Full wwPDB X-ray Structure Validation Report (i)

May 19, 2020 – 03:31 am BST

PDB ID	:	6C1K
Title	:	HypoPP mutant with ligand1
Authors	:	Catterall, W.A.; Zheng, N.; Jiang, D.; Gamal El-Din, T.M.
Deposited on	:	2018-01-04
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

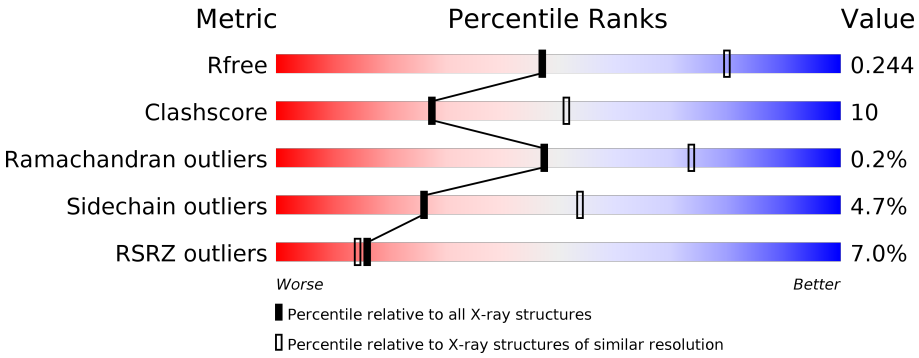
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	285	5% 59% 16% • 22%
1	B	285	6% 59% 18% • 22%

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
2	GAI	A	1301	-	X	-	-
3	PX4	A	1308	-	-	-	X
5	SO4	A	1313	-	-	X	-
5	SO4	B	2312	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4059 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1802	1228	267	294	13			
1	B	221	Total	C	N	O	S	0	0	0
			1803	1229	267	294	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	initiating methionine	UNP A8EVM5
A	984	ASP	-	expression tag	UNP A8EVM5
A	985	TYR	-	expression tag	UNP A8EVM5
A	986	LYS	-	expression tag	UNP A8EVM5
A	987	ASP	-	expression tag	UNP A8EVM5
A	988	ASP	-	expression tag	UNP A8EVM5
A	989	ASP	-	expression tag	UNP A8EVM5
A	990	ASP	-	expression tag	UNP A8EVM5
A	991	LYS	-	expression tag	UNP A8EVM5
A	992	GLY	-	expression tag	UNP A8EVM5
A	993	SER	-	expression tag	UNP A8EVM5
A	994	LEU	-	expression tag	UNP A8EVM5
A	995	VAL	-	expression tag	UNP A8EVM5
A	996	PRO	-	expression tag	UNP A8EVM5
A	997	ARG	-	expression tag	UNP A8EVM5
A	998	GLY	-	expression tag	UNP A8EVM5
A	999	SER	-	expression tag	UNP A8EVM5
A	1000	HIS	-	expression tag	UNP A8EVM5
A	1102	GLY	ARG	engineered mutation	UNP A8EVM5
A	1217	CYS	ILE	engineered mutation	UNP A8EVM5
B	1983	MET	-	initiating methionine	UNP A8EVM5
B	1984	ASP	-	expression tag	UNP A8EVM5
B	1985	TYR	-	expression tag	UNP A8EVM5
B	1986	LYS	-	expression tag	UNP A8EVM5
B	1987	ASP	-	expression tag	UNP A8EVM5

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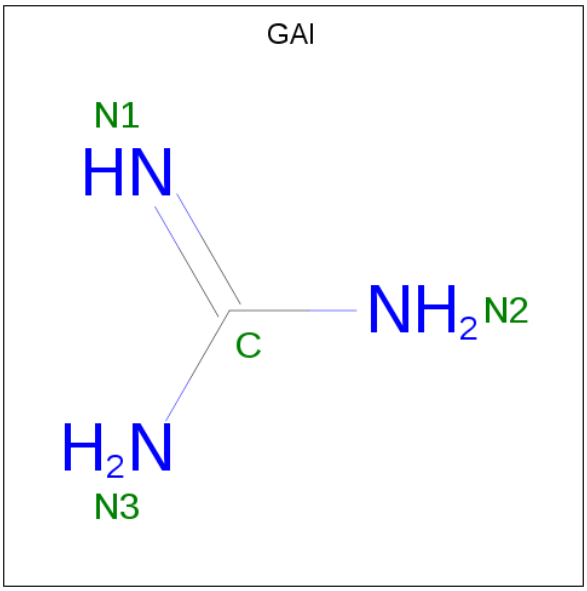
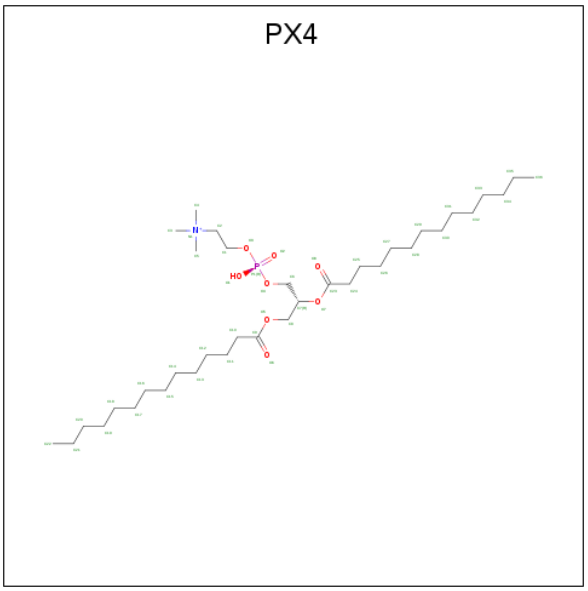
Chain	Residue	Modelled	Actual	Comment	Reference
B	1988	ASP	-	expression tag	UNP A8EVM5
B	1989	ASP	-	expression tag	UNP A8EVM5
B	1990	ASP	-	expression tag	UNP A8EVM5
B	1991	LYS	-	expression tag	UNP A8EVM5
B	1992	GLY	-	expression tag	UNP A8EVM5
B	1993	SER	-	expression tag	UNP A8EVM5
B	1994	LEU	-	expression tag	UNP A8EVM5
B	1995	VAL	-	expression tag	UNP A8EVM5
B	1996	PRO	-	expression tag	UNP A8EVM5
B	1997	ARG	-	expression tag	UNP A8EVM5
B	1998	GLY	-	expression tag	UNP A8EVM5
B	1999	SER	-	expression tag	UNP A8EVM5
B	2000	HIS	-	expression tag	UNP A8EVM5
B	2102	GLY	ARG	engineered mutation	UNP A8EVM5
B	2217	CYS	ILE	engineered mutation	UNP A8EVM5

- Molecule 2 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 4 1 3	0	0
2	B	1	Total C N 4 1 3	0	0

- Molecule 3 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
3	A	1	Total C O P 10 3 6 1	0	0
3	A	1	Total C N O P 46 36 1 8 1	0	0
3	A	1	Total C O 16 14 2	0	0
3	A	1	Total C O P 23 16 6 1	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C O P 41 32 8 1	0	0
3	A	1	Total C O 20 17 3	0	0
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C O 17 15 2	0	0
3	B	1	Total C N O P 37 27 1 8 1	0	0
3	B	1	Total C N O P 46 36 1 8 1	0	0
3	B	1	Total C O 16 14 2	0	0
3	B	1	Total C O 17 15 2	0	0
3	B	1	Total C N O P 38 28 1 8 1	0	0

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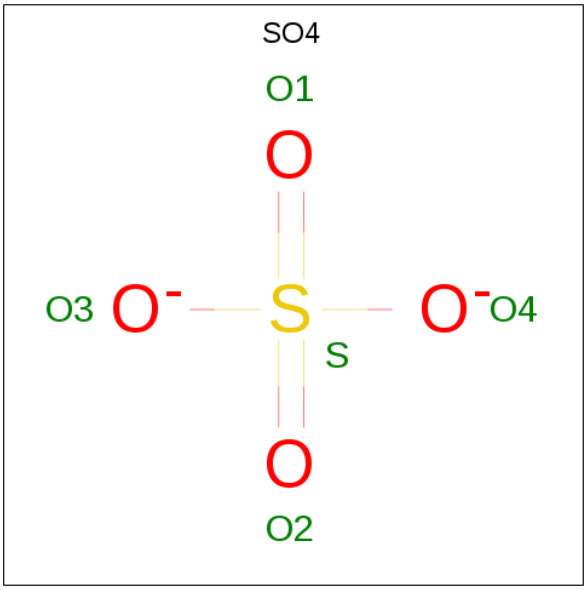
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O P 46 36 1 8 1	0	0
3	B	1	Total C O P 25 17 7 1	0	0
3	B	1	Total C 6 6	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Na 2 2	0	0
4	A	2	Total Na 2 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

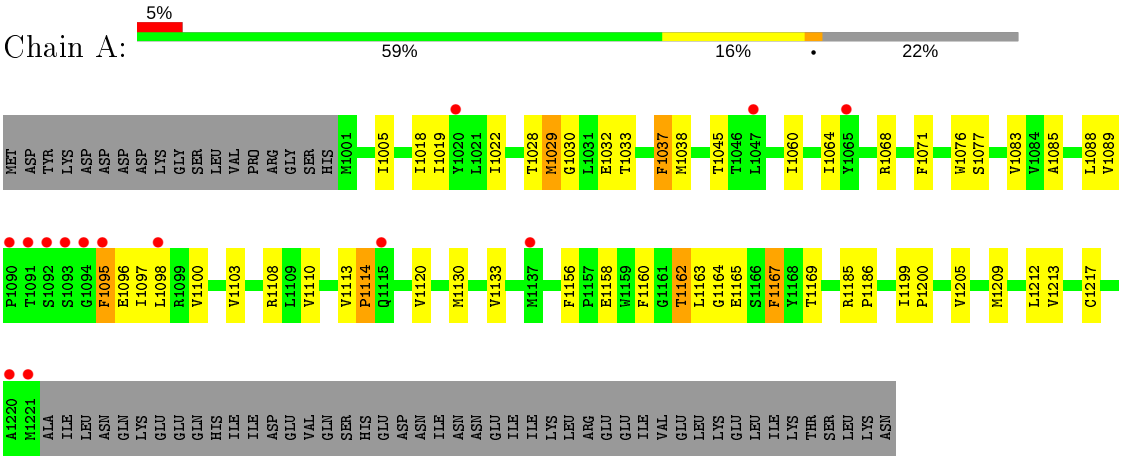
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	B	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

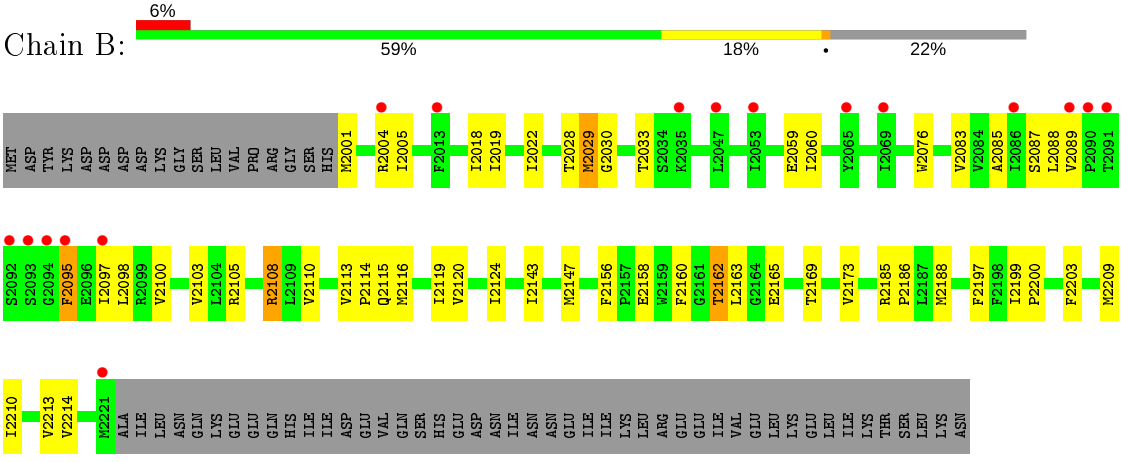
- Molecule 1: Ion transport protein

Chain A:



- Molecule 1: Ion transport protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	126.39Å 126.23Å 191.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.31 – 2.70 42.31 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (42.31-2.70) 97.0 (42.31-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.246 0.214 , 0.244	Depositor DCC
R_{free} test set	1981 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 82.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.469 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4059	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: NA, SO4, GAI, PX4

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	0.51	0/1852	0.58	1/2519 (0.0%)
1	B	0.50	0/1854	0.58	0/2522
All	All	0.50	0/3706	0.58	1/5041 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1037	PHE	CG-CD1-CE1	5.58	126.94	120.80

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	1802	0	1870	37	0
1	B	1803	0	1873	38	0
2	A	4	0	5	0	0
2	B	4	0	4	0	0
3	A	196	0	281	9	0
3	B	231	0	339	17	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	2	0
5	B	5	0	0	2	0
6	A	1	0	0	0	0
6	B	4	0	0	0	0
All	All	4059	0	4372	84	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (84) 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:1162:THR:HG22	1:A:1165:GLU:H	1.41	0.84
1:B:2162:THR:HG22	1:B:2165:GLU:H	1.43	0.83
1:B:2197:PHE:HB2	3:B:2307:PX4:H50	1.64	0.80
1:A:1085:ALA:HA	1:A:1088:LEU:HD12	1.74	0.70
3:A:1308:PX4:H45	3:B:2307:PX4:H40	1.75	0.69
1:A:1100:VAL:O	1:A:1103:VAL:HG12	1.96	0.66
1:B:2089:VAL:HG11	1:B:2098:LEU:HD13	1.78	0.66
1:B:2100:VAL:O	1:B:2103:VAL:HG12	1.97	0.65
1:B:2085:ALA:HA	1:B:2088:LEU:HD12	1.80	0.62
1:A:1037:PHE:CD2	1:A:1037:PHE:CZ	2.86	0.62
1:B:2087:SER:OG	1:B:2105:ARG:NH2	2.32	0.61
1:A:1089:VAL:HG11	1:A:1098:LEU:HD13	1.82	0.61
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.83	0.60
3:B:2301:PX4:H19	3:B:2301:PX4:H46	1.84	0.60
1:A:1103:VAL:HG11	1:B:2147:MET:HG2	1.85	0.57
1:B:2199:ILE:HB	1:B:2200:PRO:HD3	1.87	0.56
1:A:1217:CYS:SG	1:B:2214:VAL:HG22	2.45	0.56
1:B:2018:ILE:O	1:B:2022:ILE:HG12	2.07	0.55
1:A:1130:MET:HE2	1:A:1212:LEU:HD11	1.90	0.54
1:B:2076:TRP:CZ2	3:B:2308:PX4:H19	2.42	0.54
1:A:1209:MET:O	1:A:1213:VAL:HG23	2.07	0.54
3:B:2307:PX4:H17	3:B:2307:PX4:O2	2.08	0.54
1:A:1167:PHE:HB3	3:B:2301:PX4:H47	1.91	0.53
1:B:2124:ILE:HD12	3:B:2308:PX4:H20	1.90	0.52
1:B:2097:ILE:HD13	3:B:2302:PX4:H49	1.91	0.52
1:B:2076:TRP:CH2	3:B:2308:PX4:H19	2.45	0.51
1:A:1018:ILE:O	1:A:1022:ILE:HG12	2.10	0.51
1:B:2156:PHE:HD1	5:B:2312:SO4:O3	1.94	0.50
1:A:1030:GLY:O	1:A:1033:THR:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2022:ILE:HD12	1:B:2108:ARG:HB3	1.94	0.49
1:A:1032:GLU:HG3	1:A:1045:THR:HG21	1.95	0.49
1:A:1095:PHE:HB2	1:A:1097:ILE:HG13	1.95	0.49
1:B:2113:VAL:HG12	1:B:2114:PRO:O	2.13	0.49
1:A:1213:VAL:HG13	1:B:2210:ILE:HG23	1.95	0.49
1:A:1038:MET:HE2	1:A:1038:MET:HA	1.93	0.48
1:A:1185:ARG:HB2	1:A:1186:PRO:HD3	1.94	0.48
1:B:2188:MET:SD	3:B:2301:PX4:H7	2.53	0.48
1:B:2019:ILE:HD13	1:B:2113:VAL:HG22	1.95	0.48
1:B:2029:MET:HE1	1:B:2103:VAL:HA	1.95	0.47
3:B:2301:PX4:H64	3:B:2301:PX4:H59	1.50	0.47
1:B:2209:MET:O	1:B:2213:VAL:HG23	2.13	0.47
1:A:1076:TRP:CZ2	3:A:1305:PX4:H46	2.49	0.47
1:A:1029:MET:HE3	1:A:1103:VAL:HG23	1.96	0.47
1:B:2059:GLU:OE1	1:B:2108:ARG:NH2	2.48	0.47
1:A:1019:ILE:HD13	1:A:1113:VAL:HG22	1.96	0.46
3:A:1307:PX4:H24	3:A:1307:PX4:H55	1.97	0.46
1:A:1033:THR:HG21	1:B:2163:LEU:HB2	1.98	0.45
1:B:2059:GLU:CD	1:B:2108:ARG:HH22	2.20	0.45
1:B:2095:PHE:HB2	1:B:2097:ILE:HG13	1.97	0.45
1:B:2160:PHE:CZ	1:B:2169:THR:HG21	2.52	0.45
1:A:1160:PHE:CZ	1:A:1169:THR:HG21	2.52	0.45
1:B:2114:PRO:O	1:B:2116:MET:N	2.44	0.45
1:B:2185:ARG:HB2	1:B:2186:PRO:HD3	1.99	0.45
3:B:2307:PX4:H37	3:B:2307:PX4:H32	1.47	0.45
1:A:1029:MET:HE3	1:A:1103:VAL:HA	1.99	0.45
1:A:1156:PHE:HD1	5:A:1313:SO4:O4	1.99	0.45
1:B:2115:GLN:O	1:B:2119:ILE:HG12	2.17	0.45
3:B:2307:PX4:H66	3:B:2307:PX4:H35	1.99	0.45
1:B:2001:MET:HG3	1:B:2004:ARG:HD3	1.99	0.44
1:A:1110:VAL:HG11	1:A:1120:VAL:HG21	1.98	0.44
1:A:1158:GLU:N	5:A:1313:SO4:O3	2.50	0.44
1:A:1071:PHE:CE2	1:A:1077:SER:HB3	2.52	0.44
1:B:2030:GLY:O	1:B:2033:THR:HB	2.17	0.44
1:B:2143:ILE:O	1:B:2147:MET:HG3	2.17	0.43
1:A:1113:VAL:HG12	1:A:1114:PRO:O	2.19	0.43
1:A:1064:ILE:O	1:A:1068:ARG:N	2.43	0.43
1:A:1209:MET:CE	3:B:2301:PX4:H71	2.49	0.43
3:A:1309:PX4:H22	3:A:1309:PX4:H27	1.83	0.43
1:A:1018:ILE:HD13	1:A:1018:ILE:HA	1.82	0.42
3:A:1307:PX4:H59	3:A:1307:PX4:H29	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2095:PHE:CD1	1:B:2097:ILE:HD12	2.55	0.42
3:B:2302:PX4:H25	3:B:2302:PX4:H20	1.77	0.42
3:A:1307:PX4:H49	3:A:1307:PX4:H19	2.02	0.41
3:B:2307:PX4:H19	3:B:2307:PX4:H47	2.01	0.41
1:A:1076:TRP:CZ3	3:A:1305:PX4:H50	2.54	0.41
1:B:2169:THR:O	1:B:2173:VAL:HG23	2.20	0.41
1:A:1133:VAL:HG11	1:A:1212:LEU:HD12	2.02	0.41
1:A:1164:GLY:HA2	3:B:2301:PX4:H17	2.03	0.41
1:A:1029:MET:CE	1:A:1103:VAL:HA	2.51	0.41
3:A:1303:PX4:H17	3:A:1303:PX4:H19	1.83	0.41
1:B:2110:VAL:HG11	1:B:2120:VAL:HG21	2.03	0.41
3:A:1310:PX4:H37	1:B:2203:PHE:HD2	1.87	0.40
1:B:2158:GLU:N	5:B:2312:SO4:O4	2.55	0.40
1:A:1096:GLU:O	1:A:1096:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	219/285 (77%)	202 (92%)	16 (7%)	1 (0%)	29 54
1	B	219/285 (77%)	203 (93%)	16 (7%)	0	100 100
All	All	438/570 (77%)	405 (92%)	32 (7%)	1 (0%)	47 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1114	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	202/263 (77%)	191 (95%)	11 (5%)	22 47
1	B	202/263 (77%)	194 (96%)	8 (4%)	31 60
All	All	404/526 (77%)	385 (95%)	19 (5%)	26 54

