wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 10:22 PM EDT

PDB ID	:	5MRW
Title	:	Structure of the KdpFABC complex
Authors	:	Huang, C.; Pedersen, B.P.; Stokes, D.L.
Deposited on	:	2016-12-27
Resolution	:	2.90 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:

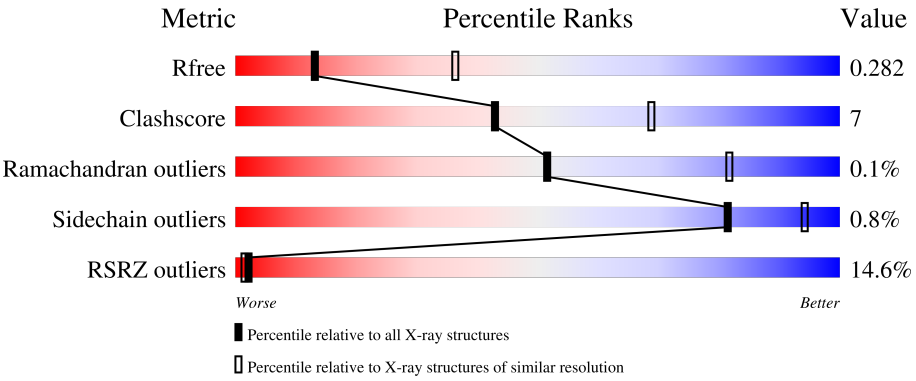
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	557	10% 78% 21%
1	E	557	8% 79% 20%
1	I	557	10% 81% 18%
2	B	674	14% 82% 18%
2	F	674	21% 83% 17%

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Mol	Chain	Length	Quality of chain
2	J	674	28% 84% 16%
3	C	187	5% 83% 17%
3	G	187	9% 86% 14%
3	K	187	8% 86% 14%
4	D	27	7% 96%
4	H	27	7% 96%
4	L	27	15% 96%

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
6	PX4	A	602	-	-	-	X
6	PX4	A	603	-	-	-	X
6	PX4	E	602	-	-	-	X
6	PX4	H	101	-	-	-	X
6	PX4	I	602	-	-	-	X
6	PX4	I	603	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 32666 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 Potassium-transporting ATPase potassium-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4157	2716	681	725	35			
1	E	557	Total	C	N	O	S	0	0	0
			4157	2716	681	725	35			
1	I	557	Total	C	N	O	S	0	0	0
			4157	2716	681	725	35			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ARG	GLN	engineered mutation	UNP P03959
E	116	ARG	GLN	engineered mutation	UNP P03959
I	116	ARG	GLN	engineered mutation	UNP P03959

- Molecule 2 is a protein called Potassium-transporting ATPase ATP-binding subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	674	Total	C	N	O	P	S	0	0	0
			5008	3187	864	932	1	24			
2	F	674	Total	C	N	O	P	S	0	0	0
			5008	3187	864	932	1	24			
2	J	674	Total	C	N	O	P	S	0	0	0
			5008	3187	864	932	1	24			

- Molecule 3 is a protein called Potassium-transporting ATPase KdpC subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	187	Total	C	N	O	S	0	0	0
			1413	903	245	264	1			
3	G	187	Total	C	N	O	S	0	0	0
			1413	903	245	264	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	187	Total	C	N	O	S	0	0	0
			1413	903	245	264	1			

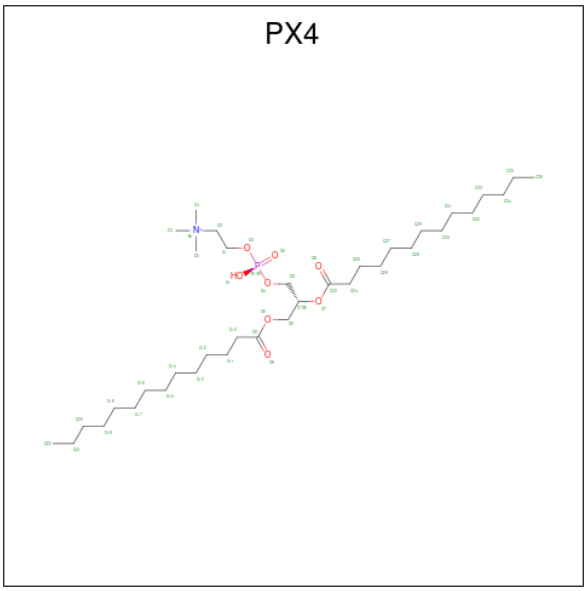
- Molecule 4 is a protein called Potassium-transporting ATPase KdpF subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	27	Total	C	N	O	S	0	0	0
			200	137	28	34	1			
4	H	27	Total	C	N	O	S	0	0	0
			200	137	28	34	1			
4	L	27	Total	C	N	O	S	0	0	0
			200	137	28	34	1			

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

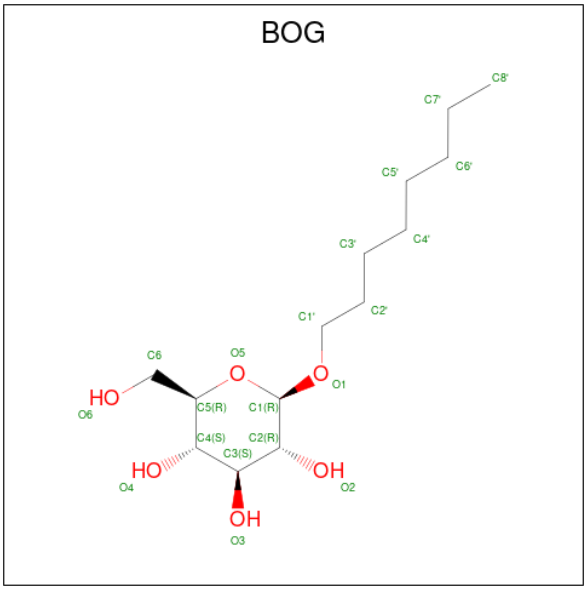
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	E	1	Total	K	0	0
			1	1		
5	I	1	Total	K	0	0
			1	1		

- Molecule 6 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			41	32	8	1		
6	A	1	Total	C	O	P	0	0
			41	32	8	1		
6	E	1	Total	C	O	P	0	0
			41	32	8	1		
6	H	1	Total	C	O	P	0	0
			41	32	8	1		
6	I	1	Total	C	O	P	0	0
			41	32	8	1		
6	I	1	Total	C	O	P	0	0
			41	32	8	1		

- Molecule 7 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			20	14	6		
7	B	1	Total	C	O	0	0
			20	14	6		
7	E	1	Total	C	O	0	0
			20	14	6		
7	I	1	Total	C	O	0	0
			20	14	6		

- Molecule 8 is water.

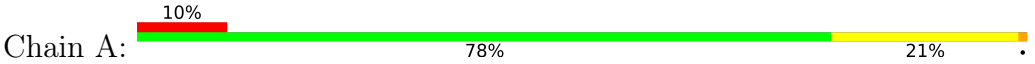
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total O 1 1	0	0
8	F	1	Total O 1 1	0	0
8	J	1	Total O 1 1	0	0

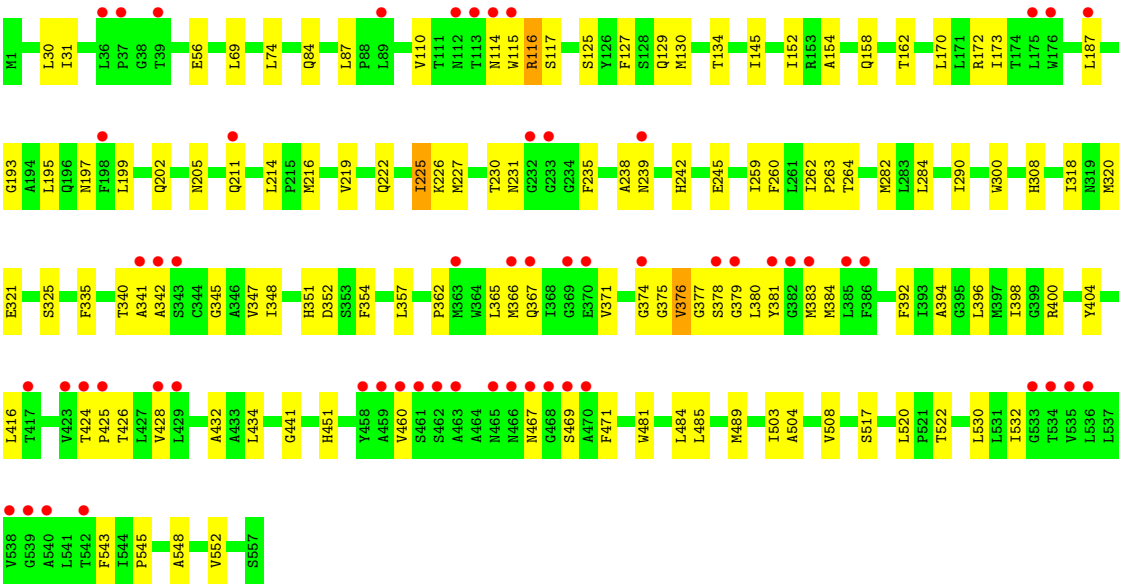
3 Residue-property plots (i)

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: Potassium-transporting ATPase potassium-binding subunit

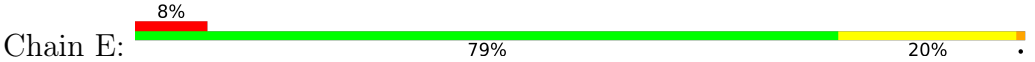
Chain A:

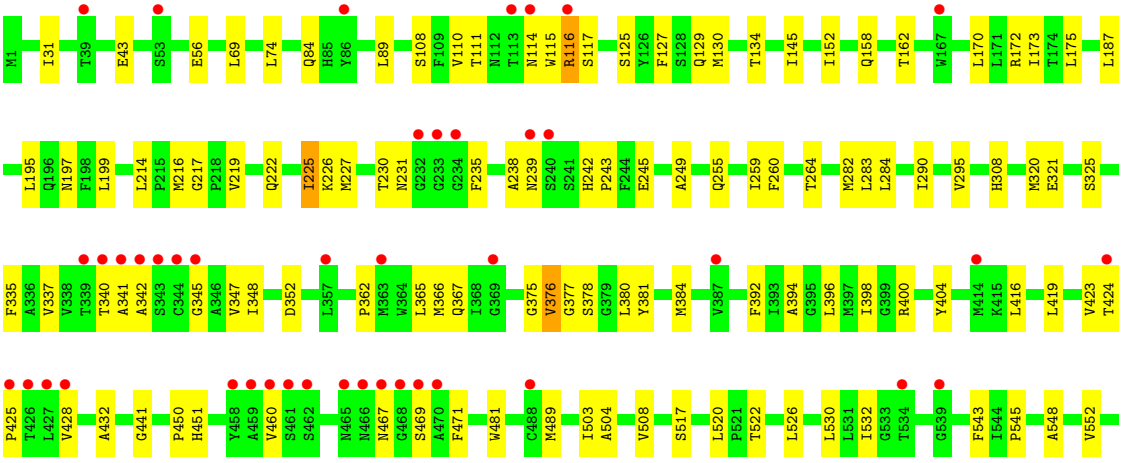




• Molecule 1: Potassium-transporting ATPase potassium-binding subunit

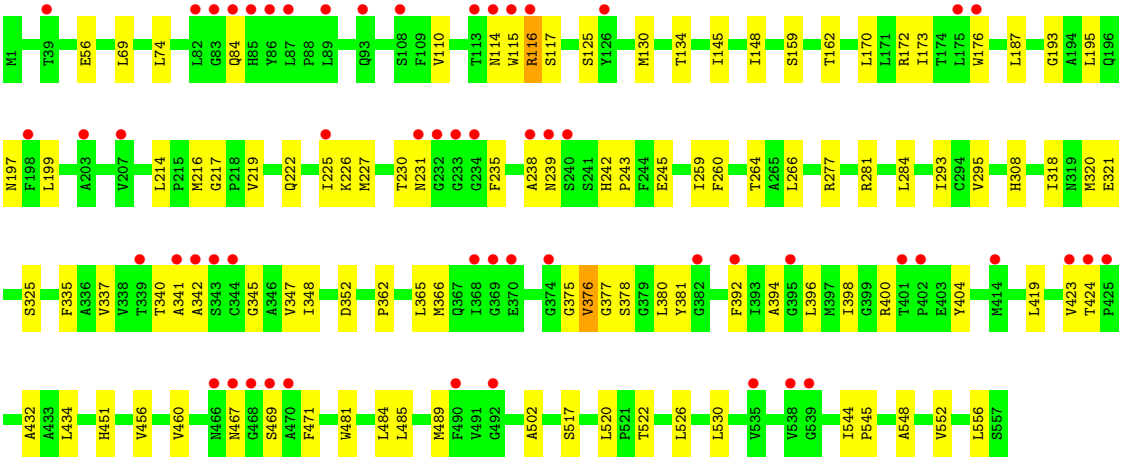
Chain E:





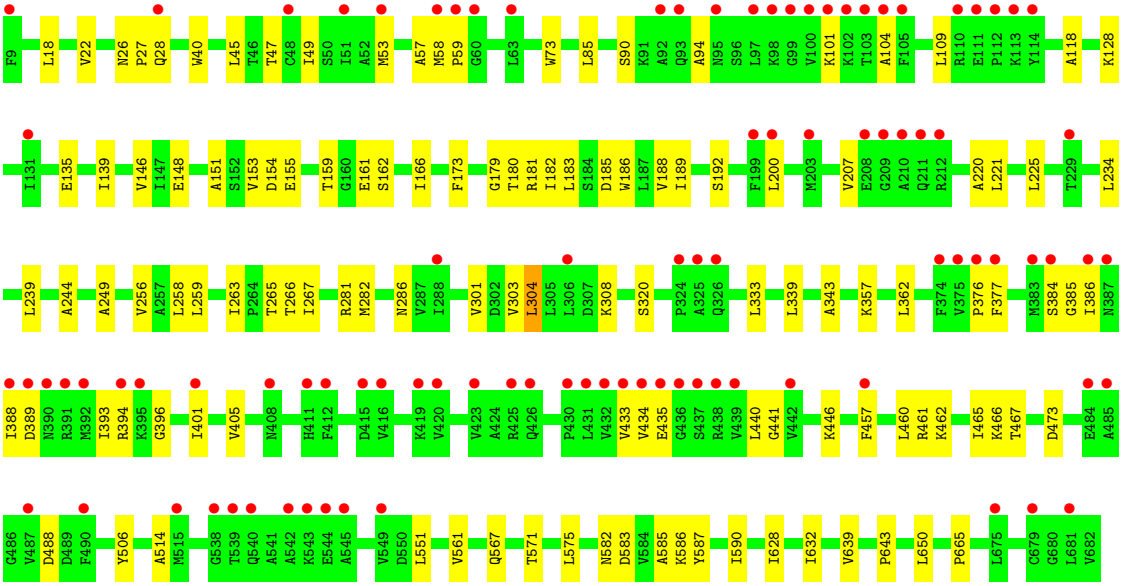
• Molecule 1: Potassium-transporting ATPase potassium-binding subunit

Chain I:



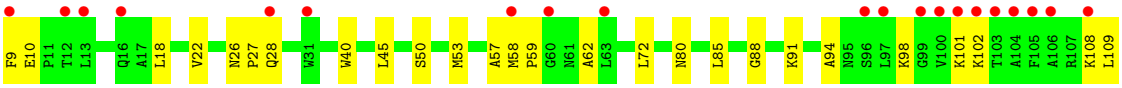
• Molecule 2: Potassium-transporting ATPase ATP-binding subunit

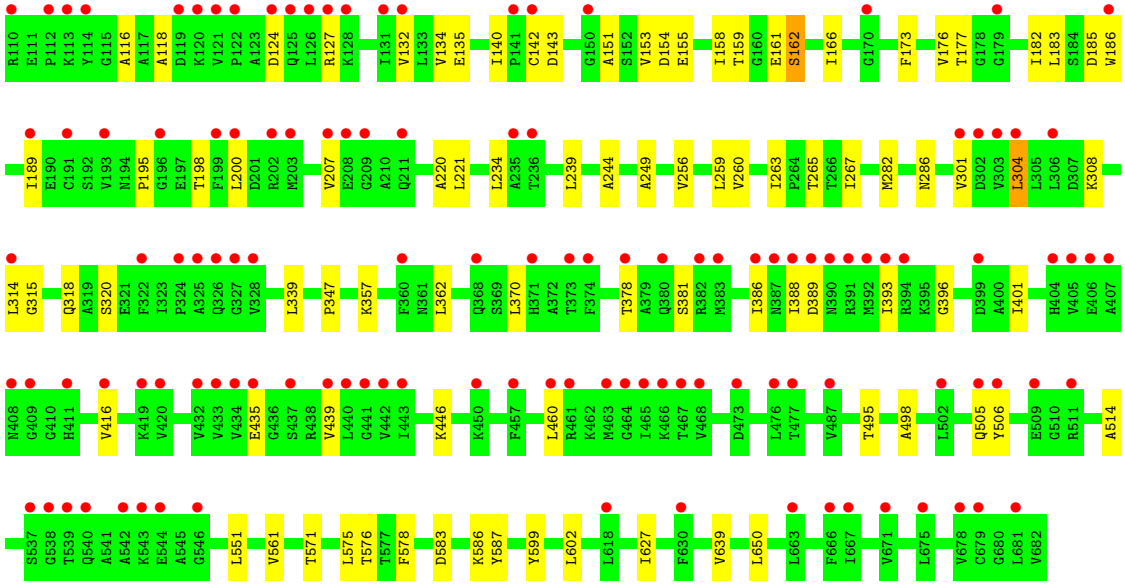
Chain B:



• Molecule 2: Potassium-transporting ATPase ATP-binding subunit

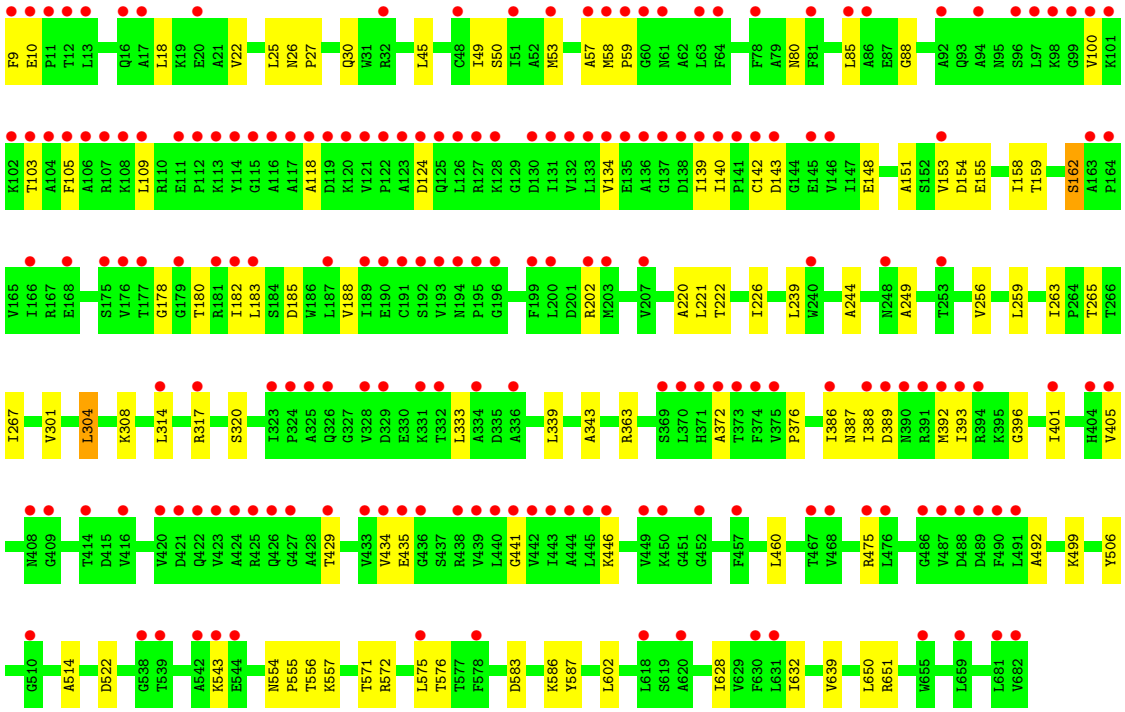
Chain F:





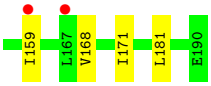
• Molecule 2: Potassium-transporting ATPase ATP-binding subunit

Chain J:



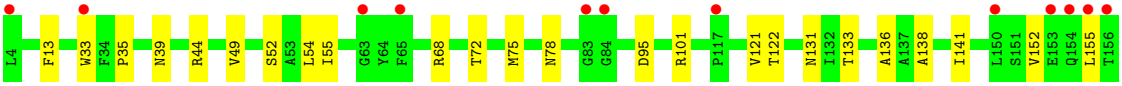
• Molecule 3: Potassium-transporting ATPase KdpC subunit

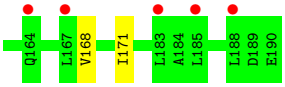
Chain C:



• Molecule 3: Potassium-transporting ATPase KdpC subunit

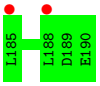
Chain G:





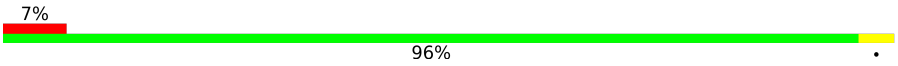
• Molecule 3: Potassium-transporting ATPase KdpC subunit

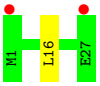
Chain K:



• Molecule 4: Potassium-transporting ATPase KdpF subunit

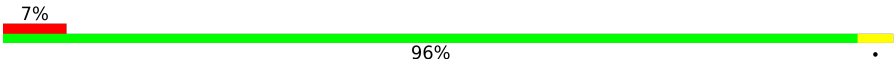
Chain D:

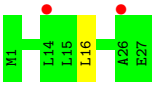




• Molecule 4: Potassium-transporting ATPase KdpF subunit

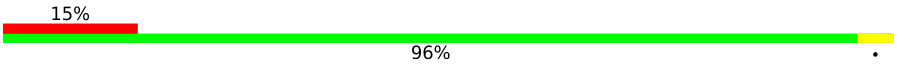
Chain H:

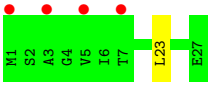




• Molecule 4: Potassium-transporting ATPase KdpF subunit

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.72Å 166.29Å 196.30Å 90.00° 107.41° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 49.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.90) 99.4 (49.88-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.243 , 0.275 0.252 , 0.282	Depositor DCC
R_{free} test set	8397 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	94.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 92.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32666	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: K, BOG, PX4, SEP

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	0.25	0/4249	0.39	0/5784
1	E	0.27	1/4249 (0.0%)	0.39	0/5784
1	I	0.26	1/4249 (0.0%)	0.39	0/5784
2	B	0.24	0/5072	0.40	0/6889
2	F	0.24	0/5072	0.40	0/6889
2	J	0.24	0/5072	0.40	0/6889
3	C	0.24	0/1444	0.40	0/1977
3	G	0.24	0/1444	0.39	0/1977
3	K	0.24	0/1444	0.38	0/1977
4	D	0.23	0/202	0.37	0/275
4	H	0.23	0/202	0.36	0/275
4	L	0.23	0/202	0.37	0/275
All	All	0.25	2/32901 (0.0%)	0.39	0/44775

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	217	GLY	C-N	7.48	1.48	1.34
1	I	217	GLY	C-N	5.58	1.44	1.34

There are no bond angle outliers.

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	4157	0	4286	78	0
1	E	4157	0	4286	78	0
1	I	4157	0	4286	70	0
2	B	5008	0	5195	71	0
2	F	5008	0	5195	72	0
2	J	5008	0	5195	66	0
3	C	1413	0	1428	24	0
3	G	1413	0	1428	22	0
3	K	1413	0	1428	21	0
4	D	200	0	221	1	0
4	H	200	0	221	1	0
4	L	200	0	221	1	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
6	A	82	0	118	1	0
6	E	41	0	59	1	0
6	H	41	0	59	0	0
6	I	82	0	118	3	0
7	A	20	0	28	0	0
7	B	20	0	28	0	0
7	E	20	0	28	1	0
7	I	20	0	28	1	0
8	B	1	0	0	0	0
8	F	1	0	0	0	0
8	J	1	0	0	0	0
All	All	32666	0	33856	453	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 7.

The worst 5 of 453 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:545:PRO:HB2	2:B:239:LEU:HD21	1.65	0.79
1:I:545:PRO:HB2	2:J:239:LEU:HD21	1.65	0.76
1:E:545:PRO:HB2	2:F:239:LEU:HD21	1.69	0.72
1:E:340:THR:HG21	1:E:362:PRO:HB3	1.72	0.72
1:A:116:ARG:NH1	1:A:345:GLY:O	2.23	0.71

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	555/557 (100%)	529 (95%)	24 (4%)	2 (0%)	34	66
1	E	555/557 (100%)	531 (96%)	22 (4%)	2 (0%)	34	66
1	I	555/557 (100%)	529 (95%)	24 (4%)	2 (0%)	34	66
2	B	671/674 (100%)	648 (97%)	23 (3%)	0	100	100
2	F	671/674 (100%)	647 (96%)	24 (4%)	0	100	100
2	J	671/674 (100%)	647 (96%)	24 (4%)	0	100	100
3	C	185/187 (99%)	174 (94%)	11 (6%)	0	100	100
3	G	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
3	K	185/187 (99%)	174 (94%)	11 (6%)	0	100	100
4	D	25/27 (93%)	25 (100%)	0	0	100	100
4	H	25/27 (93%)	25 (100%)	0	0	100	100
4	L	25/27 (93%)	25 (100%)	0	0	100	100
All	All	4308/4335 (99%)	4129 (96%)	173 (4%)	6 (0%)	51	82

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	GLY
1	I	377	GLY
1	E	377	GLY
1	A	376	VAL
1	E	376	VAL

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	439/439 (100%)	435 (99%)	4 (1%)	78 93
1	E	439/439 (100%)	435 (99%)	4 (1%)	78 93
1	I	439/439 (100%)	436 (99%)	3 (1%)	84 95
2	B	523/523 (100%)	518 (99%)	5 (1%)	76 92
2	F	523/523 (100%)	519 (99%)	4 (1%)	81 94
2	J	523/523 (100%)	519 (99%)	4 (1%)	81 94
3	C	149/149 (100%)	148 (99%)	1 (1%)	84 95
3	G	149/149 (100%)	149 (100%)	0	100 100
3	K	149/149 (100%)	148 (99%)	1 (1%)	84 95
4	D	21/21 (100%)	21 (100%)	0	100 100
4	H	21/21 (100%)	21 (100%)	0	100 100
4	L	21/21 (100%)	21 (100%)	0	100 100
All	All	3396/3396 (100%)	3370 (99%)	26 (1%)	81 94

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	259	LEU
2	F	587	TYR
2	J	587	TYR
2	F	506	TYR
1	I	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	624	ASN
2	F	624	ASN
1	E	114	ASN
1	A	239	ASN

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Mol	Chain	Res	Type
1	E	239	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	$\#\|Z\| > 2$
2	SEP	F	162	2	8,9,10	1.56	1 (12%)	8,12,14	1.66	2 (25%)
2	SEP	J	162	2	8,9,10	1.56	1 (12%)	8,12,14	1.79	2 (25%)
2	SEP	B	162	2	8,9,10	1.55	1 (12%)	8,12,14	1.82	2 (25%)

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
2	SEP	F	162	2	-	0/5/8/10	-
2	SEP	J	162	2	-	0/5/8/10	-
2	SEP	B	162	2	-	1/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	162	SEP	P-O1P	3.39	1.61	1.50
2	B	162	SEP	P-O1P	3.37	1.61	1.50
2	F	162	SEP	P-O1P	3.36	1.61	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	162	SEP	OG-CB-CA	3.41	111.46	108.14
2	J	162	SEP	OG-CB-CA	3.36	111.42	108.14
2	B	162	SEP	P-OG-CB	-3.36	109.03	118.30
2	J	162	SEP	P-OG-CB	-3.26	109.30	118.30
2	F	162	SEP	P-OG-CB	-3.18	109.54	118.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	162	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	162	SEP	1	0
2	J	162	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
6	PX4	I	602	-	40,40,45	1.27	5 (12%)	43,45,53	1.07	2 (4%)
6	PX4	E	602	-	40,40,45	1.26	5 (12%)	43,45,53	1.11	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PX4	A	603	-	40,40,45	1.27	5 (12%)	43,45,53	1.10	2 (4%)
6	PX4	A	602	-	40,40,45	1.26	5 (12%)	43,45,53	1.15	2 (4%)
7	BOG	E	603	-	20,20,20	1.22	1 (5%)	25,25,25	0.82	0
7	BOG	I	604	-	20,20,20	1.21	1 (5%)	25,25,25	0.82	0
6	PX4	I	603	-	40,40,45	1.26	5 (12%)	43,45,53	1.15	2 (4%)
7	BOG	B	701	-	20,20,20	1.22	1 (5%)	25,25,25	0.80	0
7	BOG	A	604	-	20,20,20	1.21	1 (5%)	25,25,25	0.79	0
6	PX4	H	101	-	40,40,45	1.27	5 (12%)	43,45,53	1.12	2 (4%)

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
6	PX4	I	602	-	-	8/44/44/49	-
6	PX4	E	602	-	-	17/44/44/49	-
6	PX4	A	603	-	-	18/44/44/49	-
6	PX4	A	602	-	-	22/44/44/49	-
7	BOG	E	603	-	-	3/11/31/31	0/1/1/1
7	BOG	I	604	-	-	4/11/31/31	0/1/1/1
6	PX4	I	603	-	-	15/44/44/49	-
7	BOG	B	701	-	-	1/11/31/31	0/1/1/1
7	BOG	A	604	-	-	3/11/31/31	0/1/1/1
6	PX4	H	101	-	-	19/44/44/49	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	604	BOG	O5-C1	3.56	1.50	1.41
7	A	604	BOG	O5-C1	3.53	1.50	1.41
7	E	603	BOG	O5-C1	3.53	1.50	1.41
7	B	701	BOG	O5-C1	3.51	1.50	1.41
6	H	101	PX4	O5-C9	3.29	1.43	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	603	PX4	O7-C23-C24	4.49	121.19	111.50
6	A	602	PX4	O7-C23-C24	4.05	120.24	111.50
6	H	101	PX4	O7-C23-C24	3.90	119.90	111.50
6	A	603	PX4	O7-C23-C24	3.81	119.72	111.50
6	E	602	PX4	O7-C23-C24	3.81	119.71	111.50

There are no chirality outliers.

5 of 110 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	PX4	C6-O4-P1-O1
6	A	602	PX4	O8-C23-O7-C7
6	A	602	PX4	C24-C23-O7-C7
6	A	603	PX4	C1-O3-P1-O1
6	E	602	PX4	C1-O3-P1-O1

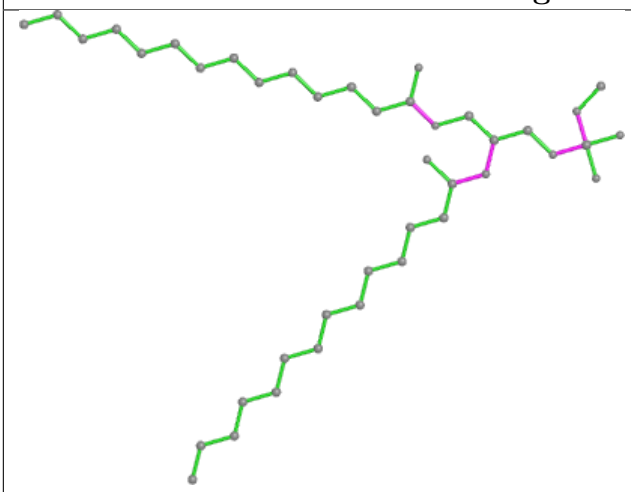
There are no ring outliers.

6 monomers are involved in 7 short contacts:

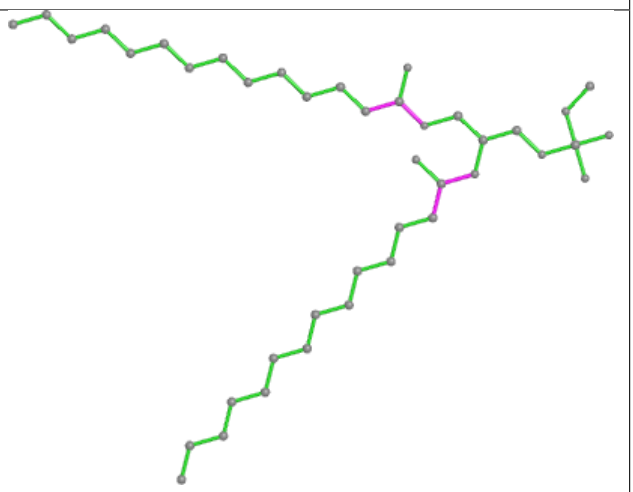
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	602	PX4	1	0
6	E	602	PX4	1	0
6	A	602	PX4	1	0
7	E	603	BOG	1	0
7	I	604	BOG	1	0
6	I	603	PX4	2	0

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 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.

