



Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2026 – 08:19 PM JST

PDB ID : 9VDQ / pdb_00009vdq
Title : Crystal structure of voltage-gated sodium channel NavAb N49K mutant
Authors : Irie, K.
Deposited on : 2025-06-09
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

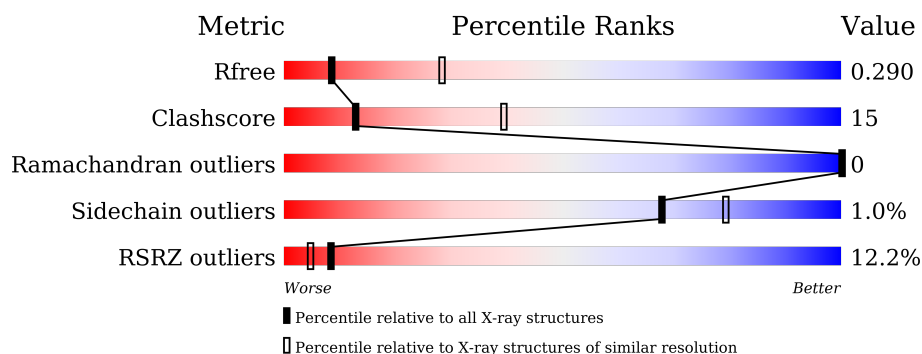
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	269	<div> <div>10%</div> <div>62%</div> <div>22%</div> <div>15%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2281 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	229	Total	C	N	O	S	0	0	0
			1870	1273	281	304	12			

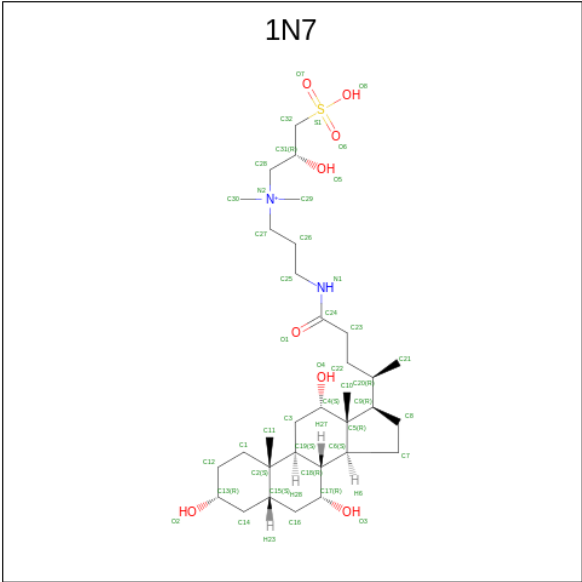
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	999	GLY	-	expression tag	UNP A8EVM5
A	1000	SER	-	expression tag	UNP A8EVM5
A	1049	LYS	ASN	engineered mutation	UNP A8EVM5

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

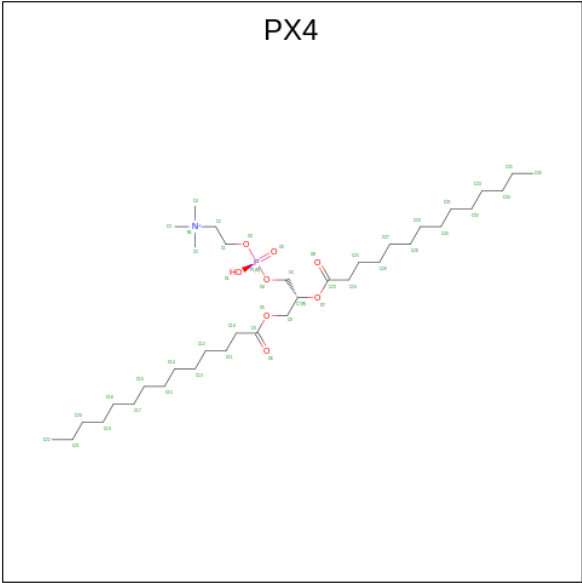
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Na	0	0
			3	3		

- Molecule 3 is CHAPSO (CCD ID: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	25	1	4		

- Molecule 4 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PX4) (formula: C₃₆H₇₃NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		

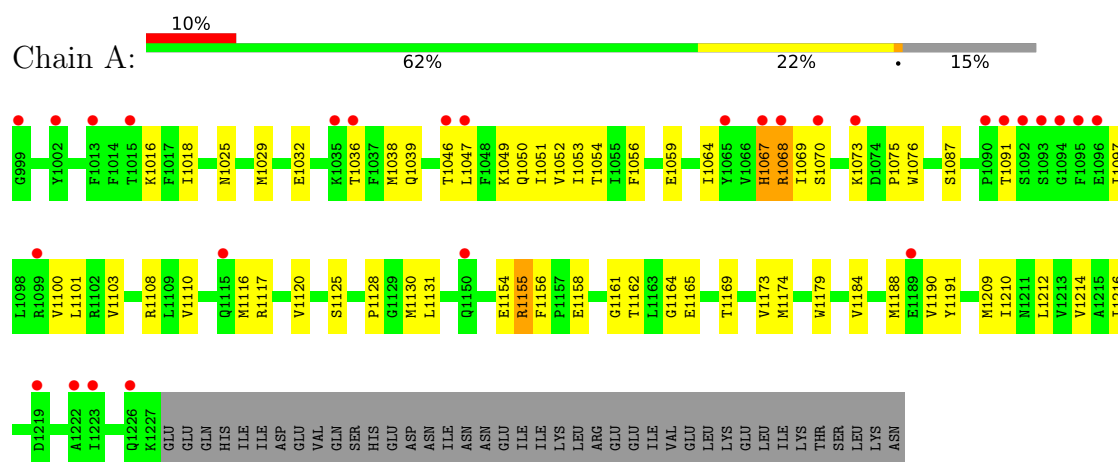
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		

3 Residue-property plots [i](#)

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

- Molecule 1: Ion transport protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	127.18Å 127.18Å 201.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.93 – 3.10 43.93 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.2 (43.93-3.10) 96.2 (43.93-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.241 , 0.289 0.246 , 0.290	Depositor DCC
R_{free} test set	1480 reflections (7.96%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2281	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: 1N7, NA, PX4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/1921	0.79	5/2610 (0.2%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1068	ARG	N-CA-C	8.05	119.84	111.14
1	A	1067	HIS	N-CA-C	-6.37	94.89	107.69
1	A	1155	ARG	CB-CG-CD	6.18	125.51	111.30
1	A	1068	ARG	CB-CA-C	-5.49	102.22	110.90
1	A	1069	ILE	N-CA-C	-5.27	107.69	112.96

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	1870	0	1958	54	5
2	A	3	0	0	0	0
3	A	30	0	40	5	0
4	A	368	0	576	20	6
5	A	10	0	0	0	1
All	All	2281	0	2574	73	8

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.

All (73) 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:1025:ASN:ND2	1:A:1052:VAL:HG21	1.76	1.00
1:A:1025:ASN:HD22	1:A:1052:VAL:HG21	1.28	0.98
1:A:1162:THR:HB	1:A:1165:GLU:HG2	1.61	0.81
3:A:1304:1N7:H35	3:A:1304:1N7:H14	1.66	0.77
1:A:1155:ARG:CZ	1:A:1190:VAL:HG21	2.17	0.75
1:A:1155:ARG:HD2	1:A:1190:VAL:HG11	1.67	0.74
1:A:1155:ARG:HD3	1:A:1156:PHE:CE1	2.24	0.72
1:A:1076:TRP:HE1	4:A:1305:PX4:H12	1.54	0.72
4:A:1311:PX4:H61	4:A:1311:PX4:H39	1.73	0.71
4:A:1305:PX4:H69	4:A:1306:PX4:H61	1.72	0.70
1:A:1032:GLU:OE1	1:A:1049:LYS:HE2	1.93	0.68
4:A:1306:PX4:H47	4:A:1307:PX4:H26	1.77	0.66
1:A:1032:GLU:HA	1:A:1038:MET:HE3	1.77	0.64
1:A:1130:MET:HE3	1:A:1212:LEU:HD21	1.81	0.63
1:A:1067:HIS:HB3	1:A:1070:SER:HB2	1.81	0.62
4:A:1305:PX4:H17	4:A:1306:PX4:H49	1.82	0.62
1:A:1076:TRP:NE1	4:A:1305:PX4:H12	2.14	0.61
1:A:1191:TYR:HD1	4:A:1312:PX4:H15	1.67	0.60
1:A:1076:TRP:CZ3	1:A:1117:ARG:HG2	2.37	0.59
4:A:1305:PX4:H53	4:A:1306:PX4:H19	1.84	0.58
3:A:1304:1N7:O4	3:A:1304:1N7:H33	2.03	0.58
1:A:1025:ASN:O	1:A:1029:MET:HG3	2.03	0.58
1:A:1162:THR:HG22	1:A:1164:GLY:H	1.67	0.58
1:A:1162:THR:HG22	1:A:1164:GLY:N	2.19	0.58
1:A:1128:PRO:HA	1:A:1131:LEU:HD13	1.86	0.57
1:A:1100:VAL:O	1:A:1103:VAL:HG12	2.05	0.57
1:A:1155:ARG:NE	1:A:1190:VAL:HG21	2.19	0.56
4:A:1308:PX4:H7	4:A:1308:PX4:P1	2.47	0.54
4:A:1308:PX4:H37	4:A:1308:PX4:H70	1.90	0.54
1:A:1047:LEU:O	1:A:1051:ILE:HG12	2.08	0.53
1:A:1052:VAL:HG23	1:A:1053:ILE:N	2.22	0.53
4:A:1306:PX4:H5	4:A:1307:PX4:H7	1.90	0.53
1:A:1155:ARG:CD	1:A:1190:VAL:HG11	2.37	0.53
1:A:1125:SER:O	1:A:1128:PRO:HD2	2.09	0.53
1:A:1191:TYR:CD1	4:A:1312:PX4:H15	2.44	0.53
1:A:1059:GLU:OE2	1:A:1108:ARG:NH2	2.42	0.52
1:A:1038:MET:HA	1:A:1038:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1306:PX4:H39	4:A:1307:PX4:H72	1.91	0.52
1:A:1188:MET:HA	1:A:1191:TYR:O	2.11	0.51
1:A:1029:MET:HG2	1:A:1049:LYS:HE3	1.93	0.50
1:A:1169:THR:O	1:A:1173:VAL:HG23	2.12	0.50
1:A:1050:GLN:O	1:A:1054:THR:HG23	2.12	0.49
1:A:1070:SER:O	1:A:1073:LYS:HG2	2.13	0.49
4:A:1308:PX4:H12	4:A:1308:PX4:H1	1.66	0.48
1:A:1110:VAL:HG11	1:A:1120:VAL:HG21	1.96	0.46
4:A:1305:PX4:H64	4:A:1305:PX4:H71	1.76	0.46
1:A:1097:ILE:O	1:A:1101:LEU:HG	2.16	0.46
3:A:1304:1N7:H17	3:A:1304:1N7:H4	1.71	0.45
1:A:1053:ILE:HD12	1:A:1053:ILE:HA	1.81	0.45
3:A:1304:1N7:H16	3:A:1304:1N7:H20	1.98	0.44
1:A:1018:ILE:HG13	1:A:1059:GLU:OE1	2.18	0.44
1:A:1210:ILE:O	1:A:1214:VAL:HG23	2.17	0.44
1:A:1029:MET:HE1	1:A:1103:VAL:HA	1.99	0.44
1:A:1056:PHE:HA	1:A:1059:GLU:HG2	2.00	0.44
1:A:1075:PRO:HG3	4:A:1307:PX4:H20	2.00	0.43
1:A:1158:GLU:O	1:A:1158:GLU:HG2	2.18	0.42
1:A:1212:LEU:O	1:A:1216:ILE:HG12	2.19	0.42
1:A:1064:ILE:O	1:A:1068:ARG:HA	2.20	0.42
1:A:1046:THR:O	1:A:1050:GLN:HG2	2.19	0.42
1:A:1108:ARG:HE	1:A:1108:ARG:HB3	1.65	0.42
1:A:1209:MET:HE3	1:A:1209:MET:HB3	1.73	0.42
1:A:1018:ILE:HD13	1:A:1018:ILE:HA	1.84	0.41
1:A:1179:TRP:O	1:A:1184:VAL:HG23	2.20	0.41
1:A:1073:LYS:HE2	4:A:1307:PX4:H3	2.02	0.41
1:A:1053:ILE:HD11	1:A:1087:SER:HB2	2.03	0.41
1:A:1016:LYS:HE2	1:A:1016:LYS:HB3	1.77	0.41
1:A:1110:VAL:HA	1:A:1116:MET:HB3	2.03	0.41
1:A:1049:LYS:O	1:A:1052:VAL:HG22	2.22	0.40
4:A:1310:PX4:H1	4:A:1310:PX4:H9	1.75	0.40
1:A:1036:THR:O	1:A:1039:GLN:HG2	2.20	0.40
3:A:1304:1N7:H10	3:A:1304:1N7:H31	1.78	0.40
4:A:1307:PX4:H12	4:A:1307:PX4:H1	1.82	0.40
4:A:1309:PX4:H54	4:A:1309:PX4:H48	1.86	0.40

