



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:19 am BST

PDB ID : 5VB2  
Title : Crystal structure of the NavAb voltage-gated sodium channel in a closed conformation  
Authors : Lenaeus, M.J.; Catterall, W.A.  
Deposited on : 2017-03-28  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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

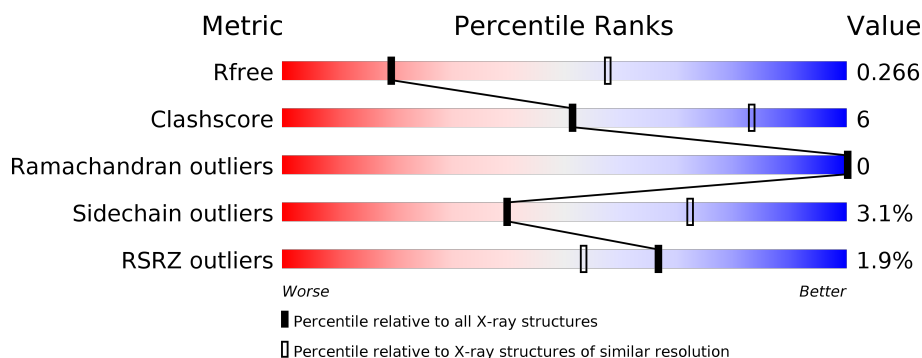
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	285	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>8%</div> </div> </div>
1	B	285	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>9%</div> </div> </div>
1	C	285	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>8%</div> </div> </div>
1	D	285	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PX4	B	2303	-	-	-	X
5	CL	C	1307	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17438 atoms, of which 8667 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	262	Total	C	H	N	O	S	0	0	0
			4078	1383	2022	310	351	12			
1	B	259	Total	C	H	N	O	S	0	0	0
			3938	1347	1930	299	351	11			
1	C	261	Total	C	H	N	O	S	0	0	0
			3895	1340	1897	299	348	11			
1	D	268	Total	C	H	N	O	S	0	0	0
			4218	1422	2101	321	362	12			

There are 80 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	1206	PHE	THR	engineered mutation	UNP A8EVM5
A	1213	TYR	VAL	engineered mutation	UNP A8EVM5
B	1983	MET	-	initiating methionine	UNP A8EVM5

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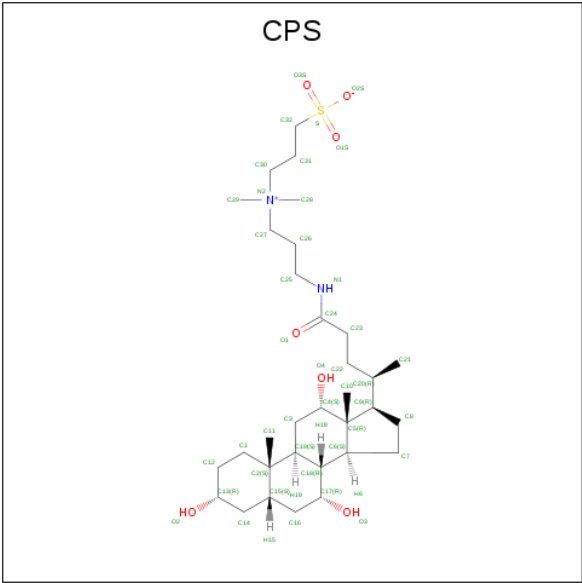
Chain	Residue	Modelled	Actual	Comment	Reference
B	1984	ASP	-	expression tag	UNP A8EVM5
B	1985	TYR	-	expression tag	UNP A8EVM5
B	1986	LYS	-	expression tag	UNP A8EVM5
B	1987	ASP	-	expression tag	UNP A8EVM5
B	1988	ASP	-	expression tag	UNP A8EVM5
B	1989	ASP	-	expression tag	UNP A8EVM5
B	1990	ASP	-	expression tag	UNP A8EVM5
B	1991	LYS	-	expression tag	UNP A8EVM5
B	1992	GLY	-	expression tag	UNP A8EVM5
B	1993	SER	-	expression tag	UNP A8EVM5
B	1994	LEU	-	expression tag	UNP A8EVM5
B	1995	VAL	-	expression tag	UNP A8EVM5
B	1996	PRO	-	expression tag	UNP A8EVM5
B	1997	ARG	-	expression tag	UNP A8EVM5
B	1998	GLY	-	expression tag	UNP A8EVM5
B	1999	SER	-	expression tag	UNP A8EVM5
B	2000	HIS	-	expression tag	UNP A8EVM5
B	2206	PHE	THR	engineered mutation	UNP A8EVM5
B	2213	TYR	VAL	engineered mutation	UNP A8EVM5
C	983	MET	-	initiating methionine	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	1206	PHE	THR	engineered mutation	UNP A8EVM5
C	1213	TYR	VAL	engineered mutation	UNP A8EVM5
D	1983	MET	-	initiating methionine	UNP A8EVM5
D	1984	ASP	-	expression tag	UNP A8EVM5
D	1985	TYR	-	expression tag	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1986	LYS	-	expression tag	UNP A8EVM5
D	1987	ASP	-	expression tag	UNP A8EVM5
D	1988	ASP	-	expression tag	UNP A8EVM5
D	1989	ASP	-	expression tag	UNP A8EVM5
D	1990	ASP	-	expression tag	UNP A8EVM5
D	1991	LYS	-	expression tag	UNP A8EVM5
D	1992	GLY	-	expression tag	UNP A8EVM5
D	1993	SER	-	expression tag	UNP A8EVM5
D	1994	LEU	-	expression tag	UNP A8EVM5
D	1995	VAL	-	expression tag	UNP A8EVM5
D	1996	PRO	-	expression tag	UNP A8EVM5
D	1997	ARG	-	expression tag	UNP A8EVM5
D	1998	GLY	-	expression tag	UNP A8EVM5
D	1999	SER	-	expression tag	UNP A8EVM5
D	2000	HIS	-	expression tag	UNP A8EVM5
D	2206	PHE	THR	engineered mutation	UNP A8EVM5
D	2213	TYR	VAL	engineered mutation	UNP A8EVM5

- Molecule 2 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: C<sub>32</sub>H<sub>58</sub>N<sub>2</sub>O<sub>7</sub>S).



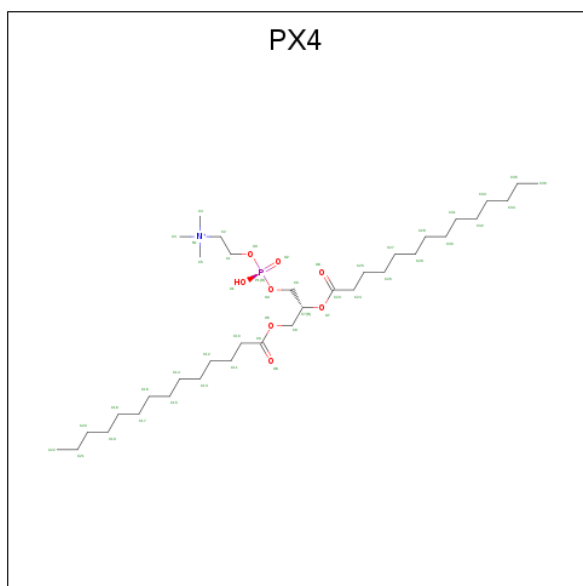
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			63	23	37	3		
2	A	1	Total	C	H	O	0	0
			65	23	39	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			65	23	39	3		
2	B	1	Total	C	H	O	0	0
			65	23	39	3		
2	C	1	Total	C	H	O	0	0
			65	23	39	3		
2	C	1	Total	C	H	O	0	0
			65	23	39	3		
2	D	1	Total	C	H	O	0	0
			65	23	39	3		
2	D	1	Total	C	H	O	0	0
			65	23	39	3		

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



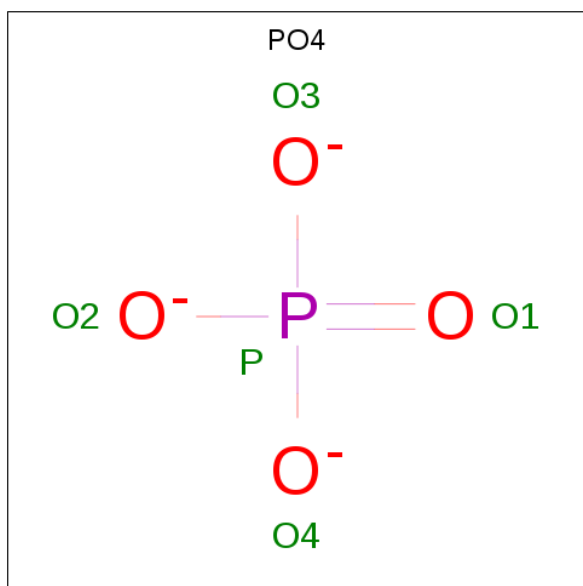
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			60	17	34	1	7	1		
3	A	1	Total	C	H	N	O	P	0	0
			53	15	28	1	8	1		
3	A	1	Total	C	H	N	O	P	0	0
			77	23	44	1	8	1		
3	B	1	Total	C	H	N	O	P	0	0
			60	18	32	1	8	1		
3	B	1	Total	C	H	N	O	P	0	0
			76	22	45	1	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	O	P	0	0
			43	13	21	8	1		
3	B	1	Total	C	H	N	O	P	0
			60	17	34	1	7	1	
3	C	1	Total	C	H	O	P	0	0
			37	11	17	8	1		
3	C	1	Total	C	H	N	O	P	0
			63	18	36	1	7	1	
3	C	1	Total	C	H	N	O	P	0
			86	26	50	1	8	1	
3	D	1	Total	C	H	O	P	0	0
			34	10	15	8	1		
3	D	1	Total	C	H	N	O	P	0
			59	17	32	1	8	1	
3	D	1	Total	C	H	O	P	0	0
			40	12	19	8	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		

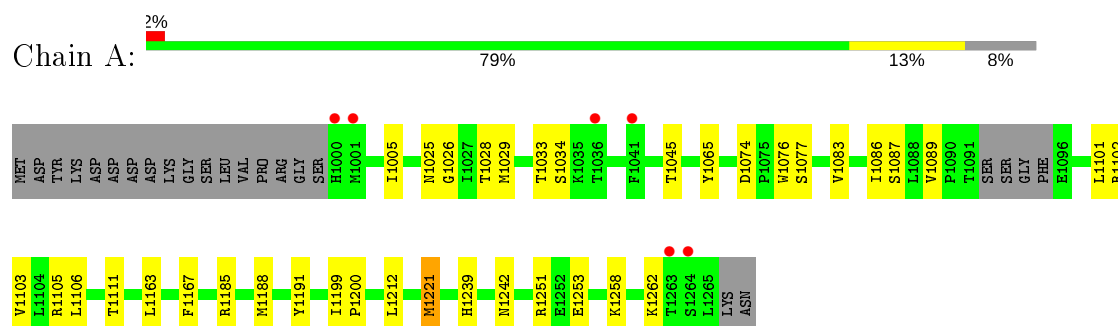
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	6	Total	O	0	0
			6	6		
6	C	5	Total	O	0	0
			5	5		
6	D	3	Total	O	0	0
			3	3		

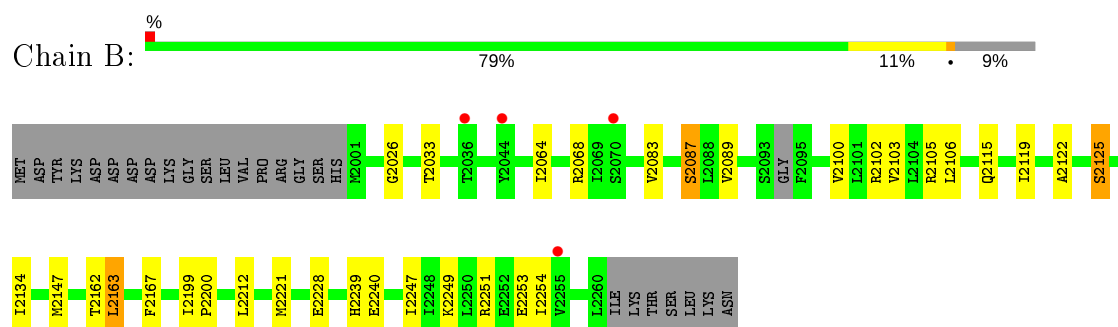
### 3 Residue-property plots [i](#)

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.

