



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:07 am BST

PDB ID : 6P6X
Title : Crystal structure of voltage-gated sodium channel NavAb G94C/Q150C mutant in the activated state
Authors : Wisedchaisri, G.; Tonggu, L.; McCord, E.; Gamal El-Din, T.M.; Wang, L.; Zheng, N.; Catterall, W.A.
Deposited on : 2019-06-04
Resolution : 2.75 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 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 : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

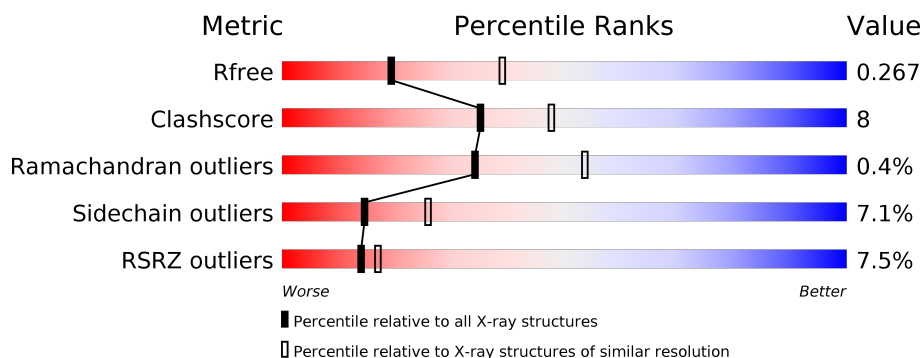
1 Overall quality at a glance

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	257	

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	A	2007	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2167 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.

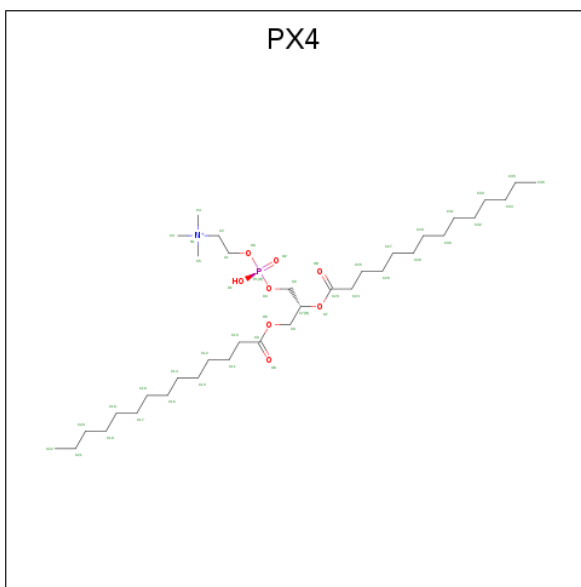
- Molecule 1 is a protein called Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	1	0
			1825	1238	277	297	13			

There are 20 discrepancies between the modelled and reference sequences:

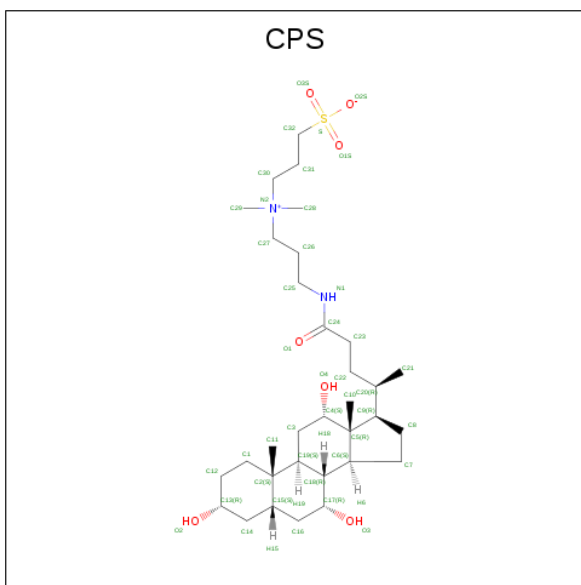
Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	initiating methionine	UNP A8EVM5
A	984	ASP	-	expression tag	UNP A8EVM5
A	985	TYR	-	expression tag	UNP A8EVM5
A	986	LYS	-	expression tag	UNP A8EVM5
A	987	ASP	-	expression tag	UNP A8EVM5
A	988	ASP	-	expression tag	UNP A8EVM5
A	989	ASP	-	expression 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	1094	CYS	GLY	engineered mutation	UNP A8EVM5
A	1150	CYS	GLN	engineered mutation	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	C	N	O	P	0	0
			44	34	1	8	1		
2	A	1	Total	C	O	P		0	0
			42	33	8	1			
2	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
2	A	1	Total	C	O	P		0	0
			40	31	8	1			
2	A	1	Total	C	N	O	P	0	0
			36	26	1	8	1		
2	A	1	Total	C	O	P		0	0
			32	23	8	1			
2	A	1	Total	C	O	P		0	0
			19	11	7	1			
2	A	1	Total	C				0	0
			8	8					
2	A	1	Total	C	O			0	0
			21	17	4				

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: C₃₂H₅₈N₂O₇S).

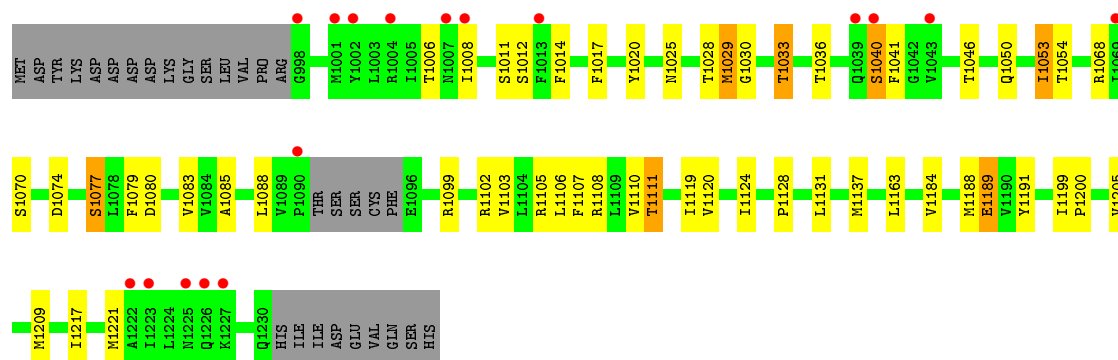


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 22 3	0	0
3	A	1	Total C N O 29 24 1 4	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ion transport protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.45Å 124.45Å 193.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.04 – 2.75 44.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	83.2 (44.04-2.75) 83.3 (44.00-2.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.213 , 0.265 0.218 , 0.267	Depositor DCC
R_{free} test set	851 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2167	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CPS, 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	0.77	2/1876 (0.1%)	0.90	0/2554

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1189	GLU	CD-OE1	7.76	1.34	1.25
1	A	1189	GLU	CD-OE2	6.24	1.32	1.25

There are no bond angle outliers.

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	1825	0	1869	33	1
2	A	288	0	401	6	0
3	A	54	0	74	1	0
All	All	2167	0	2344	37	1

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 8.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:VAL:HG11	1:A:1105:ARG:HA	1.50	0.89
1:A:1008:ILE:O	1:A:1011:SER:HB3	1.73	0.89
1:A:1036:THR:HG22	3:A:2010:CPS:H7	1.61	0.80
1:A:1080:ASP:OD1	1:A:1111:THR:HG21	1.83	0.78
1:A:1029:MET:HE3	1:A:1103:VAL:HG23	1.67	0.75
1:A:1137:MET:HE1	1:A:1205:VAL:HA	1.73	0.71
1:A:1083:VAL:CG1	1:A:1105:ARG:HA	2.23	0.67
1:A:1184:VAL:O	1:A:1188:MET:HG3	2.01	0.60
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.83	0.60
1:A:1029:MET:HE2	1:A:1106:LEU:HD21	1.84	0.58
1:A:1217:ILE:O	1:A:1221:MET:HG2	2.07	0.54
1:A:1083:VAL:HG11	1:A:1105:ARG:CA	2.32	0.54
1:A:1209:MET:HE1	2:A:2001:PX4:H43	1.90	0.53
1:A:1074:ASP:OD2	1:A:1077:SER:OG	2.26	0.53
1:A:1030:GLY:O	1:A:1033:THR:HB	2.10	0.51
2:A:2003:PX4:H17	2:A:2003:PX4:H46	1.92	0.51
2:A:2001:PX4:O8	2:A:2002:PX4:H50	2.11	0.50
1:A:1029:MET:HE1	1:A:1106:LEU:HG	1.94	0.50
1:A:1108:ARG:O	1:A:1111:THR:HG22	2.12	0.49
1:A:1079:PHE:CZ	1:A:1083:VAL:HG21	2.48	0.48
1:A:1120:VAL:HG12	1:A:1124:ILE:HD12	1.95	0.48
1:A:1188:MET:HA	1:A:1191:TYR:O	2.14	0.48
1:A:1050:GLN:HA	1:A:1053:ILE:HG22	1.95	0.47
1:A:1083:VAL:CG1	1:A:1105:ARG:CA	2.90	0.47
1:A:1099:ARG:O	1:A:1102[B]:ARG:HD3	2.15	0.46
1:A:1017:PHE:O	1:A:1020:TYR:HB3	2.15	0.46
1:A:1029:MET:HE2	1:A:1106:LEU:HD11	1.98	0.46
2:A:2006:PX4:H19	2:A:2006:PX4:H55	1.99	0.44
1:A:1085:ALA:O	1:A:1088:LEU:HB2	2.17	0.44
1:A:1107:PHE:O	1:A:1110:VAL:HB	2.18	0.43
1:A:1025:ASN:OD1	1:A:1105:ARG:NH1	2.36	0.42
1:A:1131:LEU:HB3	2:A:2005:PX4:H47	2.02	0.41
1:A:1040:SER:HB2	1:A:1041:PHE:CD1	2.55	0.41
2:A:2001:PX4:O8	2:A:2002:PX4:C26	2.69	0.41
1:A:1006:THR:HG22	1:A:1006:THR:O	2.20	0.41
1:A:1014:PHE:O	1:A:1017:PHE:HB3	2.21	0.41
1:A:1025:ASN:OD1	1:A:1105:ARG:HD2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:GLU:OE1	1:A:1189:GLU:OE1[5_454]	2.01	0.19