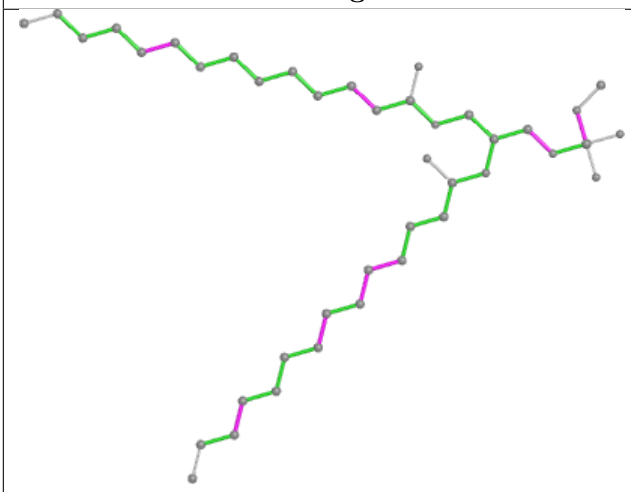
Ligand PX4 I 602



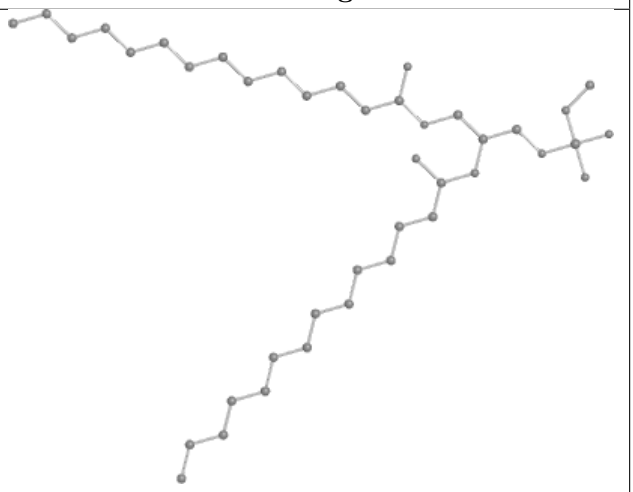
Bond lengths



Bond angles

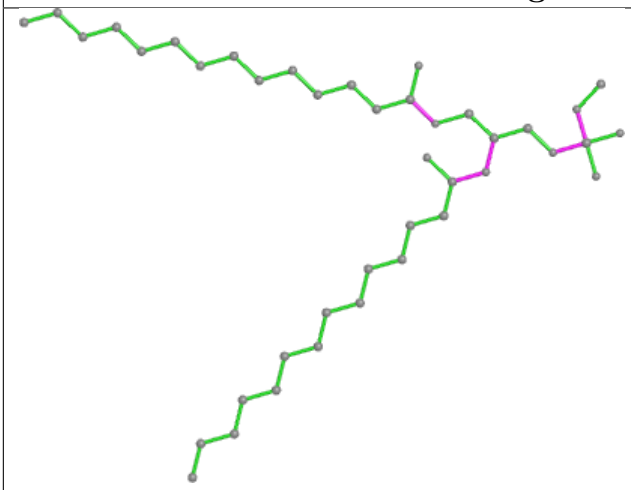


Torsions



Rings

Ligand PX4 E 602



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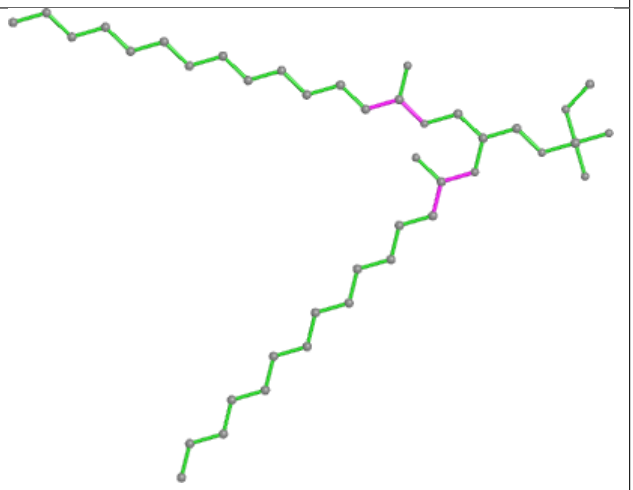

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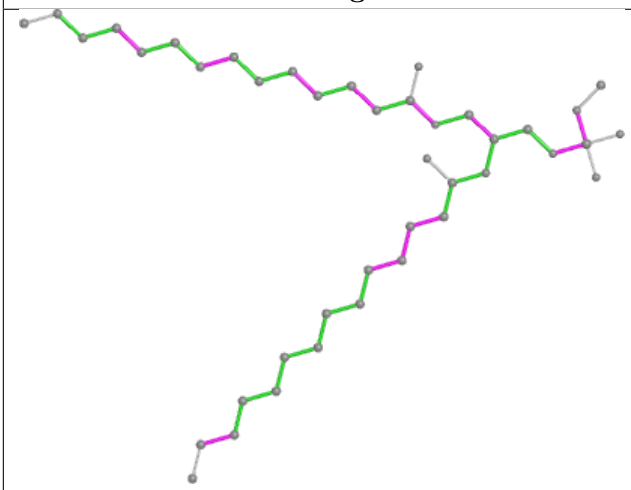

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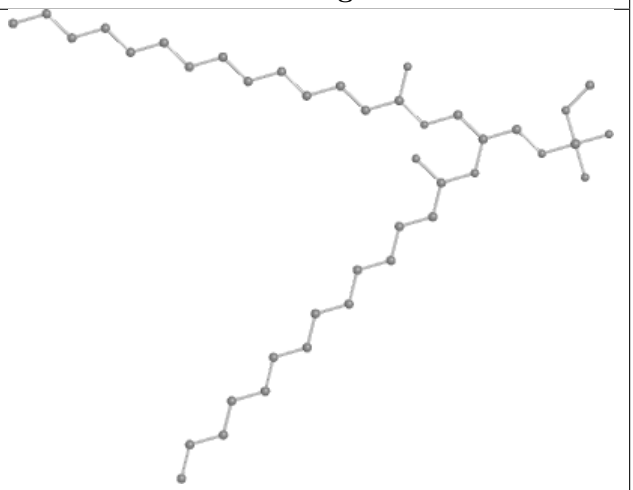
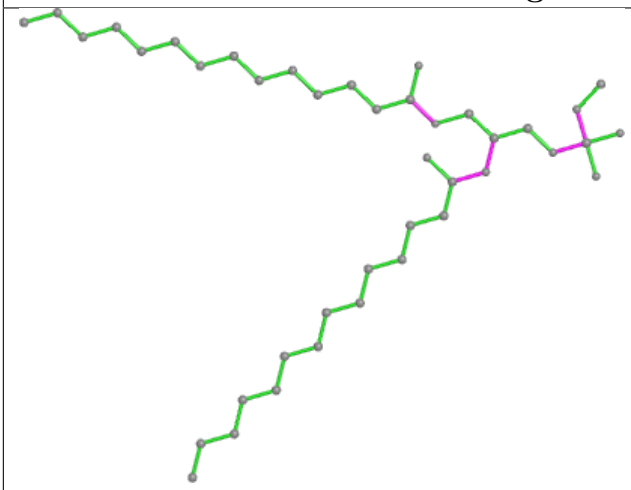


Rings

Ligand PX4 A 603



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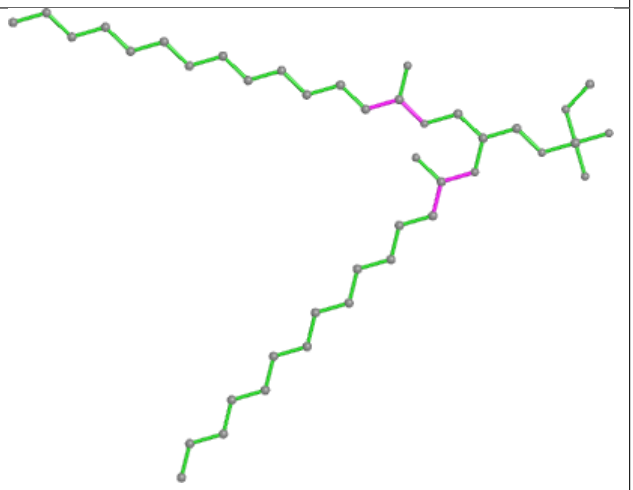

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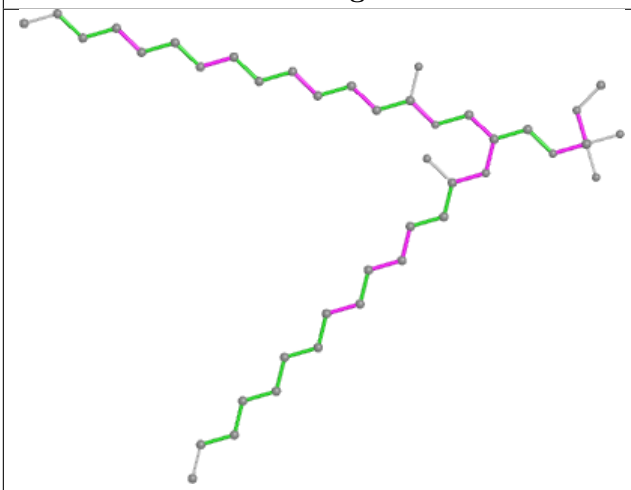

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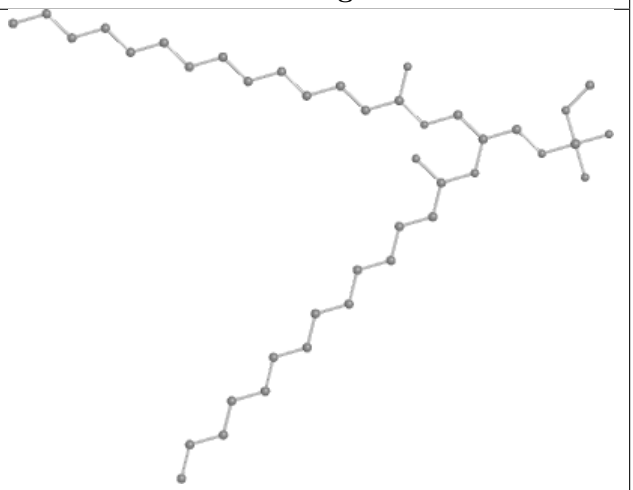
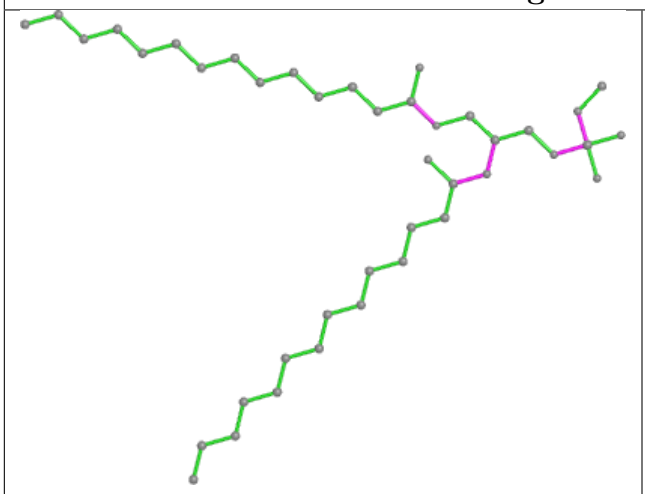