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1005	ILE
1	A	1028	THR
1	A	1029	MET
1	A	1060	ILE
1	A	1083	VAL
1	A	1095	PHE
1	A	1108	ARG
1	A	1162	THR
1	A	1163	LEU
1	A	1167	PHE
1	A	1205	VAL
1	B	2005	ILE
1	B	2028	THR
1	B	2029	MET
1	B	2060	ILE
1	B	2083	VAL
1	B	2095	PHE
1	B	2108	ARG
1	B	2162	THR

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

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
3	PX4	A	1304	-	12,15,45	0.79	0	11,15,53	0.74	0
3	PX4	B	2304	-	16,16,45	1.21	1 (6%)	16,16,53	0.90	1 (6%)
3	PX4	B	2301	-	36,36,45	1.31	5 (13%)	42,44,53	1.31	3 (7%)
3	PX4	B	2308	-	24,24,45	1.10	1 (4%)	27,28,53	1.15	1 (3%)
3	PX4	A	1305	-	22,22,45	1.06	2 (9%)	25,26,53	1.43	2 (8%)
5	SO4	A	1313	-	4,4,4	0.21	0	6,6,6	0.36	0
3	PX4	A	1308	-	19,19,45	1.22	1 (5%)	19,19,53	1.10	2 (10%)
3	PX4	B	2309	-	5,5,45	0.77	0	4,4,53	0.48	0
3	PX4	A	1306	-	5,5,45	0.75	0	4,4,53	0.49	0
5	SO4	B	2312	-	4,4,4	0.19	0	6,6,6	0.26	0
3	PX4	B	2302	-	45,45,45	1.14	3 (6%)	51,53,53	1.04	3 (5%)
3	PX4	A	1302	-	9,9,45	0.94	1 (11%)	11,12,53	0.64	0
3	PX4	A	1309	-	16,16,45	1.33	2 (12%)	16,16,53	0.94	1 (6%)
3	PX4	B	2306	-	37,37,45	1.22	3 (8%)	43,45,53	1.14	2 (4%)
3	PX4	A	1307	-	40,40,45	1.07	2 (5%)	43,45,53	1.17	3 (6%)
3	PX4	B	2303	-	12,15,45	0.76	0	11,15,53	0.84	0
2	GAI	B	2305	-	3,3,3	2.97	2 (66%)	3,3,3	1.27	0
3	PX4	A	1310	-	16,16,45	1.17	1 (6%)	16,16,53	1.00	1 (6%)
2	GAI	A	1301	-	3,3,3	4.27	3 (100%)	3,3,3	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PX4	B	2307	-	45,45,45	1.15	3 (6%)	51,53,53	1.42	6 (11%)
3	PX4	A	1303	-	45,45,45	1.19	3 (6%)	51,53,53	1.08	2 (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
3	PX4	A	1304	-	-	5/11/13/49	-
3	PX4	B	2304	-	-	6/15/15/49	-
3	PX4	B	2301	-	-	15/40/40/49	-
3	PX4	B	2308	-	-	15/24/24/49	-
3	PX4	A	1305	-	-	8/22/22/49	-
3	PX4	A	1308	-	-	10/18/18/49	-
3	PX4	B	2309	-	-	2/3/3/49	-
3	PX4	A	1306	-	-	1/3/3/49	-
3	PX4	B	2302	-	-	31/49/49/49	-
3	PX4	A	1302	-	-	8/8/8/49	-
3	PX4	A	1309	-	-	6/15/15/49	-
3	PX4	B	2306	-	-	15/41/41/49	-
3	PX4	A	1307	-	-	21/44/44/49	-
3	PX4	B	2303	-	-	5/11/13/49	-
3	PX4	A	1310	-	-	6/15/15/49	-
3	PX4	B	2307	-	-	31/49/49/49	-
3	PX4	A	1303	-	-	25/49/49/49	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	GAI	C-N1	5.81	1.42	1.30
3	B	2301	PX4	O5-C9	4.25	1.45	1.33
3	A	1308	PX4	O5-C9	4.01	1.45	1.33
2	A	1301	GAI	C-N2	3.90	1.43	1.36
3	A	1307	PX4	O5-C9	3.89	1.44	1.33
3	A	1309	PX4	O5-C9	3.87	1.45	1.33
3	B	2302	PX4	O5-C9	3.82	1.44	1.33
3	B	2308	PX4	O5-C9	3.81	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1303	PX4	O5-C9	3.78	1.44	1.33
3	B	2304	PX4	O5-C9	3.77	1.45	1.33
3	B	2307	PX4	O7-C23	3.71	1.44	1.34
2	B	2305	GAI	C-N3	3.71	1.42	1.36
3	B	2307	PX4	O5-C9	3.71	1.44	1.33
3	A	1310	PX4	O5-C9	3.67	1.44	1.33
3	A	1303	PX4	O7-C23	3.56	1.44	1.34
3	B	2306	PX4	O5-C9	3.54	1.43	1.33
2	B	2305	GAI	C-N2	3.53	1.42	1.36
3	B	2301	PX4	O7-C23	3.27	1.43	1.34
3	B	2302	PX4	O7-C23	3.18	1.43	1.34
3	A	1307	PX4	O7-C23	3.17	1.43	1.34
3	B	2306	PX4	O7-C23	3.16	1.43	1.34
3	A	1305	PX4	O7-C23	3.10	1.43	1.34
3	A	1303	PX4	C4-N1	-2.91	1.41	1.50
3	B	2301	PX4	C4-N1	-2.77	1.41	1.50
3	B	2306	PX4	C4-N1	-2.75	1.42	1.50
3	B	2307	PX4	C4-N1	-2.66	1.42	1.50
3	A	1302	PX4	P1-O2	2.65	1.59	1.50
3	B	2302	PX4	C4-N1	-2.58	1.42	1.50
2	A	1301	GAI	C-N3	-2.41	1.31	1.36
3	B	2301	PX4	C10-C9	2.16	1.57	1.50
3	A	1305	PX4	O7-C7	-2.14	1.43	1.47
3	A	1309	PX4	C10-C9	2.02	1.56	1.50
3	B	2301	PX4	C3-N1	-2.02	1.44	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2307	PX4	O7-C23-C24	5.74	123.86	111.50
3	B	2301	PX4	O7-C23-C24	4.91	122.09	111.50
3	A	1303	PX4	O7-C23-C24	4.72	121.66	111.50
3	A	1307	PX4	O7-C23-C24	4.22	120.59	111.50
3	A	1305	PX4	O7-C23-C24	4.13	120.41	111.50
3	B	2306	PX4	O7-C23-C24	3.74	119.55	111.50
3	A	1305	PX4	C7-O7-C23	-3.70	113.11	117.88
3	B	2302	PX4	O7-C23-C24	3.51	119.06	111.50
3	B	2308	PX4	O5-C9-C10	3.46	122.75	111.91
3	B	2307	PX4	O5-C9-C10	3.05	121.47	111.91
3	B	2306	PX4	O5-C9-C10	2.97	121.22	111.91
3	B	2301	PX4	O5-C9-C10	2.74	120.52	111.91
3	A	1308	PX4	O5-C9-C10	2.72	120.45	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1307	PX4	O5-C9-C10	2.71	120.40	111.91
3	A	1303	PX4	O5-C9-C10	2.70	120.37	111.91
3	B	2302	PX4	O5-C9-C10	2.63	120.15	111.91
3	A	1310	PX4	O5-C9-C10	2.49	122.06	112.23
3	B	2307	PX4	O8-C23-C24	-2.39	114.40	123.73
3	B	2304	PX4	O5-C9-C10	2.32	121.41	112.23
3	A	1309	PX4	O5-C9-C10	2.27	121.21	112.23
3	B	2307	PX4	C8-C7-C6	-2.17	106.66	111.79
3	A	1307	PX4	O7-C23-O8	-2.12	118.58	123.70
3	A	1308	PX4	C8-C7-C6	-2.12	109.34	113.95
3	B	2301	PX4	C25-C24-C23	-2.10	105.99	113.62
3	B	2302	PX4	O7-C23-O8	-2.04	118.76	123.70
3	B	2307	PX4	C26-C25-C24	-2.03	105.90	113.19
3	B	2307	PX4	C25-C24-C23	-2.02	106.28	113.62

There are no chirality outliers.

All (210) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2301	PX4	C6-O4-P1-O1
3	B	2301	PX4	C24-C23-O7-C7
3	A	1305	PX4	C6-O4-P1-O1
3	A	1305	PX4	C6-O4-P1-O2
3	A	1305	PX4	C6-O4-P1-O3
3	A	1305	PX4	O4-C6-C7-C8
3	A	1305	PX4	O4-C6-C7-O7
3	A	1303	PX4	O3-C1-C2-N1
3	A	1308	PX4	O6-C9-O5-C8
3	A	1308	PX4	C10-C9-O5-C8
3	A	1304	PX4	C9-C10-C11-C12
3	B	2302	PX4	O3-C1-C2-N1
3	B	2302	PX4	C7-C6-O4-P1
3	A	1302	PX4	C6-O4-P1-O3
3	A	1302	PX4	C7-C6-O4-P1
3	A	1302	PX4	C6-C7-C8-O5
3	B	2303	PX4	C9-C10-C11-C12
3	B	2308	PX4	C6-O4-P1-O1
3	B	2308	PX4	C6-O4-P1-O3
3	A	1307	PX4	C1-O3-P1-O1
3	A	1307	PX4	C1-O3-P1-O2
3	A	1307	PX4	C6-O4-P1-O1
3	B	2307	PX4	C1-O3-P1-O1