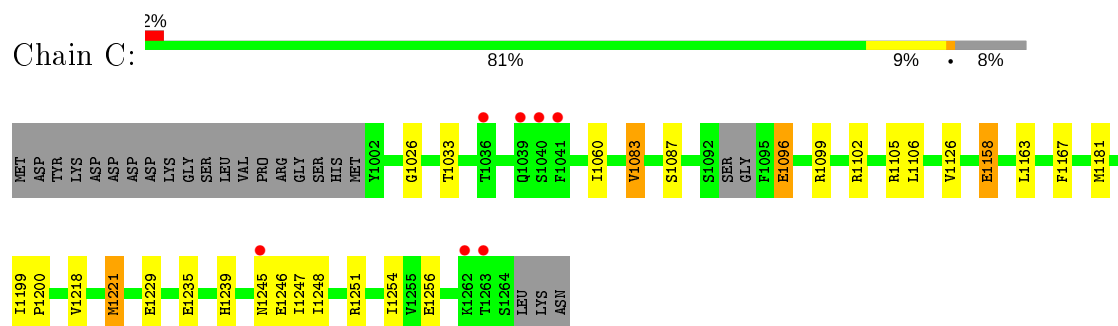
- Molecule 1: Ion transport protein



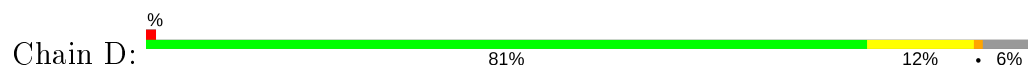
- Molecule 1: Ion transport protein

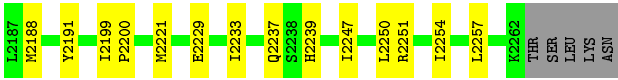
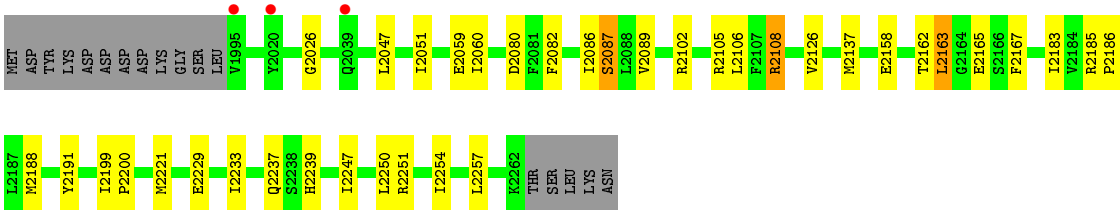


- Molecule 1: Ion transport protein



- Molecule 1: Ion transport protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.96Å 129.85Å 196.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 3.20 29.63 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.63-3.20) 99.1 (29.63-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.233 , 0.266 0.233 , 0.266	Depositor DCC
$R_{free}$ test set	1994 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.7	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 92.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CPS, CL, 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	0.26	0/2107	0.39	0/2877
1	B	0.25	0/2059	0.40	0/2815
1	C	0.25	0/2048	0.39	0/2803
1	D	0.26	0/2172	0.40	0/2966
All	All	0.26	0/8386	0.39	0/11461

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	2056	2022	2019	27	0
1	B	2008	1930	1925	25	0
1	C	1998	1897	1889	25	0
1	D	2117	2101	2095	28	0
2	A	52	76	74	2	0
2	B	52	78	74	2	0
2	C	52	78	74	2	0
2	D	52	78	74	3	0
3	A	84	106	96	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	107	132	124	3	0
3	C	83	103	93	0	0
3	D	67	66	54	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	C	1	0	0	6	0
6	A	8	0	0	2	0
6	B	6	0	0	1	0
6	C	5	0	0	0	0
6	D	3	0	0	1	0
All	All	8771	8667	8591	97	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 6.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1239:HIS:NE2	5:C:1307:CL:CL	2.44	0.87
3:A:1303:PX4:O1	6:A:1401:HOH:O	1.94	0.85
5:C:1307:CL:CL	1:D:2239:HIS:NE2	2.52	0.79
1:A:1239:HIS:NE2	5:C:1307:CL:CL	2.52	0.79
1:B:2122:ALA:O	1:B:2125:SER:OG	2.02	0.78
6:B:2401:HOH:O	1:C:1181:MET:SD	2.40	0.77
1:B:2087:SER:OG	1:B:2105:ARG:NH2	2.25	0.69
1:B:2239:HIS:NE2	5:C:1307:CL:CL	2.66	0.66
1:C:1247:ILE:O	1:C:1251:ARG:N	2.28	0.66
1:D:2158:GLU:OE2	6:D:2401:HOH:O	2.14	0.64
1:A:1242:ASN:ND2	1:B:2240:GLU:OE2	2.32	0.63
1:C:1235:GLU:OE1	1:D:2237:GLN:NE2	2.32	0.62
3:B:2306:PX4:O3	3:B:2306:PX4:H12	2.01	0.60
1:A:1089:VAL:O	1:A:1102:ARG:NH2	2.36	0.59
2:B:2302:CPS:H4	2:B:2302:CPS:H21A	1.84	0.58
1:A:1221:MET:HE1	1:B:2221:MET:HE2	1.87	0.57
1:A:1102:ARG:O	1:A:1105:ARG:HG2	2.04	0.57
1:A:1087:SER:OG	1:A:1105:ARG:NH2	2.38	0.57
1:C:1221:MET:CE	1:D:2221:MET:HG2	2.34	0.56
1:B:2100:VAL:O	1:B:2103:VAL:HG12	2.04	0.56
1:D:2089:VAL:O	1:D:2102:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1304:PX4:H17	1:B:2162:THR:HG23	1.89	0.55
1:A:1221:MET:SD	1:C:1221:MET:SD	3.06	0.54
2:D:2302:CPS:H21A	2:D:2302:CPS:H10B	1.91	0.53
3:A:1303:PX4:O3	3:A:1303:PX4:H12	2.07	0.52
1:A:1034:SER:OG	3:A:1304:PX4:O1	2.15	0.52
1:C:1221:MET:HE3	1:D:2221:MET:HG2	1.92	0.51
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.93	0.51
1:A:1221:MET:SD	1:B:2221:MET:HG3	2.51	0.50
1:B:2033:THR:HG21	1:C:1163:LEU:HB2	1.93	0.50
1:A:1258:LYS:O	1:A:1262:LYS:N	2.44	0.50
2:C:1301:CPS:H21A	2:C:1301:CPS:H4	1.92	0.50
1:D:2087:SER:OG	1:D:2105:ARG:NH1	2.44	0.50
2:A:1301:CPS:H21A	2:A:1301:CPS:H10B	1.93	0.49
1:D:2026:GLY:CA	1:D:2106:LEU:HD21	2.41	0.49
2:B:2301:CPS:H10B	2:B:2301:CPS:H21A	1.94	0.49
1:A:1239:HIS:CD2	5:C:1307:CL:CL	3.02	0.49
1:C:1083:VAL:HG11	1:C:1105:ARG:HA	1.94	0.49
1:C:1096:GLU:O	1:C:1099:ARG:N	2.43	0.49
1:B:2199:ILE:HB	1:B:2200:PRO:HD3	1.93	0.49
1:D:2080:ASP:OD2	1:D:2108:ARG:NH1	2.46	0.49
1:D:2199:ILE:HB	1:D:2200:PRO:HD3	1.95	0.48
1:A:1076:TRP:HB3	1:A:1111:THR:HG23	1.95	0.48
1:D:2082:PHE:CZ	1:D:2086:ILE:HD11	2.49	0.48
1:A:1253:GLU:HB3	1:B:2254:ILE:HG21	1.95	0.48
1:B:2221:MET:HE3	1:B:2221:MET:HA	1.96	0.48
3:A:1303:PX4:H11	1:D:2165:GLU:HG2	1.96	0.47
1:C:1199:ILE:HB	1:C:1200:PRO:HD3	1.95	0.47
1:C:1245:ASN:O	1:C:1248:ILE:N	2.46	0.47
1:B:2083:VAL:HG11	1:B:2105:ARG:HA	1.97	0.46
1:D:2233:ILE:O	1:D:2237:GLN:N	2.48	0.46
1:D:2247:ILE:O	1:D:2251:ARG:N	2.38	0.46
1:A:1083:VAL:HG11	1:A:1105:ARG:HA	1.97	0.46
1:D:2026:GLY:HA3	1:D:2106:LEU:HD21	1.97	0.46
1:A:1188:MET:HA	1:A:1191:TYR:O	2.16	0.46
1:C:1221:MET:SD	1:D:2221:MET:HG2	2.56	0.46
1:C:1158:GLU:N	1:C:1158:GLU:OE1	2.49	0.46
1:D:2059:GLU:CD	1:D:2108:ARG:HH22	2.20	0.45
2:A:1302:CPS:H4	2:A:1302:CPS:H21A	1.97	0.45
1:C:1102:ARG:O	1:C:1105:ARG:HG2	2.17	0.45
1:B:2247:ILE:O	1:B:2251:ARG:N	2.40	0.44
1:A:1033:THR:HG21	1:B:2163:LEU:HB2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:ARG:NH1	6:A:1403:HOH:O	2.46	0.44
1:B:2115:GLN:O	1:B:2119:ILE:HG12	2.17	0.44
1:A:1086:ILE:HD11	1:A:1101:LEU:HB2	1.99	0.44
1:A:1074:ASP:OD2	1:A:1077:SER:N	2.48	0.44
1:B:2221:MET:SD	1:C:1221:MET:HB3	2.57	0.44
1:C:1033:THR:HG21	1:D:2163:LEU:HB2	2.00	0.44
1:B:2089:VAL:O	1:B:2102:ARG:NH2	2.51	0.44
1:B:2228:GLU:HG3	1:C:1229:GLU:HG3	2.00	0.44
1:D:2229:GLU:O	1:D:2233:ILE:HG12	2.18	0.43
1:A:1251:ARG:HA	1:D:2250:LEU:HD11	2.00	0.43
1:A:1026:GLY:HA2	1:A:1106:LEU:HD21	2.01	0.43
1:C:1026:GLY:HA3	1:C:1106:LEU:HD21	2.01	0.43
1:C:1126:VAL:HG22	2:C:1301:CPS:C16	2.49	0.43
1:B:2239:HIS:CD2	5:C:1307:CL:CL	3.08	0.43
1:A:1239:HIS:CE1	1:B:2240:GLU:HA	2.53	0.43
3:B:2303:PX4:O1	3:B:2303:PX4:H12	2.19	0.43
1:A:1005:ILE:HD11	1:A:1065:TYR:HD2	1.83	0.43
1:C:1026:GLY:CA	1:C:1106:LEU:HD21	2.49	0.43
1:D:2087:SER:HA	1:D:2102:ARG:HG2	2.02	0.42
1:A:1025:ASN:O	1:A:1029:MET:HG3	2.19	0.42
1:C:1218:VAL:O	1:C:1221:MET:HB2	2.19	0.42
1:D:2185:ARG:HB2	1:D:2186:PRO:HD3	2.02	0.42
1:B:2249:LYS:O	1:B:2253:GLU:N	2.53	0.41
1:B:2064:ILE:O	1:B:2068:ARG:N	2.48	0.41
1:C:1254:ILE:HG12	1:D:2254:ILE:HD13	2.02	0.41
1:D:2126:VAL:HG22	2:D:2302:CPS:H16A	2.03	0.41
1:D:2188:MET:HA	1:D:2191:TYR:O	2.21	0.41
1:D:2126:VAL:HG22	2:D:2302:CPS:C16	2.51	0.41
3:B:2304:PX4:O3	3:B:2304:PX4:H12	2.21	0.41
1:D:2047:LEU:O	1:D:2051:ILE:N	2.53	0.41
1:C:1087:SER:HA	1:C:1102:ARG:HG2	2.03	0.41
1:A:1028:THR:CG2	1:A:1045:THR:HG23	2.52	0.40
1:B:2026:GLY:CA	1:B:2106:LEU:HD11	2.51	0.40
1:A:1103:VAL:HG11	1:B:2147:MET:CG	2.51	0.40
1:C:1246:GLU:HB3	1:D:2247:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	258/285 (90%)	252 (98%)	6 (2%)	0	100	100
1	B	255/285 (90%)	248 (97%)	7 (3%)	0	100	100
1	C	257/285 (90%)	251 (98%)	6 (2%)	0	100	100
1	D	266/285 (93%)	258 (97%)	8 (3%)	0	100	100
All	All	1036/1140 (91%)	1009 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	216/264 (82%)	212 (98%)	4 (2%)	57	81
1	B	207/264 (78%)	201 (97%)	6 (3%)	42	74
1	C	200/264 (76%)	193 (96%)	7 (4%)	36	69
1	D	226/264 (86%)	217 (96%)	9 (4%)	31	66
All	All	849/1056 (80%)	823 (97%)	26 (3%)	40	72

