Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 10:03 PM EDT

PDB ID	:	6C1E
Title	:	NavAb NormoPP mutant
Authors	:	Catterall, W.A.; Zheng, N.; Jiang, D.; Gamal El-Din, T.M.
Deposited on	:	2018-01-04
Resolution	:	2.86 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

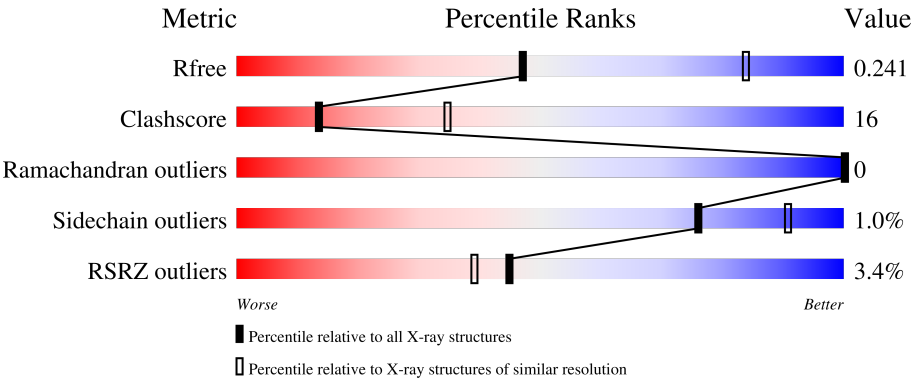
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.86 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	285	3% 59% 18% · 22%
1	B	285	2% 54% 23% · 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	PX4	B	3002	-	-	-	X
2	PX4	B	3006	-	-	-	X
3	BNC	A	1308	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4118 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
			1803	1229	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	1105	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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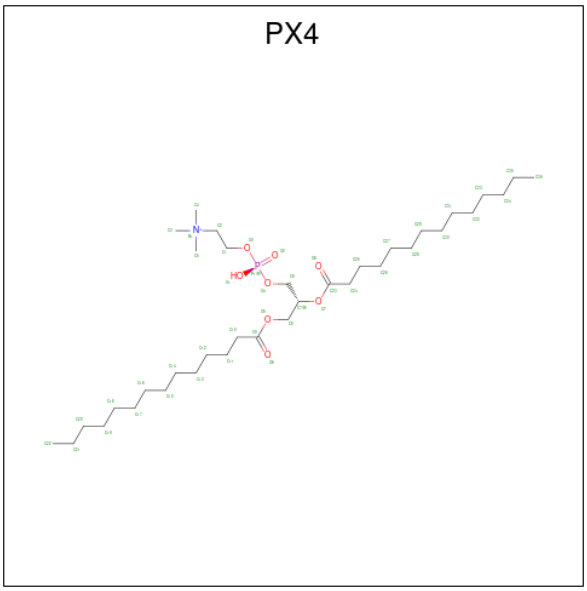
Chain	Residue	Modelled	Actual	Comment	Reference
B	1988	ASP	-	expression tag	UNP A8EVM5
B	1989	ASP	-	expression tag	UNP A8EVM5
B	1990	ASP	-	expression tag	UNP A8EVM5
B	1991	LYS	-	expression tag	UNP A8EVM5
B	1992	GLY	-	expression tag	UNP A8EVM5
B	1993	SER	-	expression tag	UNP A8EVM5
B	1994	LEU	-	expression 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	2105	GLY	ARG	engineered mutation	UNP A8EVM5
B	2217	CYS	ILE	engineered mutation	UNP A8EVM5

- Molecule 2 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
2	A	1	Total C O P 40 31 8 1	0	0
2	A	1	Total C N O P 45 35 1 8 1	0	0
2	A	1	Total C O P 24 17 6 1	0	0

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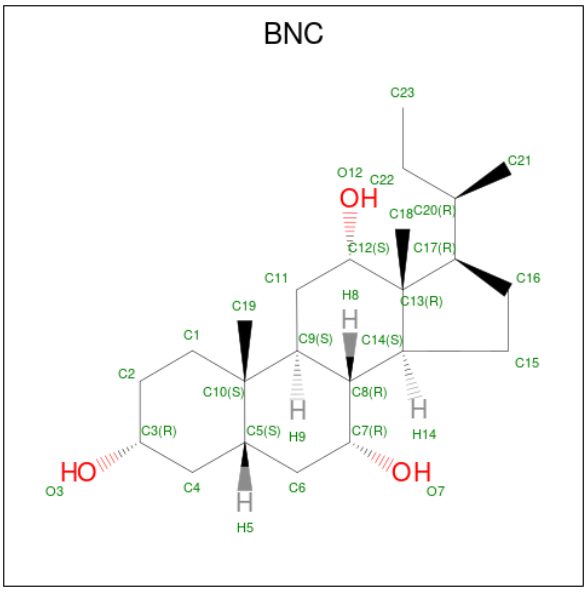
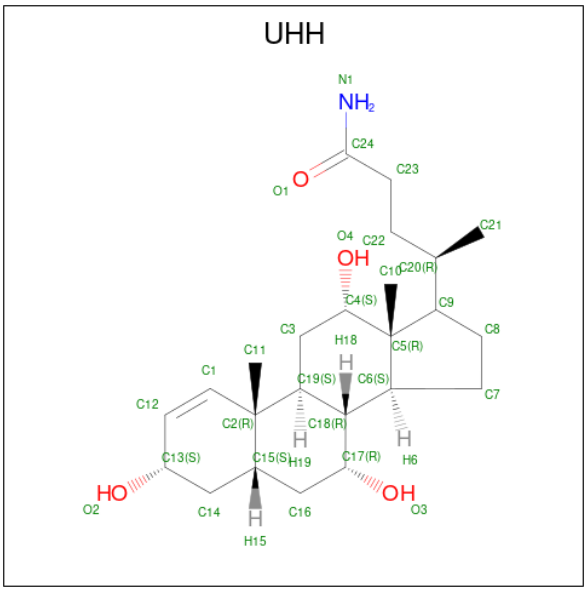
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 11 5 1 4 1	0	0
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C O P 29 20 8 1	0	0
2	A	1	Total C O P 39 30 8 1	0	0
2	A	1	Total C O P 24 17 6 1	0	0
2	A	1	Total C O 16 14 2	0	0
2	B	1	Total C N O P 40 30 1 8 1	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C N O P 33 23 1 8 1	0	0
2	B	1	Total C N O P 46 36 1 8 1	0	0
2	B	1	Total C N O P 11 5 1 4 1	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C O P 29 20 8 1	0	0

- Molecule 3 is 5-BETA-24-NOR-CHOLANE-3(ALPHA),7(ALPHA),12(ALPHA)-TRIOL (three-letter code: BNC) (formula: $C_{23}H_{40}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			26	23	3		

- Molecule 4 is (3ALPHA,5ALPHA,7ALPHA,8ALPHA,12ALPHA,14BETA,17ALPHA)-3,7,12-TRIHYDROXYCHOL-1-EN-24-AMIDE (three-letter code: UHH) (formula: $C_{24}H_{39}NO_4$).



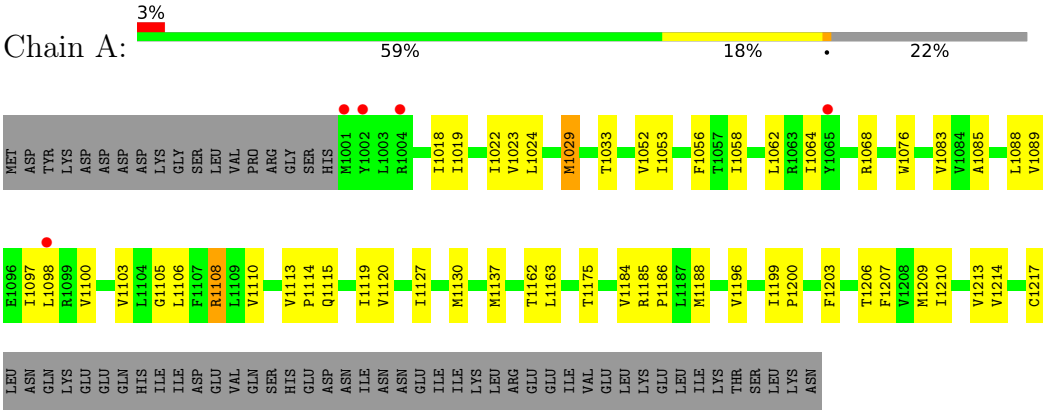
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			29	24	1	4		

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.

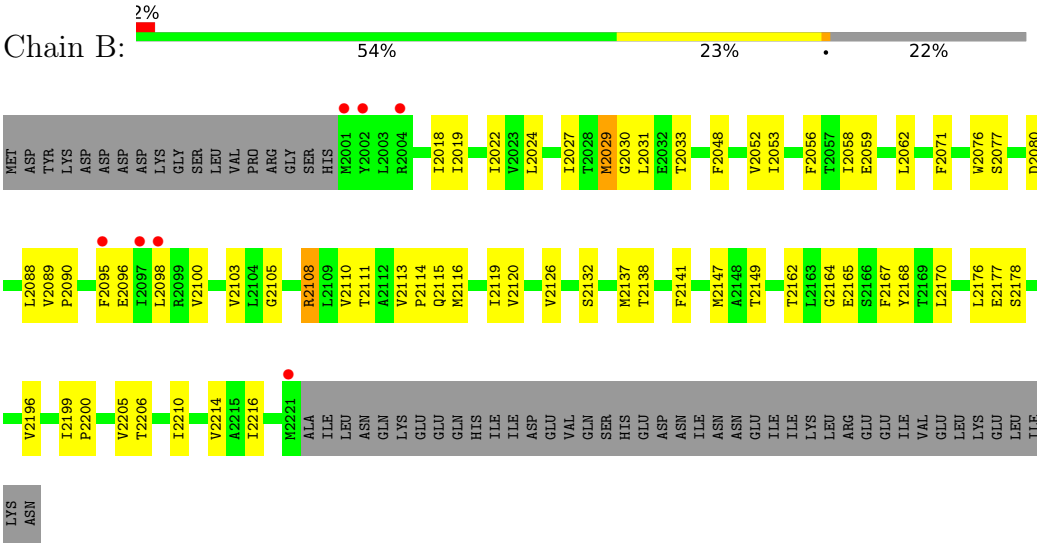
• Molecule 1: Ion transport protein

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	126.78Å 127.00Å 192.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.50 – 2.86 42.50 – 2.86	Depositor EDS
% Data completeness (in resolution range)	96.6 (42.50-2.86) 96.7 (42.50-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.240 0.216 , 0.241	Depositor DCC
R_{free} test set	1763 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	83.1	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 77.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.469 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4118	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: UHH, PX4, BNC

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	0.48	0/1854	0.58	0/2522
1	B	0.50	0/1854	0.59	0/2522
All	All	0.49	0/3708	0.59	0/5044

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1803	0	1873	59	0
1	B	1803	0	1873	67	0
2	A	260	0	363	17	0
2	B	197	0	284	24	0
3	A	26	0	0	0	0
4	B	29	0	0	0	0
All	All	4118	0	4393	136	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 16.

