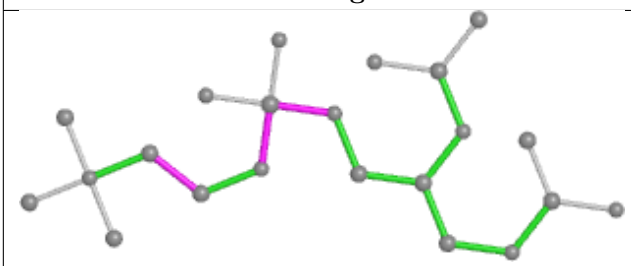
Ligand PCW A 1009



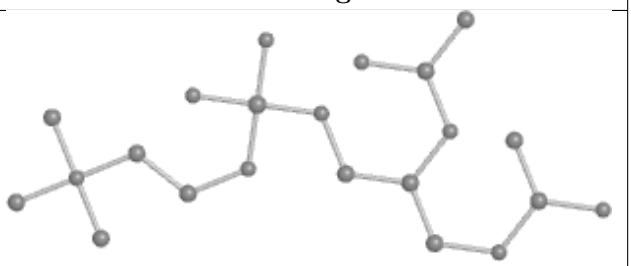
Bond lengths



Bond angles

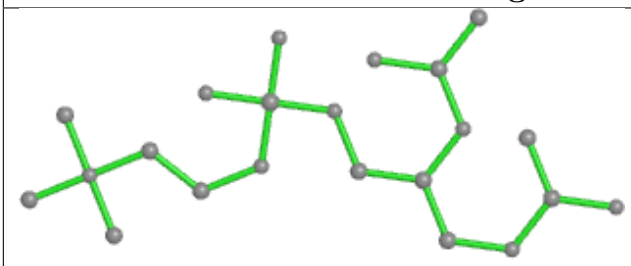


Torsions

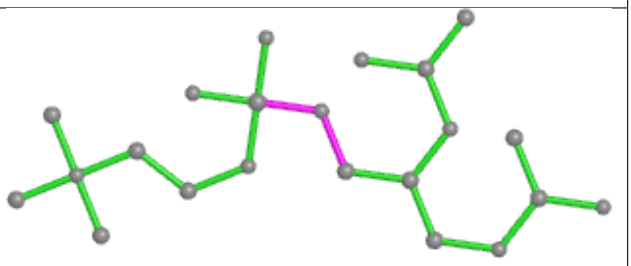


Rings

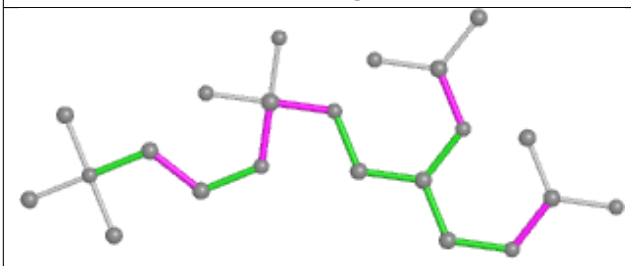
Ligand PCW A 1031



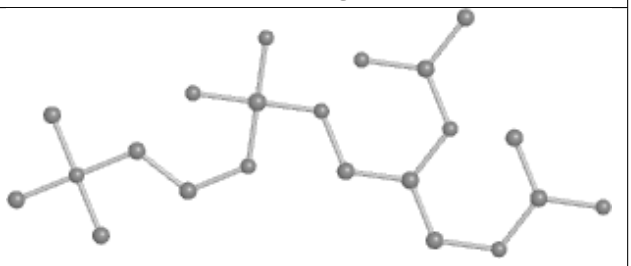
Bond lengths



Bond angles

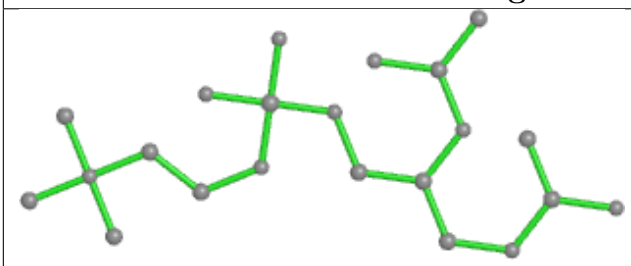


Torsions

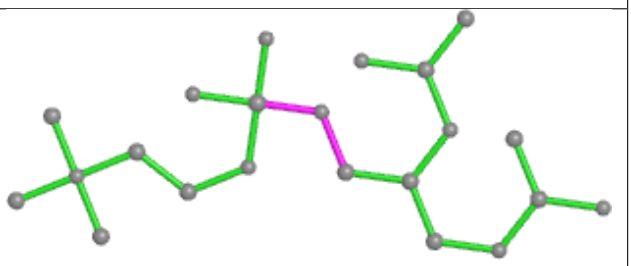


Rings

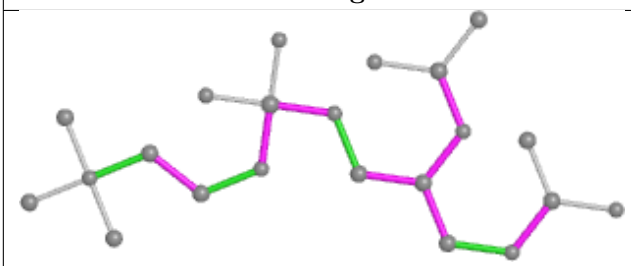
Ligand PCW A 1014



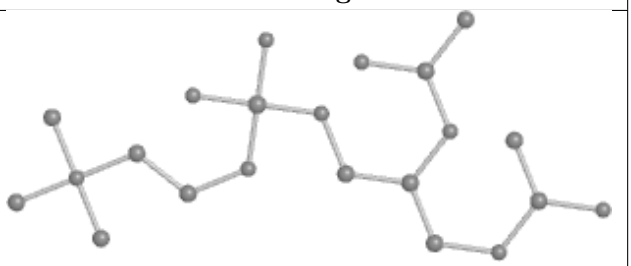
Bond lengths



Bond angles

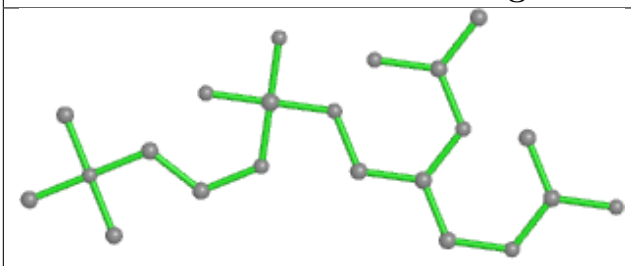


Torsions

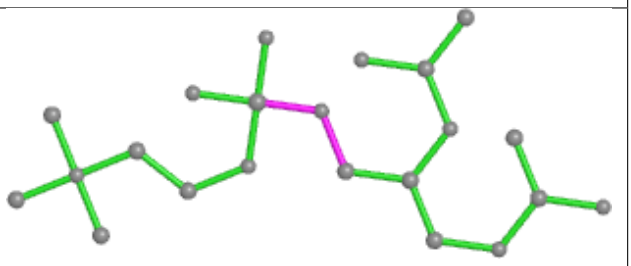


Rings

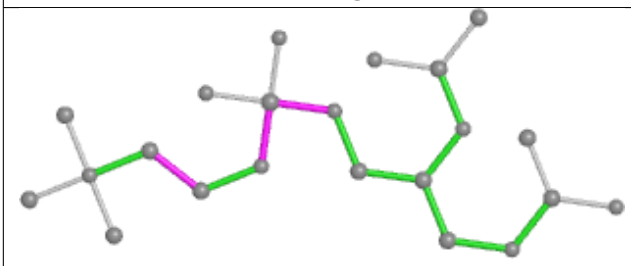
Ligand PCW A 1026



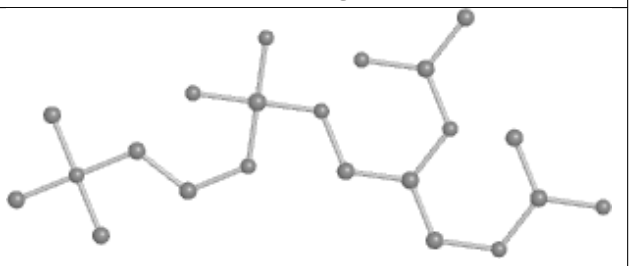
Bond lengths



Bond angles

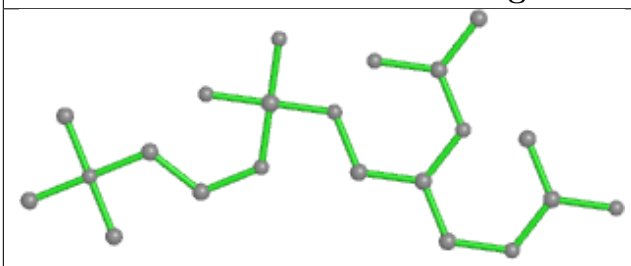


Torsions

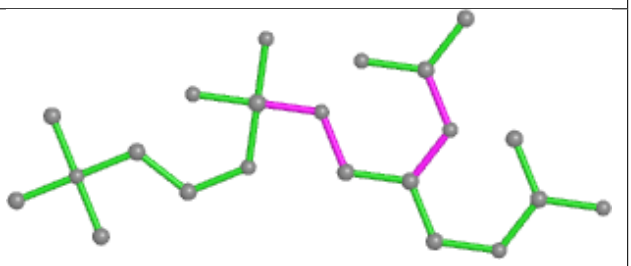


Rings

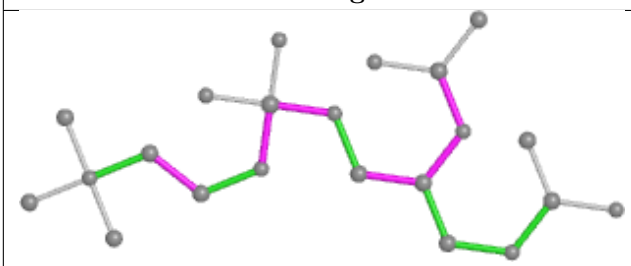
Ligand PCW A 1005



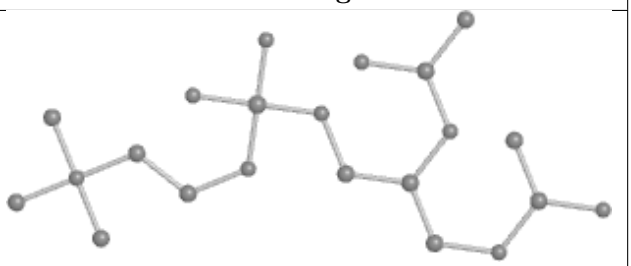
Bond lengths



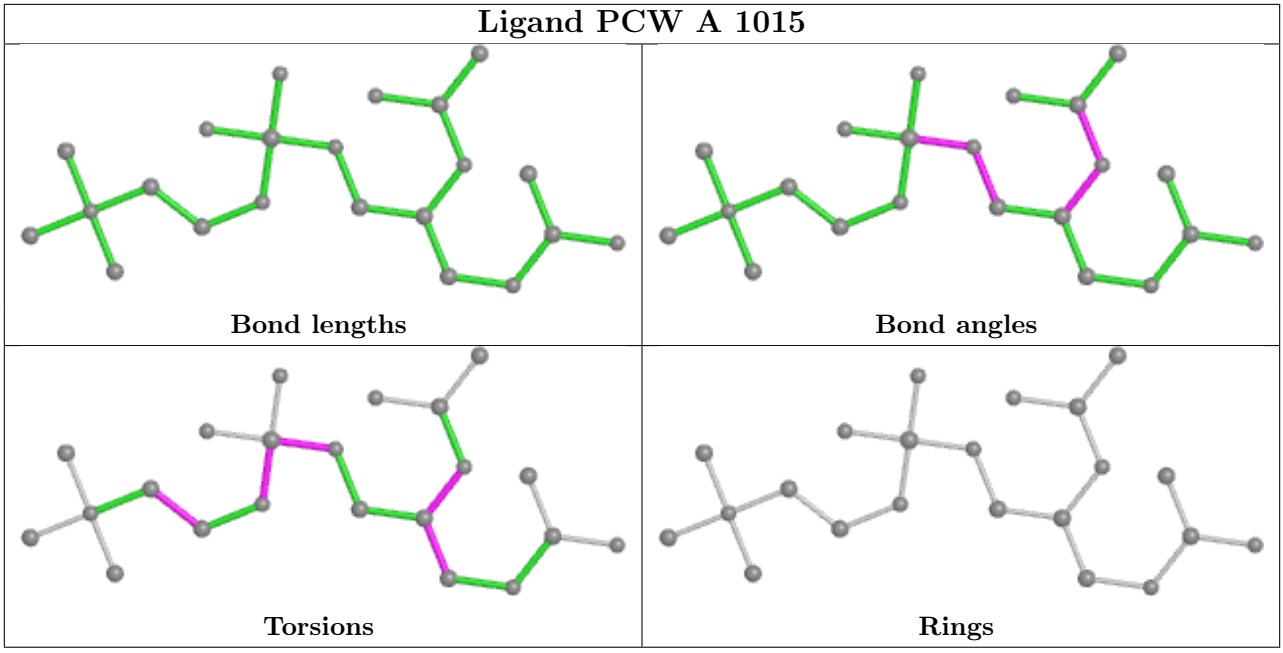
Bond angles

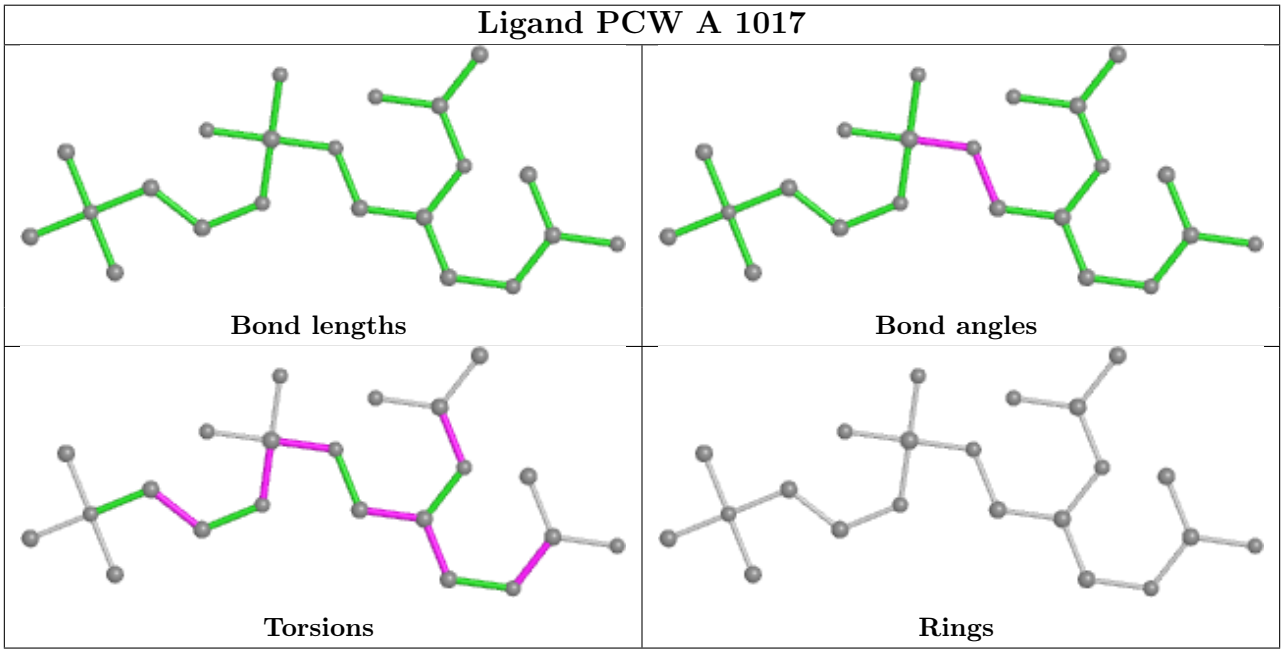


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	994/995 (99%)	-0.07	13 (1%)	77	65	21, 61, 134, 202	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	884	GLU	3.7
1	A	887	ASP	3.4
1	A	46	GLY	3.3
1	A	885	GLY	3.2
1	A	994	GLY	2.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PCW	A	1009	22/54	0.09	0.88	219,219,219,219	0
4	PCW	A	1017	22/54	0.12	1.20	212,212,212,212	0

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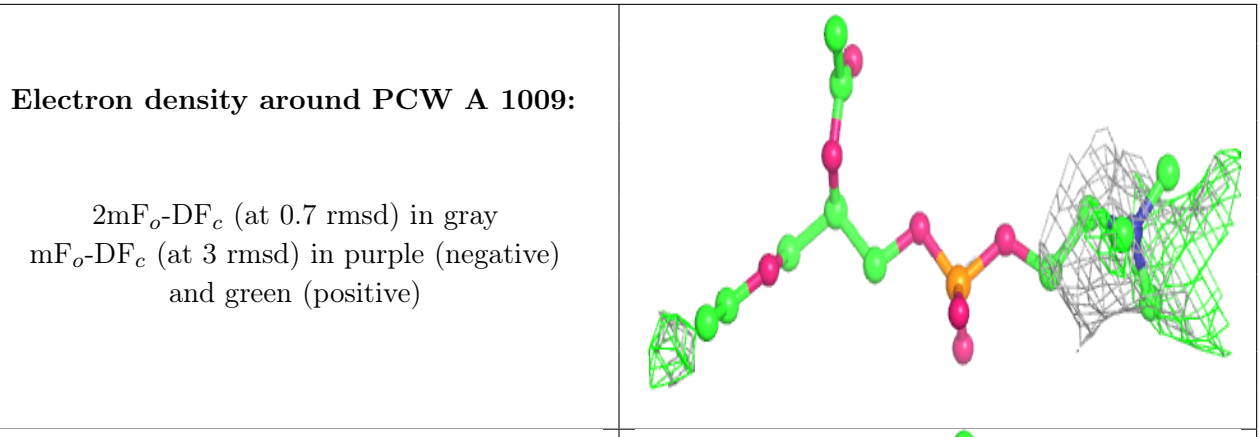
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PCW	A	1034	22/54	0.14	0.99	238,238,238,238	0
4	PCW	A	1010	22/54	0.26	0.75	195,195,195,195	0
4	PCW	A	1028	22/54	0.27	1.14	192,192,192,192	0
4	PCW	A	1035	22/54	0.28	0.70	208,208,208,208	0
4	PCW	A	1018	22/54	0.29	0.72	164,164,164,164	0
4	PCW	A	1029	22/54	0.29	1.19	191,191,191,191	0