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1163	LEU
1	A	1167	PHE

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Mol	Chain	Res	Type
1	A	1212	LEU
1	A	1221	MET
1	B	2087	SER
1	B	2125	SER
1	B	2134	ILE
1	B	2163	LEU
1	B	2167	PHE
1	B	2212	LEU
1	C	1060	ILE
1	C	1083	VAL
1	C	1096	GLU
1	C	1158	GLU
1	C	1167	PHE
1	C	1221	MET
1	C	1256	GLU
1	D	2060	ILE
1	D	2087	SER
1	D	2108	ARG
1	D	2137	MET
1	D	2162	THR
1	D	2163	LEU
1	D	2167	PHE
1	D	2183	ILE
1	D	2257	LEU

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	CPS	A	1301	-	29,29,45	0.50	0	47,47,70	1.30	5 (10%)
3	PX4	B	2306	-	25,25,45	1.11	1 (4%)	30,32,53	1.00	2 (6%)
2	CPS	A	1302	-	29,29,45	0.49	0	47,47,70	1.41	8 (17%)
3	PX4	A	1303	-	25,25,45	1.14	2 (8%)	30,32,53	0.78	1 (3%)
4	PO4	C	1306	-	4,4,4	0.97	0	6,6,6	0.45	0
3	PX4	A	1304	-	24,24,45	1.28	3 (12%)	30,32,53	1.11	1 (3%)
3	PX4	D	2303	-	18,18,45	1.48	4 (22%)	22,23,53	1.21	2 (9%)
2	CPS	D	2301	-	29,29,45	0.51	0	47,47,70	1.49	9 (19%)
2	CPS	B	2302	-	29,29,45	0.52	0	47,47,70	1.41	5 (10%)
2	CPS	D	2302	-	29,29,45	0.50	0	47,47,70	1.36	5 (10%)
3	PX4	D	2304	-	26,26,45	1.30	4 (15%)	32,34,53	1.02	2 (6%)
3	PX4	D	2305	-	20,20,45	1.42	4 (20%)	24,25,53	1.49	3 (12%)
3	PX4	C	1304	-	26,26,45	1.12	2 (7%)	31,33,53	0.76	1 (3%)
4	PO4	D	2306	-	4,4,4	0.98	0	6,6,6	0.55	0
3	PX4	C	1305	-	35,35,45	1.12	4 (11%)	41,43,53	0.98	2 (4%)
3	PX4	B	2303	-	27,27,45	1.28	4 (14%)	33,35,53	1.06	2 (6%)
3	PX4	C	1303	-	19,19,45	1.45	4 (21%)	23,24,53	1.24	2 (8%)
4	PO4	B	2307	-	4,4,4	0.98	0	6,6,6	0.57	0
2	CPS	C	1302	-	29,29,45	0.53	0	47,47,70	1.30	5 (10%)
3	PX4	A	1305	-	32,32,45	1.18	4 (12%)	38,40,53	1.05	2 (5%)
2	CPS	B	2301	-	29,29,45	0.52	0	47,47,70	1.50	9 (19%)
3	PX4	B	2304	-	30,30,45	1.04	2 (6%)	35,37,53	1.11	1 (2%)
2	CPS	C	1301	-	29,29,45	0.50	0	47,47,70	1.37	8 (17%)
3	PX4	B	2305	-	21,21,45	1.39	5 (23%)	25,26,53	1.19	2 (8%)
4	PO4	A	1306	-	4,4,4	0.97	0	6,6,6	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPS	A	1301	-	-	2/6/71/90	0/4/4/4
3	PX4	D	2305	-	-	7/22/22/49	-
3	PX4	B	2306	-	-	9/27/27/49	-
2	CPS	C	1302	-	-	1/6/71/90	0/4/4/4
2	CPS	A	1302	-	-	2/6/71/90	0/4/4/4
3	PX4	D	2304	-	-	15/30/30/49	-
3	PX4	A	1304	-	-	9/27/27/49	-
3	PX4	D	2303	-	-	3/20/20/49	-
3	PX4	A	1303	-	-	12/27/27/49	-
3	PX4	C	1305	-	-	21/39/39/49	-
2	CPS	D	2301	-	-	2/6/71/90	0/4/4/4
2	CPS	B	2301	-	-	2/6/71/90	0/4/4/4
3	PX4	B	2304	-	-	18/33/33/49	-
3	PX4	A	1305	-	-	16/36/36/49	-
2	CPS	B	2302	-	-	0/6/71/90	0/4/4/4
2	CPS	C	1301	-	-	1/6/71/90	0/4/4/4
2	CPS	D	2302	-	-	6/6/71/90	0/4/4/4
3	PX4	C	1304	-	-	14/28/28/49	-
3	PX4	B	2305	-	-	10/23/23/49	-
3	PX4	B	2303	-	-	10/31/31/49	-
3	PX4	C	1303	-	-	6/21/21/49	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1303	PX4	P1-O3	2.69	1.65	1.54
3	D	2305	PX4	P1-O3	2.67	1.65	1.54
3	D	2303	PX4	P1-O3	2.67	1.65	1.54
3	B	2305	PX4	P1-O3	2.66	1.65	1.54
3	C	1305	PX4	O7-C7	-2.66	1.40	1.46
3	B	2303	PX4	O7-C7	-2.56	1.40	1.46
3	A	1305	PX4	O5-C9	2.54	1.40	1.33
3	C	1304	PX4	O5-C9	2.54	1.40	1.33
3	D	2303	PX4	O5-C9	2.52	1.40	1.33
3	D	2305	PX4	O5-C9	2.52	1.40	1.33
3	A	1304	PX4	O7-C7	-2.50	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2306	PX4	O5-C9	2.49	1.40	1.33
3	C	1303	PX4	O7-C7	-2.48	1.40	1.46
3	C	1303	PX4	O5-C9	2.47	1.40	1.33
3	D	2304	PX4	O7-C7	-2.47	1.40	1.46
3	A	1303	PX4	O5-C9	2.44	1.40	1.33
3	B	2305	PX4	O7-C23	2.44	1.41	1.34
3	D	2305	PX4	O7-C23	2.42	1.41	1.34
3	B	2305	PX4	O7-C7	-2.40	1.40	1.46
3	A	1304	PX4	O7-C23	2.37	1.41	1.34
3	D	2303	PX4	O7-C23	2.36	1.41	1.34
3	B	2304	PX4	O7-C23	2.35	1.41	1.34
3	D	2303	PX4	O7-C7	-2.35	1.40	1.46
3	B	2305	PX4	O5-C9	2.34	1.40	1.33
3	D	2304	PX4	O7-C23	2.33	1.40	1.34
3	B	2304	PX4	O7-C7	-2.32	1.40	1.46
3	A	1305	PX4	O7-C7	-2.32	1.40	1.46
3	A	1305	PX4	O7-C23	2.31	1.40	1.34
3	D	2305	PX4	O7-C7	-2.31	1.40	1.46
3	D	2304	PX4	O5-C9	2.31	1.40	1.33
3	C	1305	PX4	O5-C9	2.30	1.40	1.33
3	B	2303	PX4	O5-C9	2.29	1.40	1.33
3	C	1303	PX4	O7-C23	2.26	1.40	1.34
3	B	2303	PX4	O7-C23	2.25	1.40	1.34
3	D	2304	PX4	O5-C8	-2.23	1.40	1.45
3	B	2303	PX4	O5-C8	-2.22	1.40	1.45
3	C	1305	PX4	O5-C8	-2.15	1.40	1.45
3	A	1303	PX4	O5-C8	-2.13	1.40	1.45
3	C	1305	PX4	O7-C23	2.12	1.40	1.34
3	C	1304	PX4	O5-C8	-2.11	1.40	1.45
3	B	2305	PX4	O5-C8	-2.10	1.40	1.45
3	A	1305	PX4	O5-C8	-2.04	1.40	1.45
3	A	1304	PX4	O5-C8	-2.01	1.40	1.45