All (136) 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:B:2095:PHE:CZ	2:B:3006:PX4:H48	1.67	1.27
1:B:2095:PHE:CZ	2:B:3006:PX4:C25	2.50	0.94
1:A:1052:VAL:CG1	1:A:1056:PHE:HE1	1.90	0.83
1:B:2052:VAL:CG1	1:B:2056:PHE:HE1	1.94	0.81
1:A:1052:VAL:HG13	1:A:1056:PHE:HE1	1.48	0.78
1:A:1052:VAL:CG1	1:A:1056:PHE:CE1	2.69	0.76
1:B:2085:ALA:HA	1:B:2088:LEU:HD12	1.70	0.74
1:B:2052:VAL:CG1	1:B:2056:PHE:CE1	2.71	0.73
1:B:2052:VAL:HG13	1:B:2056:PHE:HE1	1.54	0.71
1:B:2095:PHE:CE2	2:B:3006:PX4:H48	2.24	0.71
1:B:2080:ASP:OD2	1:B:2111:THR:HG21	1.91	0.71
1:B:2095:PHE:CE1	2:B:3006:PX4:H48	2.24	0.71
1:A:1022:ILE:HD12	1:A:1108:ARG:HB3	1.71	0.71
1:A:1052:VAL:HG13	1:A:1056:PHE:CE1	2.28	0.69
2:B:3001:PX4:H28	2:B:3001:PX4:H56	1.75	0.68
1:A:1085:ALA:HA	1:A:1088:LEU:HD12	1.77	0.67
2:A:1301:PX4:H64	2:A:1301:PX4:H37	1.76	0.66
1:B:2022:ILE:HD12	1:B:2108:ARG:HB3	1.78	0.66
1:B:2052:VAL:O	1:B:2056:PHE:HD1	1.81	0.63
1:A:1029:MET:HE2	1:A:1106:LEU:HD11	1.80	0.63
1:A:1029:MET:CE	1:A:1106:LEU:HG	2.30	0.62
1:B:2108:ARG:HG2	1:B:2108:ARG:NH1	2.14	0.62
1:A:1105:GLY:O	1:A:1108:ARG:HB2	2.00	0.61
1:B:2164:GLY:HA3	2:B:3003:PX4:O1	2.00	0.61
2:A:1301:PX4:H23	2:B:3001:PX4:H46	1.83	0.61
1:B:2089:VAL:HG11	1:B:2098:LEU:HD13	1.82	0.61
1:A:1033:THR:HG23	1:B:2149:THR:HG21	1.82	0.60
1:A:1029:MET:HE3	1:A:1103:VAL:HG23	1.82	0.60
1:B:2052:VAL:HG13	1:B:2056:PHE:CE1	2.35	0.60
1:A:1029:MET:CE	1:A:1106:LEU:HD11	2.31	0.60
1:B:2108:ARG:CG	1:B:2108:ARG:HH11	2.16	0.59
1:A:1052:VAL:O	1:A:1056:PHE:HD1	1.86	0.58
1:B:2206:THR:O	1:B:2210:ILE:HG13	2.03	0.58
1:A:1029:MET:CE	1:A:1106:LEU:CG	2.81	0.58
1:A:1100:VAL:O	1:A:1103:VAL:HG12	2.03	0.58
2:A:1302:PX4:H30	2:A:1302:PX4:H59	1.85	0.58
1:A:1019:ILE:HD13	1:A:1113:VAL:HG22	1.85	0.58
1:B:2029:MET:HE3	1:B:2103:VAL:HA	1.84	0.58
1:A:1029:MET:HE2	1:A:1106:LEU:HD21	1.85	0.57
1:A:1113:VAL:HG12	1:A:1114:PRO:O	2.05	0.56
1:B:2052:VAL:HG12	1:B:2056:PHE:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:THR:HG23	2:A:1301:PX4:H18	1.87	0.56
1:A:1089:VAL:HG11	1:A:1098:LEU:HD13	1.87	0.54
1:A:1108:ARG:NH1	1:A:1108:ARG:HG2	2.22	0.54
1:B:2113:VAL:HG12	1:B:2114:PRO:O	2.07	0.54
1:A:1052:VAL:HG12	1:A:1056:PHE:CE1	2.42	0.54
1:B:2108:ARG:HG2	1:B:2108:ARG:HH11	1.72	0.54
1:A:1110:VAL:HG11	1:A:1120:VAL:HG21	1.90	0.54
1:B:2076:TRP:CZ3	2:B:3008:PX4:H19	2.43	0.53
1:B:2095:PHE:CE2	2:B:3006:PX4:C25	2.89	0.53
1:A:1018:ILE:O	1:A:1022:ILE:HG12	2.09	0.53
1:B:2115:GLN:O	1:B:2119:ILE:HG12	2.08	0.52
1:B:2052:VAL:HG12	1:B:2056:PHE:CD1	2.44	0.52
1:A:1217:CYS:SG	1:B:2214:VAL:HG22	2.49	0.52
1:B:2018:ILE:O	1:B:2022:ILE:HG12	2.09	0.52
1:A:1029:MET:HE1	1:A:1106:LEU:HG	1.91	0.52
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.91	0.51
1:B:2199:ILE:HB	1:B:2200:PRO:HD3	1.92	0.51
1:A:1206:THR:O	1:A:1210:ILE:HG13	2.11	0.51
1:A:1115:GLN:O	1:A:1119:ILE:HG12	2.11	0.51
1:A:1023:VAL:HA	2:A:1309:PX4:H40	1.92	0.50
1:A:1203:PHE:CD2	2:A:1303:PX4:H49	2.46	0.50
2:B:3001:PX4:H29	2:B:3001:PX4:H61	1.93	0.50
1:A:1175:THR:HB	1:B:2176:LEU:HD13	1.92	0.50
1:B:2168:TYR:HA	2:B:3003:PX4:H48	1.94	0.49
2:A:1301:PX4:H27	2:B:3001:PX4:H49	1.95	0.48
1:A:1097:ILE:HD11	2:B:3004:PX4:H46	1.95	0.48
1:B:2029:MET:CE	1:B:2103:VAL:HA	2.43	0.48
2:B:3001:PX4:H48	2:B:3002:PX4:H68	1.95	0.48
1:A:1033:THR:CG2	1:B:2149:THR:HG21	2.44	0.48
1:B:2100:VAL:O	1:B:2103:VAL:HG12	2.13	0.48
1:B:2110:VAL:HG11	1:B:2120:VAL:HG21	1.95	0.48
1:A:1052:VAL:HG12	1:A:1056:PHE:CD1	2.49	0.48
1:A:1064:ILE:O	1:A:1068:ARG:N	2.38	0.48
1:B:2114:PRO:O	1:B:2116:MET:N	2.45	0.47
2:B:3003:PX4:H18	2:B:3007:PX4:H63	1.97	0.47
1:A:1163:LEU:HD23	2:A:1301:PX4:H21	1.96	0.47
2:A:1309:PX4:H67	1:B:2138:THR:HG22	1.97	0.47
1:B:2059:GLU:OE1	1:B:2108:ARG:NH2	2.48	0.47
1:B:2108:ARG:O	1:B:2111:THR:N	2.48	0.47
1:A:1029:MET:CE	1:A:1106:LEU:CD1	2.92	0.47
1:B:2019:ILE:HD13	1:B:2113:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2030:GLY:O	1:B:2033:THR:HB	2.16	0.46
2:A:1306:PX4:H54	2:B:3004:PX4:H48	1.96	0.46
1:B:2052:VAL:O	1:B:2056:PHE:CD1	2.67	0.46
1:B:2080:ASP:CG	1:B:2108:ARG:NH1	2.68	0.46
1:A:1095:PHE:CE2	2:A:1306:PX4:H52	2.51	0.46
1:A:1108:ARG:HG2	1:A:1108:ARG:HH11	1.78	0.46
1:B:2210:ILE:O	1:B:2214:VAL:HG23	2.15	0.46
1:A:1108:ARG:HH11	1:A:1108:ARG:CG	2.29	0.46
1:A:1209:MET:O	1:A:1213:VAL:HG23	2.16	0.46
1:A:1210:ILE:O	1:A:1214:VAL:HG23	2.16	0.46
1:A:1119:ILE:HG13	1:B:2132:SER:HB3	1.99	0.45
1:A:1083:VAL:HG11	1:A:1105:GLY:HA2	1.98	0.45
1:B:2193:TYR:CD1	2:B:3004:PX4:H49	2.51	0.45
1:B:2105:GLY:O	1:B:2108:ARG:HB2	2.17	0.45
1:A:1029:MET:CE	1:A:1106:LEU:HD21	2.45	0.45
1:B:2162:THR:HB	1:B:2165:GLU:HB2	1.99	0.45
1:A:1137:MET:HG2	2:B:3001:PX4:H35	2.00	0.44
2:A:1309:PX4:H19	2:A:1309:PX4:H50	2.00	0.44
1:B:2096:GLU:HG2	1:B:2096:GLU:O	2.17	0.44
1:B:2029:MET:HE3	1:B:2103:VAL:HG23	1.99	0.44
1:A:1052:VAL:O	1:A:1056:PHE:CD1	2.70	0.44
1:A:1207:PHE:CD2	2:A:1303:PX4:H64	2.52	0.43
1:A:1053:ILE:HD11	1:A:1088:LEU:HA	2.01	0.43
1:B:2089:VAL:HA	1:B:2090:PRO:HD2	1.80	0.43
1:A:1103:VAL:HG11	1:B:2147:MET:CG	2.49	0.43
1:A:1196:VAL:HG11	2:A:1302:PX4:H58	2.01	0.43
2:B:3001:PX4:O1	2:B:3001:PX4:H12	2.18	0.43
2:A:1305:PX4:H72	2:A:1305:PX4:H64	1.81	0.42
1:B:2024:LEU:HD12	1:B:2024:LEU:HA	1.94	0.42
1:B:2137:MET:HE1	1:B:2205:VAL:HA	2.01	0.42
1:B:2182:GLY:C	1:B:2183:ILE:HD12	2.40	0.42
1:A:1185:ARG:HB2	1:A:1186:PRO:HD3	2.02	0.42
1:A:1127:ILE:O	1:A:1130:MET:HB2	2.20	0.42
1:A:1076:TRP:CZ2	2:A:1307:PX4:H17	2.55	0.41
1:B:2141:PHE:HB3	1:B:2167:PHE:CE2	2.55	0.41
1:B:2196:VAL:HG11	2:B:3004:PX4:H58	2.01	0.41
2:B:3004:PX4:H51	2:B:3004:PX4:O8	2.19	0.41
2:B:3006:PX4:H71	2:B:3007:PX4:H69	2.02	0.41
1:B:2058:ILE:O	1:B:2062:LEU:HG	2.20	0.41
2:B:3003:PX4:H50	2:B:3003:PX4:O8	2.20	0.41
2:A:1302:PX4:H9	2:A:1302:PX4:H2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2048:PHE:O	1:B:2052:VAL:HG23	2.20	0.41
1:B:2126:VAL:HG11	1:B:2216:ILE:HG23	2.01	0.41
1:B:2177:GLU:OE1	1:B:2178:SER:OG	2.21	0.41
1:B:2170:LEU:HD23	1:B:2170:LEU:HA	1.93	0.41
1:B:2083:VAL:HG11	1:B:2105:GLY:HA2	2.03	0.41
2:B:3001:PX4:H28	2:B:3001:PX4:H22	1.96	0.41
1:A:1024:LEU:HD12	1:A:1024:LEU:HA	1.97	0.41
1:A:1103:VAL:HG11	1:B:2147:MET:HG3	2.03	0.40
1:A:1058:ILE:O	1:A:1062:LEU:HG	2.21	0.40
1:B:2071:PHE:CE1	1:B:2077:SER:HB3	2.56	0.40
1:B:2027:ILE:O	1:B:2031:LEU:HD13	2.21	0.40
1:A:1184:VAL:O	1:A:1188:MET:HG3	2.22	0.40
1:B:2053:ILE:HD11	1:B:2088:LEU:HA	2.03	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%)	204 (93%)	15 (7%)	0	100	100
1	B	219/285 (77%)	204 (93%)	15 (7%)	0	100	100
All	All	438/570 (77%)	408 (93%)	30 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	202/263 (77%)	200 (99%)	2 (1%)	76 91
1	B	202/263 (77%)	200 (99%)	2 (1%)	76 91
All	All	404/526 (77%)	400 (99%)	4 (1%)	76 91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1029	MET
1	A	1108	ARG
1	B	2029	MET
1	B	2108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2211	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 ligands 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	PX4	B	3007	-	10,10,45	0.66	0	9,9,53	0.69	0
2	PX4	A	1305	-	15,15,45	1.21	1 (6%)	15,15,53	1.16	0
2	PX4	A	1310	-	23,23,45	0.94	1 (4%)	25,26,53	0.99	1 (4%)
2	PX4	A	1311	-	15,15,45	1.91	2 (13%)	15,15,53	1.04	2 (13%)
2	PX4	B	3005	-	10,10,45	1.31	1 (10%)	15,15,53	0.59	0
3	BNC	A	1308	-	29,29,29	3.18	11 (37%)	47,47,47	2.44	19 (40%)
2	PX4	B	3002	-	10,10,45	0.63	0	9,9,53	0.76	0
2	PX4	A	1306	-	15,15,45	1.25	1 (6%)	15,15,53	1.04	0
4	UHH	B	3009	-	31,32,32	3.99	15 (48%)	47,51,51	2.93	15 (31%)
2	PX4	B	3004	-	45,45,45	1.17	3 (6%)	51,53,53	1.17	6 (11%)
2	PX4	A	1304	-	10,10,45	1.28	1 (10%)	15,15,53	0.67	0
2	PX4	B	3003	-	32,32,45	1.11	3 (9%)	36,39,53	1.28	4 (11%)
2	PX4	A	1309	-	38,38,45	1.21	3 (7%)	42,43,53	1.25	3 (7%)
2	PX4	B	3001	-	39,39,45	1.21	3 (7%)	45,47,53	1.14	3 (6%)
2	PX4	B	3006	-	15,15,45	1.93	2 (13%)	15,15,53	1.06	1 (6%)
2	PX4	A	1303	-	23,23,45	0.91	1 (4%)	25,26,53	1.17	2 (8%)
2	PX4	A	1301	-	39,39,45	1.20	3 (7%)	43,44,53	1.37	3 (6%)
2	PX4	A	1307	-	28,28,45	1.30	2 (7%)	32,33,53	1.22	3 (9%)
2	PX4	A	1302	-	44,44,45	1.14	3 (6%)	50,52,53	1.19	4 (8%)
2	PX4	B	3008	-	28,28,45	1.25	2 (7%)	32,33,53	1.30	3 (9%)

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	PX4	B	3007	-	-	6/8/8/49	-
2	PX4	A	1305	-	-	5/13/13/49	-
2	PX4	A	1310	-	-	11/24/24/49	-
2	PX4	A	1311	-	-	4/13/13/49	-
2	PX4	B	3005	-	-	0/8/8/49	-
3	BNC	A	1308	-	-	2/6/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PX4	B	3002	-	-	5/8/8/49	-
2	PX4	A	1306	-	-	4/13/13/49	-
4	UHH	B	3009	-	-	3/9/74/74	0/4/4/4
2	PX4	B	3004	-	-	28/49/49/49	-
2	PX4	A	1304	-	-	4/8/8/49	-
2	PX4	B	3003	-	-	24/35/35/49	-
2	PX4	A	1309	-	-	20/40/40/49	-
2	PX4	B	3001	-	-	27/43/43/49	-
2	PX4	B	3006	-	-	8/13/13/49	-
2	PX4	A	1303	-	-	10/24/24/49	-
2	PX4	A	1301	-	-	15/41/41/49	-
2	PX4	A	1307	-	-	15/30/30/49	-
2	PX4	A	1302	-	-	24/48/48/49	-
2	PX4	B	3008	-	-	14/30/30/49	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3009	UHH	C12-C1	12.88	1.51	1.32
3	A	1308	BNC	C11-C12	8.19	1.67	1.53
4	B	3009	UHH	C3-C4	7.95	1.66	1.53
2	B	3006	PX4	O8-C23	6.57	1.43	1.22
3	A	1308	BNC	C16-C15	6.42	1.71	1.54
2	A	1311	PX4	O8-C23	6.41	1.43	1.22
4	B	3009	UHH	C8-C7	6.32	1.71	1.54
4	B	3009	UHH	C18-C19	5.81	1.65	1.53
3	A	1308	BNC	C8-C9	5.66	1.64	1.53
4	B	3009	UHH	C20-C9	-5.22	1.45	1.54
3	A	1308	BNC	C13-C17	5.10	1.64	1.55
3	A	1308	BNC	C6-C5	4.85	1.61	1.53
4	B	3009	UHH	O4-C4	-4.77	1.35	1.43
4	B	3009	UHH	C7-C6	4.65	1.64	1.54
4	B	3009	UHH	C16-C15	4.59	1.61	1.53
3	A	1308	BNC	O12-C12	-4.57	1.36	1.43
3	A	1308	BNC	C15-C14	4.42	1.63	1.54
4	B	3009	UHH	C24-N1	4.40	1.47	1.32
4	B	3009	UHH	C5-C9	4.40	1.63	1.55
3	A	1308	BNC	C20-C17	-4.34	1.46	1.54
2	A	1307	PX4	O5-C9	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1309	PX4	O5-C9	4.11	1.45	1.33
2	A	1301	PX4	O5-C9	4.05	1.45	1.33
2	B	3008	PX4	O5-C9	4.01	1.45	1.33
2	A	1305	PX4	O7-C23	3.92	1.43	1.30
2	A	1306	PX4	O7-C23	3.90	1.43	1.30
3	A	1308	BNC	C6-C7	3.67	1.59	1.52
2	B	3004	PX4	O5-C9	3.64	1.44	1.33
2	A	1309	PX4	O7-C23	3.62	1.44	1.34
2	A	1301	PX4	O7-C23	3.62	1.44	1.34
2	B	3001	PX4	O5-C9	3.58	1.43	1.33
2	A	1310	PX4	O7-C23	3.45	1.43	1.33
2	B	3001	PX4	O7-C23	3.42	1.44	1.34
4	B	3009	UHH	C16-C17	3.38	1.58	1.52
2	B	3004	PX4	O7-C23	3.36	1.43	1.34
2	B	3008	PX4	O7-C23	3.35	1.43	1.34
2	A	1302	PX4	O7-C23	3.32	1.43	1.34
2	A	1302	PX4	O5-C9	3.32	1.43	1.33
2	A	1307	PX4	O7-C23	3.27	1.43	1.34
2	A	1303	PX4	O7-C23	3.14	1.42	1.33
2	B	3001	PX4	C4-N1	-2.87	1.41	1.50
2	B	3003	PX4	O7-C23	2.74	1.42	1.34
2	B	3003	PX4	O5-C9	2.74	1.43	1.33
2	A	1302	PX4	C4-N1	-2.73	1.42	1.50
2	B	3003	PX4	C4-N1	-2.73	1.42	1.50
4	B	3009	UHH	C13-C12	2.70	1.53	1.49
2	B	3005	PX4	C4-N1	-2.66	1.42	1.50
4	B	3009	UHH	C2-C19	-2.66	1.54	1.55
2	A	1304	PX4	C4-N1	-2.65	1.42	1.50
2	B	3004	PX4	C4-N1	-2.58	1.42	1.50
4	B	3009	UHH	C3-C19	-2.55	1.49	1.53
4	B	3009	UHH	C5-C4	-2.48	1.50	1.54
2	A	1301	PX4	C10-C9	2.40	1.57	1.50
3	A	1308	BNC	C13-C12	-2.37	1.50	1.54
2	A	1311	PX4	O7-C23	-2.23	1.23	1.30
3	A	1308	BNC	C11-C9	-2.22	1.50	1.53
2	A	1309	PX4	C10-C9	2.21	1.57	1.50
2	B	3006	PX4	O7-C23	-2.09	1.23	1.30

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	3009	UHH	C13-C12-C1	-10.15	114.68	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	3009	UHH	C6-C5-C4	9.04	115.82	107.40
4	B	3009	UHH	C9-C5-C4	6.97	124.03	117.67
3	A	1308	BNC	C17-C13-C12	6.63	123.72	117.67
3	A	1308	BNC	C14-C13-C12	6.28	113.25	107.40
4	B	3009	UHH	C10-C5-C4	-5.40	103.56	109.07
2	A	1301	PX4	O7-C23-C24	5.39	123.11	111.50
2	B	3004	PX4	O7-C23-C24	4.76	121.77	111.50
2	A	1309	PX4	O7-C23-C24	4.65	121.52	111.50
3	A	1308	BNC	C18-C13-C12	-4.64	104.34	109.07
2	B	3008	PX4	O7-C23-C24	4.53	121.26	111.50
2	A	1302	PX4	O7-C23-C24	4.42	121.03	111.50
3	A	1308	BNC	C18-C13-C14	-4.42	104.30	111.21
4	B	3009	UHH	C19-C2-C1	-4.26	106.14	112.23
3	A	1308	BNC	C1-C10-C5	4.15	113.90	107.77
4	B	3009	UHH	C16-C15-C14	-3.88	106.73	111.19
3	A	1308	BNC	C10-C9-C8	3.86	115.97	111.82
2	A	1307	PX4	O5-C9-C10	3.76	123.71	111.91
4	B	3009	UHH	C10-C5-C6	-3.73	105.38	111.21
2	B	3003	PX4	O7-C23-C24	3.66	119.38	111.50
2	A	1303	PX4	O7-C23-C24	3.51	122.94	111.91
2	A	1301	PX4	O5-C9-C10	3.49	122.87	111.91
3	A	1308	BNC	C9-C10-C5	3.46	113.45	108.58
2	A	1302	PX4	O5-C9-C10	3.40	122.58	111.91
2	B	3004	PX4	O5-C9-C10	3.22	122.01	111.91
2	A	1309	PX4	O5-C9-C10	3.21	122.00	111.91
4	B	3009	UHH	C11-C2-C19	-3.19	107.45	111.62
3	A	1308	BNC	C9-C11-C12	-3.15	110.14	114.30
3	A	1308	BNC	C1-C10-C9	-3.09	106.49	111.35
2	B	3001	PX4	O7-C23-C24	3.01	117.99	111.50
4	B	3009	UHH	C2-C19-C18	2.87	113.53	111.12
4	B	3009	UHH	C10-C5-C9	-2.87	106.72	111.21
2	A	1307	PX4	O7-C23-C24	2.85	117.64	111.50
2	B	3004	PX4	O7-C23-O8	-2.84	116.85	123.70
4	B	3009	UHH	C23-C22-C20	-2.78	109.44	114.52
3	A	1308	BNC	C18-C13-C17	-2.78	106.86	111.21
4	B	3009	UHH	C19-C2-C15	2.78	111.38	107.53
2	B	3001	PX4	O5-C9-C10	2.75	120.55	111.91
2	B	3008	PX4	O5-C9-C10	2.74	120.52	111.91
2	B	3003	PX4	C8-C7-C6	-2.72	105.35	111.79
3	A	1308	BNC	C17-C13-C14	2.66	102.78	100.09
3	A	1308	BNC	C6-C7-C8	2.64	114.30	111.48
3	A	1308	BNC	C15-C14-C8	2.59	121.96	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1308	BNC	C6-C5-C4	-2.59	108.21	111.19
4	B	3009	UHH	C7-C6-C18	2.59	121.95	118.33
4	B	3009	UHH	C19-C3-C4	-2.59	110.89	114.30
3	A	1308	BNC	C19-C10-C9	-2.50	107.74	111.18
2	A	1309	PX4	O5-C8-C7	2.48	115.65	108.43
2	A	1301	PX4	O5-C9-O6	-2.46	117.37	123.59
2	A	1310	PX4	O7-C23-C24	2.45	119.59	111.91
2	A	1302	PX4	O5-C9-O6	-2.44	117.43	123.59
3	A	1308	BNC	C13-C14-C8	2.40	117.80	114.74
2	A	1302	PX4	C25-C24-C23	-2.38	104.96	113.62
2	B	3003	PX4	O7-C23-O8	-2.32	118.11	123.70
2	A	1303	PX4	O7-C23-O8	-2.31	117.76	123.59
3	A	1308	BNC	C16-C17-C20	-2.31	108.58	112.15
2	B	3006	PX4	C25-C24-C23	-2.30	108.68	114.47
2	B	3004	PX4	O5-C9-O6	-2.29	117.81	123.59
4	B	3009	UHH	C5-C6-C18	2.17	117.51	114.74
2	A	1311	PX4	O7-C23-C24	2.16	120.98	114.03
2	A	1307	PX4	O6-C9-C10	-2.16	115.30	123.73
3	A	1308	BNC	C4-C5-C10	2.16	114.95	112.66
2	B	3001	PX4	C11-C10-C9	-2.10	106.00	113.62
2	B	3008	PX4	O7-C23-O8	-2.08	118.67	123.70
3	A	1308	BNC	C19-C10-C5	-2.07	106.85	110.36
2	B	3004	PX4	C11-C10-C9	-2.06	106.11	113.62
2	B	3003	PX4	O3-P1-O2	2.06	117.10	109.07
2	A	1311	PX4	O7-C23-O8	-2.02	118.26	123.30
2	B	3004	PX4	C7-O7-C23	-2.01	112.83	117.79

There are no chirality outliers.