4	PCW	A	1014	22/54	0.30	0.78	218,218,218,218	0
4	PCW	A	1026	22/54	0.34	0.87	205,205,205,205	0
4	PCW	A	1023	22/54	0.35	0.51	228,228,228,228	0
4	PCW	A	1012	22/54	0.36	0.79	190,190,190,190	0
4	PCW	A	1015	22/54	0.37	0.69	181,181,181,181	0
4	PCW	A	1032	22/54	0.37	1.02	186,186,186,186	0
4	PCW	A	1030	22/54	0.39	0.74	189,189,189,189	0
4	PCW	A	1013	22/54	0.41	0.45	191,191,191,191	0
4	PCW	A	1033	22/54	0.41	1.16	224,224,224,224	0
4	PCW	A	1016	22/54	0.43	0.56	176,176,176,176	0
4	PCW	A	1024	22/54	0.48	0.60	206,206,206,206	0
4	PCW	A	1008	22/54	0.49	0.74	185,185,185,185	0
4	PCW	A	1021	22/54	0.49	0.54	179,179,179,179	0
4	PCW	A	1037	22/54	0.50	0.61	195,195,195,195	0
4	PCW	A	1022	22/54	0.51	0.59	181,181,181,181	0
4	PCW	A	1027	22/54	0.54	0.56	220,220,220,220	0
4	PCW	A	1031	22/54	0.55	0.58	221,221,221,221	0
4	PCW	A	1019	22/54	0.55	0.47	203,203,203,203	0
4	PCW	A	1004	22/54	0.56	0.92	206,206,206,206	0
4	PCW	A	1006	22/54	0.57	0.70	173,173,173,173	0
4	PCW	A	1005	22/54	0.57	0.63	218,218,218,218	0
4	PCW	A	1020	22/54	0.57	0.47	208,208,208,208	0
4	PCW	A	1025	22/54	0.60	0.52	198,198,198,198	0
4	PCW	A	1007	22/54	0.73	0.37	139,139,139,139	0
4	PCW	A	1011	22/54	0.79	0.31	125,125,125,125	0
4	PCW	A	1036	22/54	0.83	0.26	136,136,136,136	0
2	CA	A	1002	1/1	0.94	0.09	39,39,39,39	0
3	NA	A	1003	1/1	0.97	0.09	32,32,32,32	0
2	CA	A	1001	1/1	0.98	0.15	37,37,37,37	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.

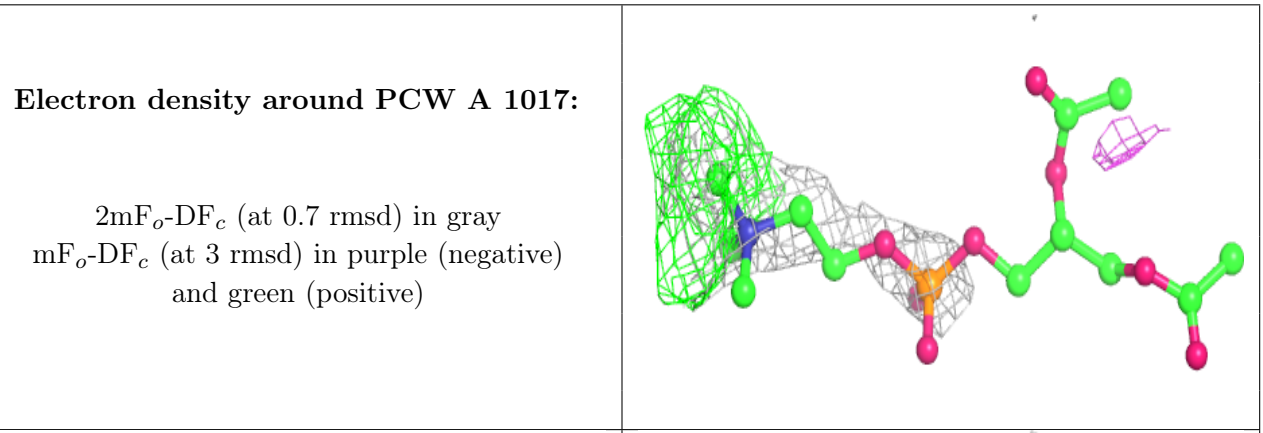
Electron density around PCW A 1009:

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



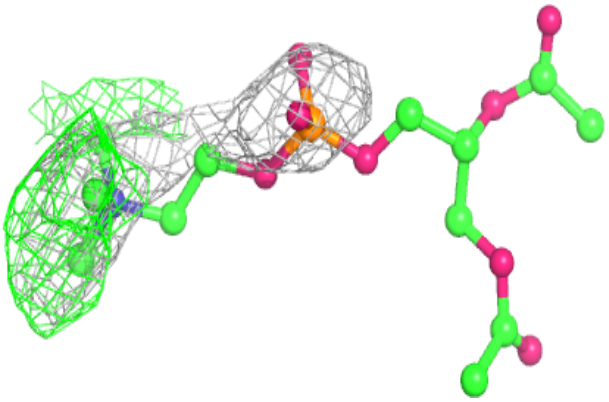
Electron density around PCW A 1017:

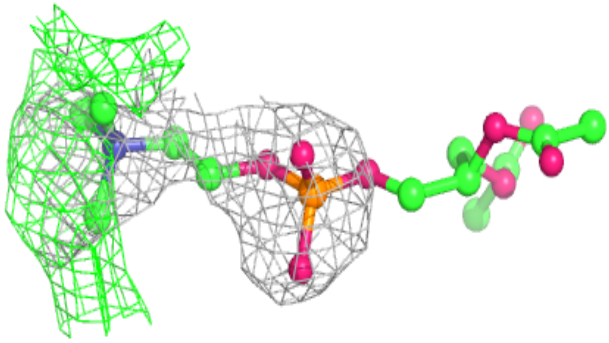
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

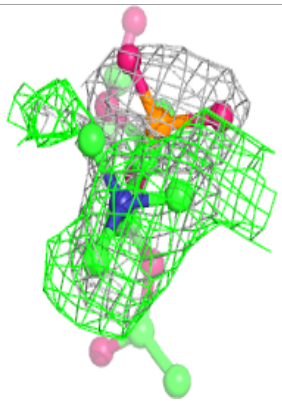


Electron density around PCW A 1034:

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

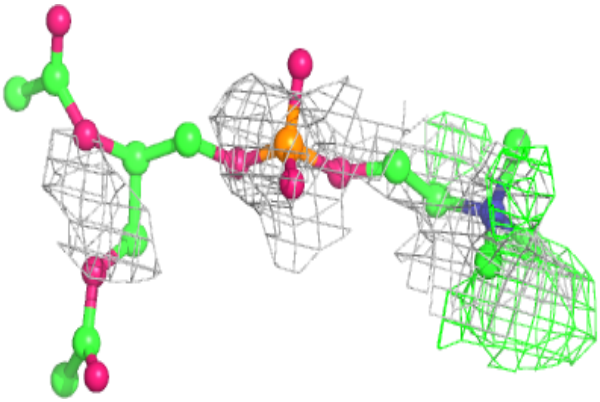


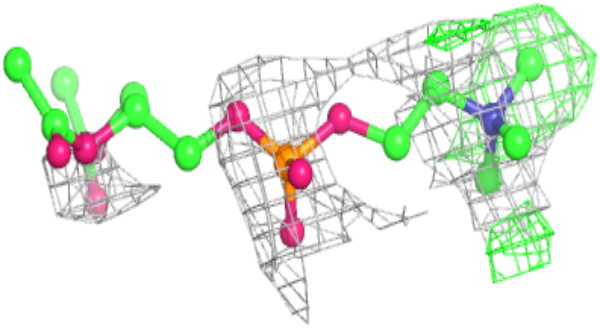


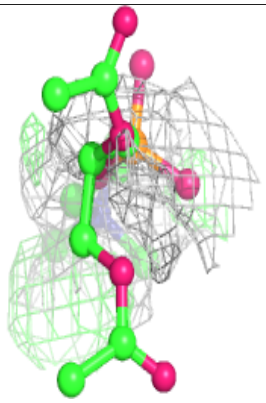


Electron density around PCW A 1010:

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

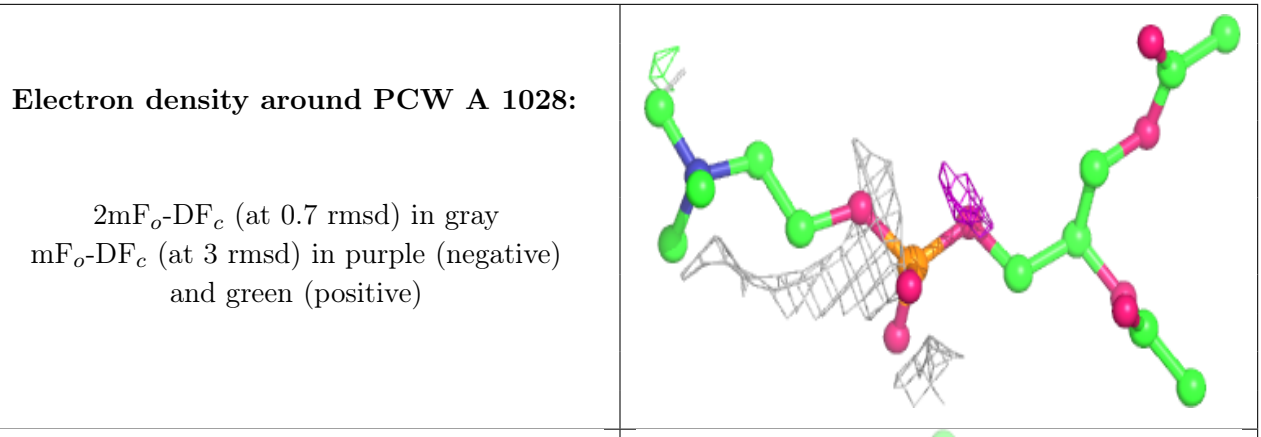






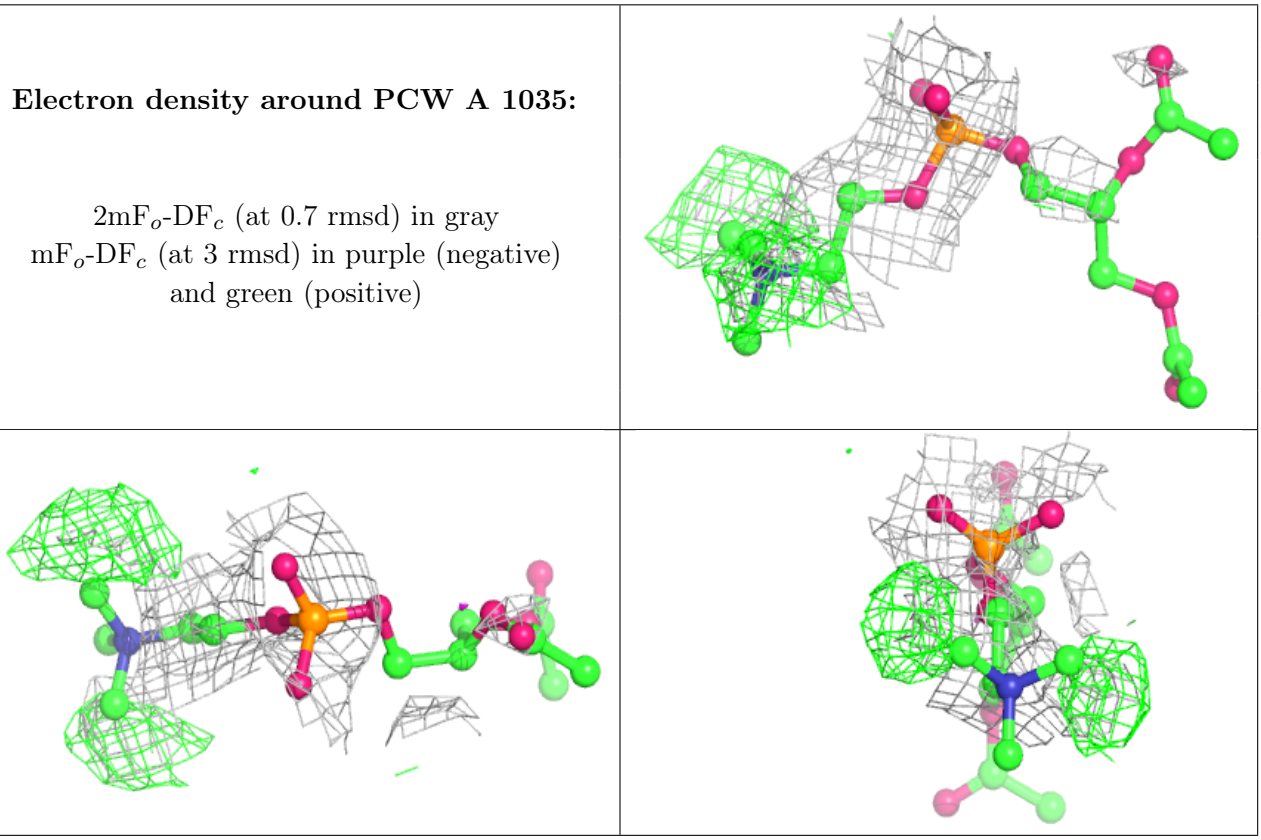
Electron density around PCW A 1028:

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



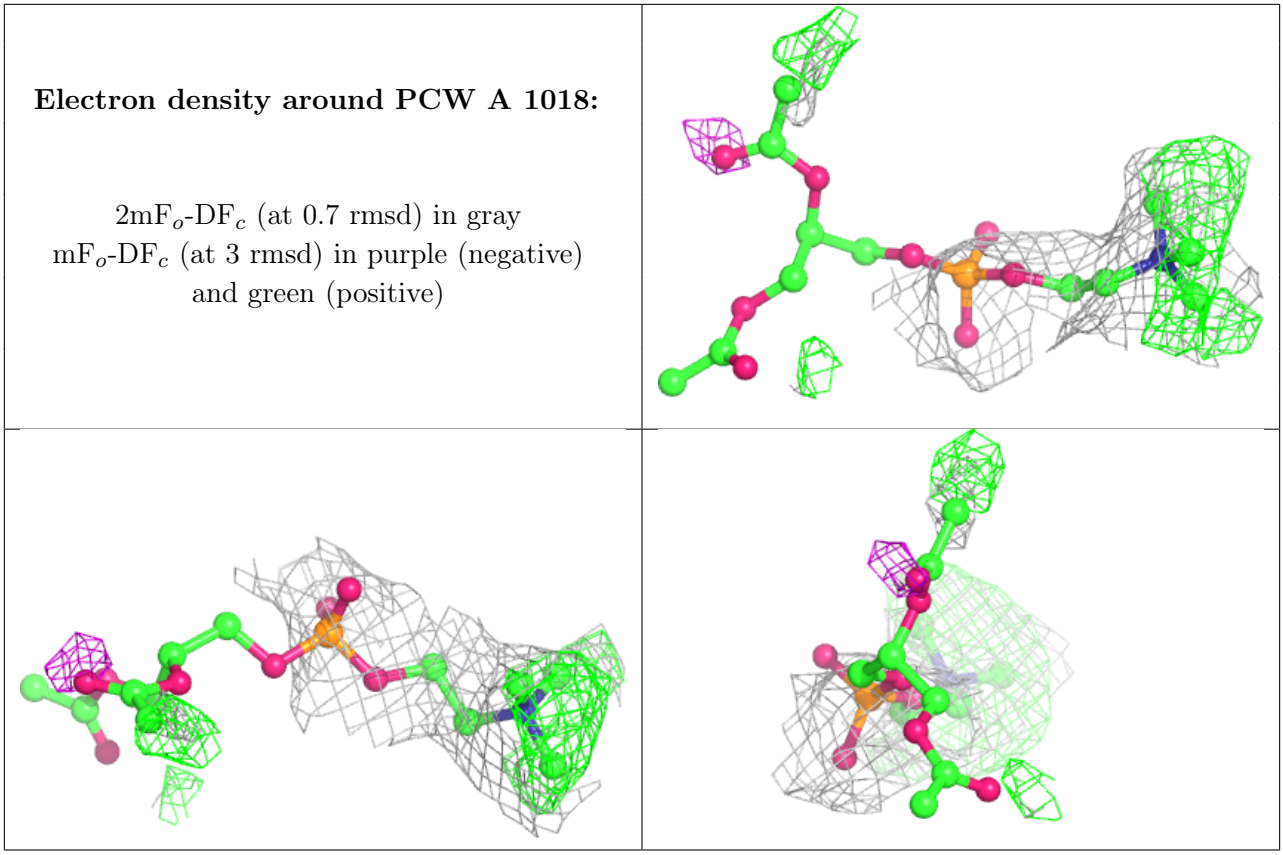
Electron density around PCW A 1035:

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



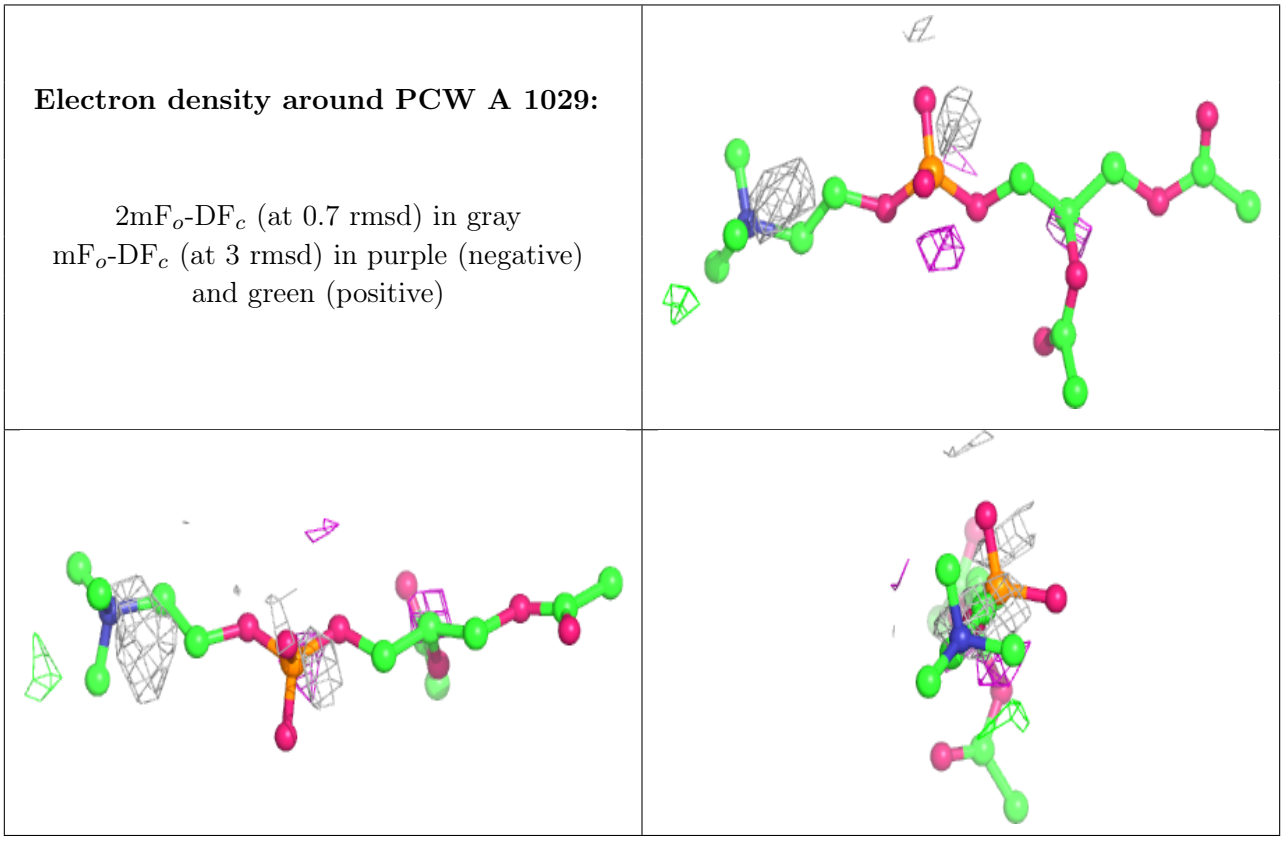
Electron density around PCW A 1018:

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



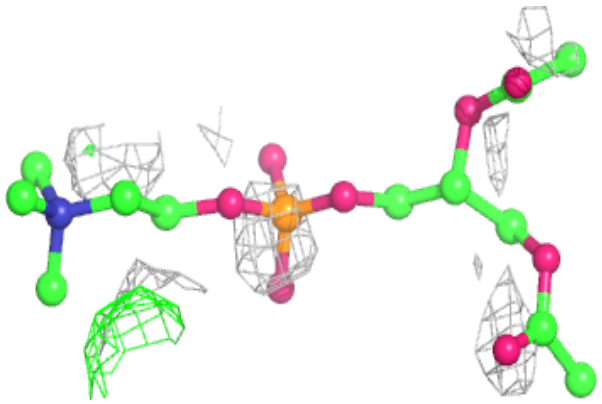
Electron density around PCW A 1029:

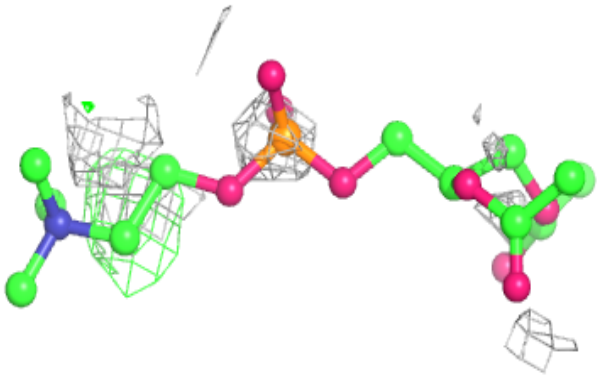
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PCW A 1014:

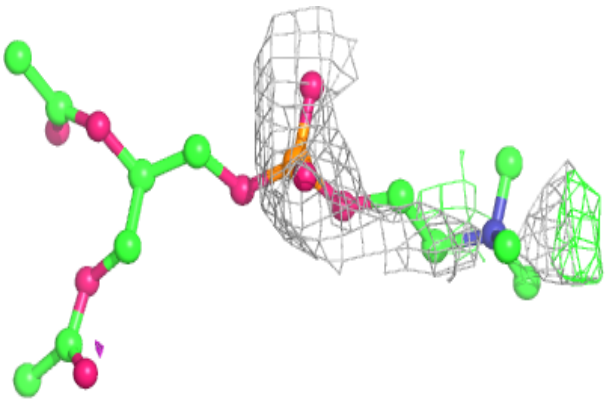
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

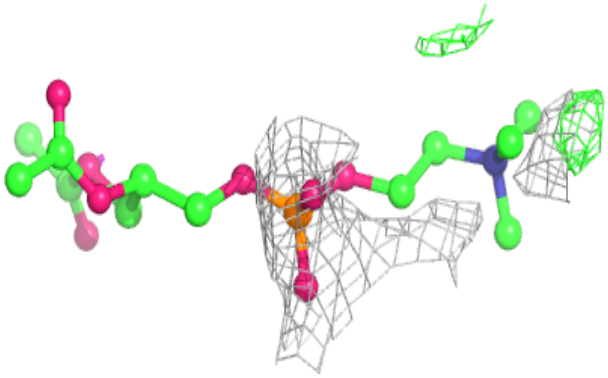


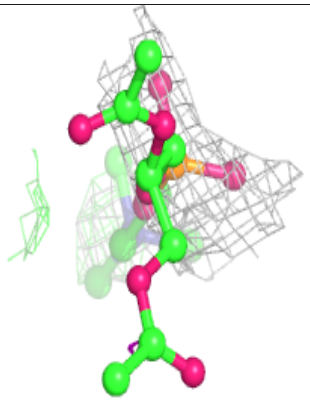


Electron density around PCW A 1026:

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

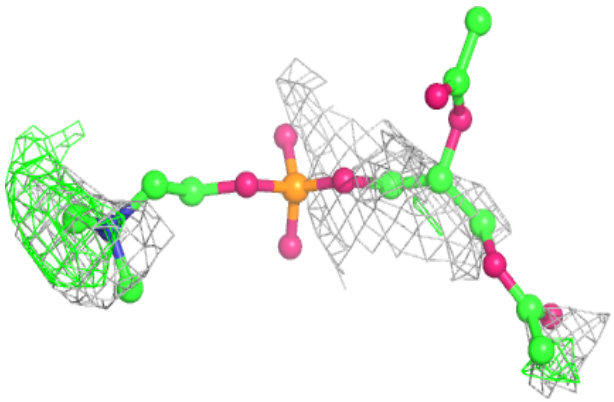


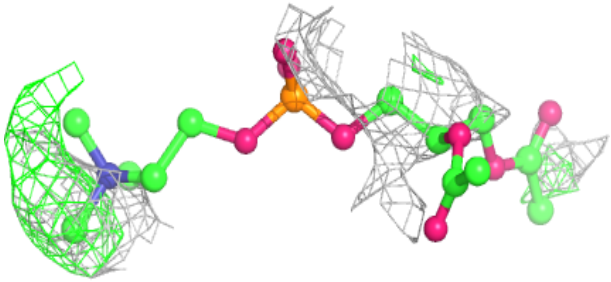


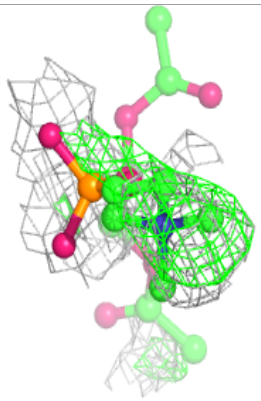


Electron density around PCW A 1023:

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

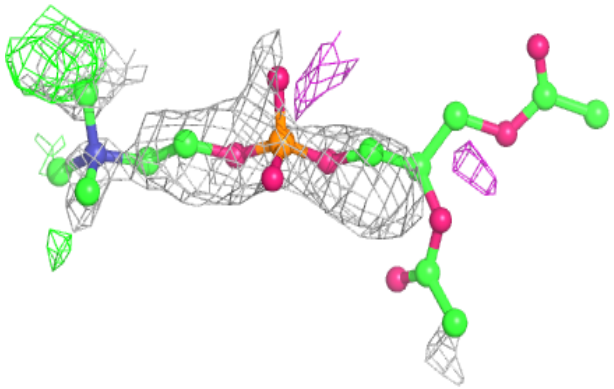


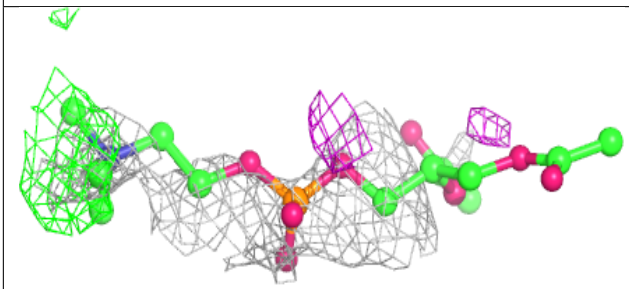


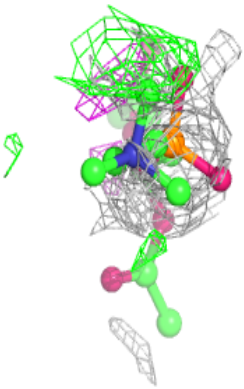


Electron density around PCW A 1012:

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

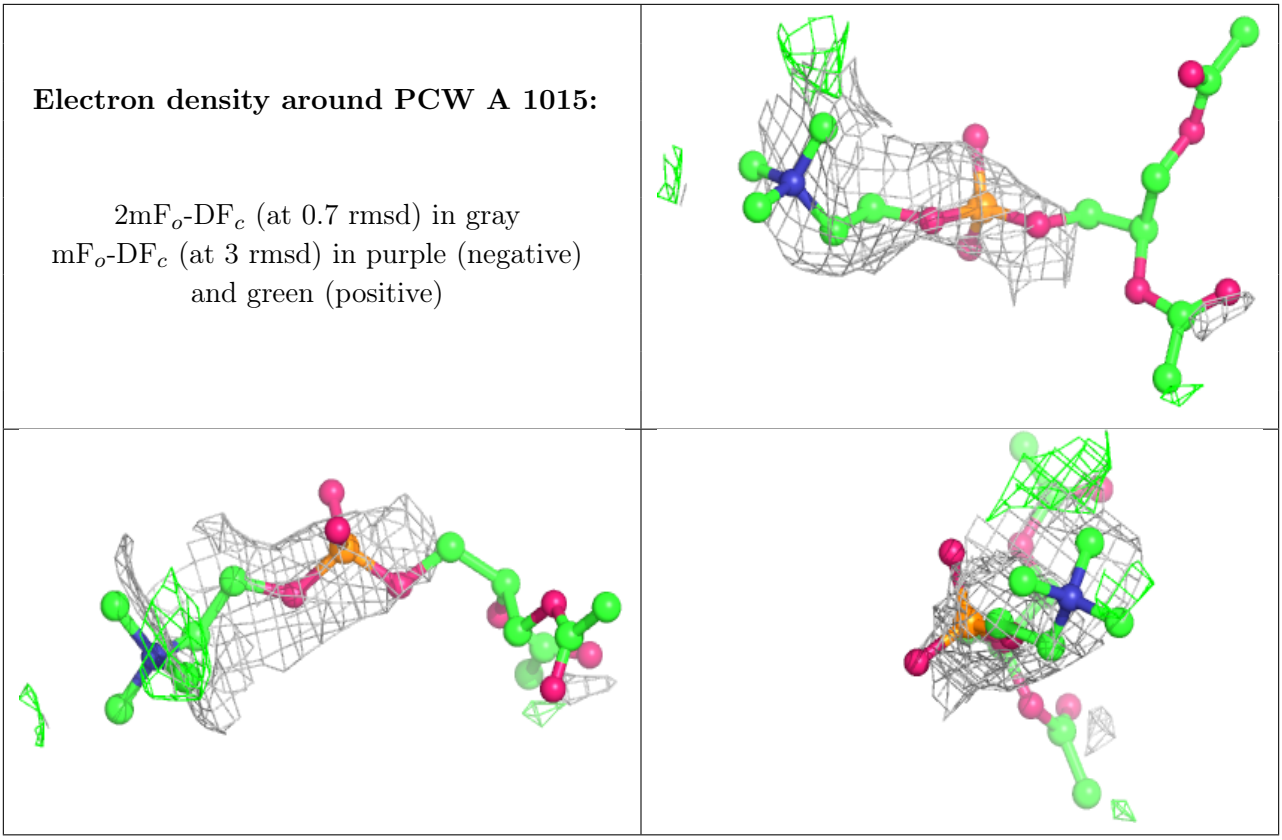






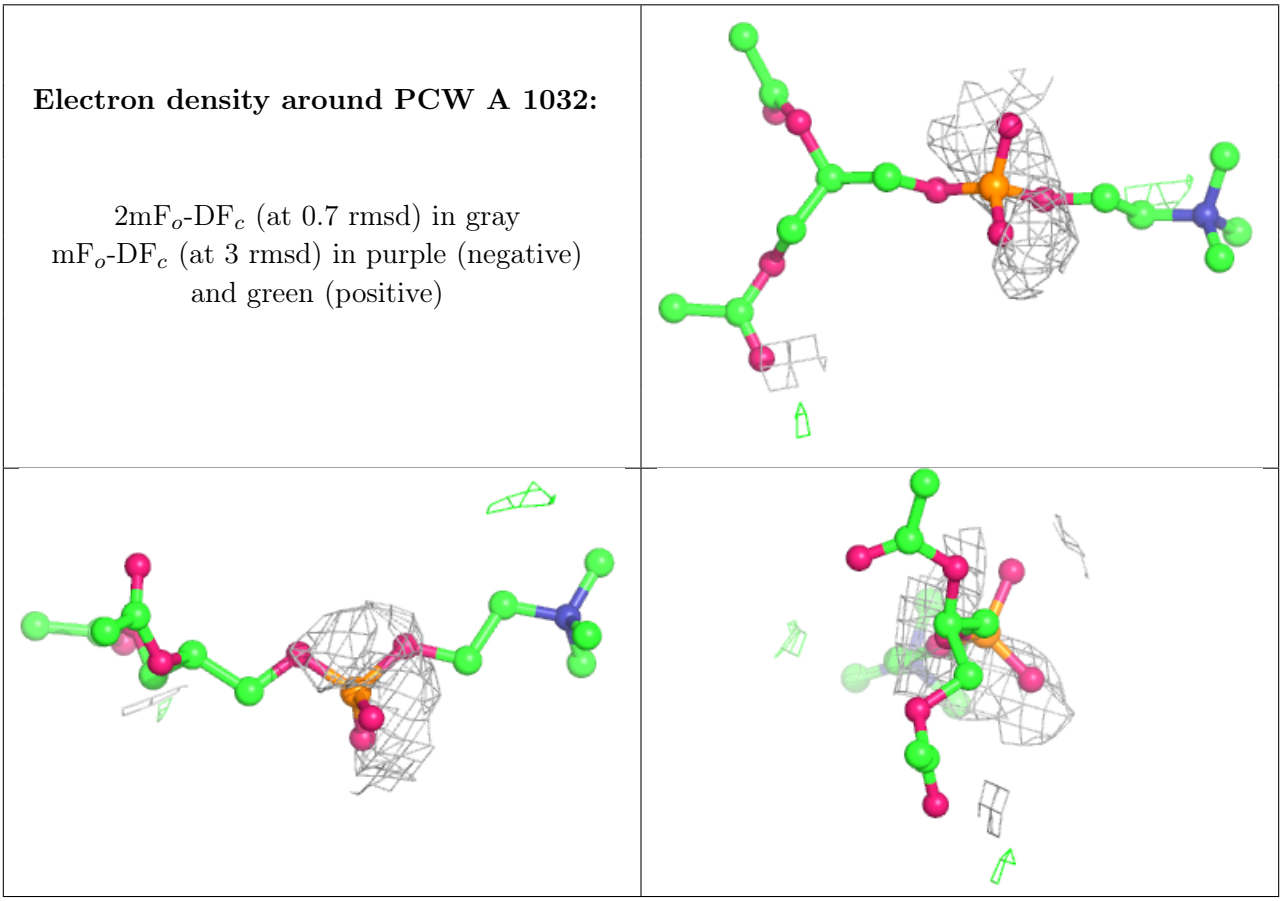
Electron density around PCW A 1015:

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



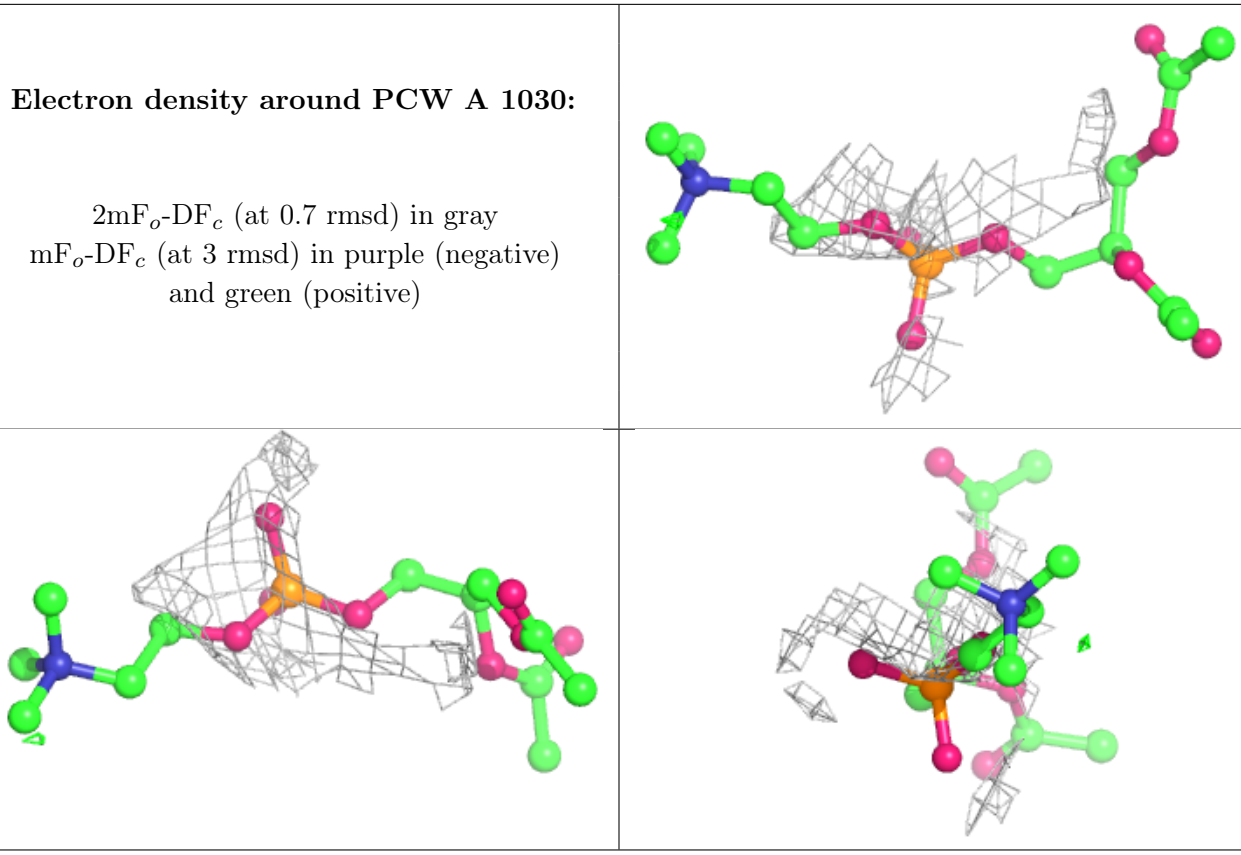
Electron density around PCW A 1032:

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



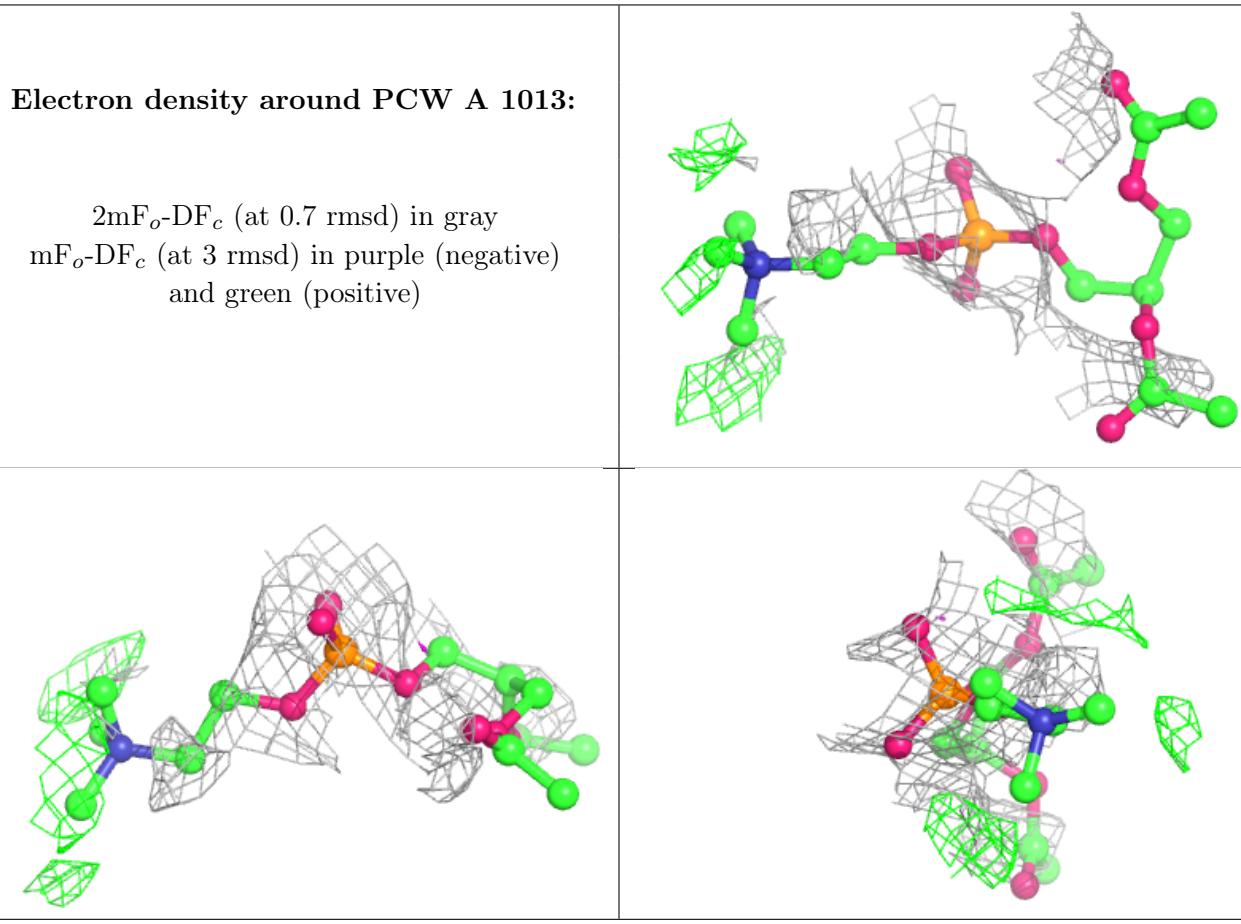
Electron density around PCW A 1030:

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



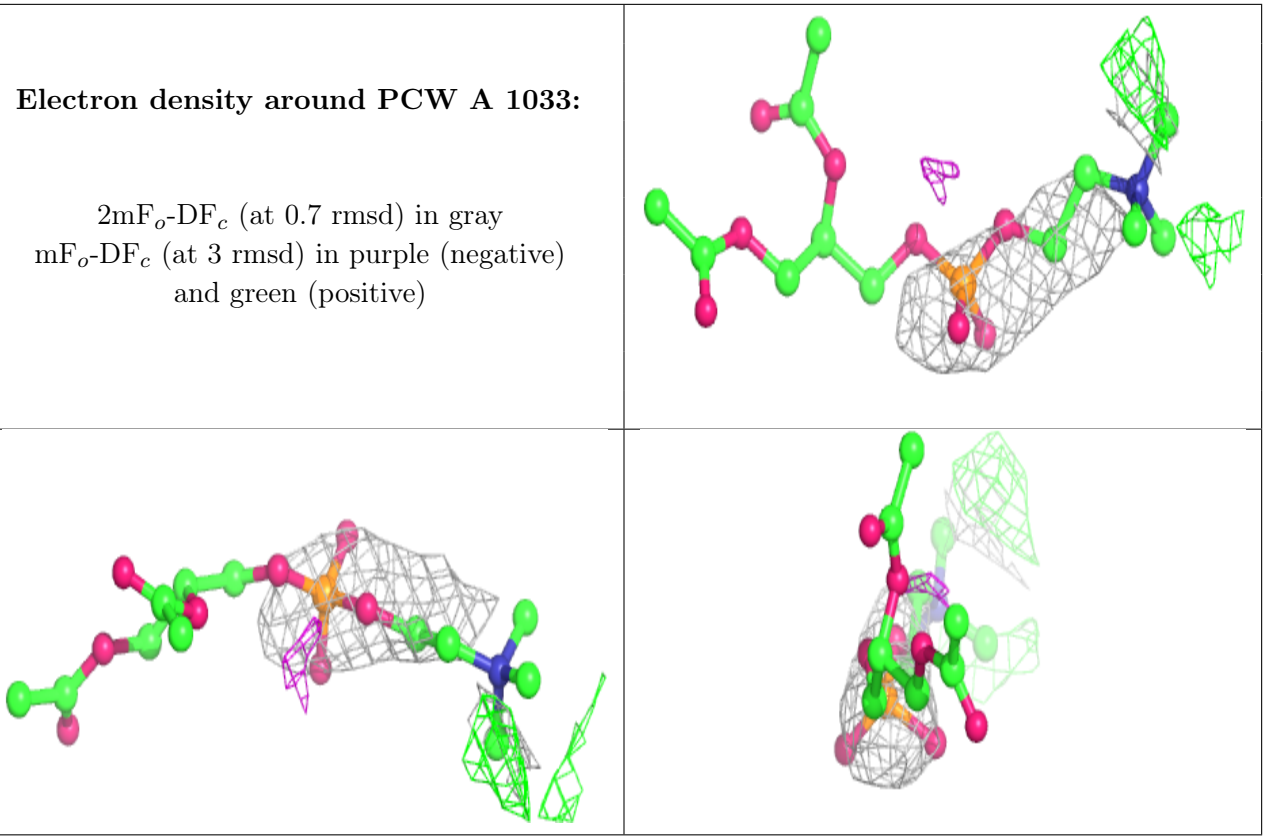
Electron density around PCW A 1013:

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



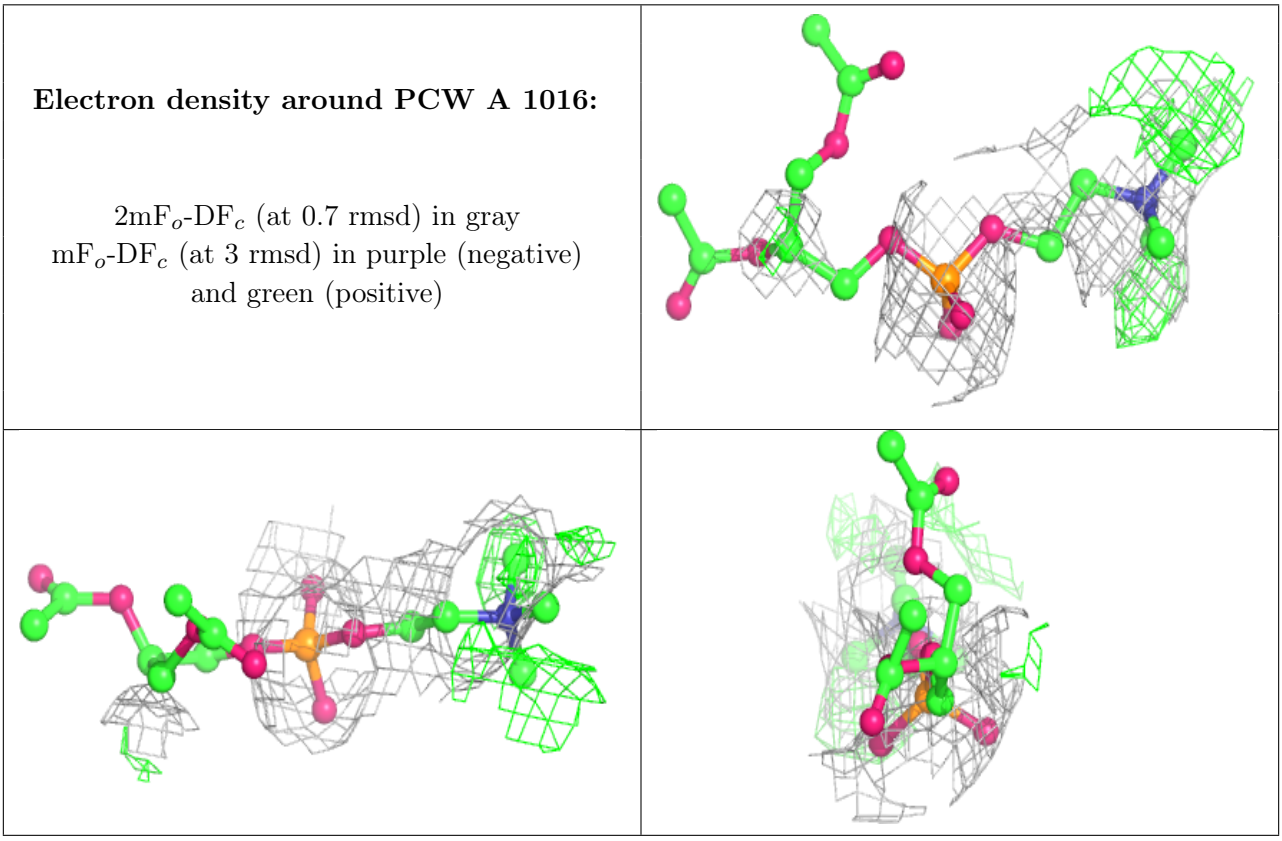
Electron density around PCW A 1033:

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



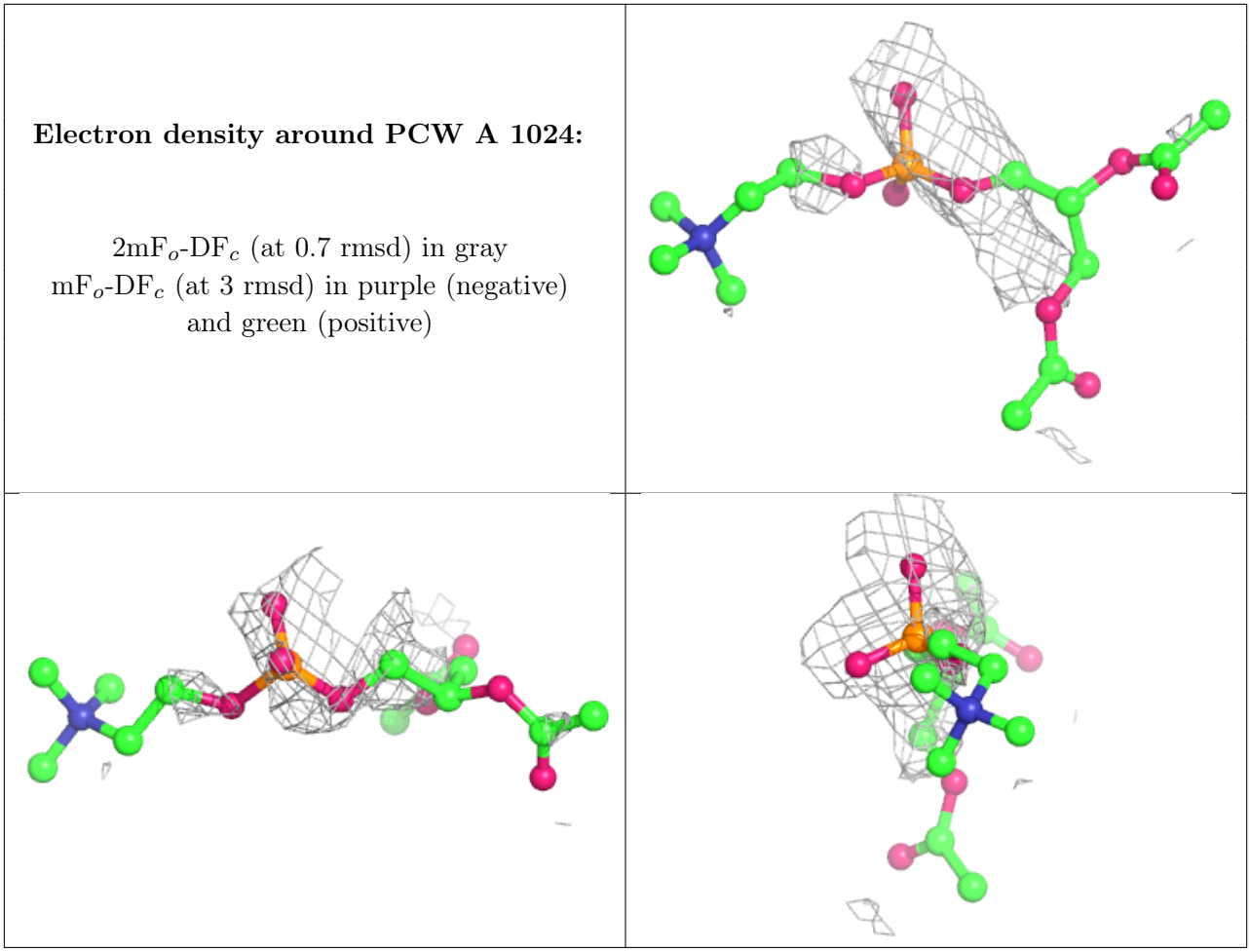
Electron density around PCW A 1016:

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



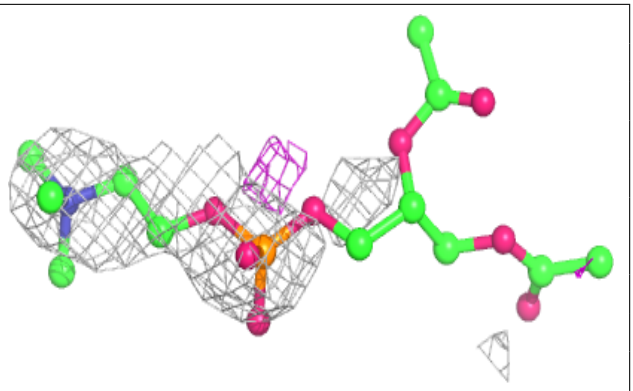
Electron density around PCW A 1024:

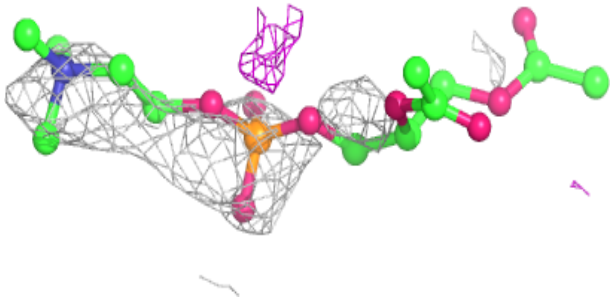
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

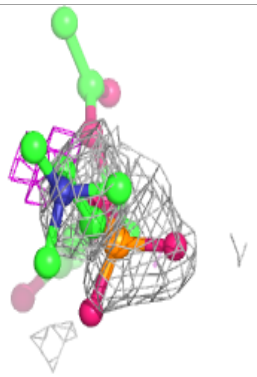


Electron density around PCW A 1008:

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

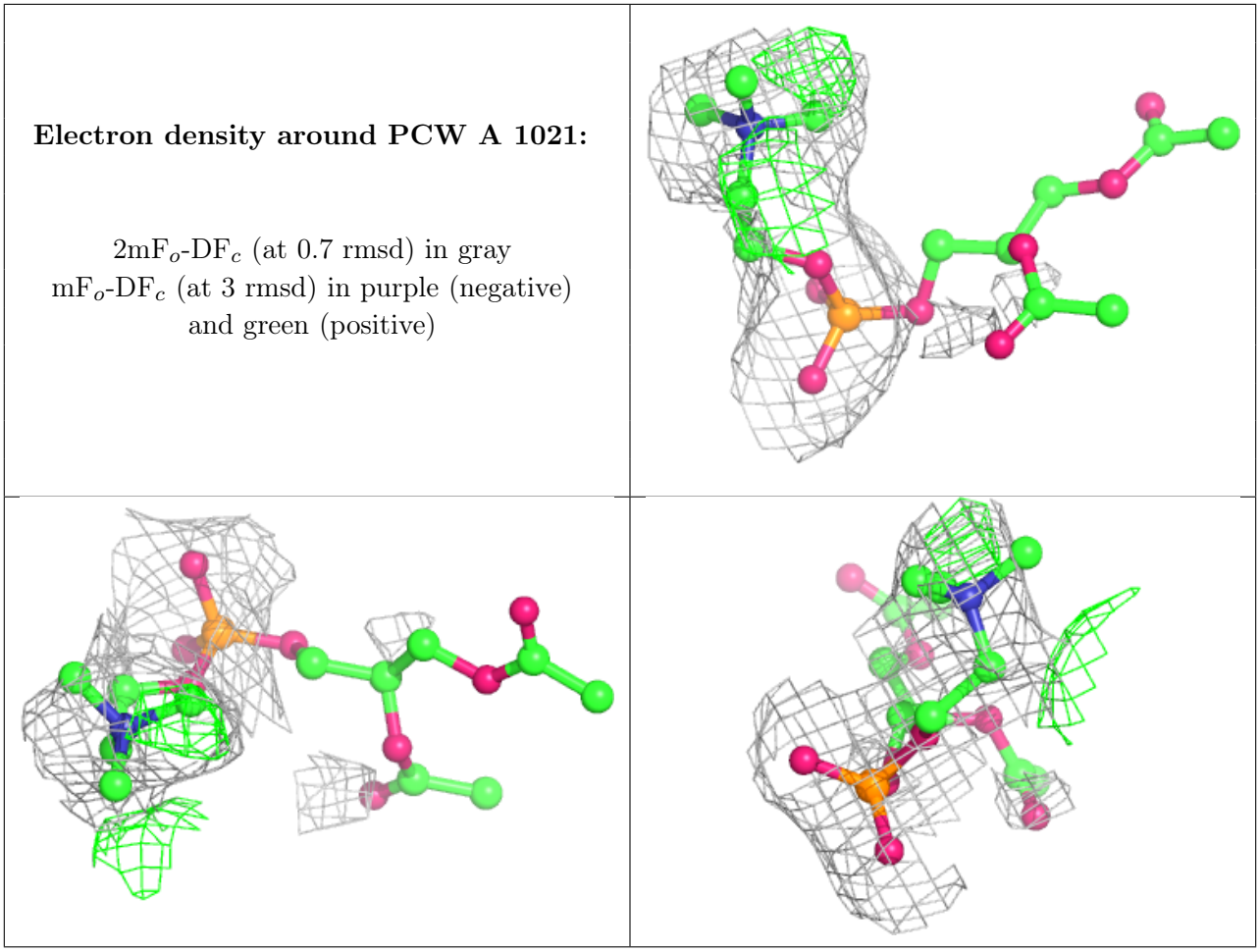






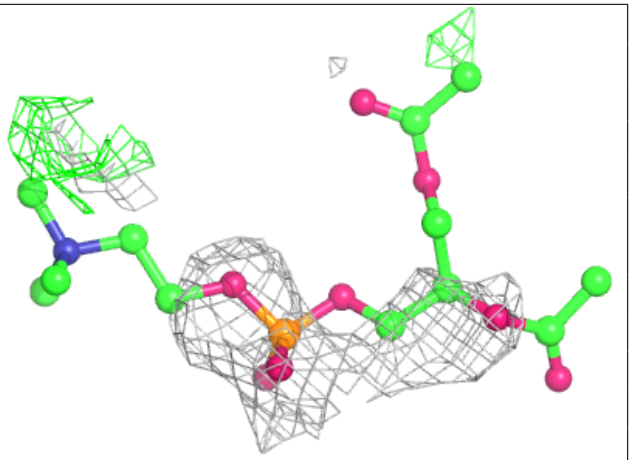
Electron density around PCW A 1021:

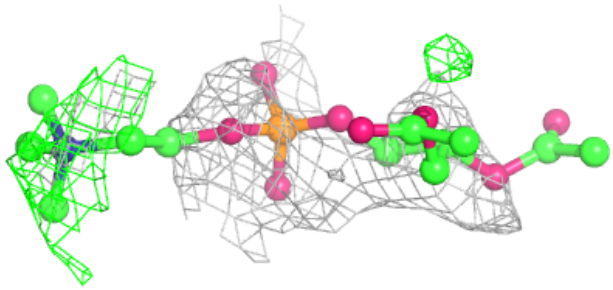
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

