



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 02:43 PM BST

PDB ID : 4MW8  
Title : Structural Basis for Ca<sup>2+</sup> Selectivity of a Voltage-gated Calcium Channel  
Authors : Tang, L.; Gamal El-Din, T.M.; Payandeh, J.; Martinez, G.Q.; Heard, T.M.;  
Scheuer, T.; Zheng, N.; Catterall, W.A.  
Deposited on : 2013-09-24  
Resolution : 3.26 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

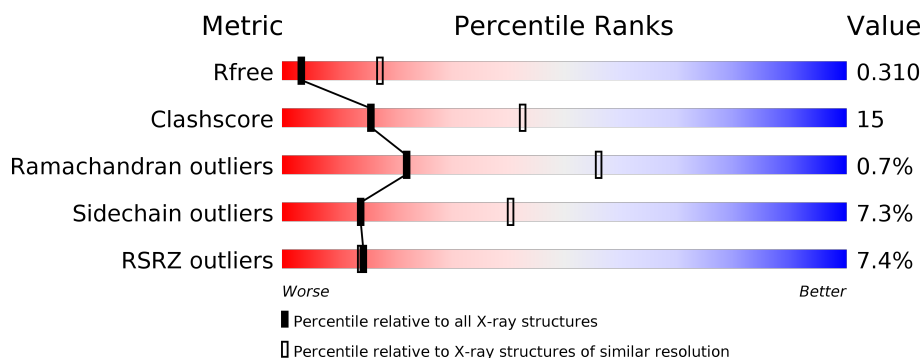
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.26 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	<div> <div>6%</div> <div> <div>54%</div> <div>34%</div> <div>8%</div> </div> </div>
1	B	237	<div> <div>8%</div> <div> <div>57%</div> <div>32%</div> <div>8%</div> </div> </div>
1	C	237	<div> <div>9%</div> <div> <div>60%</div> <div>30%</div> <div>8%</div> </div> </div>
1	D	237	<div> <div>4%</div> <div> <div>59%</div> <div>30%</div> <div>8%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PX4	B	1303	-	-	-	X
3	PX4	C	1306	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7378 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	219	Total	C	N	O	S	0	0	0
			1797	1225	268	292	12			
1	B	219	Total	C	N	O	S	0	0	0
			1797	1225	268	292	12			
1	C	219	Total	C	N	O	S	0	0	0
			1797	1225	268	292	12			
1	D	219	Total	C	N	O	S	0	0	0
			1797	1225	268	292	12			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	EXPRESSION TAG	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	1217	CYS	ILE	CONFLICT	UNP A8EVM5
B	983	MET	-	EXPRESSION TAG	UNP A8EVM5
B	984	ASP	-	EXPRESSION TAG	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	985	TYR	-	EXPRESSION TAG	UNP A8EVM5
B	986	LYS	-	EXPRESSION TAG	UNP A8EVM5
B	987	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	988	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	989	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	990	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	991	LYS	-	EXPRESSION TAG	UNP A8EVM5
B	992	GLY	-	EXPRESSION TAG	UNP A8EVM5
B	993	SER	-	EXPRESSION TAG	UNP A8EVM5
B	994	LEU	-	EXPRESSION TAG	UNP A8EVM5
B	995	VAL	-	EXPRESSION TAG	UNP A8EVM5
B	996	PRO	-	EXPRESSION TAG	UNP A8EVM5
B	997	ARG	-	EXPRESSION TAG	UNP A8EVM5
B	998	GLY	-	EXPRESSION TAG	UNP A8EVM5
B	999	SER	-	EXPRESSION TAG	UNP A8EVM5
B	1000	HIS	-	EXPRESSION TAG	UNP A8EVM5
B	1217	CYS	ILE	CONFLICT	UNP A8EVM5
C	983	MET	-	EXPRESSION TAG	UNP A8EVM5
C	984	ASP	-	EXPRESSION TAG	UNP A8EVM5
C	985	TYR	-	EXPRESSION TAG	UNP A8EVM5
C	986	LYS	-	EXPRESSION TAG	UNP A8EVM5
C	987	ASP	-	EXPRESSION TAG	UNP A8EVM5
C	988	ASP	-	EXPRESSION TAG	UNP A8EVM5
C	989	ASP	-	EXPRESSION TAG	UNP A8EVM5
C	990	ASP	-	EXPRESSION TAG	UNP A8EVM5
C	991	LYS	-	EXPRESSION TAG	UNP A8EVM5
C	992	GLY	-	EXPRESSION TAG	UNP A8EVM5
C	993	SER	-	EXPRESSION TAG	UNP A8EVM5
C	994	LEU	-	EXPRESSION TAG	UNP A8EVM5
C	995	VAL	-	EXPRESSION TAG	UNP A8EVM5
C	996	PRO	-	EXPRESSION TAG	UNP A8EVM5
C	997	ARG	-	EXPRESSION TAG	UNP A8EVM5
C	998	GLY	-	EXPRESSION TAG	UNP A8EVM5
C	999	SER	-	EXPRESSION TAG	UNP A8EVM5
C	1000	HIS	-	EXPRESSION TAG	UNP A8EVM5
C	1217	CYS	ILE	CONFLICT	UNP A8EVM5
D	983	MET	-	EXPRESSION TAG	UNP A8EVM5
D	984	ASP	-	EXPRESSION TAG	UNP A8EVM5
D	985	TYR	-	EXPRESSION TAG	UNP A8EVM5
D	986	LYS	-	EXPRESSION TAG	UNP A8EVM5
D	987	ASP	-	EXPRESSION TAG	UNP A8EVM5
D	988	ASP	-	EXPRESSION TAG	UNP A8EVM5

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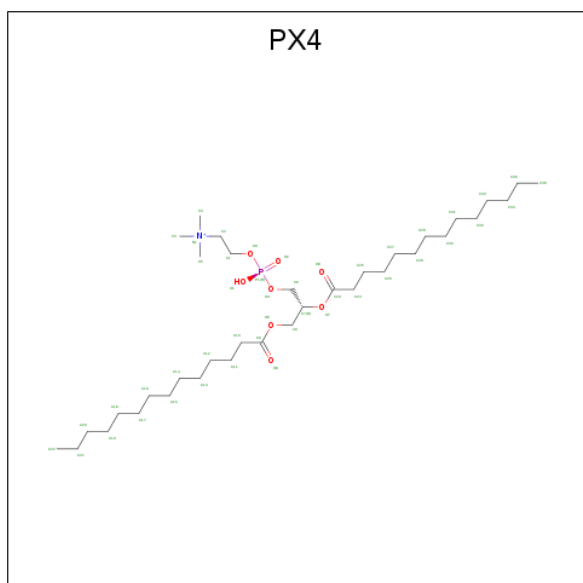
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Chain	Residue	Modelled	Actual	Comment	Reference
D	989	ASP	-	EXPRESSION TAG	UNP A8EVM5
D	990	ASP	-	EXPRESSION TAG	UNP A8EVM5
D	991	LYS	-	EXPRESSION TAG	UNP A8EVM5
D	992	GLY	-	EXPRESSION TAG	UNP A8EVM5
D	993	SER	-	EXPRESSION TAG	UNP A8EVM5
D	994	LEU	-	EXPRESSION TAG	UNP A8EVM5
D	995	VAL	-	EXPRESSION TAG	UNP A8EVM5
D	996	PRO	-	EXPRESSION TAG	UNP A8EVM5
D	997	ARG	-	EXPRESSION TAG	UNP A8EVM5
D	998	GLY	-	EXPRESSION TAG	UNP A8EVM5
D	999	SER	-	EXPRESSION TAG	UNP A8EVM5
D	1000	HIS	-	EXPRESSION TAG	UNP A8EVM5
D	1217	CYS	ILE	CONFLICT	UNP A8EVM5

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

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

- Molecule 3 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C<sub>36</sub>H<sub>73</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 10 3 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 6 6	0	0
3	A	1	Total C O P 10 3 6 1	0	0
3	B	1	Total C O P 10 3 6 1	0	0
3	B	1	Total C O P 21 13 7 1	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C O P 10 3 6 1	0	0
3	C	1	Total C O P 10 3 6 1	0	0
3	C	1	Total C O P 21 13 7 1	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C O P 10 3 6 1	0	0
3	C	1	Total C O P 21 13 7 1	0	0
3	C	1	Total C O P 10 3 6 1	0	0
3	D	1	Total C O P 21 13 7 1	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C O P 10 3 6 1	0	0

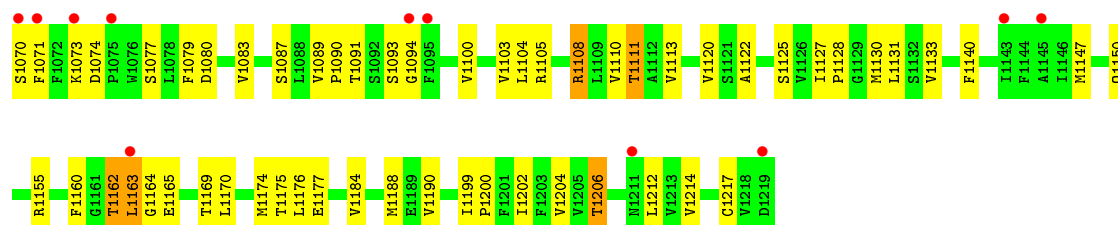
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Chain A:
- 
- 6% 54% 34% 8%
- MET ASP TPR LYS ASP ASP ASP LYS GLY SER LEU VAL PRO ARG ARG GLY SER SER HIS M1001 Y1002 L1003 L1004 L1005 T1006 M1007 L1008 Y1009 E1010 F1014 T1019 Y1020 L1021 L1024 M1025 T1028 E1032 T1033 S1034 K1035 T1036 F1037 M1038 G1042 T1045 F1048 V1052 I1053 I1058 E1059 L1062 Y1065 V1066 F1071 F1072 S1077 L1078 F1079 V1083 V1084 A1085 L1086 L1087 L1088 Y1089 P1090 T1091 S1092 S1093 G1094 Y1095 E1096 I1097 V1100 L1101 L1102 V1103 L1104 R1105 V1110 T1111 A1112 P1114 G1115 M1116 R1117 L1118 I1119 V1120 S1121 A1122 S1125 G1128 P1129 M1130 V1133 M1137 F1140

