



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 01:05 PM BST

PDB ID : 4MS2
Title : Structural basis of Ca²⁺ 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 : 2013-09-18
Resolution : 2.75 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

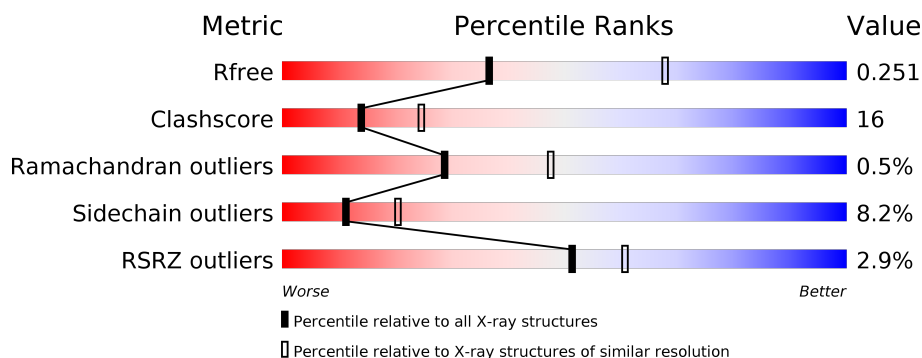
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>4%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	237	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>31%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	237	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>31%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	237	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>28%</div> <div>•</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
2	PX4	B	1301	-	-	-	X
3	CA	A	1304	-	-	-	X
3	CA	D	1303	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7889 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
			1798	1224	269	294	11			
1	B	219	Total	C	N	O	S	0	0	0
			1798	1224	269	294	11			
1	C	219	Total	C	N	O	S	0	0	0
			1798	1224	269	294	11			
1	D	219	Total	C	N	O	S	0	0	0
			1798	1224	269	294	11			

There are 88 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	1177	ASP	GLU	CONFLICT	UNP A8EVM5
A	1178	ASP	SER	CONFLICT	UNP A8EVM5
A	1181	ASN	MET	CONFLICT	UNP A8EVM5

Continued on next page...

Continued from previous page...

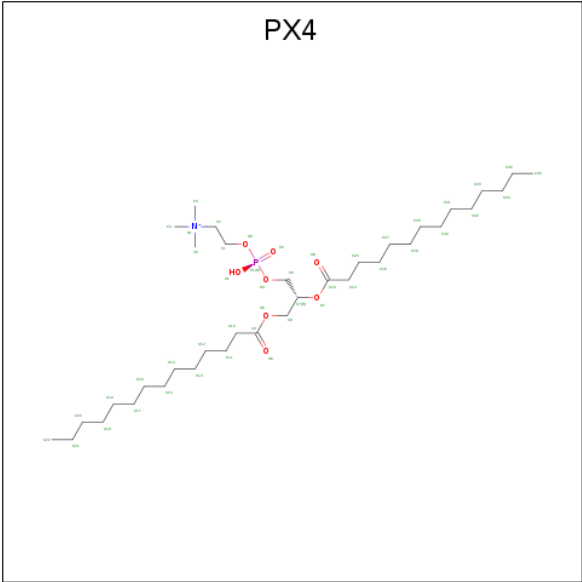
Chain	Residue	Modelled	Actual	Comment	Reference
A	1217	CYS	ILE	CONFLICT	UNP A8EVM5
B	983	MET	-	EXPRESSION TAG	UNP A8EVM5
B	984	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	985	TYR	-	EXPRESSION TAG	UNP A8EVM5
B	986	LYS	-	EXPRESSION TAG	UNP A8EVM5
B	987	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	988	ASP	-	EXPRESSION TAG	UNP 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	1177	ASP	GLU	CONFLICT	UNP A8EVM5
B	1178	ASP	SER	CONFLICT	UNP A8EVM5
B	1181	ASN	MET	CONFLICT	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	1177	ASP	GLU	CONFLICT	UNP A8EVM5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1178	ASP	SER	CONFLICT	UNP A8EVM5
C	1181	ASN	MET	CONFLICT	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
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	1177	ASP	GLU	CONFLICT	UNP A8EVM5
D	1178	ASP	SER	CONFLICT	UNP A8EVM5
D	1181	ASN	MET	CONFLICT	UNP A8EVM5
D	1217	CYS	ILE	CONFLICT	UNP A8EVM5

- Molecule 2 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C₃₆H₇₃NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total 21	C 13	O 7	P 1	0	0		
2	A	1	Total 41	C 32	O 8	P 1	0	0		
2	A	1	Total 41	C 31	N 1	O 8	P 1	0	0	
2	A	1	Total 46	C 36	N 1	O 8	P 1	0	0	
2	B	1	Total 21	C 13	O 7	P 1	0	0		
2	B	1	Total 41	C 32	O 8	P 1	0	0		
2	B	1	Total 40	C 30	N 1	O 8	P 1	0	0	
2	B	1	Total 46	C 36	N 1	O 8	P 1	0	0	
2	B	1	Total 14		C 14				0	0
2	B	1	Total 14		C 14				0	0
2	C	1	Total 21	C 13	O 7	P 1	0	0		
2	C	1	Total 41	C 32	O 8	P 1	0	0		
2	C	1	Total 43	C 33	N 1	O 8	P 1	0	0	
2	C	1	Total 42	C 32	N 1	O 8	P 1	0	0	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 46 36 1 8 1	0	0
2	C	1	Total C 14 14	0	0
2	D	1	Total C O P 21 13 7 1	0	0
2	D	1	Total C O P 41 32 8 1	0	0
2	D	1	Total C N O P 46 36 1 8 1	0	0
2	D	1	Total C 14 14	0	0

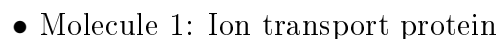
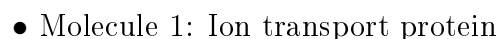
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

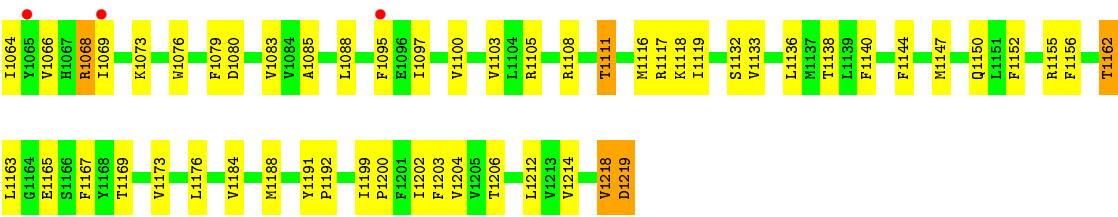
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0
3	D	2	Total Ca 2 2	0	0

- Molecule 4 is water.

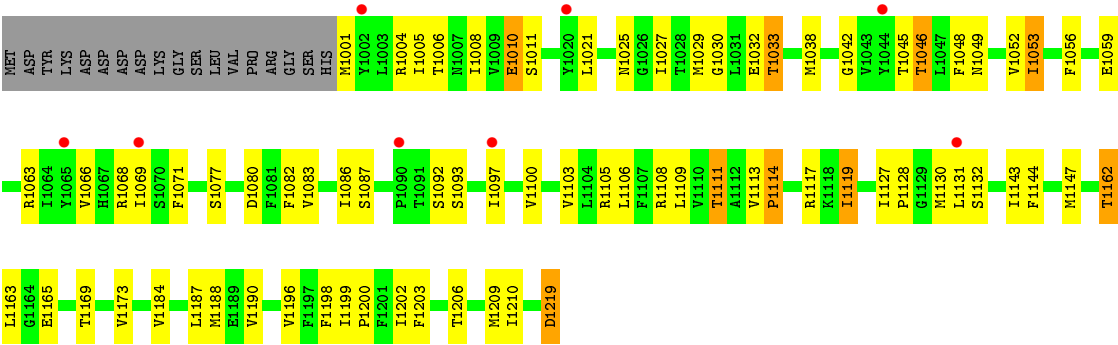
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	B	8	Total O 8 8	0	0
4	C	9	Total O 9 9	0	0
4	D	11	Total O 11 11	0	0

- Molecule 1: Ion transport protein





● 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, α , β , γ	177.79Å 177.54Å 131.14Å 90.00° 132.69° 90.00°	Depositor
Resolution (Å)	40.37 – 2.75 40.37 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.0 (40.37-2.75) 93.8 (40.37-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.232 , 0.255 0.230 , 0.251	Depositor DCC
R_{free} test set	3664 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.447 for -k,-h,-1/2*h+1/2*k-l 0.457 for k,h,-1/2*h-1/2*k-l 0.457 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7889	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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	0.60	0/1849	0.68	1/2517 (0.0%)
1	B	0.57	0/1849	0.65	0/2517
1	C	0.61	0/1849	0.67	0/2517
1	D	0.57	0/1849	0.63	0/2517
All	All	0.59	0/7396	0.66	1/10068 (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	1187	LEU	CB-CG-CD2	-5.77	101.19	111.00

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	1798	0	1863	62	0
1	B	1798	0	1863	61	0
1	C	1798	0	1863	58	0
1	D	1798	0	1863	54	0
2	A	149	0	206	24	0
2	B	176	0	258	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	207	0	298	25	0
2	D	122	0	177	22	0
3	A	3	0	0	0	0
3	D	2	0	0	0	0
4	A	10	0	0	0	0
4	B	8	0	0	0	0
4	C	9	0	0	0	0
4	D	11	0	0	0	0
All	All	7889	0	8391	255	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.

The worst 5 of 255 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)
2:B:1302:PX4:H51	2:C:1304:PX4:O8	1.49	1.12
2:A:1305:PX4:H51	2:C:1303:PX4:O8	1.51	1.10
1:C:1155:ARG:HH21	2:C:1305:PX4:H11	1.36	0.89
1:A:1027:ILE:HG12	2:A:1305:PX4:H33	1.53	0.89
1:D:1092:SER:HB3	1:D:1093:SER:HB2	1.54	0.89

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%)	194 (89%)	22 (10%)	1 (0%)	29	47
1	B	217/237 (92%)	197 (91%)	19 (9%)	1 (0%)	29	47
1	C	217/237 (92%)	199 (92%)	17 (8%)	1 (0%)	29	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	217/237 (92%)	197 (91%)	19 (9%)	1 (0%)	29	47
All	All	868/948 (92%)	787 (91%)	77 (9%)	4 (0%)	29	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1218	VAL
1	A	1063	ARG
1	B	1216	ILE
1	D	1114	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/218 (93%)	187 (93%)	15 (7%)	13	24
1	B	202/218 (93%)	182 (90%)	20 (10%)	8	13
1	C	202/218 (93%)	186 (92%)	16 (8%)	12	22
1	D	202/218 (93%)	187 (93%)	15 (7%)	13	24
All	All	808/872 (93%)	742 (92%)	66 (8%)	11	20

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1162	THR
1	C	1024	LEU
1	D	1132	SER
1	B	1163	LEU
1	B	1214	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1211	ASN
1	D	1150	GLN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 5 are monoatomic - leaving 20 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$
2	PX4	B	1302	-	40,40,45	1.44	4 (10%)	43,45,53	1.86	6 (13%)
2	PX4	D	1306	-	13,13,45	0.77	0	12,12,53	0.40	0
2	PX4	A	1307	-	45,45,45	1.66	5 (11%)	51,53,53	1.55	5 (9%)
2	PX4	B	1303	-	39,39,45	1.85	5 (12%)	45,47,53	1.79	7 (15%)
2	PX4	C	1303	-	42,42,45	1.73	5 (11%)	48,50,53	1.83	8 (16%)
2	PX4	C	1306	-	13,13,45	0.73	0	12,12,53	0.41	0
2	PX4	A	1306	-	40,40,45	1.63	6 (15%)	46,48,53	1.86	6 (13%)
2	PX4	B	1304	-	45,45,45	1.60	5 (11%)	51,53,53	1.62	6 (11%)
2	PX4	C	1302	-	40,40,45	1.63	4 (10%)	43,45,53	1.55	4 (9%)
2	PX4	D	1304	-	40,40,45	1.47	4 (10%)	43,45,53	1.63	4 (9%)
2	PX4	D	1301	-	20,20,45	1.67	2 (10%)	22,24,53	1.51	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PX4	A	1305	-	40,40,45	1.50	4 (10%)	43,45,53	1.49	4 (9%)
2	PX4	B	1305	-	13,13,45	0.77	0	12,12,53	0.40	0
2	PX4	C	1305	-	45,45,45	1.53	6 (13%)	51,53,53	1.76	5 (9%)
2	PX4	D	1305	-	45,45,45	1.66	5 (11%)	51,53,53	1.55	5 (9%)
2	PX4	A	1301	-	20,20,45	1.58	2 (10%)	22,24,53	1.66	2 (9%)
2	PX4	B	1301	-	20,20,45	1.63	2 (10%)	22,24,53	1.53	2 (9%)
2	PX4	C	1301	-	20,20,45	1.60	2 (10%)	22,24,53	1.51	2 (9%)
2	PX4	B	1306	-	13,13,45	0.78	0	12,12,53	0.43	0
2	PX4	C	1304	-	41,41,45	1.73	5 (12%)	47,49,53	1.62	5 (10%)

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	1302	-	-	21/44/44/49	-
2	PX4	D	1306	-	-	3/11/11/49	-
2	PX4	A	1307	-	-	30/49/49/49	-
2	PX4	B	1303	-	-	21/43/43/49	-
2	PX4	C	1303	-	-	27/46/46/49	-
2	PX4	C	1306	-	-	8/11/11/49	-
2	PX4	A	1306	-	-	25/44/44/49	-
2	PX4	B	1304	-	-	23/49/49/49	-
2	PX4	C	1302	-	-	20/44/44/49	-
2	PX4	D	1304	-	-	23/44/44/49	-
2	PX4	D	1301	-	-	9/22/22/49	-
2	PX4	A	1305	-	-	23/44/44/49	-
2	PX4	B	1305	-	-	3/11/11/49	-
2	PX4	C	1305	-	-	22/49/49/49	-
2	PX4	D	1305	-	-	27/49/49/49	-
2	PX4	A	1301	-	-	11/22/22/49	-
2	PX4	B	1301	-	-	10/22/22/49	-
2	PX4	C	1301	-	-	13/22/22/49	-
2	PX4	B	1306	-	-	4/11/11/49	-
2	PX4	C	1304	-	-	22/45/45/49	-

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	PX4	O6-C9	6.52	1.41	1.22
2	B	1303	PX4	O8-C23	6.52	1.41	1.22
2	C	1303	PX4	O6-C9	6.29	1.41	1.22
2	B	1301	PX4	O6-C9	6.26	1.41	1.22
2	C	1301	PX4	O6-C9	6.25	1.41	1.22

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1305	PX4	O5-C9-O6	-7.14	105.57	123.59
2	C	1303	PX4	O5-C9-O6	-7.09	105.71	123.59
2	B	1302	PX4	O5-C9-O6	-6.89	106.21	123.59
2	B	1302	PX4	O7-C23-O8	-6.61	107.73	123.70
2	A	1306	PX4	O5-C9-O6	-6.36	107.53	123.59

There are no chirality outliers.