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Mol	Chain	Res	Type	Atoms
3	B	2307	PX4	C1-O3-P1-O2
3	B	2307	PX4	C1-O3-P1-O4
3	B	2307	PX4	C7-C6-O4-P1
3	B	2307	PX4	C24-C23-O7-C7
3	A	1303	PX4	O6-C9-O5-C8
3	A	1303	PX4	C10-C9-O5-C8
3	B	2302	PX4	O6-C9-O5-C8
3	B	2301	PX4	O8-C23-O7-C7
3	B	2306	PX4	O8-C23-O7-C7
3	B	2307	PX4	O8-C23-O7-C7
3	B	2302	PX4	C10-C9-O5-C8
3	B	2307	PX4	C10-C9-O5-C8
3	B	2307	PX4	O6-C9-O5-C8
3	B	2306	PX4	C24-C23-O7-C7
3	A	1308	PX4	C6-C7-C8-O5
3	B	2301	PX4	C10-C9-O5-C8
3	B	2308	PX4	C12-C13-C14-C15
3	A	1302	PX4	O4-C6-C7-C8
3	B	2301	PX4	O6-C9-O5-C8
3	B	2301	PX4	C30-C31-C32-C33
3	B	2302	PX4	C10-C11-C12-C13
3	B	2308	PX4	C10-C9-O5-C8
3	B	2307	PX4	C9-C10-C11-C12
3	B	2307	PX4	C16-C17-C18-C19
3	B	2301	PX4	C23-C24-C25-C26
3	B	2307	PX4	C23-C24-C25-C26
3	A	1302	PX4	O4-C6-C7-O7
3	B	2301	PX4	C6-O4-P1-O3
3	A	1303	PX4	C1-O3-P1-O4
3	B	2302	PX4	C6-O4-P1-O3
3	A	1307	PX4	C6-O4-P1-O3
3	A	1308	PX4	C15-C16-C17-C18
3	B	2302	PX4	C18-C19-C20-C21
3	B	2307	PX4	C10-C11-C12-C13
3	B	2307	PX4	C29-C30-C31-C32
3	A	1310	PX4	C14-C15-C16-C17
3	A	1307	PX4	C9-C10-C11-C12
3	B	2307	PX4	C25-C26-C27-C28
3	B	2302	PX4	C27-C28-C29-C30
3	A	1307	PX4	C26-C27-C28-C29
3	A	1307	PX4	C10-C9-O5-C8
3	A	1303	PX4	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	B	2306	PX4	C24-C25-C26-C27
3	B	2308	PX4	O6-C9-O5-C8
3	B	2302	PX4	C12-C13-C14-C15
3	B	2302	PX4	C26-C27-C28-C29
3	B	2306	PX4	C23-C24-C25-C26
3	B	2308	PX4	C16-C17-C18-C19
3	A	1307	PX4	C24-C25-C26-C27
3	A	1303	PX4	C17-C18-C19-C20
3	B	2302	PX4	C28-C29-C30-C31
3	A	1309	PX4	C17-C18-C19-C20
3	A	1308	PX4	C17-C18-C19-C20
3	A	1307	PX4	C25-C26-C27-C28
3	B	2307	PX4	C26-C27-C28-C29
3	A	1307	PX4	C30-C31-C32-C33
3	B	2301	PX4	C31-C32-C33-C34
3	A	1303	PX4	C29-C30-C31-C32
3	A	1304	PX4	C11-C12-C13-C14
3	B	2304	PX4	C15-C16-C17-C18
3	A	1308	PX4	C11-C12-C13-C14
3	A	1303	PX4	C23-C24-C25-C26
3	A	1302	PX4	O7-C7-C8-O5
3	A	1307	PX4	C17-C18-C19-C20
3	A	1309	PX4	C14-C15-C16-C17
3	B	2307	PX4	C28-C29-C30-C31
3	A	1307	PX4	O6-C9-O5-C8
3	B	2308	PX4	C14-C15-C16-C17
3	B	2308	PX4	C15-C16-C17-C18
3	A	1310	PX4	C15-C16-C17-C18
3	A	1309	PX4	C10-C11-C12-C13
3	A	1305	PX4	C31-C32-C33-C34
3	A	1307	PX4	C23-C24-C25-C26
3	B	2301	PX4	C29-C30-C31-C32
3	B	2302	PX4	C24-C23-O7-C7
3	B	2306	PX4	O4-C6-C7-O7
3	B	2302	PX4	O8-C23-O7-C7
3	A	1307	PX4	C27-C28-C29-C30
3	A	1310	PX4	C16-C17-C18-C19
3	B	2307	PX4	C11-C12-C13-C14
3	B	2302	PX4	C1-O3-P1-O4
3	A	1303	PX4	O4-C6-C7-C8
3	B	2302	PX4	C7-C8-O5-C9
3	B	2302	PX4	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	B	2302	PX4	C24-C25-C26-C27
3	B	2307	PX4	C33-C34-C35-C36
3	B	2307	PX4	C24-C25-C26-C27
3	B	2306	PX4	C10-C11-C12-C13
3	A	1309	PX4	C13-C14-C15-C16
3	A	1305	PX4	C29-C30-C31-C32
3	A	1303	PX4	C11-C12-C13-C14
3	A	1303	PX4	C15-C16-C17-C18
3	A	1308	PX4	C18-C19-C20-C21
3	B	2306	PX4	C25-C26-C27-C28
3	A	1302	PX4	C6-O4-P1-O2
3	B	2308	PX4	C6-O4-P1-O2
3	B	2307	PX4	C12-C13-C14-C15
3	B	2302	PX4	O4-C6-C7-O7
3	B	2308	PX4	C17-C18-C19-C20
3	A	1306	PX4	C30-C31-C32-C33
3	A	1303	PX4	C28-C29-C30-C31
3	B	2306	PX4	O4-C6-C7-C8
3	A	1308	PX4	O4-C6-C7-C8
3	A	1307	PX4	C14-C15-C16-C17
3	A	1303	PX4	C12-C13-C14-C15
3	B	2301	PX4	C33-C34-C35-C36
3	B	2306	PX4	C10-C9-O5-C8
3	A	1303	PX4	C6-C7-C8-O5
3	A	1307	PX4	C13-C14-C15-C16
3	A	1303	PX4	C30-C31-C32-C33
3	B	2307	PX4	O4-C6-C7-O7
3	B	2304	PX4	C10-C9-O5-C8
3	A	1308	PX4	C19-C20-C21-C22
3	A	1303	PX4	C16-C17-C18-C19
3	B	2307	PX4	C17-C18-C19-C20
3	B	2307	PX4	C19-C20-C21-C22
3	B	2302	PX4	C11-C10-C9-O5
3	B	2302	PX4	C17-C18-C19-C20
3	A	1309	PX4	C15-C16-C17-C18
3	A	1303	PX4	C25-C26-C27-C28
3	A	1307	PX4	C15-C16-C17-C18
3	A	1302	PX4	C6-O4-P1-O1
3	B	2307	PX4	C8-C7-O7-C23
3	A	1303	PX4	O7-C7-C8-O5
3	B	2302	PX4	O7-C7-C8-O5
3	A	1310	PX4	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	B	2306	PX4	O6-C9-O5-C8
3	B	2308	PX4	O7-C7-C8-O5
3	B	2302	PX4	C15-C16-C17-C18
3	B	2301	PX4	C6-O4-P1-O2
3	A	1303	PX4	C1-O3-P1-O1
3	A	1303	PX4	C1-O3-P1-O2
3	B	2302	PX4	C1-O3-P1-O1
3	B	2302	PX4	C6-O4-P1-O1
3	B	2302	PX4	O4-C6-C7-C8
3	B	2302	PX4	C14-C15-C16-C17
3	A	1303	PX4	O4-C6-C7-O7
3	B	2304	PX4	C16-C17-C18-C19
3	A	1303	PX4	C18-C19-C20-C21
3	B	2306	PX4	C1-C2-N1-C5
3	B	2307	PX4	C1-C2-N1-C4
3	B	2302	PX4	C6-C7-C8-O5
3	B	2303	PX4	C11-C12-C13-C14
3	B	2308	PX4	C18-C19-C20-C21
3	B	2307	PX4	C1-C2-N1-C5
3	B	2303	PX4	C18-C19-C20-C21
3	B	2308	PX4	C11-C10-C9-O5
3	A	1303	PX4	C9-C10-C11-C12
3	B	2302	PX4	C8-C7-O7-C23
3	B	2307	PX4	O4-C6-C7-C8
3	B	2307	PX4	C14-C15-C16-C17
3	B	2306	PX4	C1-C2-N1-C3
3	B	2307	PX4	C6-O4-P1-O3
3	B	2304	PX4	C10-C11-C12-C13
3	A	1310	PX4	C10-C11-C12-C13
3	B	2307	PX4	C13-C14-C15-C16
3	A	1303	PX4	C19-C20-C21-C22
3	B	2302	PX4	C13-C14-C15-C16
3	B	2302	PX4	C9-C10-C11-C12
3	B	2303	PX4	C10-C11-C12-C13
3	A	1308	PX4	C13-C14-C15-C16
3	A	1310	PX4	C9-C10-C11-C12
3	B	2306	PX4	C1-C2-N1-C4
3	B	2307	PX4	C1-C2-N1-C3
3	B	2309	PX4	C10-C11-C12-C13
3	A	1304	PX4	C10-C11-C12-C13
3	B	2304	PX4	O6-C9-O5-C8
3	A	1304	PX4	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
3	B	2306	PX4	C27-C28-C29-C30
3	A	1303	PX4	C32-C33-C34-C35
3	A	1307	PX4	O8-C23-O7-C7
3	B	2306	PX4	C6-O4-P1-O3
3	B	2308	PX4	C10-C11-C12-C13
3	B	2308	PX4	C6-C7-C8-O5
3	B	2309	PX4	C9-C10-C11-C12
3	A	1309	PX4	C11-C12-C13-C14
3	B	2303	PX4	C13-C14-C15-C16
3	A	1304	PX4	C16-C17-C18-C19
3	A	1307	PX4	C24-C23-O7-C7
3	A	1307	PX4	C16-C17-C18-C19
3	A	1307	PX4	C1-O3-P1-O4
3	B	2301	PX4	C32-C33-C34-C35
3	B	2301	PX4	C2-C1-O3-P1
3	B	2302	PX4	C2-C1-O3-P1
3	A	1305	PX4	C32-C33-C34-C35
3	B	2304	PX4	C18-C19-C20-C21
3	B	2301	PX4	C24-C25-C26-C27

There are no ring outliers.

12 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2301	PX4	6	0
3	B	2308	PX4	3	0
3	A	1305	PX4	2	0
5	A	1313	SO4	2	0
3	A	1308	PX4	1	0
5	B	2312	SO4	2	0
3	B	2302	PX4	2	0
3	A	1309	PX4	1	0
3	A	1307	PX4	3	0
3	A	1310	PX4	1	0
3	B	2307	PX4	6	0
3	A	1303	PX4	1	0

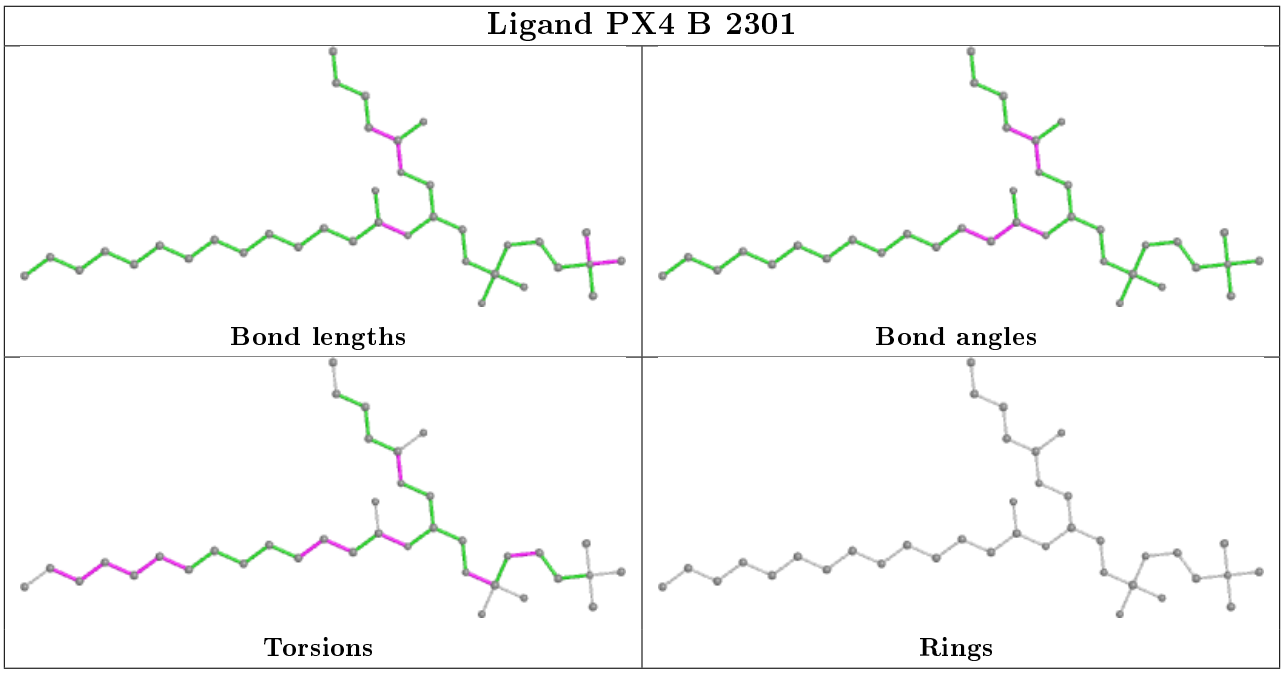
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