All (8) 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:1154:GLU:OE2	4:A:1312:PX4:C4[7_555]	1.38	0.82
1:A:1161:GLY:O	4:A:1311:PX4:C5[4_555]	1.38	0.82
1:A:1165:GLU:OE1	4:A:1310:PX4:C5[3_555]	1.38	0.82
4:A:1308:PX4:C2	4:A:1310:PX4:C4[2_555]	1.49	0.71
4:A:1309:PX4:C22	4:A:1311:PX4:C22[4_555]	1.49	0.71
1:A:1155:ARG:O	1:A:1155:ARG:NH2[7_555]	1.89	0.31
1:A:1165:GLU:CD	4:A:1310:PX4:C5[3_555]	1.89	0.31
5:A:1408:HOH:O	5:A:1408:HOH:O[4_555]	2.16	0.04

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	227/269 (84%)	225 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/249 (84%)	207 (99%)	2 (1%)	68	79

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1091	THR

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Mol	Chain	Res	Type
1	A	1174	MET

Sometimes 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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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
4	PX4	A	1307	-	45,45,45	1.04	2 (4%)	51,53,53	0.90	2 (3%)
4	PX4	A	1312	-	45,45,45	1.14	2 (4%)	51,53,53	1.10	3 (5%)
4	PX4	A	1309	-	45,45,45	1.04	2 (4%)	51,53,53	1.04	2 (3%)
4	PX4	A	1310	-	45,45,45	1.16	2 (4%)	51,53,53	1.28	4 (7%)
4	PX4	A	1308	-	45,45,45	1.10	2 (4%)	51,53,53	1.12	3 (5%)
4	PX4	A	1311	-	45,45,45	1.00	2 (4%)	51,53,53	1.31	5 (9%)
3	1N7	A	1304	-	33,33,46	0.62	0	52,52,72	2.04	13 (25%)
4	PX4	A	1305	-	45,45,45	1.00	2 (4%)	51,53,53	1.16	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PX4	A	1306	-	45,45,45	1.05	2 (4%)	51,53,53	0.90	3 (5%)

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
4	PX4	A	1307	-	-	19/49/49/49	-
4	PX4	A	1312	-	-	28/49/49/49	-
4	PX4	A	1309	-	-	26/49/49/49	-
4	PX4	A	1310	-	-	22/49/49/49	-
4	PX4	A	1308	-	-	21/49/49/49	-
4	PX4	A	1311	-	-	21/49/49/49	-
3	1N7	A	1304	-	-	10/11/76/92	0/4/4/4
4	PX4	A	1305	-	-	23/49/49/49	-
4	PX4	A	1306	-	-	18/49/49/49	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1310	PX4	O5-C9	5.14	1.48	1.33
4	A	1312	PX4	O5-C9	4.95	1.47	1.33
4	A	1310	PX4	O7-C23	4.77	1.47	1.34
4	A	1308	PX4	O5-C9	4.75	1.47	1.33
4	A	1308	PX4	O7-C23	4.73	1.47	1.34
4	A	1306	PX4	O7-C23	4.61	1.47	1.34
4	A	1312	PX4	O7-C23	4.51	1.47	1.34
4	A	1309	PX4	O5-C9	4.46	1.46	1.33
4	A	1307	PX4	O7-C23	4.42	1.46	1.34
4	A	1311	PX4	O7-C23	4.31	1.46	1.34
4	A	1306	PX4	O5-C9	4.29	1.45	1.33
4	A	1305	PX4	O7-C23	4.28	1.46	1.34
4	A	1307	PX4	O5-C9	4.25	1.45	1.33
4	A	1309	PX4	O7-C23	4.25	1.46	1.34
4	A	1311	PX4	O5-C9	4.19	1.45	1.33
4	A	1305	PX4	O5-C9	3.92	1.44	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1304	1N7	C9-C5-C4	5.32	122.52	117.67
4	A	1311	PX4	O7-C23-C24	5.09	122.47	111.50
3	A	1304	1N7	C19-C18-C6	-5.01	102.84	109.71
4	A	1310	PX4	O7-C23-C24	4.94	122.14	111.50
3	A	1304	1N7	C7-C6-C18	4.83	125.09	118.33
4	A	1312	PX4	O7-C23-C24	4.81	121.86	111.50
3	A	1304	1N7	C5-C9-C20	4.69	125.10	119.50
3	A	1304	1N7	C6-C18-C17	4.66	117.99	111.81
4	A	1308	PX4	O7-C23-C24	4.59	121.40	111.50
4	A	1305	PX4	O7-C23-C24	4.31	120.79	111.50
4	A	1309	PX4	O7-C23-C24	4.05	120.22	111.50
4	A	1307	PX4	O7-C23-C24	3.78	119.65	111.50
4	A	1311	PX4	C7-O7-C23	-3.62	108.89	117.79
3	A	1304	1N7	C8-C7-C6	-3.35	98.49	105.13
4	A	1311	PX4	O5-C9-C10	3.31	122.30	111.91
4	A	1312	PX4	O5-C9-C10	3.28	122.20	111.91
4	A	1310	PX4	O5-C9-C10	3.27	122.17	111.91
4	A	1305	PX4	O5-C9-C10	3.26	122.13	111.91
3	A	1304	1N7	C2-C19-C18	3.24	115.29	111.82
4	A	1308	PX4	O5-C9-C10	2.98	121.24	111.91
4	A	1305	PX4	O5-C9-O6	-2.88	116.31	123.59
4	A	1306	PX4	O7-C23-C24	2.77	117.48	111.50
4	A	1309	PX4	O5-C9-C10	2.68	120.31	111.91
3	A	1304	1N7	C6-C5-C4	-2.67	104.92	107.40
3	A	1304	1N7	C9-C5-C6	-2.62	97.46	100.09
4	A	1306	PX4	O5-C9-C10	2.55	119.91	111.91
4	A	1311	PX4	O5-C9-O6	-2.50	117.29	123.59
3	A	1304	1N7	C19-C18-C17	2.41	114.76	111.88
4	A	1310	PX4	O5-C8-C7	2.39	115.38	108.43
4	A	1306	PX4	C8-C7-C6	-2.30	106.34	111.79
4	A	1308	PX4	C8-C7-C6	-2.25	106.47	111.79
4	A	1312	PX4	O7-C23-O8	-2.22	118.34	123.70
4	A	1311	PX4	O7-C23-O8	-2.20	118.39	123.70
4	A	1310	PX4	O8-C23-C24	-2.19	115.19	123.73
3	A	1304	1N7	C12-C1-C2	2.17	116.51	112.78
4	A	1307	PX4	O5-C9-C10	2.10	118.51	111.91
3	A	1304	1N7	C14-C15-C2	2.06	114.84	112.66
3	A	1304	1N7	C15-C16-C17	-2.04	112.21	114.46

There are no chirality outliers.