5 of 345 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1307	PX4	C1-O3-P1-O1
2	A	1307	PX4	C1-O3-P1-O2
2	A	1307	PX4	C6-O4-P1-O1
2	A	1307	PX4	O3-C1-C2-N1
2	A	1307	PX4	O8-C23-O7-C7

There are no ring outliers.

17 monomers are involved in 80 short contacts:

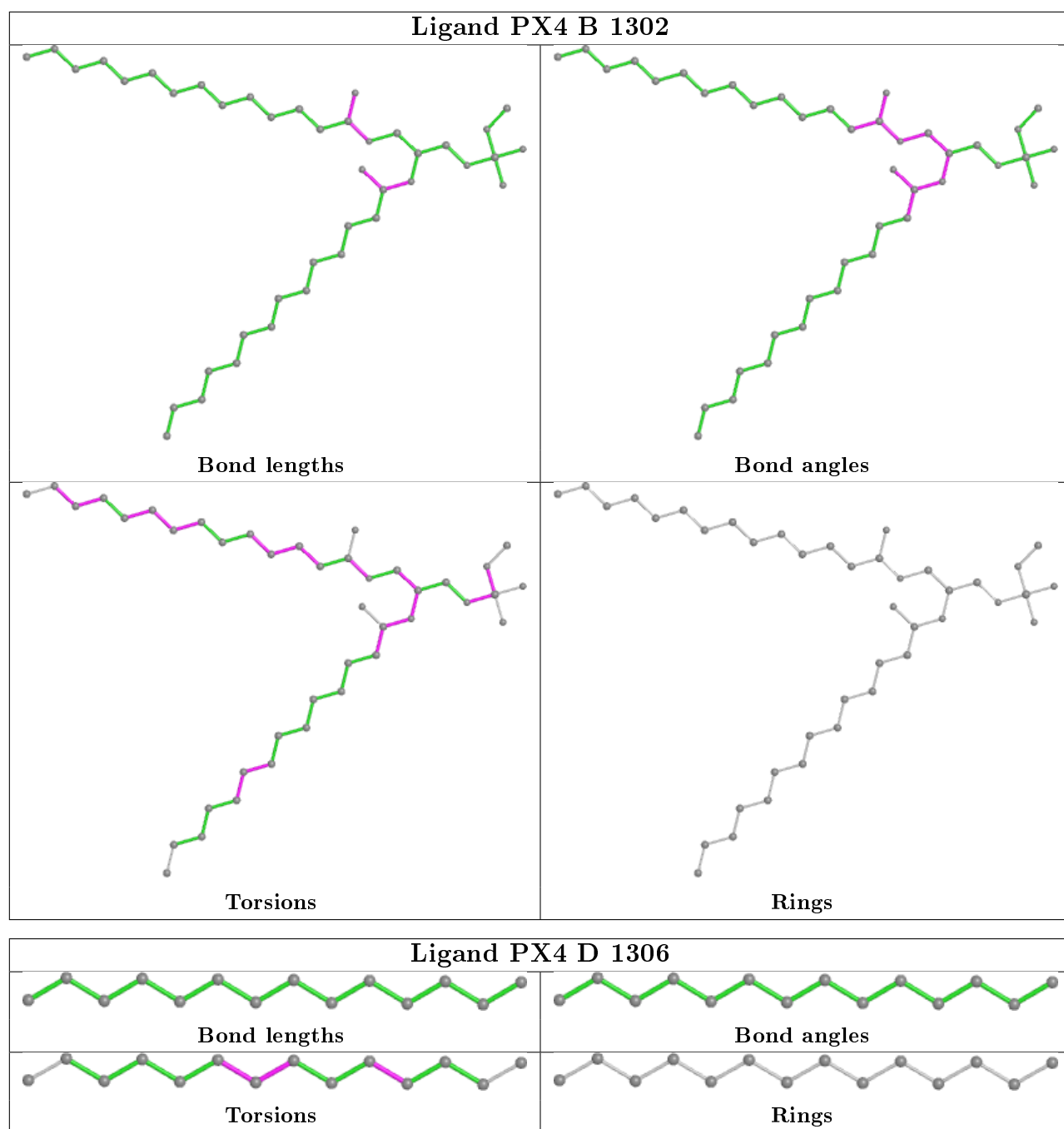
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1302	PX4	8	0
2	D	1306	PX4	2	0
2	A	1307	PX4	6	0
2	B	1303	PX4	2	0
2	C	1303	PX4	7	0
2	C	1306	PX4	3	0
2	A	1306	PX4	11	0
2	B	1304	PX4	5	0
2	C	1302	PX4	2	0
2	D	1304	PX4	11	0
2	A	1305	PX4	5	0

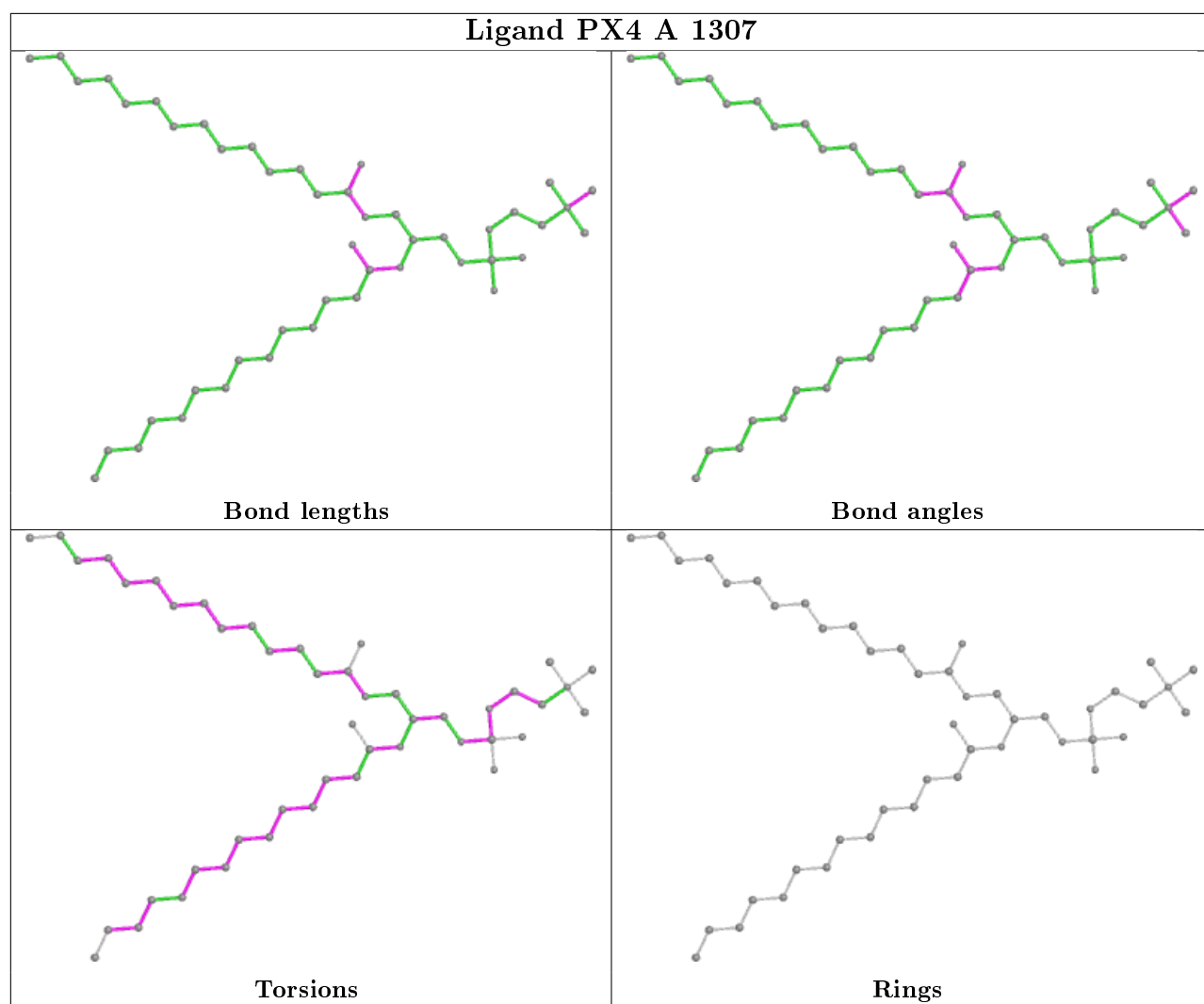
Continued on next page...

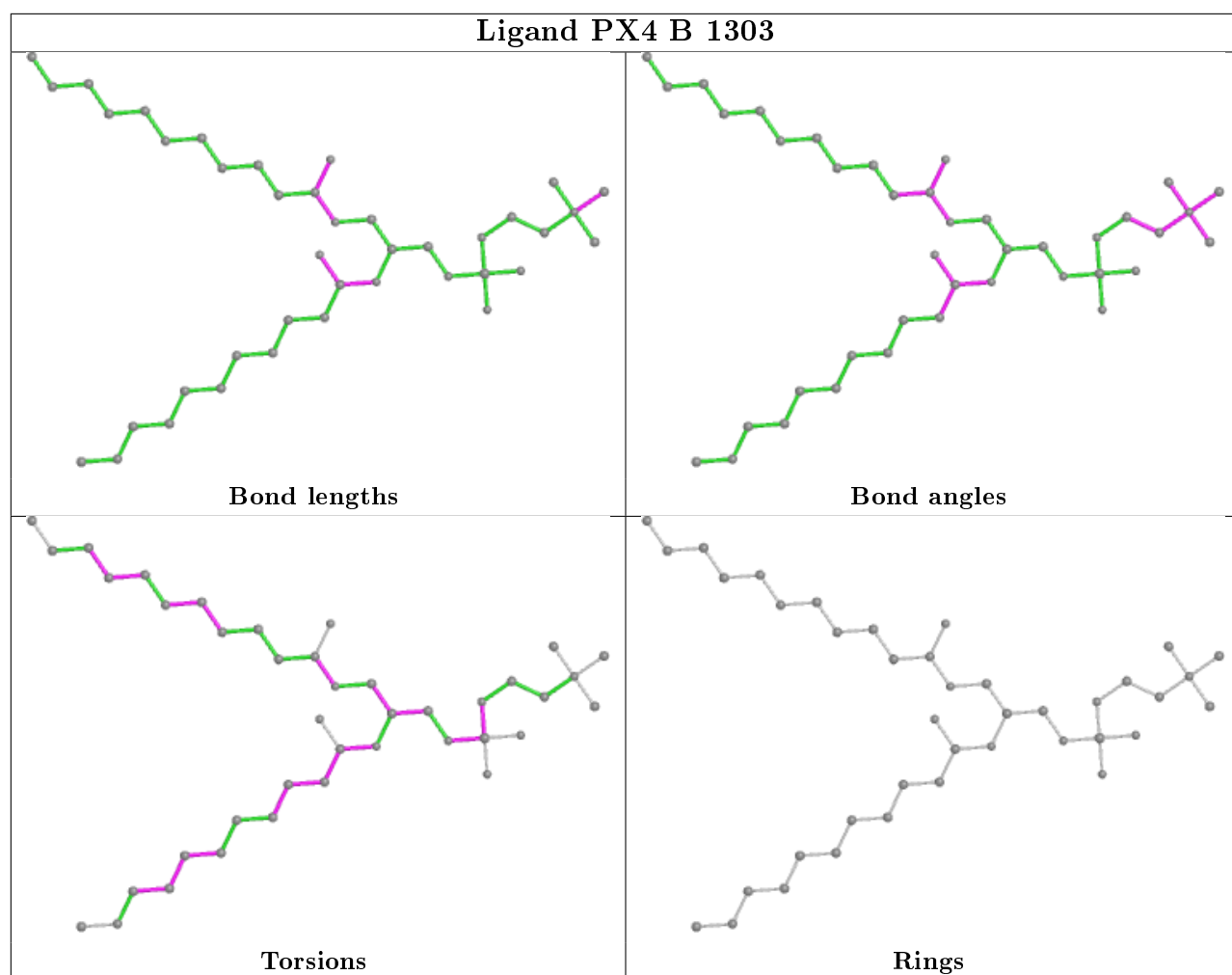
Continued from previous page...