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	225/257 (88%)	200 (89%)	24 (11%)	1 (0%)	34 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1012	SER

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	198/237 (84%)	184 (93%)	14 (7%)	14 26

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1028	THR
1	A	1029	MET
1	A	1033	THR
1	A	1040	SER
1	A	1046	THR

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Mol	Chain	Res	Type
1	A	1053	ILE
1	A	1054	THR
1	A	1068	ARG
1	A	1070	SER
1	A	1077	SER
1	A	1111	THR
1	A	1119	ILE
1	A	1128	PRO
1	A	1163	LEU

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

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
3	CPS	A	2010	-	28,28,45	0.53	0	46,46,70	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PX4	A	2006	-	31,31,45	0.48	0	35,36,53	0.71	1 (2%)
2	PX4	A	2008	-	7,7,45	0.29	0	6,6,53	0.22	0
2	PX4	A	2001	-	43,43,45	0.51	0	49,51,53	0.58	0
3	CPS	A	2011	-	32,32,45	0.44	0	51,51,70	0.71	0
2	PX4	A	2005	-	35,35,45	0.44	0	41,43,53	0.66	1 (2%)
2	PX4	A	2004	-	39,39,45	0.51	0	43,44,53	0.85	1 (2%)
2	PX4	A	2003	-	45,45,45	0.44	0	51,53,53	0.72	1 (1%)
2	PX4	A	2007	-	18,18,45	0.58	0	21,22,53	0.69	1 (4%)
2	PX4	A	2009	-	20,20,45	0.51	0	21,21,53	0.38	0
2	PX4	A	2002	-	41,41,45	0.44	0	44,46,53	0.72	1 (2%)

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	CPS	A	2010	-	-	0/4/69/90	0/4/4/4
2	PX4	A	2006	-	-	18/33/33/49	-
2	PX4	A	2008	-	-	2/5/5/49	-
2	PX4	A	2001	-	-	26/47/47/49	-
3	CPS	A	2011	-	-	6/9/74/90	0/4/4/4
2	PX4	A	2005	-	-	16/39/39/49	-
2	PX4	A	2004	-	-	15/41/41/49	-
2	PX4	A	2003	-	-	27/49/49/49	-
2	PX4	A	2007	-	-	7/18/18/49	-
2	PX4	A	2009	-	-	16/20/20/49	-
2	PX4	A	2002	-	-	23/45/45/49	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2003	PX4	O7-C23-C24	3.64	119.34	111.50
3	A	2010	CPS	C15-C16-C17	3.09	117.87	114.46
2	A	2006	PX4	O1-P1-O2	2.70	121.27	110.68
2	A	2005	PX4	O7-C23-C24	2.53	116.95	111.50
2	A	2004	PX4	O4-P1-O2	2.33	113.00	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2007	PX4	O1-P1-O2	2.05	118.72	110.68
3	A	2010	CPS	C5-C6-C18	2.03	117.33	114.74
2	A	2002	PX4	O7-C23-O8	-2.01	118.84	123.70

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	PX4	C6-O4-P1-O1
2	A	2001	PX4	C6-O4-P1-O2
2	A	2001	PX4	C6-O4-P1-O3
2	A	2001	PX4	O7-C7-C8-O5
2	A	2001	PX4	C24-C23-O7-C7
2	A	2005	PX4	C6-O4-P1-O1
2	A	2004	PX4	C6-O4-P1-O1
2	A	2003	PX4	O8-C23-O7-C7
2	A	2009	PX4	O4-C6-C7-C8
2	A	2009	PX4	O4-C6-C7-O7
2	A	2009	PX4	C6-C7-C8-O5
2	A	2009	PX4	O7-C7-C8-O5
2	A	2002	PX4	C1-O3-P1-O2
2	A	2002	PX4	C6-O4-P1-O1
2	A	2002	PX4	C6-O4-P1-O2
2	A	2009	PX4	O6-C9-O5-C8
2	A	2009	PX4	C10-C9-O5-C8
2	A	2003	PX4	O6-C9-O5-C8
2	A	2003	PX4	C24-C23-O7-C7
2	A	2003	PX4	C10-C9-O5-C8
2	A	2001	PX4	O8-C23-O7-C7
3	A	2011	CPS	C9-C20-C22-C23
2	A	2007	PX4	C7-C6-O4-P1
2	A	2001	PX4	C10-C9-O5-C8
2	A	2001	PX4	O6-C9-O5-C8
2	A	2003	PX4	C23-C24-C25-C26
2	A	2009	PX4	C9-C10-C11-C12
2	A	2002	PX4	C23-C24-C25-C26
2	A	2004	PX4	C23-C24-C25-C26
2	A	2005	PX4	C1-O3-P1-O4
2	A	2005	PX4	C6-O4-P1-O3
2	A	2002	PX4	C6-O4-P1-O3
2	A	2004	PX4	C14-C15-C16-C17
2	A	2006	PX4	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
2	A	2003	PX4	C30-C31-C32-C33
2	A	2007	PX4	C12-C13-C14-C15
2	A	2002	PX4	C25-C26-C27-C28
2	A	2001	PX4	C29-C30-C31-C32
2	A	2004	PX4	C18-C19-C20-C21
2	A	2009	PX4	C12-C13-C14-C15
2	A	2006	PX4	C27-C28-C29-C30
2	A	2004	PX4	C32-C33-C34-C35
2	A	2009	PX4	C17-C18-C19-C20
2	A	2001	PX4	C10-C11-C12-C13
2	A	2007	PX4	C9-C10-C11-C12
2	A	2003	PX4	C17-C18-C19-C20
2	A	2006	PX4	C25-C26-C27-C28
2	A	2005	PX4	C26-C27-C28-C29
3	A	2011	CPS	C21-C20-C22-C23
2	A	2006	PX4	C26-C27-C28-C29
2	A	2003	PX4	C25-C26-C27-C28
2	A	2007	PX4	C10-C11-C12-C13
2	A	2002	PX4	C26-C27-C28-C29
2	A	2006	PX4	C10-C9-O5-C8
2	A	2007	PX4	C10-C9-O5-C8
2	A	2003	PX4	C31-C32-C33-C34
2	A	2002	PX4	C17-C18-C19-C20
2	A	2001	PX4	C12-C13-C14-C15
2	A	2001	PX4	C13-C14-C15-C16
2	A	2001	PX4	C26-C27-C28-C29
2	A	2007	PX4	O6-C9-O5-C8
2	A	2002	PX4	C27-C28-C29-C30
2	A	2003	PX4	C16-C17-C18-C19
2	A	2009	PX4	C10-C11-C12-C13
2	A	2006	PX4	O6-C9-O5-C8
2	A	2006	PX4	O8-C23-O7-C7
2	A	2001	PX4	C23-C24-C25-C26
2	A	2003	PX4	C29-C30-C31-C32
2	A	2008	PX4	C27-C28-C29-C30
2	A	2004	PX4	C12-C13-C14-C15
2	A	2009	PX4	C13-C14-C15-C16
2	A	2006	PX4	C24-C23-O7-C7
2	A	2005	PX4	C13-C14-C15-C16
2	A	2004	PX4	O7-C7-C8-O5
2	A	2002	PX4	C14-C15-C16-C17
2	A	2009	PX4	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
2	A	2002	PX4	C30-C31-C32-C33
2	A	2005	PX4	C24-C25-C26-C27
2	A	2003	PX4	C27-C28-C29-C30
2	A	2004	PX4	C25-C26-C27-C28
2	A	2003	PX4	C28-C29-C30-C31
2	A	2004	PX4	C11-C12-C13-C14
2	A	2004	PX4	C24-C25-C26-C27
2	A	2005	PX4	C25-C26-C27-C28
2	A	2006	PX4	C13-C14-C15-C16
2	A	2001	PX4	C18-C19-C20-C21
2	A	2002	PX4	C12-C13-C14-C15
2	A	2004	PX4	C6-O4-P1-O2
2	A	2001	PX4	C25-C26-C27-C28
2	A	2005	PX4	O4-C6-C7-O7
2	A	2002	PX4	O4-C6-C7-O7
2	A	2009	PX4	C19-C20-C21-C22
2	A	2003	PX4	C32-C33-C34-C35
2	A	2004	PX4	C33-C34-C35-C36
2	A	2005	PX4	C6-C7-C8-O5
2	A	2004	PX4	C6-C7-C8-O5
2	A	2003	PX4	C19-C20-C21-C22
2	A	2006	PX4	O4-C6-C7-O7
3	A	2011	CPS	C22-C23-C24-N1
3	A	2011	CPS	C22-C23-C24-O1
2	A	2007	PX4	C13-C14-C15-C16
2	A	2005	PX4	O7-C7-C8-O5
2	A	2003	PX4	C7-C6-O4-P1
2	A	2002	PX4	C24-C23-O7-C7
2	A	2003	PX4	C26-C27-C28-C29
2	A	2002	PX4	O8-C23-O7-C7
2	A	2006	PX4	C23-C24-C25-C26
2	A	2008	PX4	C26-C27-C28-C29
2	A	2003	PX4	C15-C16-C17-C18
2	A	2001	PX4	C6-C7-C8-O5
2	A	2001	PX4	O4-C6-C7-O7
2	A	2002	PX4	C19-C20-C21-C22
2	A	2006	PX4	C11-C12-C13-C14
2	A	2003	PX4	C1-O3-P1-O4
2	A	2005	PX4	C1-O3-P1-O2
2	A	2003	PX4	C1-O3-P1-O1
2	A	2001	PX4	O4-C6-C7-C8
2	A	2005	PX4	O4-C6-C7-C8