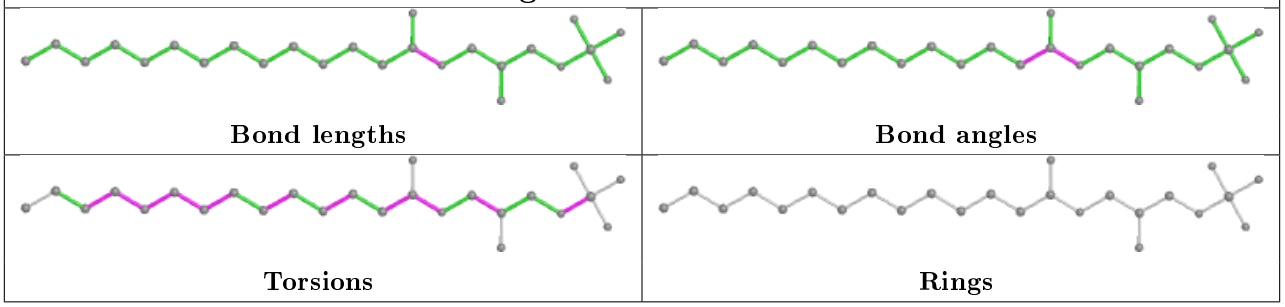
Ligand PX4 A 1304

Ligand PX4 B 2304

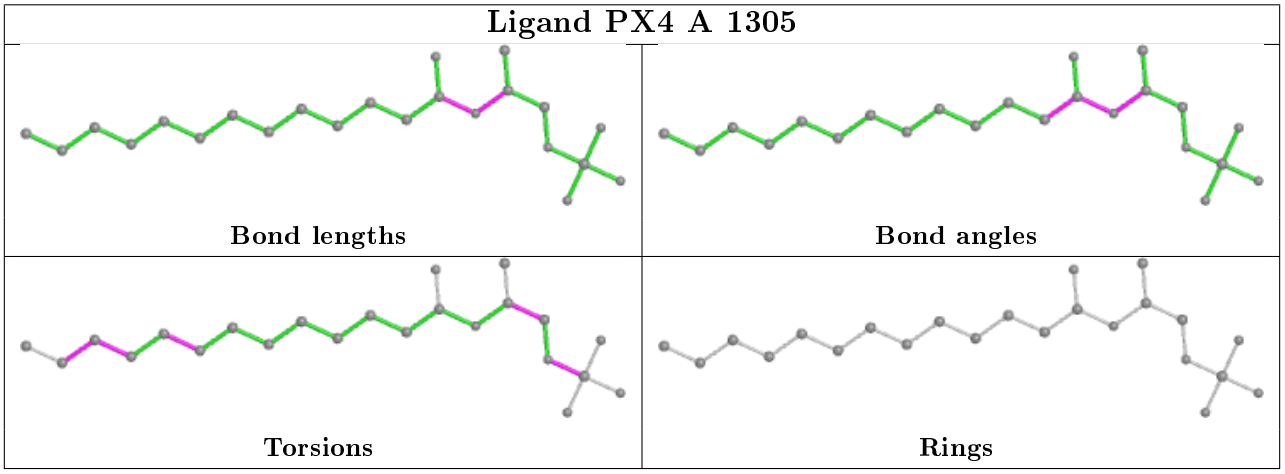
Ligand PX4 B 2301



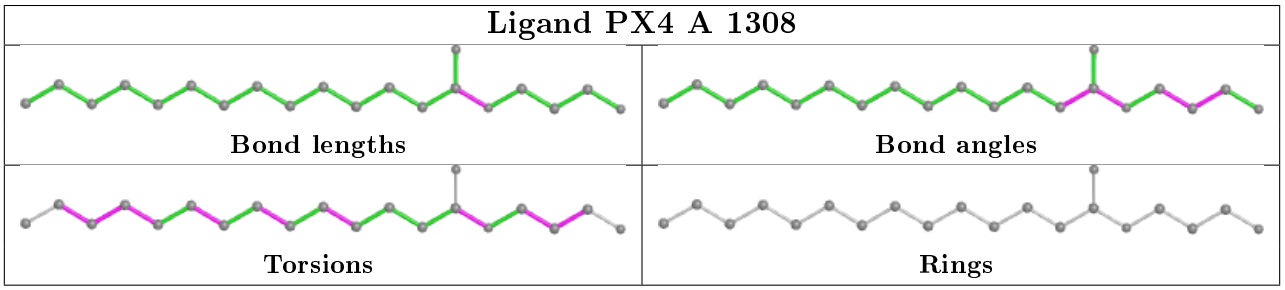
Ligand PX4 B 2308



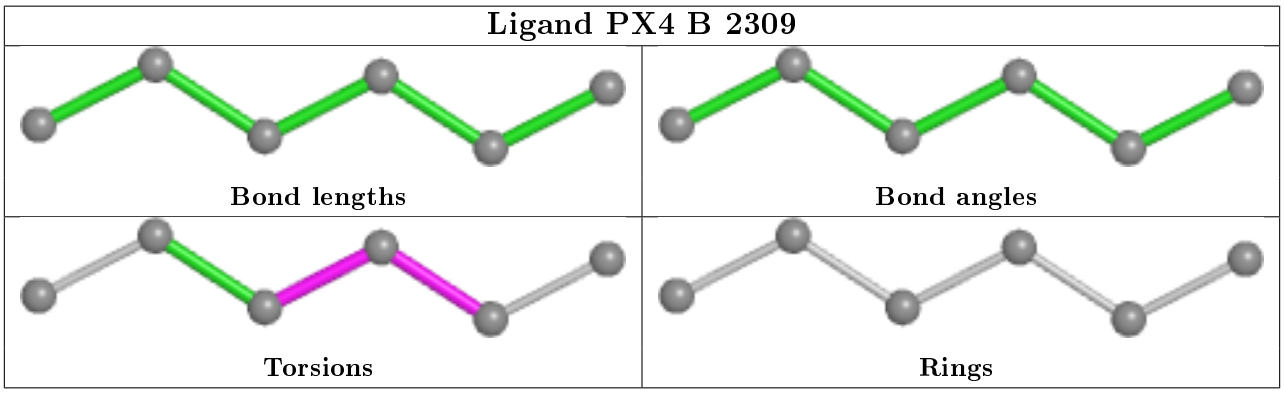
Ligand PX4 A 1305



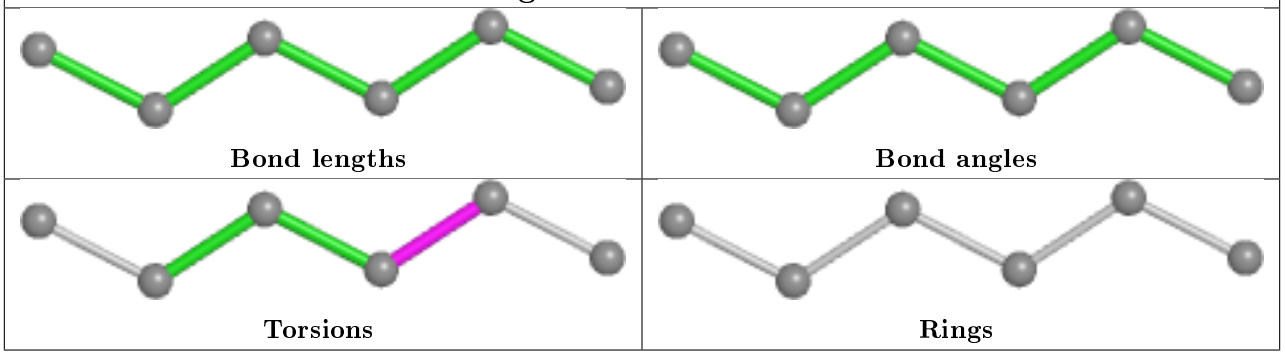
Ligand PX4 A 1308



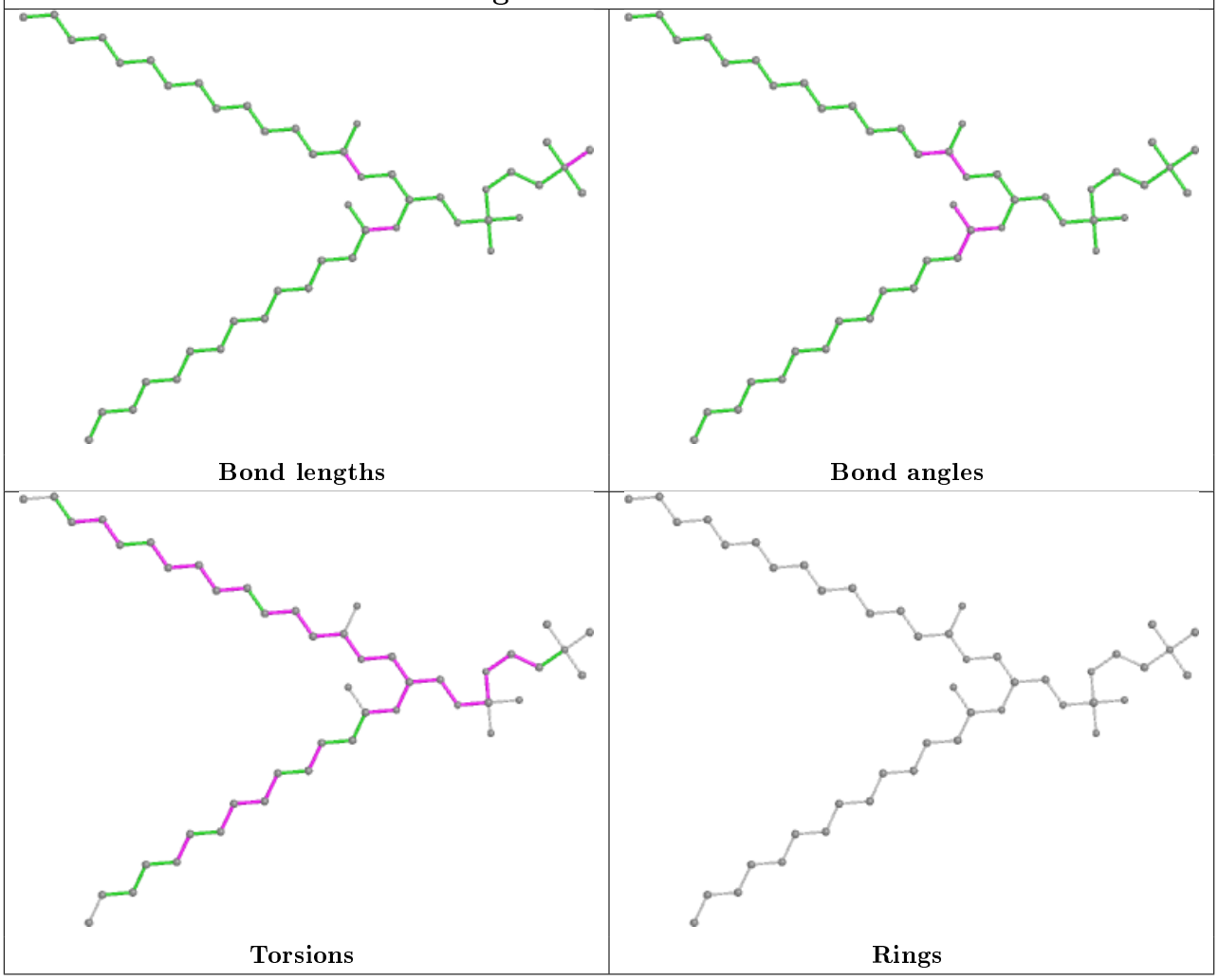
Ligand PX4 B 2309



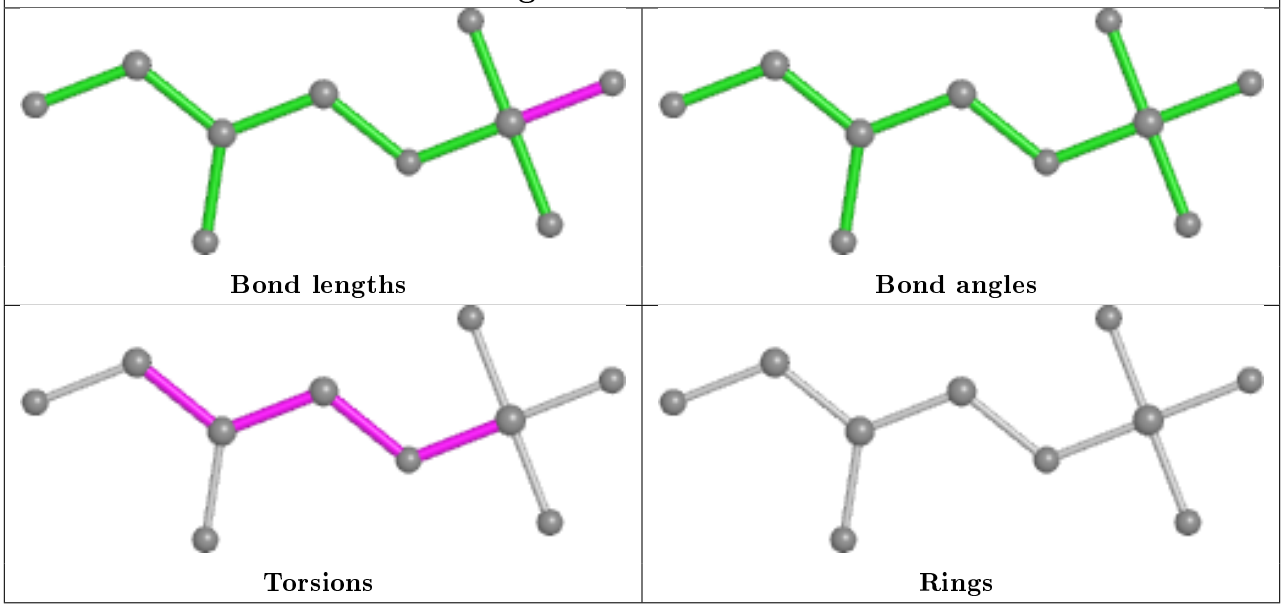
Ligand PX4 A 1306



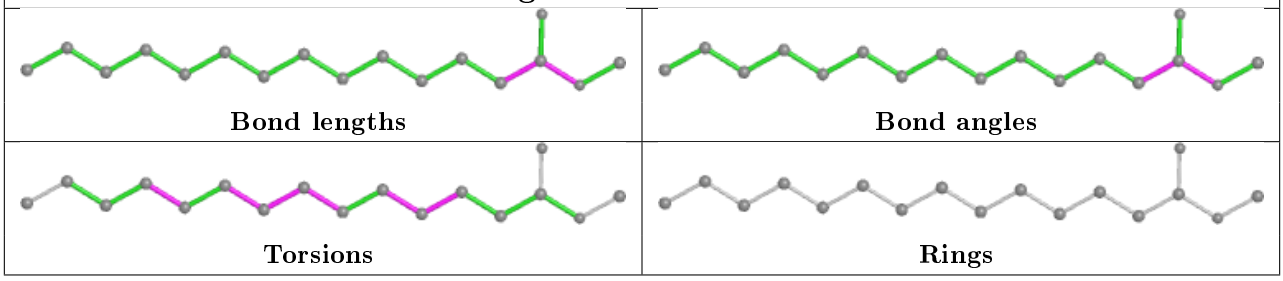
Ligand PX4 B 2302



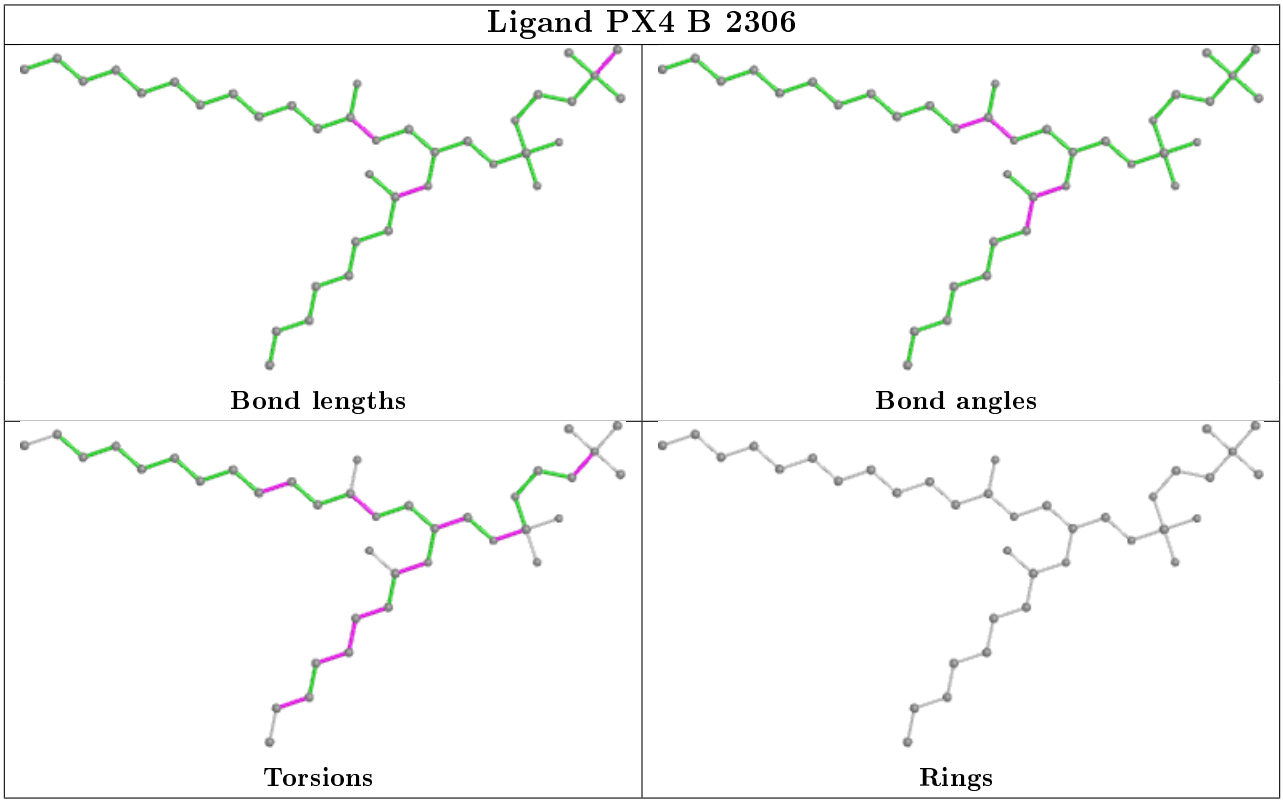
Ligand PX4 A 1302



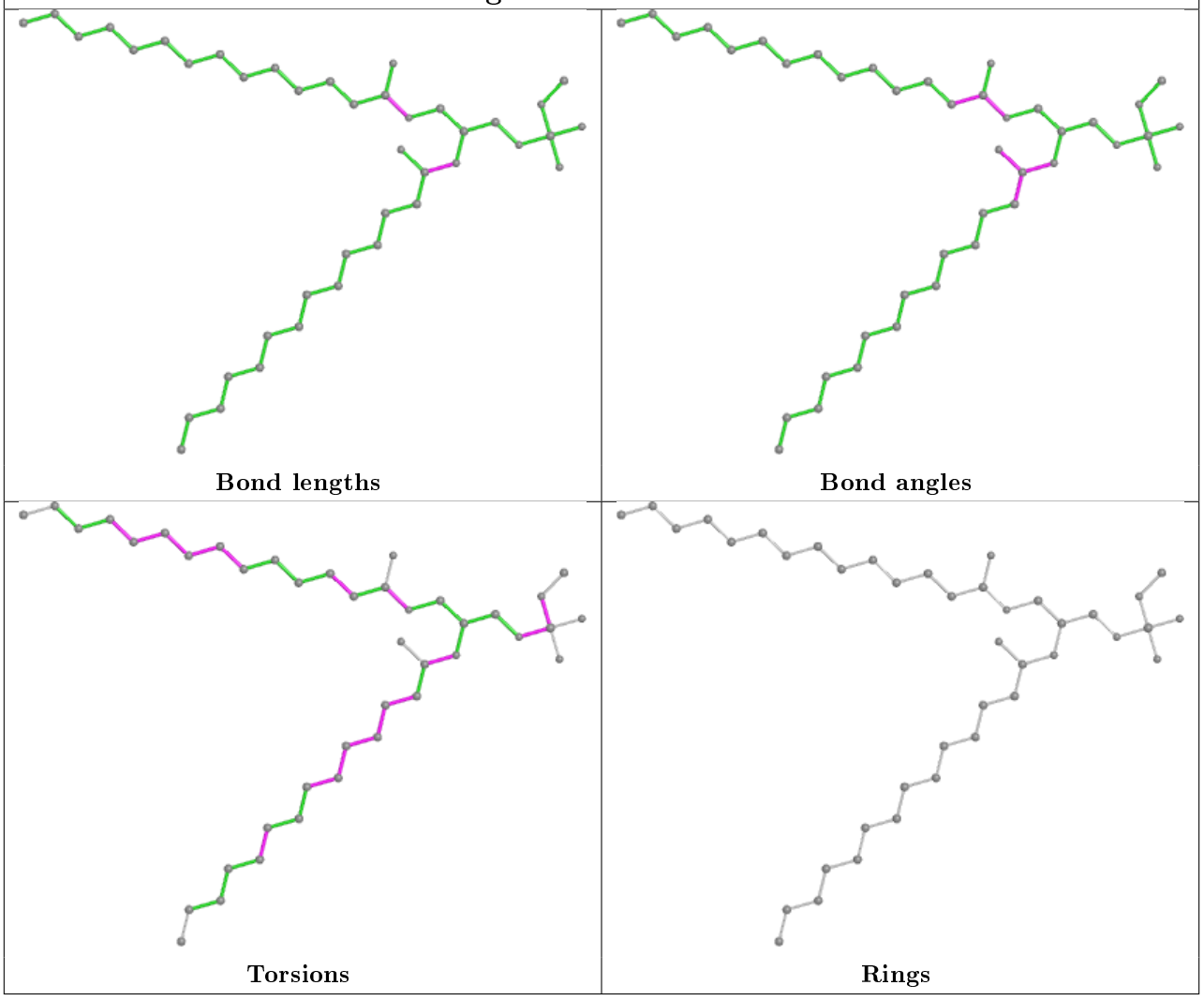
Ligand PX4 A 1309



Ligand PX4 B 2306

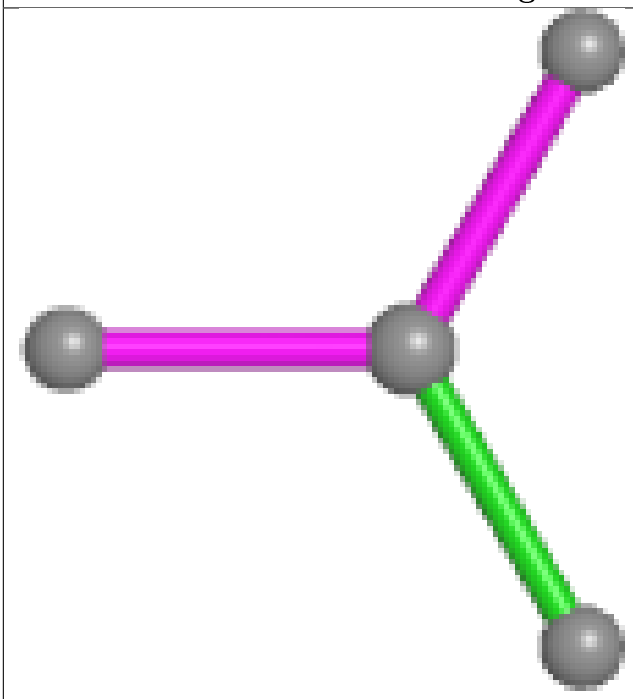


Ligand PX4 A 1307

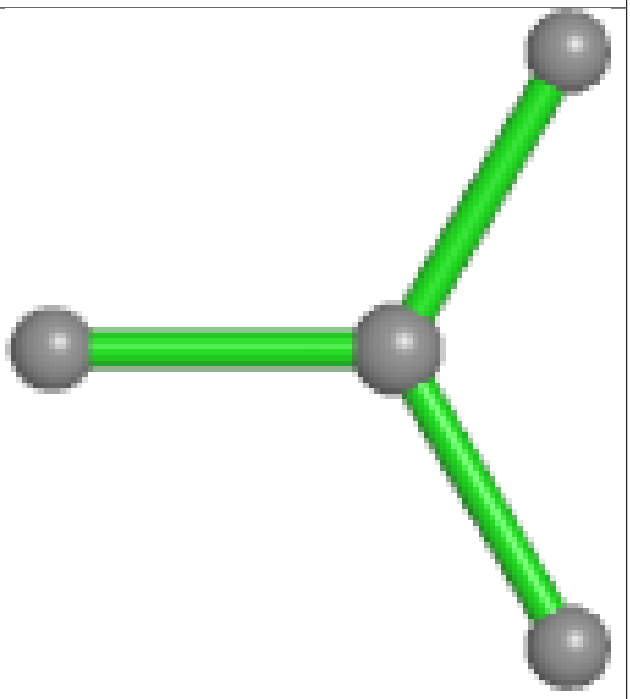


Ligand PX4 B 2303

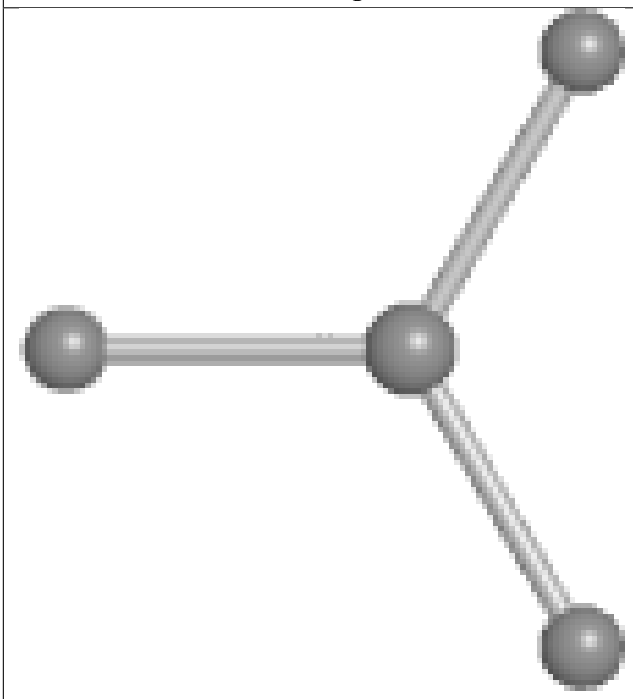
Ligand GAI B 2305



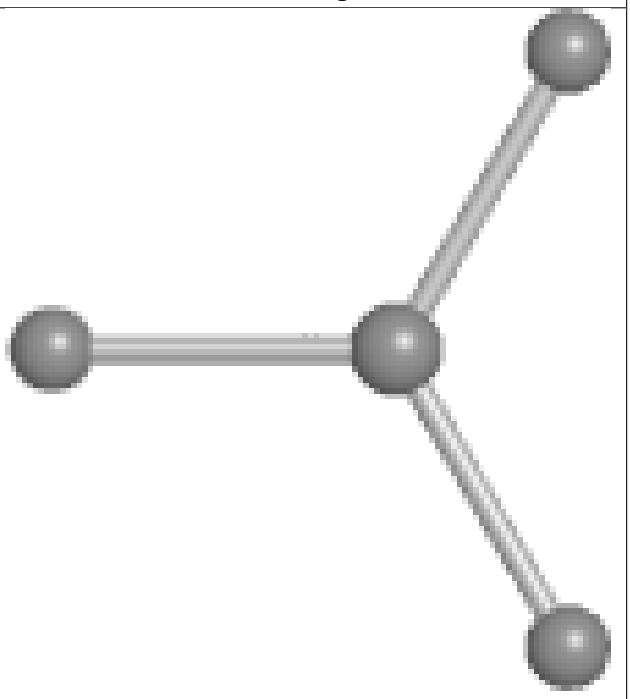
Bond lengths



Bond angles

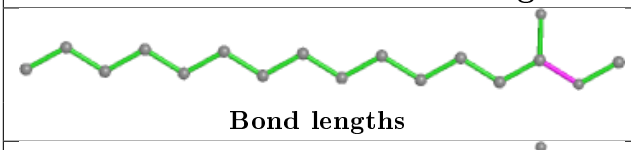


Torsions

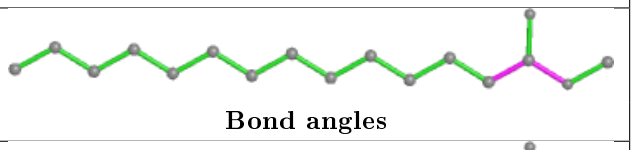


Rings

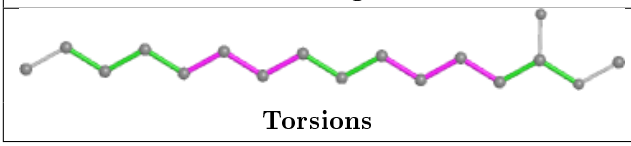
Ligand PX4 A 1310



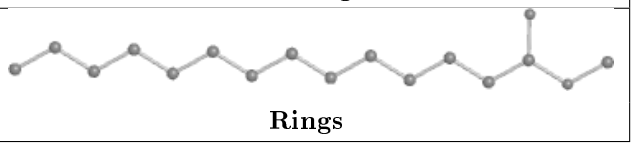
Bond lengths



Bond angles

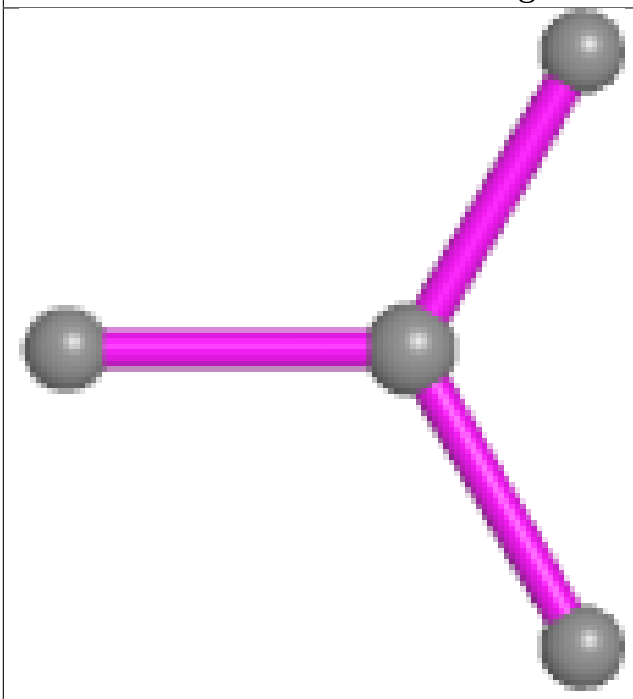


Torsions

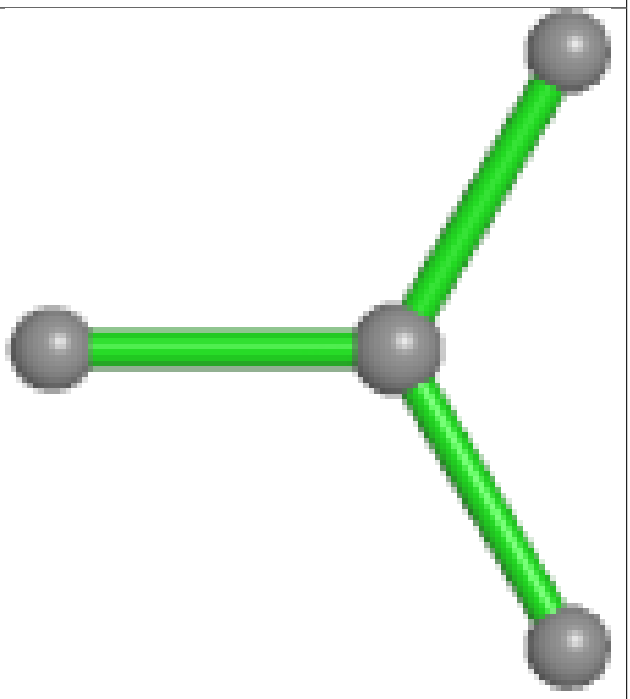


Rings

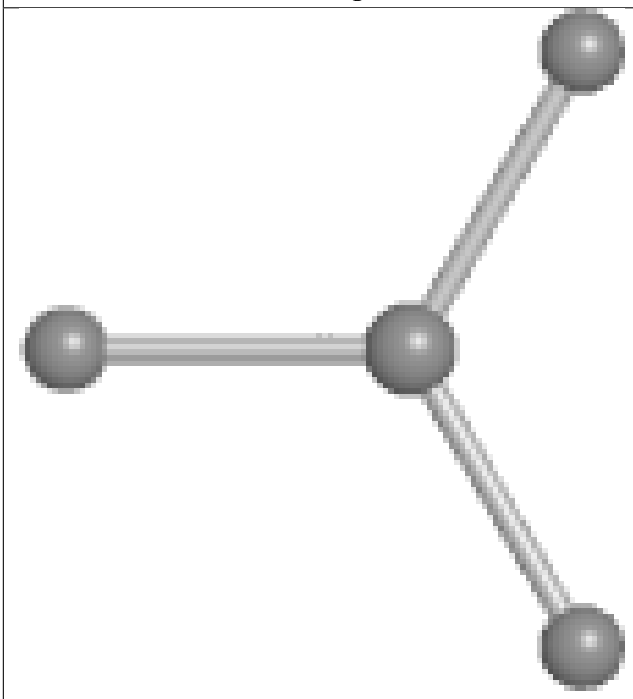
Ligand GAI A 1301



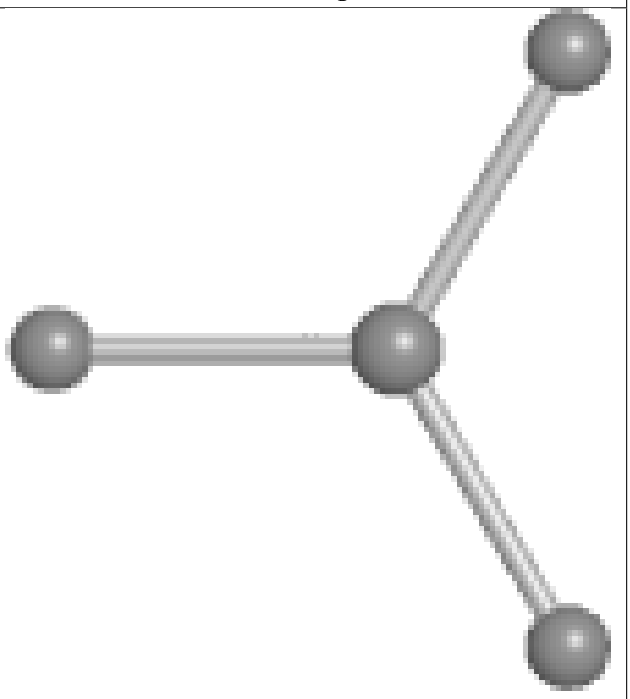
Bond lengths



Bond angles

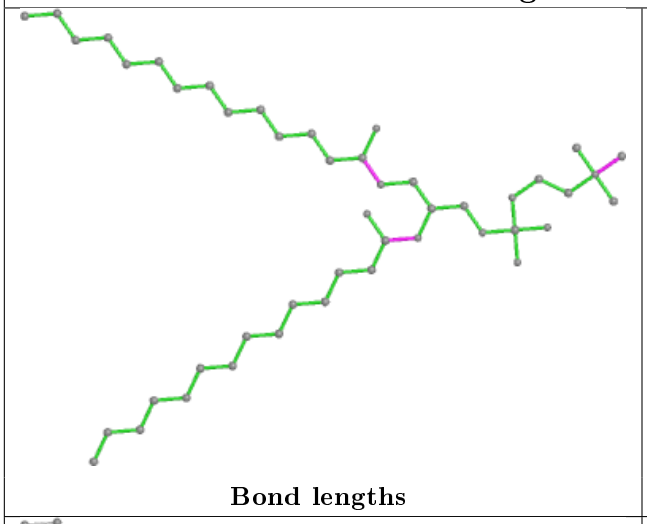


Torsions

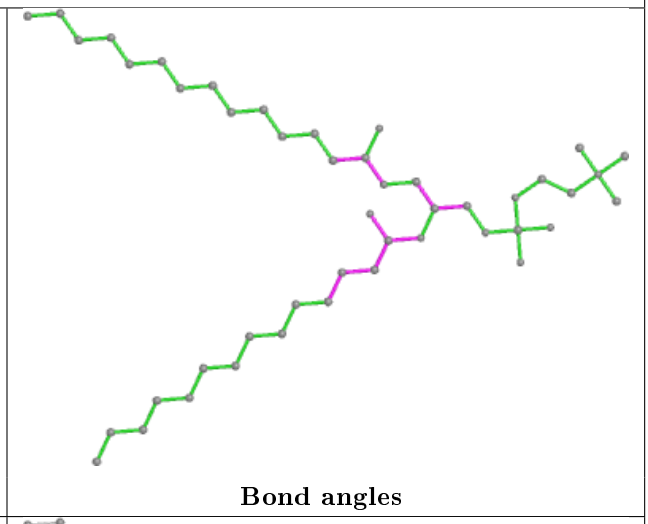


Rings

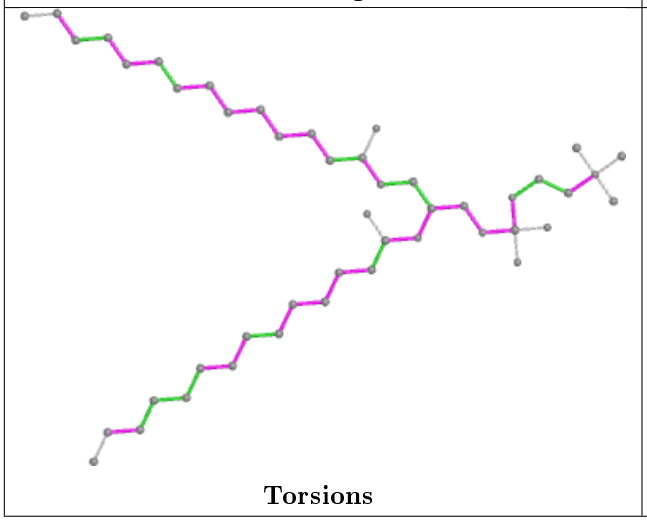
Ligand PX4 B 2307



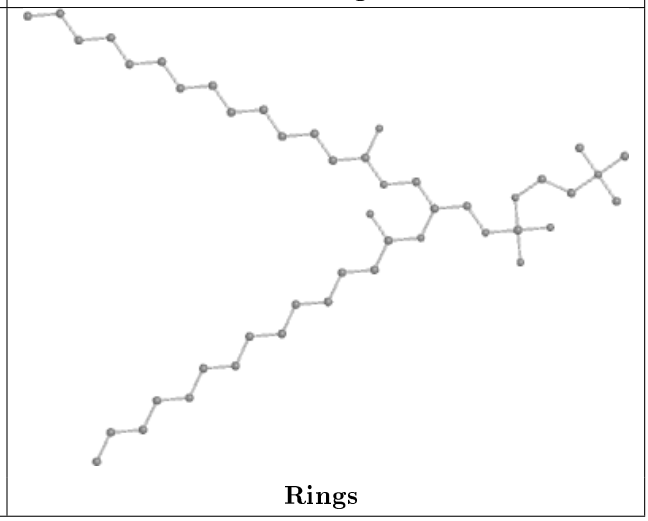
Bond lengths



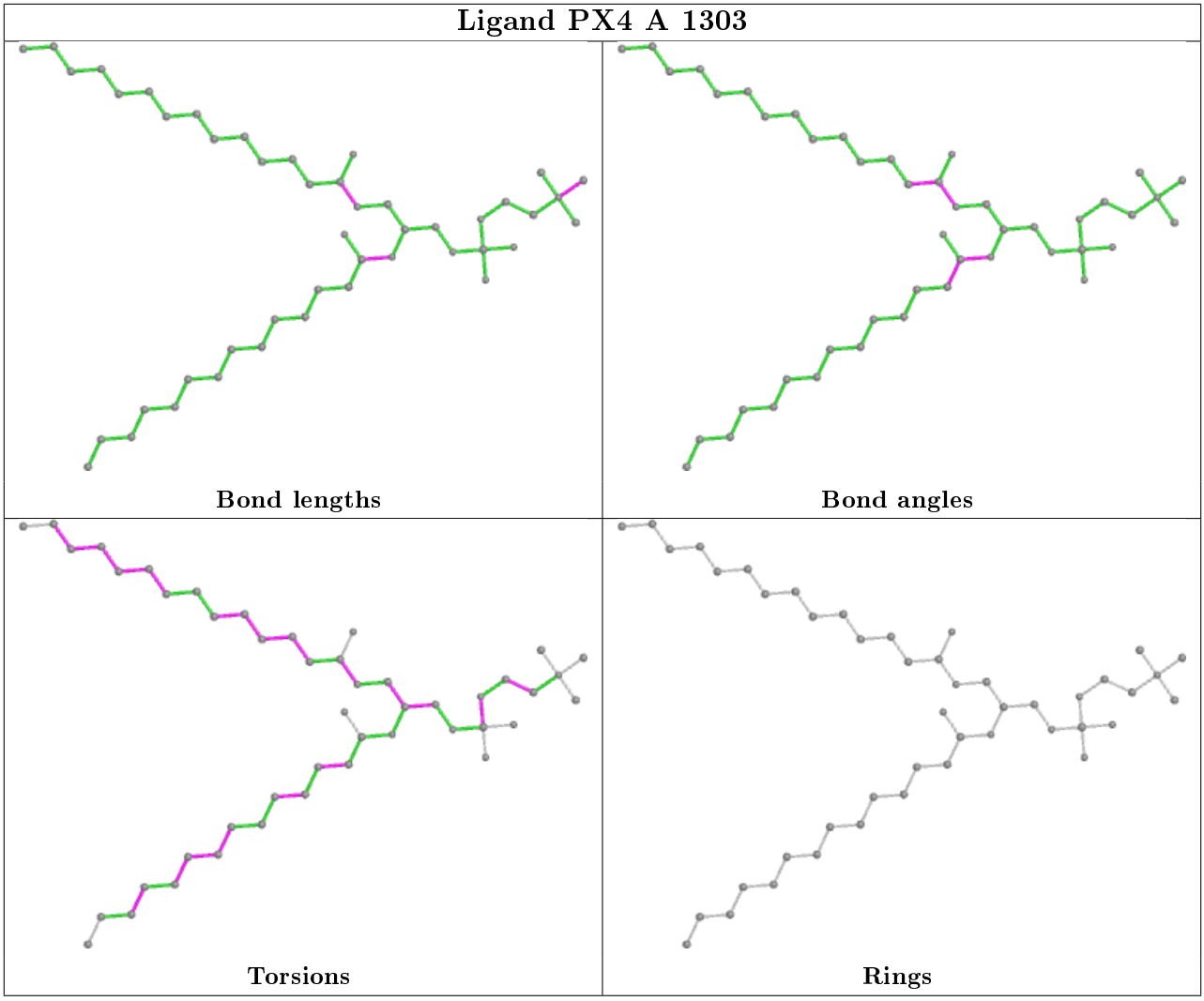