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2305	PX4	O7-C23-C24	4.75	121.74	111.50
3	B	2304	PX4	O7-C23-C24	4.74	121.72	111.50
2	B	2302	CPS	C5-C9-C20	-4.52	114.09	119.50
3	A	1305	PX4	O7-C23-C24	4.26	120.68	111.50
3	A	1304	PX4	O7-C23-C24	4.15	120.45	111.50
3	C	1303	PX4	O7-C23-C24	3.83	119.76	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2303	PX4	O7-C23-C24	3.74	119.55	111.50
3	B	2306	PX4	O5-C9-C10	3.60	123.22	111.91
3	D	2304	PX4	O7-C23-C24	3.57	119.19	111.50
3	B	2305	PX4	O7-C23-C24	3.55	120.69	110.80
2	D	2302	CPS	C9-C5-C6	-3.47	96.60	100.09
3	D	2303	PX4	O7-C23-C24	3.40	120.29	110.80
2	B	2301	CPS	C7-C6-C5	-3.36	100.25	103.55
3	C	1305	PX4	O7-C23-C24	3.32	118.66	111.50
2	D	2301	CPS	C10-C5-C4	3.32	112.44	109.07
2	B	2301	CPS	C10-C5-C4	3.26	112.38	109.07
2	D	2302	CPS	C6-C18-C17	-3.17	107.60	111.81
2	A	1301	CPS	C7-C6-C5	-3.16	100.45	103.55
2	B	2301	CPS	C1-C12-C13	-3.12	106.46	110.47
2	A	1302	CPS	C7-C6-C18	-3.10	114.00	118.33
2	C	1301	CPS	C9-C5-C6	-3.01	97.06	100.09
2	A	1302	CPS	C7-C6-C5	-2.99	100.62	103.55
2	A	1302	CPS	C6-C18-C17	-2.92	107.94	111.81
3	D	2305	PX4	O5-C9-C10	2.91	121.05	111.91
2	B	2302	CPS	C5-C6-C18	-2.88	111.06	114.74
2	C	1302	CPS	C7-C6-C5	-2.86	100.75	103.55
2	C	1301	CPS	C6-C18-C17	-2.79	108.10	111.81
2	D	2302	CPS	C7-C6-C18	-2.73	114.52	118.33
2	B	2302	CPS	C19-C18-C6	-2.72	105.97	109.71
2	D	2301	CPS	C9-C5-C4	-2.67	115.22	117.67
2	D	2301	CPS	C1-C12-C13	-2.64	107.07	110.47
2	B	2301	CPS	C19-C18-C17	-2.64	108.72	111.88
2	A	1302	CPS	C19-C3-C4	-2.64	110.82	114.30
2	C	1302	CPS	C19-C3-C4	-2.59	110.88	114.30
2	D	2301	CPS	C5-C6-C18	-2.59	111.43	114.74
3	C	1303	PX4	O5-C9-C10	2.58	120.01	111.91
3	D	2303	PX4	O5-C9-C10	2.57	119.97	111.91
3	C	1305	PX4	O5-C9-C10	2.57	119.97	111.91
3	B	2303	PX4	O5-C9-C10	2.57	119.97	111.91
2	C	1302	CPS	C5-C9-C20	-2.54	116.46	119.50
2	C	1301	CPS	C7-C6-C18	-2.52	114.81	118.33
3	D	2304	PX4	O5-C9-C10	2.50	119.76	111.91
2	C	1301	CPS	C19-C3-C4	-2.50	111.00	114.30
2	A	1302	CPS	C9-C5-C6	-2.47	97.60	100.09
2	D	2302	CPS	C19-C3-C4	-2.47	111.04	114.30
2	B	2301	CPS	C19-C3-C4	-2.45	111.06	114.30
3	A	1305	PX4	O5-C9-C10	2.45	119.59	111.91
2	A	1301	CPS	C5-C9-C20	-2.43	116.59	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1303	PX4	O5-C9-C10	2.43	119.53	111.91
2	B	2301	CPS	C9-C5-C4	-2.42	115.45	117.67
2	D	2301	CPS	C7-C6-C5	-2.42	101.18	103.55
2	A	1302	CPS	C5-C9-C20	-2.41	116.62	119.50
3	B	2305	PX4	O5-C9-C10	2.39	119.41	111.91
2	C	1301	CPS	C5-C9-C20	-2.36	116.67	119.50
2	C	1302	CPS	C10-C5-C4	2.36	111.47	109.07
2	D	2301	CPS	C5-C9-C20	-2.35	116.69	119.50
2	D	2302	CPS	C7-C6-C5	-2.33	101.26	103.55
2	D	2301	CPS	C14-C13-C12	-2.33	107.78	110.55
2	A	1301	CPS	C9-C5-C4	-2.32	115.55	117.67
2	A	1302	CPS	C21-C20-C9	-2.30	109.39	112.92
2	A	1302	CPS	C15-C14-C13	-2.29	109.40	112.76
2	C	1301	CPS	C22-C20-C9	-2.28	105.58	110.29
2	B	2301	CPS	C3-C4-C5	-2.26	108.92	111.24
2	D	2301	CPS	C3-C19-C2	-2.25	111.40	113.73
2	A	1301	CPS	C5-C6-C18	-2.19	111.95	114.74
2	C	1302	CPS	C5-C6-C18	-2.16	111.98	114.74
3	D	2305	PX4	O7-C23-O8	-2.15	118.50	123.70
2	D	2301	CPS	C8-C9-C20	-2.12	108.86	112.15
2	B	2302	CPS	C15-C14-C13	-2.11	109.66	112.76
3	C	1304	PX4	O5-C9-C10	2.11	118.53	111.91
2	B	2301	CPS	C14-C13-C12	-2.11	108.04	110.55
2	B	2302	CPS	C10-C5-C6	2.10	114.49	111.21
2	A	1301	CPS	C11-C2-C1	-2.09	104.90	108.26
2	C	1301	CPS	C21-C20-C9	-2.06	109.77	112.92
2	B	2301	CPS	C5-C9-C20	-2.05	117.05	119.50
2	C	1301	CPS	C8-C9-C20	-2.05	108.97	112.15
3	B	2306	PX4	O5-C9-O6	-2.01	118.52	123.59

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2306	PX4	C1-O3-P1-O1
3	B	2306	PX4	C1-O3-P1-O2
3	B	2306	PX4	C1-O3-P1-O4
3	B	2306	PX4	C6-O4-P1-O3
2	A	1302	CPS	C21-C20-C22-C23
3	A	1303	PX4	C1-O3-P1-O1
3	A	1303	PX4	C1-O3-P1-O2
3	A	1303	PX4	O7-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
3	D	2304	PX4	C1-O3-P1-O2
3	D	2304	PX4	C6-O4-P1-O2
3	D	2304	PX4	O3-C1-C2-N1
3	D	2304	PX4	C7-C6-O4-P1
3	D	2305	PX4	C6-O4-P1-O3
3	D	2305	PX4	O8-C23-O7-C7
3	D	2305	PX4	C24-C23-O7-C7
3	C	1304	PX4	C6-O4-P1-O1
3	C	1304	PX4	C6-O4-P1-O2
3	C	1304	PX4	O3-C1-C2-N1
3	C	1304	PX4	O7-C7-C8-O5
3	C	1305	PX4	C1-O3-P1-O1
3	C	1305	PX4	C1-O3-P1-O2
3	C	1305	PX4	C6-O4-P1-O1
3	C	1305	PX4	C6-O4-P1-O2
3	C	1305	PX4	O3-C1-C2-N1
3	C	1305	PX4	O7-C7-C8-O5
3	B	2303	PX4	C1-O3-P1-O2
3	B	2303	PX4	C1-O3-P1-O4
3	B	2303	PX4	C6-O4-P1-O2
3	C	1303	PX4	O7-C7-C8-O5
3	A	1305	PX4	C1-O3-P1-O1
3	A	1305	PX4	C1-O3-P1-O2
3	A	1305	PX4	C6-O4-P1-O1
3	A	1305	PX4	C6-O4-P1-O2
3	A	1305	PX4	C24-C23-O7-C7
3	B	2304	PX4	C1-O3-P1-O2
3	B	2304	PX4	C1-O3-P1-O4
3	B	2304	PX4	C6-O4-P1-O2
3	B	2305	PX4	C6-O4-P1-O1
3	B	2305	PX4	C6-O4-P1-O3
3	A	1305	PX4	O8-C23-O7-C7
3	D	2305	PX4	C10-C9-O5-C8
2	D	2302	CPS	C22-C20-C9-C8
3	D	2305	PX4	O6-C9-O5-C8
3	C	1304	PX4	O4-C6-C7-O7
3	B	2303	PX4	C24-C23-O7-C7
3	B	2304	PX4	C24-C23-O7-C7
2	D	2301	CPS	C21-C20-C22-C23
2	A	1302	CPS	C9-C20-C22-C23
3	B	2303	PX4	O8-C23-O7-C7
3	B	2306	PX4	O4-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	C	1305	PX4	C10-C9-O5-C8
3	C	1304	PX4	C6-C7-C8-O5
3	A	1303	PX4	O4-C6-C7-O7
3	A	1305	PX4	C9-C10-C11-C12
3	C	1305	PX4	O6-C9-O5-C8
2	B	2301	CPS	C21-C20-C22-C23
3	B	2304	PX4	C23-C24-C25-C26
3	B	2304	PX4	O8-C23-O7-C7
3	B	2306	PX4	O4-C6-C7-O7
3	B	2305	PX4	C24-C23-O7-C7
3	A	1303	PX4	C1-O3-P1-O4
3	A	1304	PX4	C1-O3-P1-O4
3	D	2304	PX4	C1-O3-P1-O4
3	C	1304	PX4	C6-O4-P1-O3
3	C	1305	PX4	C1-O3-P1-O4
3	C	1305	PX4	C6-O4-P1-O3
3	A	1305	PX4	C1-O3-P1-O4
3	A	1305	PX4	C6-O4-P1-O3
3	B	2304	PX4	C6-O4-P1-O3
3	B	2305	PX4	O8-C23-O7-C7
3	B	2303	PX4	C10-C9-O5-C8
2	D	2302	CPS	C9-C20-C22-C23
3	B	2305	PX4	C10-C11-C12-C13
3	D	2303	PX4	C24-C23-O7-C7
3	B	2304	PX4	C32-C33-C34-C35
3	A	1303	PX4	C10-C11-C12-C13
3	B	2306	PX4	C13-C14-C15-C16
3	D	2303	PX4	O8-C23-O7-C7
3	C	1304	PX4	C11-C12-C13-C14
3	A	1303	PX4	C10-C9-O5-C8
3	C	1304	PX4	C12-C13-C14-C15
3	B	2303	PX4	O6-C9-O5-C8
3	A	1305	PX4	C10-C9-O5-C8
3	A	1303	PX4	O6-C9-O5-C8
3	C	1305	PX4	O8-C23-O7-C7
3	B	2305	PX4	C9-C10-C11-C12
3	C	1305	PX4	C24-C23-O7-C7
3	B	2305	PX4	O4-C6-C7-O7
3	A	1305	PX4	O6-C9-O5-C8
2	D	2302	CPS	C21-C20-C9-C5
2	D	2302	CPS	C21-C20-C22-C23
2	D	2302	CPS	C21-C20-C9-C8