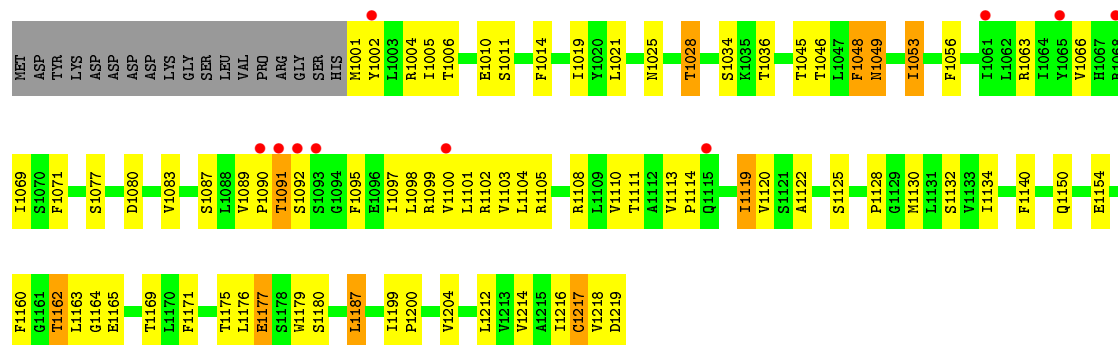
- Chain B:
- 
- 8% 57% 32% 8%
- | Category | Value |
|----------|-------|
| M1137    | 1063  |
| Q1150    | 1067  |
| F1160    | 1069  |
| G1161    | 1070  |
| T1162    | 1071  |
| L1163    | 1072  |
| G1164    | 1077  |
| E1165    | 1078  |
| S1166    | 1079  |
| F1167    | 1080  |
| T1169    | 1083  |
| Q1172    | 1084  |
| V1173    | 1089  |
| M1174    | 1090  |
| T1175    | 1091  |
| L1176    | 1092  |
| E1177    | 1093  |
| S1180    | 1094  |
| M1181    | 1095  |
| G1182    | 1096  |
| L1183    | 1097  |
| V1184    | 1098  |
| L1187    | 1099  |
| M1188    | 1100  |
| Y1193    | 1101  |
| V1196    | 1104  |
| F1197    | 1105  |
| F1198    | 1108  |
| P1200    | 1109  |
| F1201    | 1110  |
| L1202    | 1113  |
| V1205    | 1114  |
| T1206    | 1118  |
| F1207    | 1119  |
| V1208    | 1120  |
| M1209    | 1121  |
| L1210    | 1122  |
| M1211    | 1123  |
| L1212    | 1124  |
| F1213    | 1125  |
| V1214    | 1126  |
| A1215    | 1127  |
| L1216    | 1128  |
| G1217    | 1129  |
| V1218    | 1130  |
| D1219    | 1133  |
| L1062    | 1063  |
| R1063    | 1067  |
| H1067    | 1069  |
| R1068    | 1070  |
| I1069    | 1071  |
| S1070    | 1072  |
| F1071    | 1077  |
| F1072    | 1078  |
| S1077    | 1079  |
| L1078    | 1080  |
| F1079    | 1083  |
| D1080    | 1084  |
| V1083    | 1089  |
| V1084    | 1090  |
| P1090    | 1091  |
| T1091    | 1092  |
| S1092    | 1093  |
| S1093    | 1094  |
| G1094    | 1095  |
| F1095    | 1096  |
| E1096    | 1097  |
| I1097    | 1098  |
| S1011    | 1099  |
| S1012    | 1100  |
| F1013    | 1101  |
| F1014    | 1104  |
| T1015    | 1105  |
| I1019    | 1108  |
| Y1020    | 1109  |
| L1021    | 1113  |
| I1022    | 1114  |
| M1025    | 1118  |
| T1028    | 1119  |
| L1031    | 1120  |
| E1032    | 1121  |
| F1037    | 1122  |
| M1038    | 1123  |
| F1041    | 1124  |
| F1048    | 1125  |
| I1051    | 1126  |
| V1052    | 1127  |
| I1053    | 1128  |
| T1054    | 1129  |
| I1055    | 1130  |
| I1058    | 1133  |
| I1126    | 1136  |

- Chain C:
- 
- 9% 60% 30% 8%
- MET ASP TYR LYS ASP ASP ASP LYS GLY SER LEU VAL PRO ARG GLY SER HIS MI001 RI004 LI005 LI008 FI013 LI019 LI022 VI023 LI024 NI025 TI028 TI033 SI034 KI035 TI036 FI037 MI038 QI039 SI040 FI041 GI042 VI043 YI044 FI048 VI052 LI053 LI058 RI062 LI063 TI060





• Molecule 1: Ion transport protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	229.22Å 124.88Å 124.76Å 90.00° 122.95° 90.00°	Depositor
Resolution (Å)	48.13 – 3.26 48.09 – 3.26	Depositor EDS
% Data completeness (in resolution range)	85.8 (48.13-3.26) 85.8 (48.09-3.26)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.276 , 0.314 0.269 , 0.310	Depositor DCC
$R_{free}$ test set	2030 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.377 for -h-k-l,l,k 0.388 for -h+k-l,-l,-k 0.399 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.71	0/1848	0.79	1/2514 (0.0%)
1	B	0.67	0/1848	0.77	0/2514
1	C	0.69	0/1848	0.79	0/2514
1	D	0.69	0/1848	0.79	0/2514
All	All	0.69	0/7392	0.78	1/10056 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1181	MET	CA-CB-CG	-5.59	103.79	113.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1797	0	1869	63	0
1	B	1797	0	1869	63	0
1	C	1797	0	1869	57	0
1	D	1797	0	1869	58	0
2	A	2	0	0	0	0
3	A	26	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	47	0	40	9	0
3	C	78	0	64	2	0
3	D	37	0	35	5	0
All	All	7378	0	7636	220	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 15.

The worst 5 of 220 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:C:1162:THR:HG22	1:C:1165:GLU:H	1.30	0.95
1:D:1162:THR:HG22	1:D:1165:GLU:H	1.34	0.93
1:D:1164:GLY:CA	3:D:1301:PX4:H14	2.10	0.81
1:C:1089:VAL:HG13	1:C:1090:PRO:HD2	1.66	0.77
1:B:1162:THR:HG22	1:B:1165:GLU:H	1.50	0.76

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	217/237 (92%)	203 (94%)	13 (6%)	1 (0%)	29	62
1	B	217/237 (92%)	198 (91%)	19 (9%)	0	100	100
1	C	217/237 (92%)	202 (93%)	13 (6%)	2 (1%)	17	50
1	D	217/237 (92%)	197 (91%)	17 (8%)	3 (1%)	11	40
All	All	868/948 (92%)	800 (92%)	62 (7%)	6 (1%)	22	56

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1091	THR
1	D	1091	THR
1	D	1217	CYS
1	C	1093	SER
1	C	1094	GLY

### 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	202/218 (93%)	188 (93%)	14 (7%)	15	43
1	B	202/218 (93%)	185 (92%)	17 (8%)	11	35
1	C	202/218 (93%)	190 (94%)	12 (6%)	19	50
1	D	202/218 (93%)	186 (92%)	16 (8%)	12	37
All	All	808/872 (93%)	749 (93%)	59 (7%)	14	40

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1187	LEU
1	C	1035	LYS
1	D	1162	THR
1	B	1205	VAL
1	B	1209	MET

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 ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	C	1303	-	5,5,45	0.36	0	4,4,53	0.19	0
3	PX4	D	1303	-	9,9,45	0.95	0	11,12,53	1.61	4 (36%)
3	PX4	C	1302	-	20,20,45	1.40	2 (10%)	22,24,53	1.57	2 (9%)
3	PX4	B	1304	-	9,9,45	0.80	0	11,12,53	1.38	3 (27%)
3	PX4	C	1306	-	9,9,45	0.80	0	11,12,53	1.45	2 (18%)
3	PX4	B	1301	-	9,9,45	0.60	0	11,12,53	1.19	1 (9%)
3	PX4	C	1301	-	9,9,45	0.57	0	11,12,53	0.94	0
3	PX4	C	1305	-	20,20,45	1.48	2 (10%)	22,24,53	1.37	2 (9%)
3	PX4	D	1301	-	20,20,45	1.24	2 (10%)	22,24,53	1.82	2 (9%)
3	PX4	A	1305	-	9,9,45	0.97	0	11,12,53	1.37	1 (9%)
3	PX4	B	1302	-	20,20,45	1.59	2 (10%)	22,24,53	1.57	2 (9%)
3	PX4	C	1304	-	9,9,45	0.60	0	11,12,53	1.59	2 (18%)
3	PX4	D	1302	-	5,5,45	0.38	0	4,4,53	0.42	0
3	PX4	A	1304	-	5,5,45	0.34	0	4,4,53	0.34	0
3	PX4	A	1303	-	9,9,45	0.60	0	11,12,53	1.13	1 (9%)
3	PX4	B	1303	-	5,5,45	0.52	0	4,4,53	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	C	1303	-	-	3/3/3/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	D	1303	-	-	6/8/8/49	-
3	PX4	C	1302	-	-	10/22/22/49	-
3	PX4	B	1304	-	-	7/8/8/49	-
3	PX4	C	1306	-	-	5/8/8/49	-
3	PX4	B	1301	-	-	6/8/8/49	-
3	PX4	C	1301	-	-	5/8/8/49	-
3	PX4	C	1305	-	-	6/22/22/49	-
3	PX4	D	1301	-	-	11/22/22/49	-
3	PX4	A	1305	-	-	3/8/8/49	-
3	PX4	B	1302	-	-	11/22/22/49	-
3	PX4	C	1304	-	-	2/8/8/49	-
3	PX4	D	1302	-	-	0/3/3/49	-
3	PX4	A	1304	-	-	1/3/3/49	-
3	PX4	A	1303	-	-	5/8/8/49	-
3	PX4	B	1303	-	-	1/3/3/49	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	PX4	O6-C9	5.46	1.38	1.22
3	C	1305	PX4	O6-C9	5.33	1.38	1.22
3	C	1302	PX4	O6-C9	4.92	1.37	1.22
3	D	1301	PX4	O6-C9	4.56	1.36	1.22
3	B	1302	PX4	O5-C9	3.87	1.44	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1301	PX4	O5-C9-O6	-6.94	106.08	123.59
3	C	1302	PX4	O5-C9-O6	-5.45	109.84	123.59
3	B	1302	PX4	O5-C9-O6	-4.90	111.22	123.59
3	B	1302	PX4	O6-C9-C10	-4.50	106.19	123.73
3	C	1305	PX4	O5-C9-O6	-4.30	112.75	123.59