All (188) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1304	1N7	C22-C20-C9-C5
3	A	1304	1N7	C23-C24-N1-C25
4	A	1305	PX4	C1-O3-P1-O2
4	A	1305	PX4	C6-O4-P1-O1
4	A	1306	PX4	C1-O3-P1-O1
4	A	1306	PX4	C1-O3-P1-O2
4	A	1306	PX4	C1-O3-P1-O4
4	A	1306	PX4	O3-C1-C2-N1
4	A	1306	PX4	C24-C23-O7-C7
4	A	1307	PX4	O3-C1-C2-N1
4	A	1308	PX4	C1-O3-P1-O1
4	A	1308	PX4	C1-O3-P1-O2
4	A	1308	PX4	C1-O3-P1-O4
4	A	1308	PX4	C6-O4-P1-O2
4	A	1308	PX4	C24-C23-O7-C7
4	A	1309	PX4	C24-C23-O7-C7
4	A	1310	PX4	C6-O4-P1-O1
4	A	1310	PX4	C6-O4-P1-O2
4	A	1310	PX4	C6-O4-P1-O3
4	A	1310	PX4	C24-C23-O7-C7
4	A	1311	PX4	C1-O3-P1-O1
4	A	1311	PX4	C1-O3-P1-O2
4	A	1311	PX4	C1-O3-P1-O4
4	A	1312	PX4	C1-O3-P1-O2
4	A	1312	PX4	C6-O4-P1-O3
4	A	1312	PX4	O3-C1-C2-N1
4	A	1312	PX4	O8-C23-O7-C7
4	A	1308	PX4	O6-C9-O5-C8
4	A	1306	PX4	O8-C23-O7-C7
4	A	1310	PX4	O8-C23-O7-C7
4	A	1308	PX4	C10-C9-O5-C8
4	A	1312	PX4	C24-C23-O7-C7
3	A	1304	1N7	C22-C20-C9-C8
4	A	1308	PX4	O8-C23-O7-C7
4	A	1309	PX4	O8-C23-O7-C7
3	A	1304	1N7	C21-C20-C9-C8
3	A	1304	1N7	C9-C20-C22-C23
4	A	1311	PX4	C1-C2-N1-C3
3	A	1304	1N7	C21-C20-C9-C5
4	A	1311	PX4	C16-C17-C18-C19
4	A	1308	PX4	C23-C24-C25-C26
4	A	1311	PX4	C1-C2-N1-C4
4	A	1312	PX4	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
4	A	1310	PX4	C10-C9-O5-C8
3	A	1304	1N7	O1-C24-N1-C25
4	A	1307	PX4	C6-O4-P1-O3
4	A	1312	PX4	C1-O3-P1-O4
4	A	1306	PX4	C9-C10-C11-C12
4	A	1310	PX4	C17-C18-C19-C20
4	A	1307	PX4	C24-C23-O7-C7
4	A	1309	PX4	C10-C9-O5-C8
4	A	1305	PX4	C27-C28-C29-C30
4	A	1311	PX4	C31-C32-C33-C34
4	A	1307	PX4	O8-C23-O7-C7
4	A	1307	PX4	C29-C30-C31-C32
4	A	1312	PX4	C11-C12-C13-C14
4	A	1305	PX4	C24-C23-O7-C7
3	A	1304	1N7	C21-C20-C22-C23
4	A	1311	PX4	C1-C2-N1-C5
4	A	1307	PX4	C13-C14-C15-C16
4	A	1307	PX4	C27-C28-C29-C30
4	A	1309	PX4	C14-C15-C16-C17
4	A	1312	PX4	C24-C25-C26-C27
4	A	1310	PX4	O6-C9-O5-C8
4	A	1305	PX4	C10-C11-C12-C13
4	A	1305	PX4	C29-C30-C31-C32
4	A	1309	PX4	C24-C25-C26-C27
4	A	1309	PX4	C28-C29-C30-C31
4	A	1309	PX4	O6-C9-O5-C8
3	A	1304	1N7	C20-C22-C23-C24
4	A	1309	PX4	C17-C18-C19-C20
4	A	1306	PX4	C30-C31-C32-C33
4	A	1305	PX4	O8-C23-O7-C7
4	A	1307	PX4	C1-C2-N1-C5
4	A	1305	PX4	C10-C9-O5-C8
4	A	1305	PX4	C33-C34-C35-C36
4	A	1306	PX4	C15-C16-C17-C18
4	A	1306	PX4	C23-C24-C25-C26
4	A	1312	PX4	C9-C10-C11-C12
4	A	1308	PX4	C15-C16-C17-C18
4	A	1310	PX4	C26-C27-C28-C29
4	A	1312	PX4	C10-C11-C12-C13
4	A	1309	PX4	C31-C32-C33-C34
4	A	1305	PX4	O6-C9-O5-C8
4	A	1308	PX4	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	A	1309	PX4	C15-C16-C17-C18
4	A	1305	PX4	C16-C17-C18-C19
4	A	1308	PX4	C27-C28-C29-C30
4	A	1309	PX4	C16-C17-C18-C19
4	A	1307	PX4	C30-C31-C32-C33
4	A	1305	PX4	C6-O4-P1-O3
4	A	1308	PX4	C6-O4-P1-O3
4	A	1305	PX4	C17-C18-C19-C20
4	A	1310	PX4	C32-C33-C34-C35
4	A	1311	PX4	C9-C10-C11-C12
4	A	1308	PX4	C25-C26-C27-C28
4	A	1305	PX4	C25-C26-C27-C28
4	A	1312	PX4	C16-C17-C18-C19
4	A	1307	PX4	C15-C16-C17-C18
4	A	1310	PX4	C24-C25-C26-C27
4	A	1311	PX4	C10-C11-C12-C13
4	A	1307	PX4	C11-C12-C13-C14
4	A	1308	PX4	C7-C8-O5-C9
4	A	1307	PX4	C12-C13-C14-C15
4	A	1311	PX4	O4-C6-C7-C8
4	A	1312	PX4	C27-C28-C29-C30
4	A	1309	PX4	C11-C12-C13-C14
4	A	1309	PX4	C9-C10-C11-C12
4	A	1306	PX4	C26-C27-C28-C29
4	A	1309	PX4	C29-C30-C31-C32
4	A	1305	PX4	C32-C33-C34-C35
4	A	1306	PX4	C11-C12-C13-C14
4	A	1306	PX4	C14-C15-C16-C17
4	A	1306	PX4	C6-C7-C8-O5
4	A	1312	PX4	C6-C7-C8-O5
4	A	1308	PX4	C13-C14-C15-C16
4	A	1311	PX4	C13-C14-C15-C16
4	A	1306	PX4	O7-C7-C8-O5
4	A	1310	PX4	O7-C7-C8-O5
4	A	1310	PX4	C30-C31-C32-C33
4	A	1308	PX4	C12-C13-C14-C15
4	A	1310	PX4	C9-C10-C11-C12
4	A	1312	PX4	C32-C33-C34-C35
4	A	1307	PX4	O4-C6-C7-C8
4	A	1310	PX4	C11-C12-C13-C14
4	A	1309	PX4	C10-C11-C12-C13
4	A	1312	PX4	C7-C6-O4-P1

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Mol	Chain	Res	Type	Atoms
4	A	1311	PX4	O4-C6-C7-O7
4	A	1311	PX4	C32-C33-C34-C35
4	A	1309	PX4	O7-C7-C8-O5
4	A	1312	PX4	O7-C7-C8-O5
4	A	1310	PX4	C33-C34-C35-C36
4	A	1305	PX4	C18-C19-C20-C21
4	A	1305	PX4	C1-O3-P1-O4
4	A	1305	PX4	C6-O4-P1-O2
4	A	1307	PX4	C6-O4-P1-O1
4	A	1307	PX4	C1-C2-N1-C4
4	A	1312	PX4	C1-O3-P1-O1
4	A	1312	PX4	C6-O4-P1-O1
4	A	1312	PX4	C13-C14-C15-C16
4	A	1308	PX4	C24-C25-C26-C27
4	A	1312	PX4	C26-C27-C28-C29
4	A	1307	PX4	O4-C6-C7-O7
4	A	1312	PX4	C15-C16-C17-C18
4	A	1305	PX4	O3-C1-C2-N1
4	A	1309	PX4	O3-C1-C2-N1
4	A	1311	PX4	O3-C1-C2-N1
4	A	1305	PX4	C28-C29-C30-C31
4	A	1307	PX4	C1-C2-N1-C3
4	A	1309	PX4	C23-C24-C25-C26
4	A	1309	PX4	C1-O3-P1-O4
4	A	1310	PX4	C6-C7-C8-O5
4	A	1312	PX4	C12-C13-C14-C15
4	A	1306	PX4	C24-C25-C26-C27
4	A	1310	PX4	C27-C28-C29-C30
4	A	1310	PX4	C12-C13-C14-C15
4	A	1311	PX4	C18-C19-C20-C21
4	A	1309	PX4	C6-C7-C8-O5
4	A	1305	PX4	C23-C24-C25-C26
4	A	1306	PX4	C29-C30-C31-C32
4	A	1312	PX4	C31-C32-C33-C34
4	A	1308	PX4	C30-C31-C32-C33
4	A	1308	PX4	C28-C29-C30-C31
4	A	1311	PX4	C30-C31-C32-C33
4	A	1308	PX4	C18-C19-C20-C21
4	A	1309	PX4	C27-C28-C29-C30
4	A	1311	PX4	O7-C23-C24-C25
3	A	1304	1N7	C22-C23-C24-O1
4	A	1312	PX4	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	A	1309	PX4	C11-C10-C9-O5
4	A	1312	PX4	O7-C23-C24-C25
4	A	1311	PX4	O8-C23-C24-C25
4	A	1305	PX4	O7-C23-C24-C25
4	A	1309	PX4	C11-C10-C9-O6
4	A	1309	PX4	C1-O3-P1-O2
4	A	1310	PX4	C1-C2-N1-C5
4	A	1310	PX4	C28-C29-C30-C31
4	A	1306	PX4	C16-C17-C18-C19
4	A	1307	PX4	C26-C27-C28-C29
4	A	1312	PX4	O8-C23-C24-C25
4	A	1305	PX4	O8-C23-C24-C25
4	A	1307	PX4	C28-C29-C30-C31
4	A	1312	PX4	C29-C30-C31-C32
4	A	1311	PX4	C19-C20-C21-C22
4	A	1311	PX4	C12-C13-C14-C15
4	A	1310	PX4	C1-C2-N1-C4
4	A	1309	PX4	C30-C31-C32-C33
4	A	1309	PX4	C25-C26-C27-C28

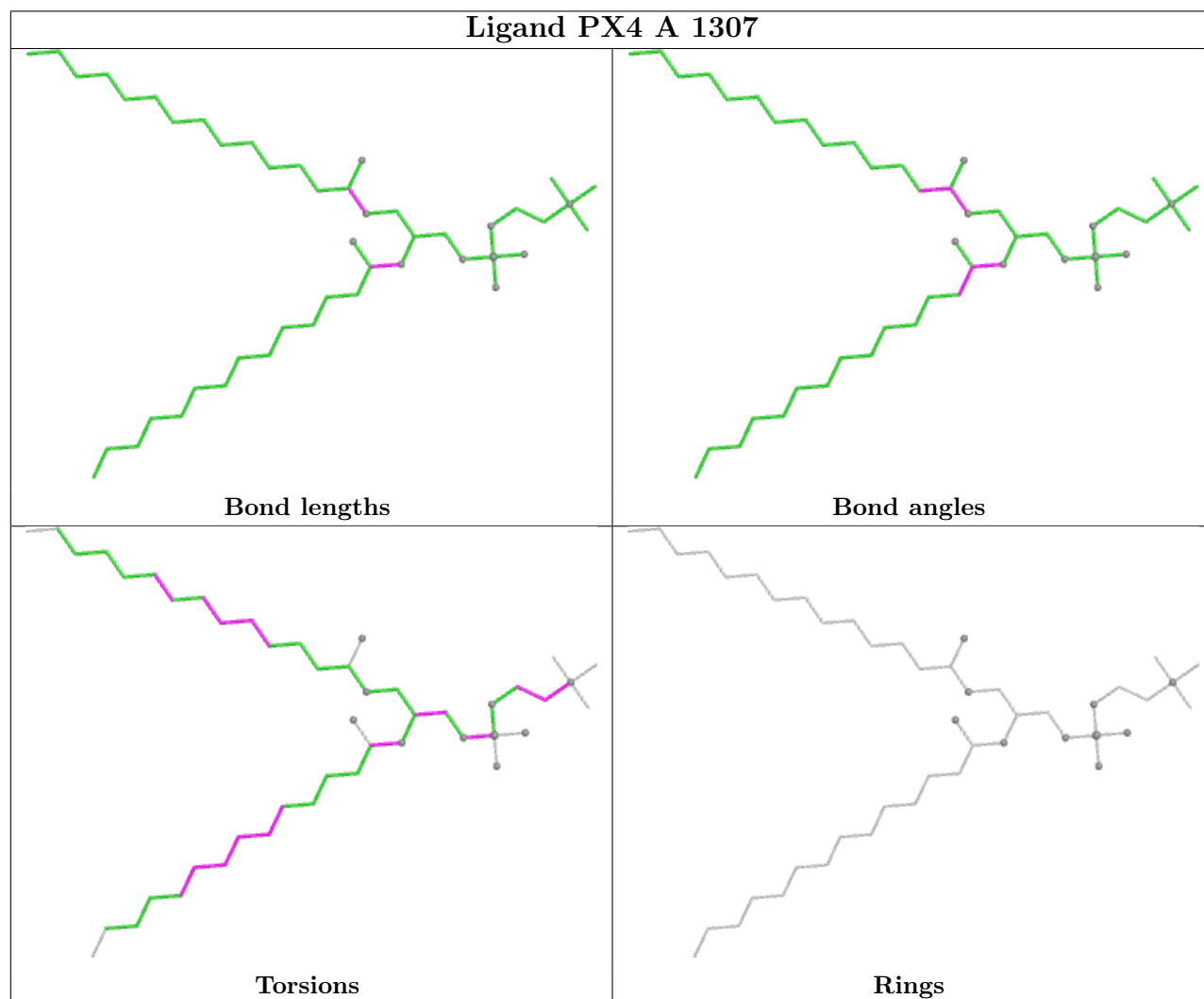
There are no ring outliers.