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	221/285 (77%)	0.54	14 (6%)	20	19	44, 94, 170, 214	0
1	B	221/285 (77%)	0.57	17 (7%)	13	11	40, 92, 171, 228	0
All	All	442/570 (77%)	0.55	31 (7%)	16	14	40, 93, 171, 228	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1095	PHE	10.1
1	A	1090	PRO	7.0
1	B	2090	PRO	6.4
1	A	1094	GLY	5.6
1	B	2091	THR	5.0
1	A	1221	MET	4.7
1	A	1091	THR	4.4
1	B	2094	GLY	4.1
1	A	1065	TYR	4.1
1	B	2095	PHE	4.0
1	A	1220	ALA	3.8
1	A	1098	LEU	3.7
1	B	2004	ARG	3.6
1	B	2089	VAL	3.6
1	B	2069	ILE	3.1
1	A	1047	LEU	2.9
1	B	2221	MET	2.9
1	B	2047	LEU	2.4
1	A	1115	GLN	2.4
1	B	2093	SER	2.4
1	B	2097	ILE	2.4
1	B	2065	TYR	2.3
1	B	2086	ILE	2.3
1	A	1020	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	2013	PHE	2.2
1	A	1092	SER	2.1
1	B	2053	ILE	2.1
1	B	2092	SER	2.1
1	A	1093	SER	2.0
1	A	1137	MET	2.0
1	B	2035	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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
5	SO4	B	2312	5/5	0.54	0.38	264,265,268,274	0
3	PX4	A	1305	23/46	0.73	0.38	69,122,246,246	0
3	PX4	B	2303	16/46	0.73	0.33	72,96,152,153	0
3	PX4	A	1308	20/46	0.74	0.45	84,103,140,141	0
3	PX4	A	1309	17/46	0.75	0.37	81,110,126,127	0
3	PX4	B	2308	25/46	0.78	0.33	71,104,261,262	0
3	PX4	A	1304	16/46	0.79	0.28	71,105,136,139	0
2	GAI	A	1301	4/4	0.80	0.15	106,108,109,111	0
4	NA	A	1312	1/1	0.81	0.32	88,88,88,88	0
4	NA	B	2311	1/1	0.82	0.24	86,86,86,86	0
3	PX4	B	2309	6/46	0.83	0.41	76,91,93,105	0
3	PX4	A	1302	10/46	0.86	0.21	123,135,168,171	0
3	PX4	A	1303	46/46	0.86	0.25	72,96,123,197	0
5	SO4	A	1313	5/5	0.87	0.24	155,155,156,162	0
3	PX4	A	1310	17/46	0.87	0.27	59,89,127,133	0
4	NA	B	2310	1/1	0.88	0.24	76,76,76,76	0