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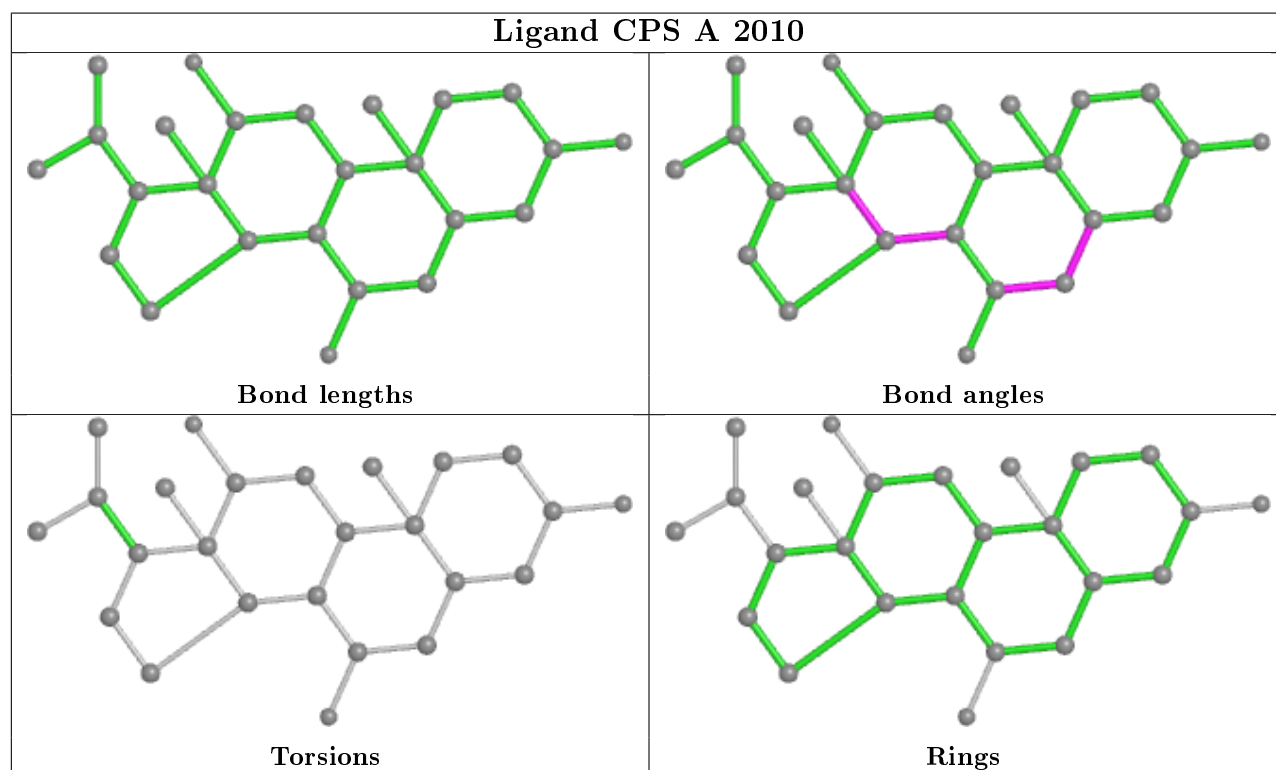
Mol	Chain	Res	Type	Atoms
2	A	2002	PX4	O4-C6-C7-C8
2	A	2005	PX4	C15-C16-C17-C18
2	A	2005	PX4	C12-C13-C14-C15
2	A	2005	PX4	O3-C1-C2-N1
2	A	2009	PX4	C16-C17-C18-C19
2	A	2003	PX4	O7-C7-C8-O5
2	A	2001	PX4	C16-C17-C18-C19
2	A	2003	PX4	C33-C34-C35-C36
2	A	2002	PX4	O6-C9-O5-C8
2	A	2003	PX4	C18-C19-C20-C21
2	A	2001	PX4	C9-C10-C11-C12
2	A	2006	PX4	O7-C7-C8-O5
2	A	2006	PX4	C9-C10-C11-C12
2	A	2002	PX4	C29-C30-C31-C32
2	A	2005	PX4	C11-C12-C13-C14
2	A	2006	PX4	C7-C6-O4-P1
2	A	2004	PX4	C16-C17-C18-C19
2	A	2009	PX4	C11-C12-C13-C14
2	A	2001	PX4	C1-C2-N1-C5
2	A	2001	PX4	C31-C32-C33-C34
2	A	2006	PX4	C29-C30-C31-C32
2	A	2003	PX4	C10-C11-C12-C13
2	A	2009	PX4	C15-C16-C17-C18
2	A	2006	PX4	O4-C6-C7-C8
2	A	2003	PX4	C7-C8-O5-C9
2	A	2004	PX4	C6-O4-P1-O3
2	A	2001	PX4	C1-C2-N1-C4
2	A	2003	PX4	C6-C7-C8-O5
2	A	2002	PX4	O7-C23-C24-C25
2	A	2002	PX4	C10-C9-O5-C8
2	A	2006	PX4	O7-C23-C24-C25
2	A	2003	PX4	C1-C2-N1-C3
2	A	2002	PX4	C1-O3-P1-O1
2	A	2001	PX4	C2-C1-O3-P1
2	A	2001	PX4	C1-C2-N1-C3
3	A	2011	CPS	C22-C20-C9-C8
2	A	2002	PX4	O8-C23-C24-C25
3	A	2011	CPS	C22-C20-C9-C5

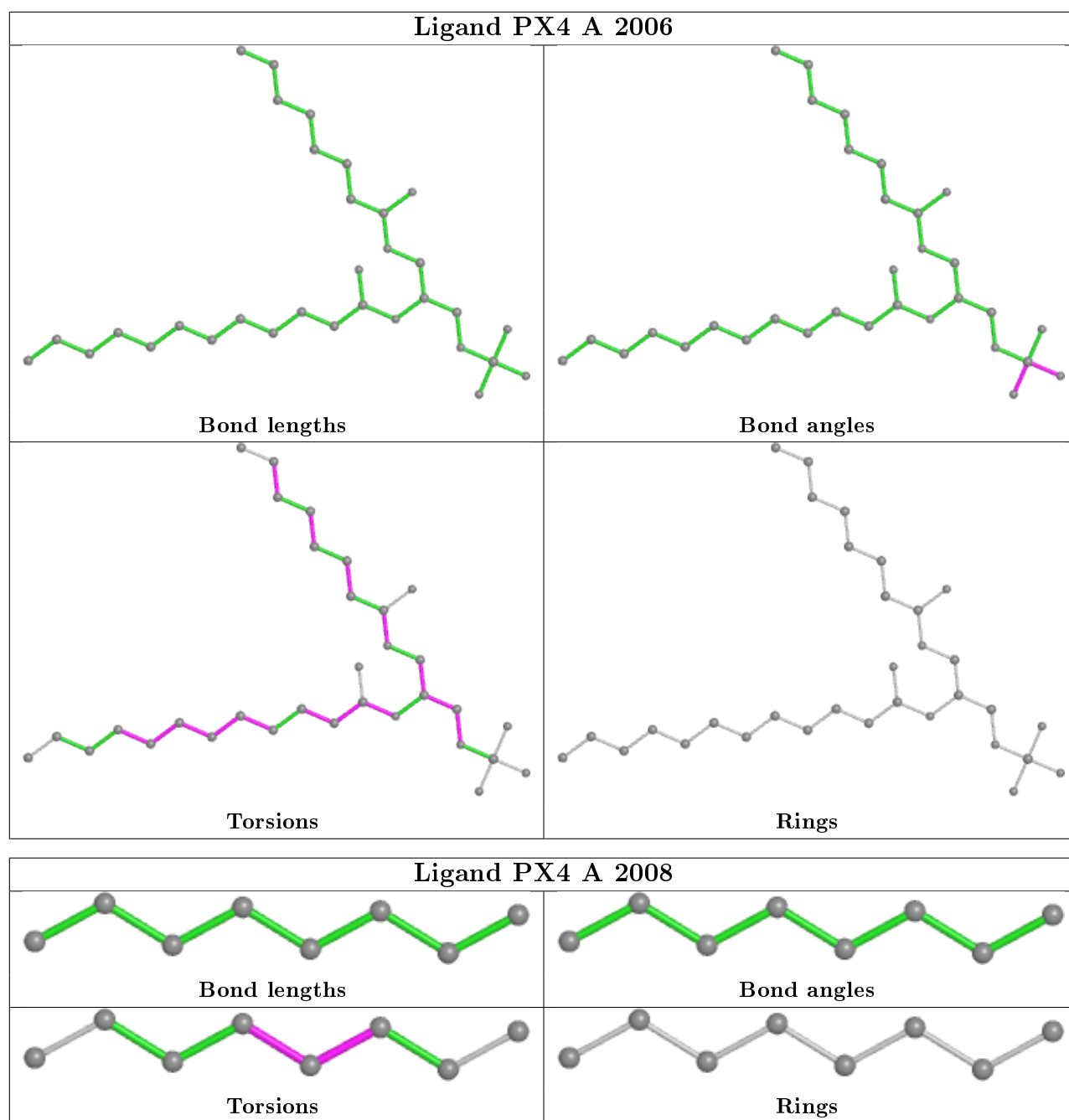
There are no ring outliers.