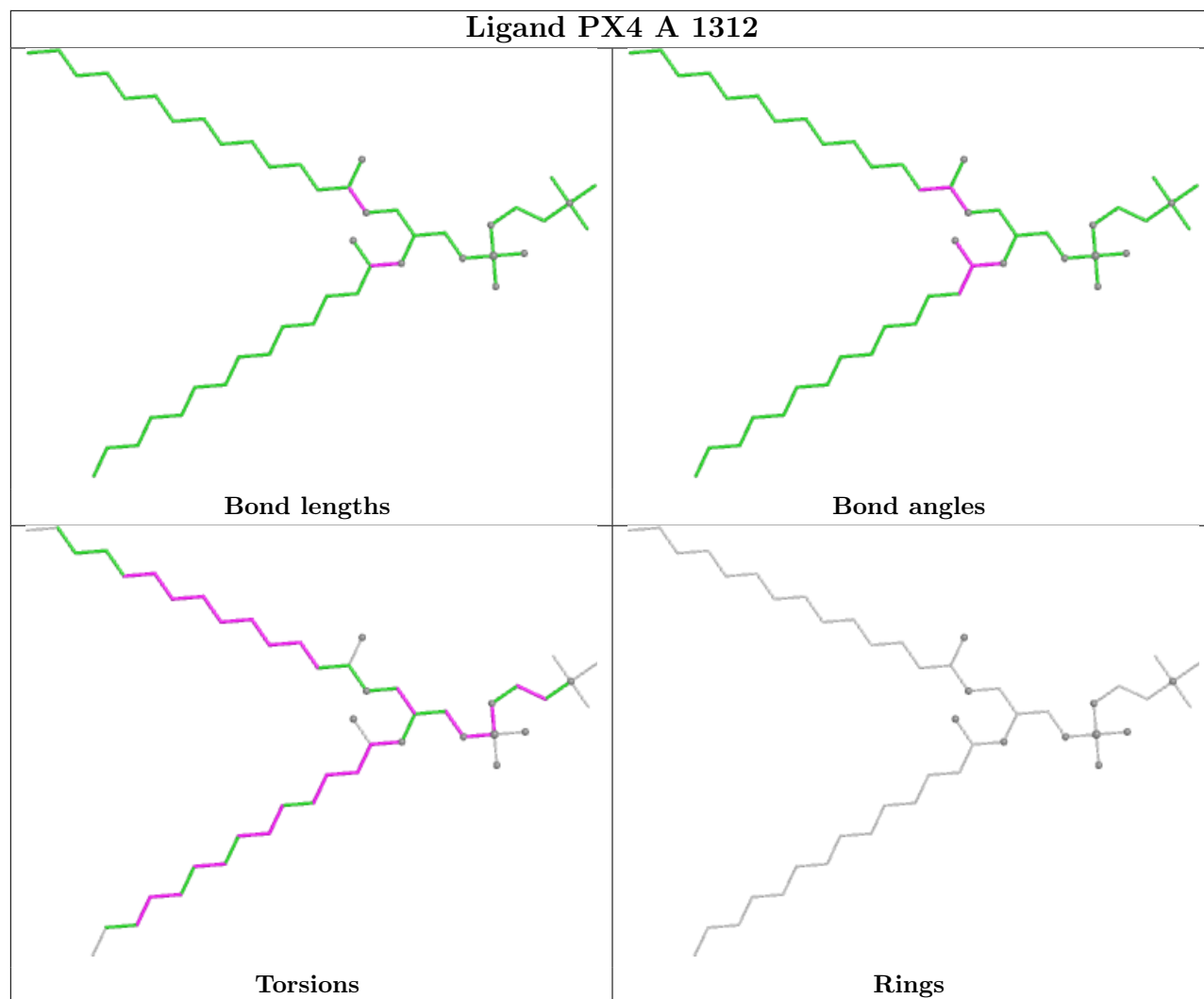
9 monomers are involved in 31 short contacts:

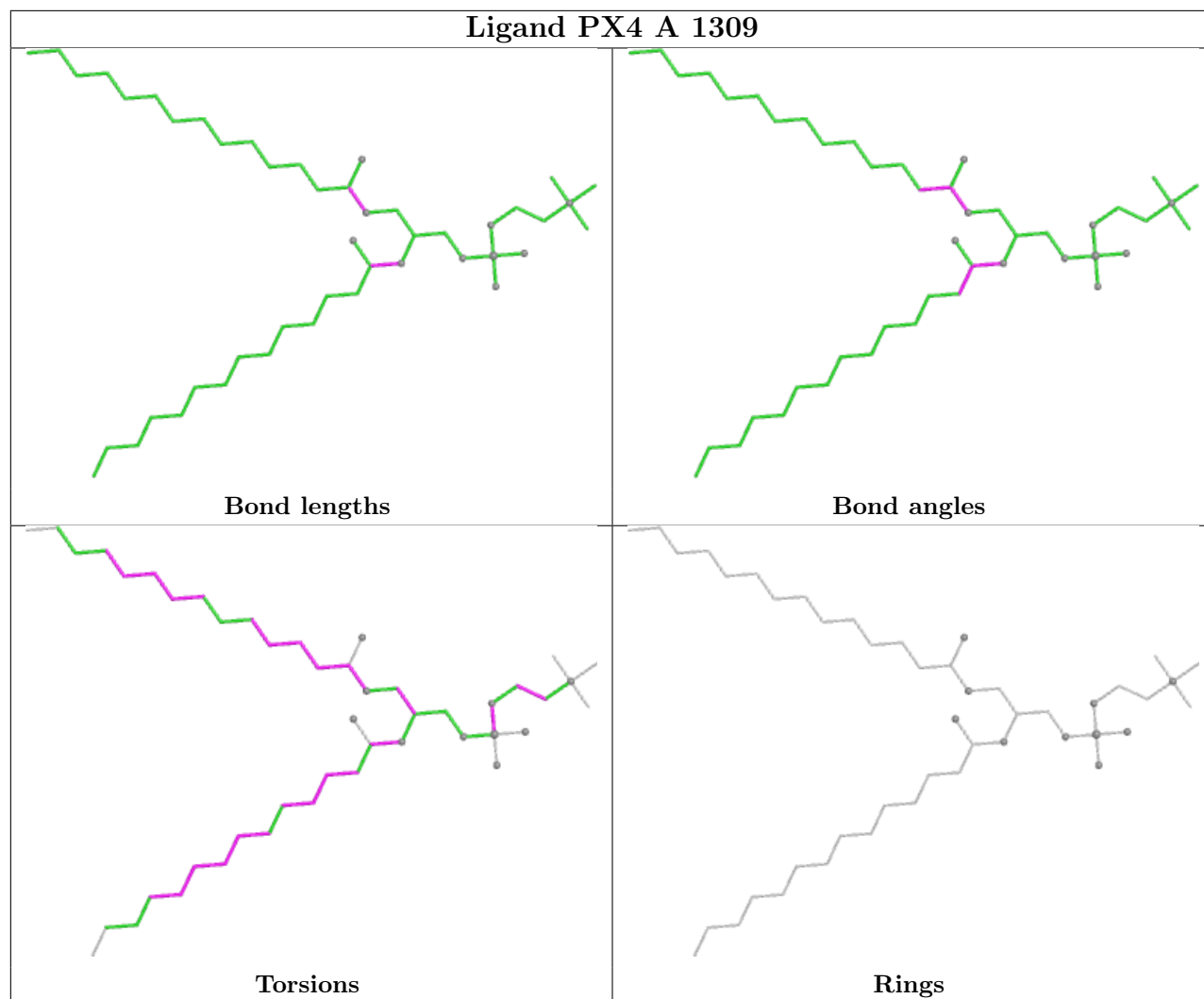
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1307	PX4	6	0
4	A	1312	PX4	2	1
4	A	1309	PX4	1	1
4	A	1310	PX4	1	3
4	A	1308	PX4	3	1
4	A	1311	PX4	1	2
3	A	1304	1N7	5	0
4	A	1305	PX4	6	0
4	A	1306	PX4	6	0