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Mol	Chain	Res	Type	Atoms
3	B	2305	PX4	C6-O4-P1-O2
3	C	1303	PX4	O7-C23-C24-C25
3	A	1303	PX4	C9-C10-C11-C12
3	D	2304	PX4	O4-C6-C7-C8
3	B	2304	PX4	O4-C6-C7-C8
3	B	2305	PX4	O4-C6-C7-C8
2	C	1302	CPS	C21-C20-C22-C23
3	A	1303	PX4	C6-C7-C8-O5
3	A	1304	PX4	O4-C6-C7-O7
3	C	1304	PX4	O4-C6-C7-C8
3	B	2304	PX4	C6-C7-C8-O5
3	D	2304	PX4	C10-C9-O5-C8
3	C	1304	PX4	C10-C9-O5-C8
3	A	1303	PX4	C14-C15-C16-C17
3	C	1305	PX4	C7-C6-O4-P1
3	C	1305	PX4	C24-C25-C26-C27
3	B	2304	PX4	O7-C7-C8-O5
3	A	1305	PX4	C11-C12-C13-C14
3	A	1305	PX4	C6-C7-O7-C23
3	C	1305	PX4	C6-C7-C8-O5
3	C	1304	PX4	O6-C9-O5-C8
3	D	2304	PX4	O4-C6-C7-O7
3	B	2304	PX4	O4-C6-C7-O7
3	A	1303	PX4	O4-C6-C7-C8
2	D	2302	CPS	C22-C20-C9-C5
3	D	2304	PX4	O6-C9-O5-C8
3	B	2306	PX4	O7-C7-C8-O5
3	D	2304	PX4	C6-O4-P1-O3
3	B	2303	PX4	C6-O4-P1-O3
3	A	1305	PX4	C10-C11-C12-C13
3	A	1304	PX4	C1-O3-P1-O1
3	A	1304	PX4	C1-O3-P1-O2
3	A	1304	PX4	C2-C1-O3-P1
3	C	1305	PX4	C26-C27-C28-C29
3	A	1304	PX4	O3-C1-C2-N1
3	C	1303	PX4	C6-C7-C8-O5
2	D	2301	CPS	C9-C20-C22-C23
3	B	2304	PX4	C28-C29-C30-C31
3	B	2304	PX4	C33-C34-C35-C36
3	D	2305	PX4	C8-C7-O7-C23
3	D	2304	PX4	C24-C25-C26-C27
3	D	2303	PX4	C6-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
3	C	1305	PX4	O4-C6-C7-O7
3	C	1304	PX4	C1-O3-P1-O4
2	C	1301	CPS	C21-C20-C22-C23
3	D	2304	PX4	C24-C23-O7-C7
3	D	2304	PX4	O8-C23-O7-C7
3	C	1303	PX4	C23-C24-C25-C26
3	C	1304	PX4	C13-C14-C15-C16
3	B	2304	PX4	C27-C28-C29-C30
3	D	2304	PX4	C8-C7-O7-C23
3	A	1305	PX4	C23-C24-C25-C26
3	A	1305	PX4	C13-C14-C15-C16
3	C	1305	PX4	C13-C14-C15-C16
3	D	2304	PX4	C23-C24-C25-C26
2	A	1301	CPS	C21-C20-C22-C23
3	A	1304	PX4	O8-C23-O7-C7
3	A	1304	PX4	O4-C6-C7-C8
3	C	1303	PX4	O8-C23-C24-C25
3	B	2303	PX4	C7-C6-O4-P1
3	C	1303	PX4	C6-O4-P1-O1
3	B	2304	PX4	O7-C23-C24-C25
3	D	2305	PX4	O4-C6-C7-O7
2	B	2301	CPS	C22-C20-C9-C8
3	C	1305	PX4	C27-C28-C29-C30
3	B	2303	PX4	C11-C10-C9-O5
2	A	1301	CPS	C9-C20-C22-C23
3	A	1304	PX4	C24-C23-O7-C7
3	B	2304	PX4	C30-C31-C32-C33
3	B	2305	PX4	O7-C7-C8-O5
3	B	2304	PX4	C6-C7-O7-C23
3	B	2306	PX4	C11-C10-C9-O5
3	C	1305	PX4	C11-C10-C9-O5
3	C	1305	PX4	C11-C10-C9-O6

There are no ring outliers.

11 monomers are involved in 17 short contacts:

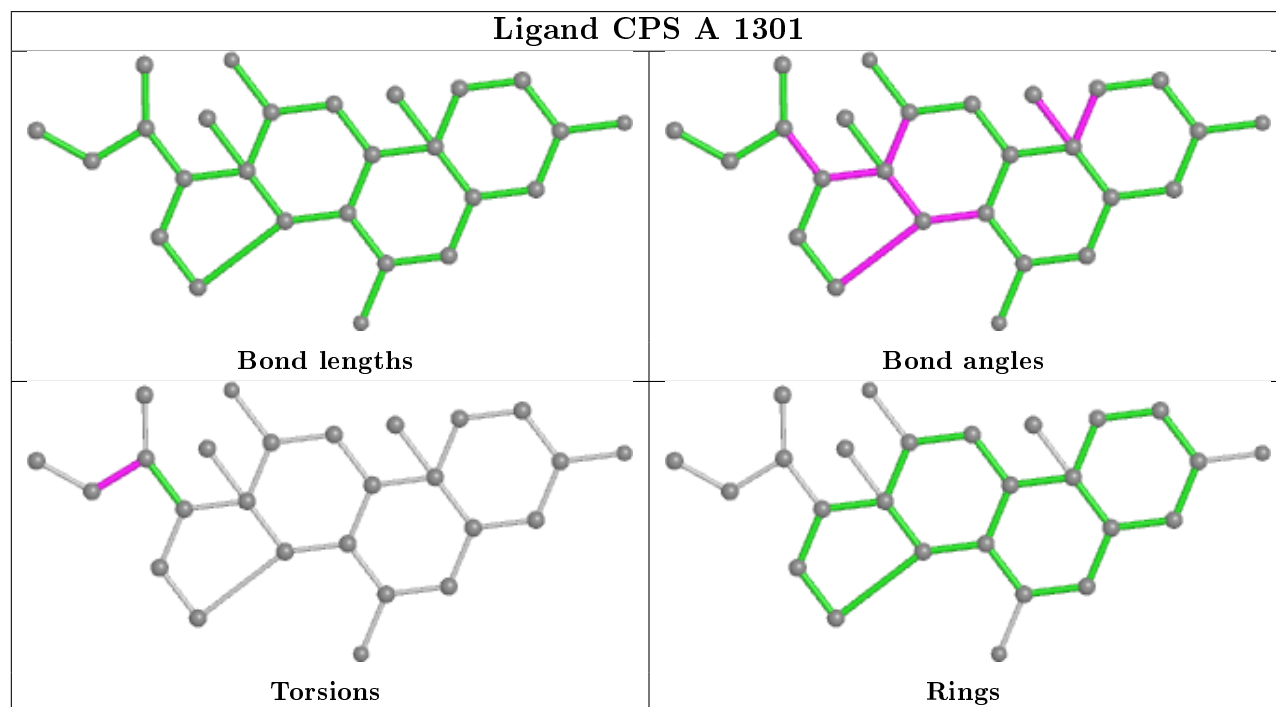
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	CPS	1	0
3	B	2306	PX4	1	0
2	A	1302	CPS	1	0
3	A	1303	PX4	3	0
3	A	1304	PX4	2	0