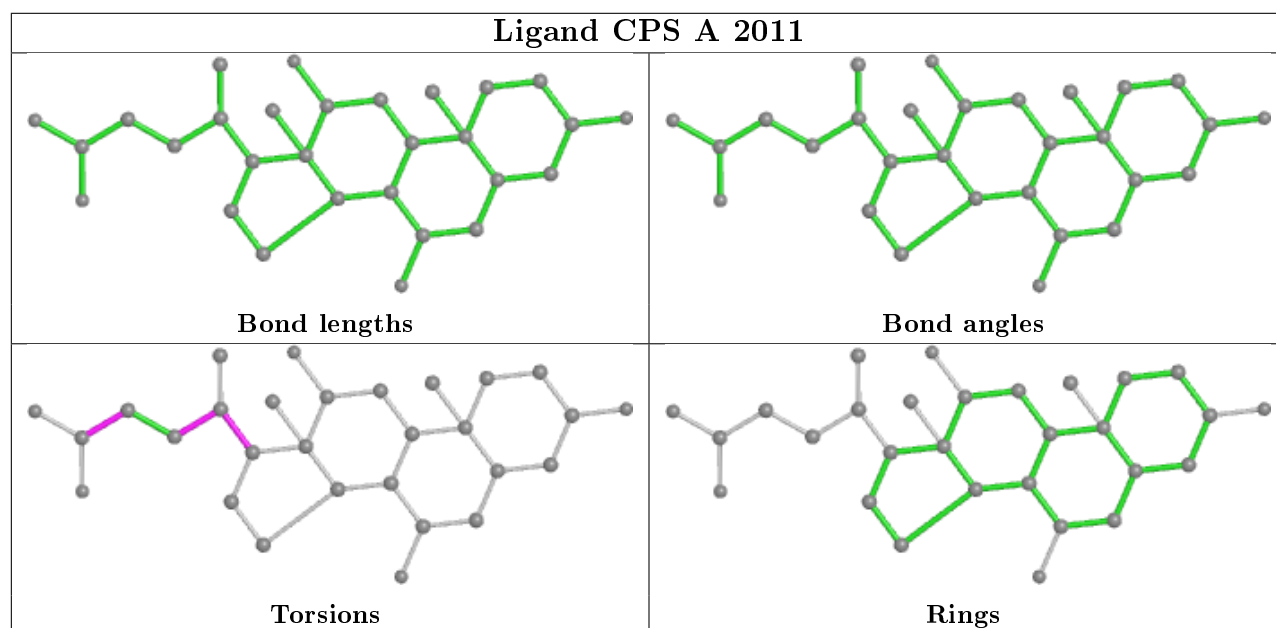
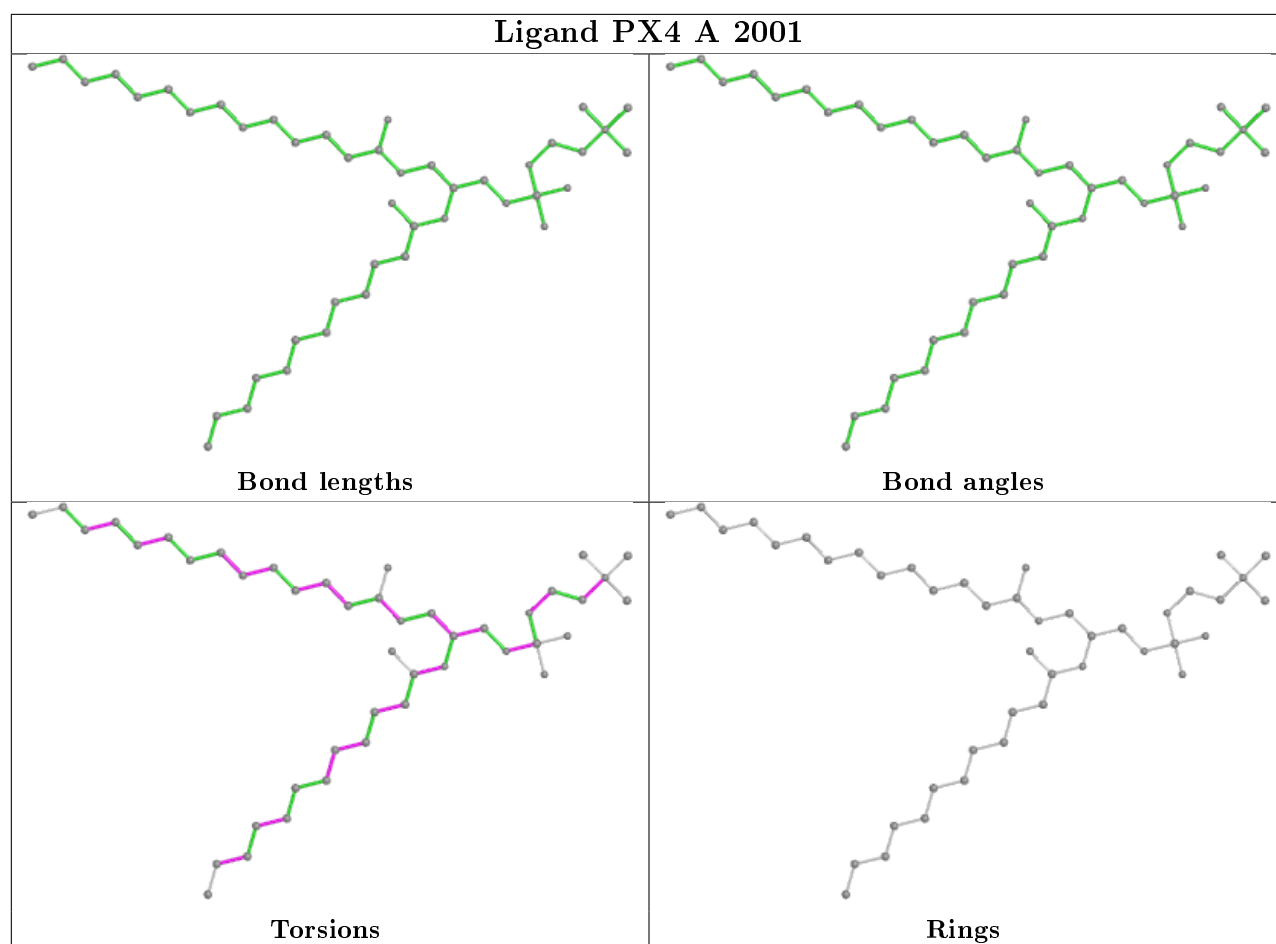
6 monomers are involved in 7 short contacts:

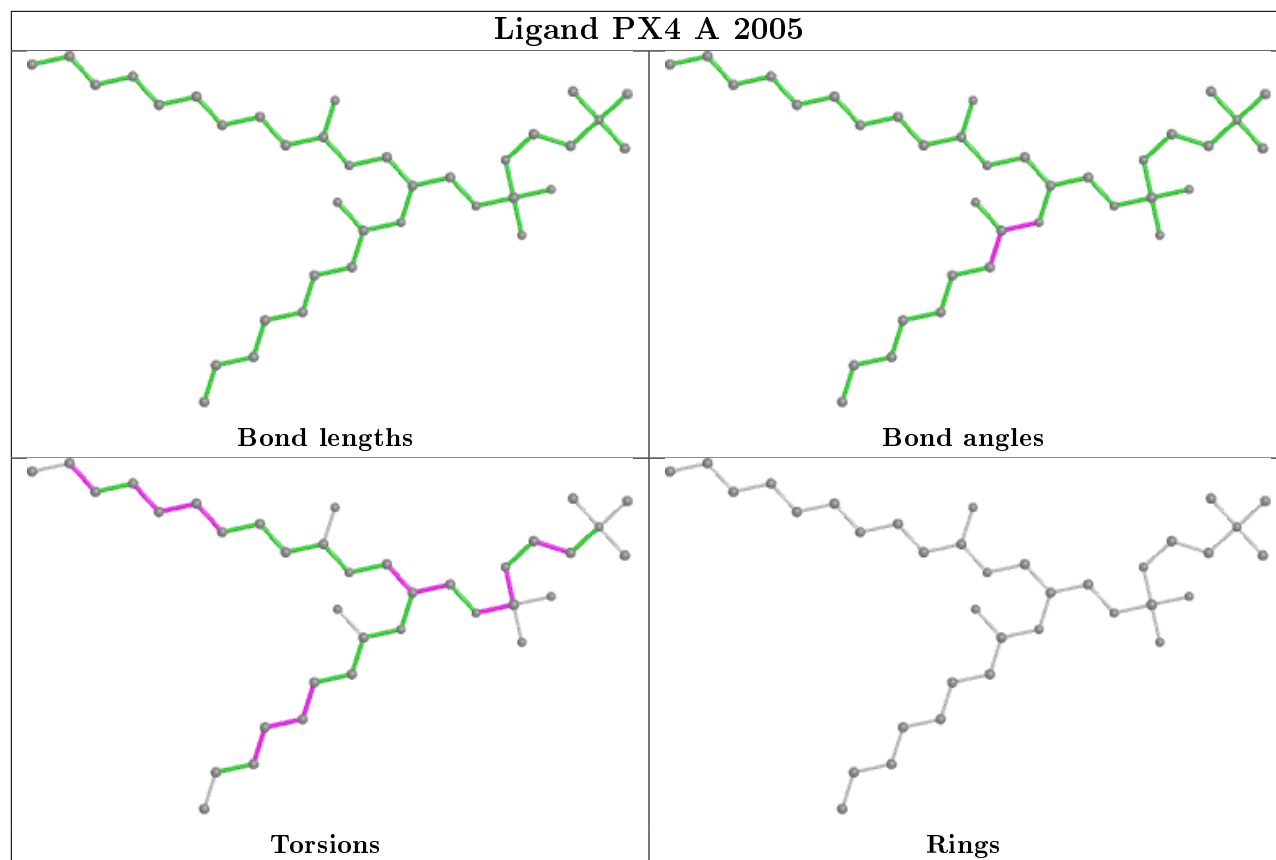
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2010	CPS	1	0
2	A	2006	PX4	1	0
2	A	2001	PX4	3	0
2	A	2005	PX4	1	0
2	A	2003	PX4	1	0
2	A	2002	PX4	2	0

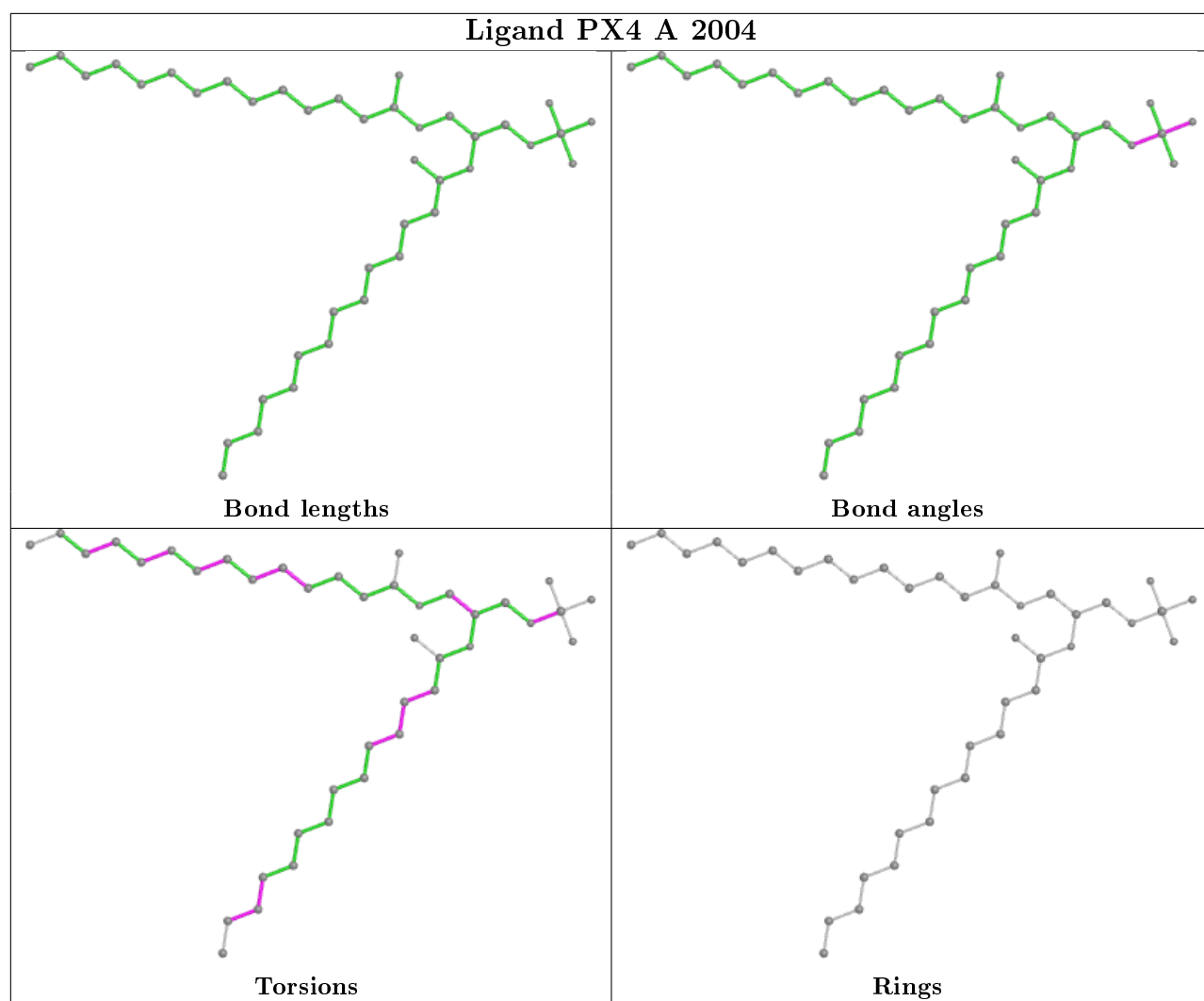
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

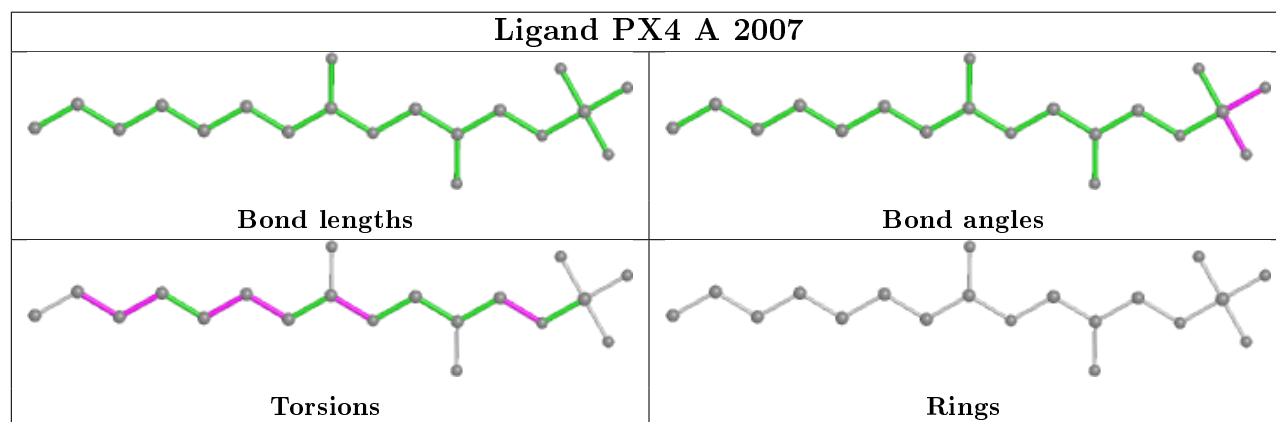
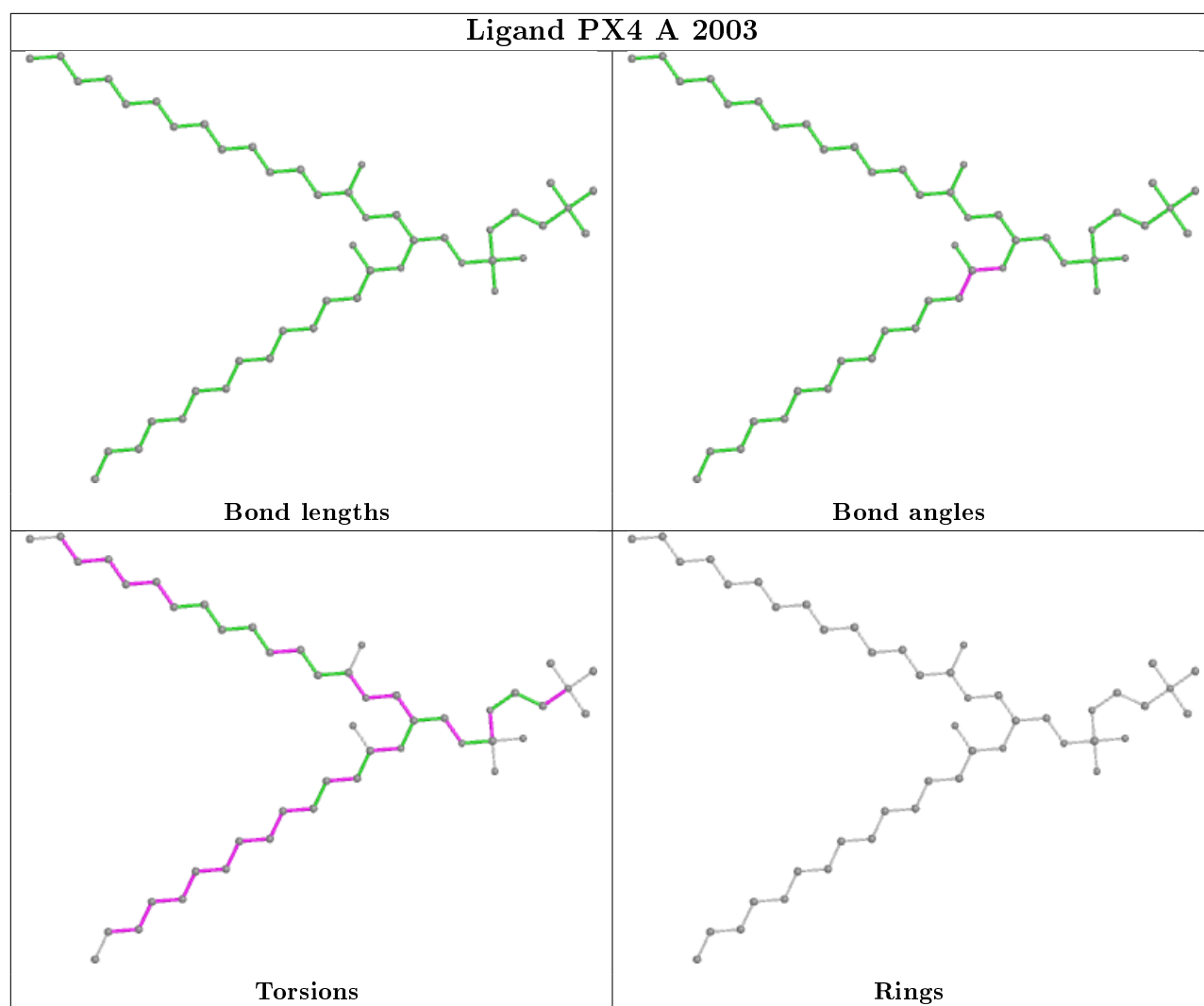