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1303	PX4	C6-O4-P1-O1

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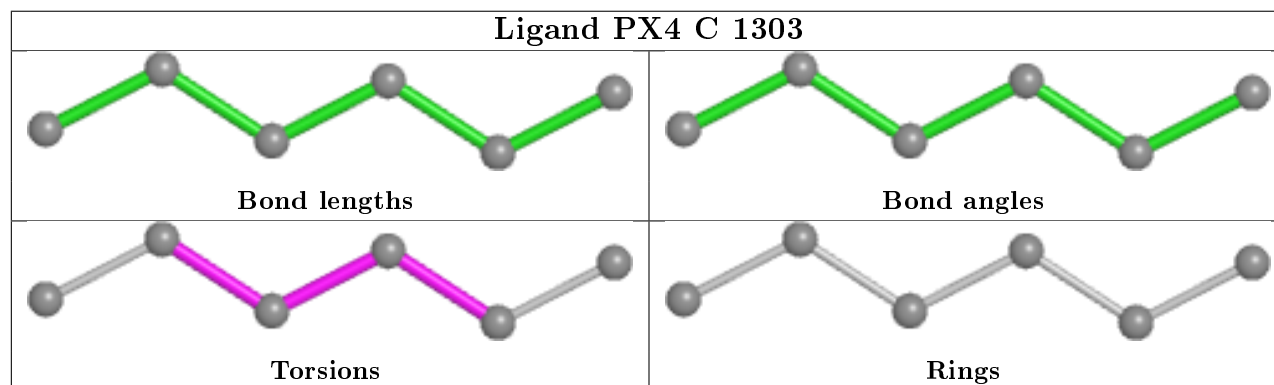
Mol	Chain	Res	Type	Atoms
3	D	1303	PX4	C6-O4-P1-O3
3	D	1303	PX4	C6-C7-C8-O5
3	C	1302	PX4	C1-O3-P1-O4
3	C	1302	PX4	C6-O4-P1-O2

There are no ring outliers.

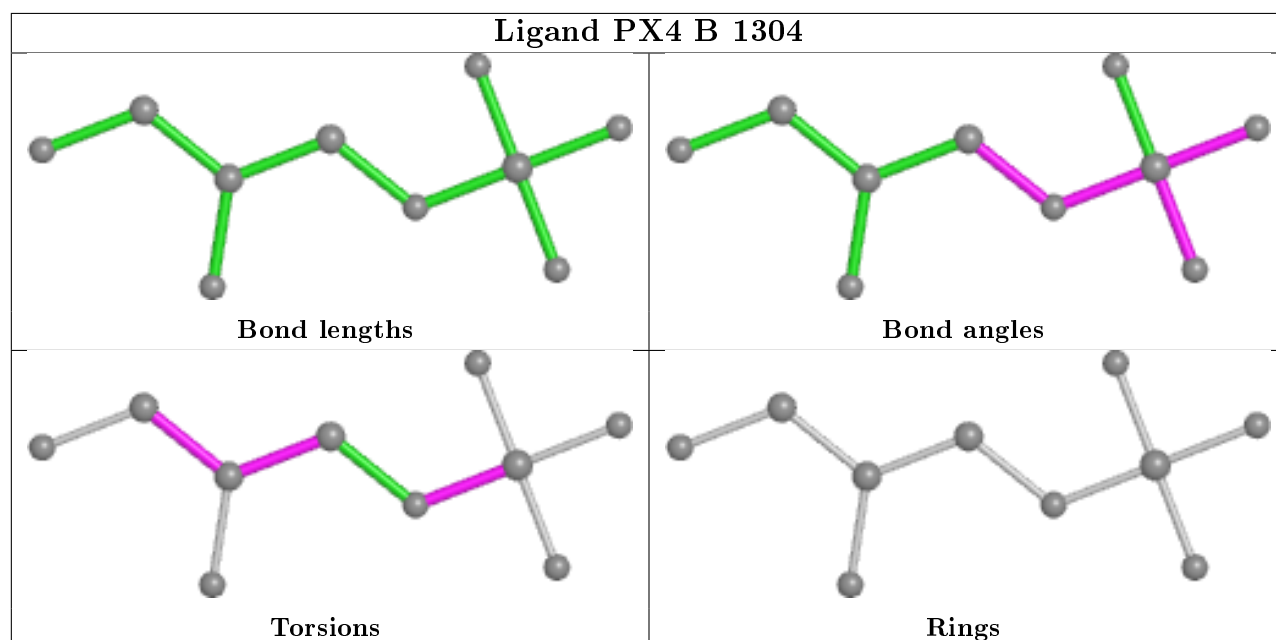
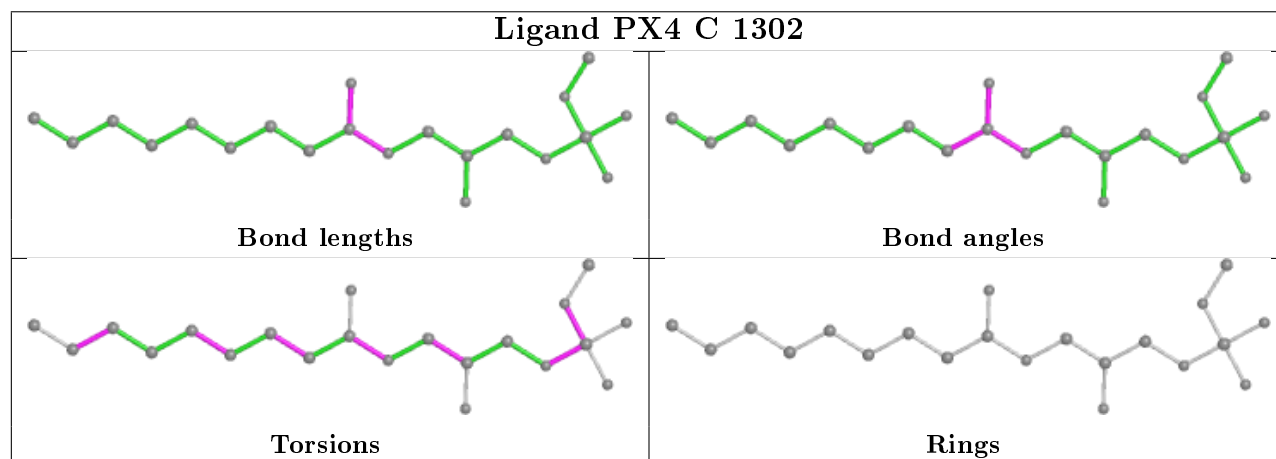
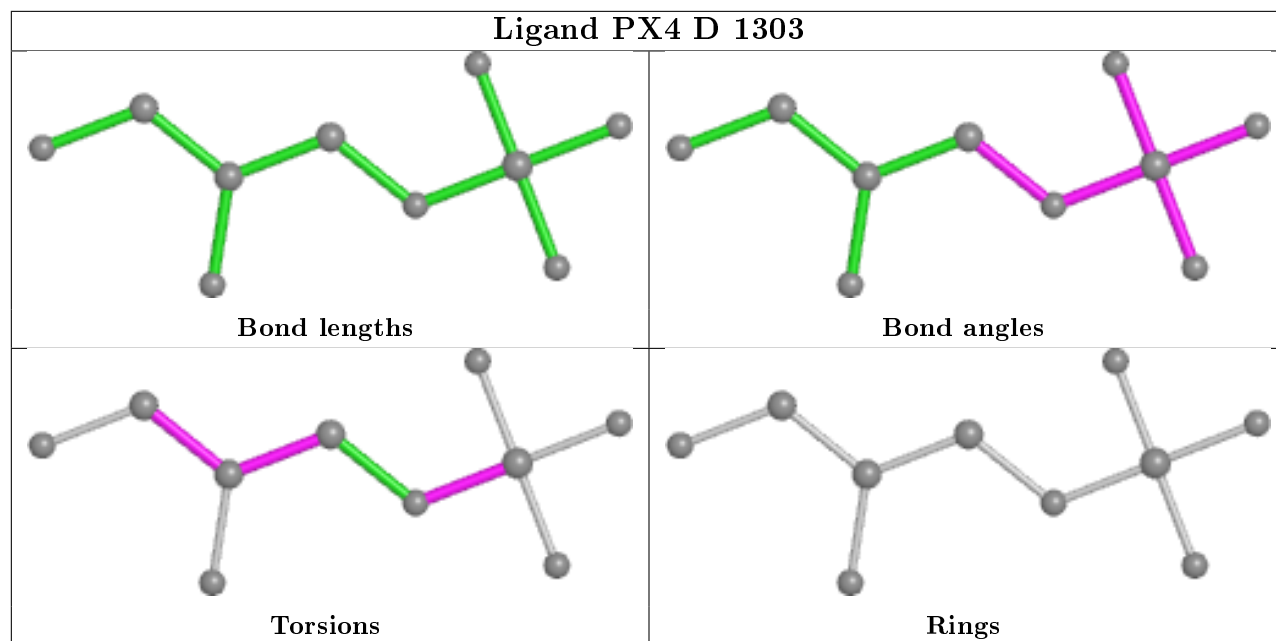
3 monomers are involved in 16 short contacts:

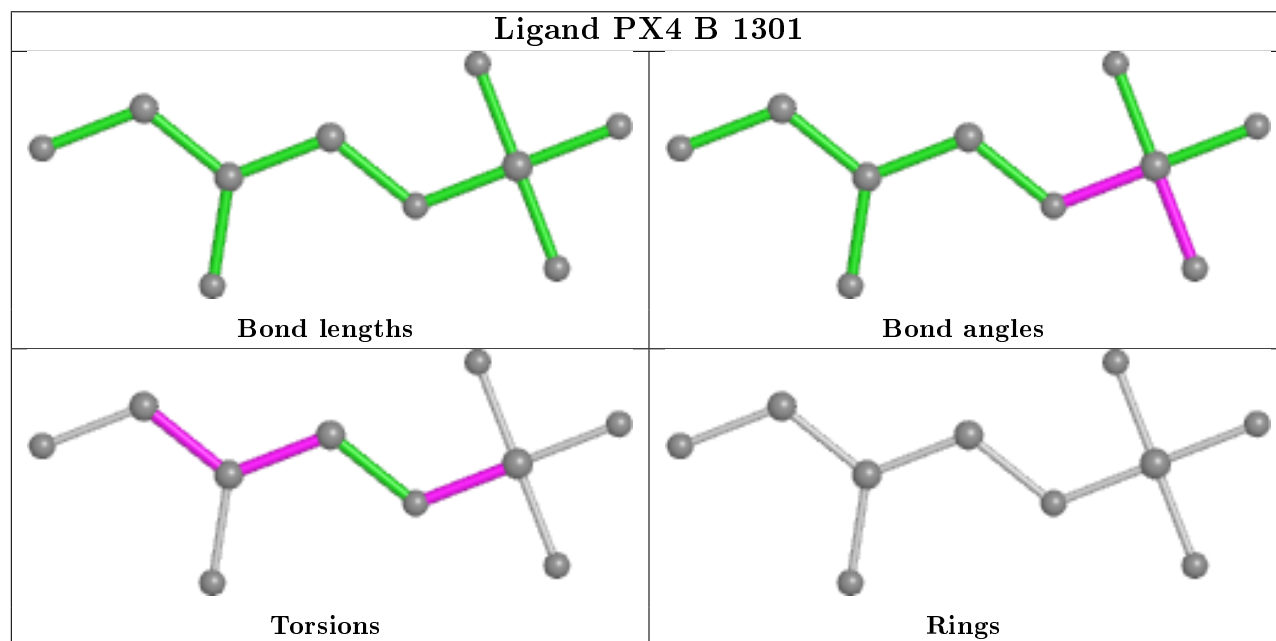
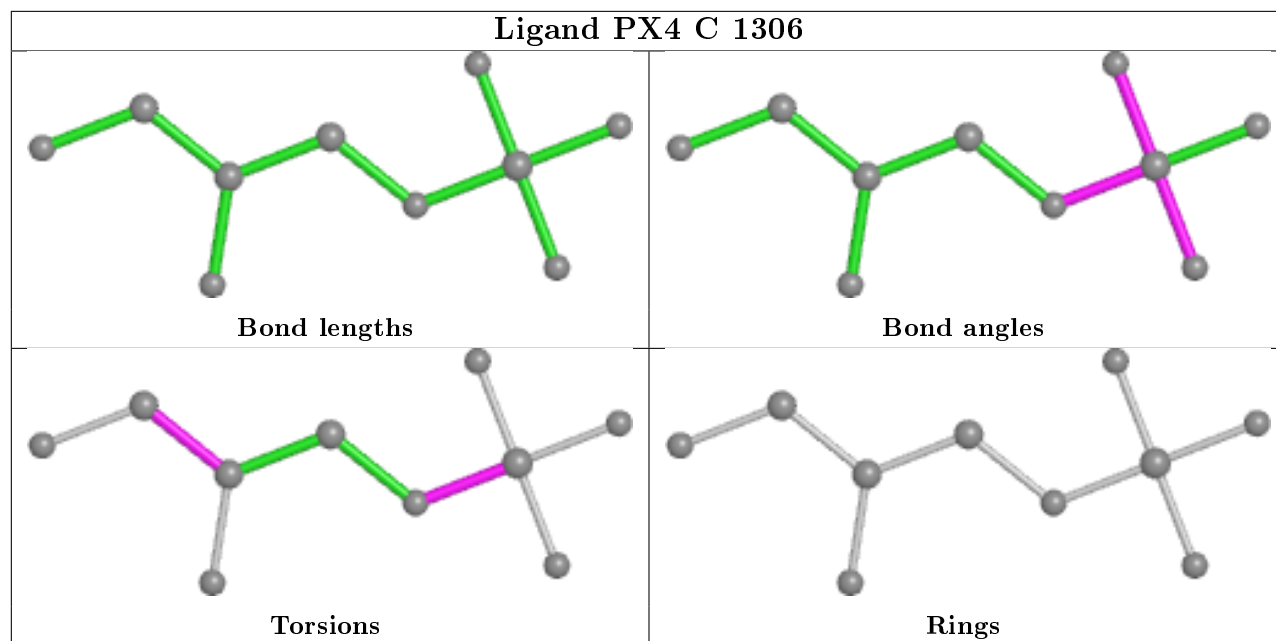
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1302	PX4	2	0
3	D	1301	PX4	5	0
3	B	1302	PX4	9	0

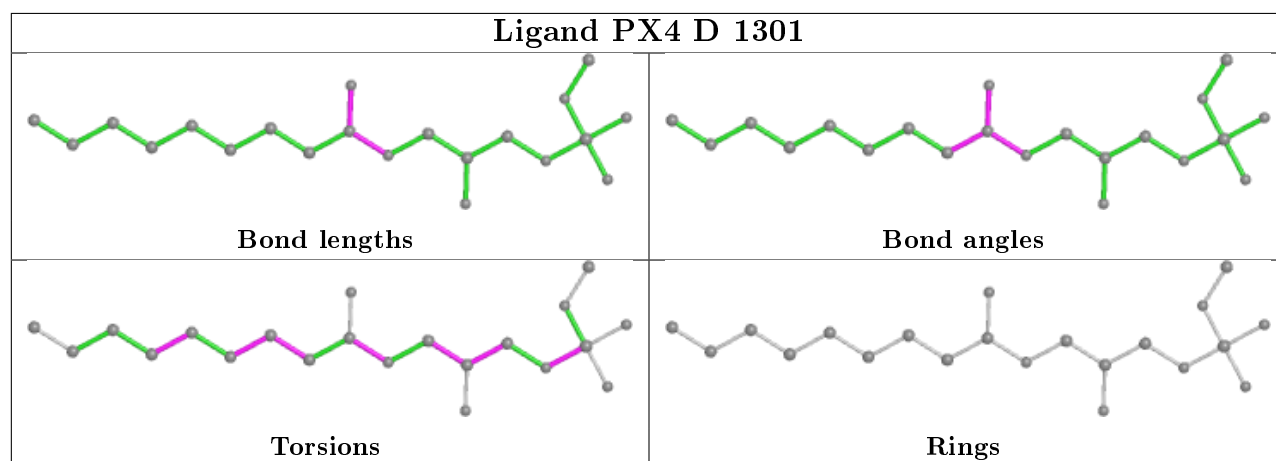
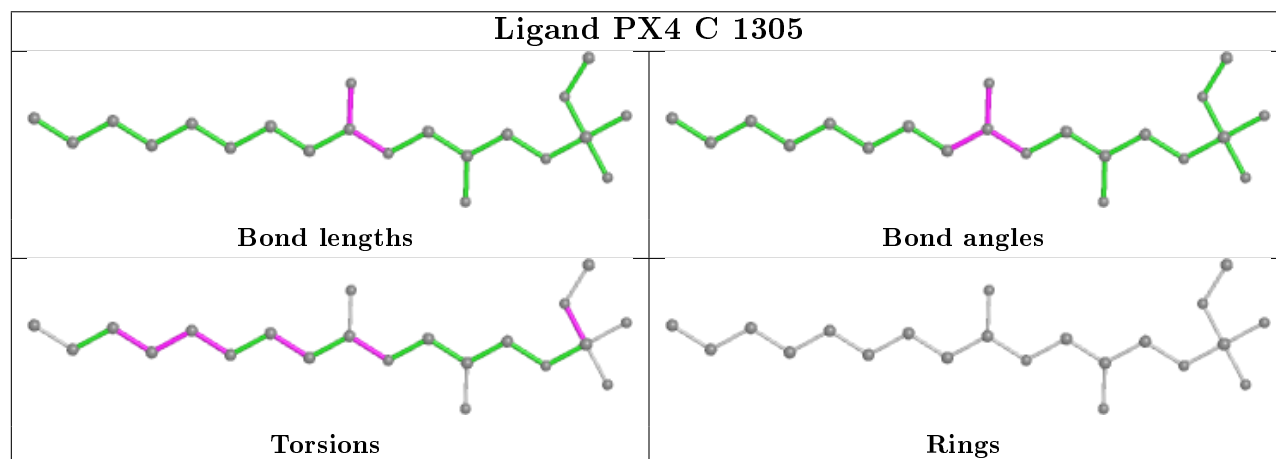
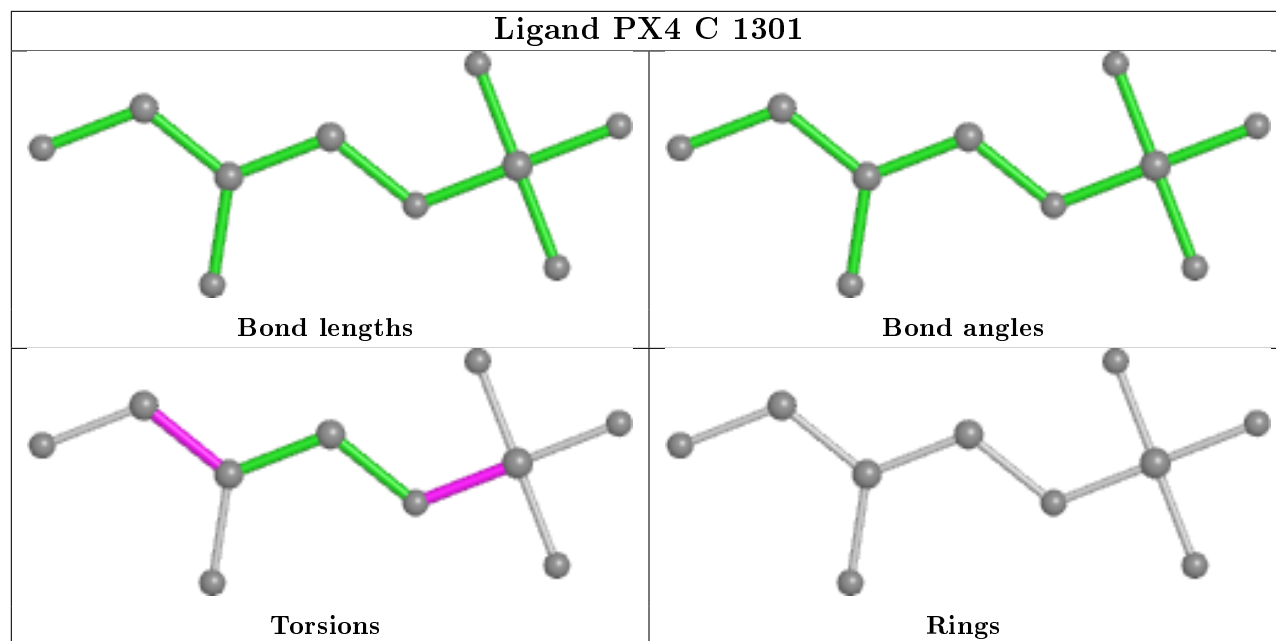
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