All (229) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1302	PX4	O7-C7-C8-O5
2	A	1303	PX4	C6-O4-P1-O2
2	A	1304	PX4	C1-O3-P1-O1
2	A	1304	PX4	C1-O3-P1-O4
2	A	1304	PX4	O3-C1-C2-N1
2	A	1307	PX4	C6-O4-P1-O1
2	A	1307	PX4	C6-O4-P1-O2
2	A	1307	PX4	C6-O4-P1-O3
2	A	1309	PX4	C6-O4-P1-O1
2	A	1309	PX4	C6-O4-P1-O2
2	A	1309	PX4	C6-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
2	A	1309	PX4	C24-C23-O7-C7
2	B	3001	PX4	C1-O3-P1-O2
2	B	3001	PX4	O3-C1-C2-N1
2	B	3003	PX4	C1-O3-P1-O1
2	B	3003	PX4	C6-O4-P1-O3
2	B	3003	PX4	O6-C9-O5-C8
2	B	3004	PX4	C6-O4-P1-O1
2	B	3004	PX4	C6-O4-P1-O2
2	B	3004	PX4	C6-O4-P1-O3
2	B	3008	PX4	C6-O4-P1-O2
2	B	3008	PX4	O8-C23-O7-C7
2	B	3008	PX4	C24-C23-O7-C7
2	A	1302	PX4	O8-C23-O7-C7
2	A	1309	PX4	O8-C23-O7-C7
2	A	1310	PX4	C24-C23-O7-C7
2	A	1310	PX4	O8-C23-O7-C7
2	A	1302	PX4	C24-C23-O7-C7
2	A	1302	PX4	C16-C17-C18-C19
2	A	1309	PX4	C10-C9-O5-C8
2	A	1309	PX4	O6-C9-O5-C8
2	A	1301	PX4	C10-C9-O5-C8
2	B	3001	PX4	C10-C9-O5-C8
4	B	3009	UHH	C21-C20-C22-C23
2	B	3004	PX4	C23-C24-C25-C26
2	A	1301	PX4	O6-C9-O5-C8
2	B	3001	PX4	O6-C9-O5-C8
2	B	3008	PX4	C9-C10-C11-C12
2	B	3008	PX4	C23-C24-C25-C26
2	A	1303	PX4	C6-O4-P1-O3
2	A	1310	PX4	C6-O4-P1-O3
2	B	3001	PX4	C1-O3-P1-O4
2	B	3003	PX4	C1-O3-P1-O4
4	B	3009	UHH	C20-C22-C23-C24
2	A	1301	PX4	C23-C24-C25-C26
2	B	3001	PX4	C1-C2-N1-C3
2	B	3001	PX4	C1-C2-N1-C4
2	B	3001	PX4	C1-C2-N1-C5
2	B	3004	PX4	C1-C2-N1-C3
2	B	3004	PX4	C1-C2-N1-C4
2	B	3004	PX4	C1-C2-N1-C5
2	A	1302	PX4	C30-C31-C32-C33
2	A	1305	PX4	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	A	1310	PX4	C29-C30-C31-C32
2	B	3004	PX4	C16-C17-C18-C19
2	B	3006	PX4	C25-C26-C27-C28
2	B	3008	PX4	C10-C11-C12-C13
2	B	3008	PX4	C16-C17-C18-C19
2	A	1302	PX4	C14-C15-C16-C17
2	B	3006	PX4	C24-C25-C26-C27
2	A	1302	PX4	C11-C12-C13-C14
2	A	1303	PX4	C27-C28-C29-C30
2	B	3003	PX4	C32-C33-C34-C35
2	B	3006	PX4	C28-C29-C30-C31
2	B	3001	PX4	C14-C15-C16-C17
2	B	3002	PX4	C28-C29-C30-C31
2	B	3001	PX4	C9-C10-C11-C12
2	B	3001	PX4	C25-C26-C27-C28
2	B	3008	PX4	C14-C15-C16-C17
2	A	1306	PX4	C23-C24-C25-C26
2	A	1301	PX4	C26-C27-C28-C29
2	B	3001	PX4	C27-C28-C29-C30
2	B	3006	PX4	C23-C24-C25-C26
2	B	3004	PX4	C14-C15-C16-C17
2	A	1303	PX4	C25-C26-C27-C28
2	A	1310	PX4	C31-C32-C33-C34
2	A	1309	PX4	C13-C14-C15-C16
2	B	3004	PX4	C15-C16-C17-C18
2	B	3003	PX4	C25-C26-C27-C28
2	B	3004	PX4	C17-C18-C19-C20
2	A	1307	PX4	C9-C10-C11-C12
2	A	1310	PX4	C27-C28-C29-C30
2	A	1303	PX4	C28-C29-C30-C31
2	B	3001	PX4	C26-C27-C28-C29
2	B	3001	PX4	C28-C29-C30-C31
2	A	1309	PX4	C10-C11-C12-C13
2	A	1309	PX4	C15-C16-C17-C18
2	B	3003	PX4	C27-C28-C29-C30
2	A	1307	PX4	C24-C23-O7-C7
2	A	1302	PX4	C12-C13-C14-C15
2	A	1307	PX4	O8-C23-O7-C7
2	A	1307	PX4	O7-C7-C8-O5
2	B	3004	PX4	O7-C7-C8-O5
2	A	1309	PX4	C23-C24-C25-C26
2	B	3003	PX4	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	A	1301	PX4	C15-C16-C17-C18
2	A	1302	PX4	C6-O4-P1-O3
2	A	1307	PX4	O4-C6-C7-C8
2	A	1309	PX4	O4-C6-C7-C8
2	B	3002	PX4	C31-C32-C33-C34
2	B	3003	PX4	C29-C30-C31-C32
3	A	1308	BNC	C17-C20-C22-C23
2	A	1301	PX4	C10-C11-C12-C13
2	A	1302	PX4	C31-C32-C33-C34
2	A	1311	PX4	C29-C30-C31-C32
2	A	1301	PX4	C6-C7-C8-O5
2	A	1302	PX4	C6-C7-C8-O5
2	B	3008	PX4	C6-C7-C8-O5
2	A	1303	PX4	C33-C34-C35-C36
2	B	3008	PX4	C24-C25-C26-C27
2	A	1307	PX4	O7-C23-C24-C25
2	A	1311	PX4	C31-C32-C33-C34
2	B	3006	PX4	C26-C27-C28-C29
3	A	1308	BNC	C21-C20-C22-C23
2	A	1303	PX4	C32-C33-C34-C35
2	A	1306	PX4	C29-C30-C31-C32
2	A	1311	PX4	C23-C24-C25-C26
2	A	1310	PX4	C32-C33-C34-C35
2	A	1302	PX4	C18-C19-C20-C21
2	A	1310	PX4	C33-C34-C35-C36
2	B	3007	PX4	C27-C28-C29-C30
2	A	1309	PX4	C8-C7-O7-C23
2	B	3008	PX4	C6-C7-O7-C23
2	A	1309	PX4	C9-C10-C11-C12
2	A	1305	PX4	C25-C26-C27-C28
2	A	1305	PX4	C32-C33-C34-C35
2	B	3003	PX4	C30-C31-C32-C33
2	A	1310	PX4	C1-O3-P1-O2
2	B	3007	PX4	C32-C33-C34-C35
2	A	1301	PX4	C32-C33-C34-C35
2	B	3002	PX4	C26-C27-C28-C29
2	A	1306	PX4	C25-C26-C27-C28
2	B	3007	PX4	C29-C30-C31-C32
2	A	1301	PX4	C17-C18-C19-C20
2	B	3004	PX4	C10-C11-C12-C13
2	B	3001	PX4	O4-C6-C7-C8
2	A	1301	PX4	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
2	A	1307	PX4	C6-C7-C8-O5
2	B	3004	PX4	C6-C7-C8-O5
2	A	1301	PX4	C27-C28-C29-C30
2	B	3001	PX4	C6-O4-P1-O3
2	B	3004	PX4	C24-C25-C26-C27
2	A	1301	PX4	O7-C7-C8-O5
2	B	3001	PX4	O7-C7-C8-O5
2	A	1310	PX4	C25-C26-C27-C28
2	B	3003	PX4	C24-C23-O7-C7
2	A	1303	PX4	C30-C31-C32-C33
2	A	1305	PX4	C29-C30-C31-C32
2	B	3004	PX4	C32-C33-C34-C35
2	B	3007	PX4	C26-C27-C28-C29
2	A	1302	PX4	C13-C14-C15-C16
2	B	3004	PX4	C28-C29-C30-C31
2	B	3004	PX4	C7-C6-O4-P1
2	B	3001	PX4	C29-C30-C31-C32
2	A	1303	PX4	C26-C27-C28-C29
2	B	3004	PX4	C24-C23-O7-C7
2	A	1309	PX4	C30-C31-C32-C33
2	A	1302	PX4	C28-C29-C30-C31
2	B	3003	PX4	C7-C6-O4-P1
2	A	1309	PX4	O4-C6-C7-O7
2	B	3001	PX4	O4-C6-C7-O7
2	B	3003	PX4	O4-C6-C7-O7
2	B	3002	PX4	C27-C28-C29-C30
2	A	1301	PX4	C18-C19-C20-C21
2	B	3003	PX4	O8-C23-O7-C7
2	A	1302	PX4	C32-C33-C34-C35
2	B	3004	PX4	C31-C32-C33-C34
2	B	3004	PX4	C27-C28-C29-C30
2	A	1302	PX4	C1-O3-P1-O1
2	A	1302	PX4	C6-O4-P1-O1
2	A	1310	PX4	C6-O4-P1-O1
2	B	3003	PX4	C1-O3-P1-O2
2	B	3003	PX4	C1-C2-N1-C3
2	B	3004	PX4	C1-O3-P1-O1
2	A	1303	PX4	C23-C24-C25-C26
2	A	1307	PX4	O4-C6-C7-O7
2	B	3003	PX4	C1-C2-N1-C5
2	A	1302	PX4	O3-C1-C2-N1
2	B	3003	PX4	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
2	A	1302	PX4	C25-C26-C27-C28
2	B	3004	PX4	C13-C14-C15-C16
2	B	3003	PX4	C1-C2-N1-C4
2	B	3007	PX4	C28-C29-C30-C31
2	A	1307	PX4	C6-C7-O7-C23
2	B	3004	PX4	O8-C23-O7-C7
2	B	3008	PX4	O7-C7-C8-O5
2	A	1309	PX4	C25-C26-C27-C28
2	B	3001	PX4	C17-C18-C19-C20
2	A	1302	PX4	C7-C6-O4-P1
2	A	1301	PX4	C11-C12-C13-C14
2	A	1302	PX4	O4-C6-C7-C8
2	A	1301	PX4	C31-C32-C33-C34
2	B	3001	PX4	C10-C11-C12-C13
2	B	3003	PX4	C26-C27-C28-C29
2	A	1302	PX4	C27-C28-C29-C30
2	B	3008	PX4	C15-C16-C17-C18
2	A	1307	PX4	O8-C23-C24-C25
2	B	3001	PX4	C16-C17-C18-C19
2	B	3006	PX4	O7-C23-C24-C25
2	B	3006	PX4	O8-C23-C24-C25
2	A	1311	PX4	C27-C28-C29-C30
2	B	3001	PX4	C13-C14-C15-C16
2	B	3003	PX4	C6-C7-O7-C23
2	A	1306	PX4	C30-C31-C32-C33
2	B	3004	PX4	C9-C10-C11-C12
4	B	3009	UHH	C21-C20-C9-C5
2	A	1302	PX4	O4-C6-C7-O7
2	A	1309	PX4	C29-C30-C31-C32
2	B	3001	PX4	C6-C7-C8-O5
2	B	3008	PX4	C6-O4-P1-O3
2	B	3001	PX4	O7-C23-C24-C25
2	A	1304	PX4	C1-O3-P1-O2
2	A	1305	PX4	C33-C34-C35-C36
2	B	3004	PX4	C19-C20-C21-C22
2	B	3002	PX4	C29-C30-C31-C32
2	A	1307	PX4	C17-C18-C19-C20
2	B	3001	PX4	O8-C23-C24-C25
2	B	3004	PX4	C10-C9-O5-C8
2	A	1307	PX4	C23-C24-C25-C26
2	A	1309	PX4	C16-C17-C18-C19
2	A	1302	PX4	C6-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
2	B	3001	PX4	C6-O4-P1-O1
2	B	3003	PX4	C6-O4-P1-O2
2	B	3003	PX4	O4-C6-C7-C8
2	B	3007	PX4	C33-C34-C35-C36
2	B	3003	PX4	C8-C7-O7-C23
2	B	3004	PX4	C11-C10-C9-O5
2	A	1309	PX4	C27-C28-C29-C30
2	B	3006	PX4	C29-C30-C31-C32

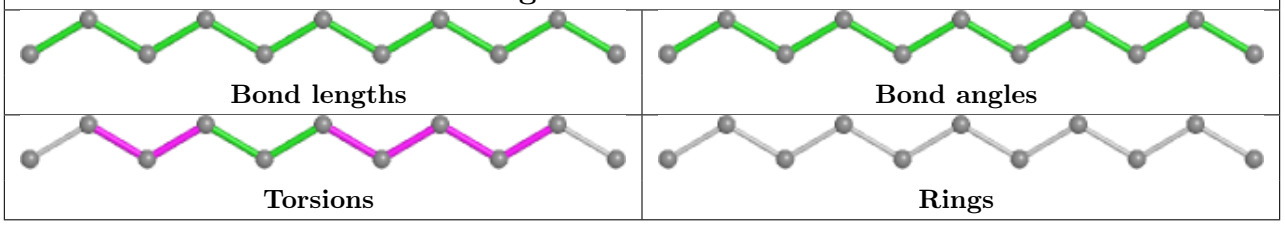
There are no ring outliers.

14 monomers are involved in 38 short contacts:

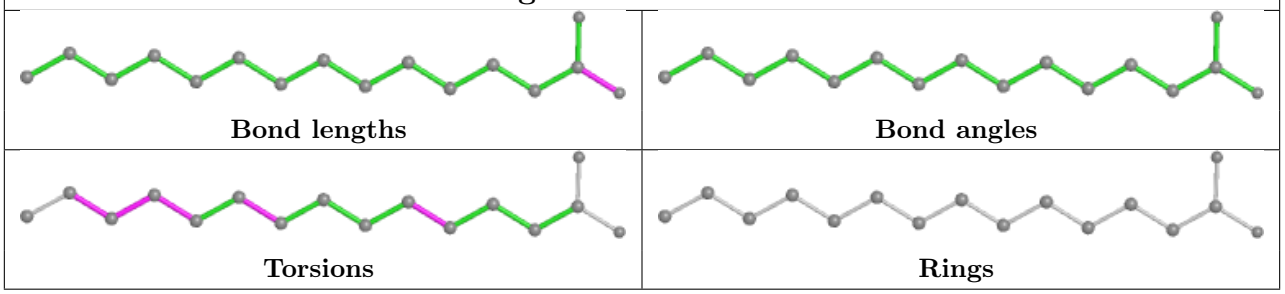
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3007	PX4	2	0
2	A	1305	PX4	1	0
2	B	3002	PX4	1	0
2	A	1306	PX4	2	0
2	B	3004	PX4	5	0
2	B	3003	PX4	4	0
2	A	1309	PX4	3	0
2	B	3001	PX4	8	0
2	B	3006	PX4	6	0
2	A	1303	PX4	2	0
2	A	1301	PX4	5	0
2	A	1307	PX4	1	0
2	A	1302	PX4	3	0
2	B	3008	PX4	1	0

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.