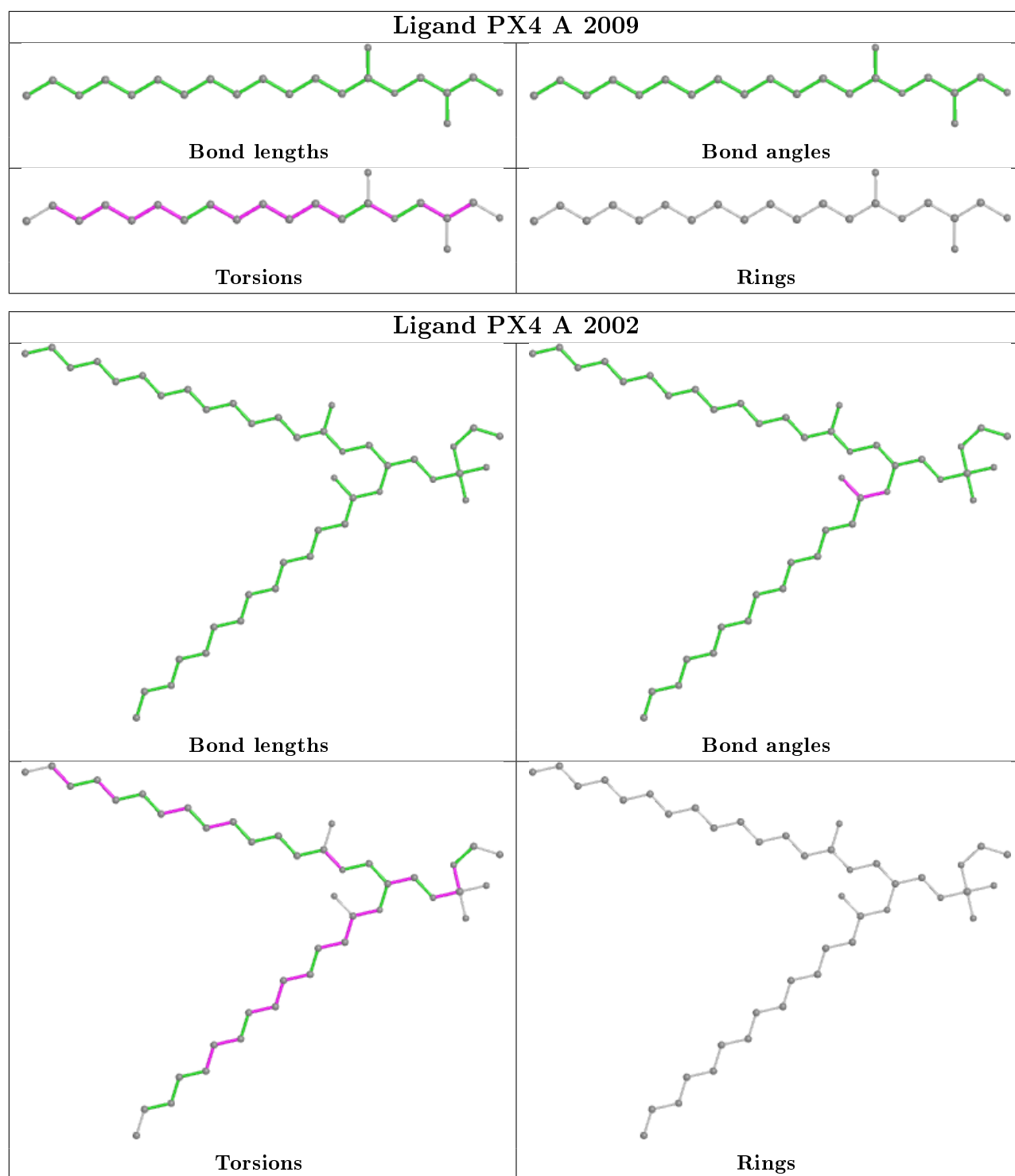












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	228/257 (88%)	-0.09	17 (7%) 14 17	8, 37, 81, 105	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1039	GLN	3.6
1	A	998	GLY	3.2
1	A	1007	ASN	2.9
1	A	1008	ILE	2.9
1	A	1002	TYR	2.7
1	A	1001	MET	2.6
1	A	1223	ILE	2.6
1	A	1069	ILE	2.5
1	A	1222	ALA	2.5
1	A	1040	SER	2.2
1	A	1227	LYS	2.2
1	A	1225	ASN	2.1
1	A	1090	PRO	2.1
1	A	1013	PHE	2.1
1	A	1226	GLN	2.1
1	A	1004	ARG	2.0
1	A	1043	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

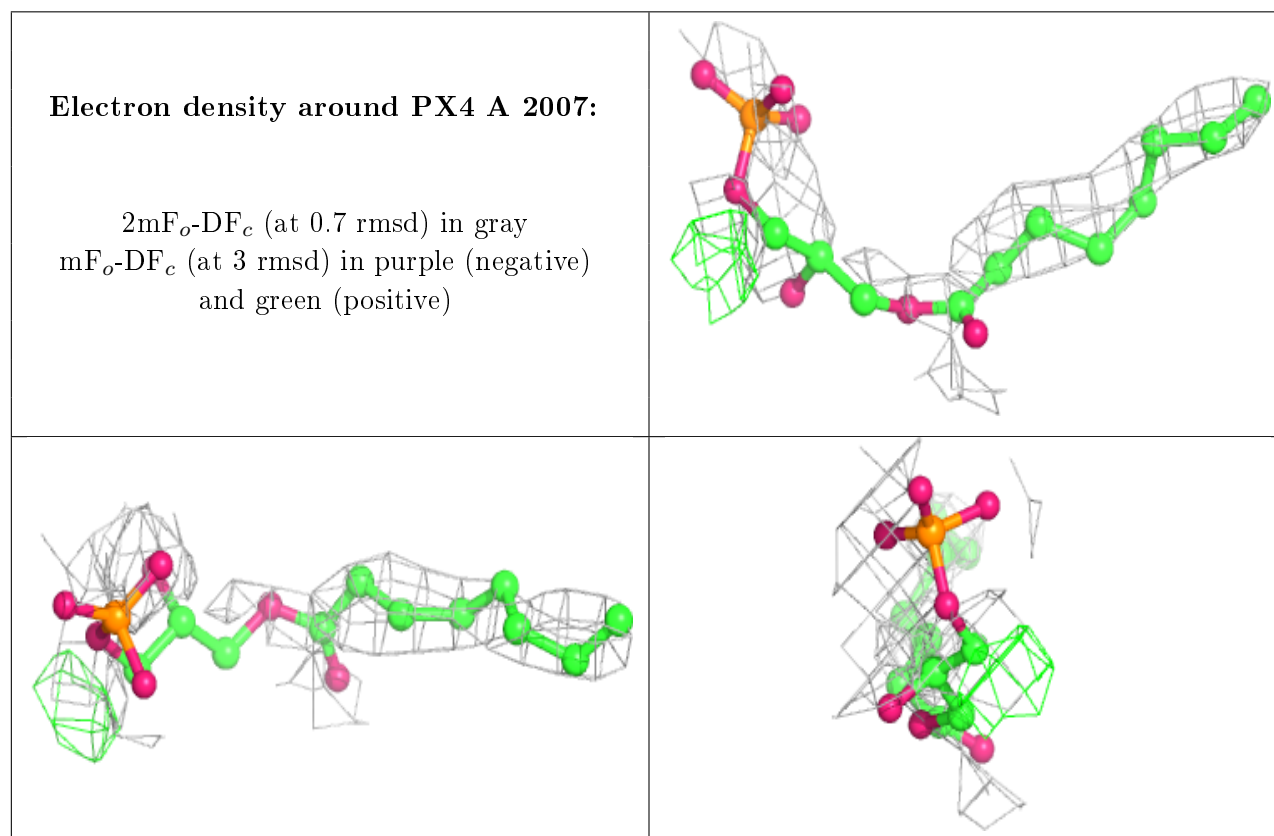
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