Rings

Ligand PX4 A 602



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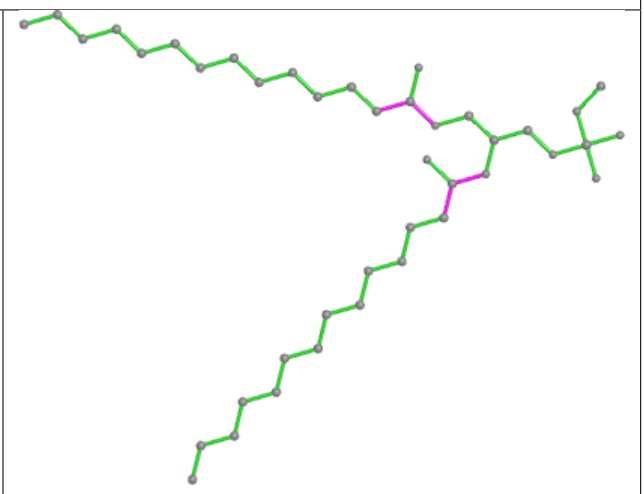

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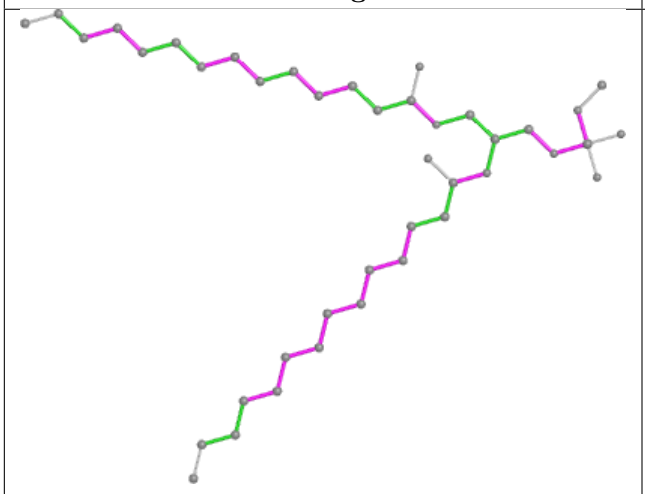

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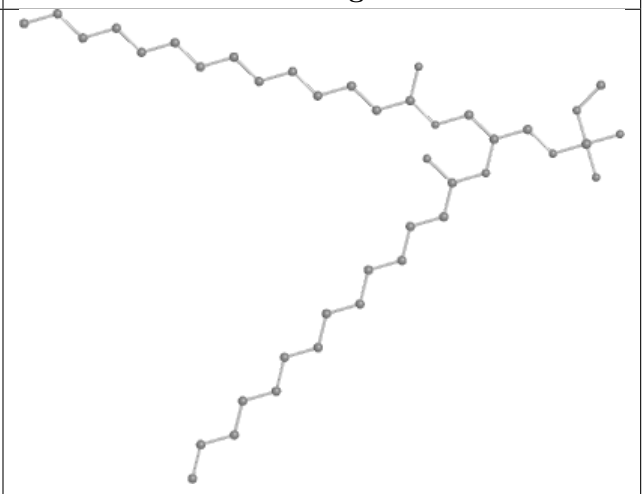
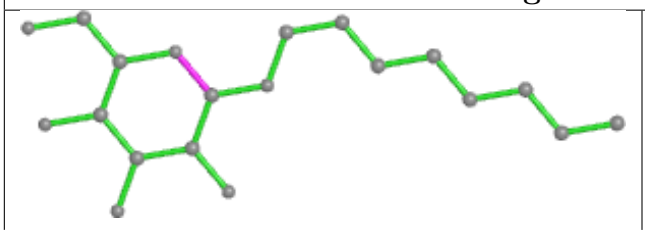


Rings

Ligand BOG E 603



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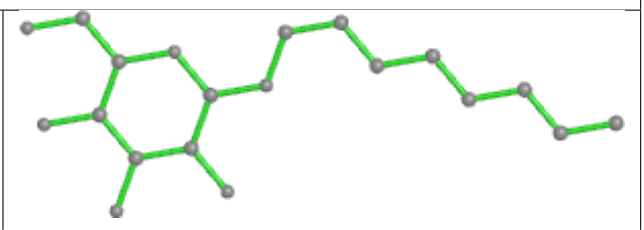

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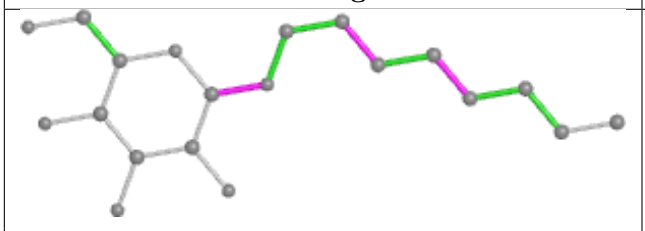

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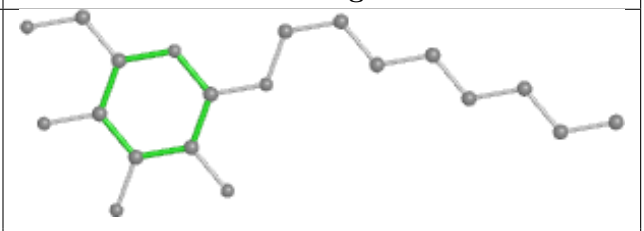

Rings

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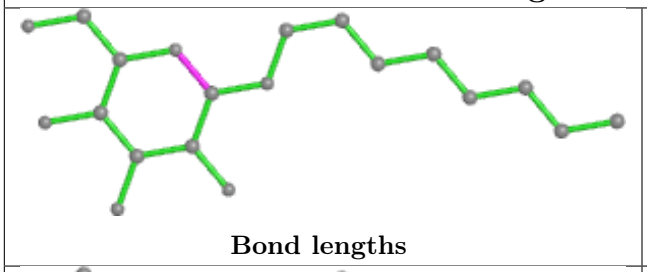

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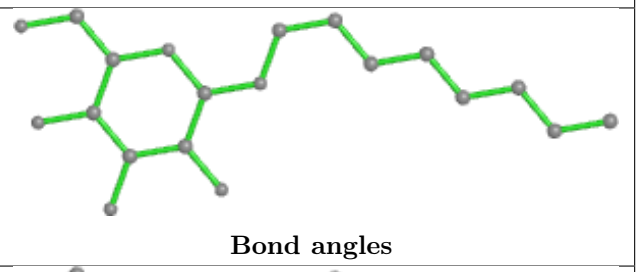
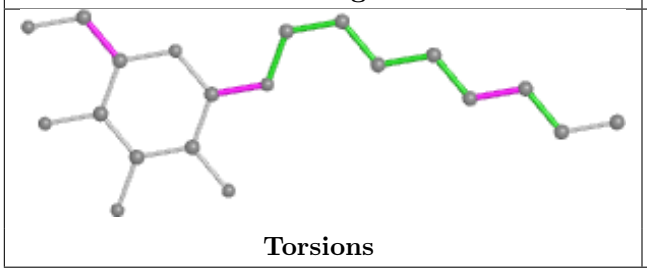


Bond angles



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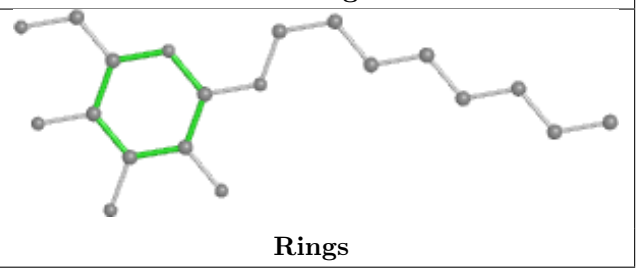
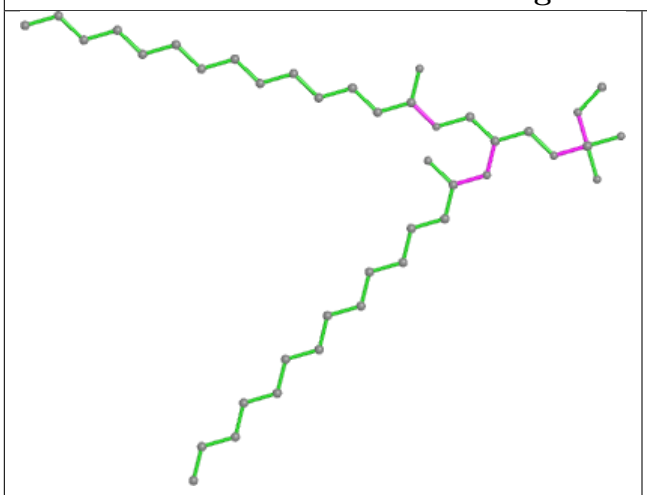
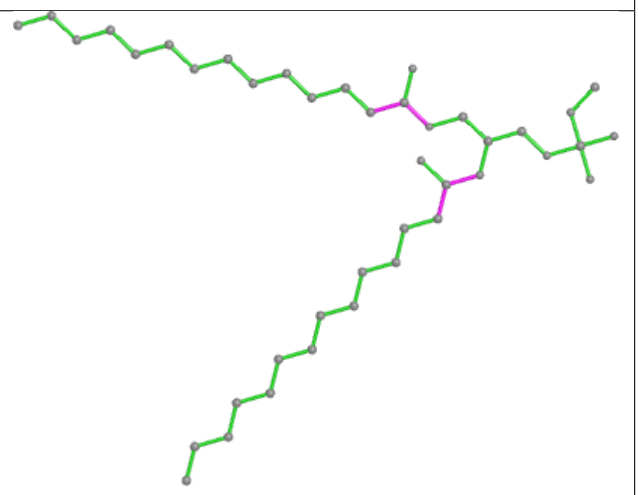