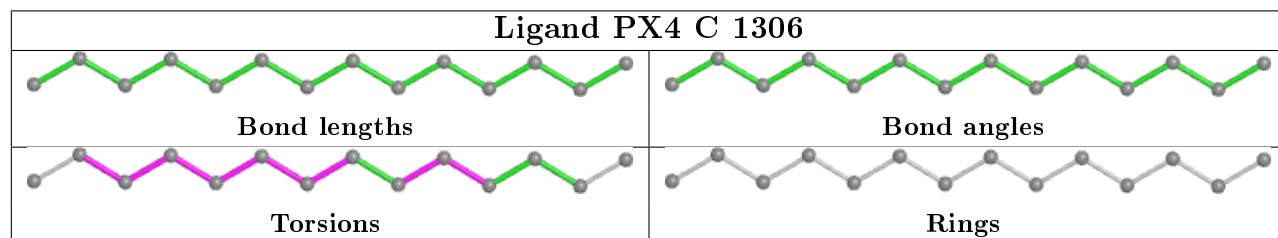
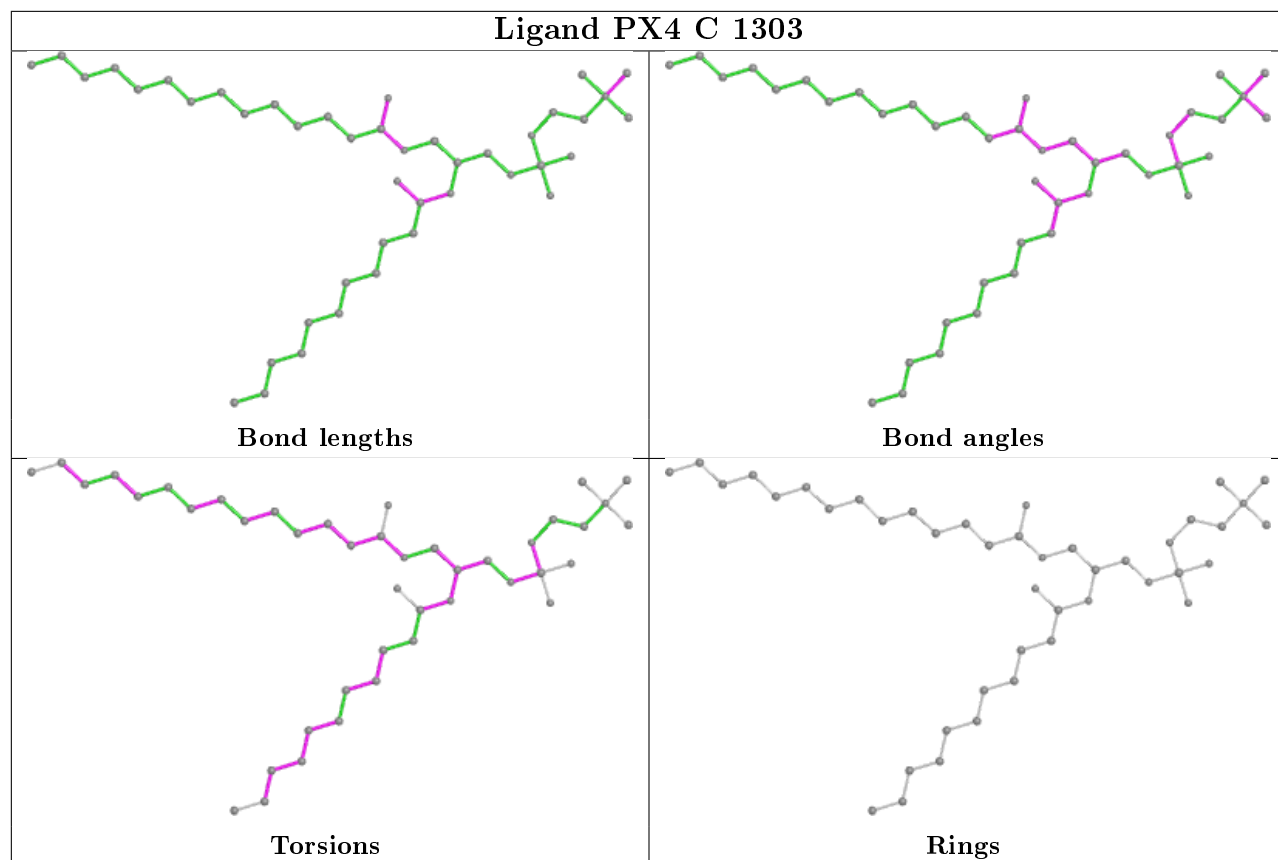
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1305	PX4	3	0
2	C	1305	PX4	8	0
2	D	1305	PX4	9	0
2	A	1301	PX4	2	0
2	B	1306	PX4	3	0
2	C	1304	PX4	5	0

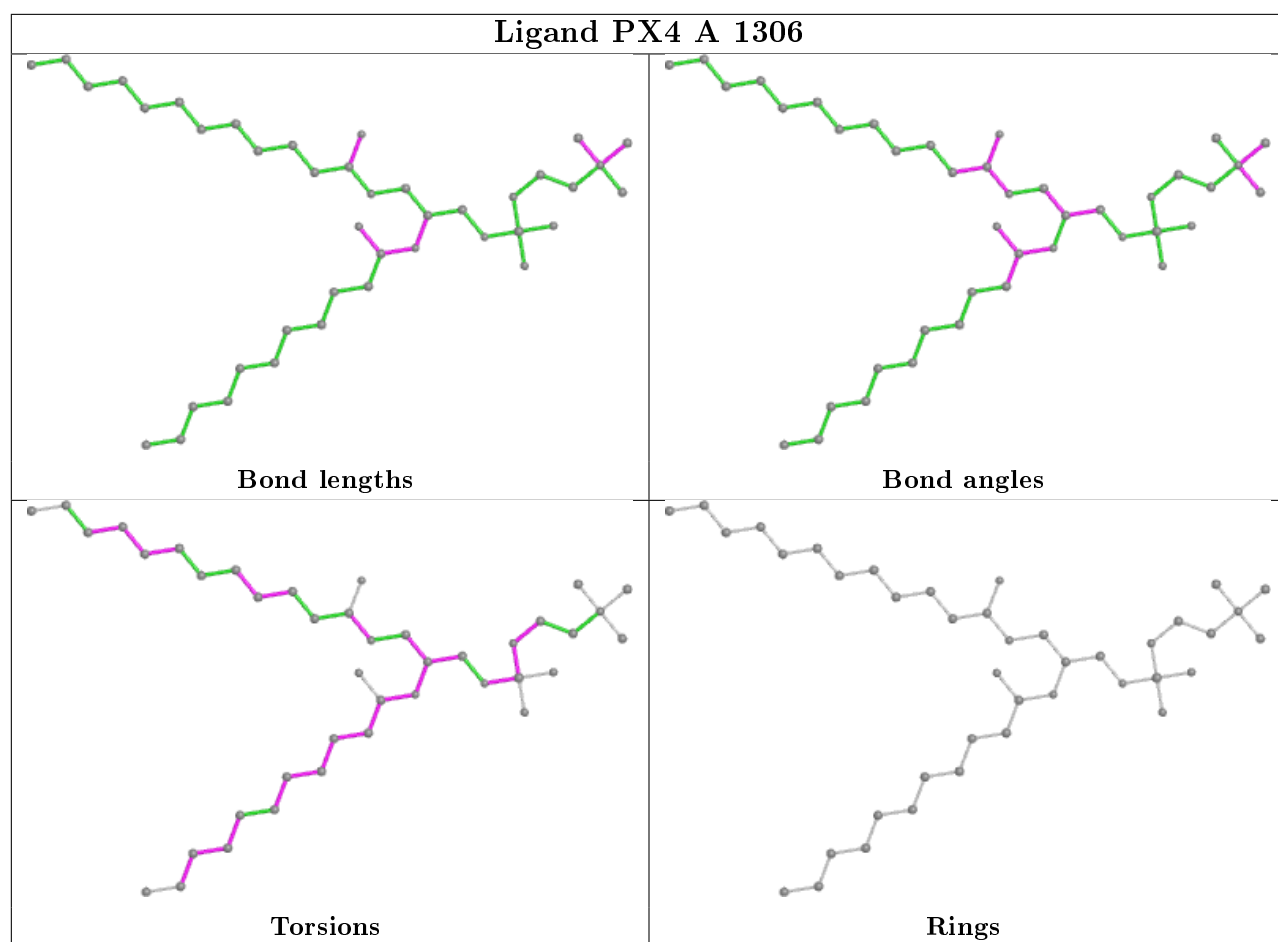
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