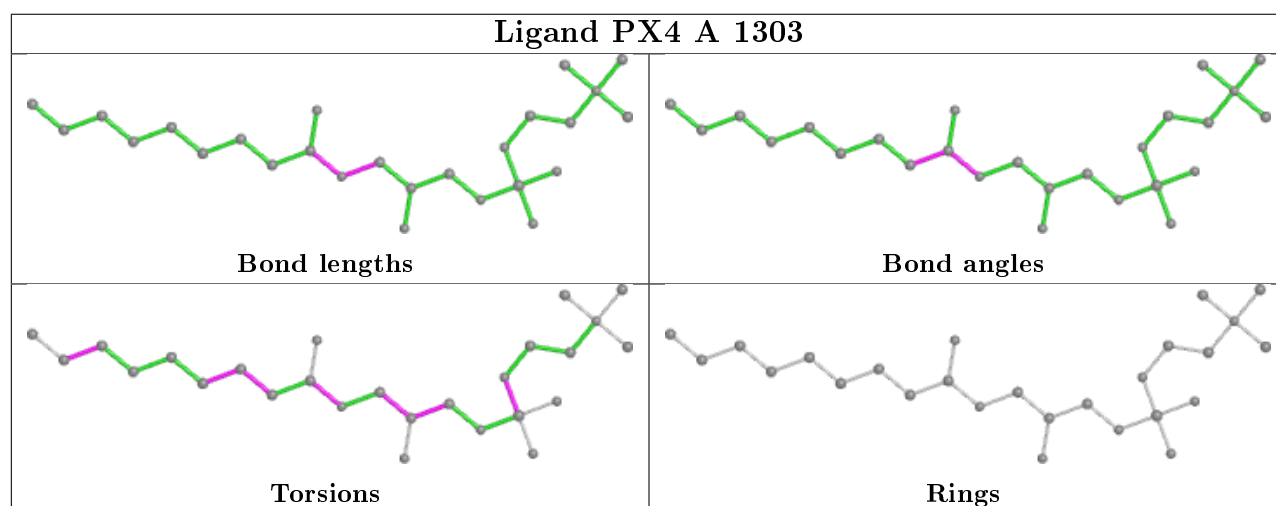
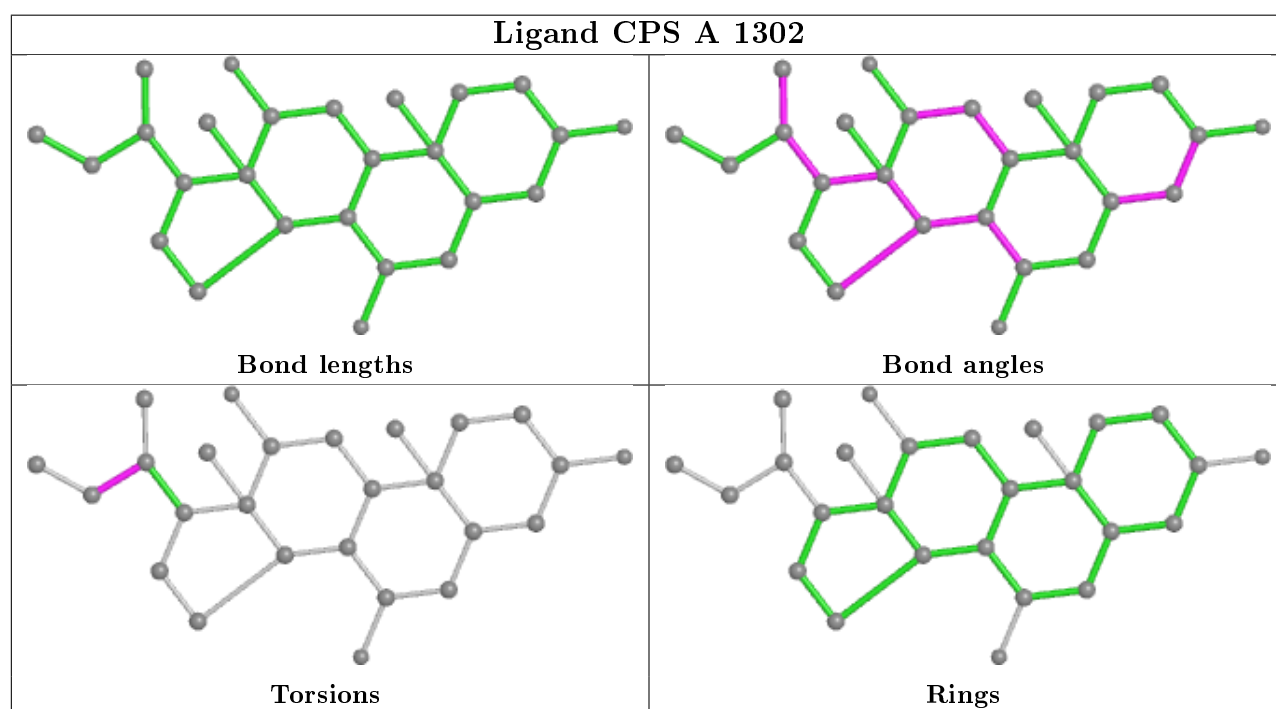
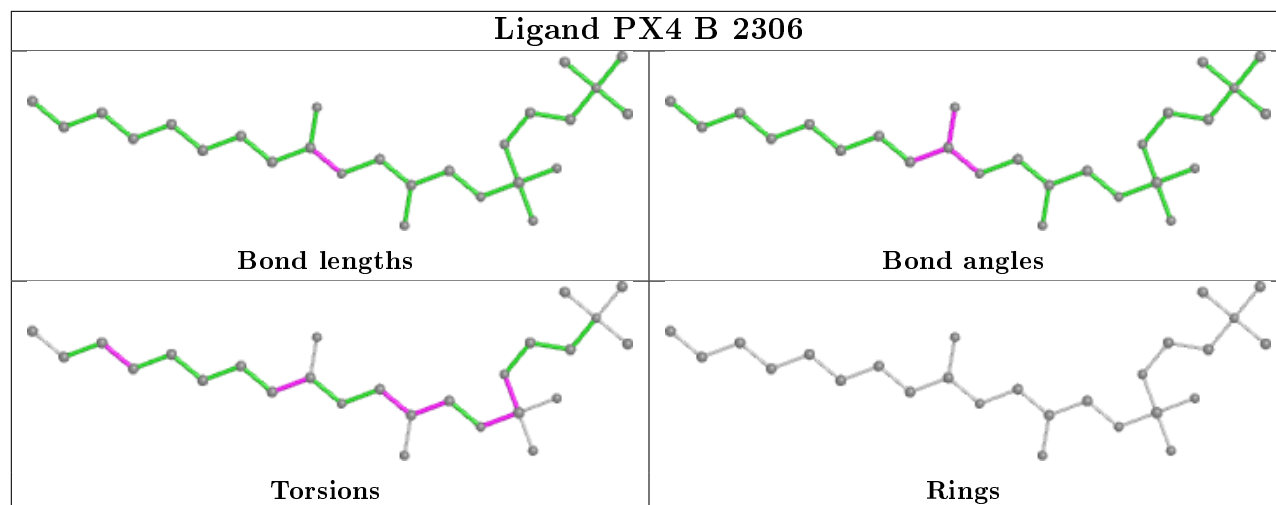
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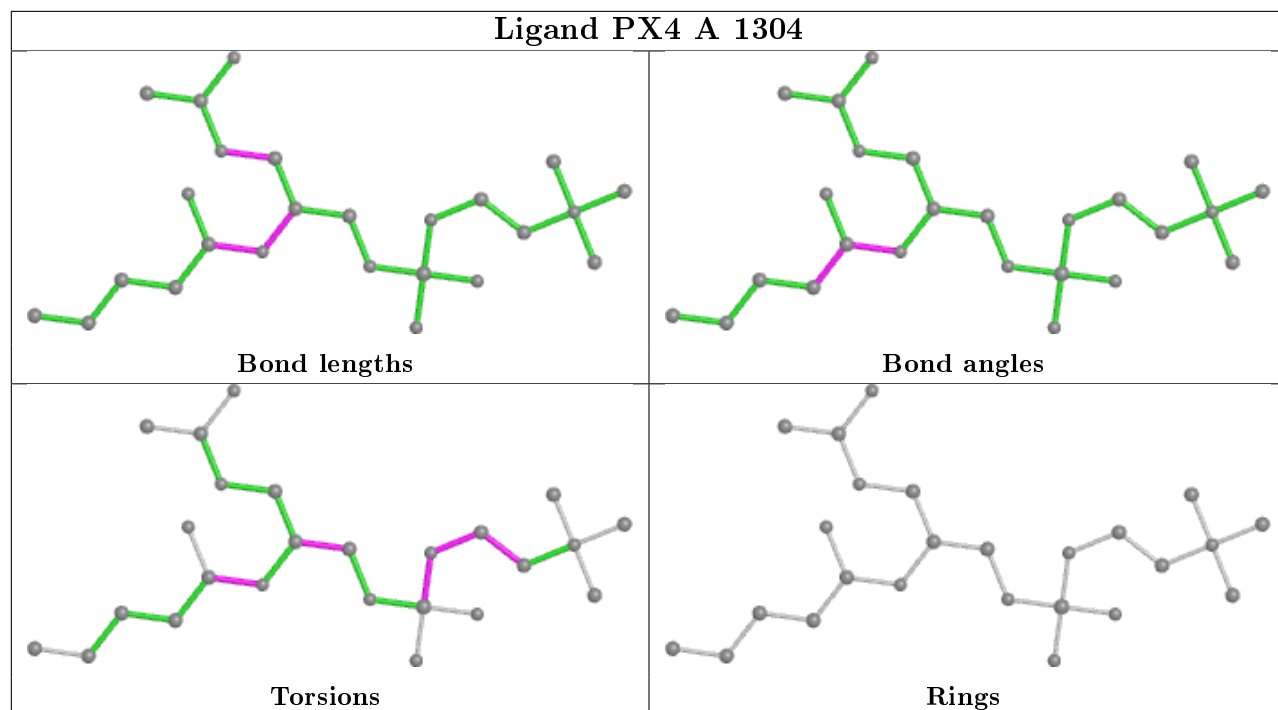
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2302	CPS	1	0
2	D	2302	CPS	3	0
3	B	2303	PX4	1	0
2	B	2301	CPS	1	0
3	B	2304	PX4	1	0
2	C	1301	CPS	2	0

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.