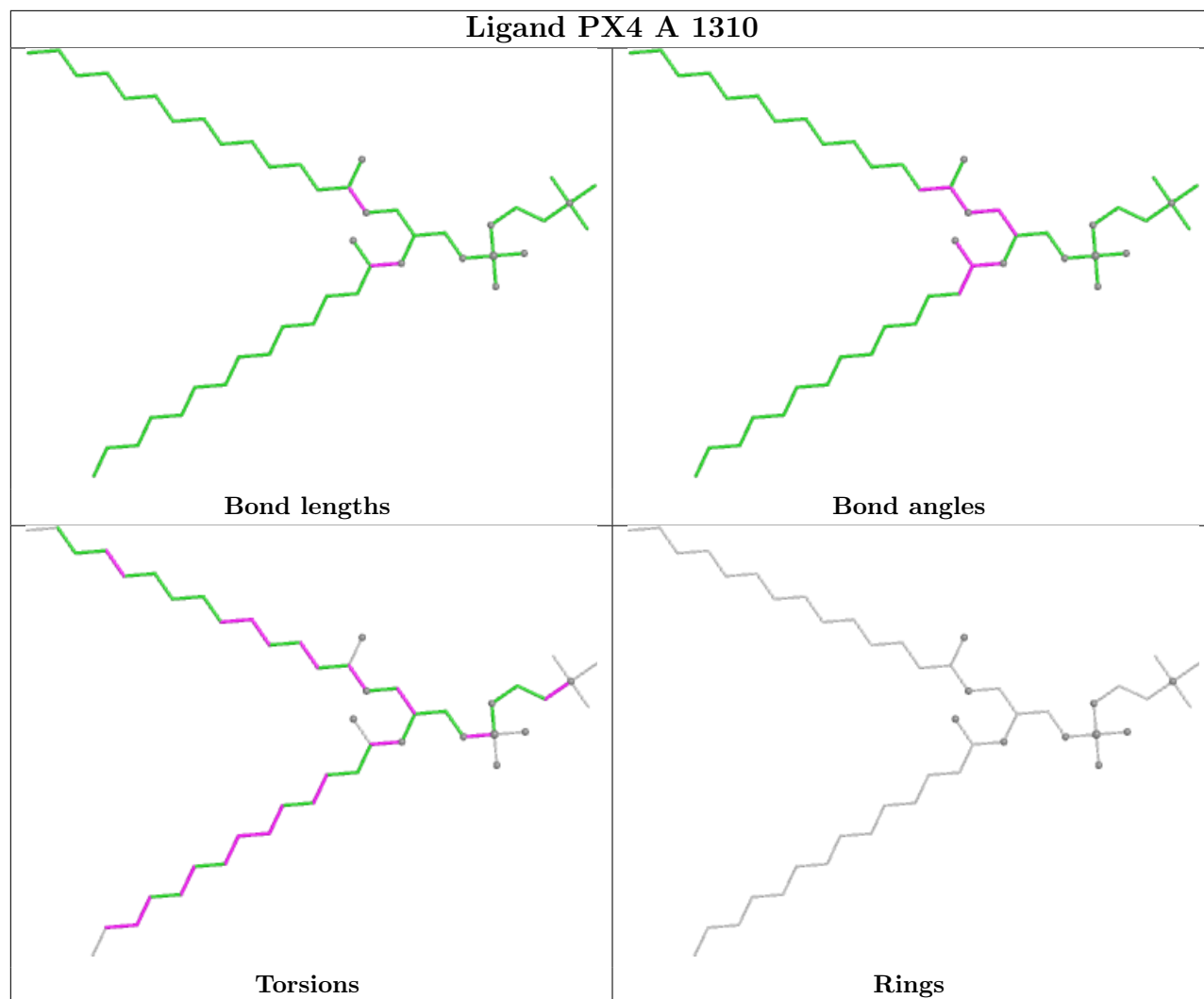
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

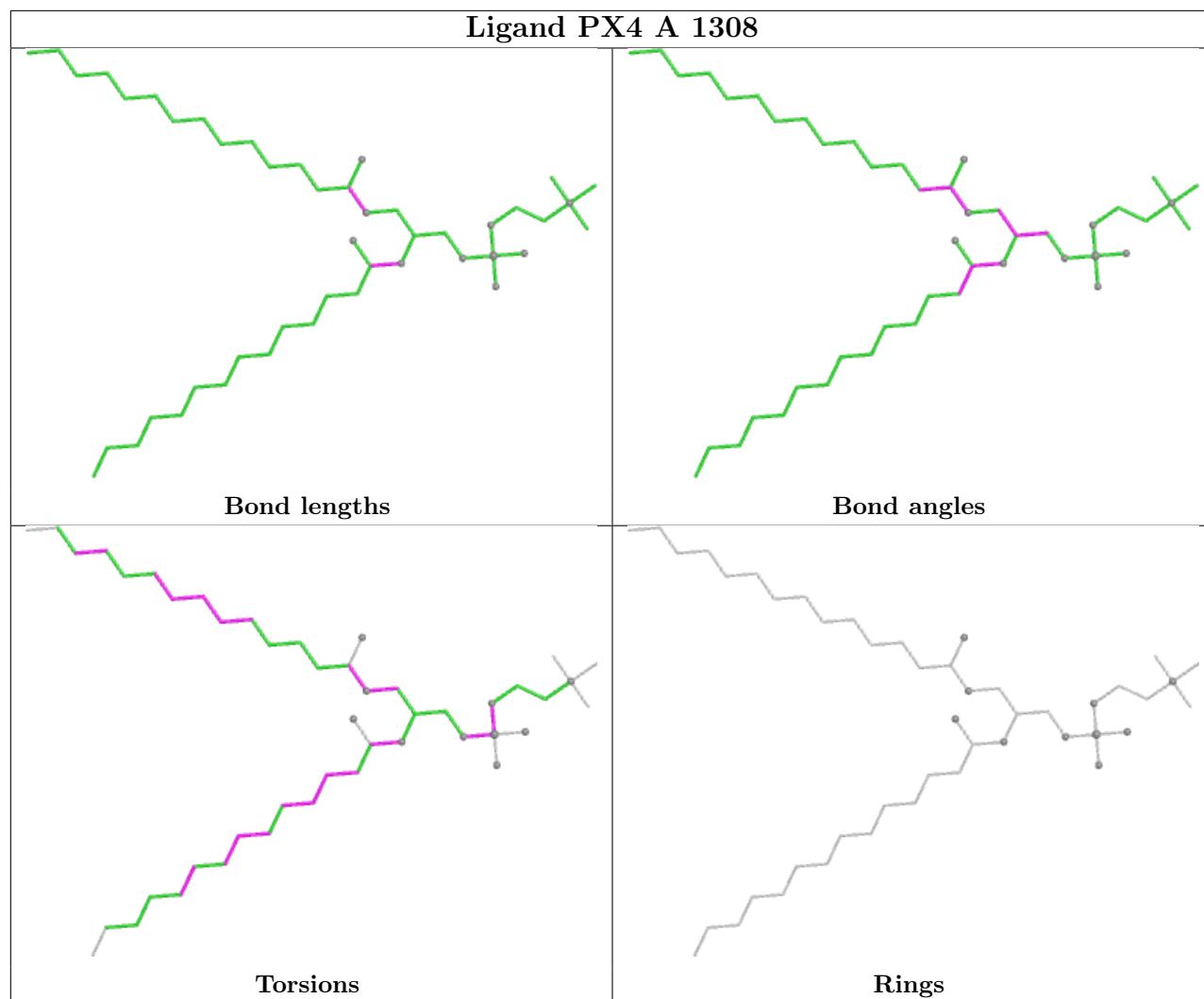
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

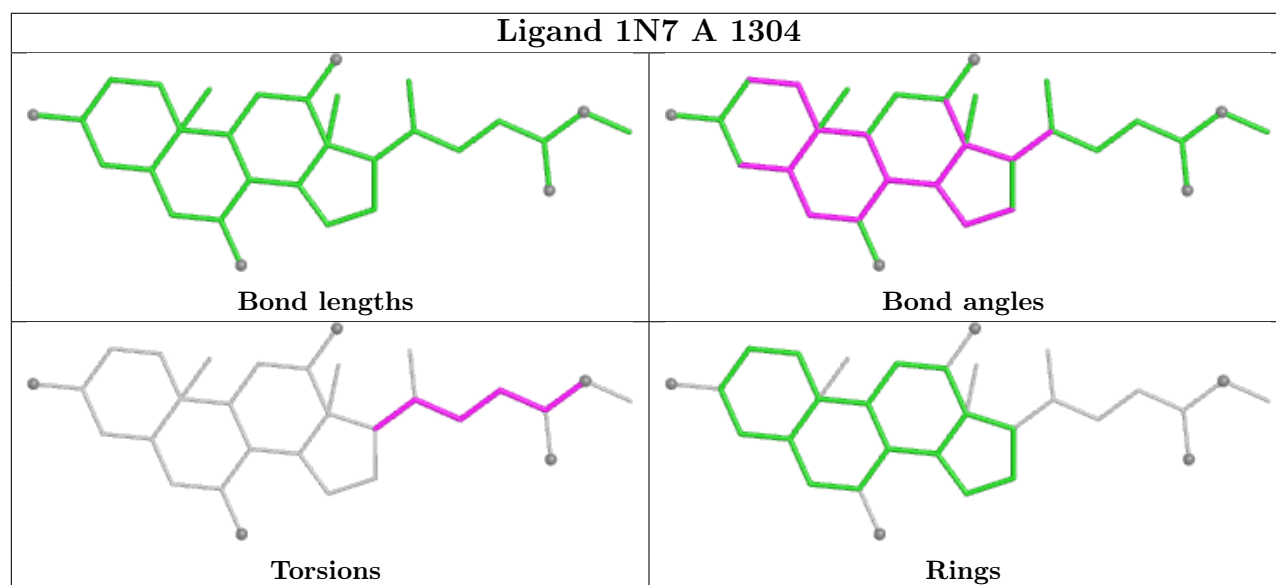
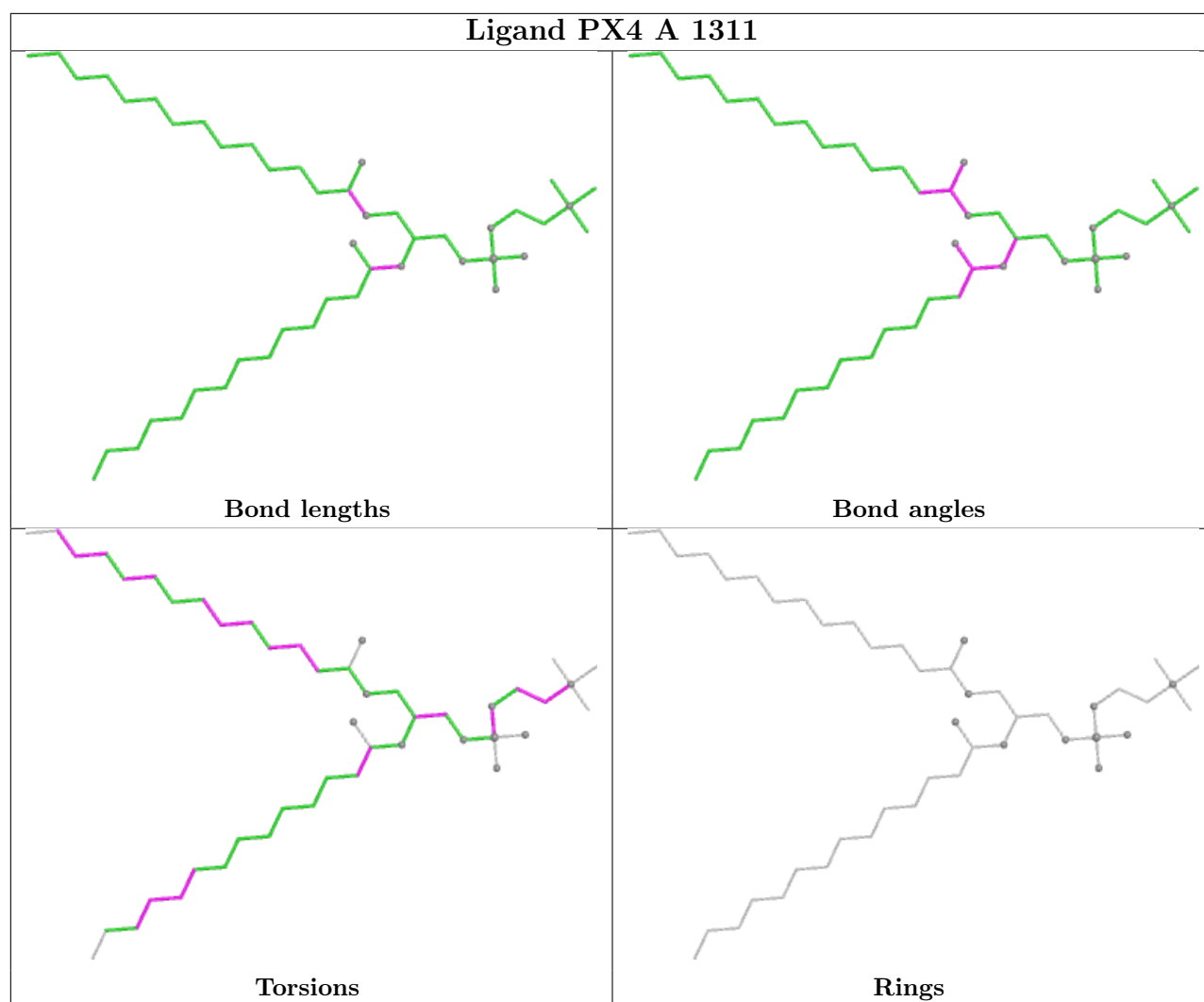