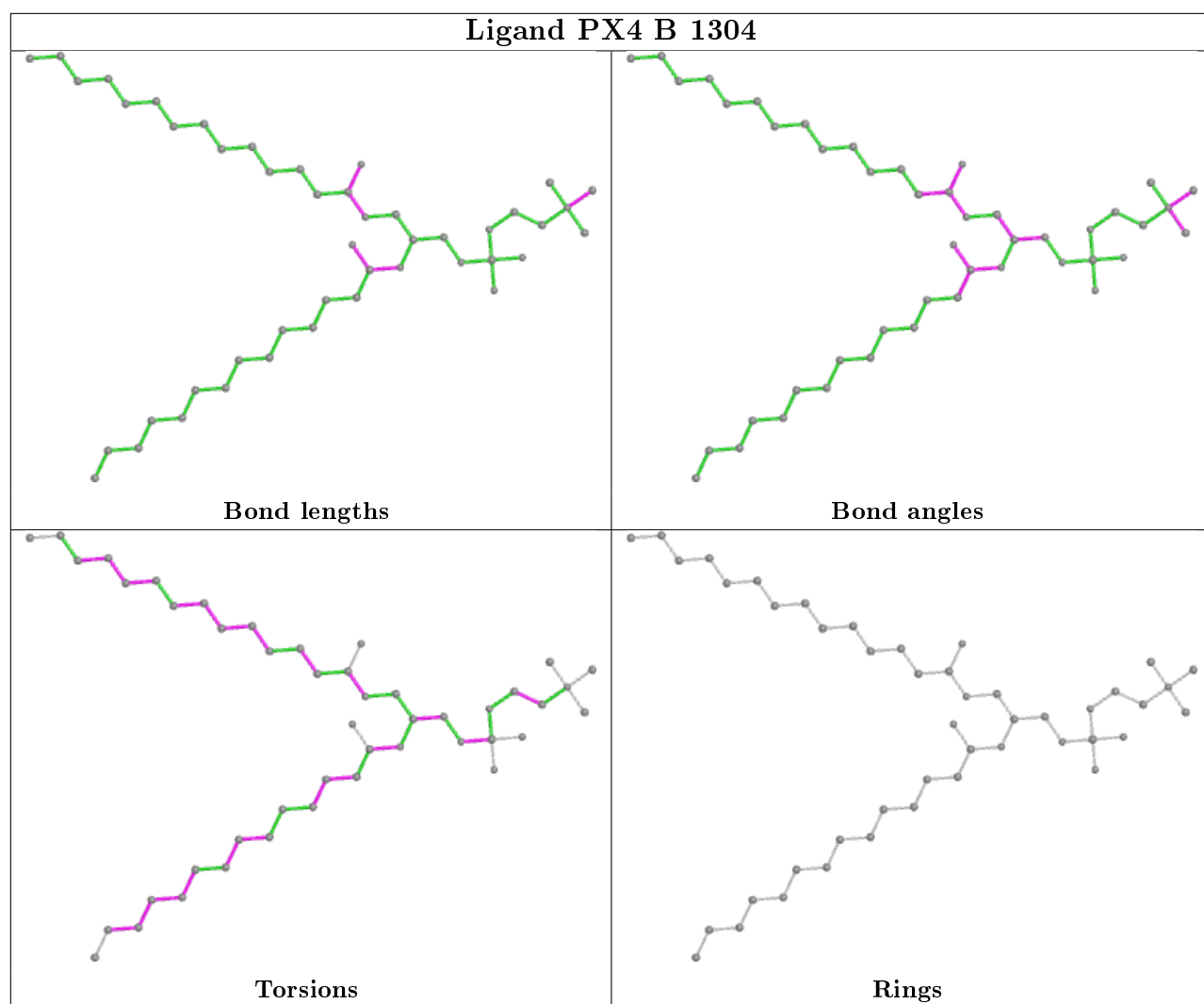


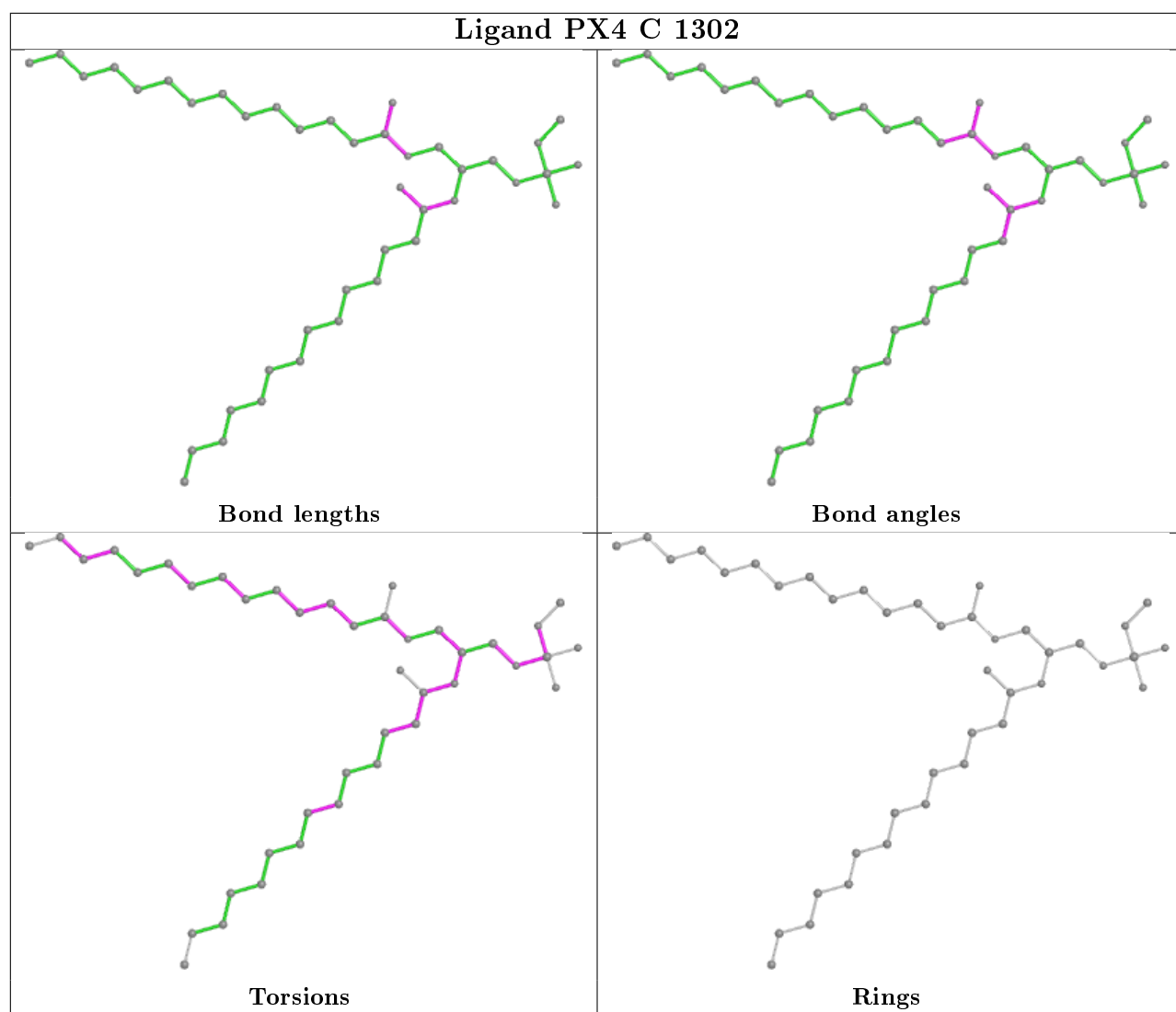


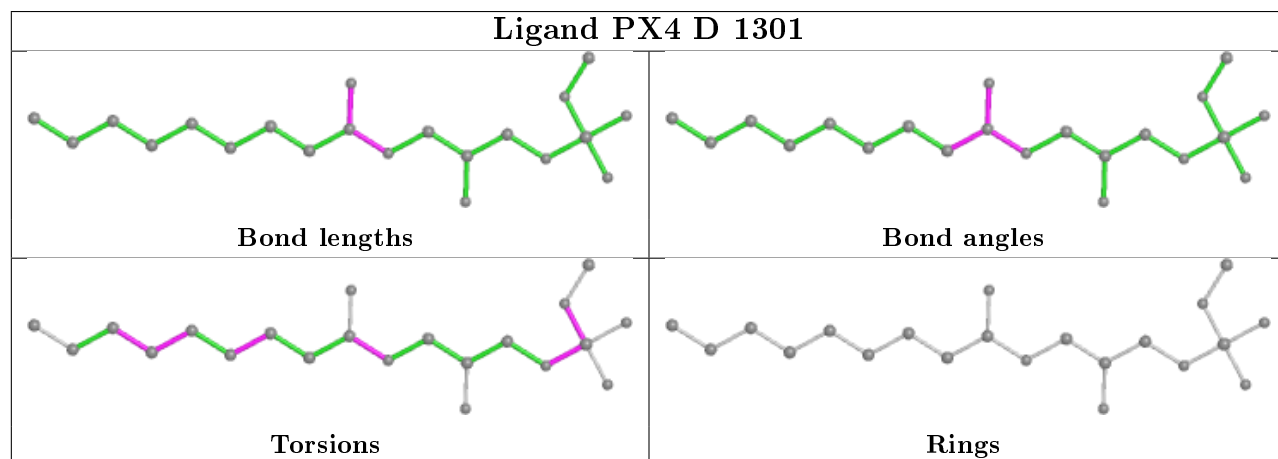
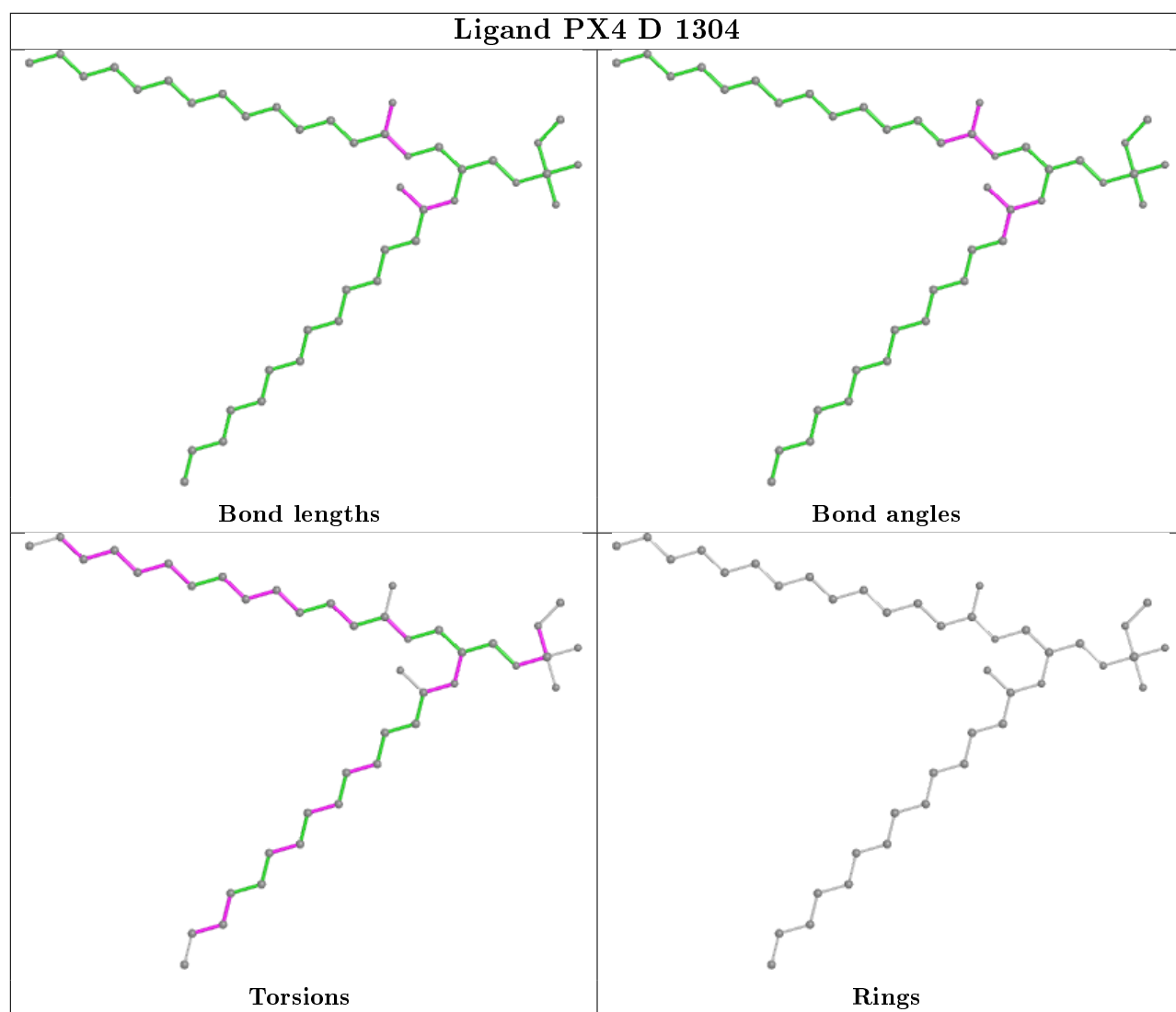