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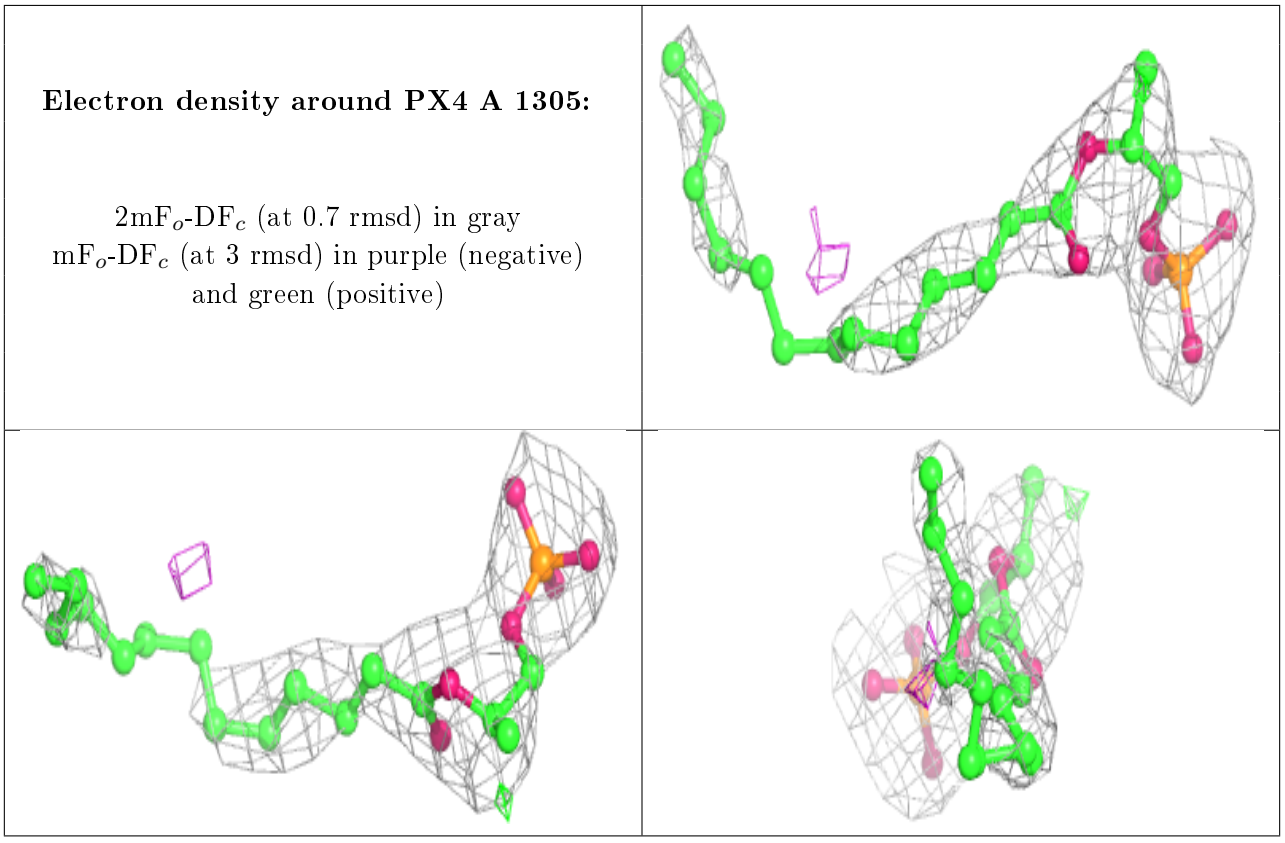
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PX4	A	1306	6/46	0.88	0.13	79,88,96,109	0
4	NA	A	1311	1/1	0.88	0.28	82,82,82,82	0
3	PX4	B	2307	46/46	0.88	0.45	79,104,138,148	0
3	PX4	B	2302	46/46	0.89	0.34	52,100,143,162	0
3	PX4	B	2304	17/46	0.91	0.27	48,91,106,113	0
2	GAI	B	2305	4/4	0.92	0.10	104,112,114,121	0
3	PX4	B	2306	38/46	0.94	0.28	49,90,114,116	0
3	PX4	B	2301	37/46	0.95	0.22	62,90,120,134	0
3	PX4	A	1307	41/46	0.95	0.30	65,97,126,139	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.

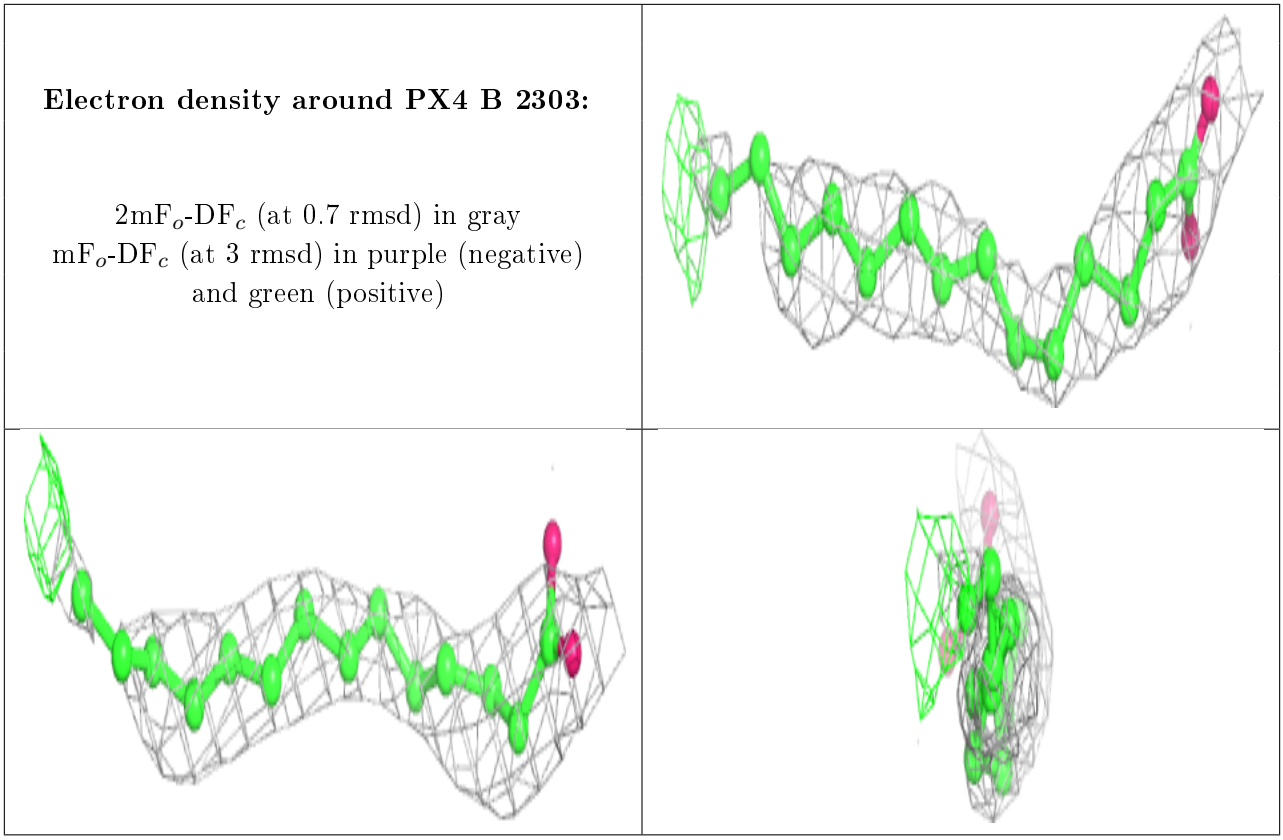
Electron density around PX4 A 1305:

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



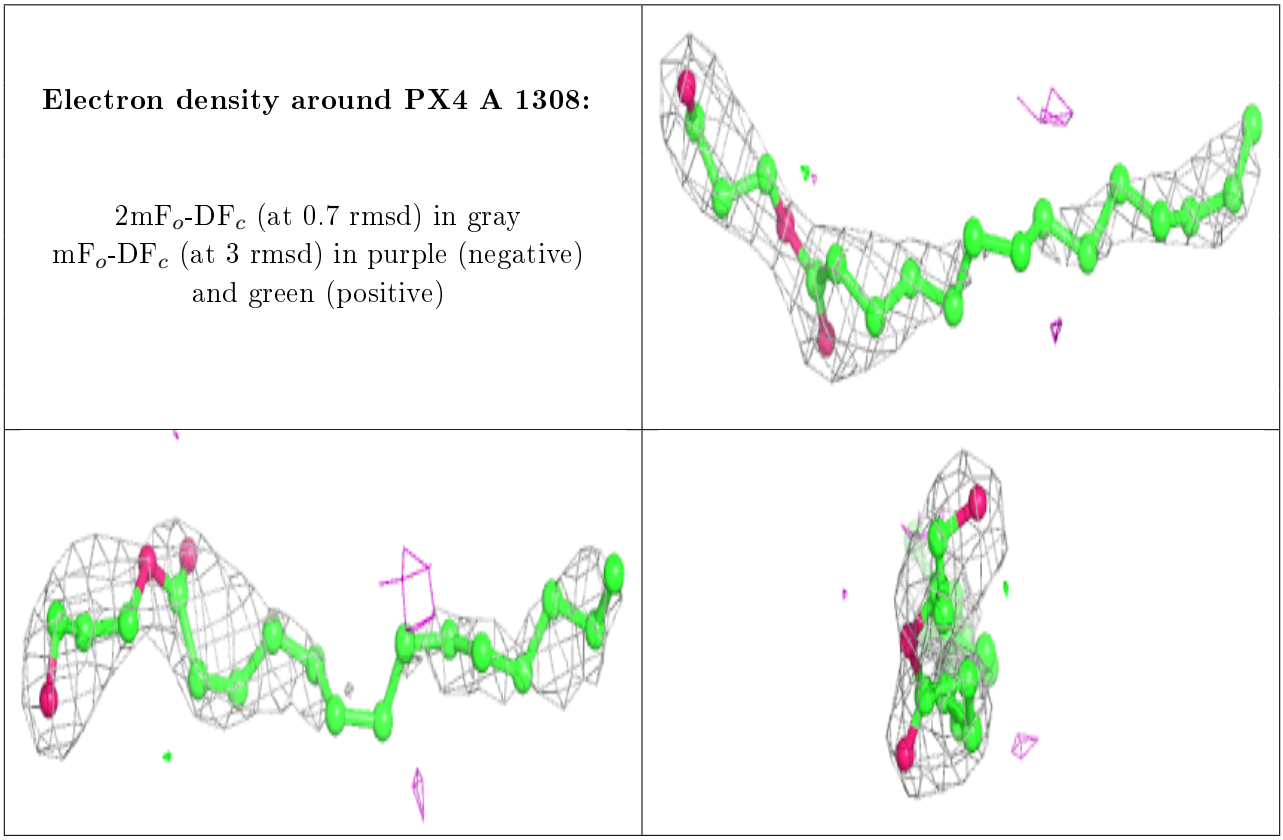
Electron density around PX4 B 2303:

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



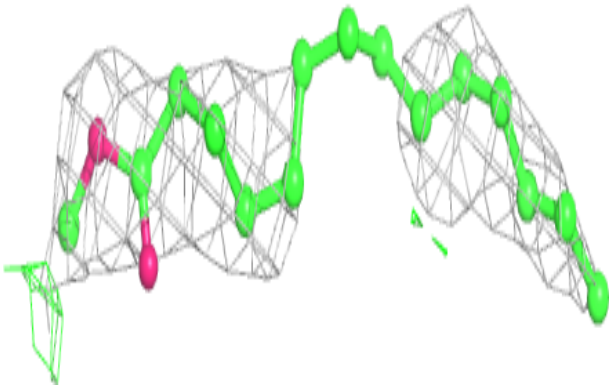
Electron density around PX4 A 1308:

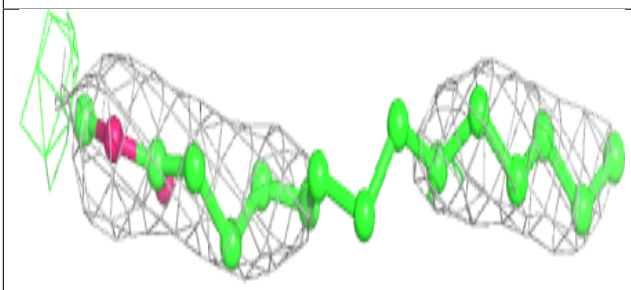
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

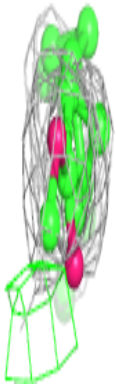


Electron density around PX4 A 1309:

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

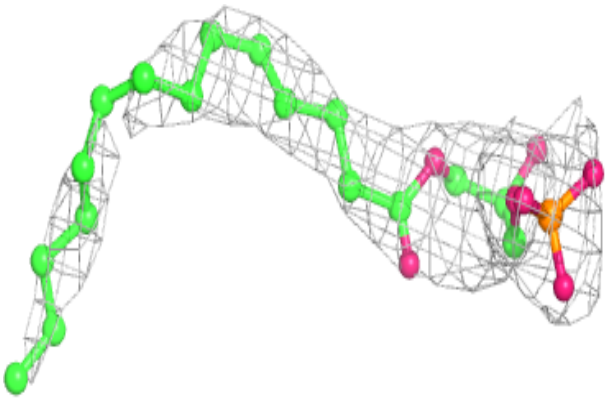


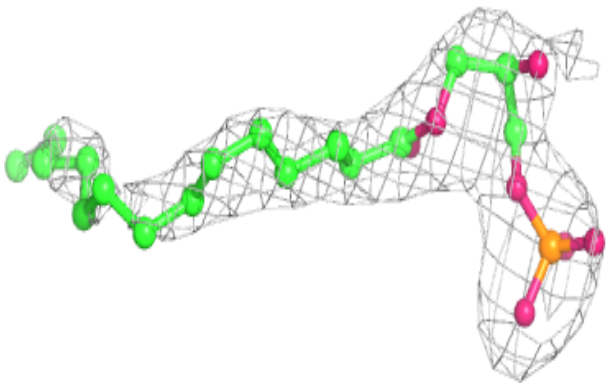


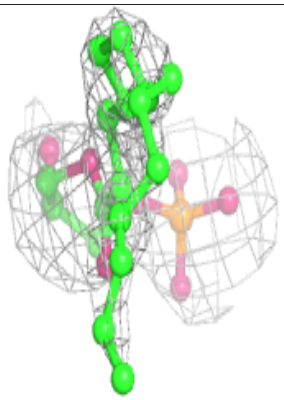


Electron density around PX4 B 2308:

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

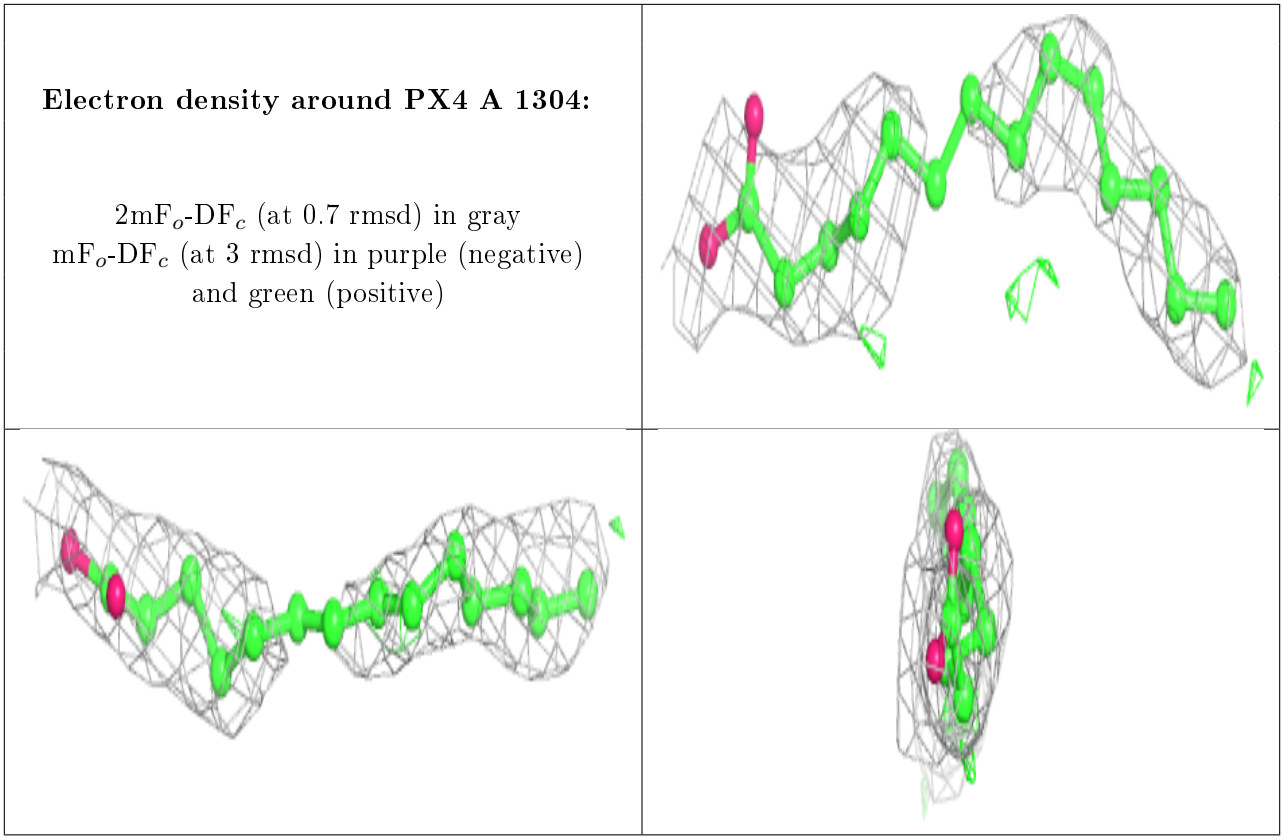






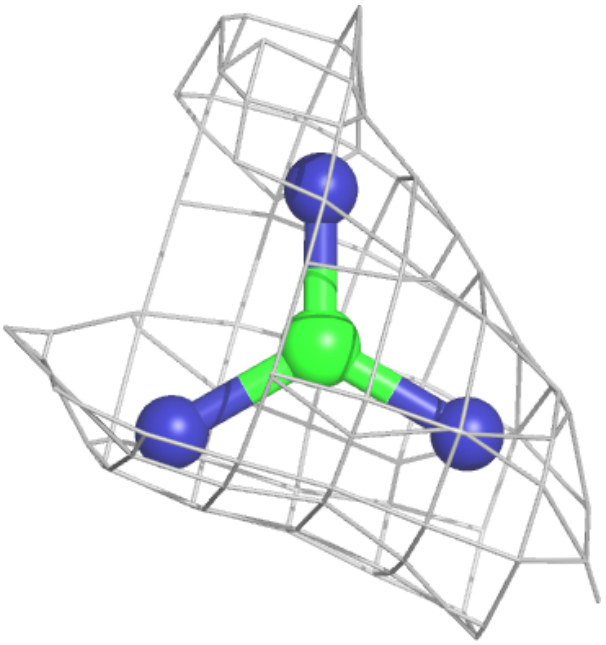
Electron density around PX4 A 1304:

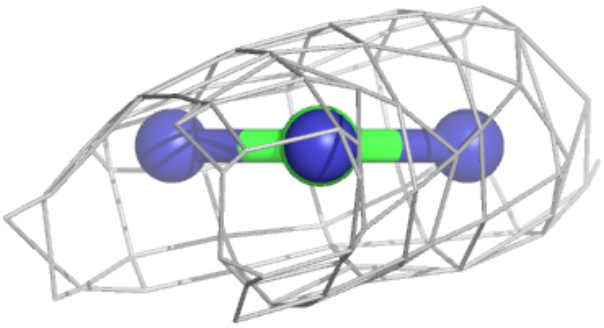
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

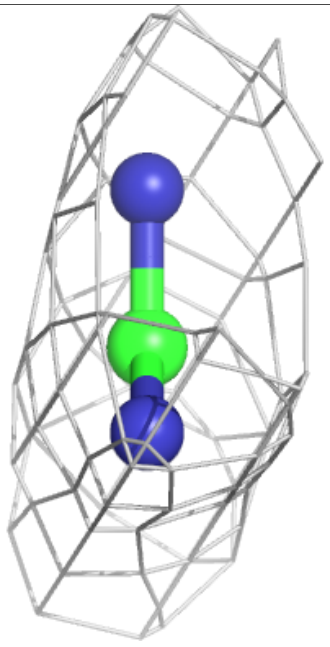


Electron density around GAI A 1301:

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

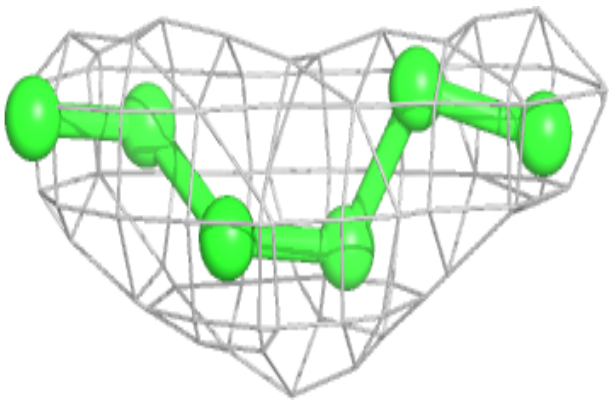


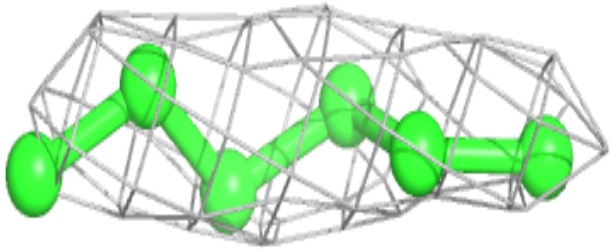


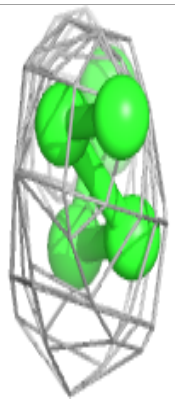


Electron density around PX4 B 2309:

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

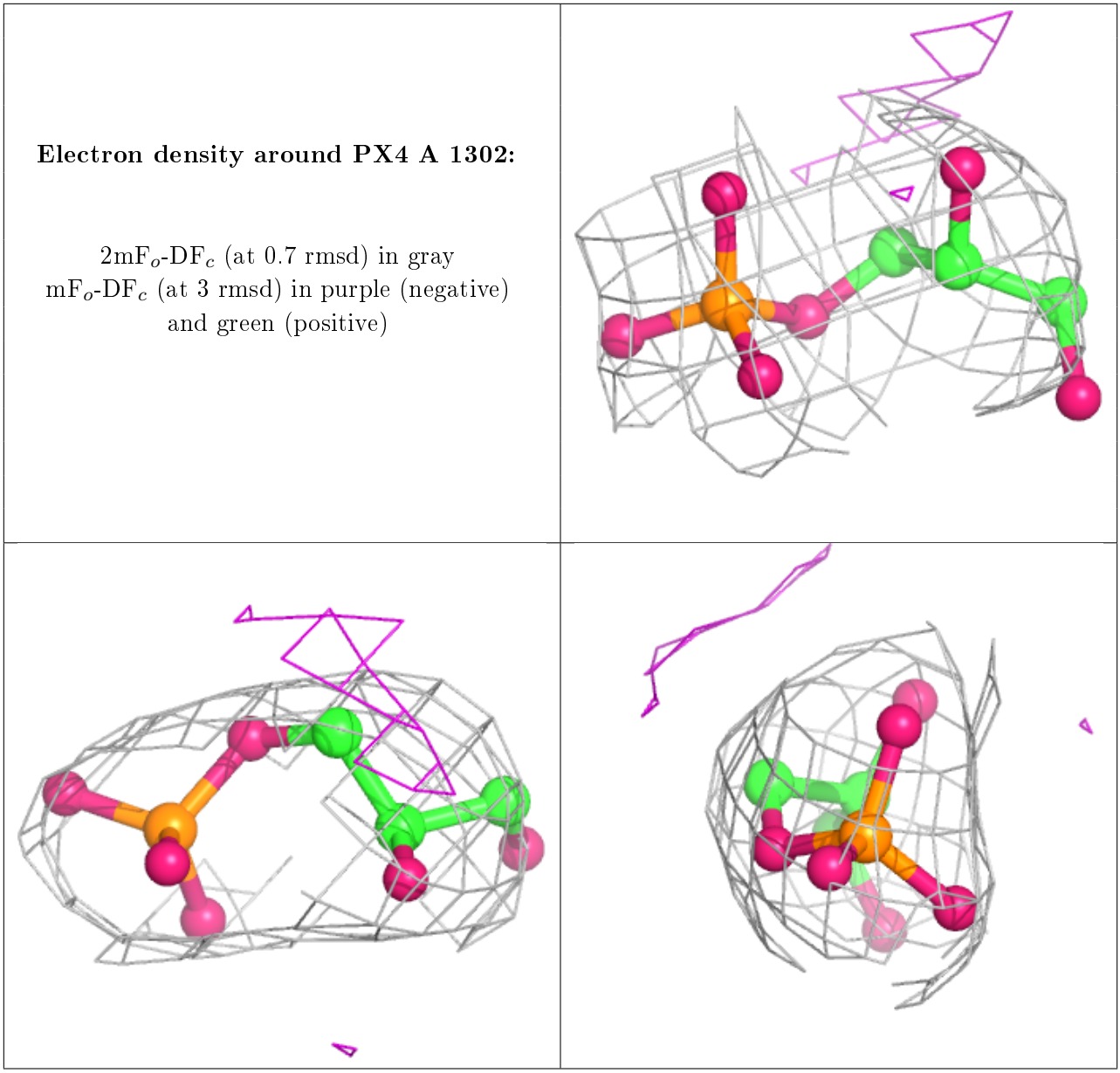






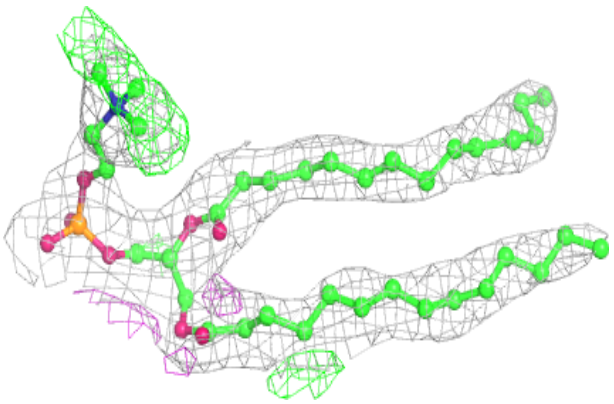
Electron density around PX4 A 1302:

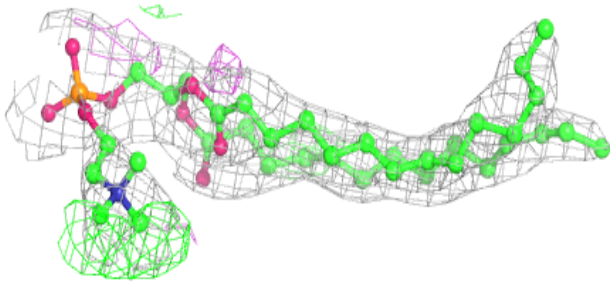
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

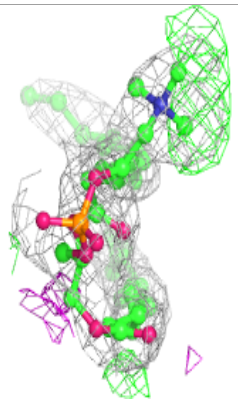


Electron density around PX4 A 1303:

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

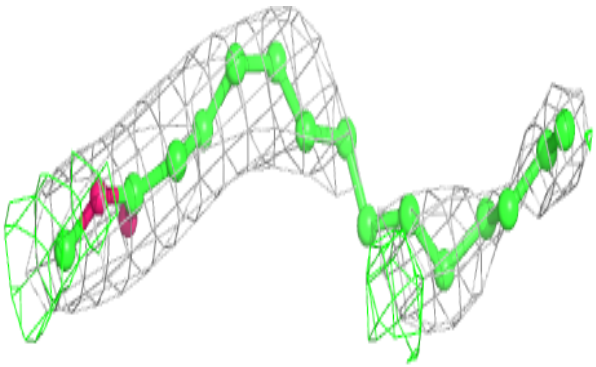


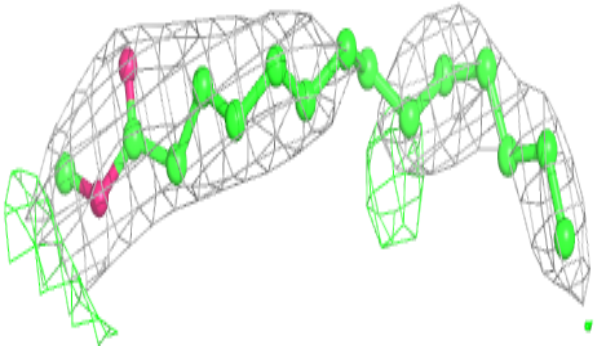


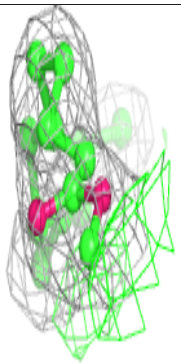


Electron density around PX4 A 1310:

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

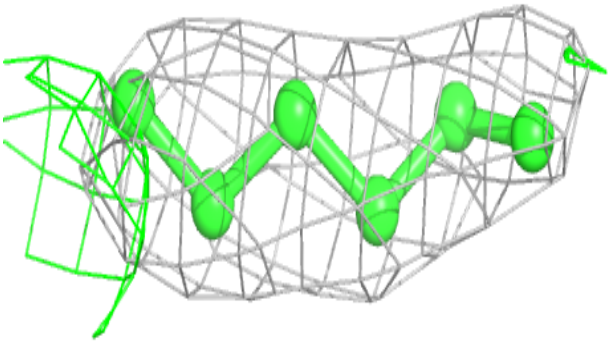


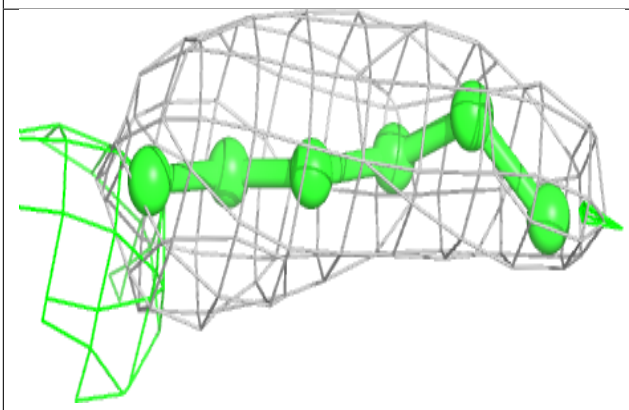


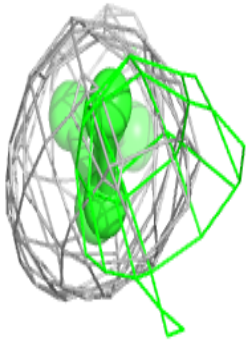


Electron density around PX4 A 1306:

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

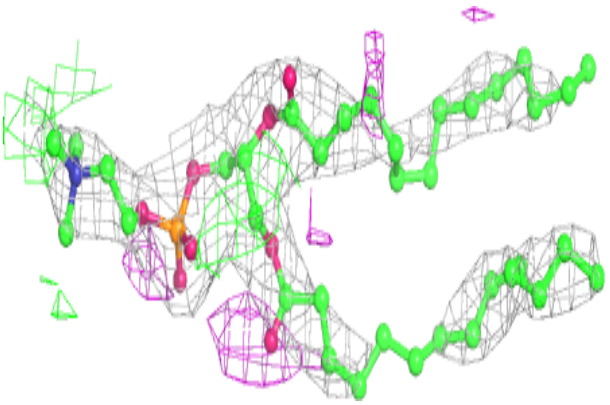


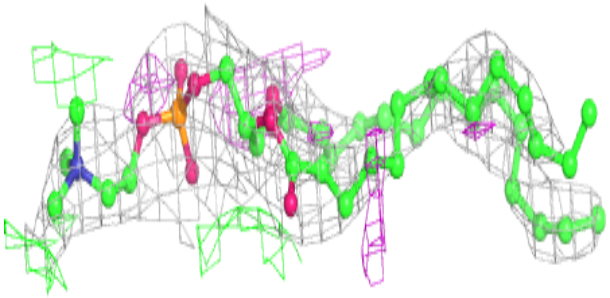


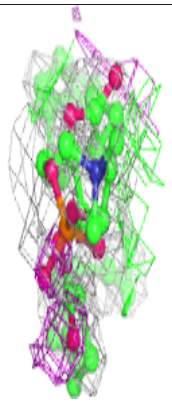


Electron density around PX4 B 2307:

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

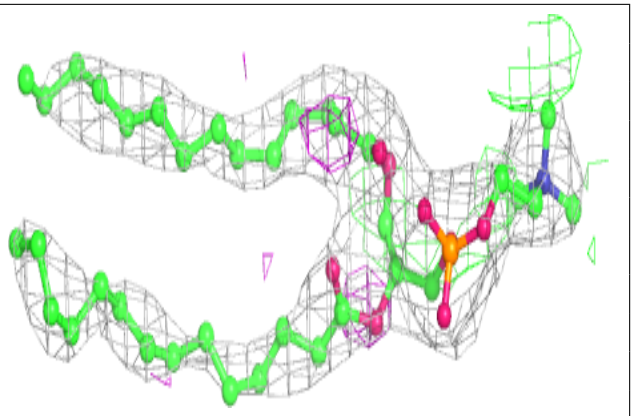


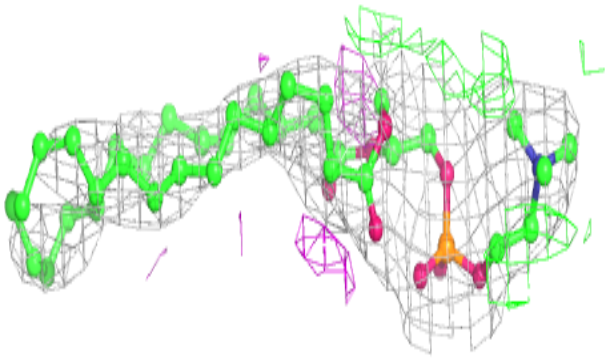


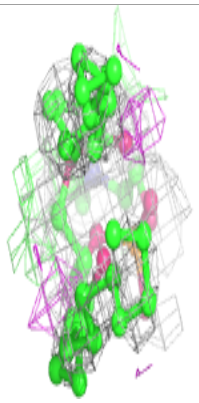


Electron density around PX4 B 2302:

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

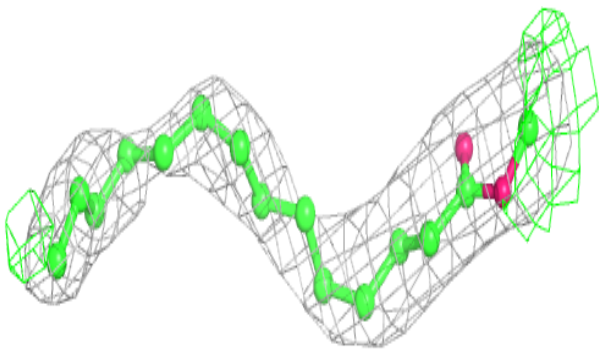


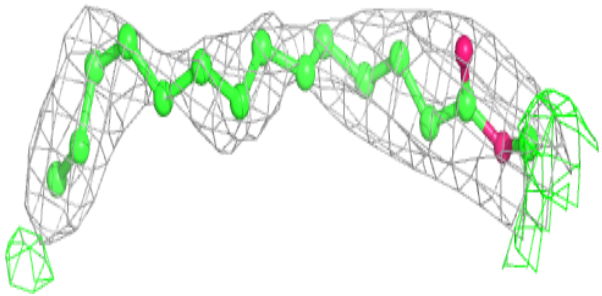


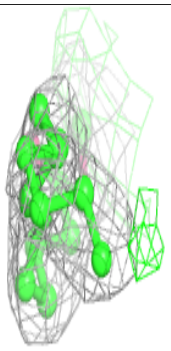


Electron density around PX4 B 2304:

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

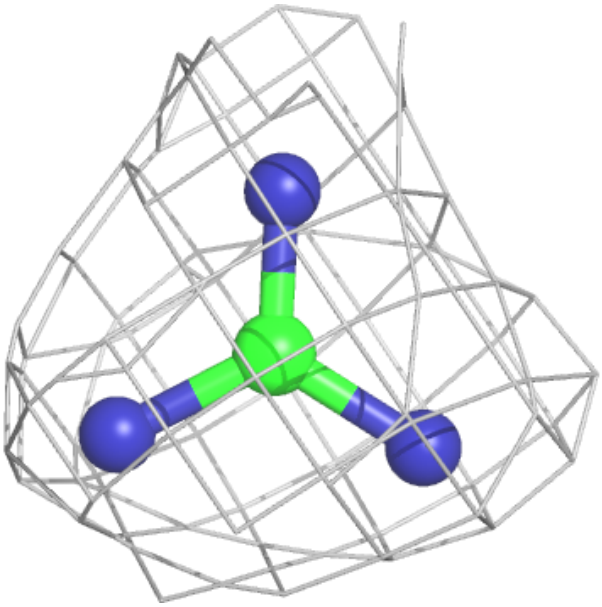


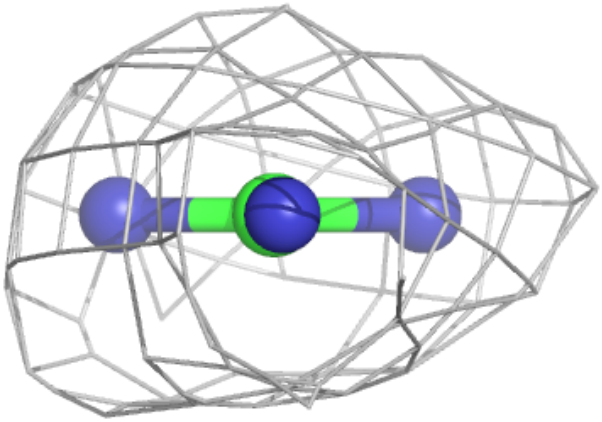


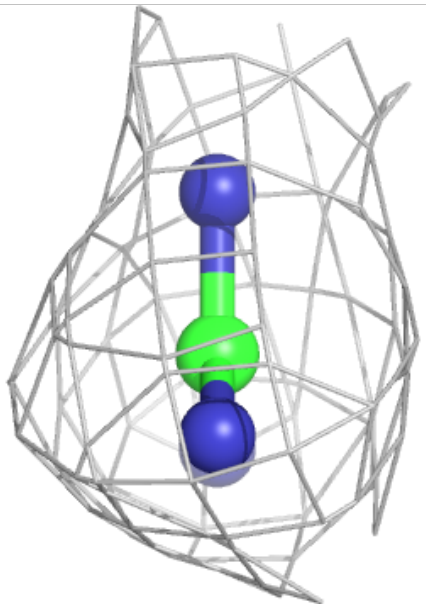


Electron density around GAI B 2305:

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

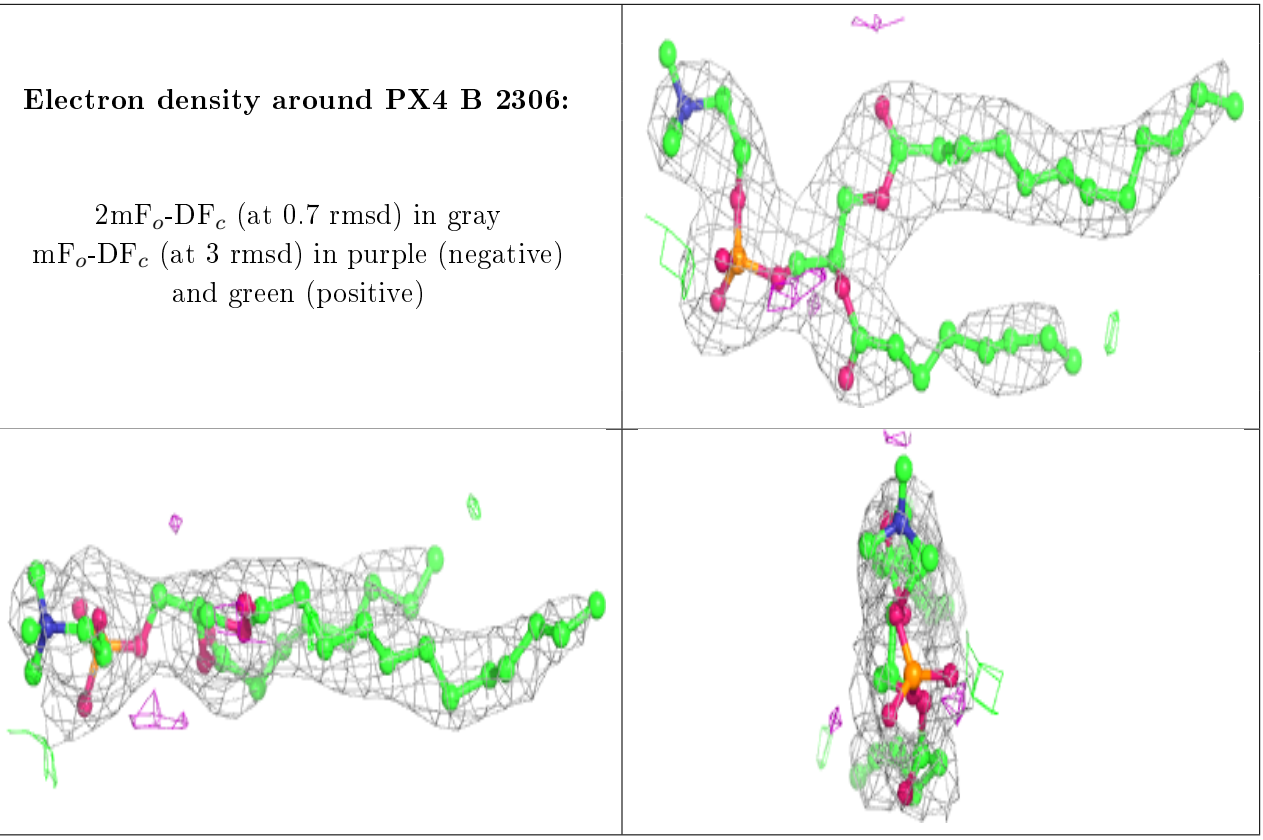






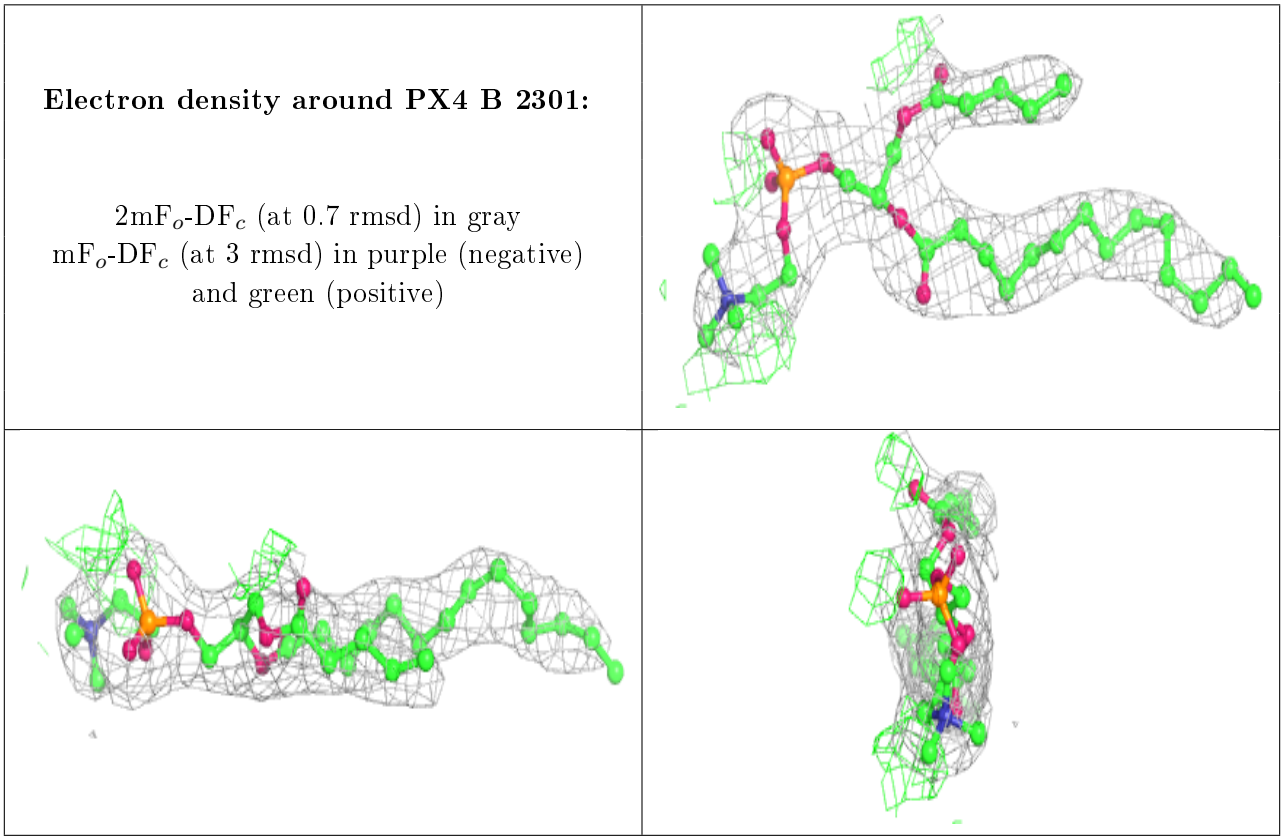
Electron density around PX4 B 2306:

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



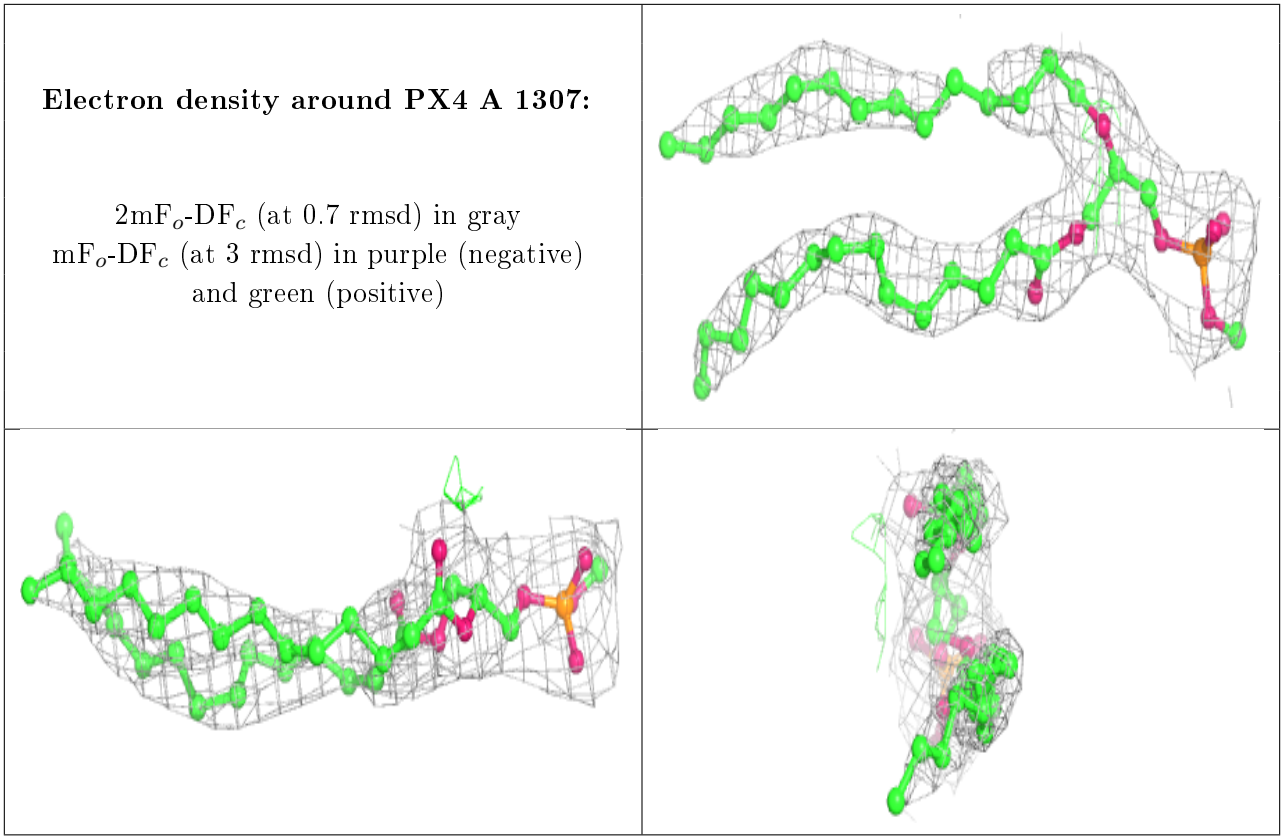
Electron density around PX4 B 2301:

$2mF_o$-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 1307:

$2mF_o$-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

There are no such residues in this entry.