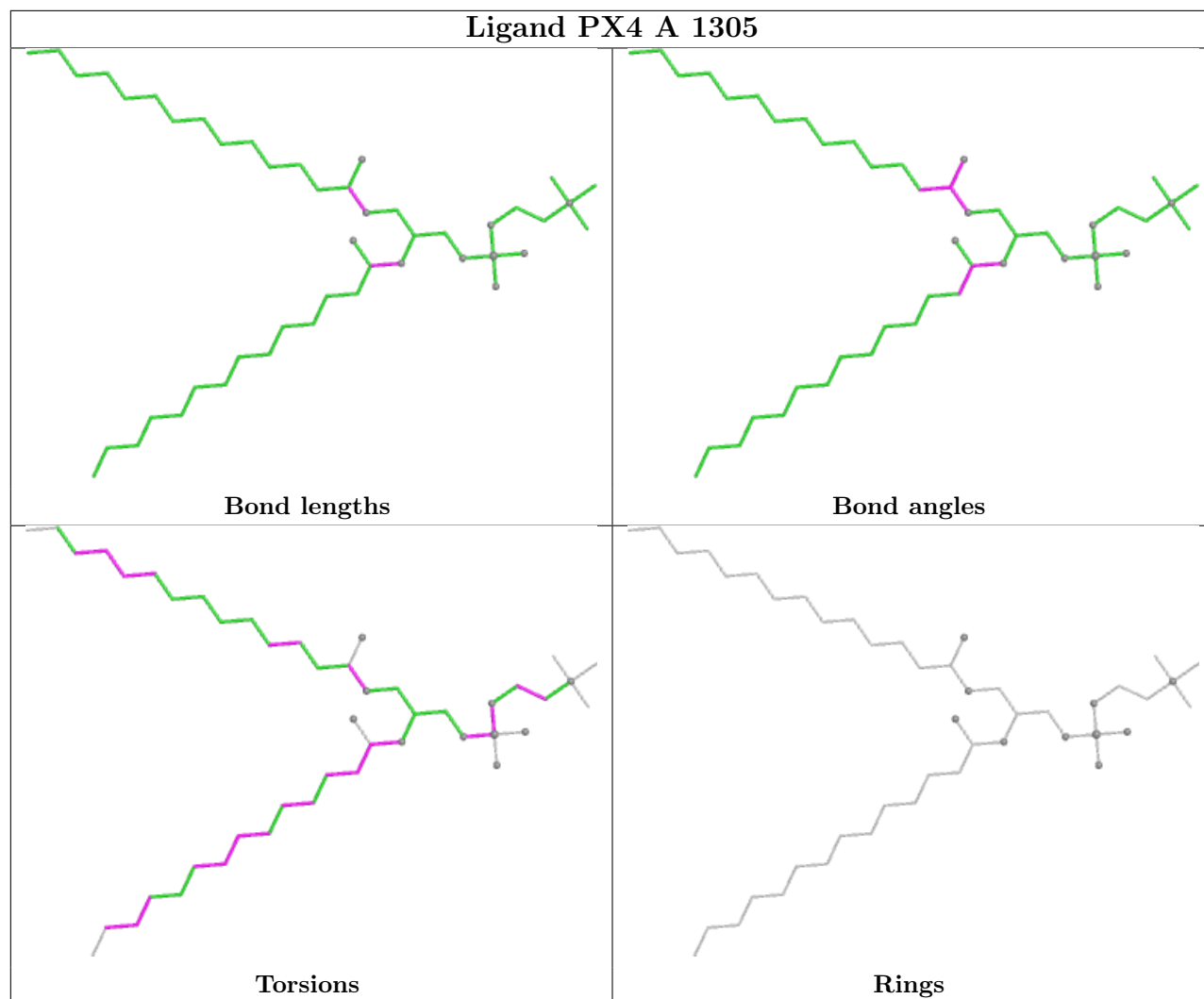


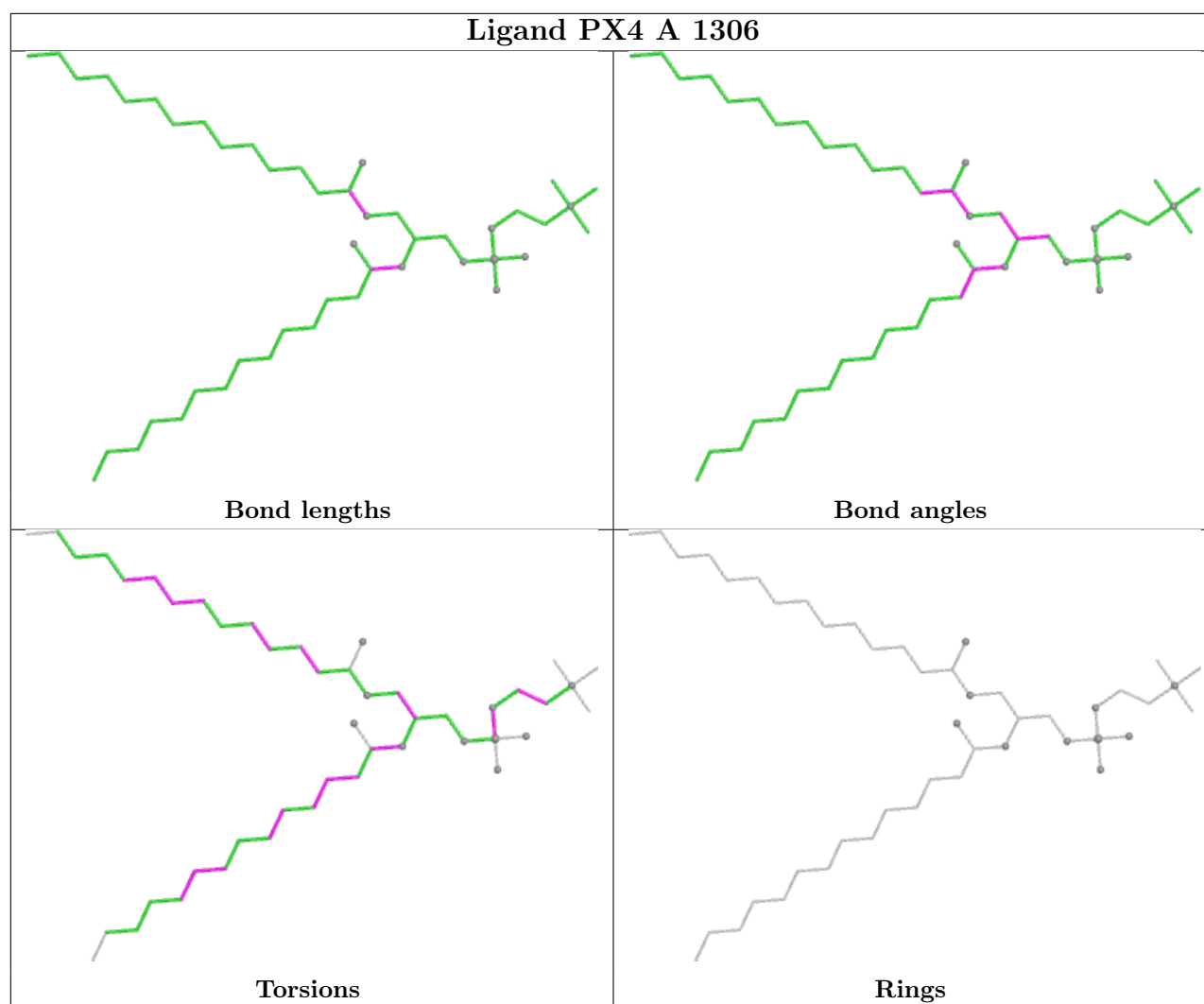












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	229/269 (85%)	0.66	28 (12%) 8 5	21, 64, 119, 151	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1096	GLU	5.7
1	A	1091	THR	5.2
1	A	1090	PRO	5.0
1	A	1095	PHE	4.6
1	A	1092	SER	4.1
1	A	1093	SER	4.0
1	A	1068	ARG	3.6
1	A	1094	GLY	3.5
1	A	1226	GLN	3.2
1	A	1099	ARG	3.2
1	A	1013	PHE	3.0
1	A	999	GLY	2.9
1	A	1115	GLN	2.8
1	A	1067	HIS	2.8
1	A	1002	TYR	2.7
1	A	1073	LYS	2.7
1	A	1150	GLN	2.5
1	A	1222	ALA	2.4
1	A	1015	THR	2.3
1	A	1070	SER	2.3
1	A	1046	THR	2.2
1	A	1035	LYS	2.1
1	A	1047	LEU	2.1
1	A	1223	ILE	2.1
1	A	1065	TYR	2.1
1	A	1036	THR	2.0
1	A	1219	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1189	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