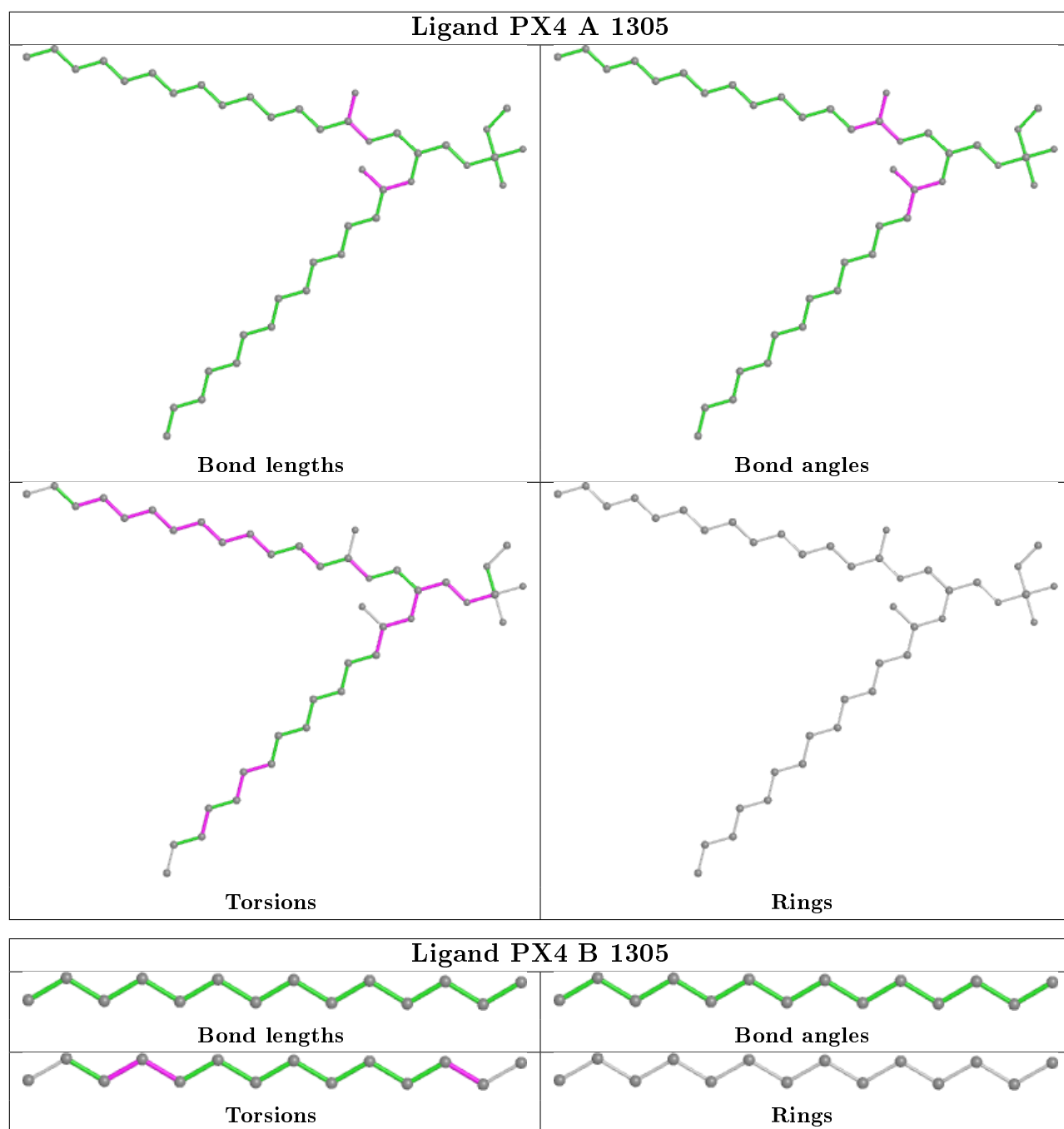


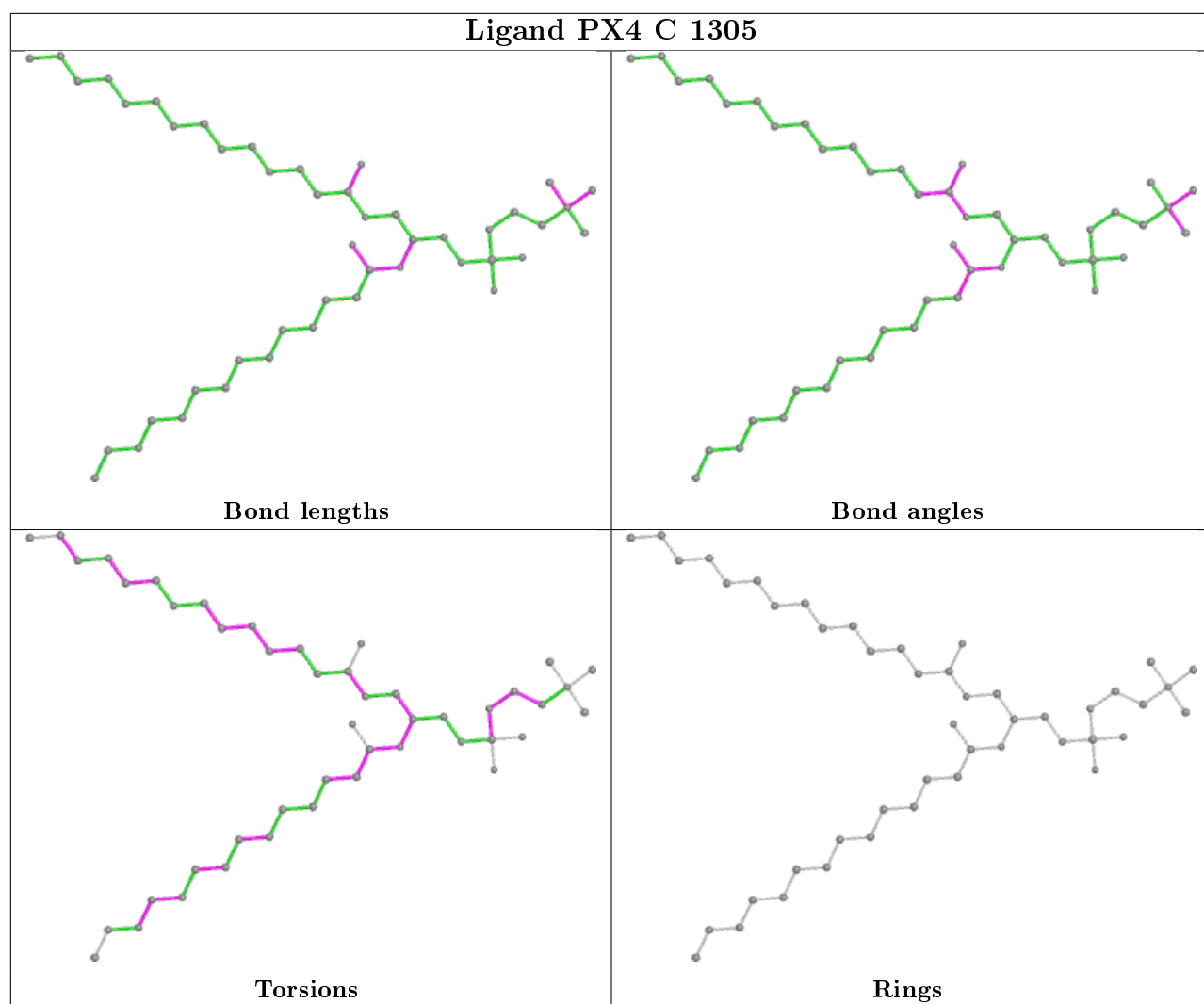


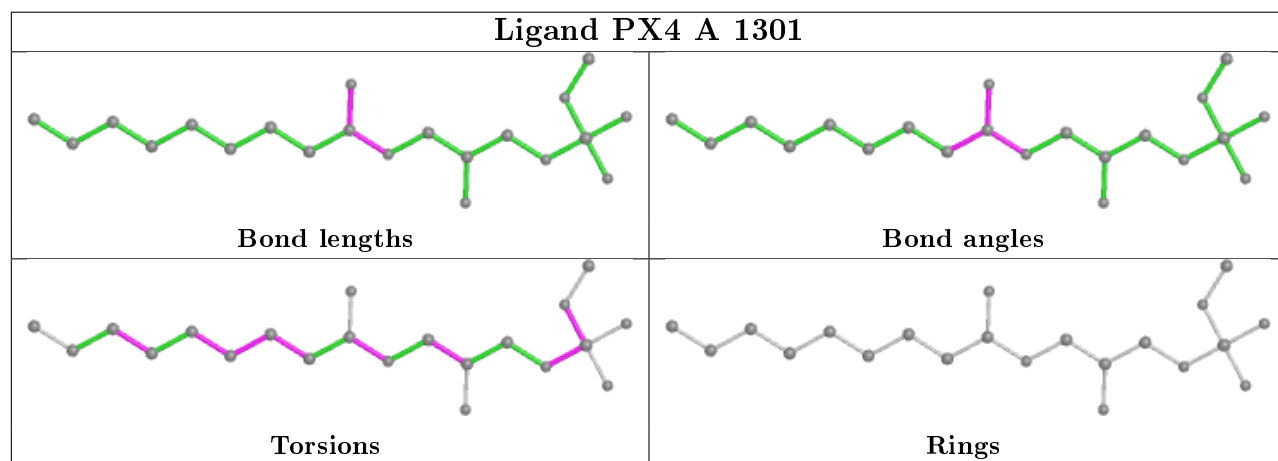
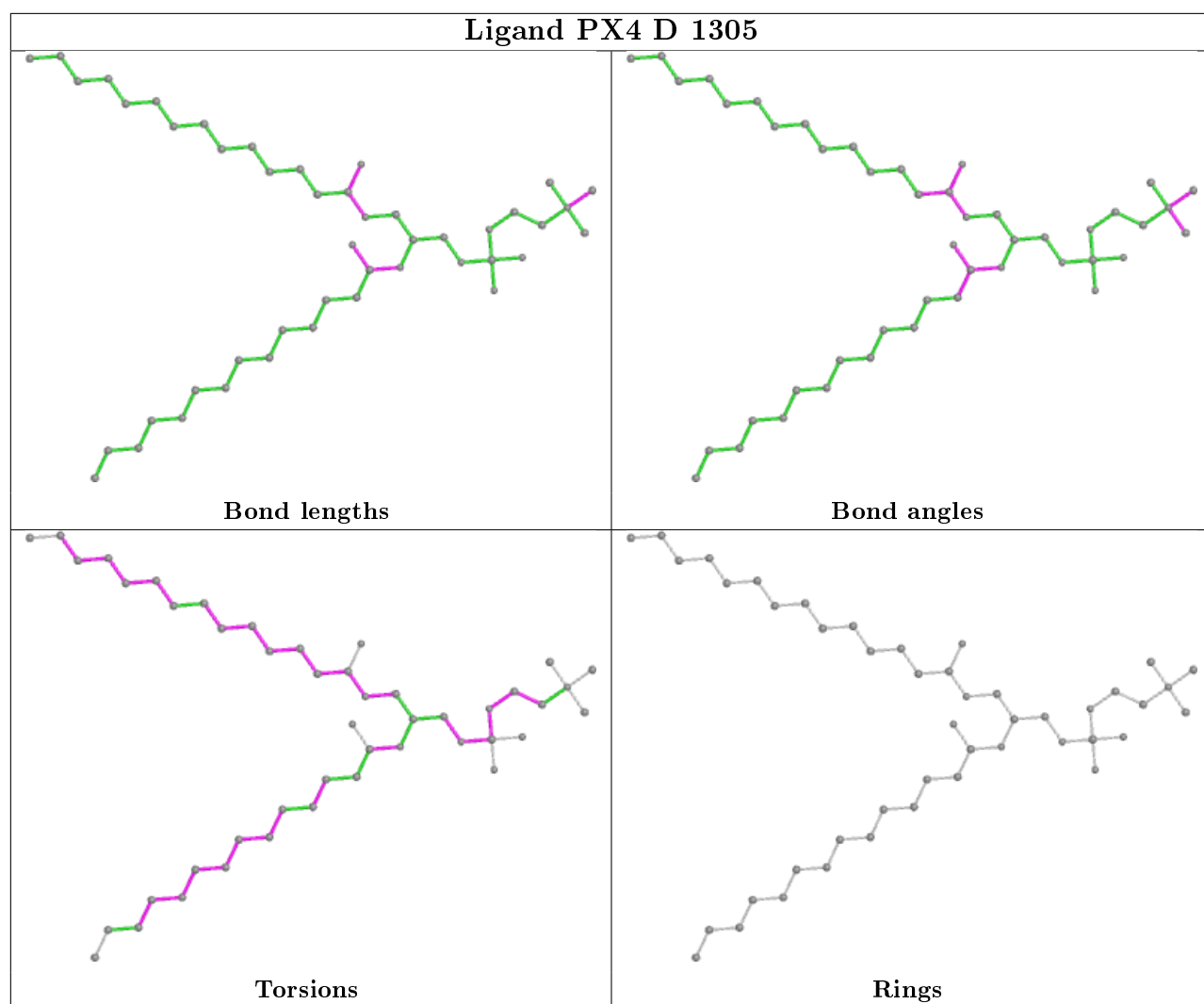


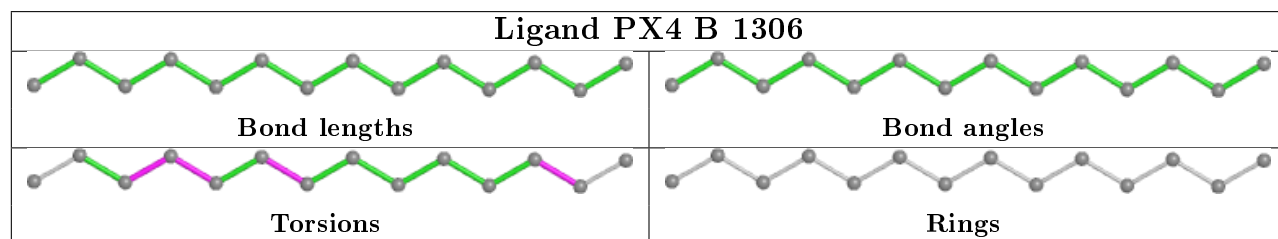
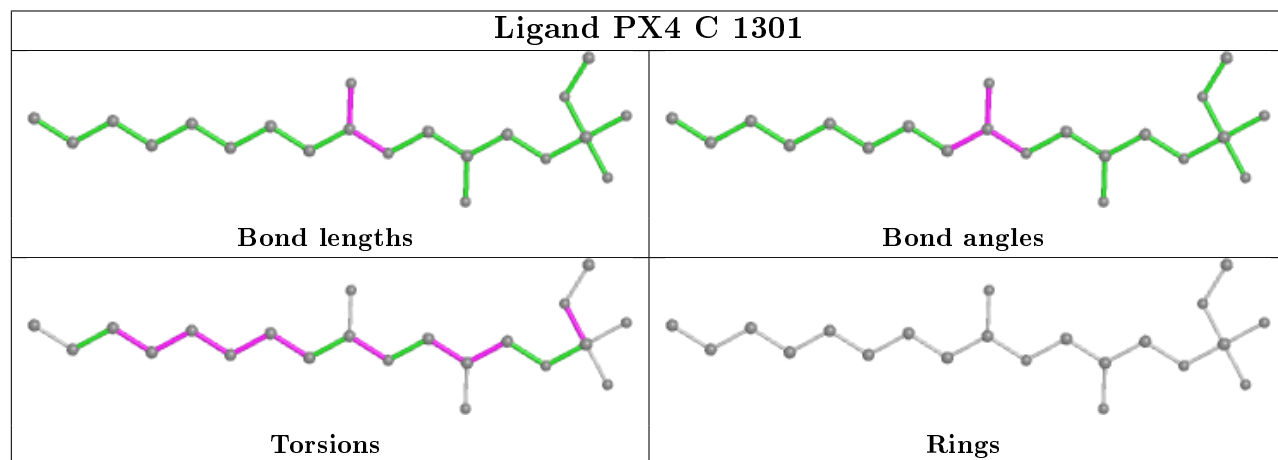
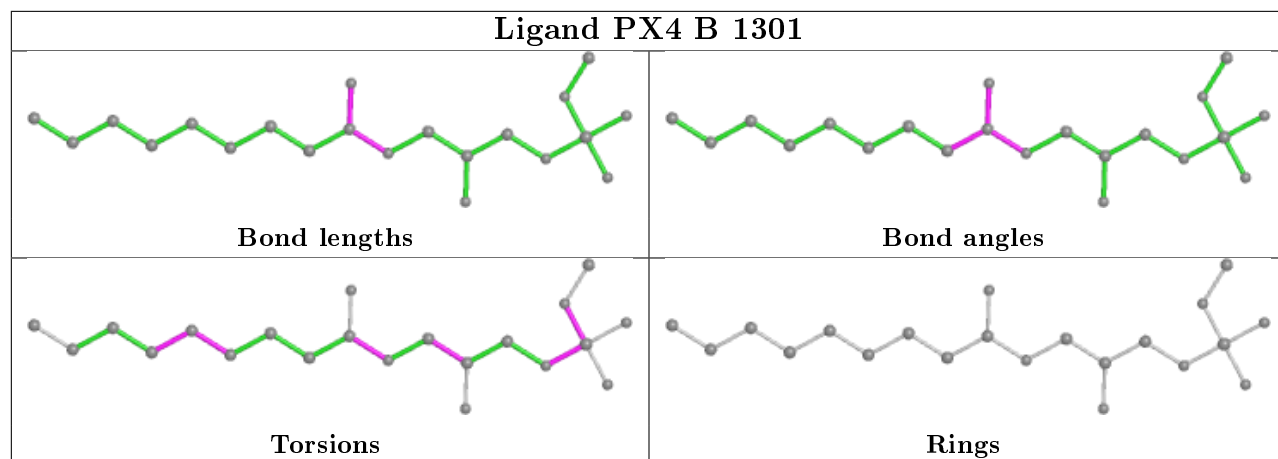