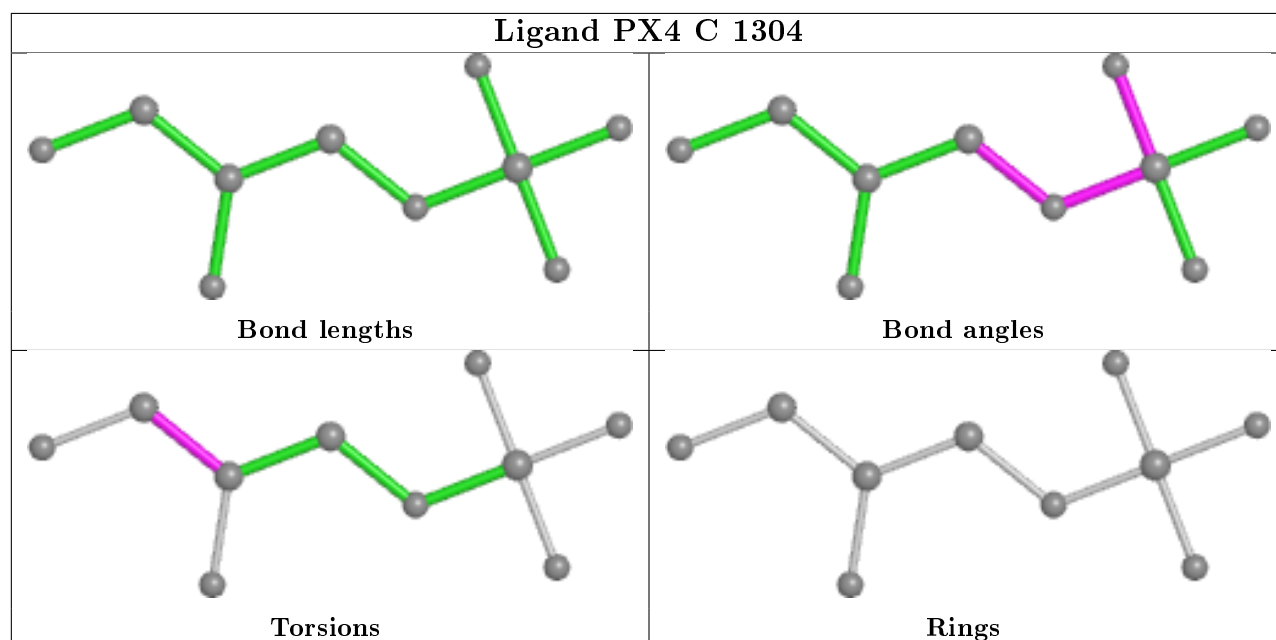
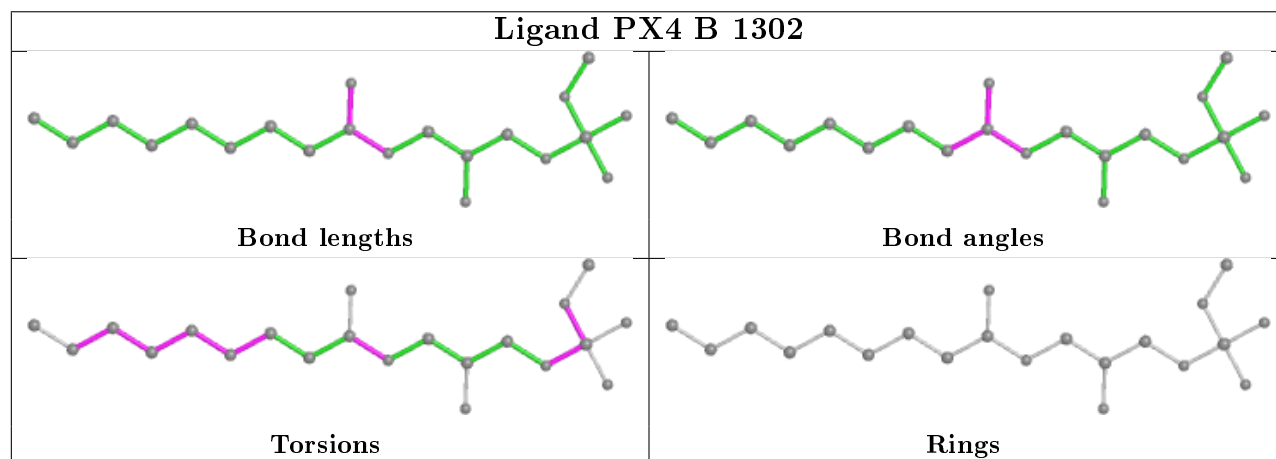
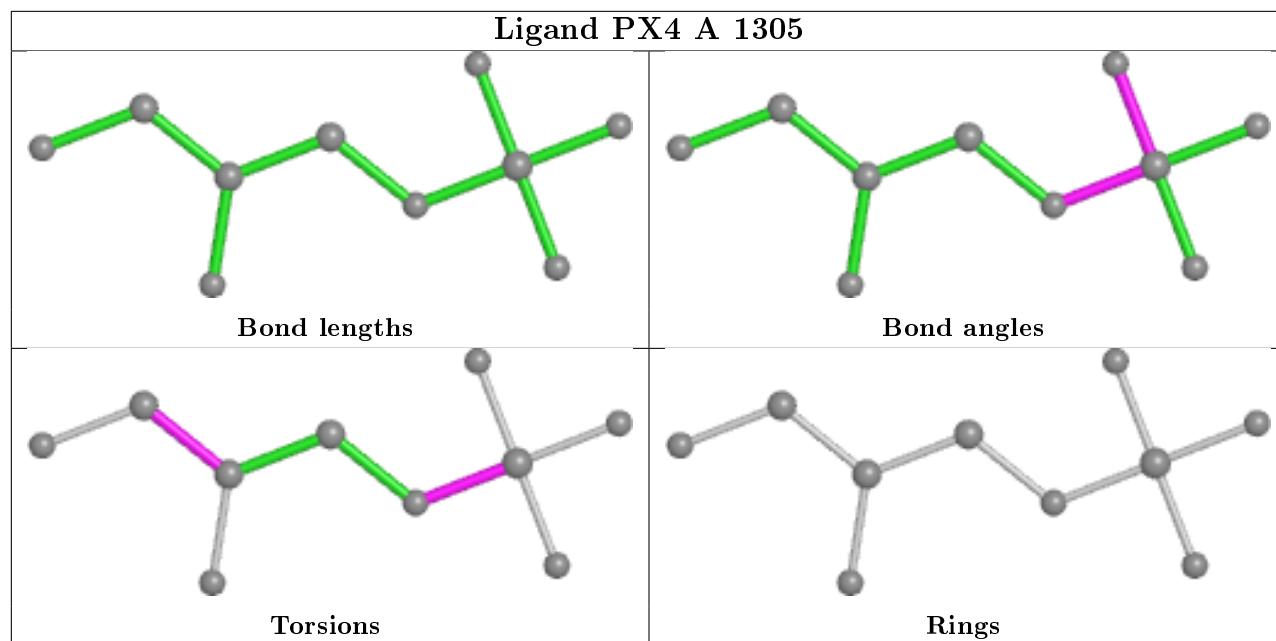


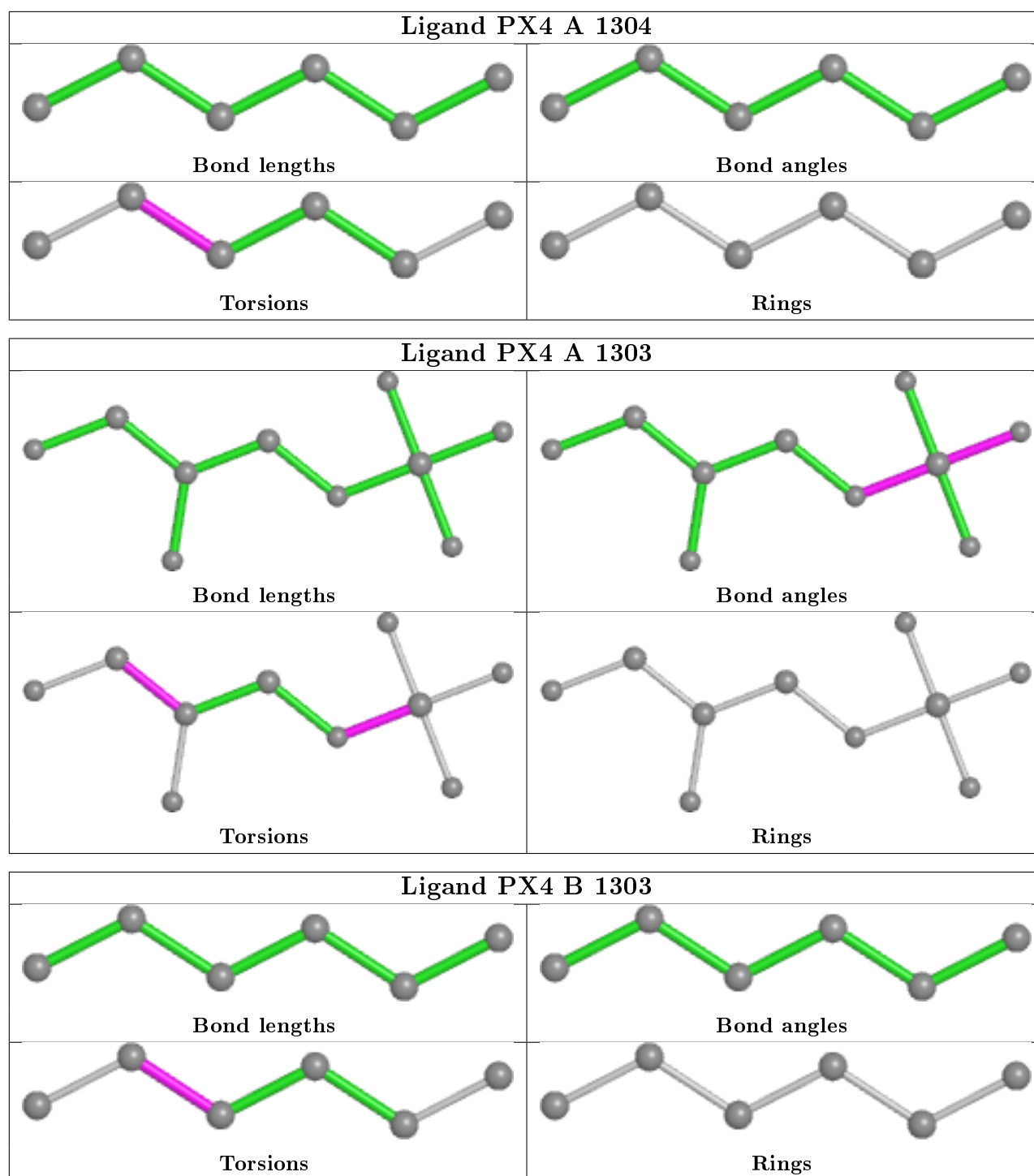












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	219/237 (92%)	0.44	15 (6%) 17 16	62, 96, 125, 151	0
1	B	219/237 (92%)	0.42	19 (8%) 10 10	62, 96, 126, 152	0
1	C	219/237 (92%)	0.42	21 (9%) 8 8	62, 95, 129, 152	0
1	D	219/237 (92%)	0.17	10 (4%) 32 30	62, 95, 125, 154	0
All	All	876/948 (92%)	0.36	65 (7%) 14 14	62, 96, 127, 154	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1095	PHE	10.3
1	A	1007	ASN	10.1
1	B	1013	PHE	7.3
1	B	1097	ILE	7.1
1	C	1040	SER	5.3