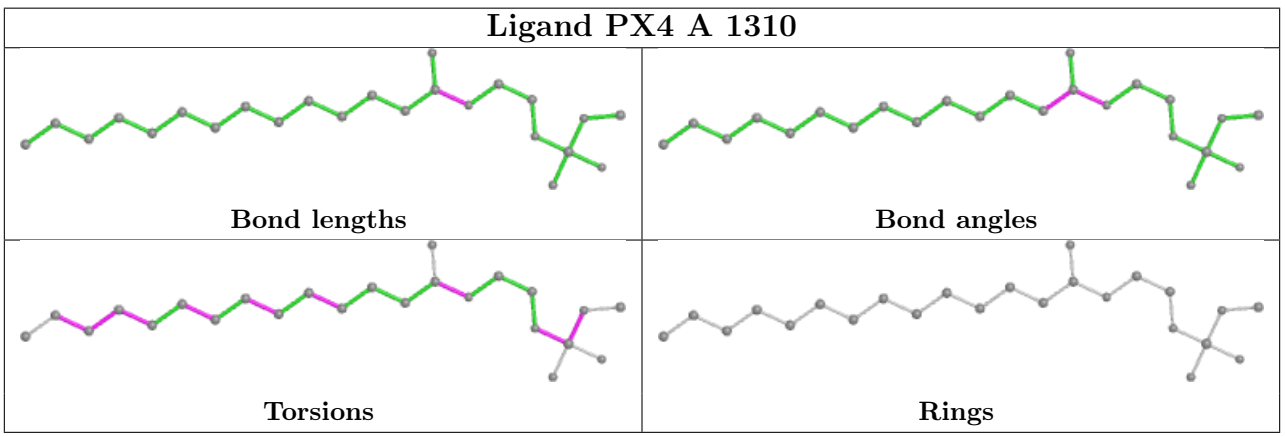
Ligand PX4 B 3007



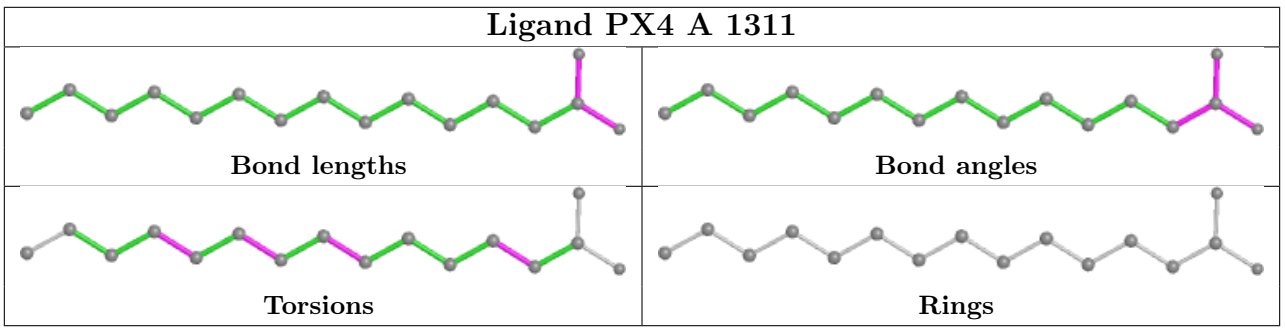
Ligand PX4 A 1305



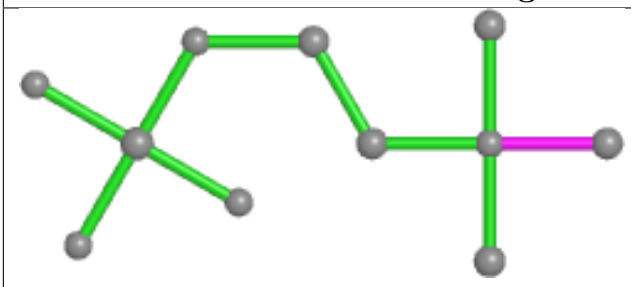
Ligand PX4 A 1310



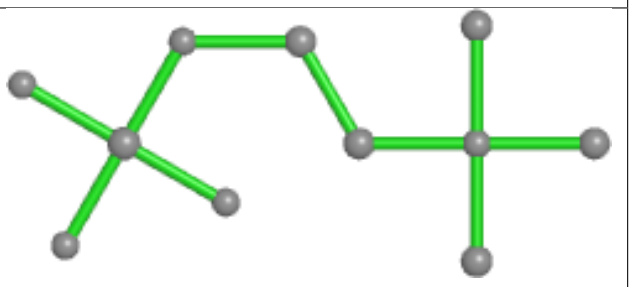
Ligand PX4 A 1311



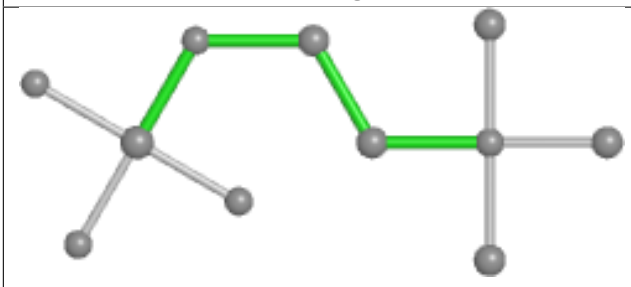
Ligand PX4 B 3005



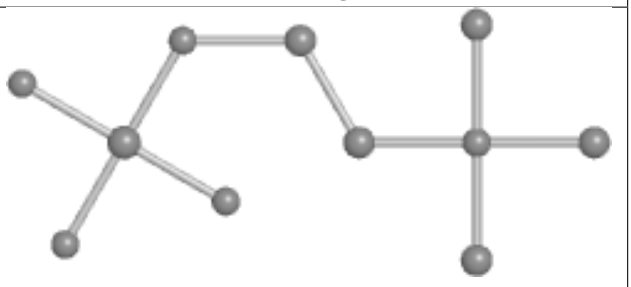
Bond lengths



Bond angles

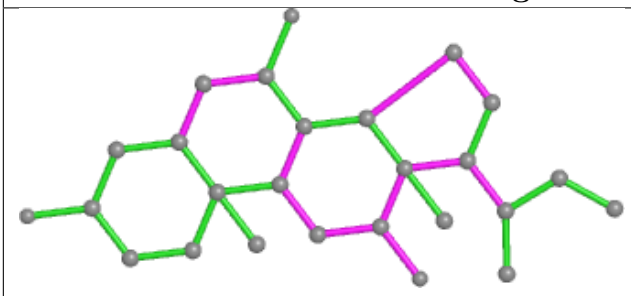


Torsions

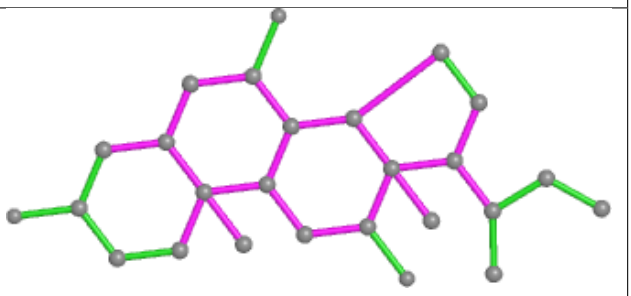


Rings

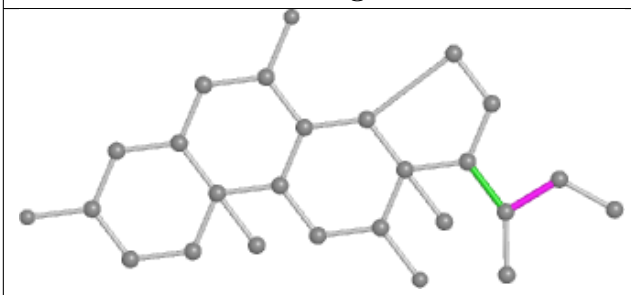
Ligand BNC A 1308



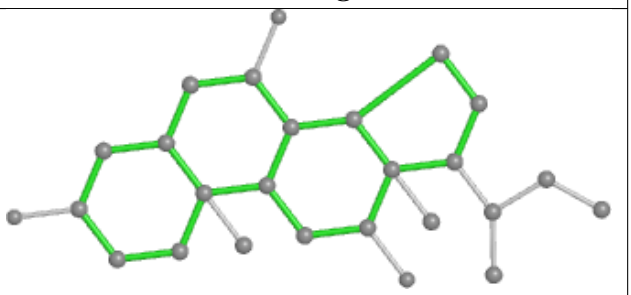
Bond lengths



Bond angles

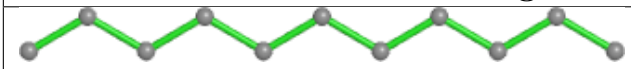


Torsions

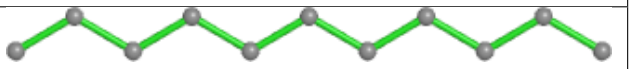


Rings

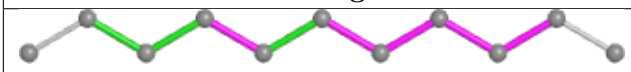
Ligand PX4 B 3002



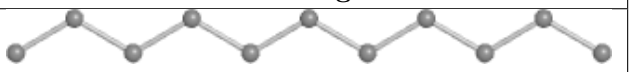
Bond lengths



Bond angles

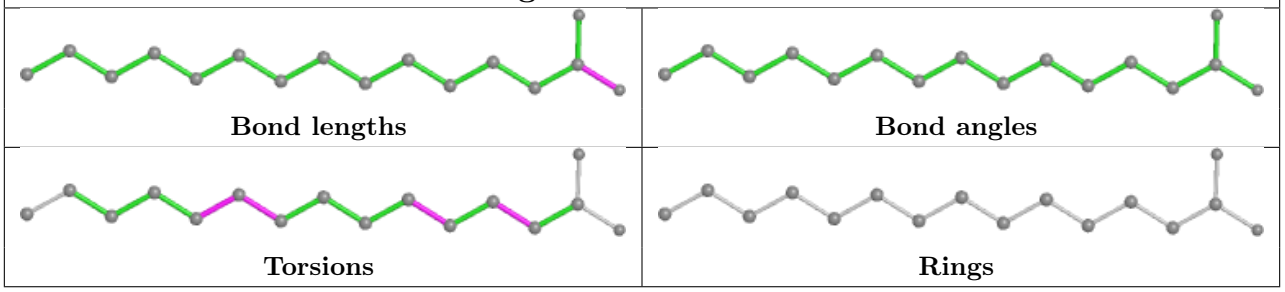


Torsions

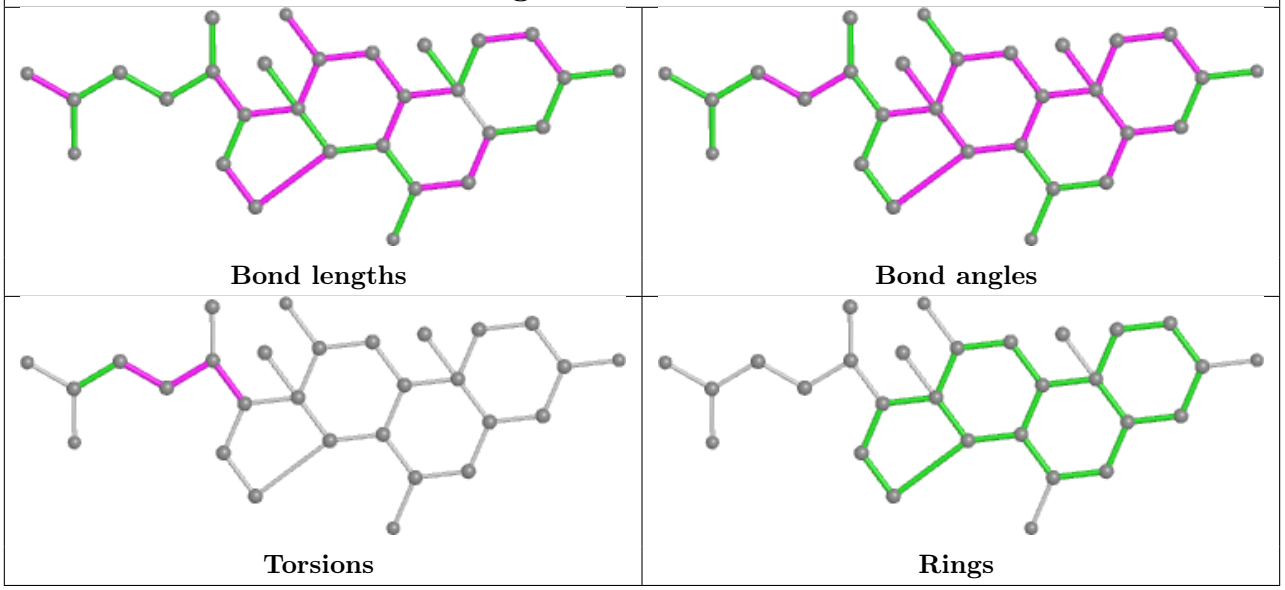


Rings

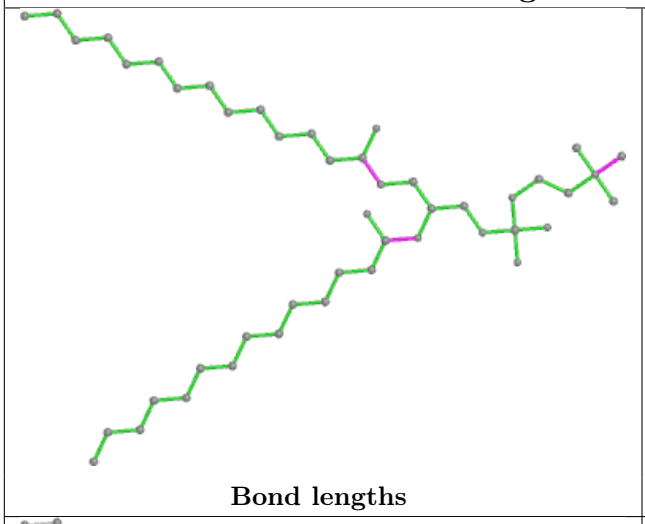
Ligand PX4 A 1306



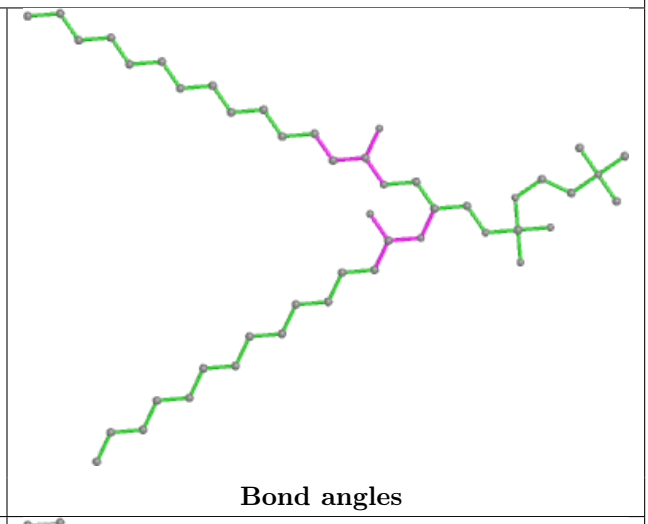
Ligand UHH B 3009



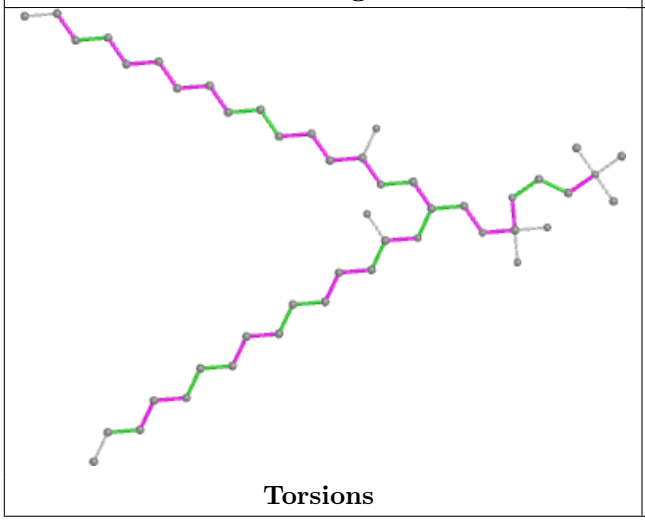
Ligand PX4 B 3004



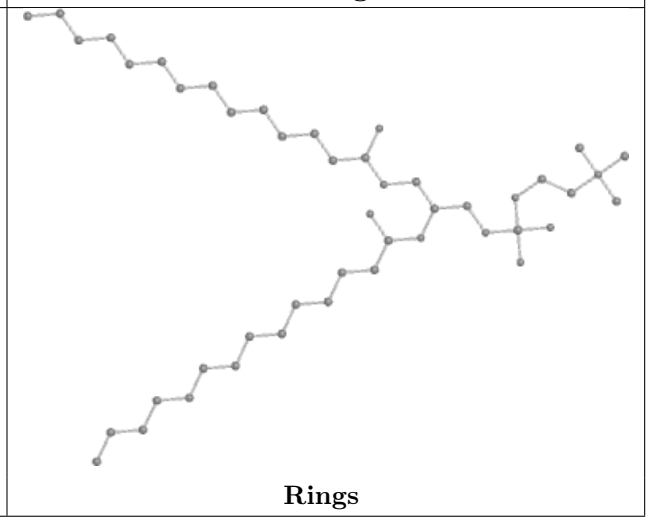
Bond lengths



Bond angles

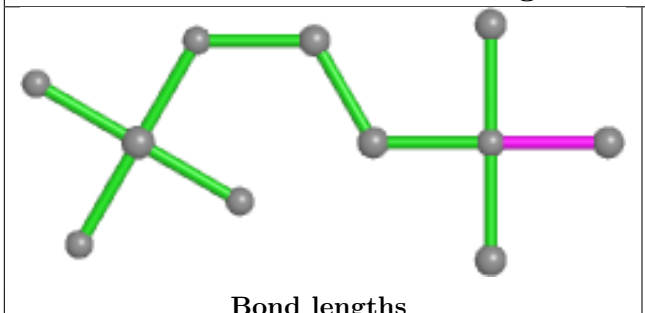


Torsions

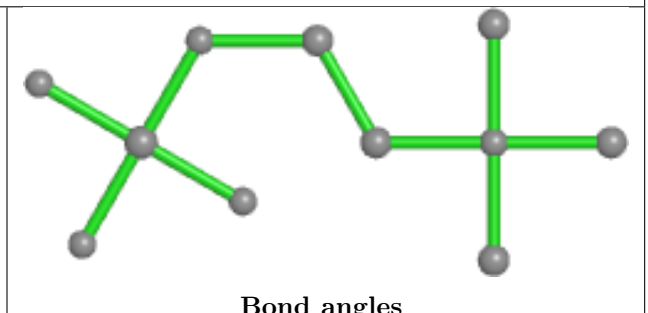


Rings

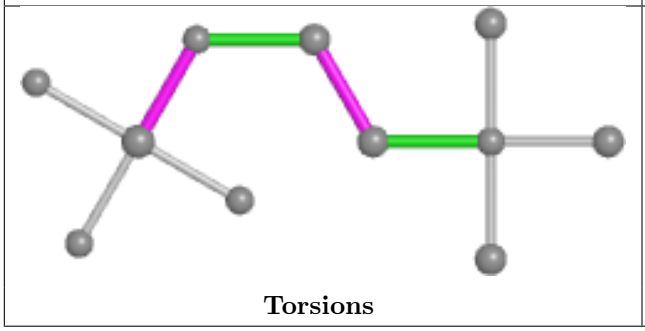
Ligand PX4 A 1304



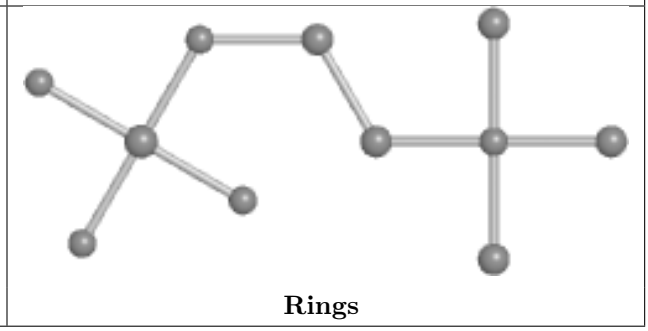
Bond lengths



Bond angles