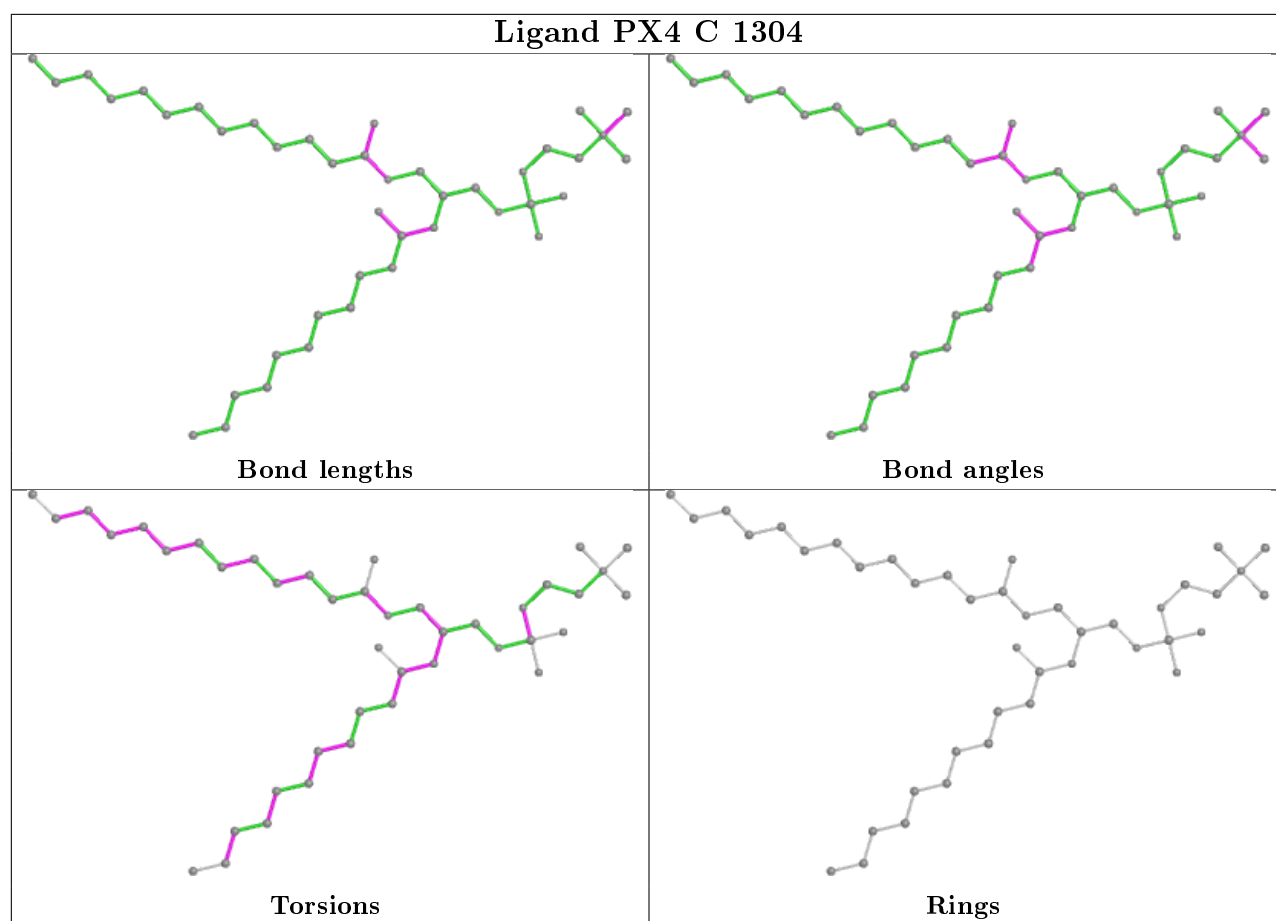












5.7 Other polymers [i](#)

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, 95th 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	219/237 (92%)	0.39	9 (4%) 37 44	29, 77, 112, 139	0
1	B	219/237 (92%)	0.37	5 (2%) 60 69	30, 76, 115, 135	0
1	C	219/237 (92%)	0.35	3 (1%) 75 82	28, 76, 112, 143	0
1	D	219/237 (92%)	0.36	8 (3%) 41 49	30, 78, 116, 137	0
All	All	876/948 (92%)	0.37	25 (2%) 51 61	28, 77, 115, 143	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1095	PHE	5.4
1	C	1065	TYR	4.2
1	D	1069	ILE	4.1
1	A	1020	TYR	3.6
1	D	1065	TYR	3.6

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](#)

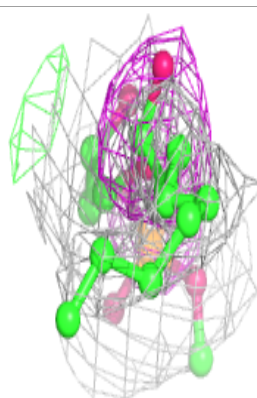
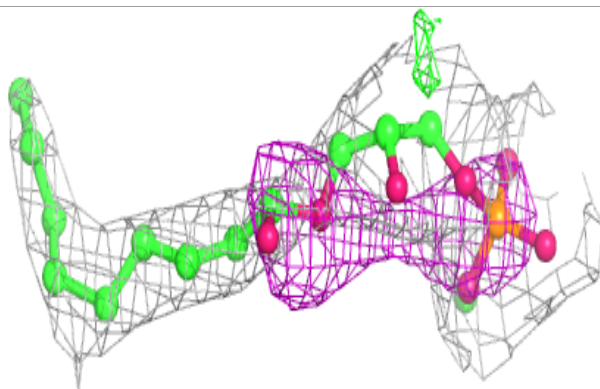
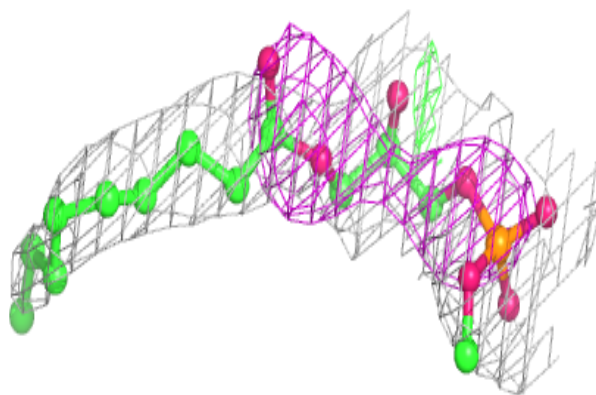
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	A	1303	1/1	0.59	0.34	81,81,81,81	0
3	CA	D	1303	1/1	0.71	0.52	113,113,113,113	0
3	CA	A	1304	1/1	0.73	1.15	99,99,99,99	0
2	PX4	C	1301	21/46	0.76	0.38	74,94,111,124	0
2	PX4	B	1305	14/46	0.77	0.32	47,65,74,79	0
2	PX4	B	1301	21/46	0.77	0.43	74,95,112,122	0
2	PX4	A	1301	21/46	0.78	0.34	68,96,111,120	0
2	PX4	D	1306	14/46	0.80	0.26	47,70,75,79	0
2	PX4	D	1301	21/46	0.81	0.41	79,99,116,123	0
2	PX4	C	1306	14/46	0.81	0.20	47,63,75,77	0
2	PX4	B	1306	14/46	0.81	0.29	51,62,82,83	0
3	CA	D	1302	1/1	0.83	0.09	59,59,59,59	0
2	PX4	A	1307	46/46	0.87	0.36	55,73,86,94	0
2	PX4	B	1302	41/46	0.89	0.29	64,75,94,105	0
2	PX4	D	1305	46/46	0.89	0.39	56,75,91,109	0
2	PX4	B	1304	46/46	0.90	0.34	53,72,82,91	0
2	PX4	C	1305	46/46	0.91	0.32	57,73,85,96	0
2	PX4	D	1304	41/46	0.92	0.26	62,74,90,100	0
2	PX4	C	1302	41/46	0.92	0.33	60,74,93,109	0
2	PX4	C	1303	43/46	0.93	0.22	48,71,76,84	0
2	PX4	B	1303	40/46	0.94	0.23	44,68,76,78	0
2	PX4	C	1304	42/46	0.94	0.26	49,68,79,83	0
2	PX4	A	1306	41/46	0.95	0.22	44,69,78,81	0
2	PX4	A	1305	41/46	0.95	0.30	62,76,92,101	0
3	CA	A	1302	1/1	0.95	0.11	63,63,63,63	0

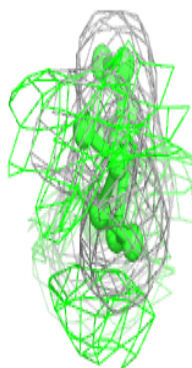
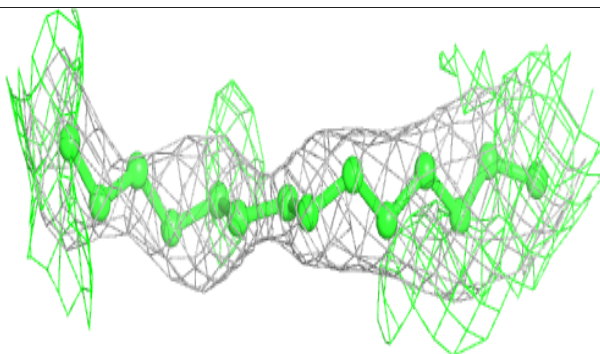
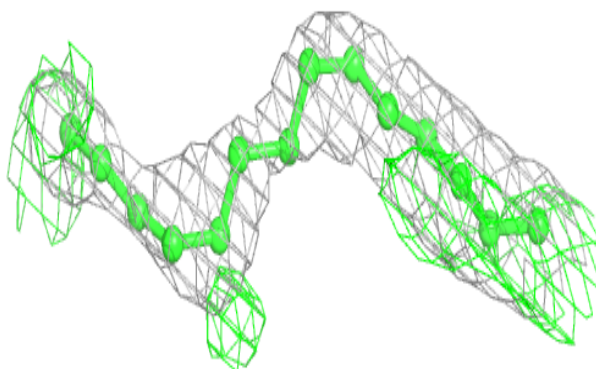
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PX4 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)

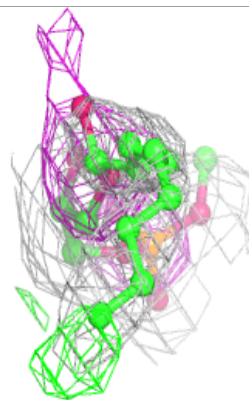
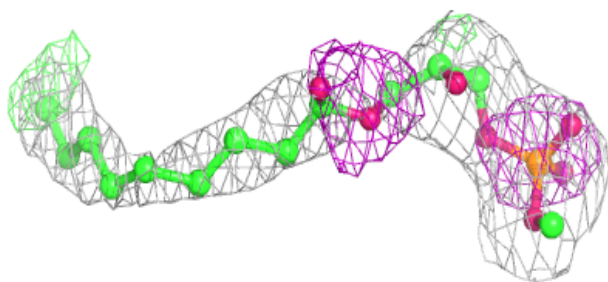
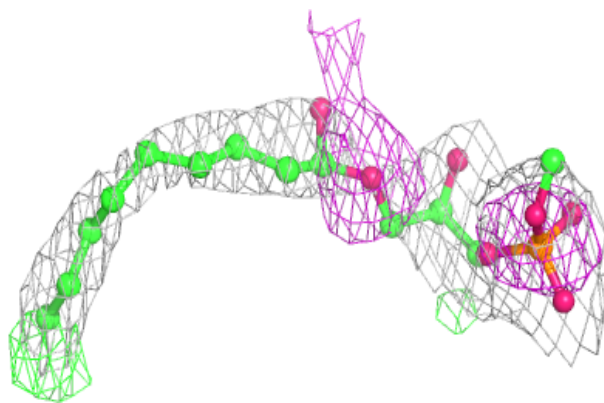
**Electron density around PX4 B 1305:**

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

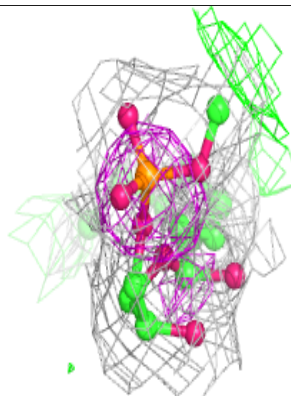
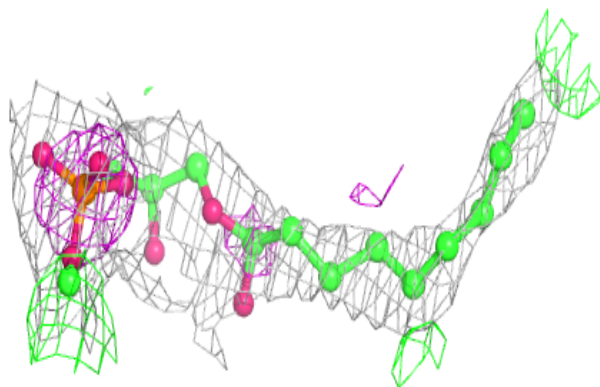
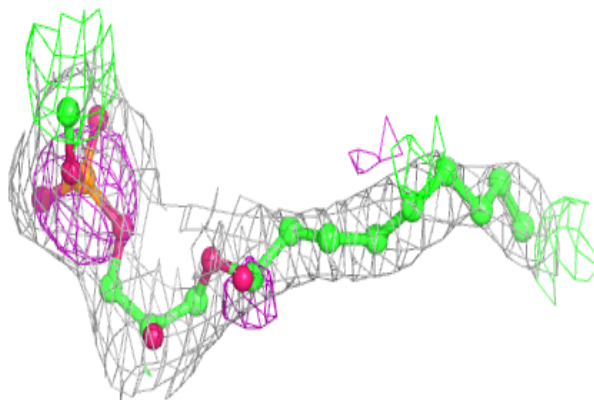


Electron density around PX4 B 1301:

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

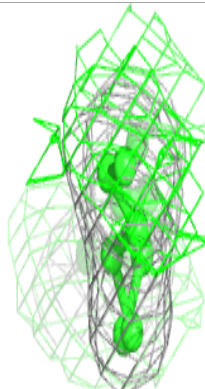
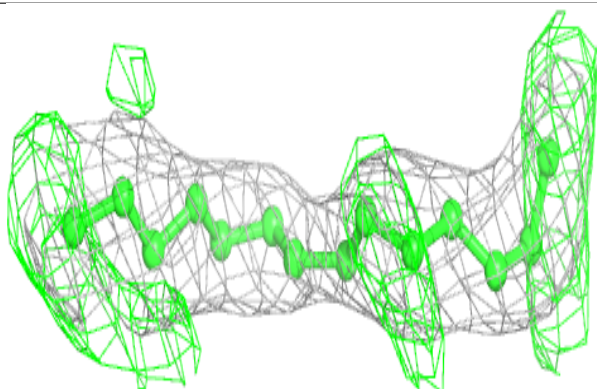
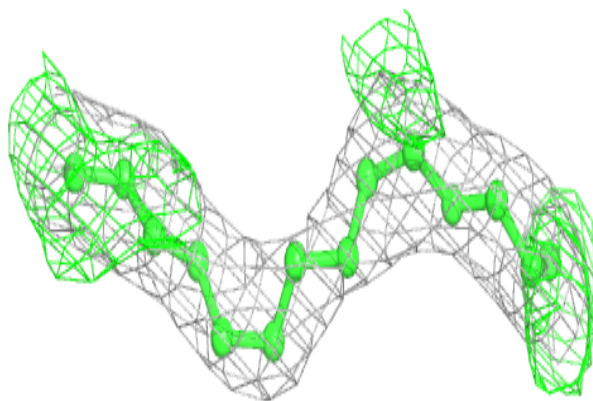
**Electron density around PX4 A 1301:**

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

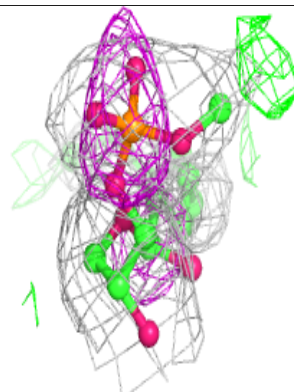
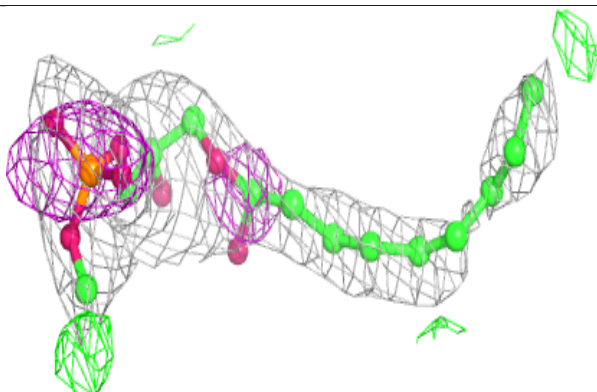
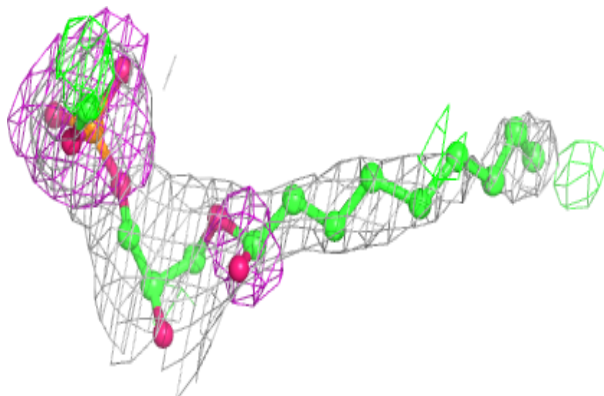


Electron density around PX4 D 1306:

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

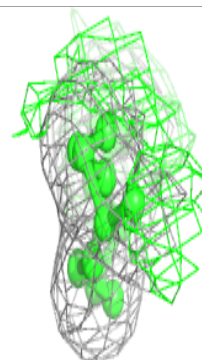
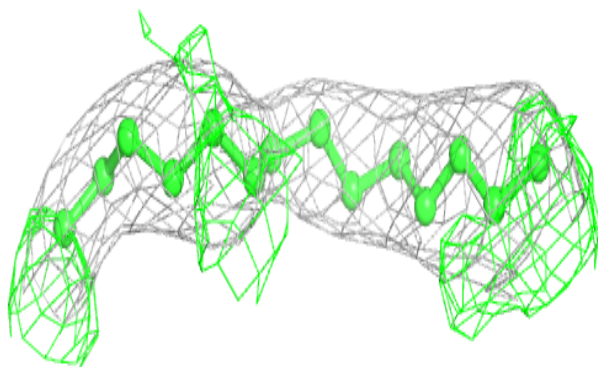
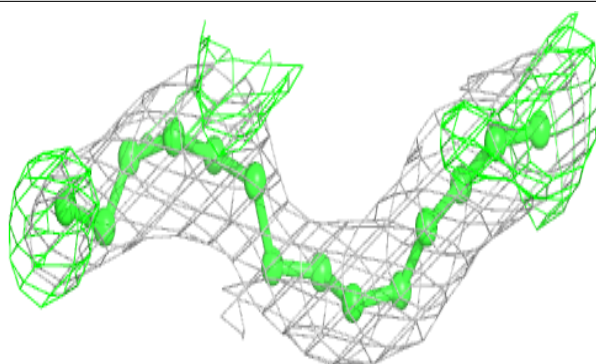
**Electron density around PX4 D 1301:**

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

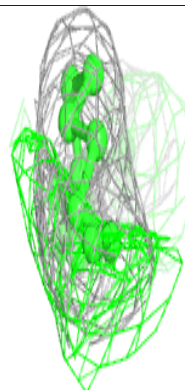
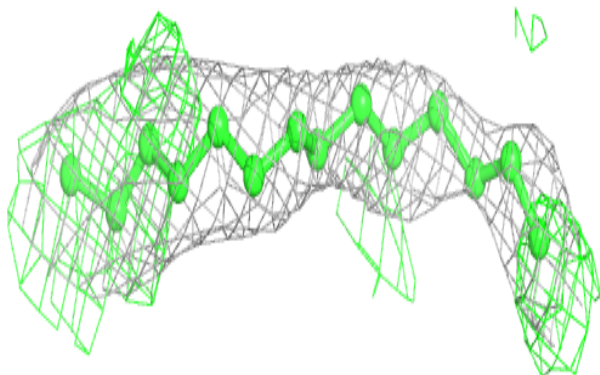
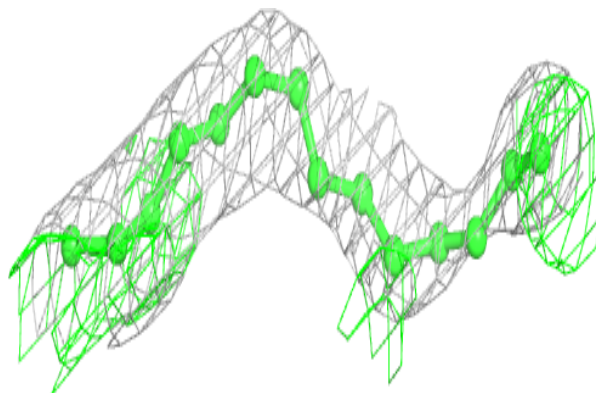


Electron density around PX4 C 1306:

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

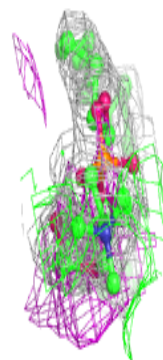
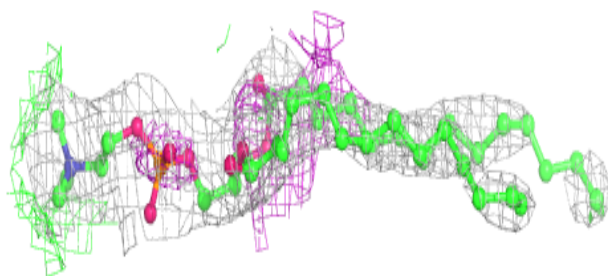
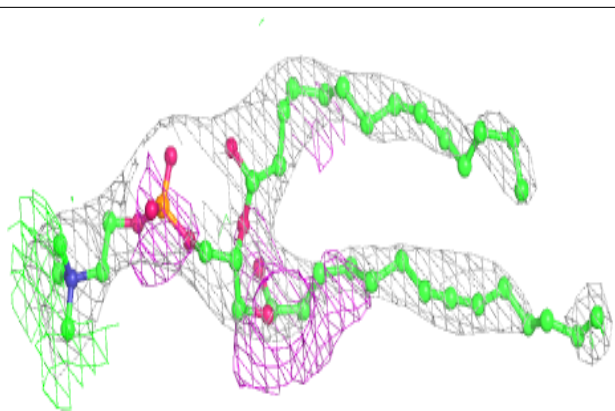
**Electron density around PX4 B 1306:**

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

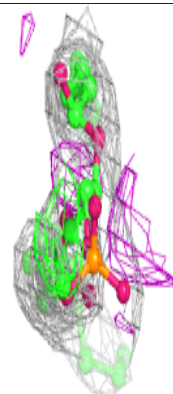
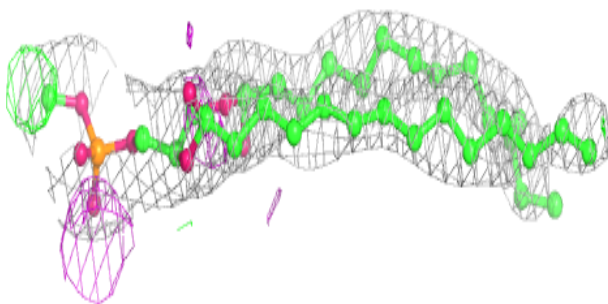
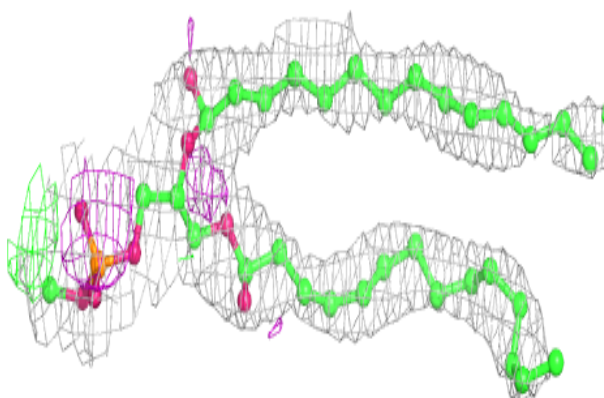


Electron density around PX4 A 1307:

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

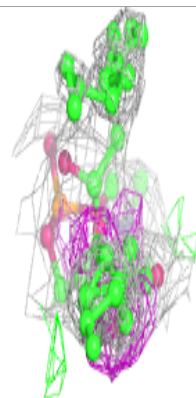
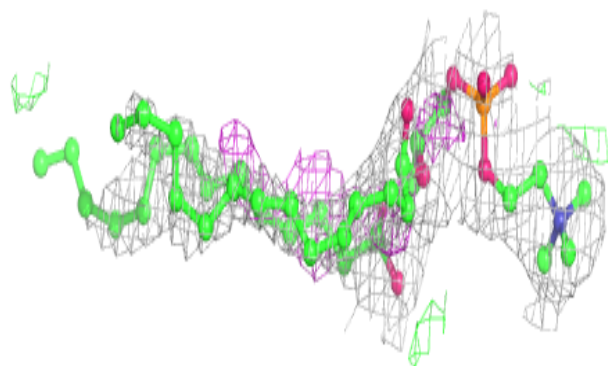
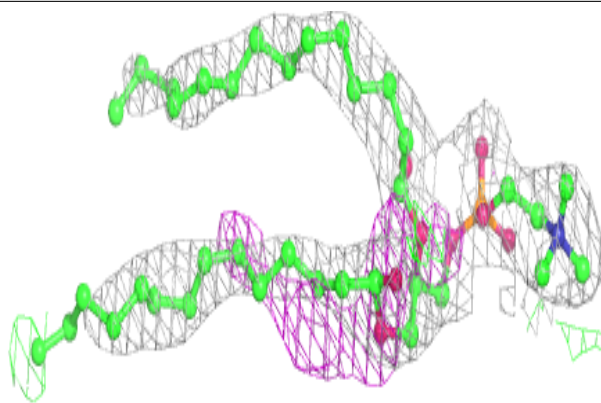
**Electron density around PX4 B 1302:**

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

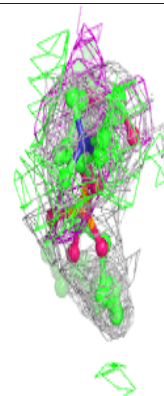
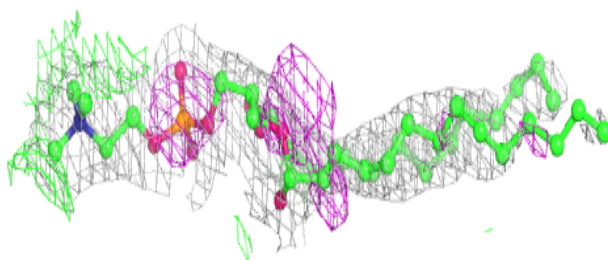
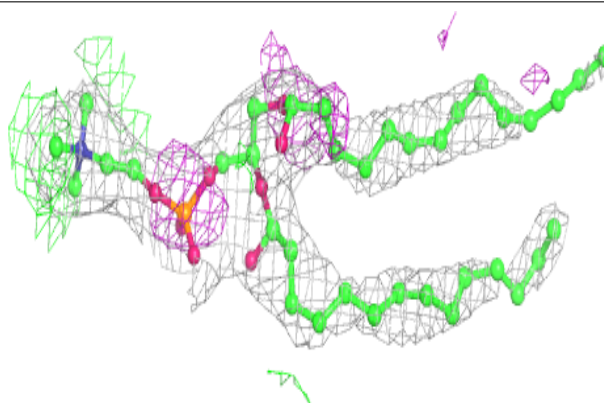