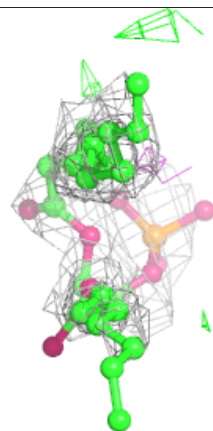
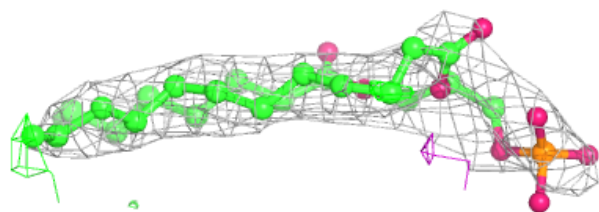
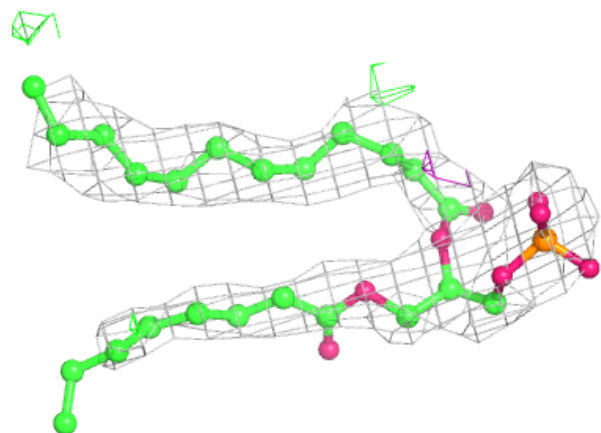
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PX4	A	2007	19/46	0.62	0.43	68,131,189,190	0
2	PX4	A	2006	32/46	0.68	0.37	62,103,143,159	0
2	PX4	A	2004	40/46	0.77	0.26	55,71,89,91	0
2	PX4	A	2005	36/46	0.83	0.23	74,88,120,128	0
2	PX4	A	2009	21/46	0.83	0.34	39,55,80,87	0
2	PX4	A	2003	46/46	0.88	0.26	43,66,81,89	0
3	CPS	A	2011	29/42	0.89	0.31	79,93,103,106	0
2	PX4	A	2002	42/46	0.89	0.20	43,53,65,70	0
2	PX4	A	2008	8/46	0.91	0.20	54,59,62,64	0
2	PX4	A	2001	44/46	0.93	0.19	30,52,74,76	0
3	CPS	A	2010	25/42	0.93	0.36	60,85,100,103	0

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

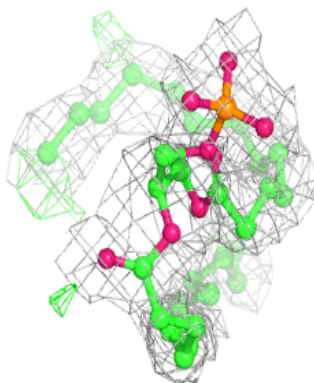
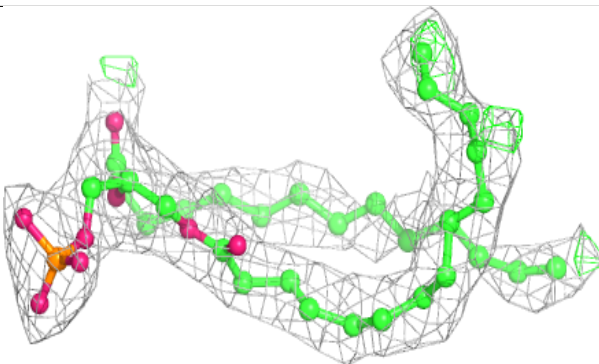
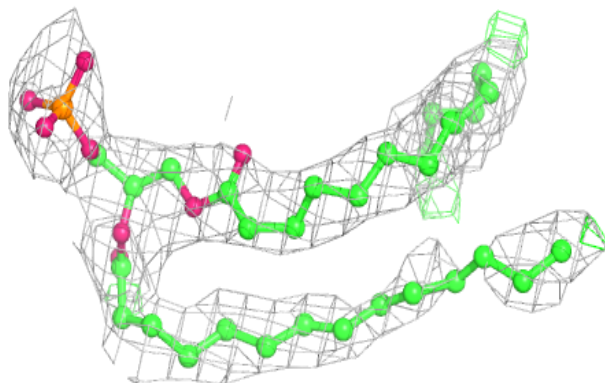


Electron density around PX4 A 2006:

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

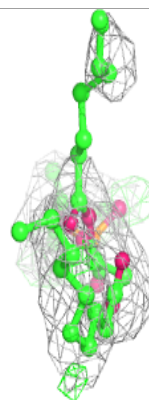
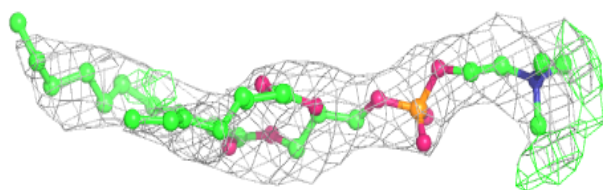
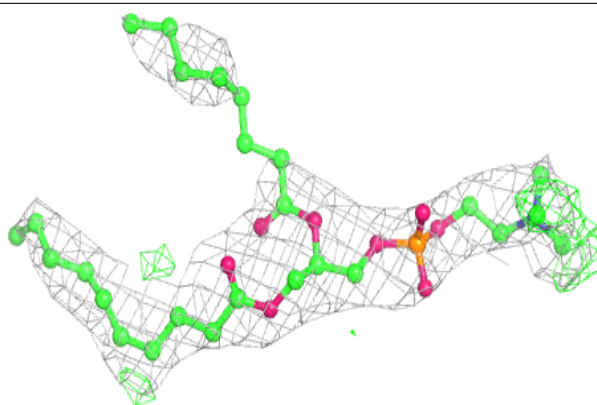
**Electron density around PX4 A 2004:**

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

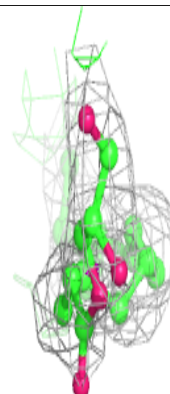
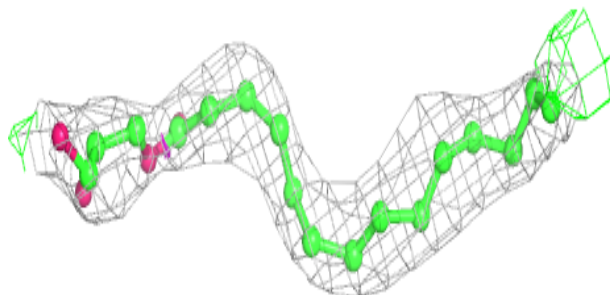
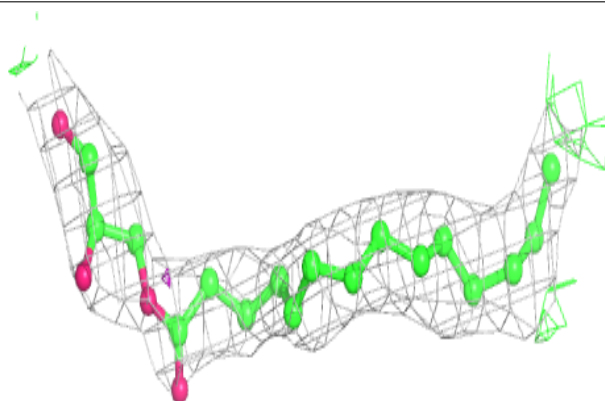


Electron density around PX4 A 2005:

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

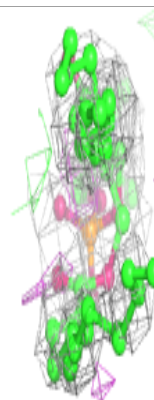
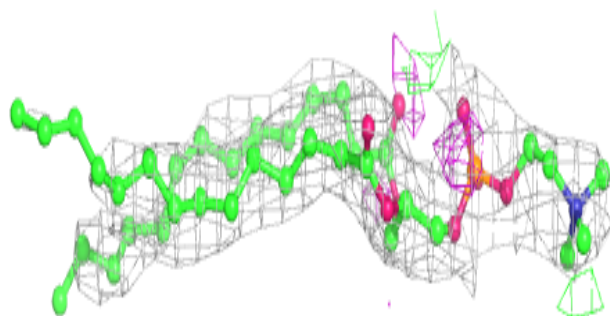
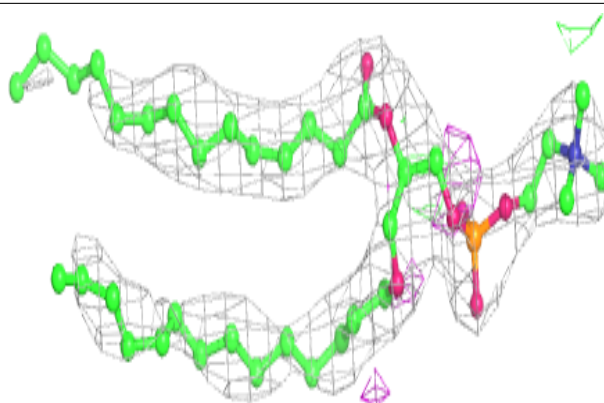
**Electron density around PX4 A 2009:**