Rings

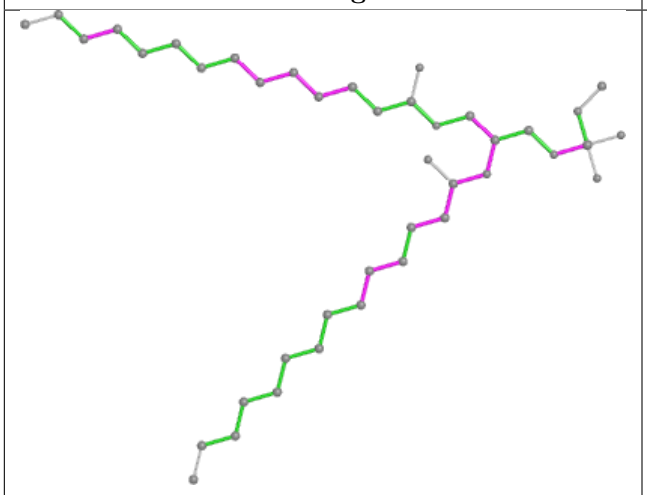
Ligand PX4 I 603



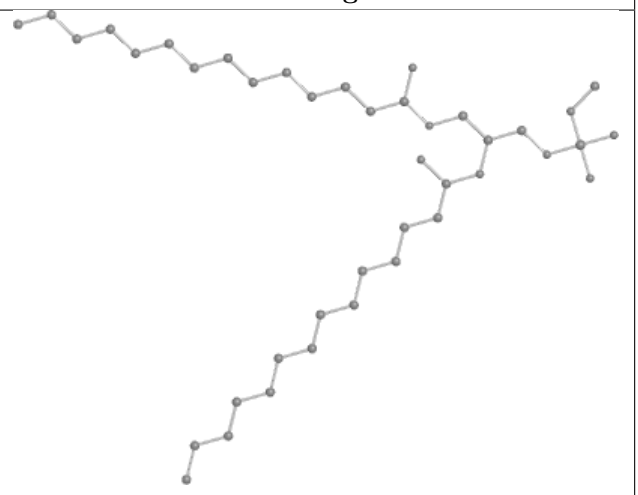
Bond lengths



Bond angles

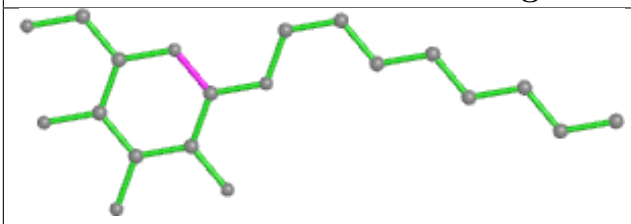


Torsions

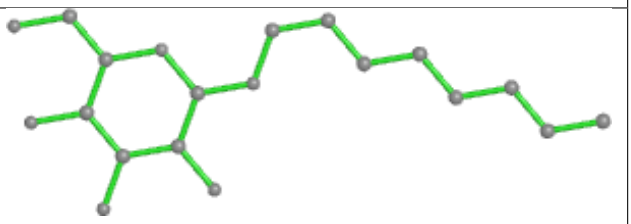


Rings

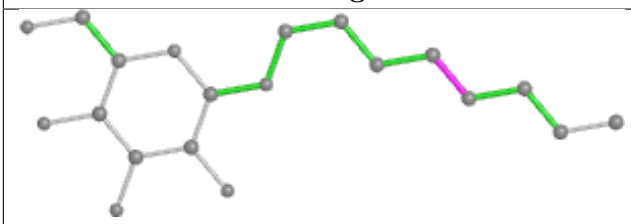
Ligand BOG B 701



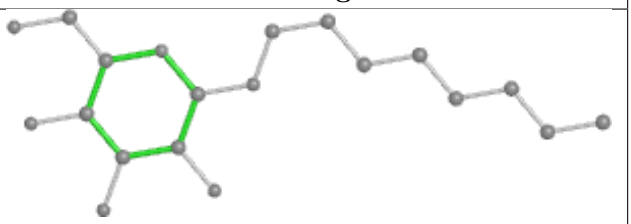
Bond lengths



Bond angles

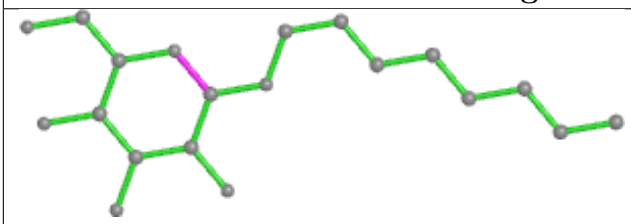


Torsions

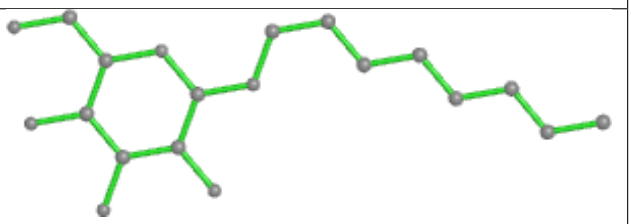


Rings

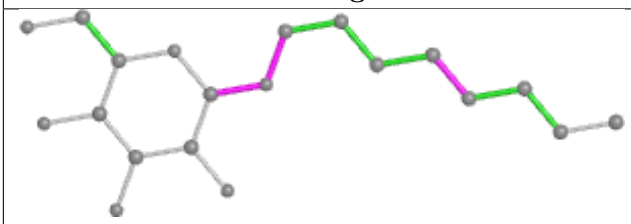
Ligand BOG A 604



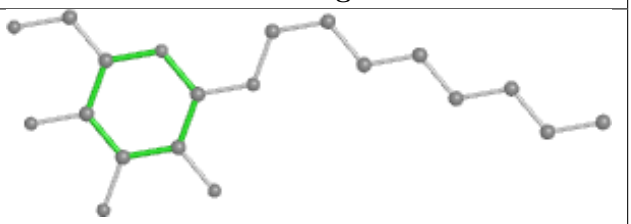
Bond lengths



Bond angles

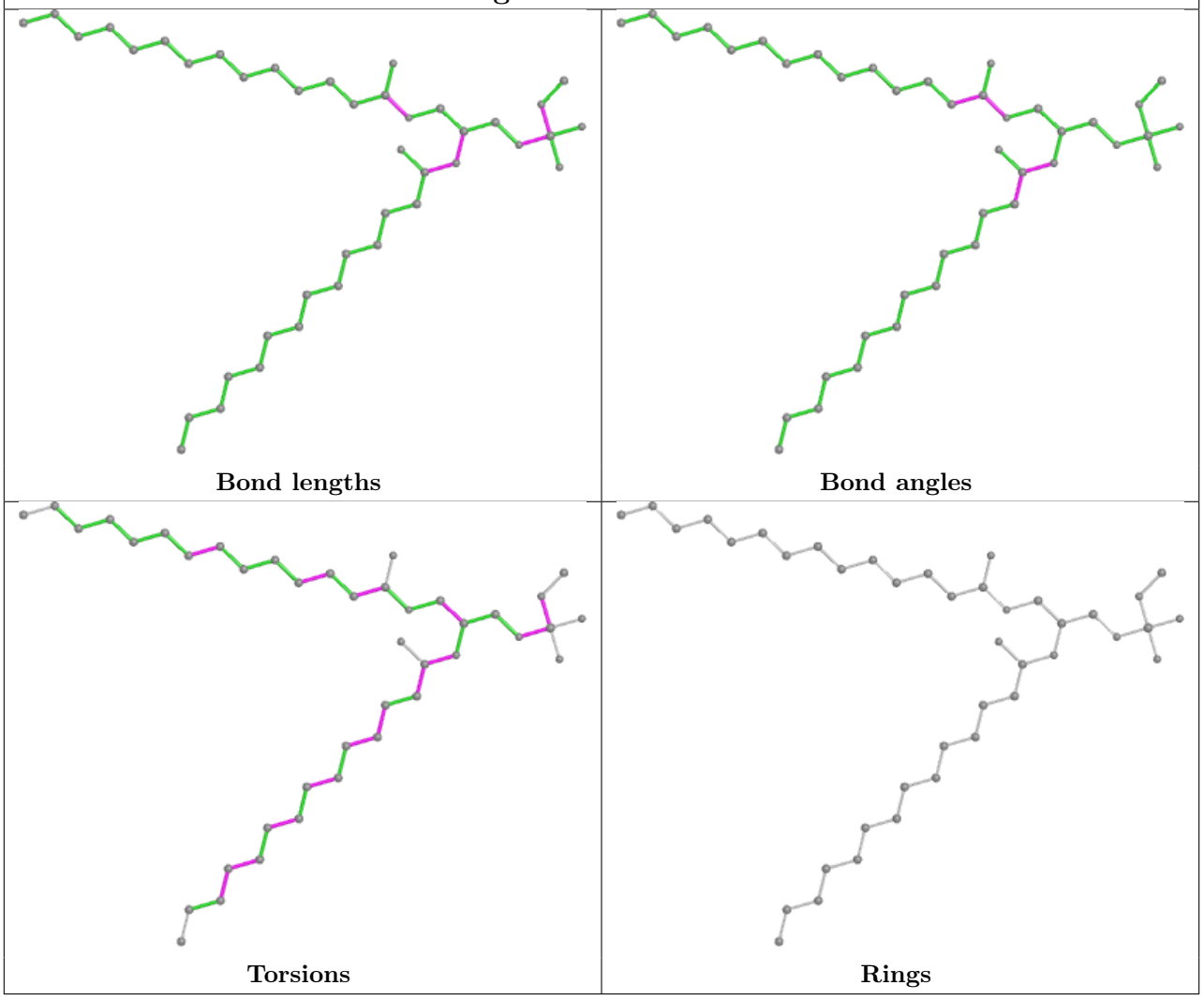


Torsions



Rings

Ligand PX4 H 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	557/557 (100%)	0.53	58 (10%) 6 5	84, 115, 153, 208	0
1	E	557/557 (100%)	0.43	43 (7%) 13 10	83, 116, 151, 232	0
1	I	557/557 (100%)	0.54	56 (10%) 7 5	92, 121, 160, 225	0
2	B	673/674 (99%)	0.71	95 (14%) 2 2	107, 152, 241, 371	0
2	F	673/674 (99%)	0.99	143 (21%) 0 0	108, 162, 253, 364	0
2	J	673/674 (99%)	1.39	188 (27%) 0 0	117, 184, 310, 484	0
3	C	187/187 (100%)	0.37	9 (4%) 30 27	102, 128, 169, 226	0
3	G	187/187 (100%)	0.40	17 (9%) 9 6	109, 134, 184, 250	0
3	K	187/187 (100%)	0.36	15 (8%) 12 9	103, 134, 191, 267	0
4	D	27/27 (100%)	0.21	2 (7%) 14 11	122, 149, 186, 203	0
4	H	27/27 (100%)	-0.02	2 (7%) 14 11	118, 143, 187, 212	0
4	L	27/27 (100%)	0.43	4 (14%) 2 1	132, 158, 231, 255	0
All	All	4332/4335 (99%)	0.73	632 (14%) 2 1	83, 138, 246, 484	0

The worst 5 of 632 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	388	ILE	11.9
2	B	539	THR	11.4
2	J	12	THR	11.2
2	J	388	ILE	11.1
2	J	103	THR	11.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
2	SEP	J	162	10/11	0.68	0.19	218,226,232,235	0
2	SEP	F	162	10/11	0.79	0.35	169,175,199,205	0
2	SEP	B	162	10/11	0.94	0.20	153,163,177,182	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