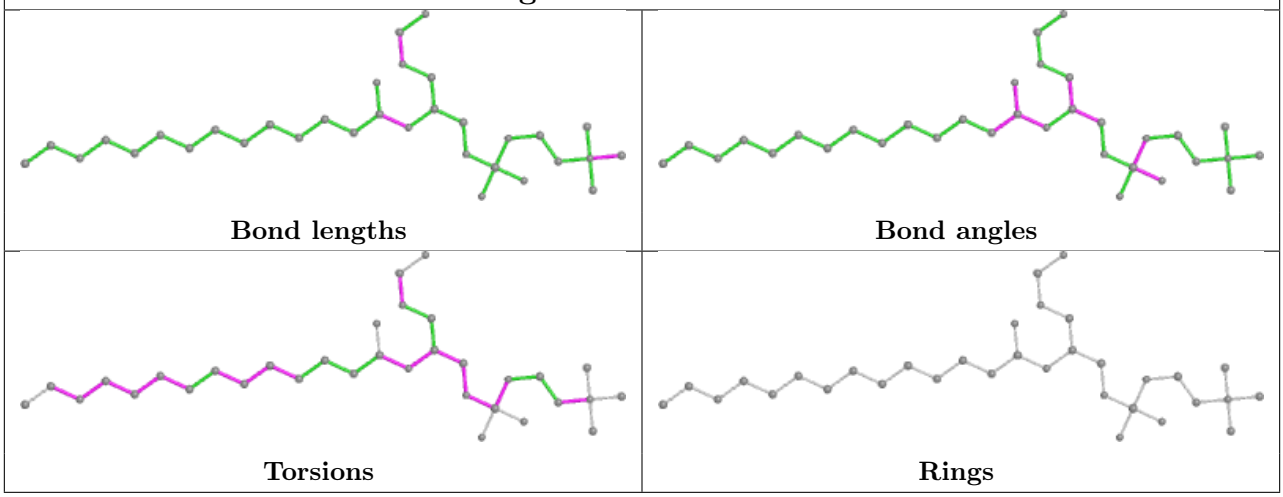


Torsions

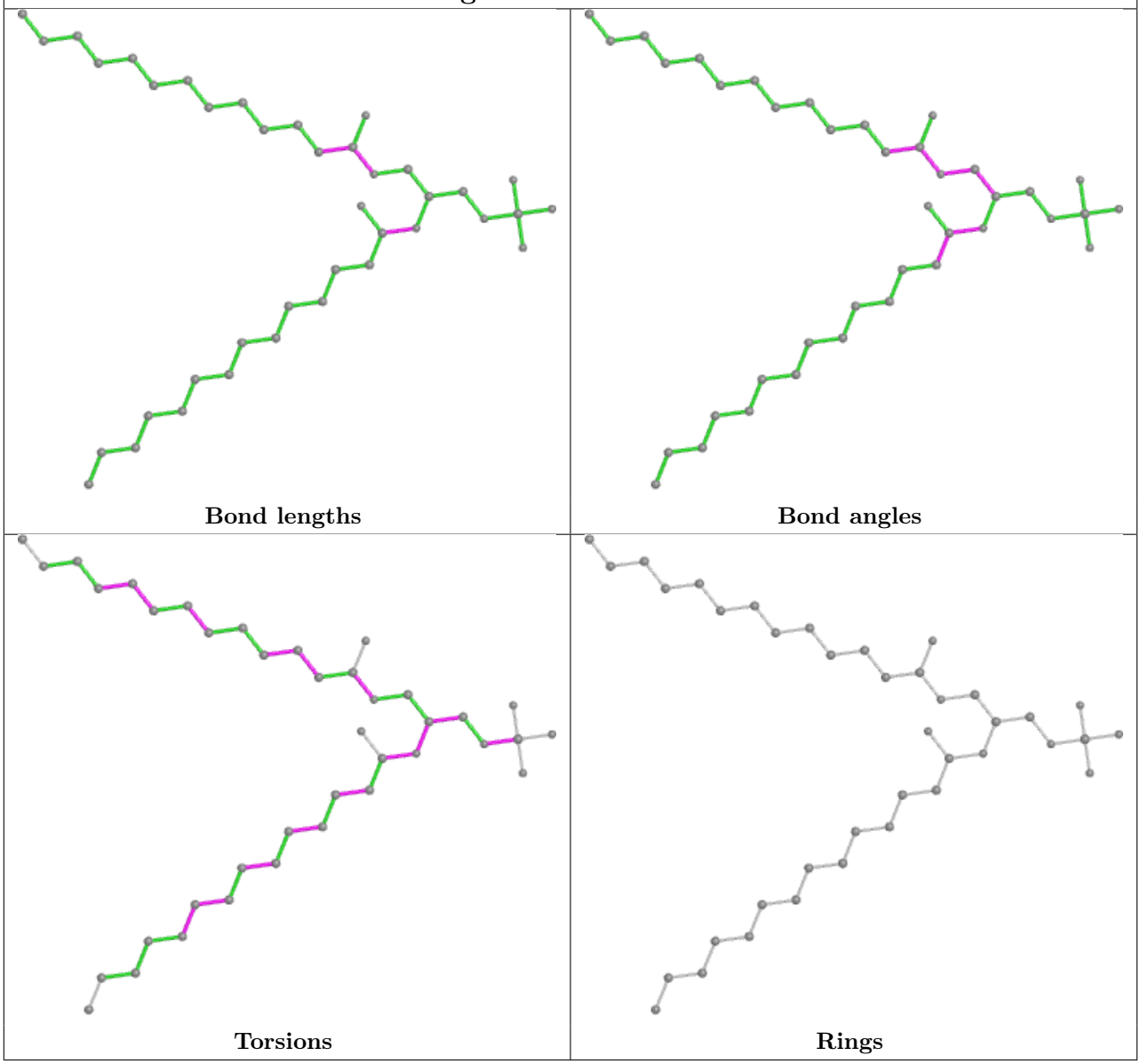


Rings

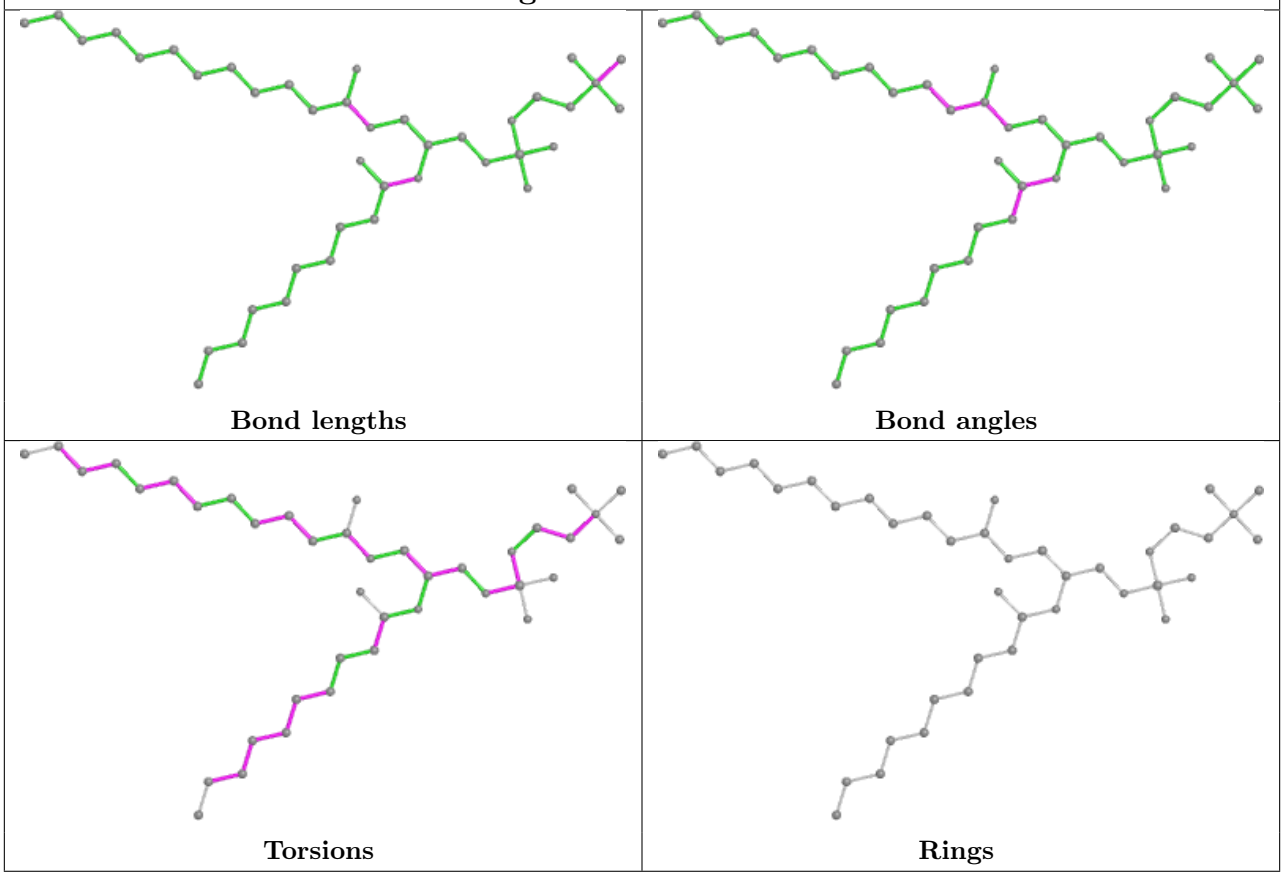
Ligand PX4 B 3003



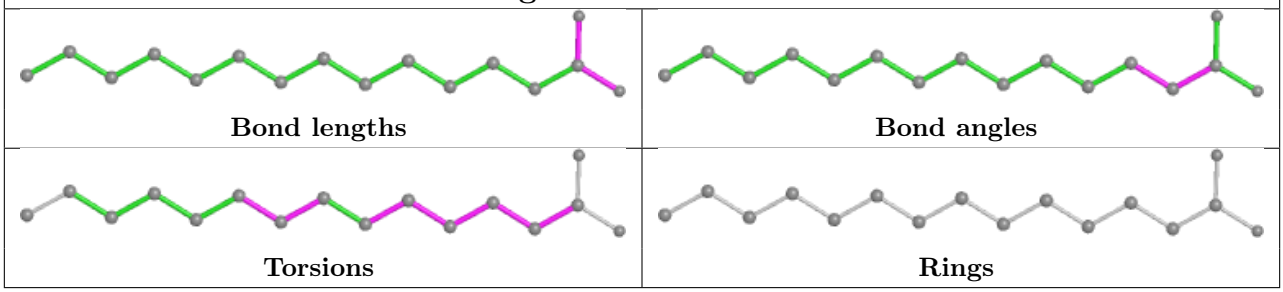
Ligand PX4 A 1309



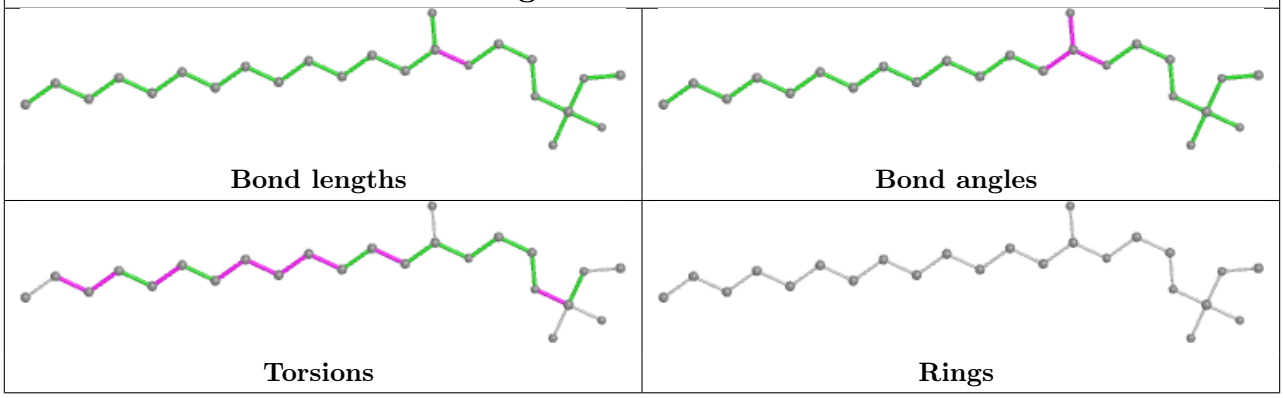
Ligand PX4 B 3001



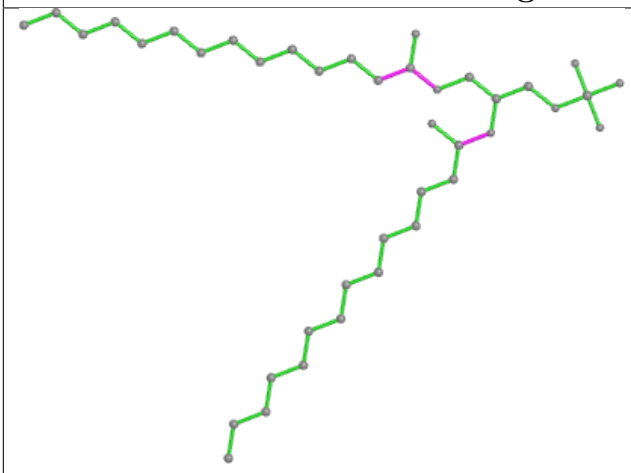
Ligand PX4 B 3006



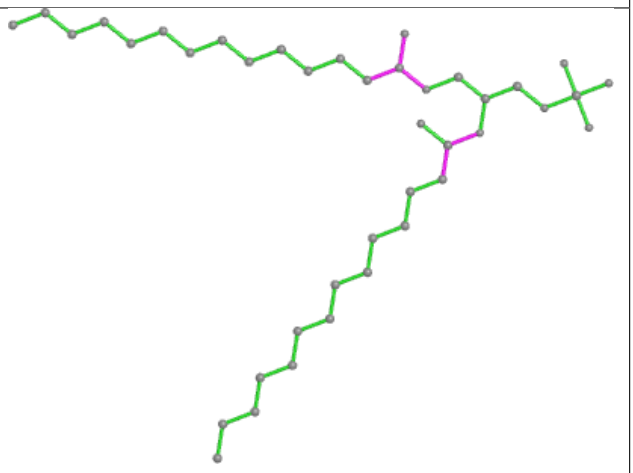
Ligand PX4 A 1303



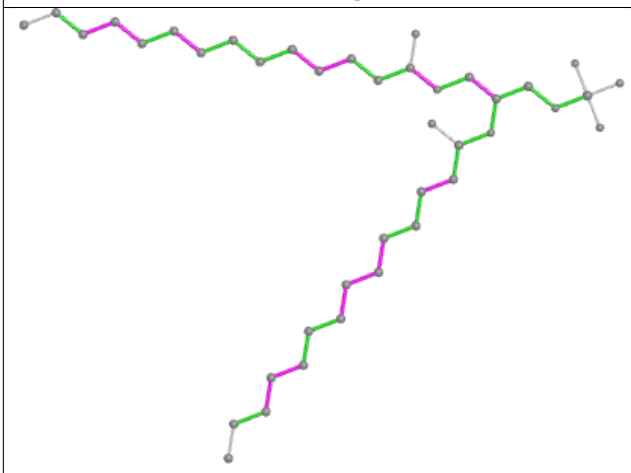
Ligand PX4 A 1301



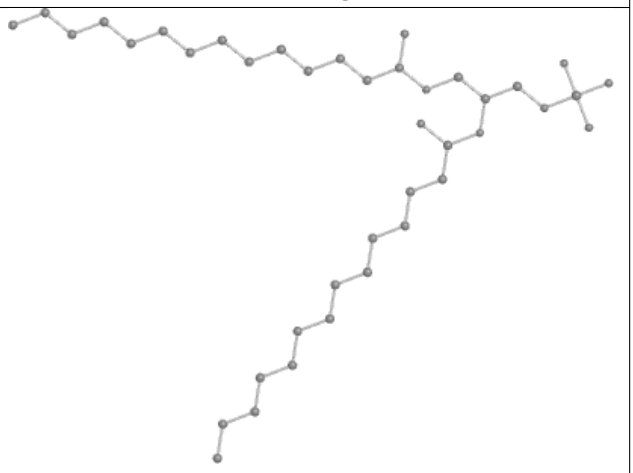
Bond lengths



Bond angles

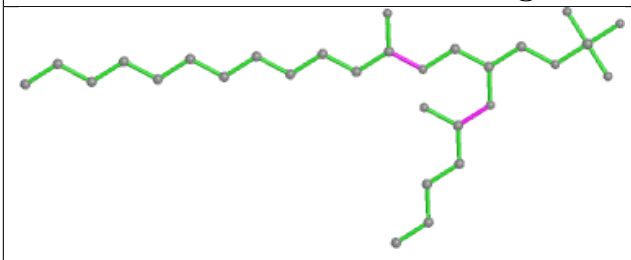


Torsions

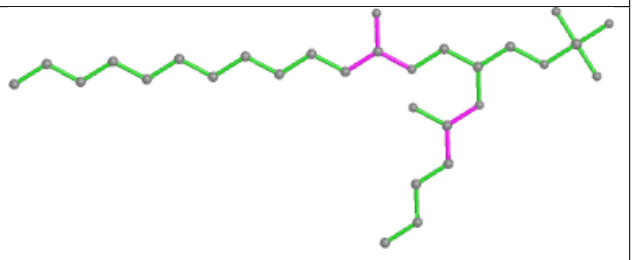


Rings

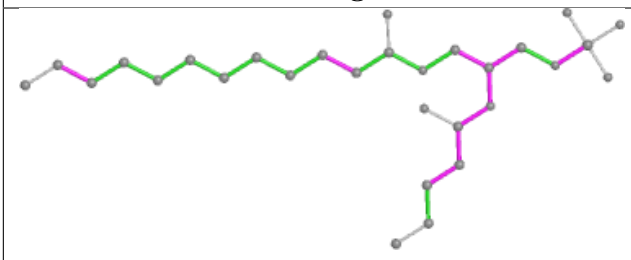
Ligand PX4 A 1307



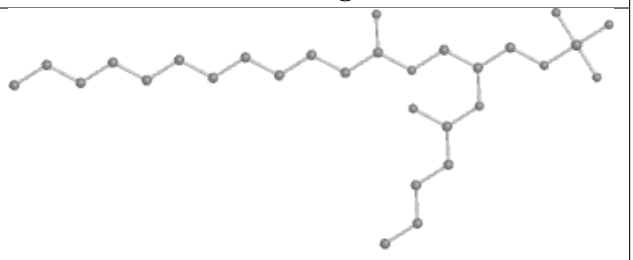
Bond lengths



Bond angles

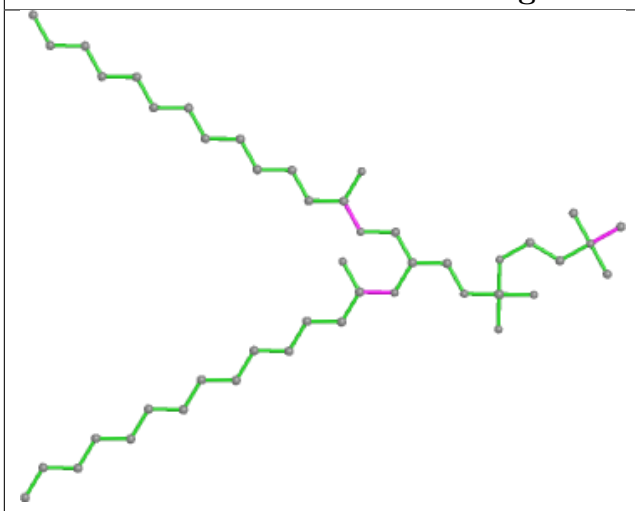


Torsions

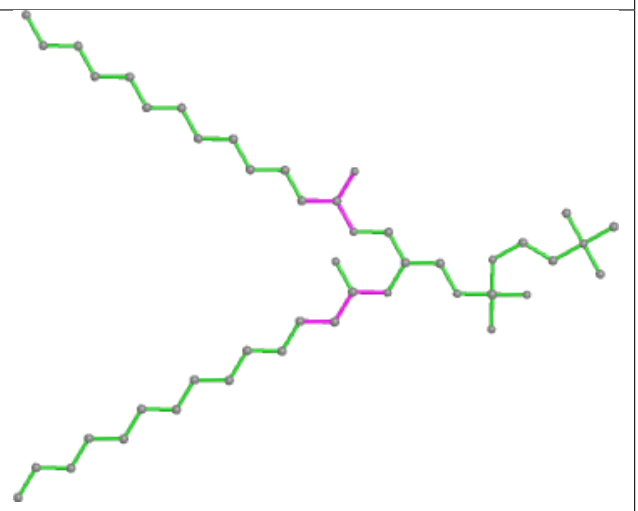


Rings

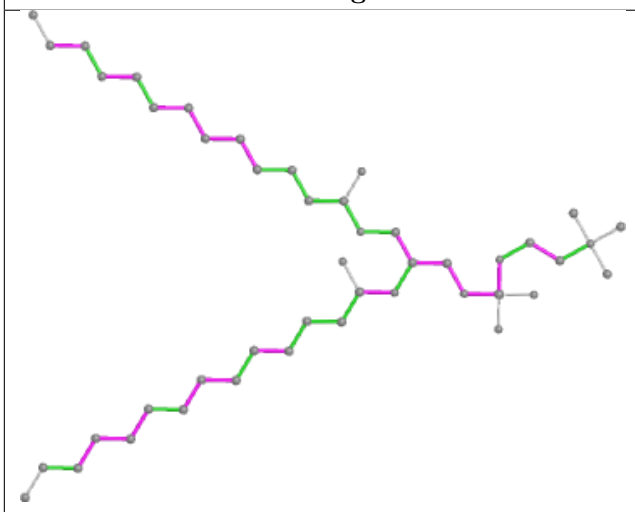
Ligand PX4 A 1302



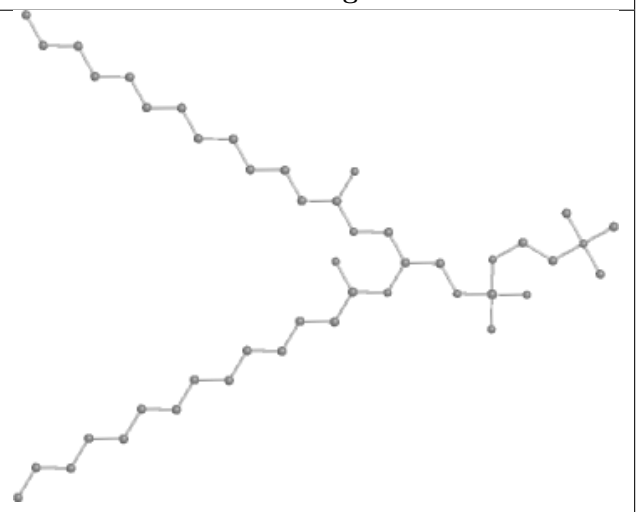
Bond lengths



Bond angles

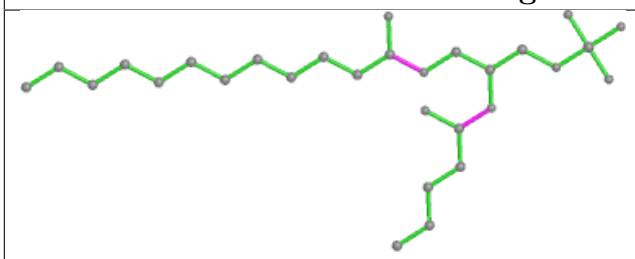


Torsions

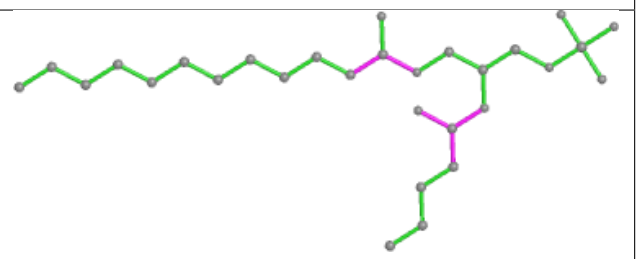


Rings

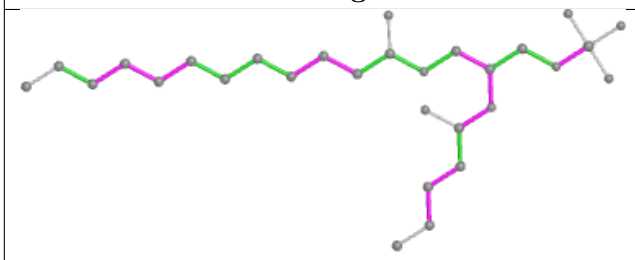
Ligand PX4 B 3008



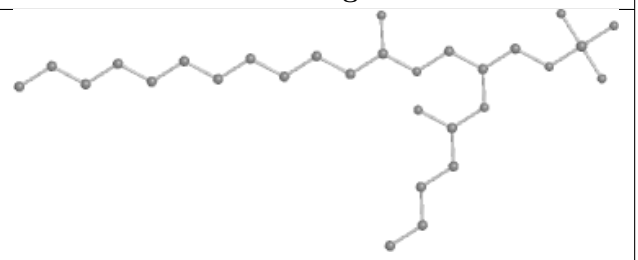
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	221/285 (77%)	0.23	8 (3%)	42	37	52, 103, 185, 236	0
1	B	221/285 (77%)	0.16	7 (3%)	47	42	50, 104, 185, 230	0