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

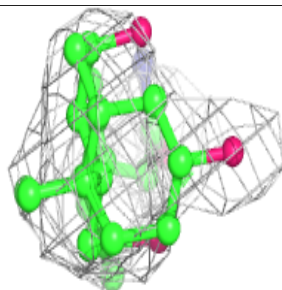
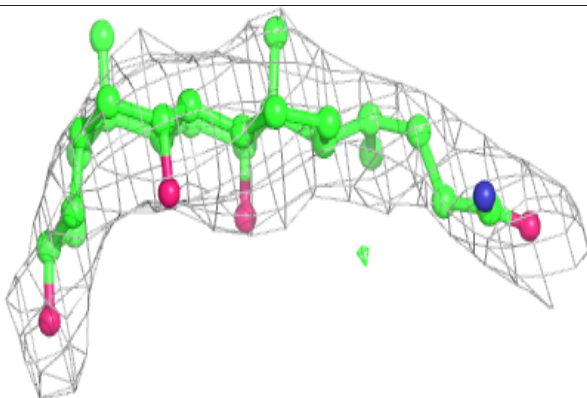
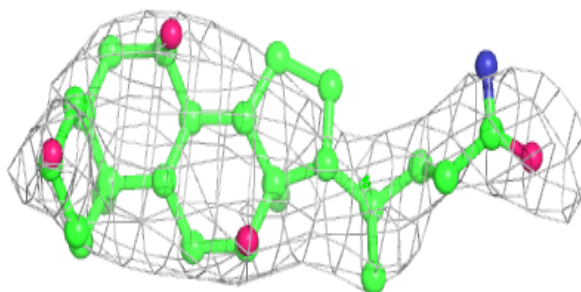


Electron density around PX4 A 2003:

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

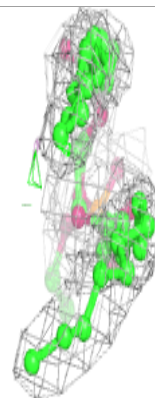
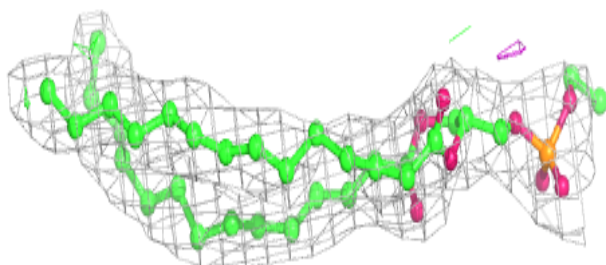
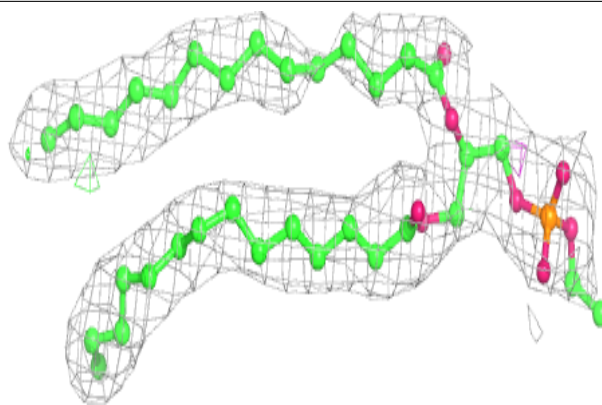
**Electron density around CPS A 2011:**

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

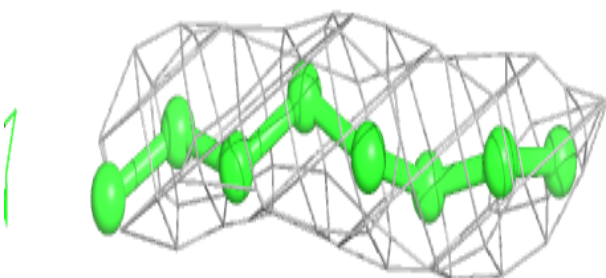
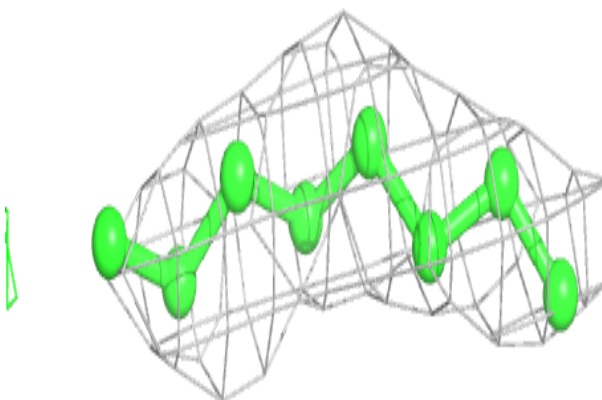


Electron density around PX4 A 2002:

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

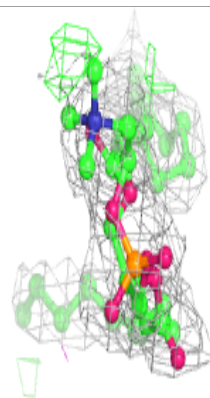
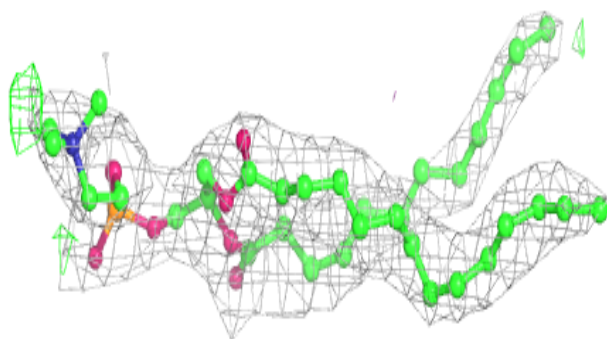
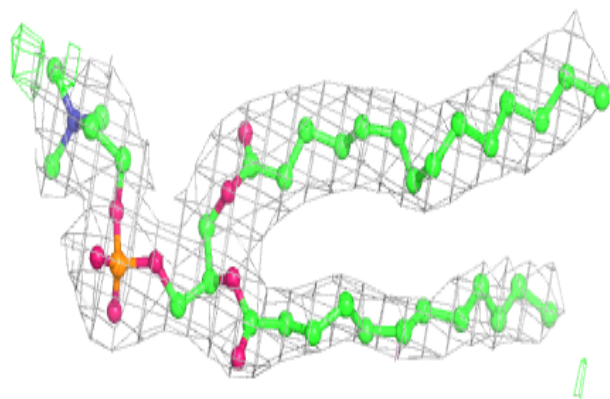
**Electron density around PX4 A 2008:**

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

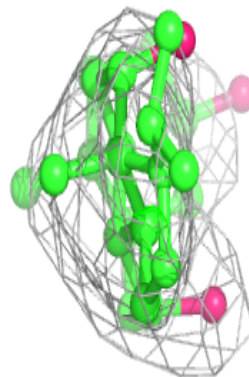
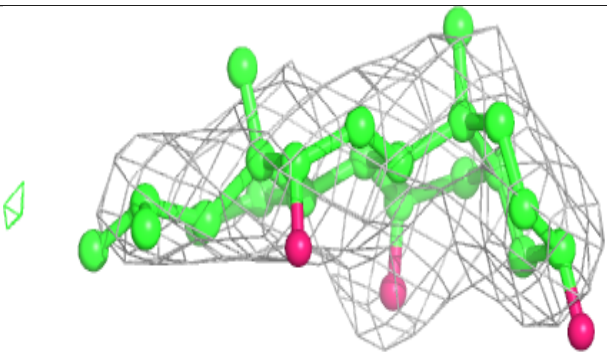
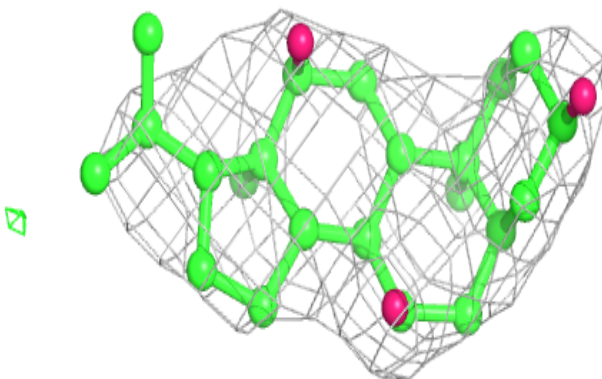


Electron density around PX4 A 2001:

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

**Electron density around CPS A 2010:**

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



6.5 Other polymers

There are no such residues in this entry.