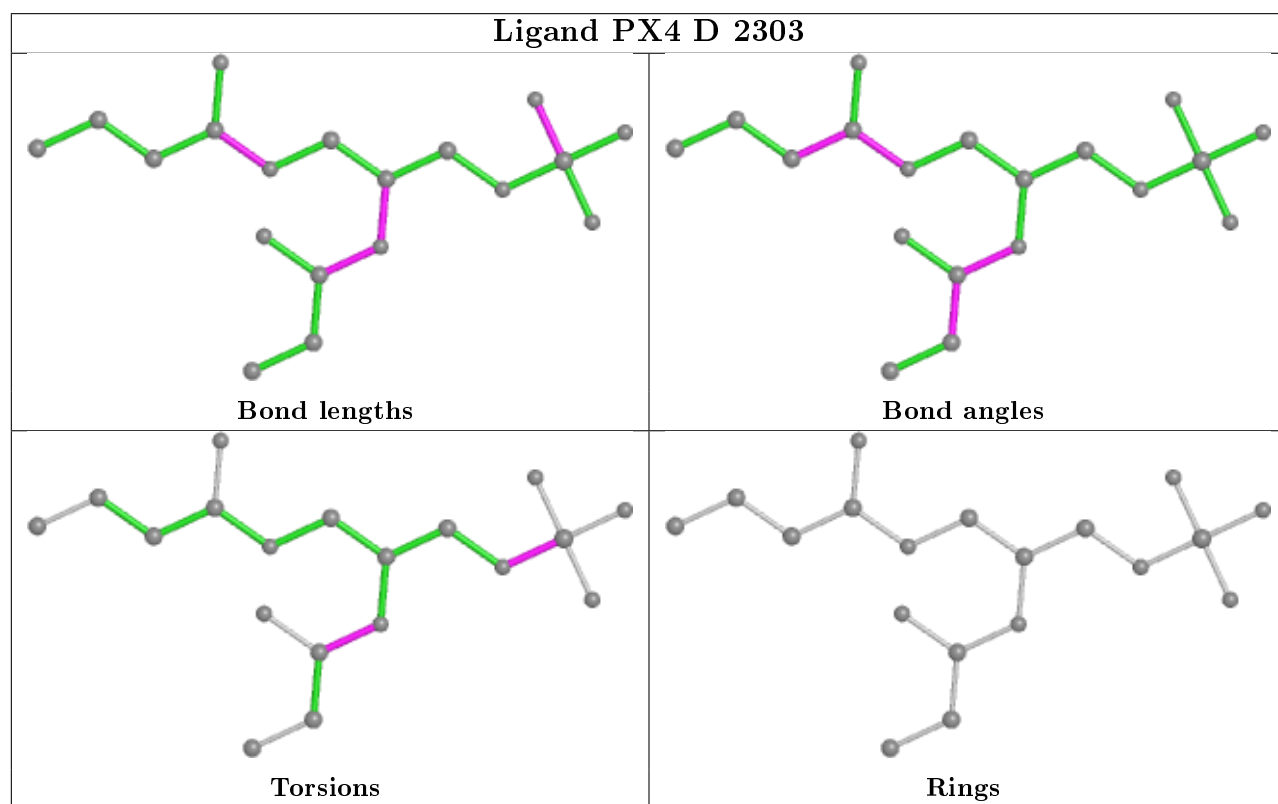


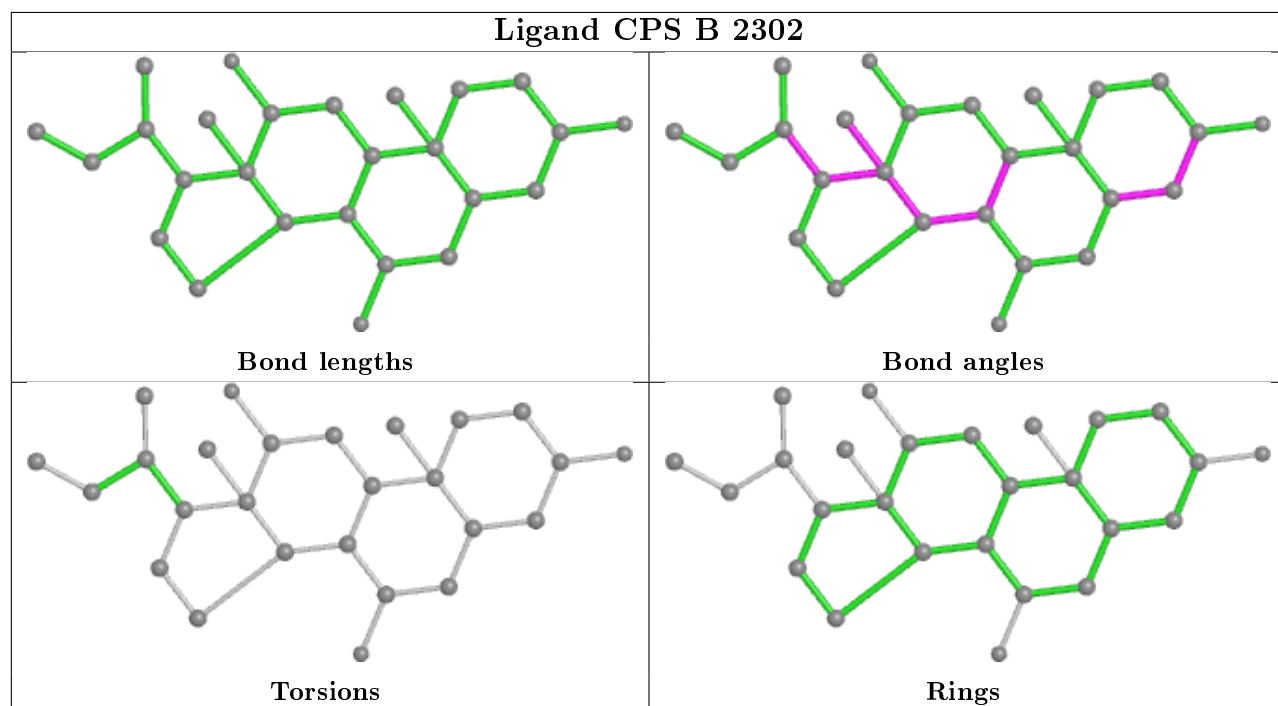
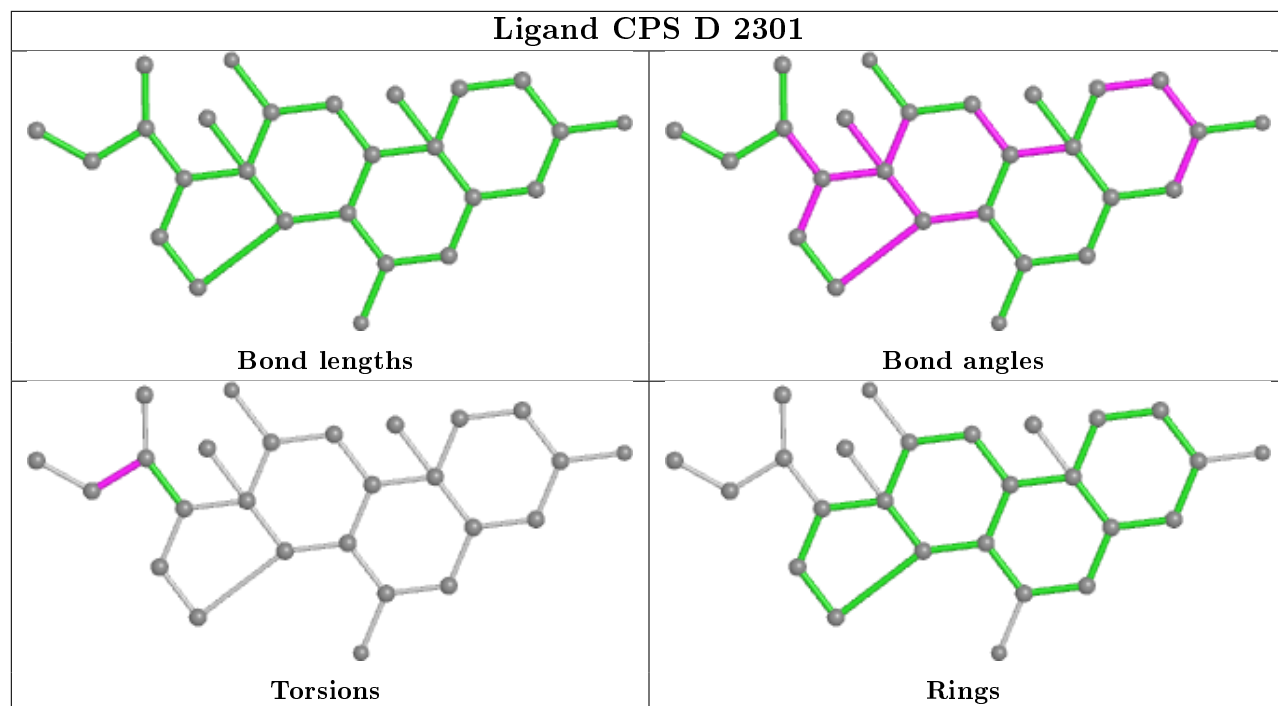


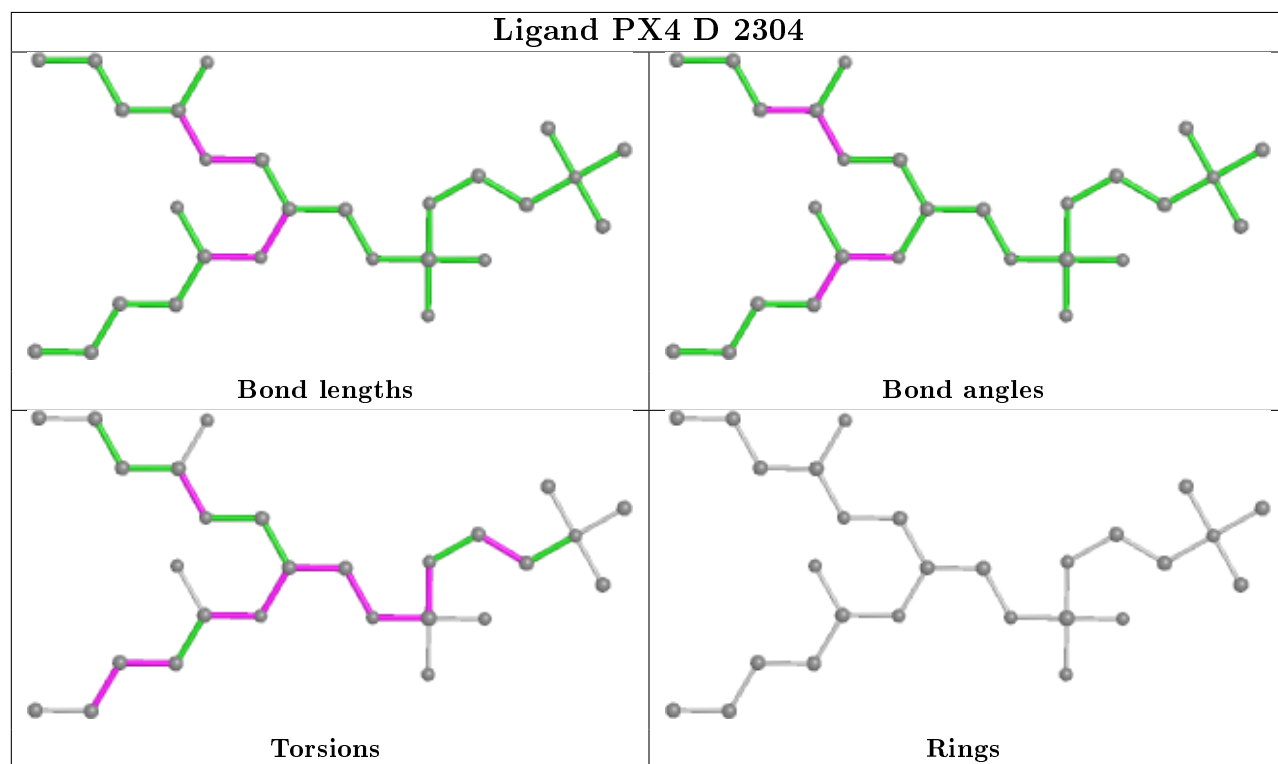
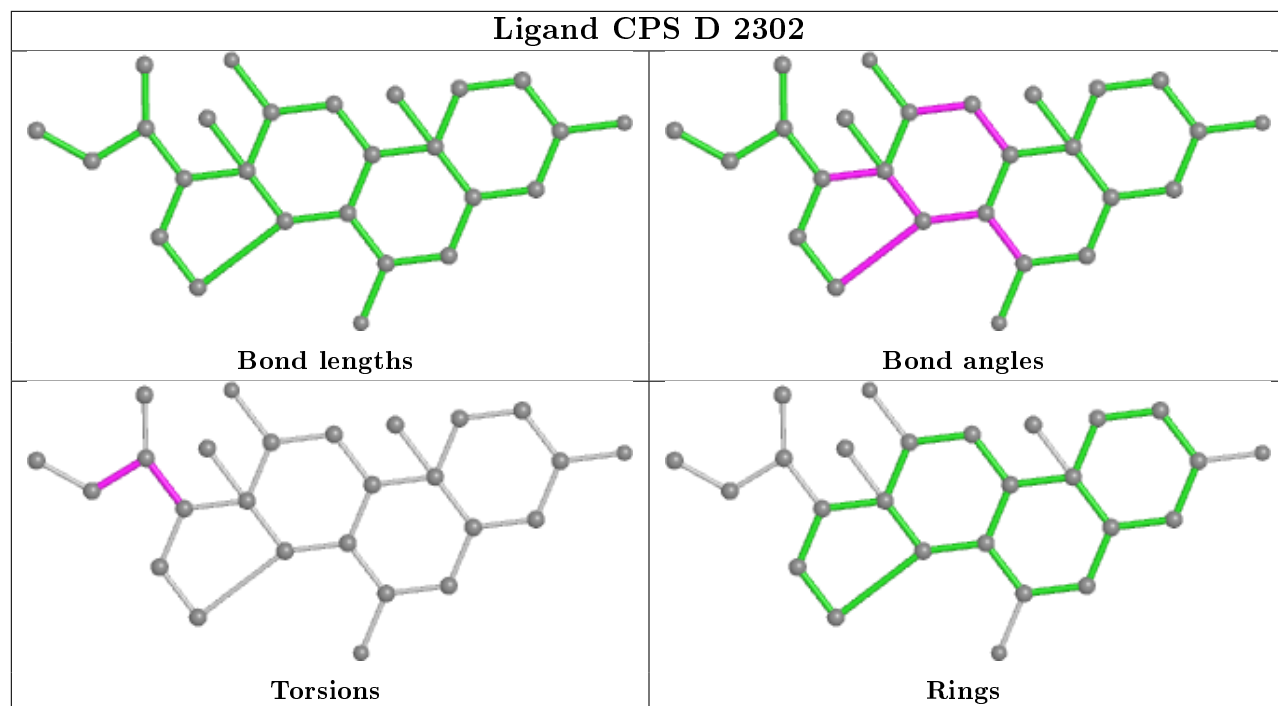
## Ligand PX4 A 1304