Electron density around PX4 D 1305:

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

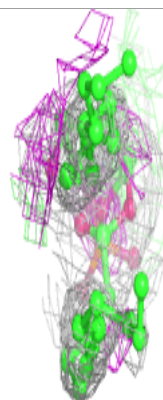
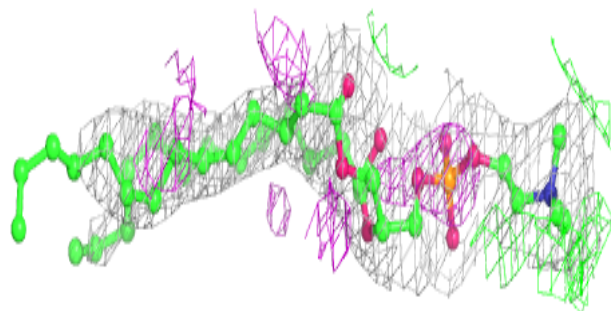
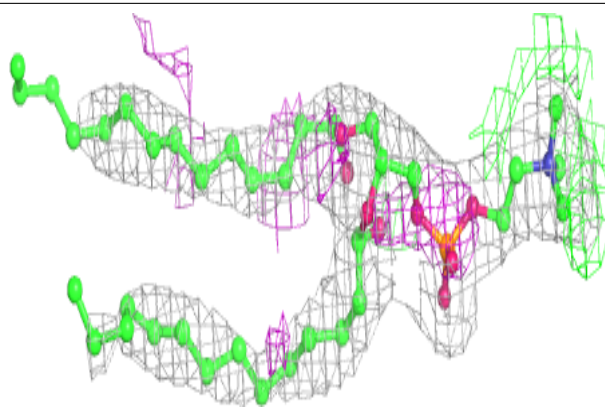
**Electron density around PX4 B 1304:**

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

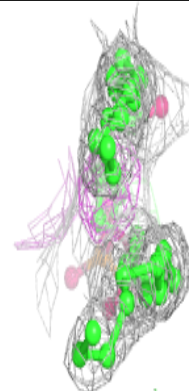
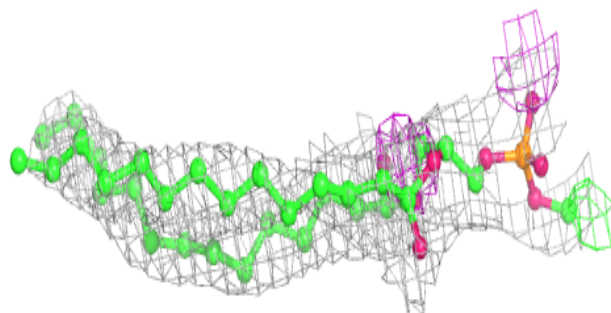
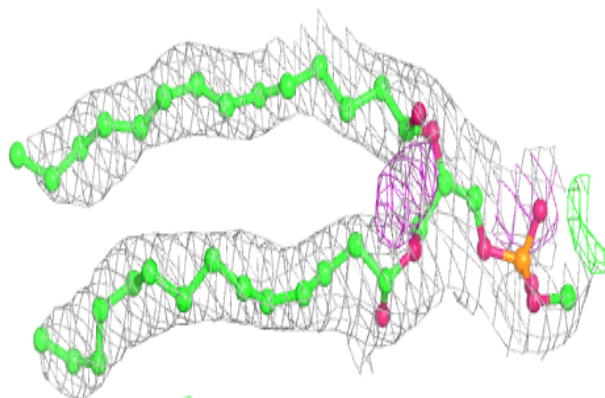


Electron density around PX4 C 1305:

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

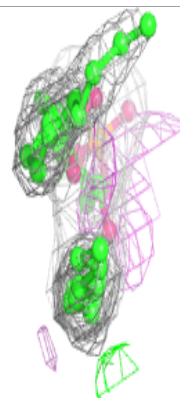
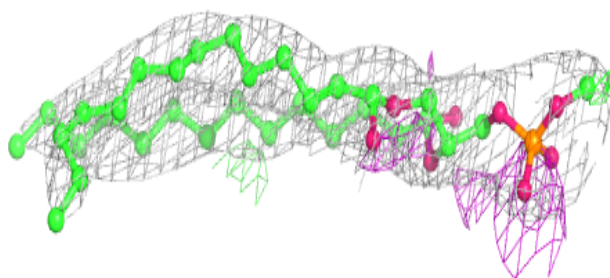
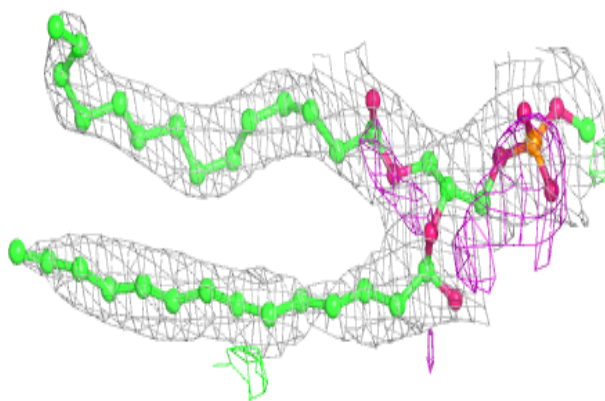
**Electron density around PX4 D 1304:**

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

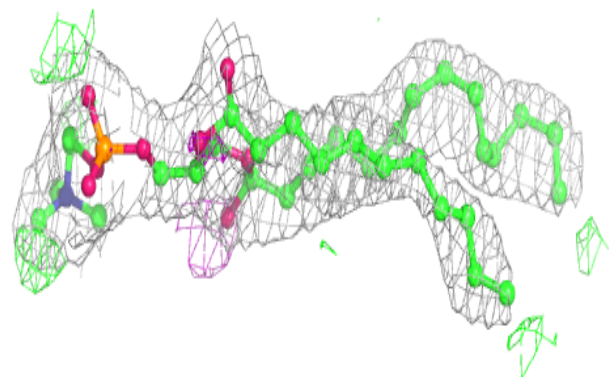
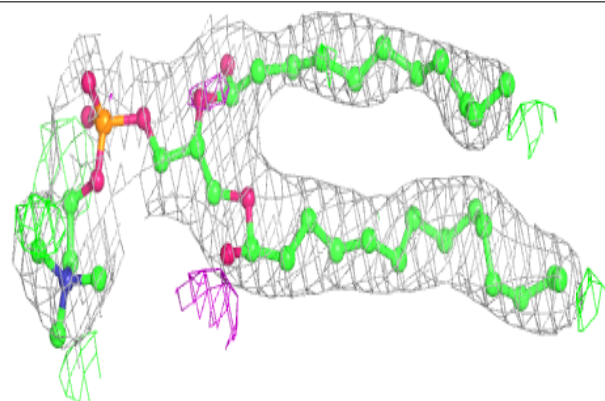


Electron density around PX4 C 1302:

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

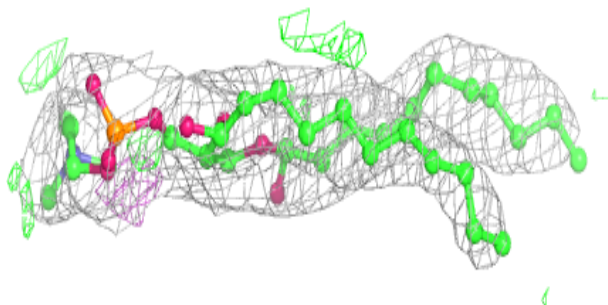
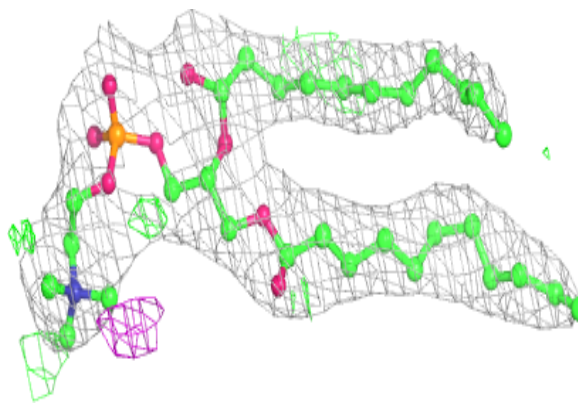
**Electron density around PX4 C 1303:**

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

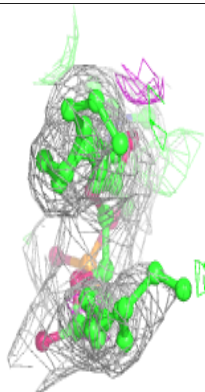
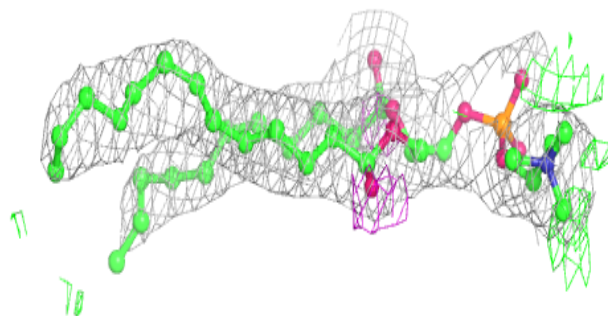
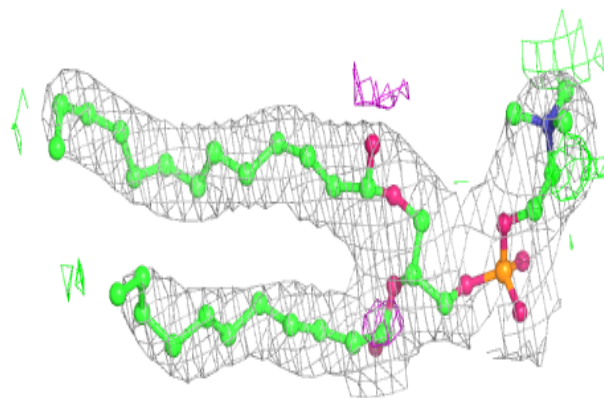


Electron density around PX4 B 1303:

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

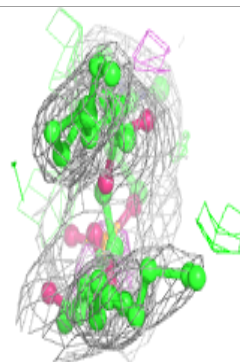
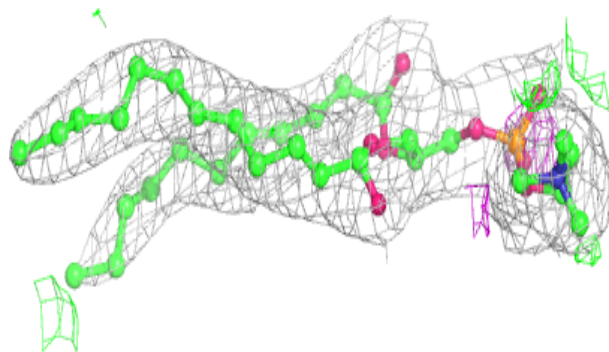
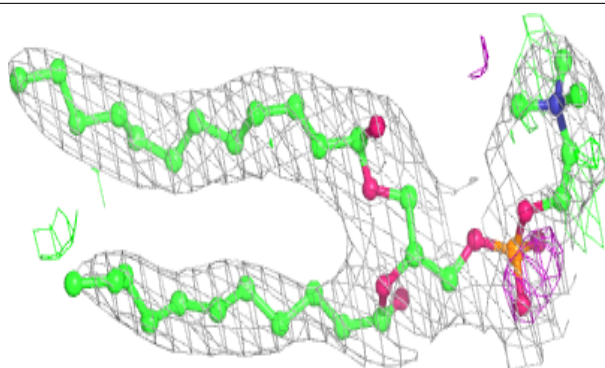
**Electron density around PX4 C 1304:**

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

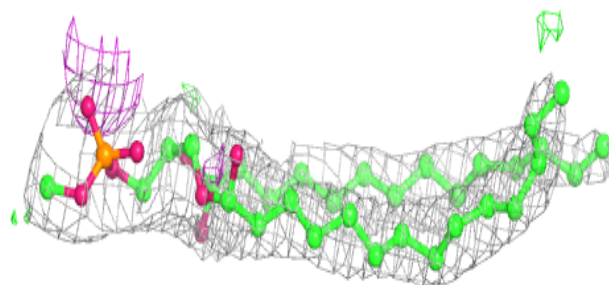
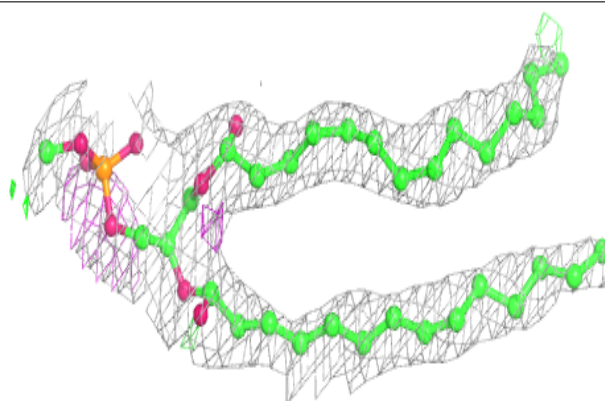


Electron density around PX4 A 1306:

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

**Electron density around PX4 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.