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

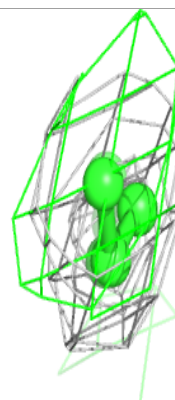
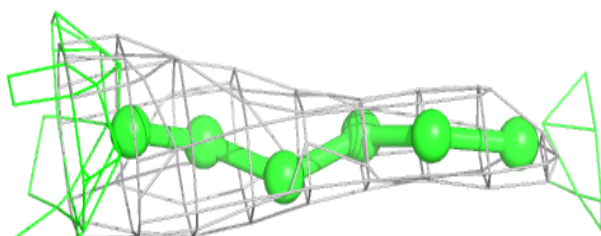
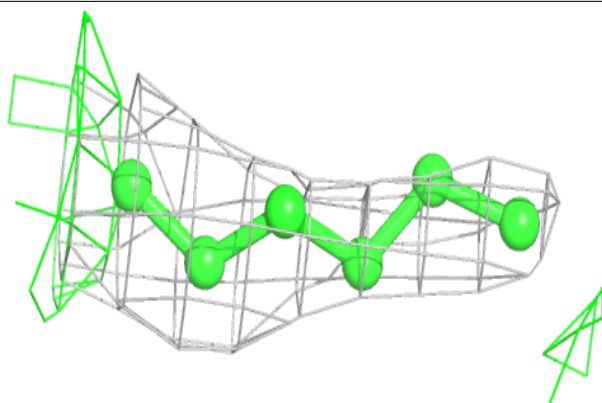
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PX4	B	1303	6/46	0.39	0.53	62,63,65,66	0
3	PX4	C	1306	10/46	0.66	0.61	86,106,133,142	0
3	PX4	D	1302	6/46	0.71	0.29	62,63,65,66	0
3	PX4	D	1303	10/46	0.72	0.21	87,106,132,137	0
3	PX4	B	1304	10/46	0.76	0.17	81,95,121,135	0
3	PX4	C	1305	21/46	0.76	0.22	65,77,92,101	0
3	PX4	A	1303	10/46	0.78	0.22	78,92,109,136	0
3	PX4	A	1304	6/46	0.81	0.27	62,63,65,65	0
3	PX4	D	1301	21/46	0.81	0.19	69,77,89,97	0
3	PX4	C	1302	21/46	0.81	0.21	64,72,85,86	0
3	PX4	C	1303	6/46	0.82	0.38	62,62,62,62	0
3	PX4	C	1301	10/46	0.82	0.18	71,81,115,133	0
3	PX4	A	1305	10/46	0.84	0.67	83,100,131,139	0
3	PX4	B	1302	21/46	0.85	0.16	66,74,98,108	0
3	PX4	B	1301	10/46	0.86	0.23	68,83,123,126	0
3	PX4	C	1304	10/46	0.88	0.14	64,78,114,121	0
2	CA	A	1302	1/1	0.94	0.45	89,89,89,89	0
2	CA	A	1301	1/1	0.97	0.47	62,62,62,62	0

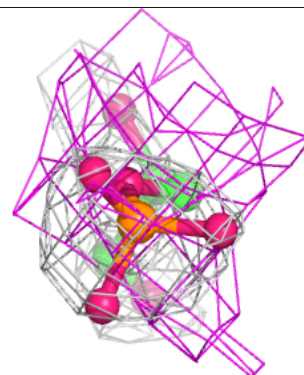
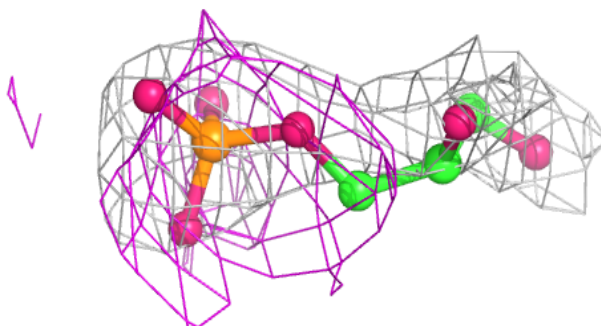
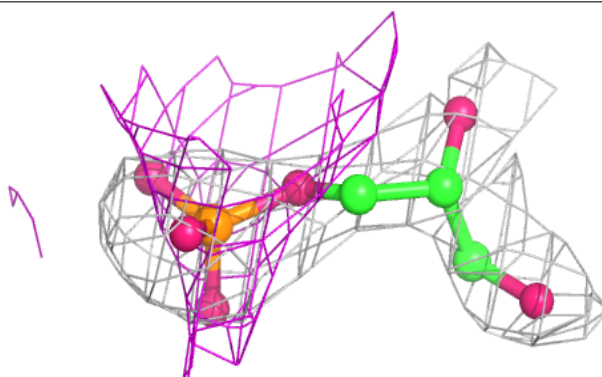
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PX4 B 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 C 1306:**

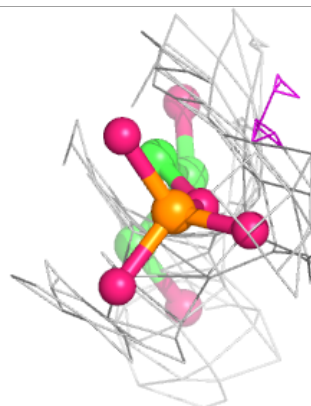
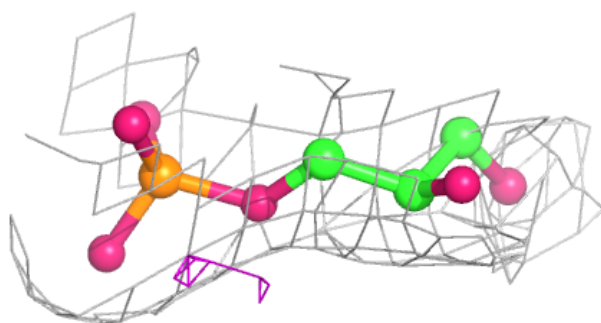
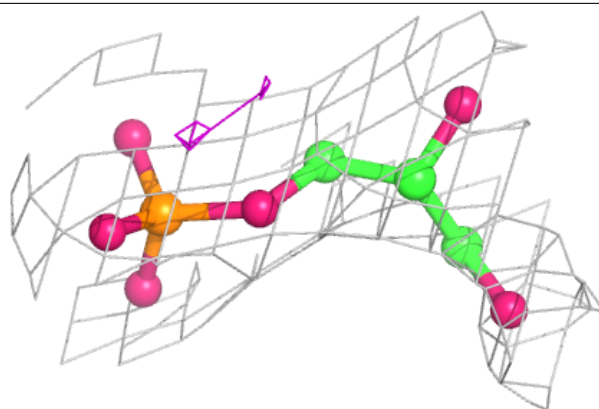
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



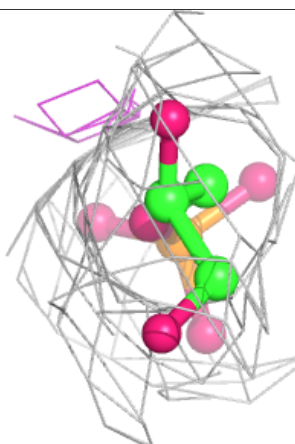
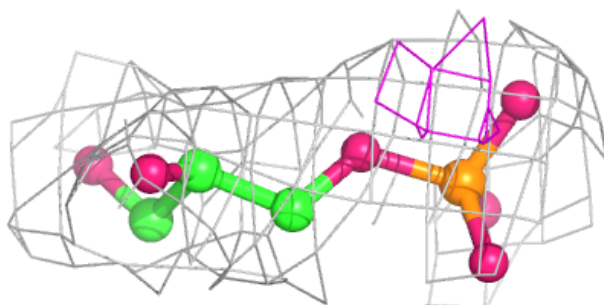
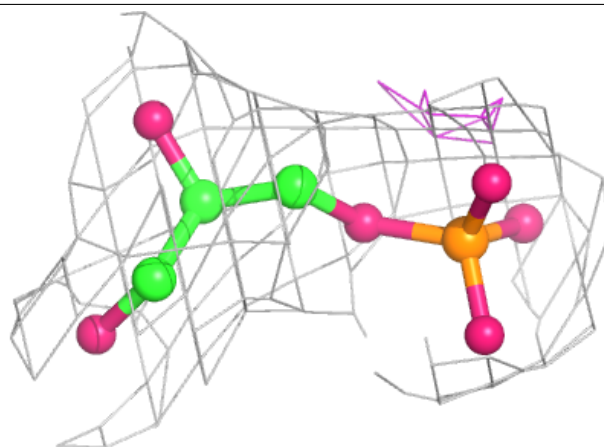