All	All	442/570 (77%)	0.20	15 (3%)	45	39	50, 104, 185, 236	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1095	PHE	6.3
1	A	1094	GLY	5.6
1	B	2001	MET	3.9
1	A	1002	TYR	3.7
1	A	1004	ARG	3.6
1	B	2095	PHE	3.4
1	B	2221	MET	3.2
1	A	1065	TYR	3.2
1	B	2004	ARG	3.0
1	B	2002	TYR	2.9
1	A	1093	SER	2.8
1	A	1098	LEU	2.8
1	A	1001	MET	2.7
1	B	2098	LEU	2.6
1	B	2097	ILE	2.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

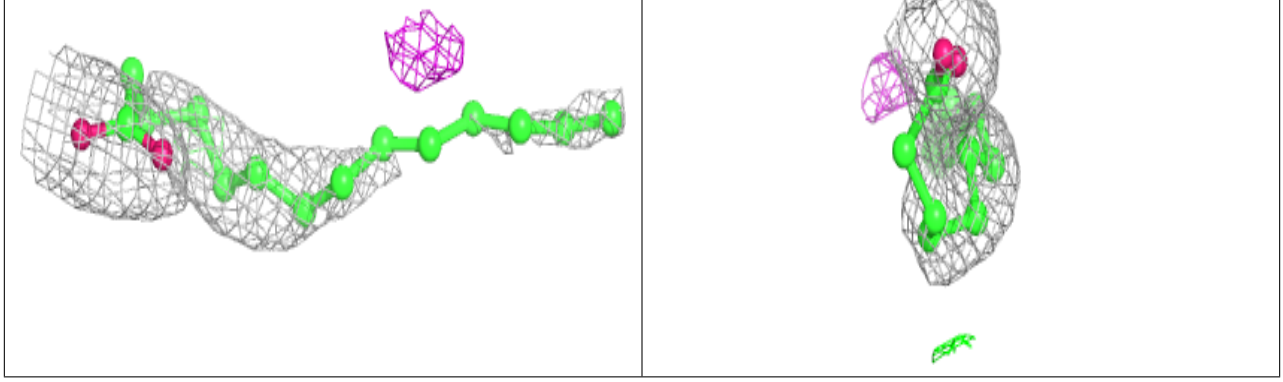
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	PX4	B	3006	16/46	0.57	0.44	88,122,153,156	0
2	PX4	A	1306	16/46	0.60	0.33	94,125,144,145	0
2	PX4	B	3002	11/46	0.66	0.56	113,120,146,146	0
2	PX4	B	3007	11/46	0.67	0.31	101,118,130,134	0
2	PX4	B	3008	29/46	0.70	0.36	97,126,271,294	0
2	PX4	A	1311	16/46	0.74	0.20	101,124,143,148	0
3	BNC	A	1308	26/26	0.77	0.42	110,161,184,188	0
2	PX4	A	1307	29/46	0.78	0.29	86,132,292,300	0
2	PX4	B	3004	46/46	0.82	0.49	65,116,177,254	0
2	PX4	A	1305	16/46	0.83	0.15	89,119,146,146	0
2	PX4	B	3005	11/46	0.83	0.23	116,133,274,282	0
2	PX4	A	1310	24/46	0.85	0.39	88,105,225,235	0
2	PX4	A	1304	11/46	0.85	0.19	121,132,307,311	0
2	PX4	A	1302	45/46	0.85	0.45	79,115,156,219	0
2	PX4	A	1303	24/46	0.88	0.47	87,122,215,221	0
4	UHH	B	3009	29/29	0.88	0.31	129,153,172,179	0
2	PX4	A	1301	40/46	0.89	0.22	74,104,172,182	0
2	PX4	A	1309	39/46	0.89	0.28	79,106,165,184	0
2	PX4	B	3003	33/46	0.91	0.24	68,112,148,149	0
2	PX4	B	3001	40/46	0.96	0.21	69,106,128,138	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.