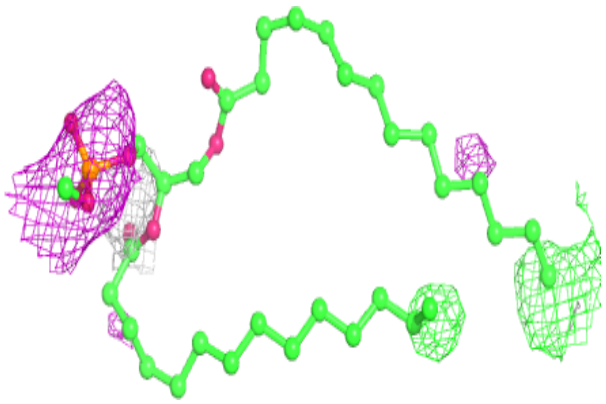
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

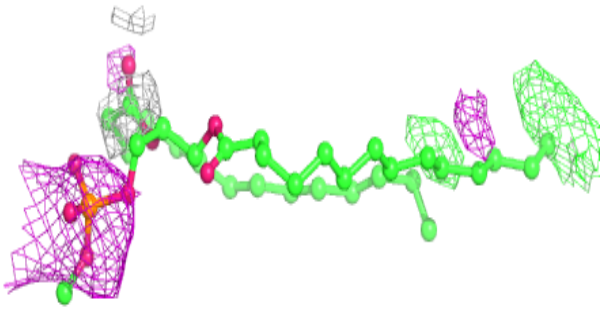
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PX4	E	602	41/46	0.31	0.75	199,227,281,284	0
6	PX4	I	602	41/46	0.48	0.67	167,183,225,228	0
6	PX4	A	602	41/46	0.59	0.46	156,188,203,205	0
6	PX4	A	603	41/46	0.67	0.44	130,169,230,232	0
6	PX4	H	101	41/46	0.69	0.42	171,197,211,214	0
5	K	E	601	1/1	0.72	0.34	124,124,124,124	0
6	PX4	I	603	41/46	0.73	0.46	164,204,226,228	0
5	K	I	601	1/1	0.77	0.37	123,123,123,123	0
7	BOG	B	701	20/20	0.78	0.33	173,185,194,195	0
7	BOG	E	603	20/20	0.78	0.23	154,184,190,194	0
7	BOG	A	604	20/20	0.85	0.32	178,191,198,198	0
5	K	A	601	1/1	0.86	0.36	123,123,123,123	0
7	BOG	I	604	20/20	0.88	0.41	205,221,224,227	0

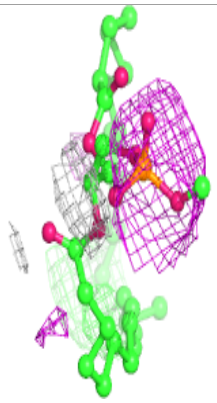
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PX4 E 602:

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

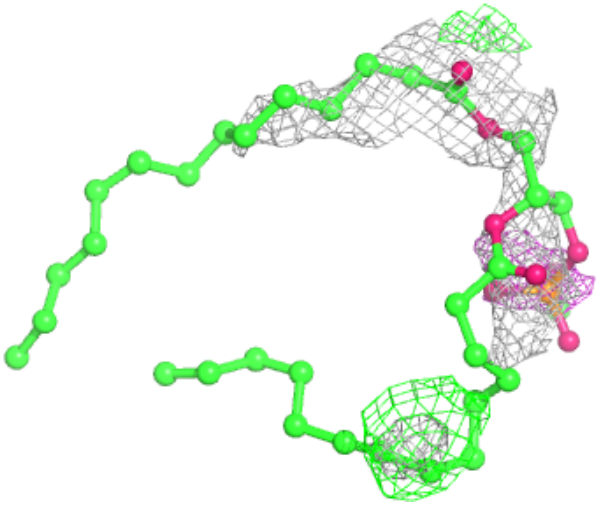


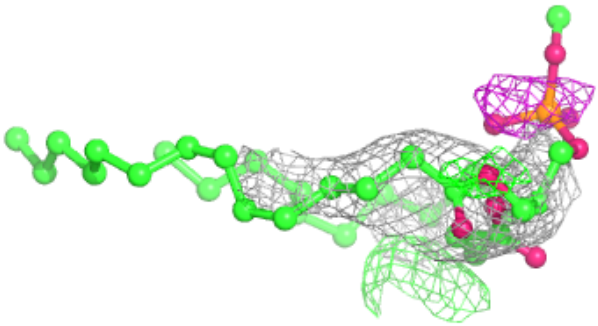


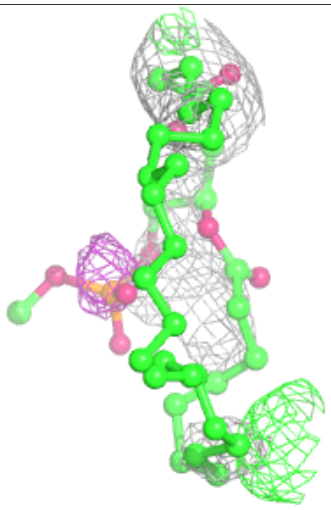


Electron density around PX4 I 602:

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

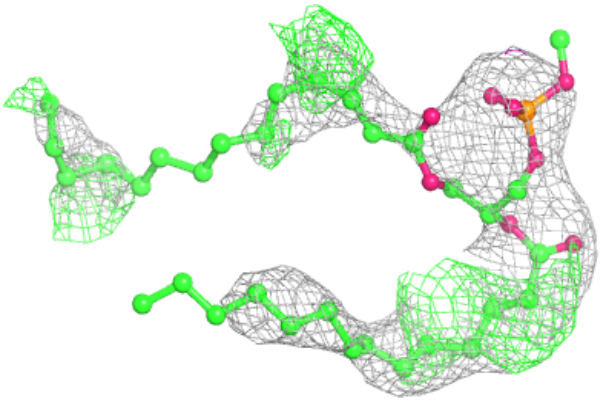


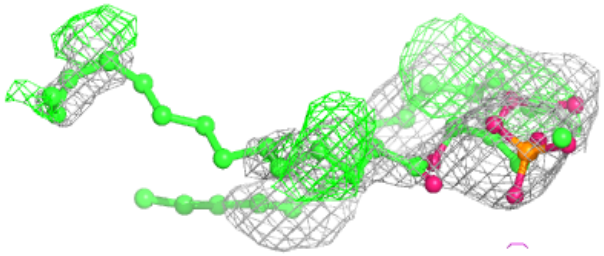


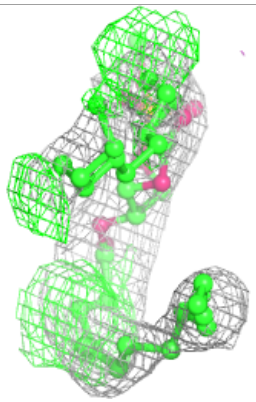


Electron density around PX4 A 602:

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

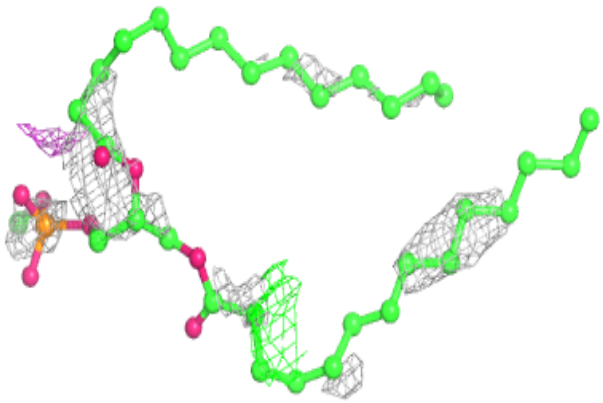


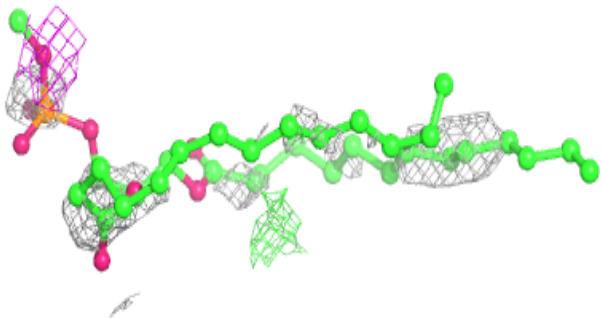


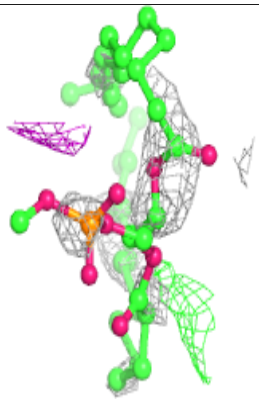


Electron density around PX4 A 603:

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

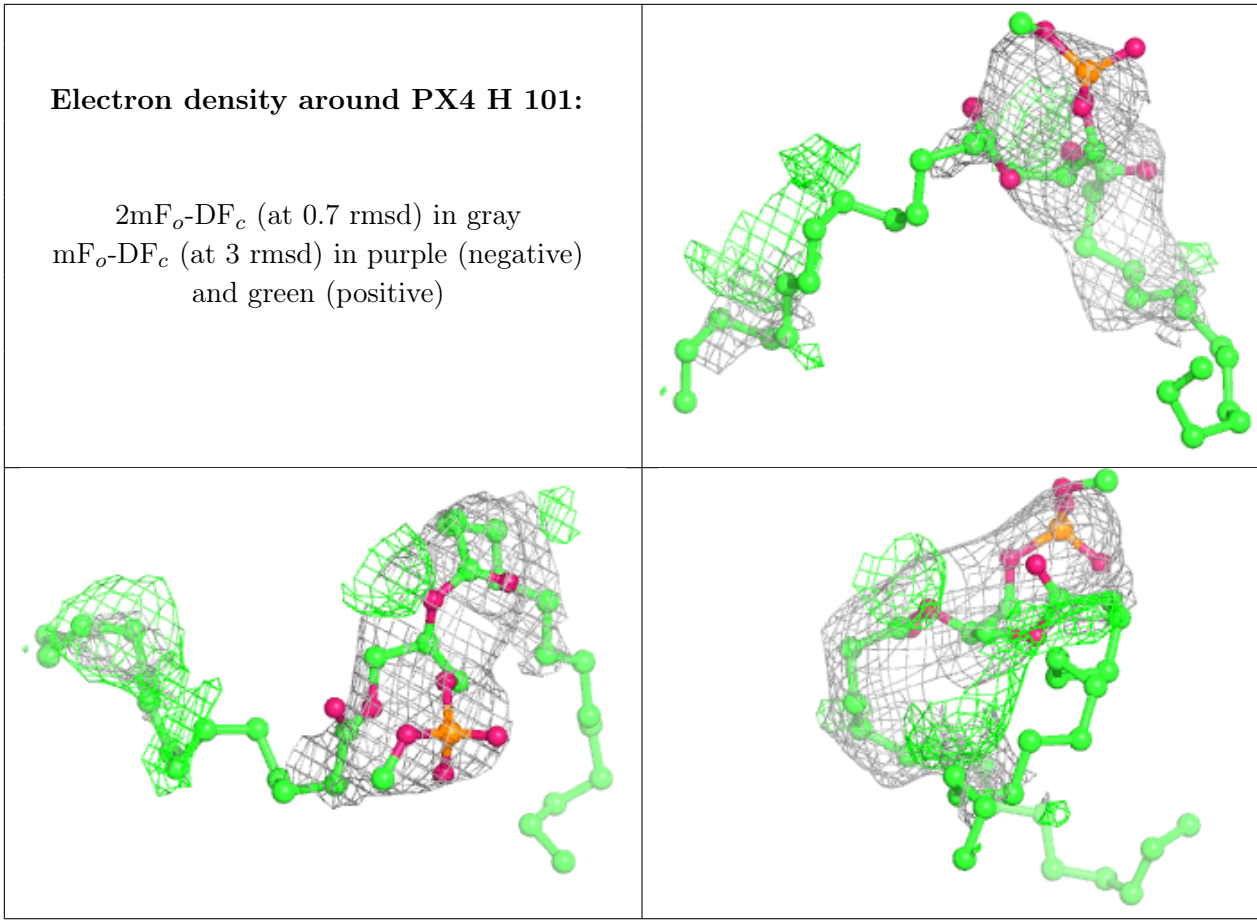






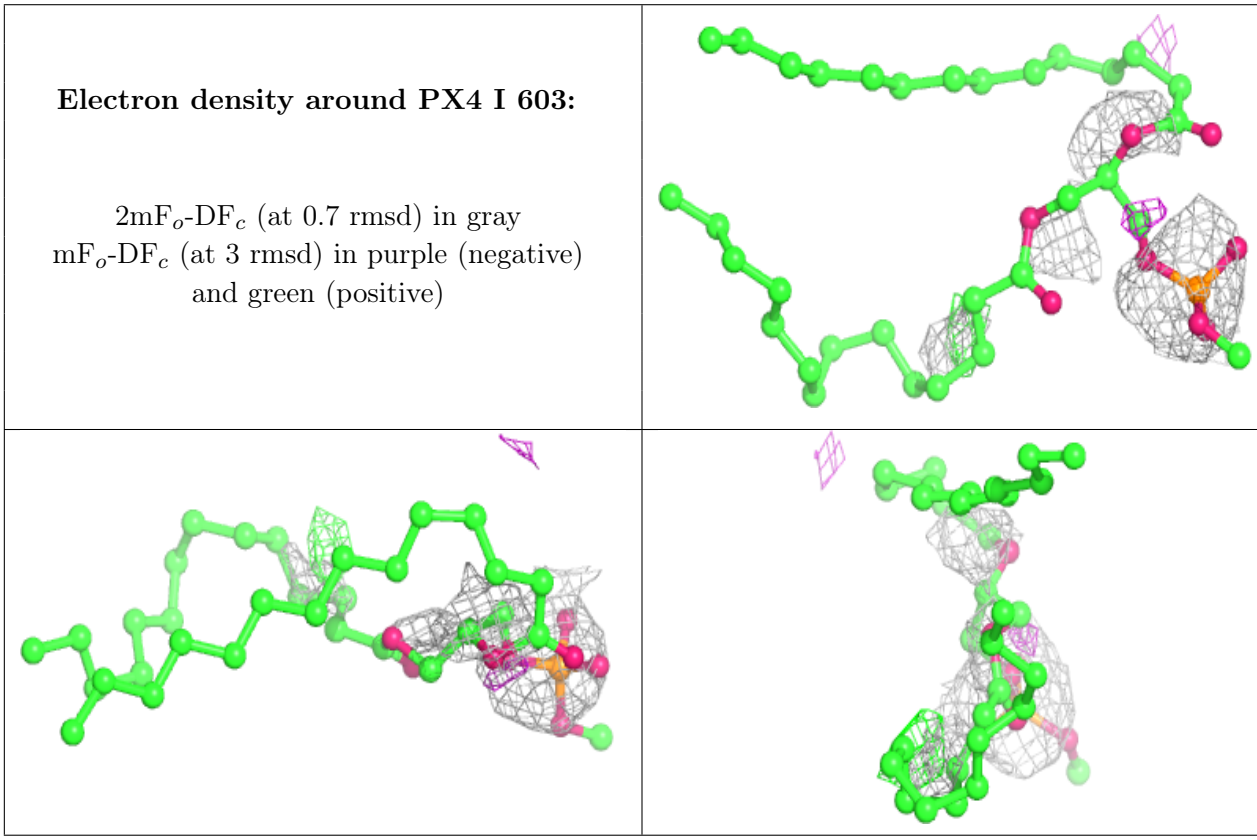
Electron density around PX4 H 101:

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



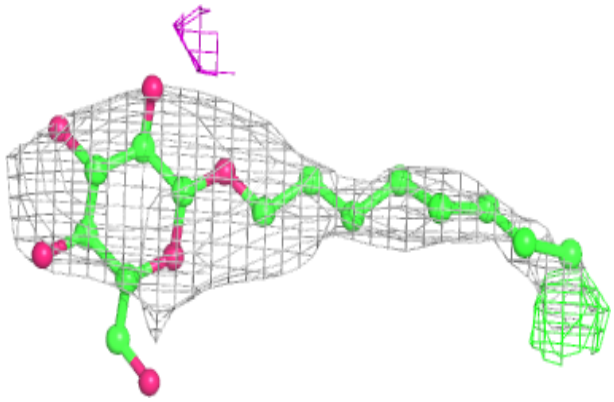
Electron density around PX4 I 603:

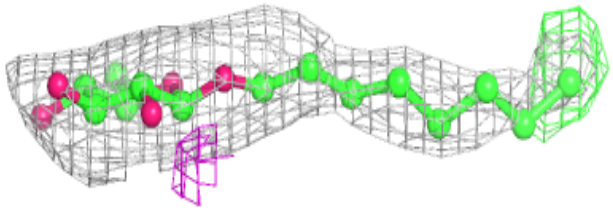
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

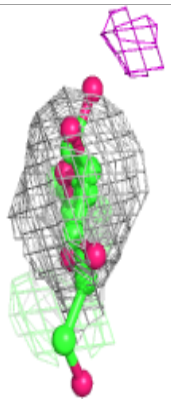


Electron density around BOG B 701:

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

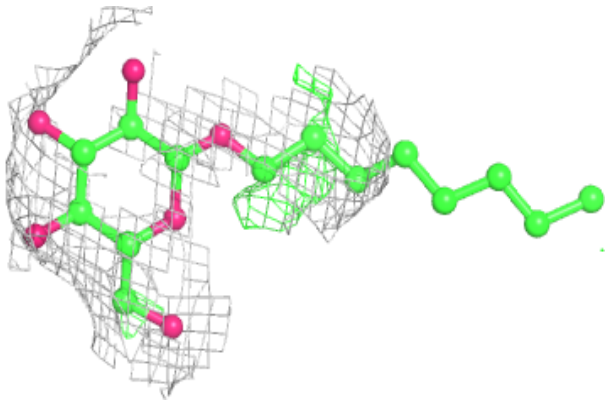


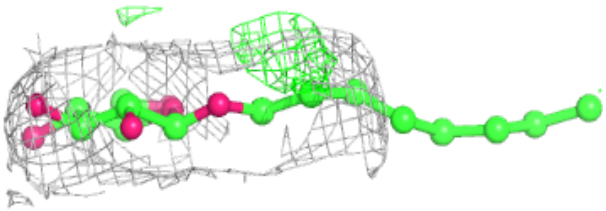


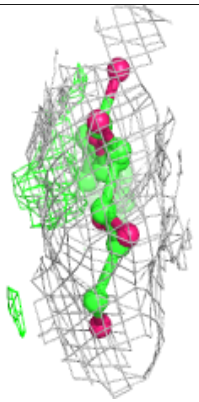


Electron density around BOG E 603:

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

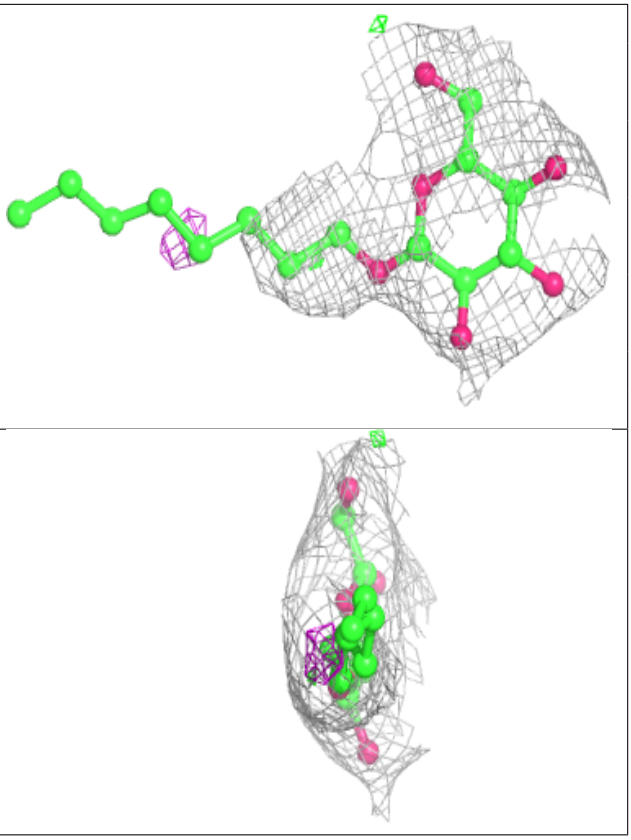






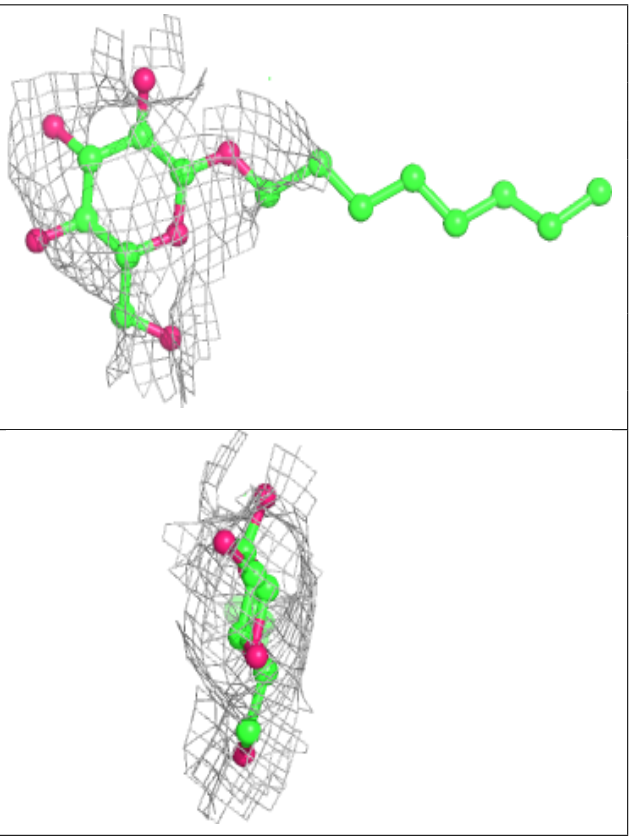
Electron density around BOG A 604:

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



Electron density around BOG I 604:

$2mF_o$-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.