**Electron density around PX4 D 1303:**

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

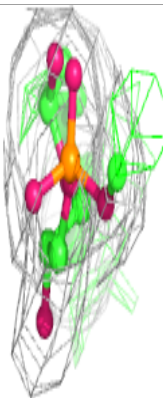
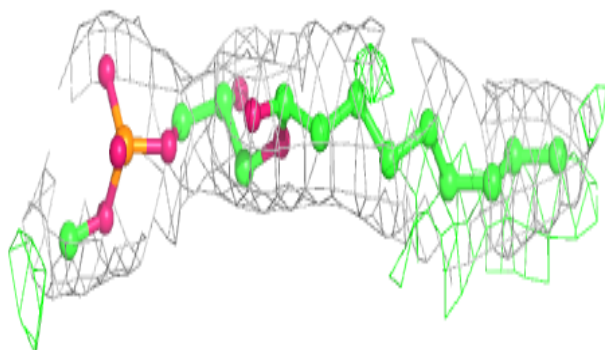
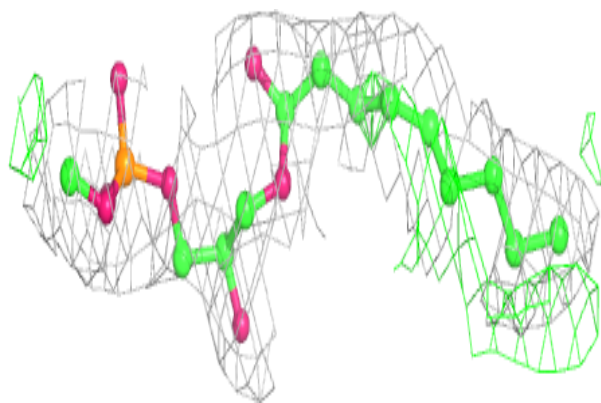
**Electron density around PX4 B 1304:**

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and green (positive)

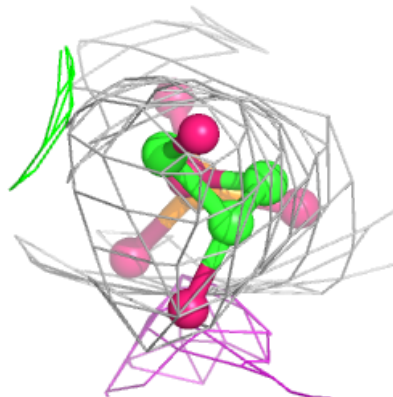
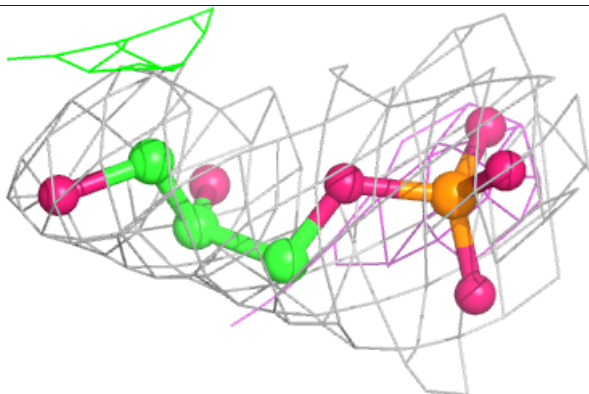
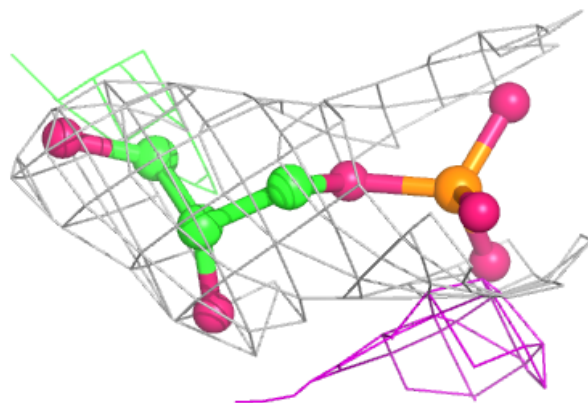


**Electron density around PX4 C 1305:**

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and green (positive)

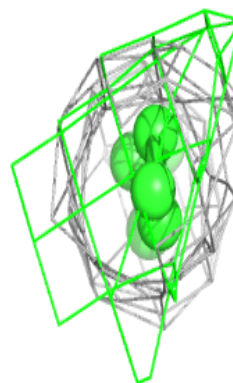
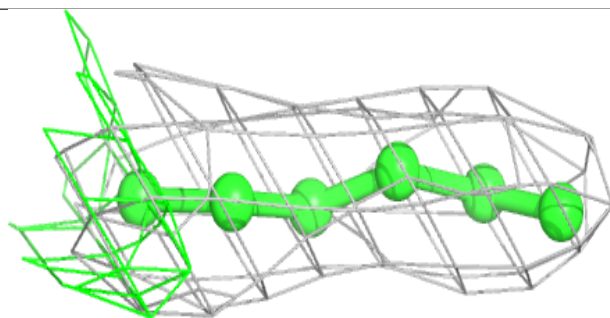
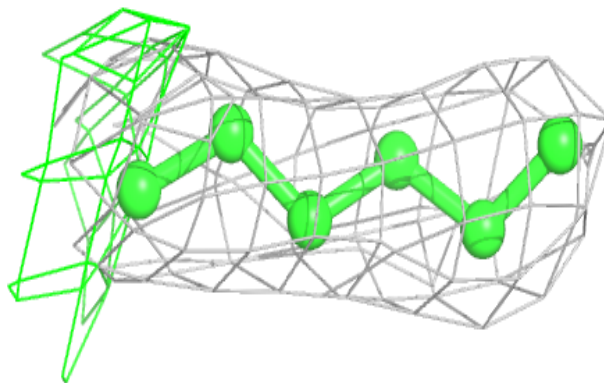
**Electron density around PX4 A 1303:**

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and green (positive)

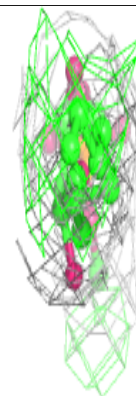
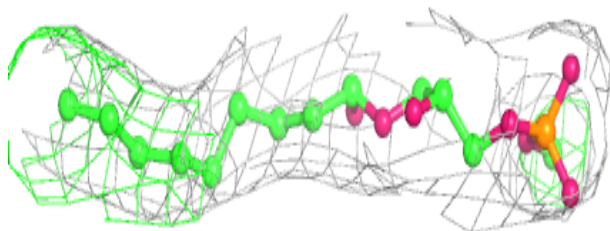
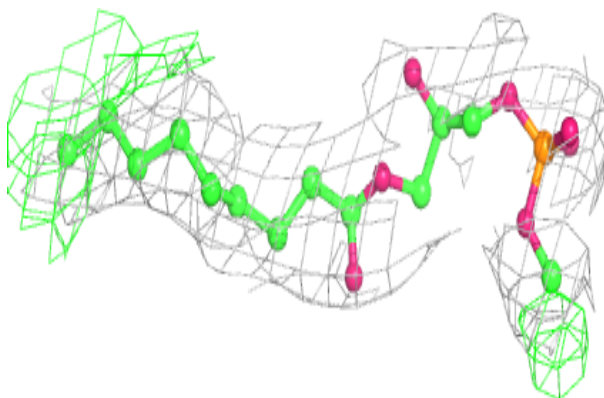


**Electron density around PX4 A 1304:**

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and green (positive)

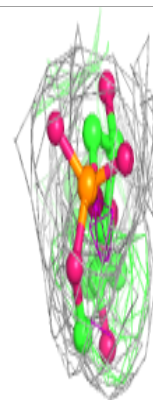
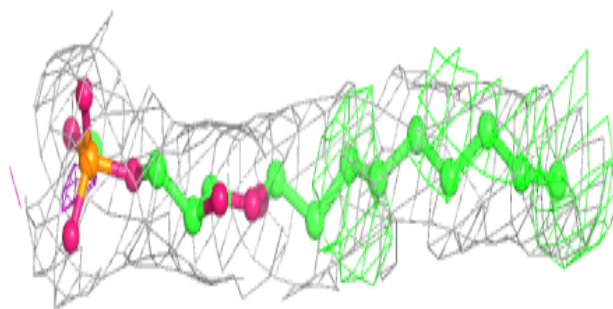
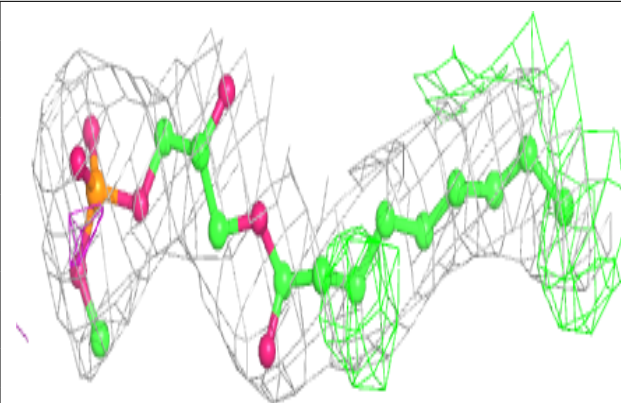
**Electron density around PX4 D 1301:**

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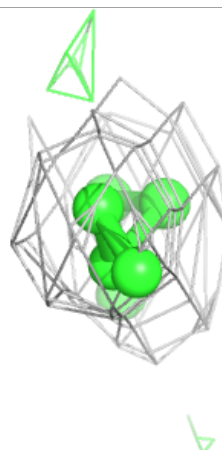
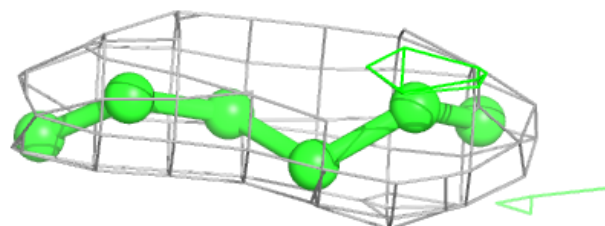
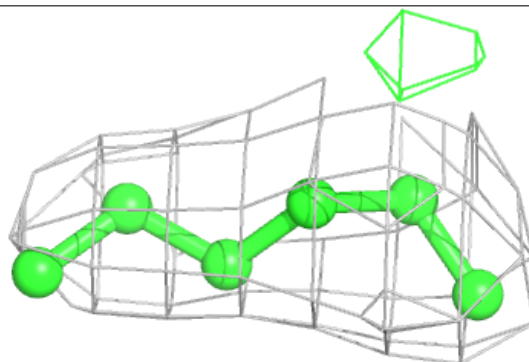