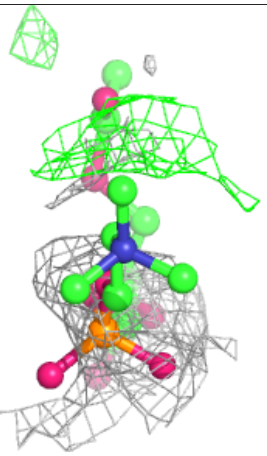


Electron density around PCW A 1037:

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

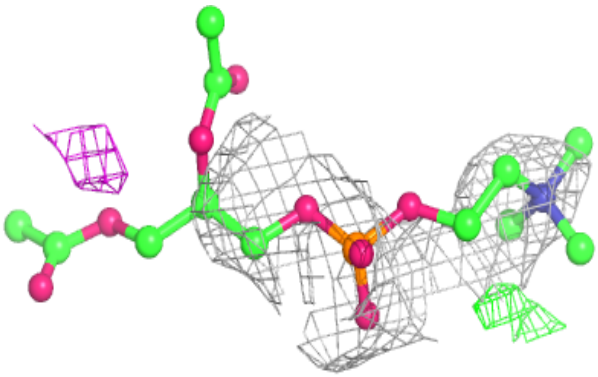


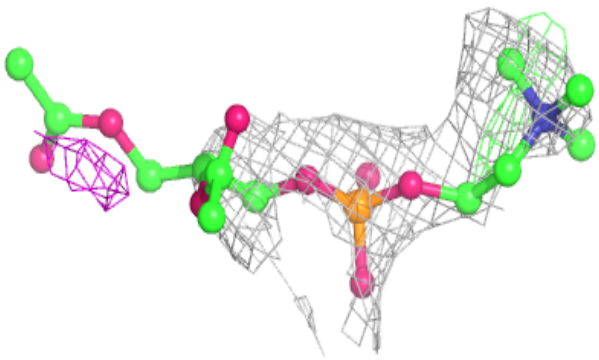


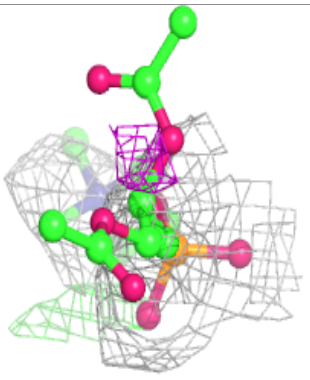


Electron density around PCW A 1022:

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

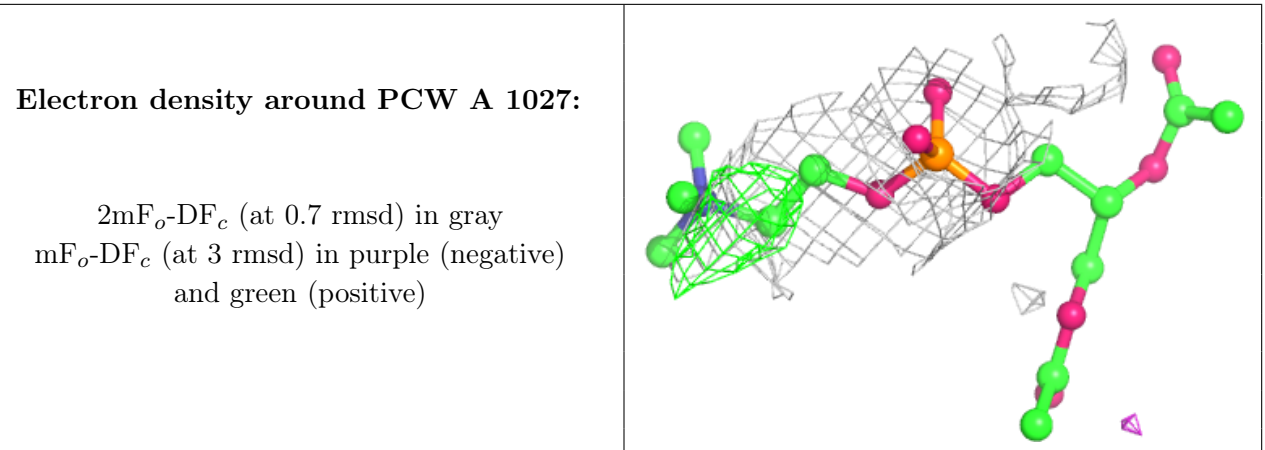


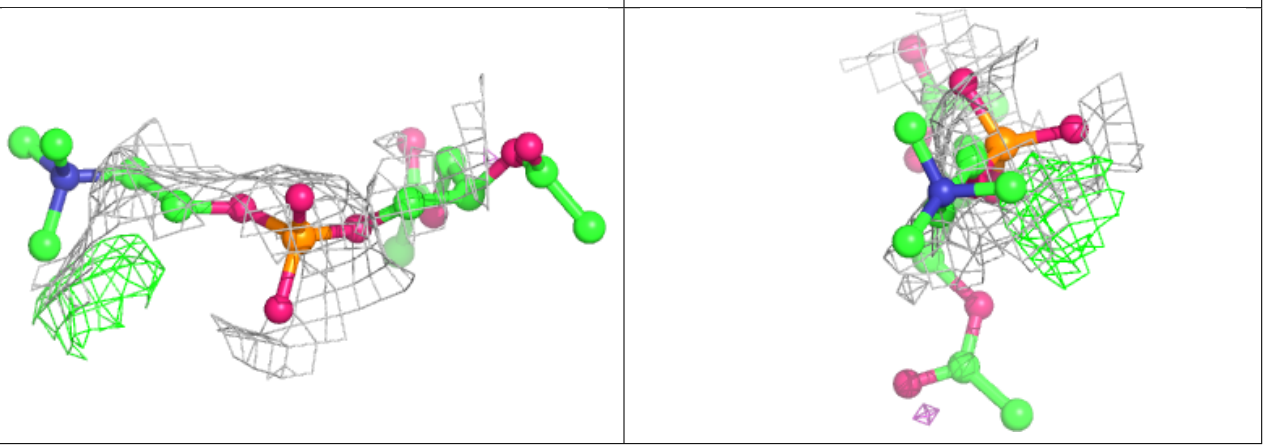




Electron density around PCW A 1027:

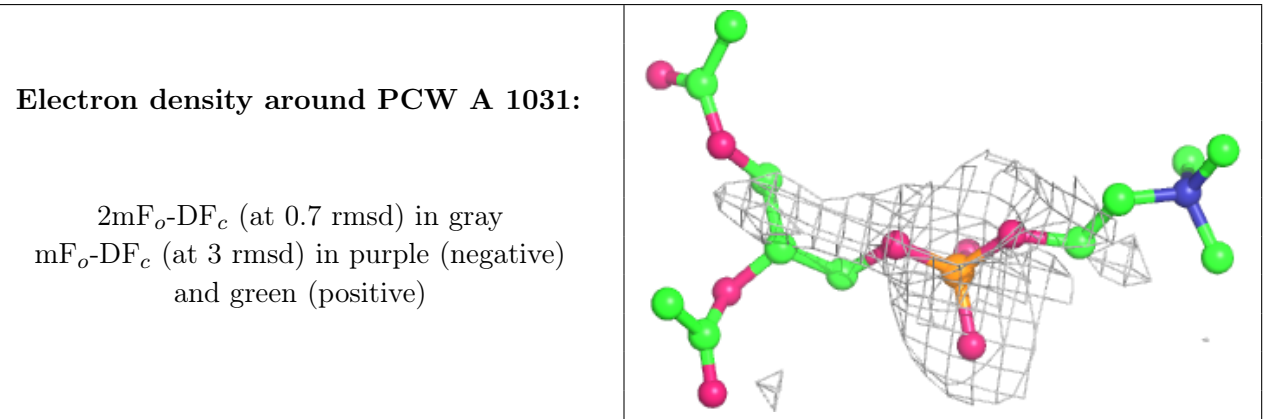
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

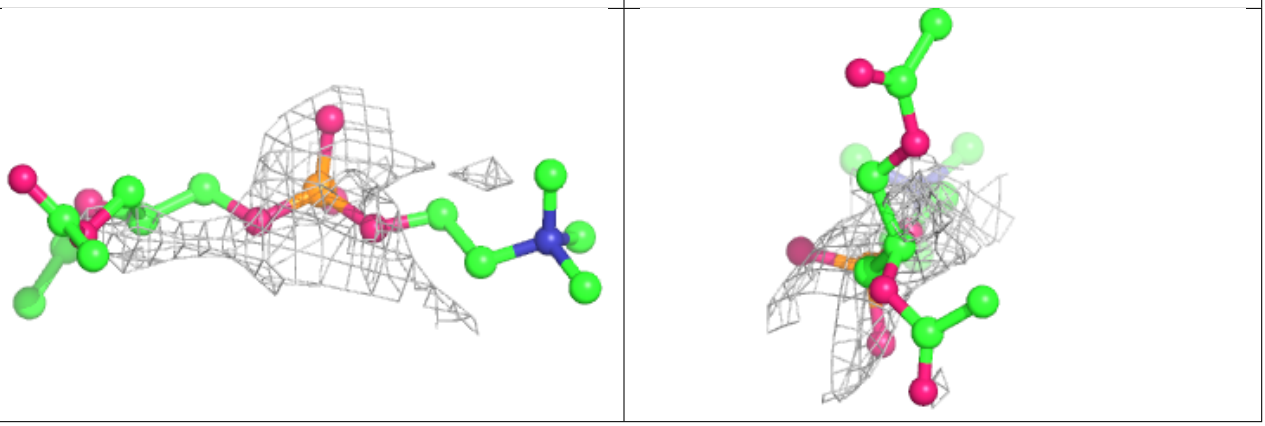




Electron density around PCW A 1031:

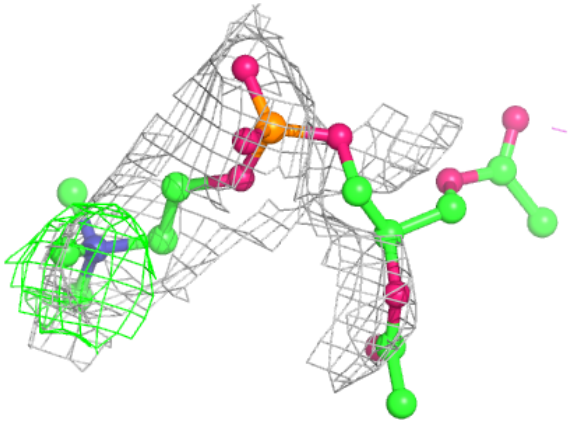
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

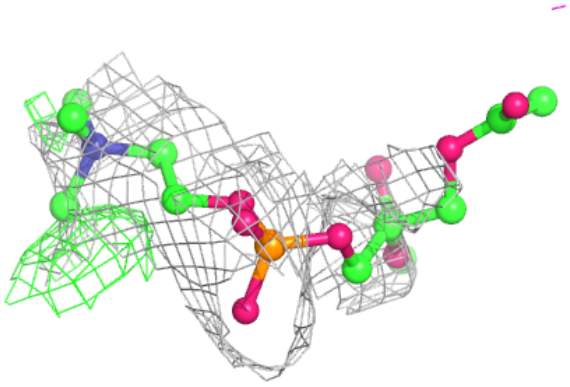


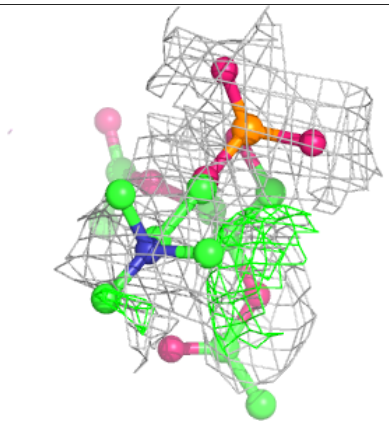


Electron density around PCW A 1019:

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

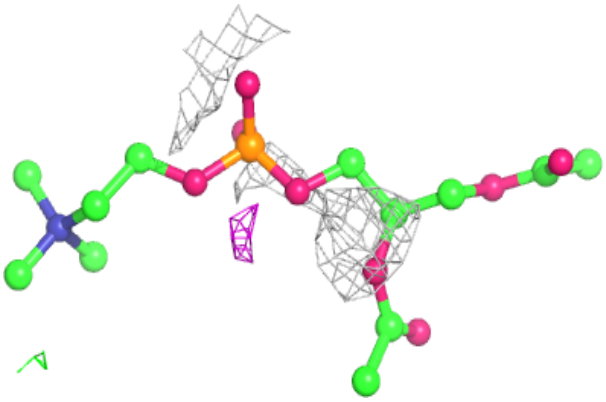


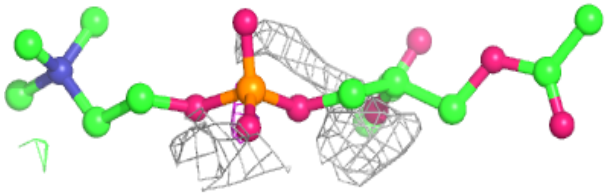




Electron density around PCW A 1004:

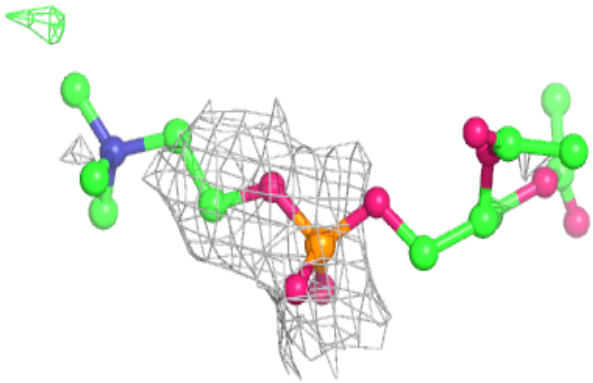
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

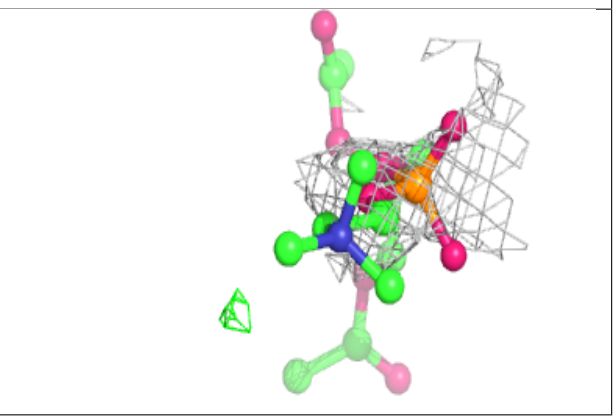




Electron density around PCW A 1006:

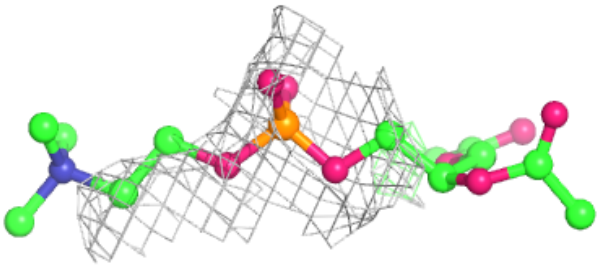
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

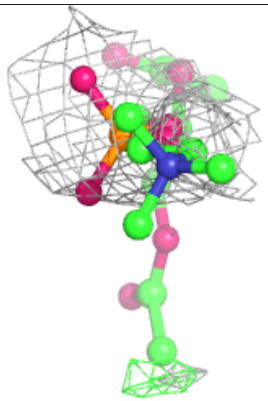




Electron density around PCW A 1005:

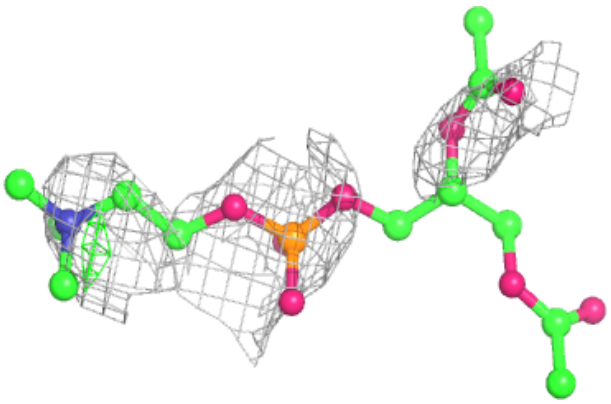
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

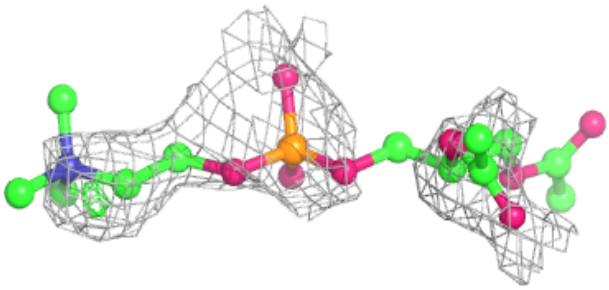


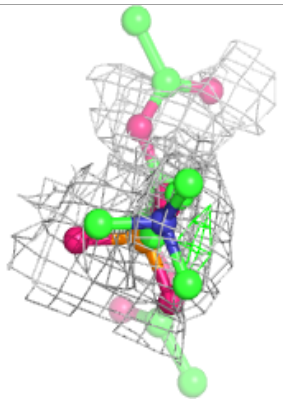


Electron density around PCW A 1020:

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

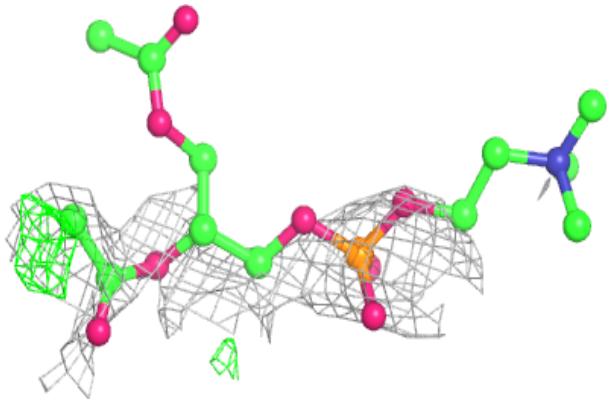


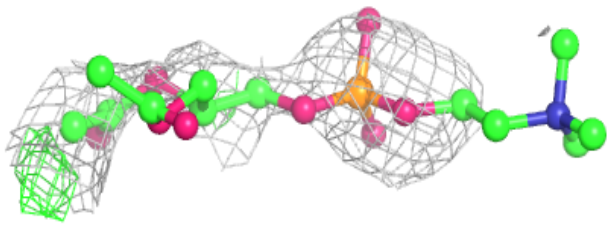


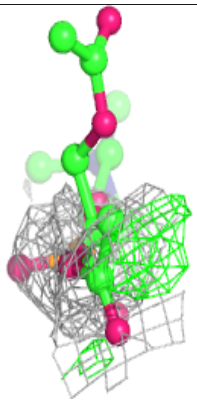


Electron density around PCW A 1025:

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

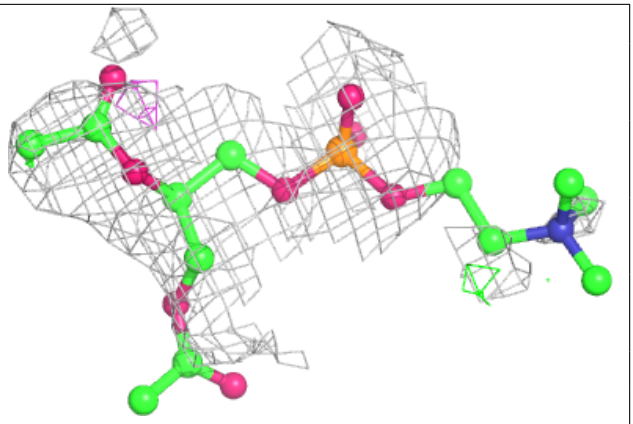


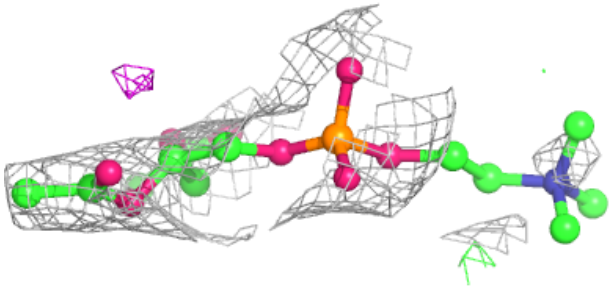


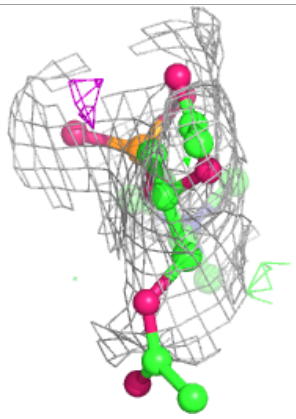


Electron density around PCW A 1007:

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

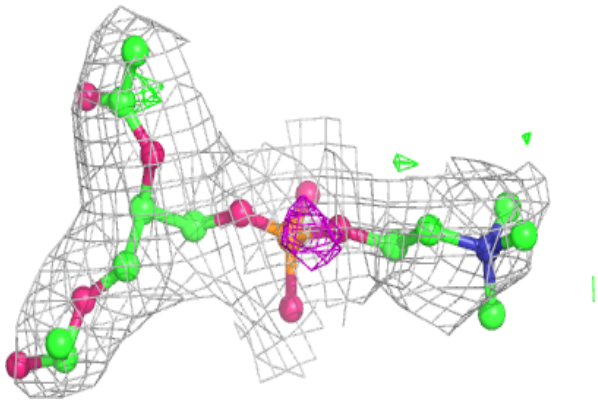


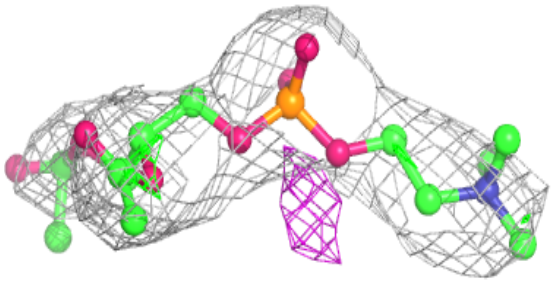


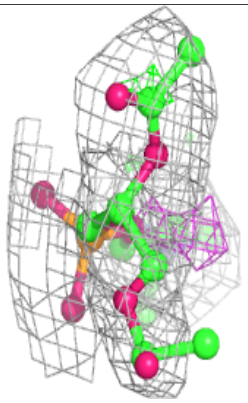


Electron density around PCW A 1011:

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

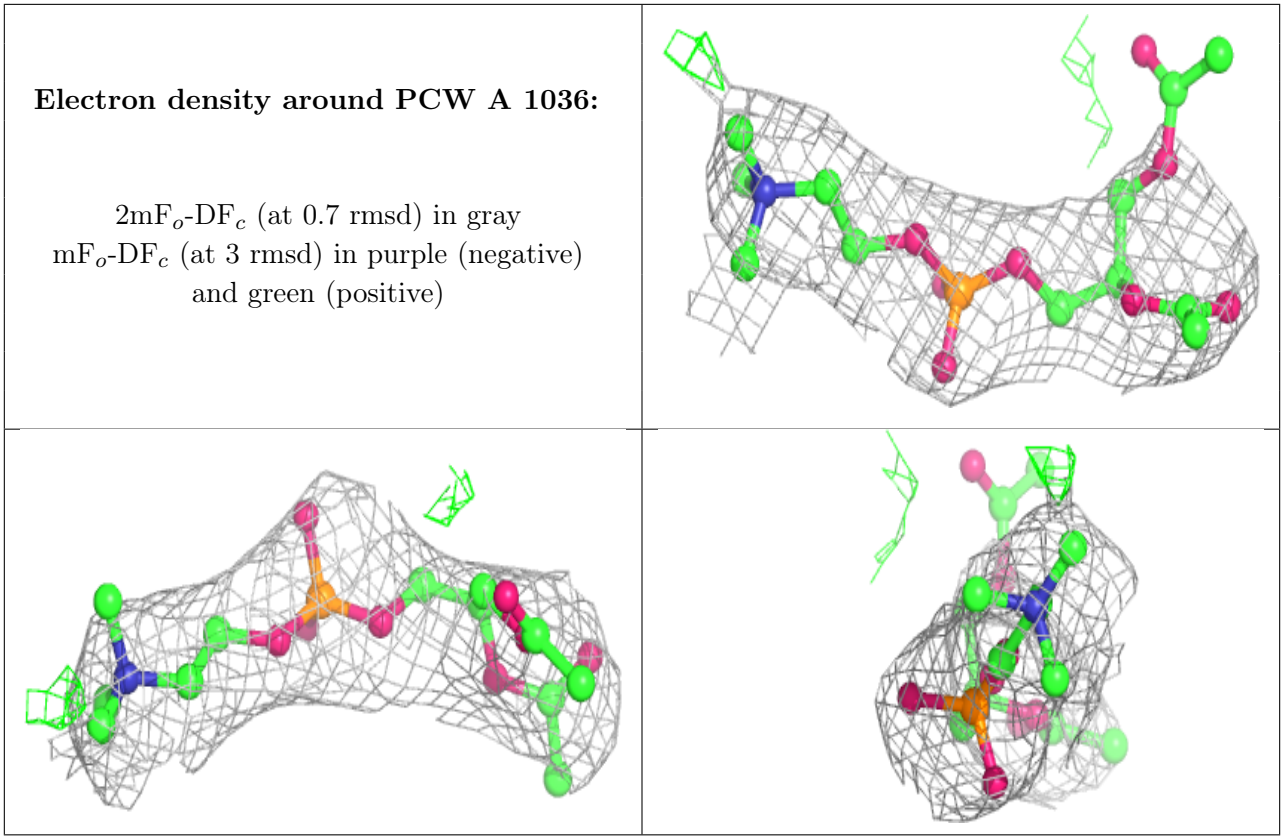






Electron density around PCW A 1036:

$2mF_o$-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.