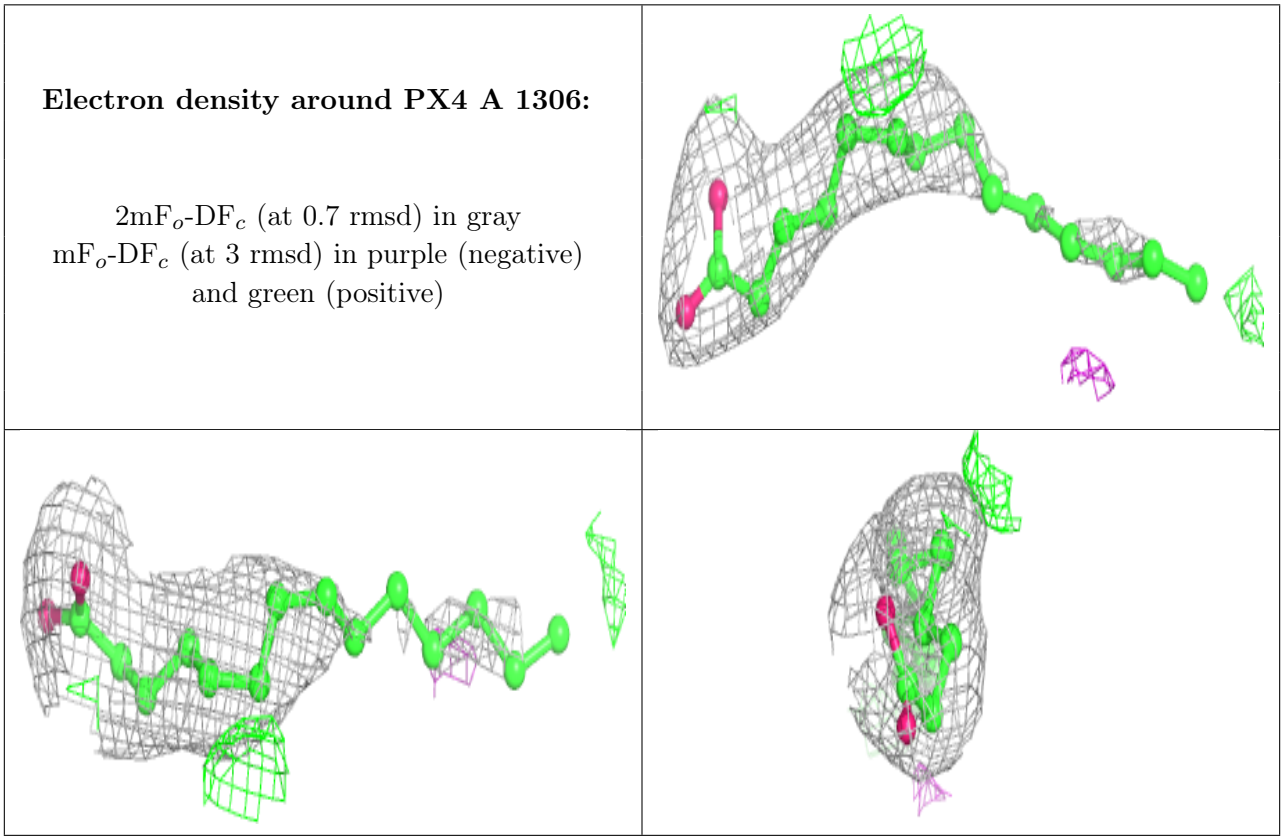
Electron density around PX4 B 3006:

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



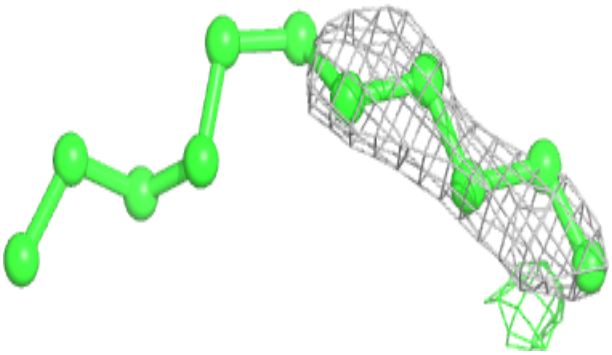
Electron density around PX4 A 1306:

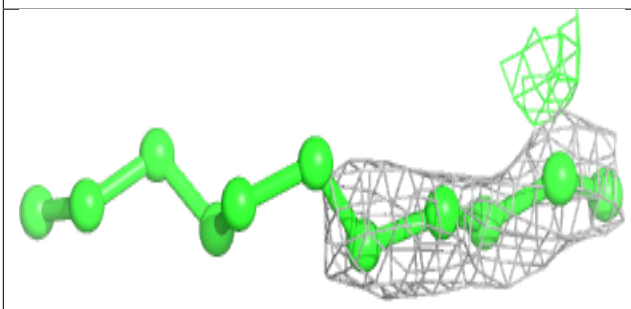
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

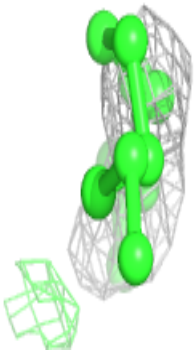


Electron density around PX4 B 3002:

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

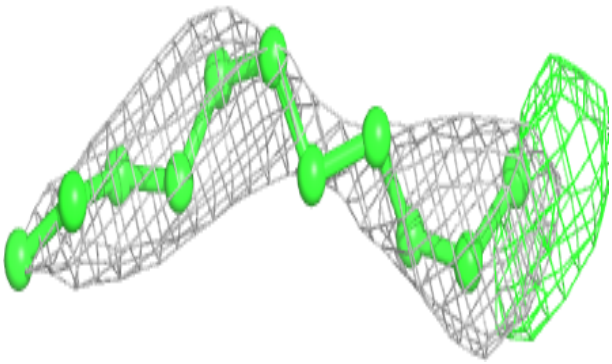


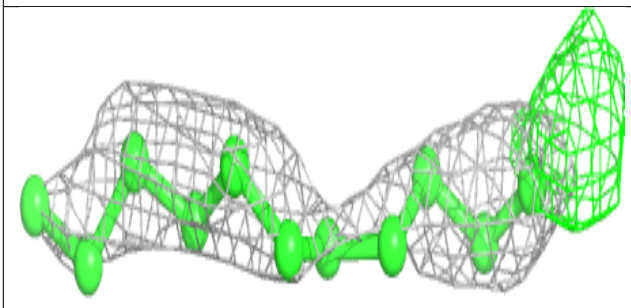


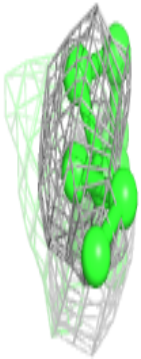


Electron density around PX4 B 3007:

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

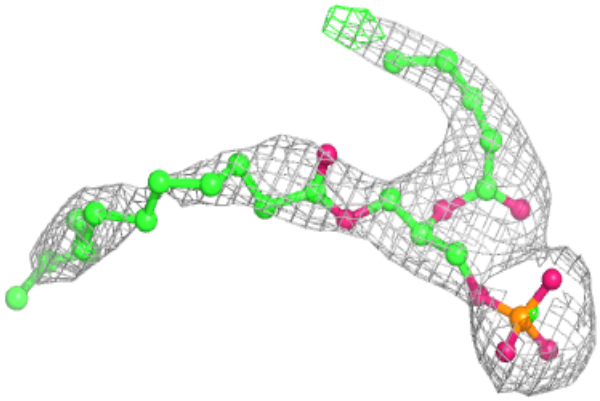


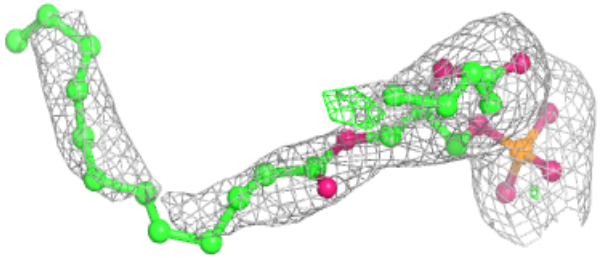


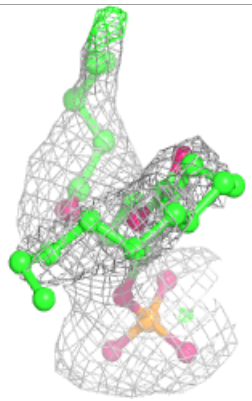


Electron density around PX4 B 3008:

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

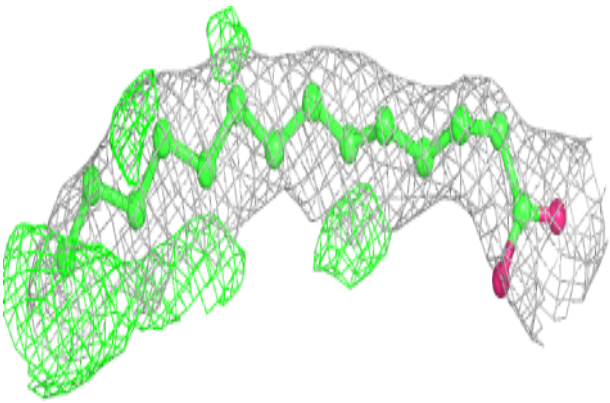


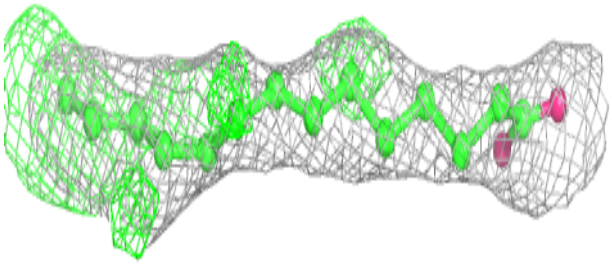


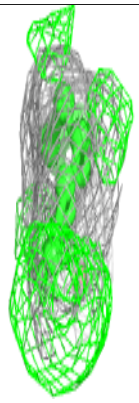


Electron density around PX4 A 1311:

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

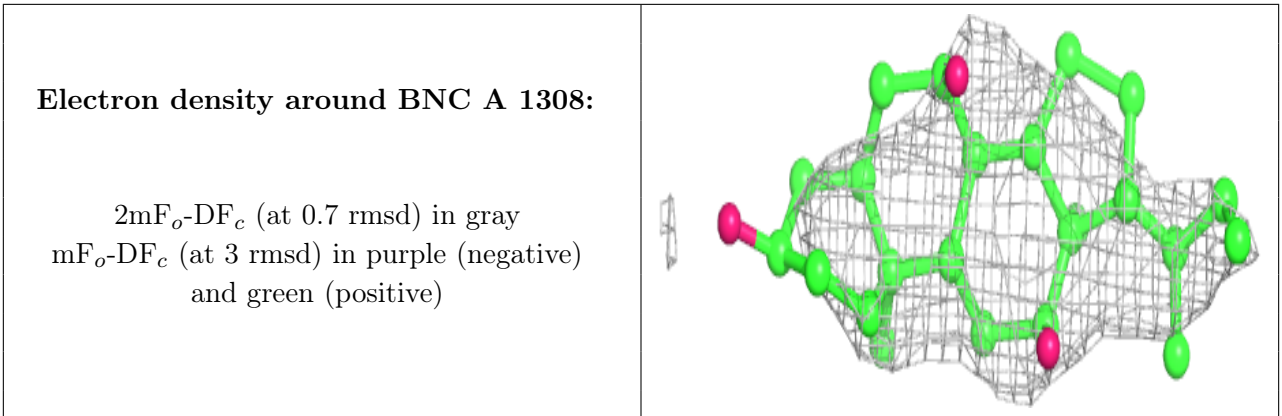






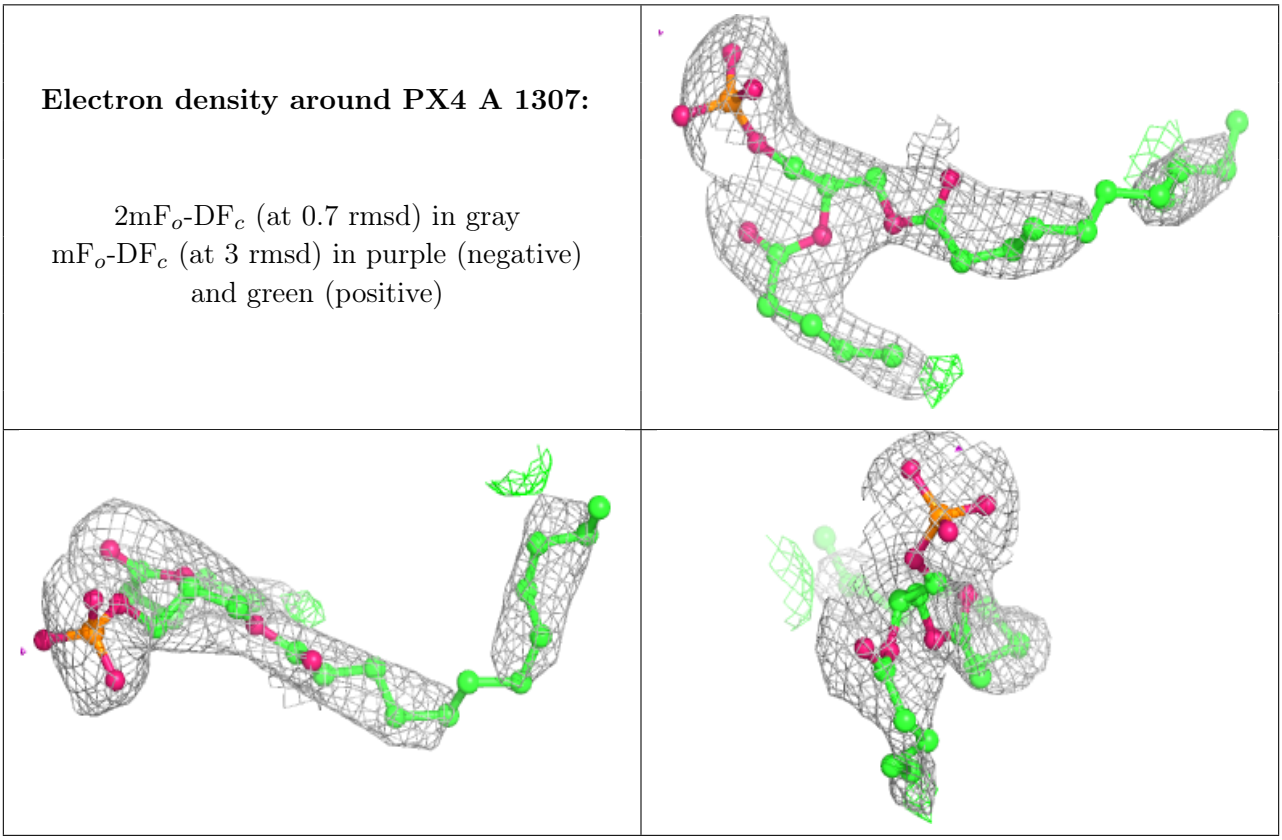
Electron density around BNC A 1308:

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



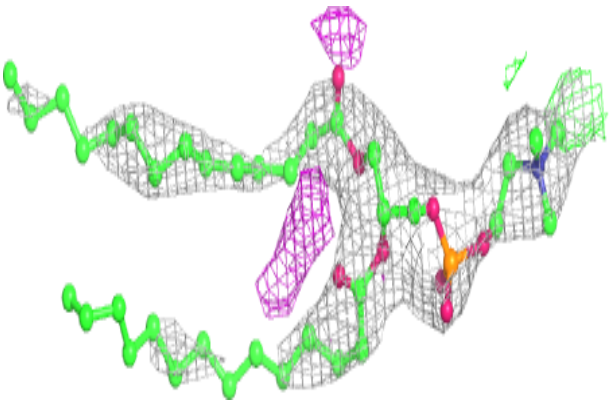
Electron density around PX4 A 1307:

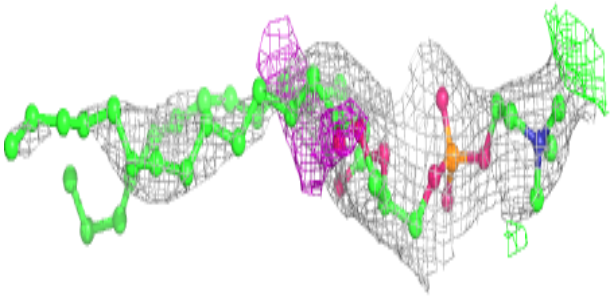
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

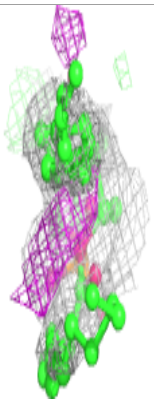


Electron density around PX4 B 3004:

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

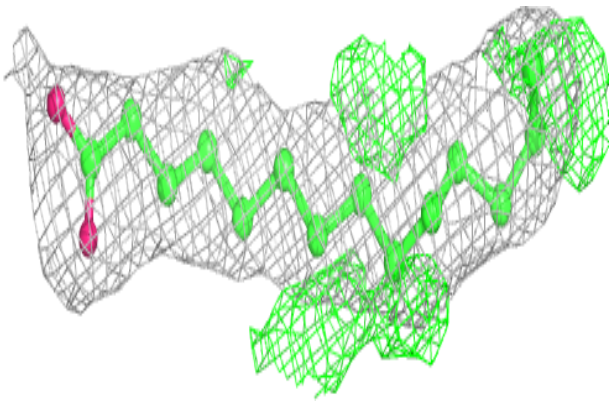


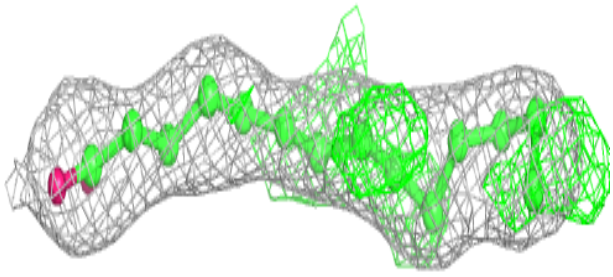


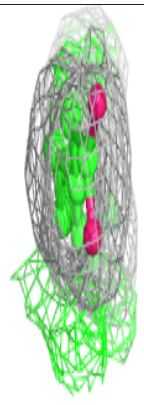


Electron density around PX4 A 1305:

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

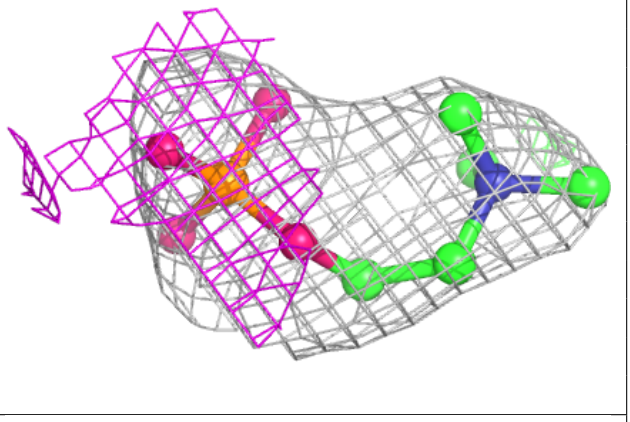


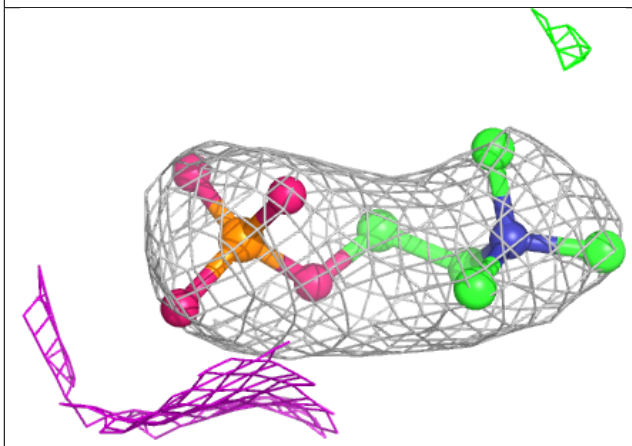


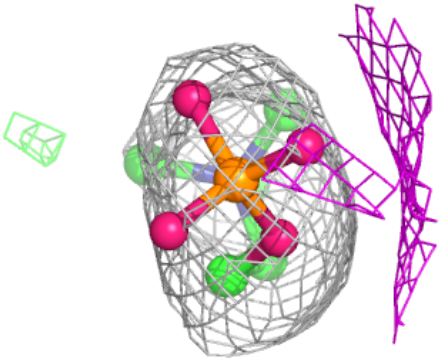


Electron density around PX4 B 3005:

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

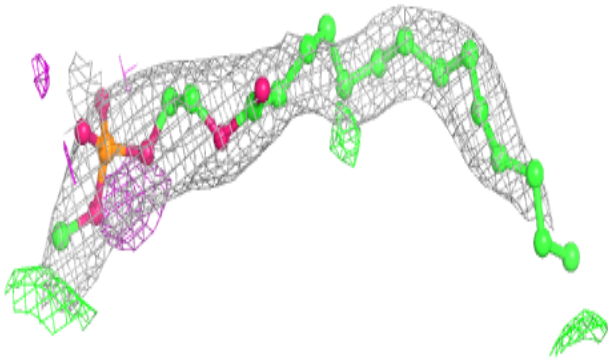


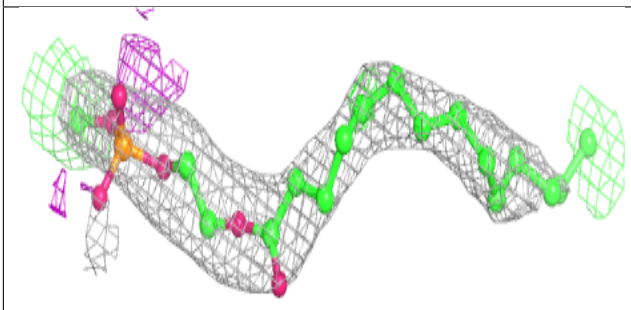


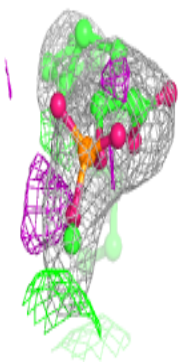


Electron density around PX4 A 1310:

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

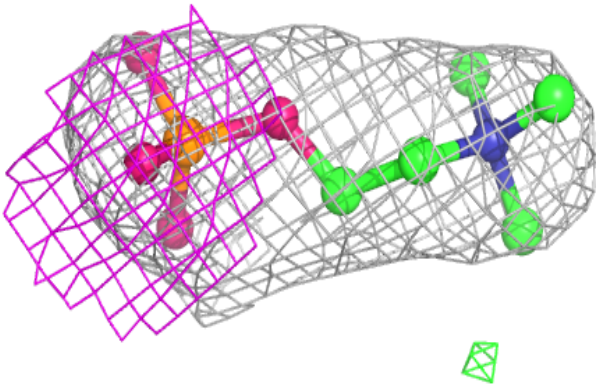


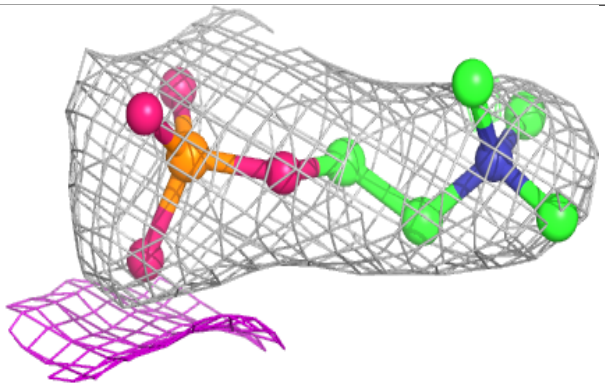


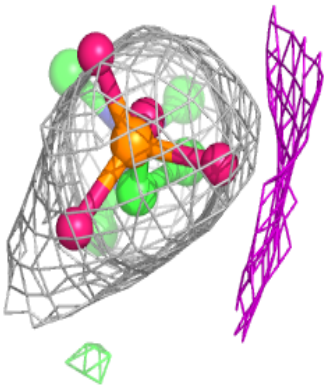


Electron density around PX4 A 1304:

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

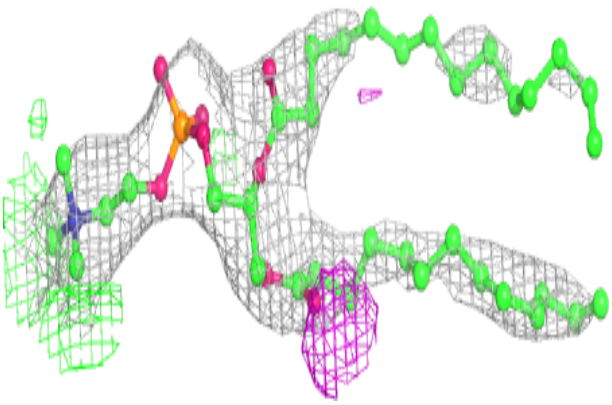


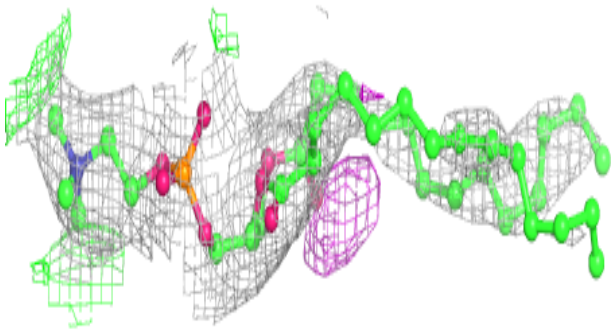


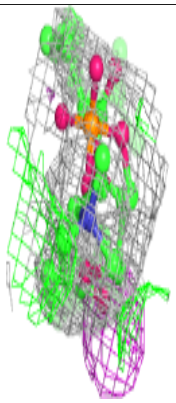


Electron density around PX4 A 1302:

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

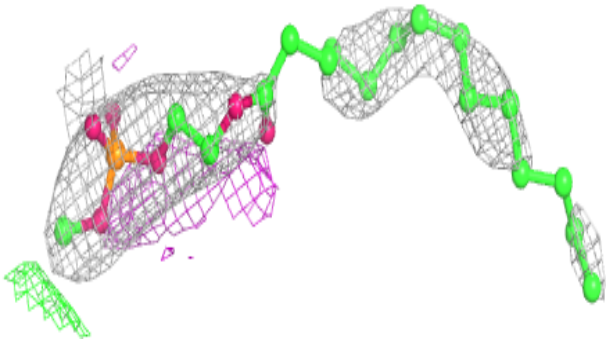


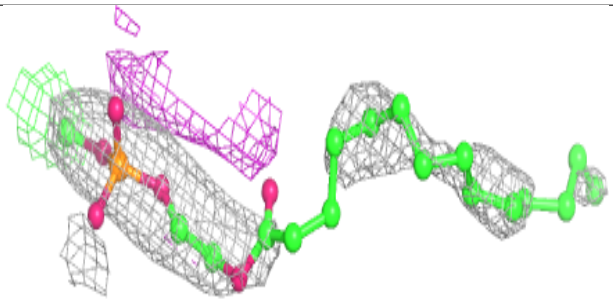


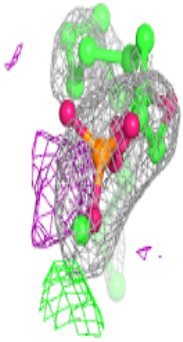


Electron density around PX4 A 1303:

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

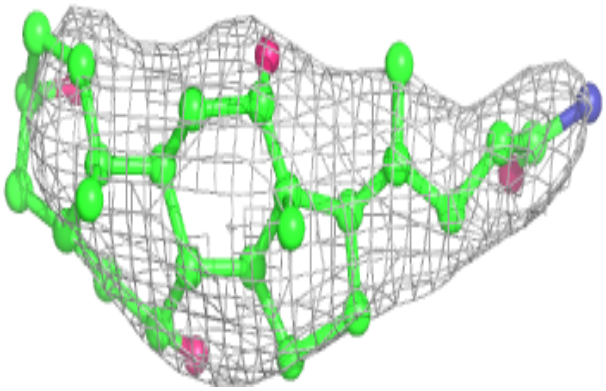


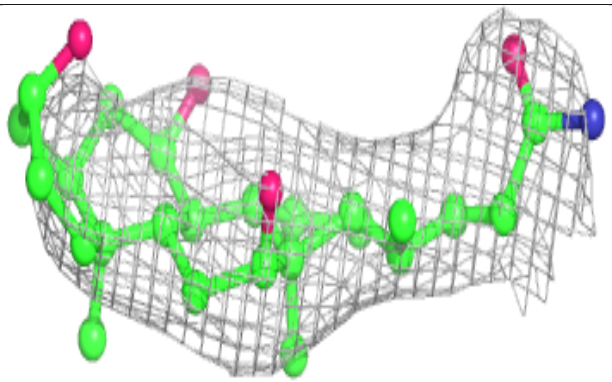


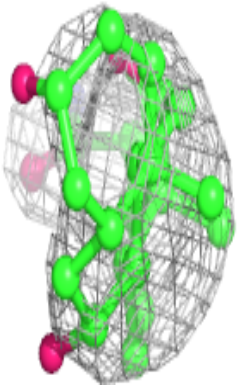


Electron density around UHH B 3009:

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

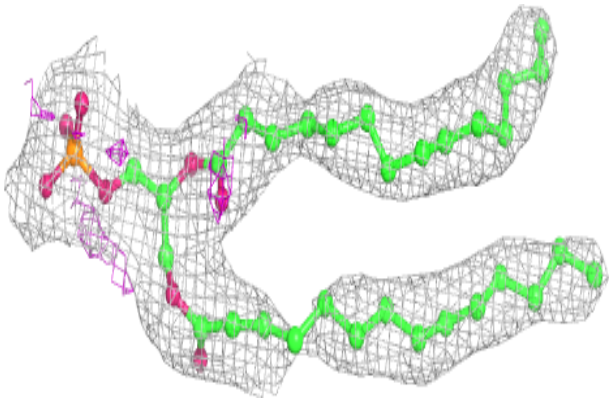


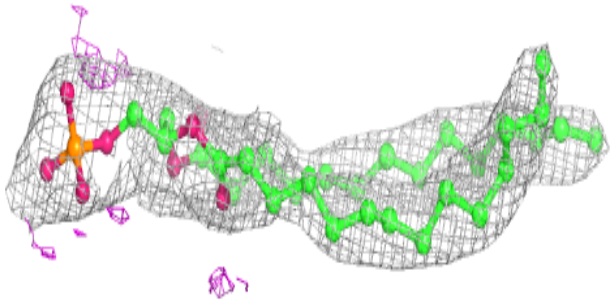


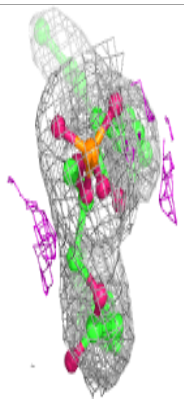


Electron density around PX4 A 1301:

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

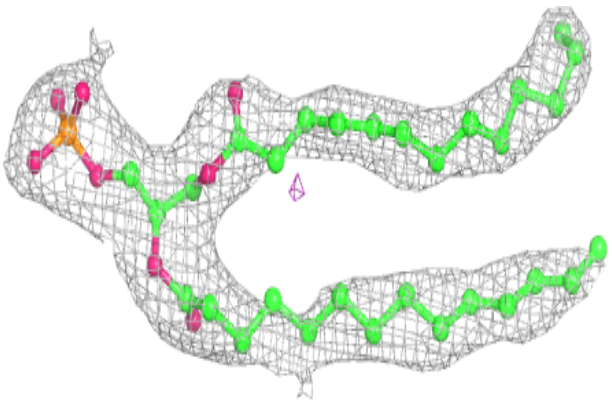


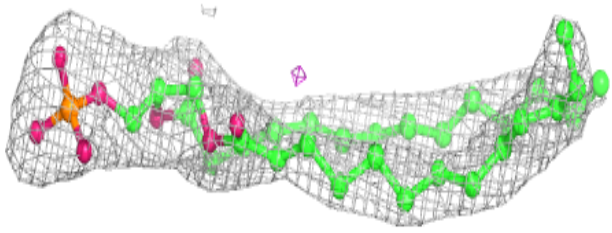


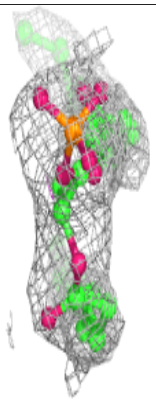


Electron density around PX4 A 1309:

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

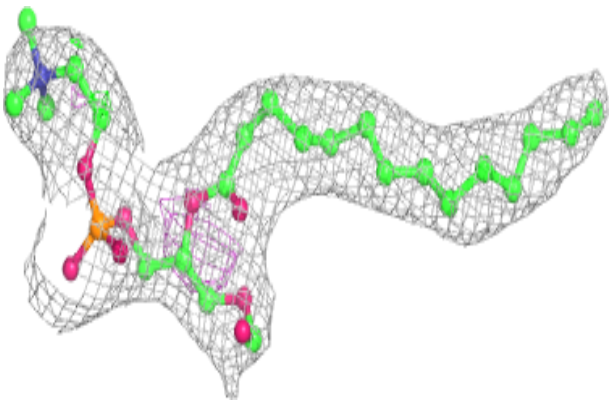


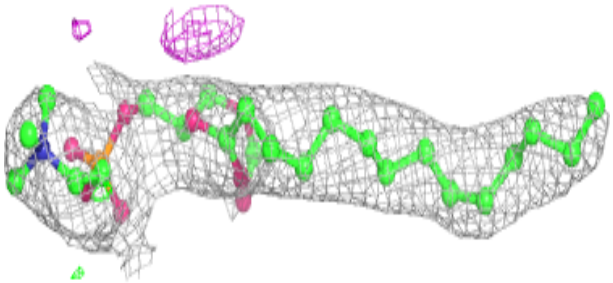


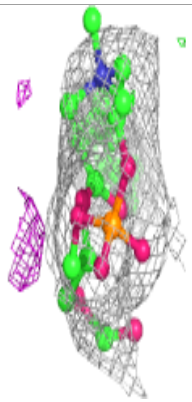


Electron density around PX4 B 3003:

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

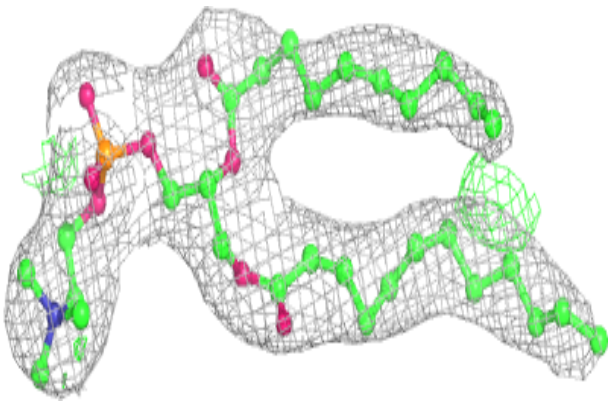


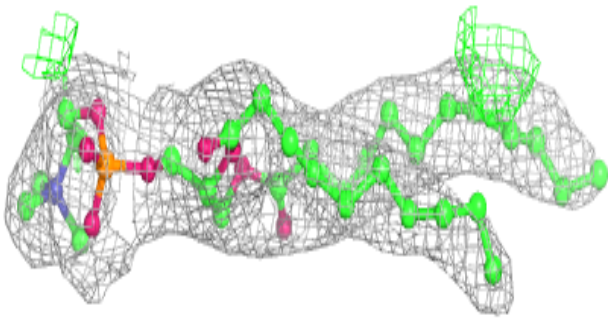


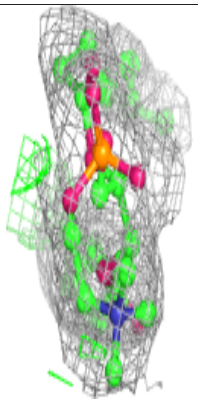


Electron density around PX4 B 3001:

$2mF_o$-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.