**Electron density around PX4 C 1302:**

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

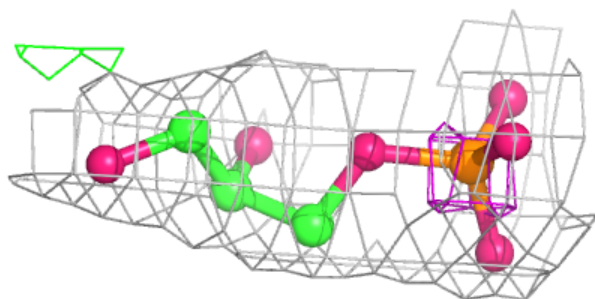
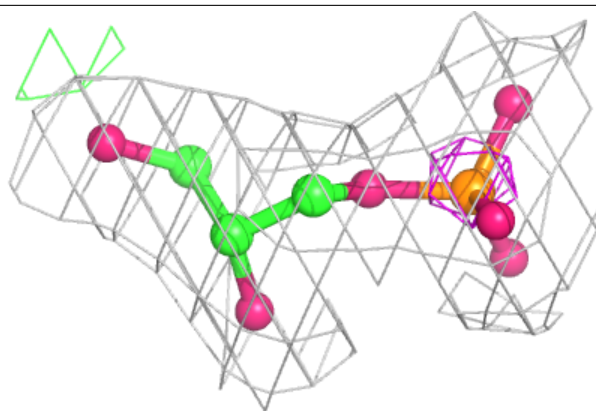
**Electron density around PX4 C 1303:**

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



**Electron density around PX4 C 1301:**

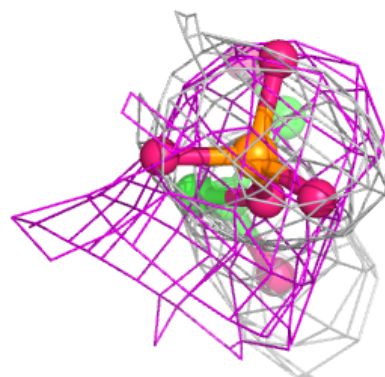
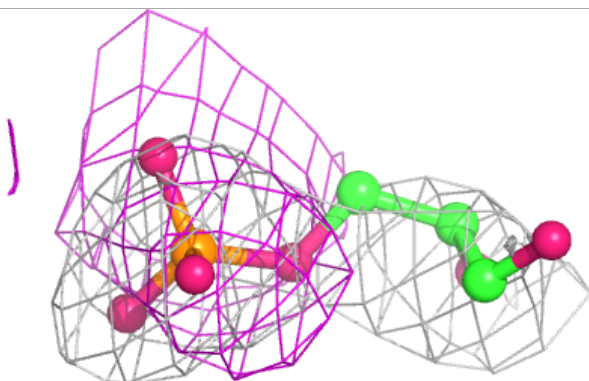
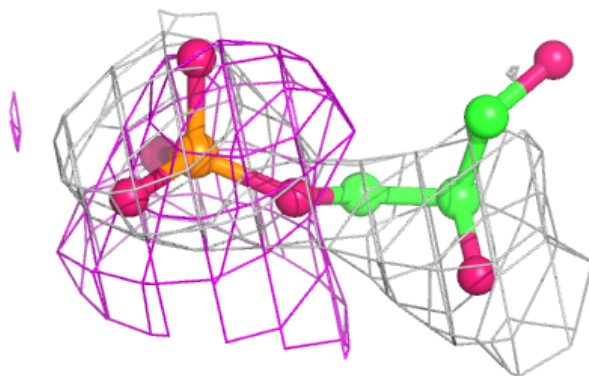
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





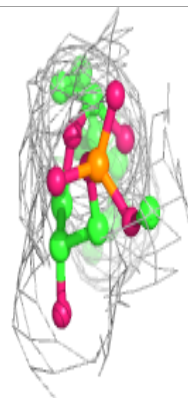
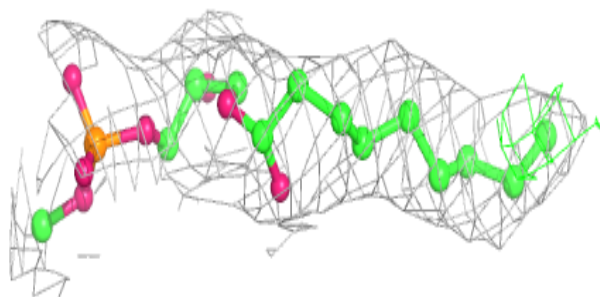
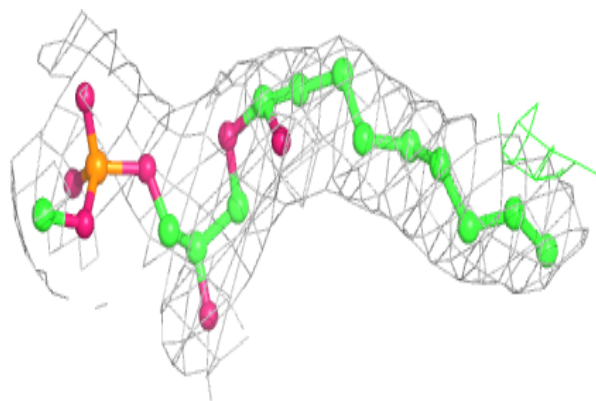
**Electron density around PX4 A 1305:**

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

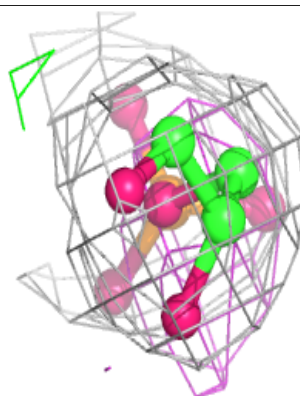
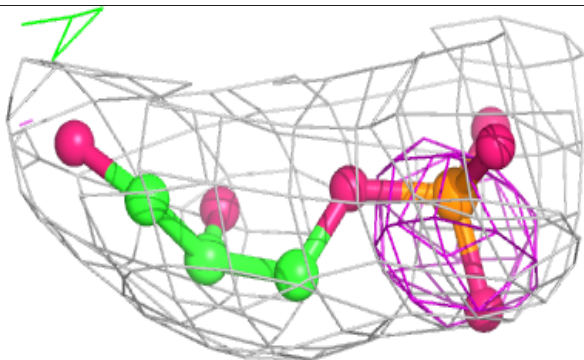
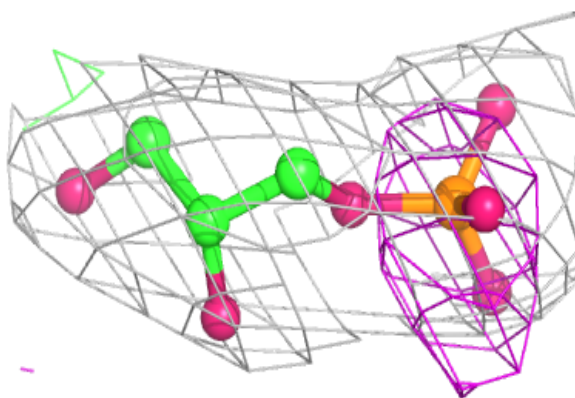


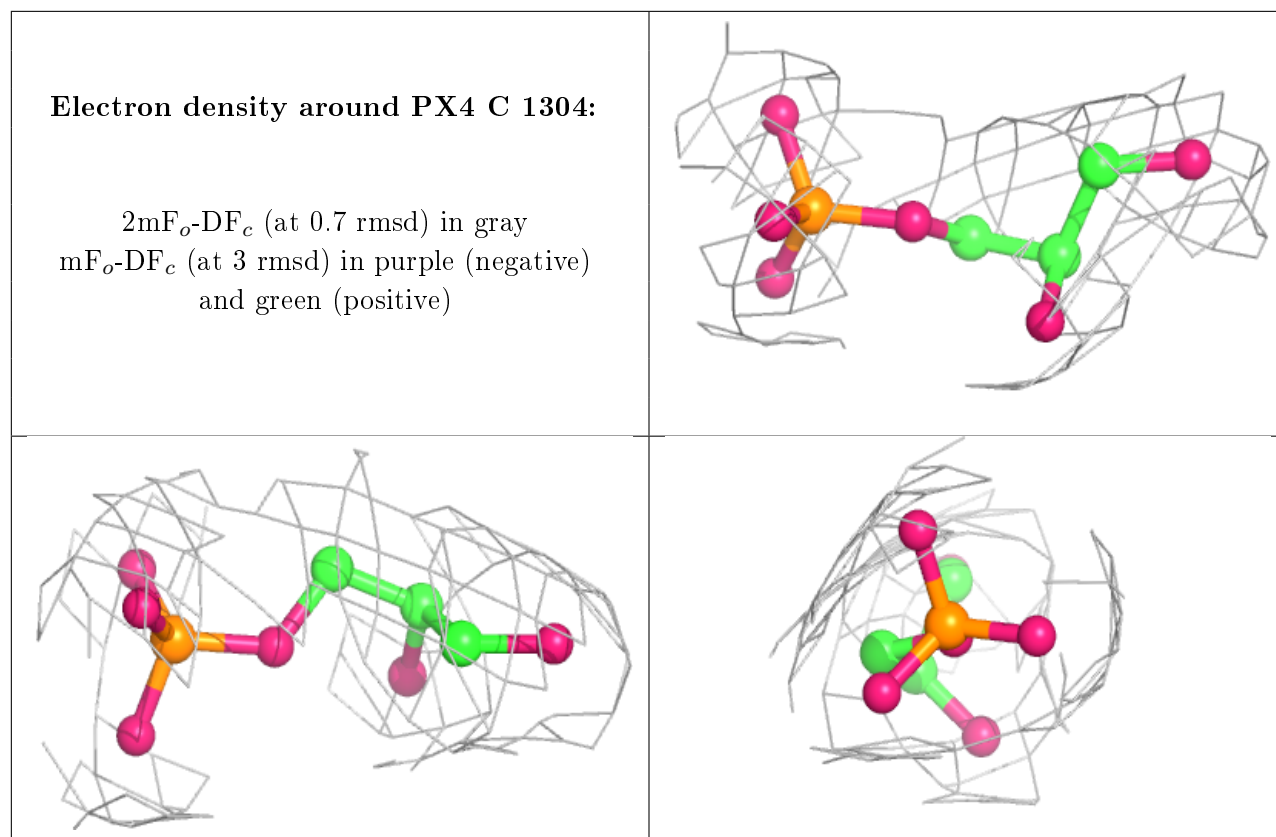
**Electron density around PX4 B 1302:**

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

**Electron density around PX4 B 1301:**

$2mF_o-DF_c$  (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.