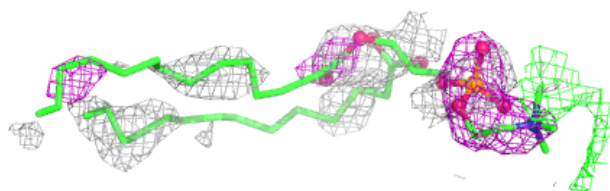
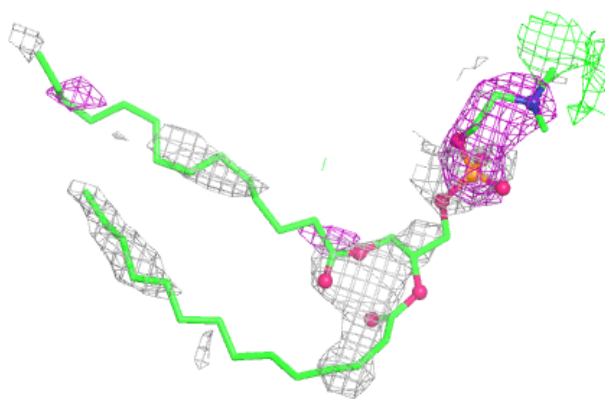
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PX4	A	1308	46/46	0.51	0.37	69,89,105,110	0
4	PX4	A	1306	46/46	0.58	0.35	69,91,124,143	0
4	PX4	A	1307	46/46	0.68	0.36	75,100,126,148	0
4	PX4	A	1312	46/46	0.72	0.25	41,66,85,99	0
4	PX4	A	1309	46/46	0.75	0.26	70,91,131,134	0
4	PX4	A	1305	46/46	0.79	0.28	49,83,102,124	0
3	1N7	A	1304	30/43	0.80	0.22	62,69,82,89	0
2	NA	A	1303	1/1	0.81	0.24	58,58,58,58	1
4	PX4	A	1311	46/46	0.85	0.20	57,66,84,89	0
4	PX4	A	1310	46/46	0.87	0.19	34,59,70,89	0
2	NA	A	1302	1/1	0.92	0.17	51,51,51,51	1
2	NA	A	1301	1/1	0.97	0.68	23,23,23,23	1

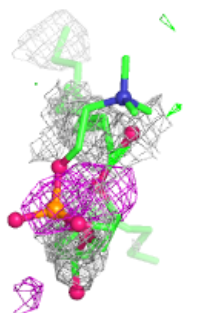
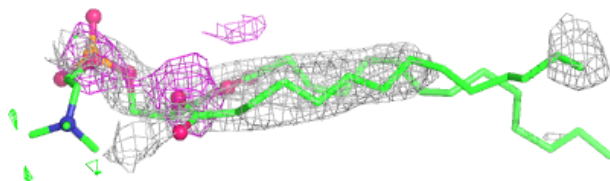
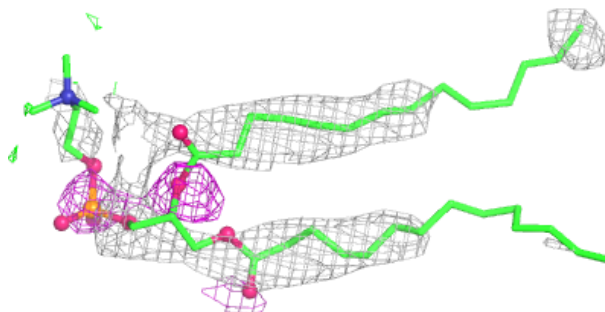
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PX4 A 1308:

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

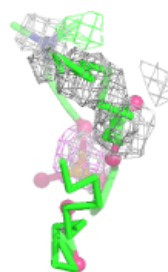
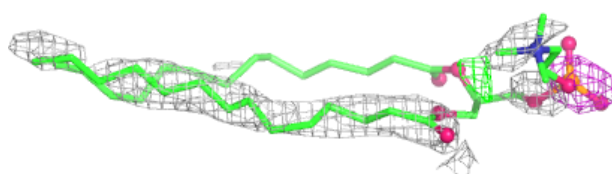
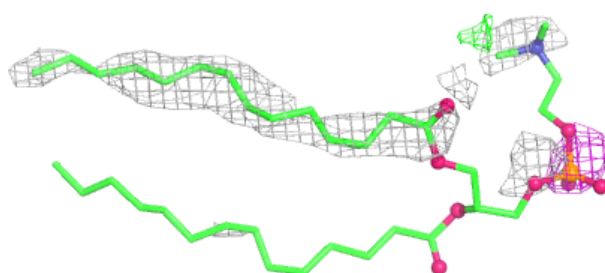
**Electron density around PX4 A 1306:**

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

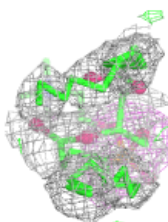
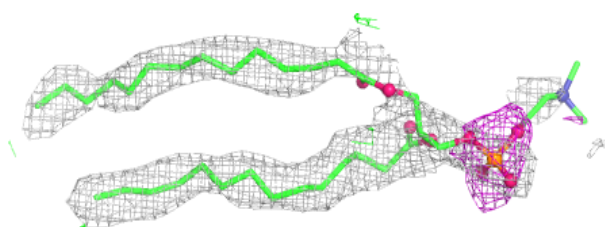


Electron density around PX4 A 1307:

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

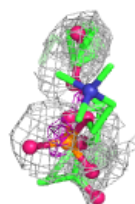
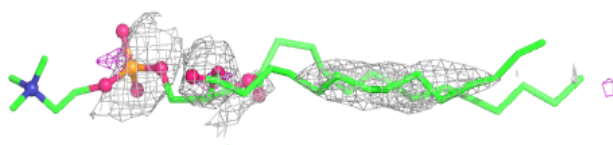
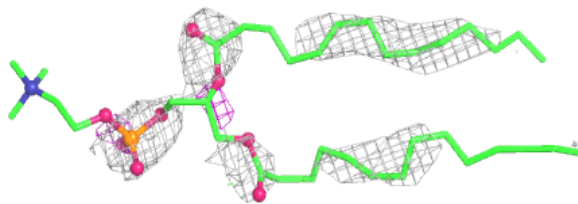
**Electron density around PX4 A 1312:**

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



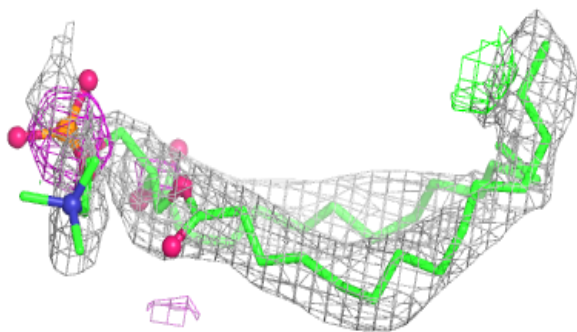
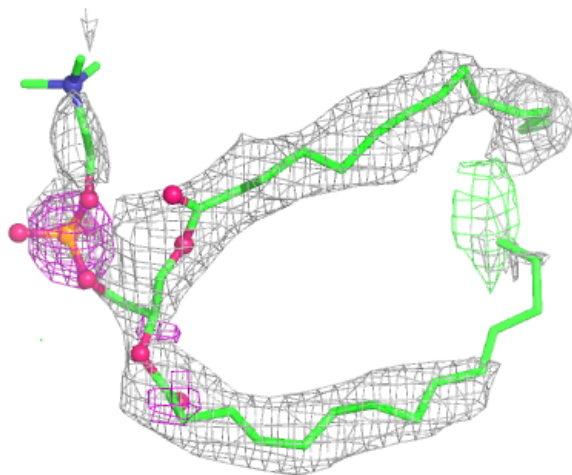
Electron density around PX4 A 1309:

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



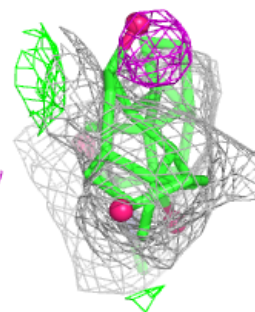
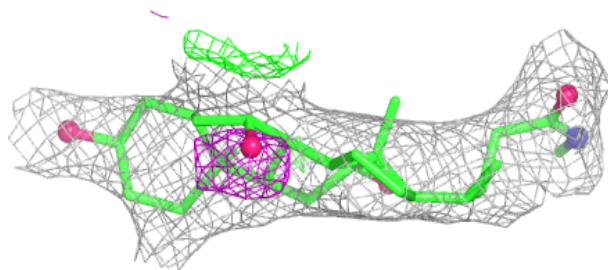
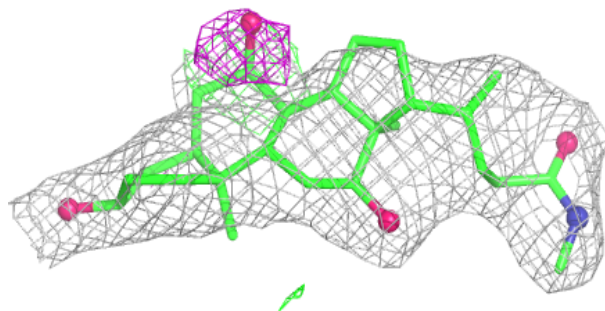
Electron density around PX4 A 1305:

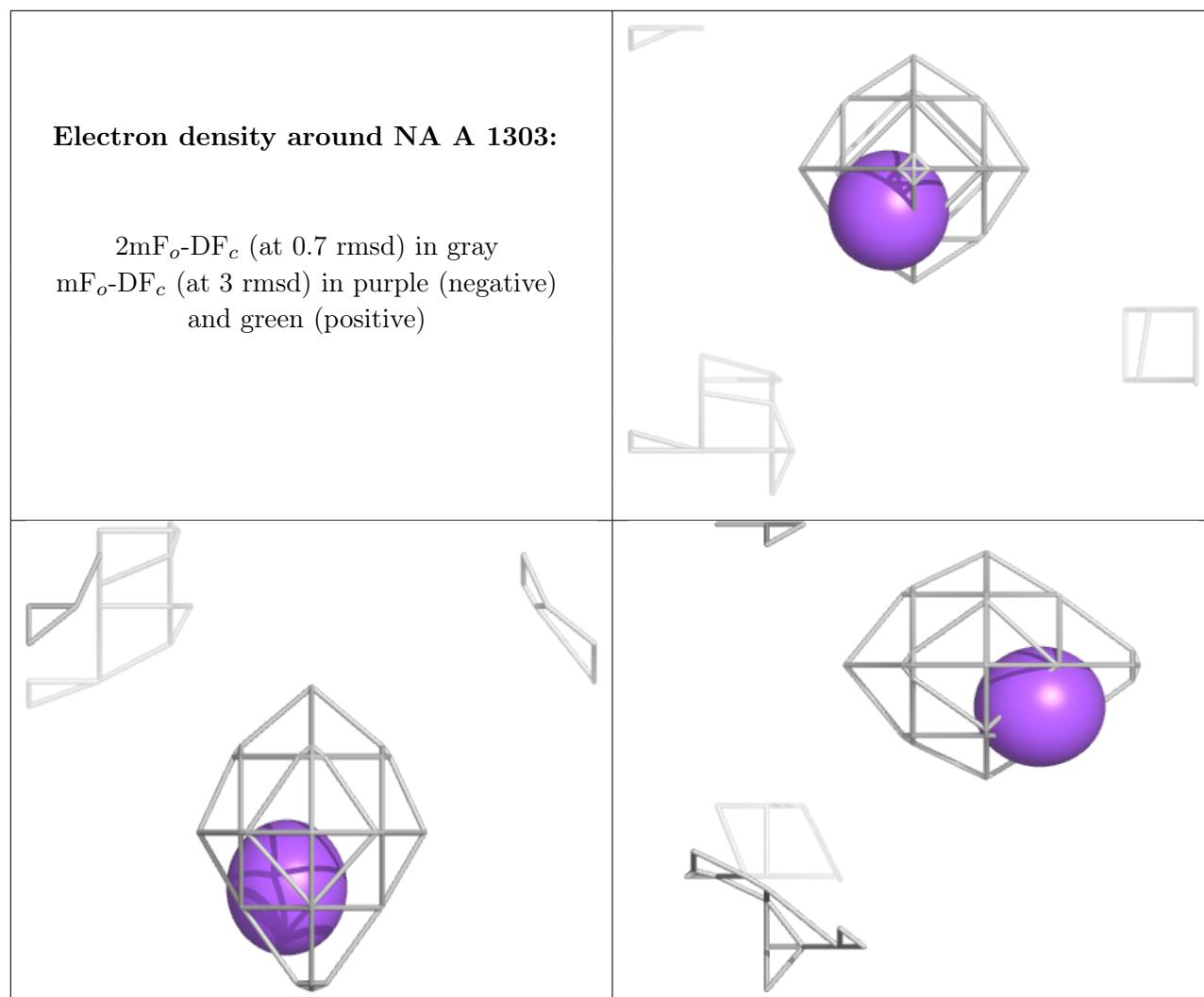
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 1N7 A 1304:

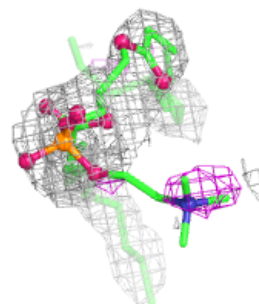
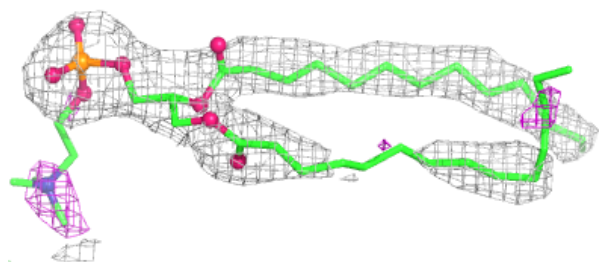
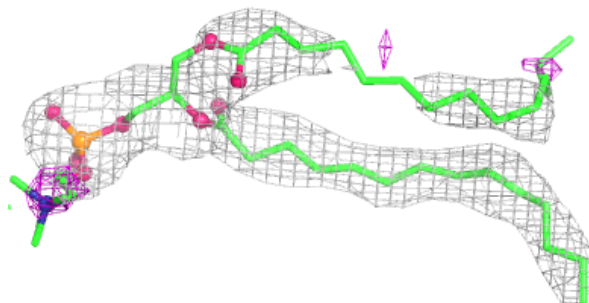
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



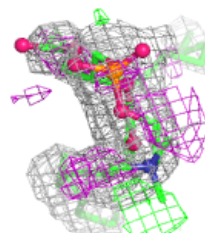
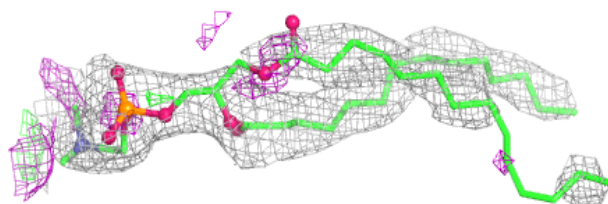
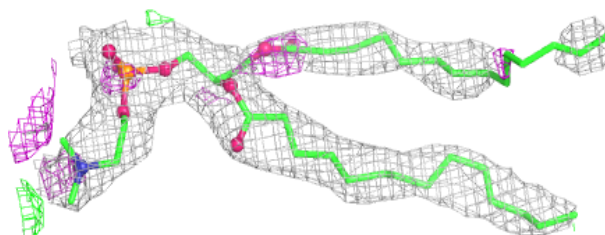


Electron density around PX4 A 1311:

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

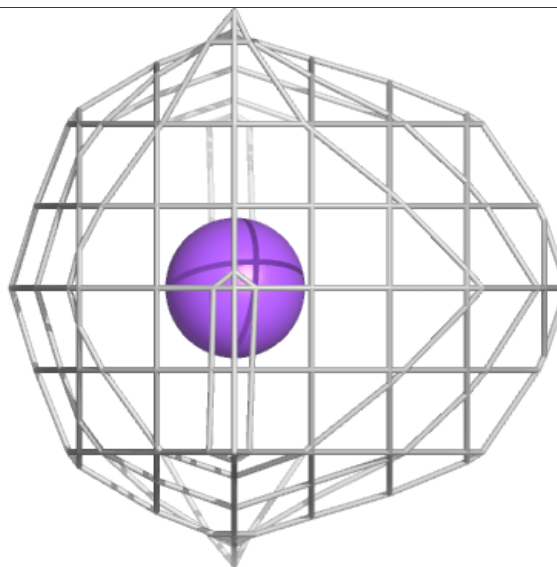
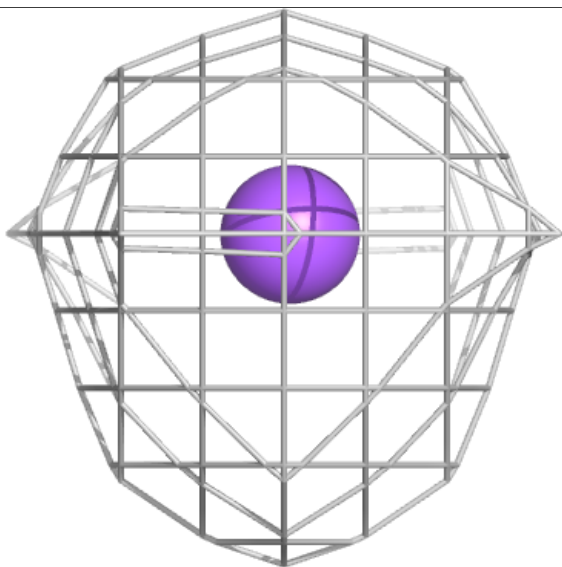
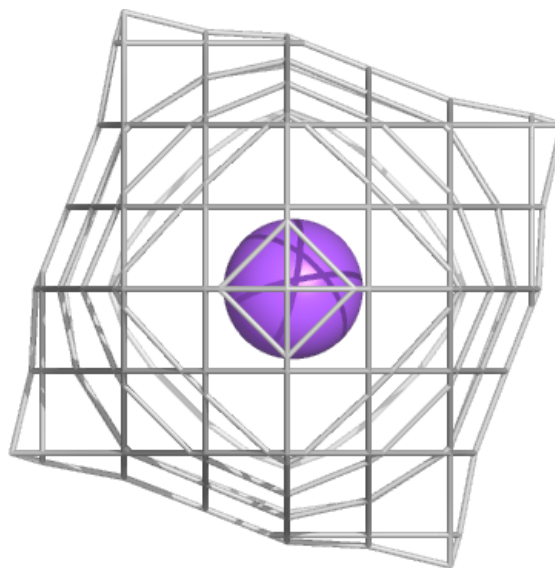
**Electron density around PX4 A 1310:**

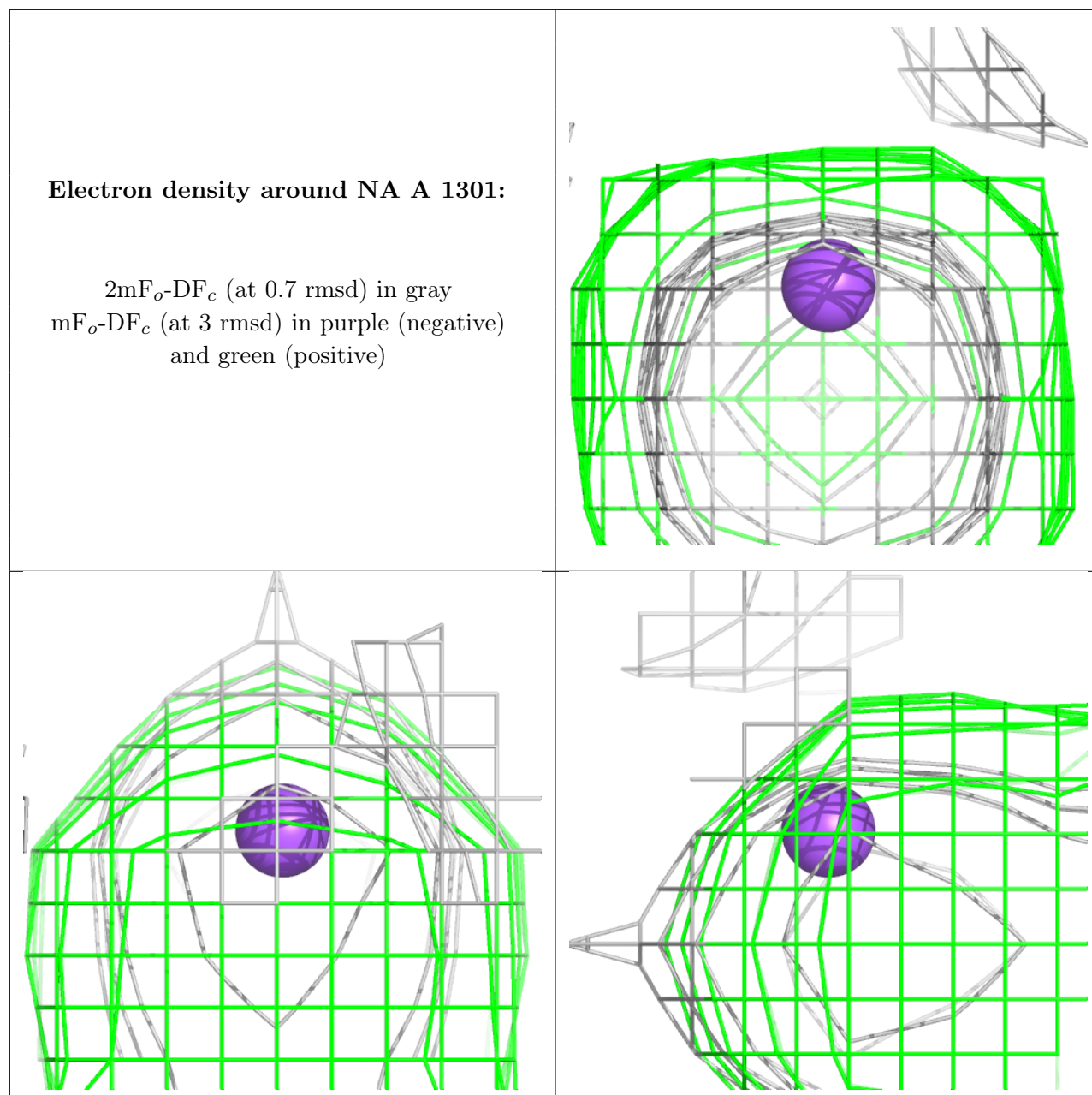
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NA A 1302:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.