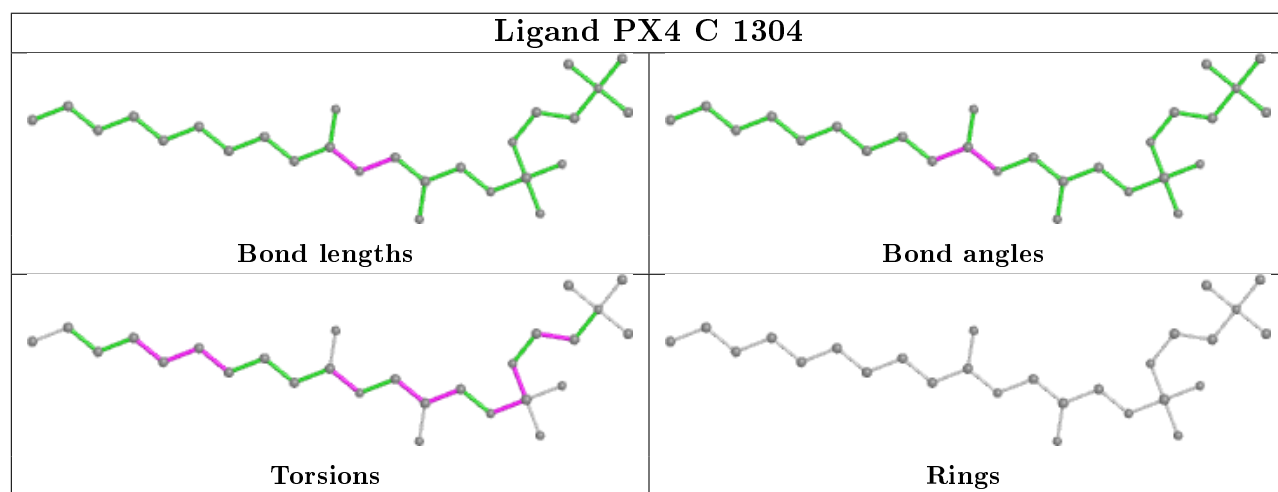
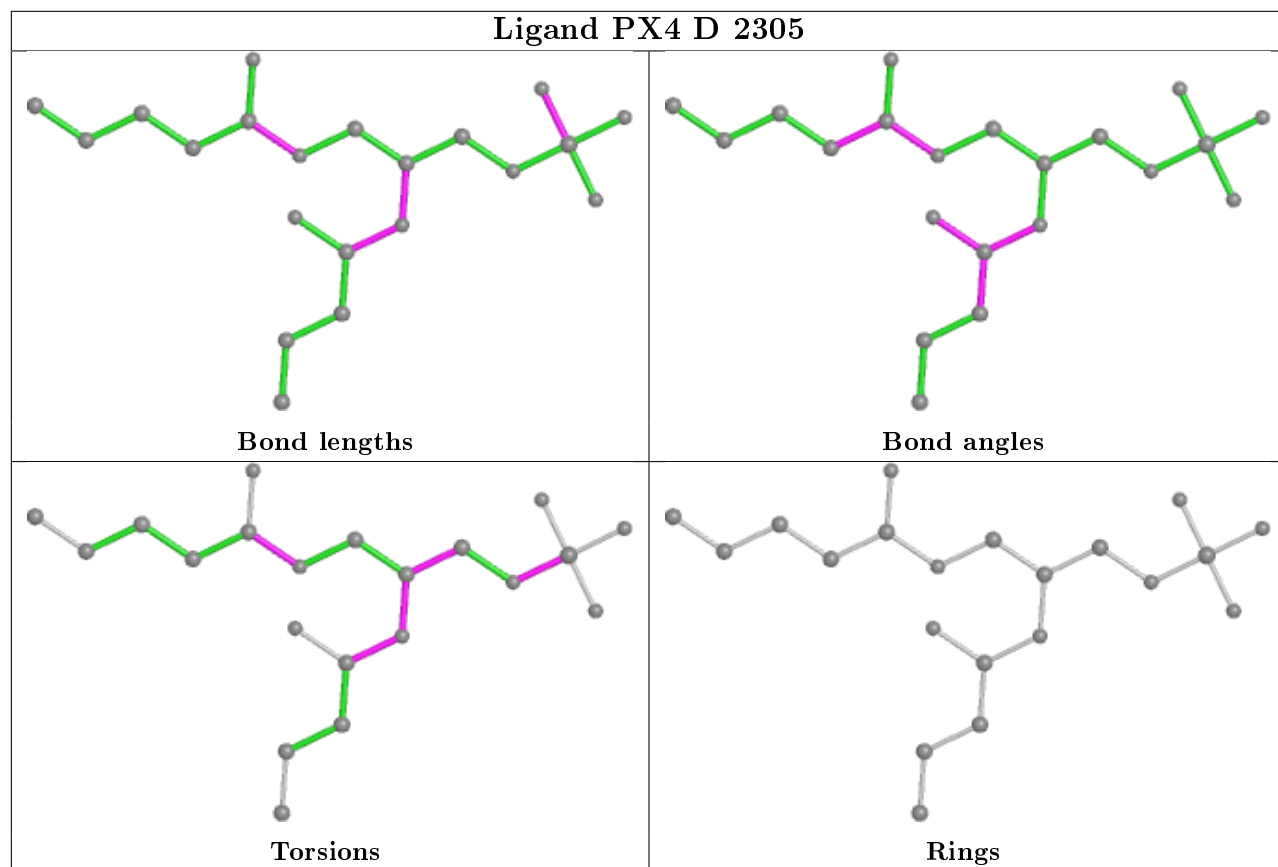
## Ligand PX4 D 2303

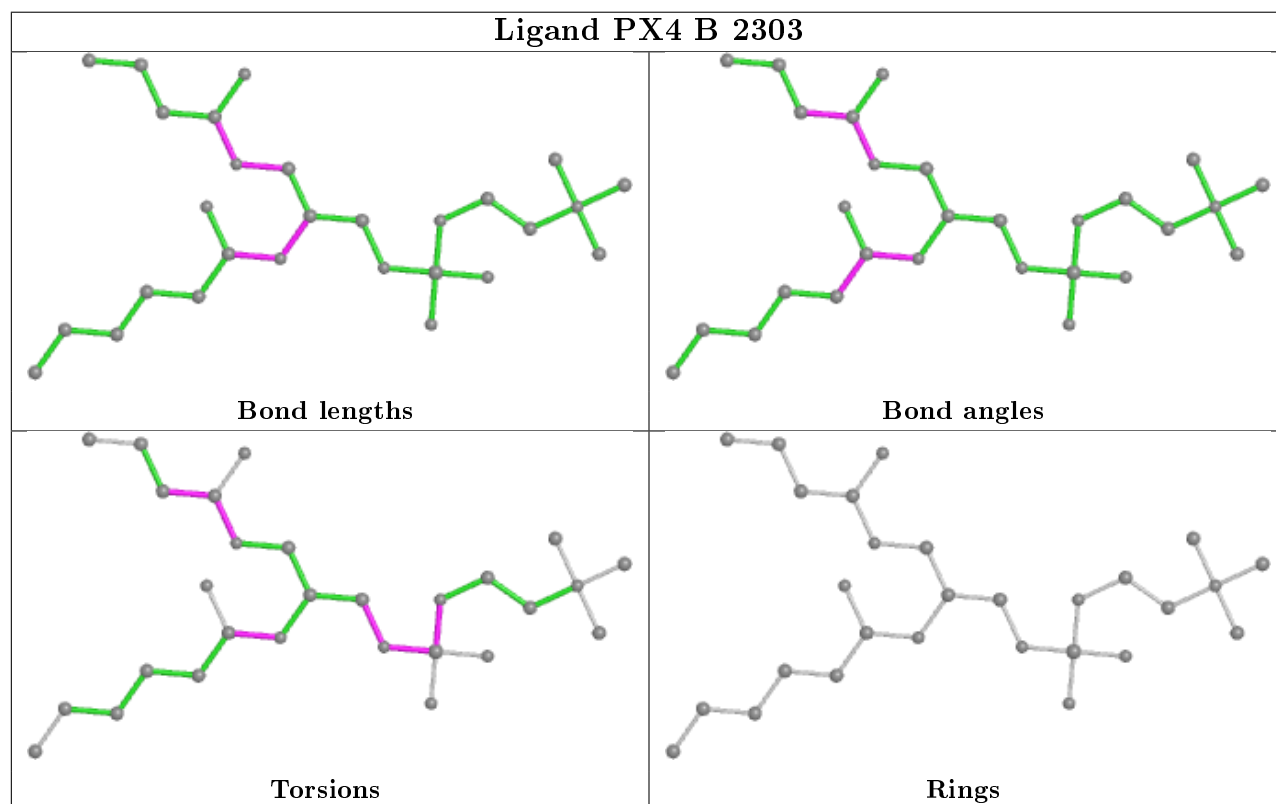
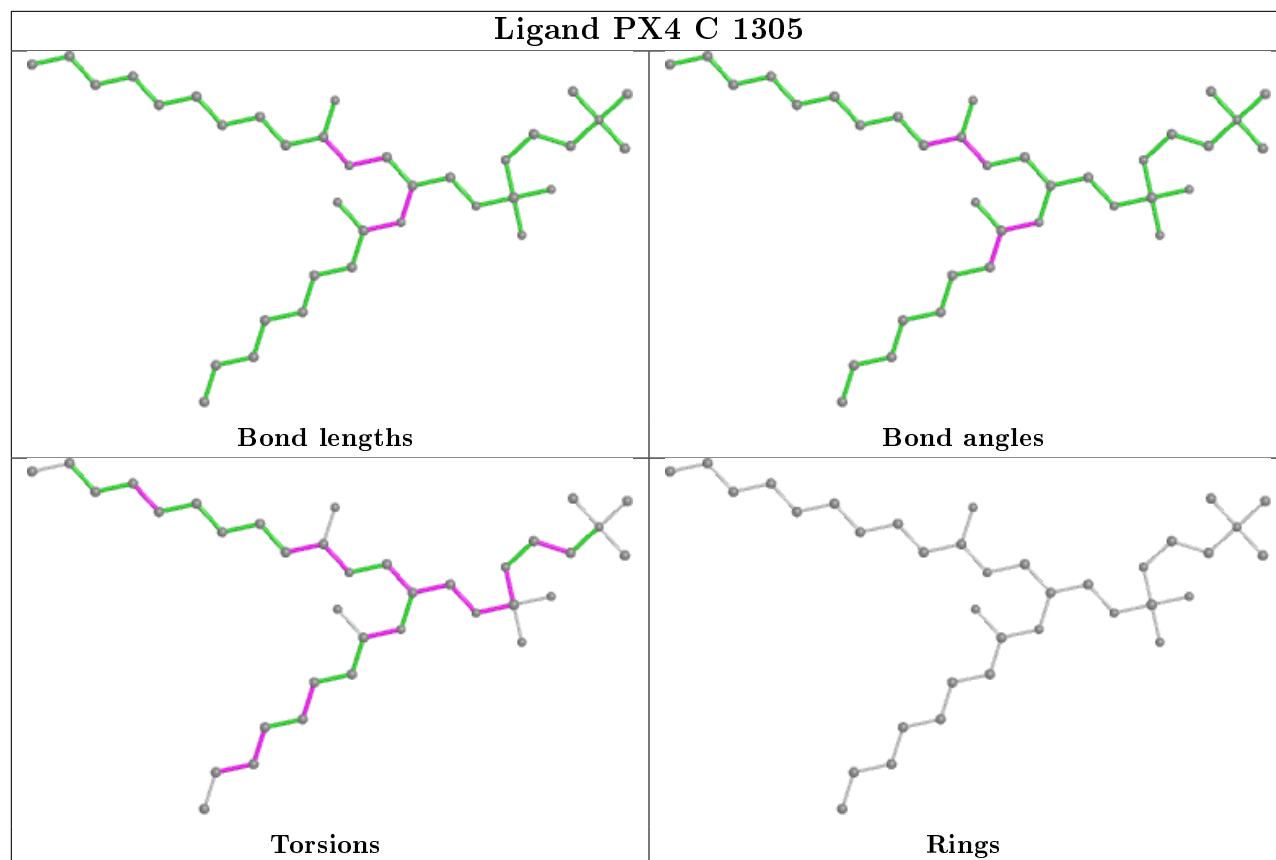




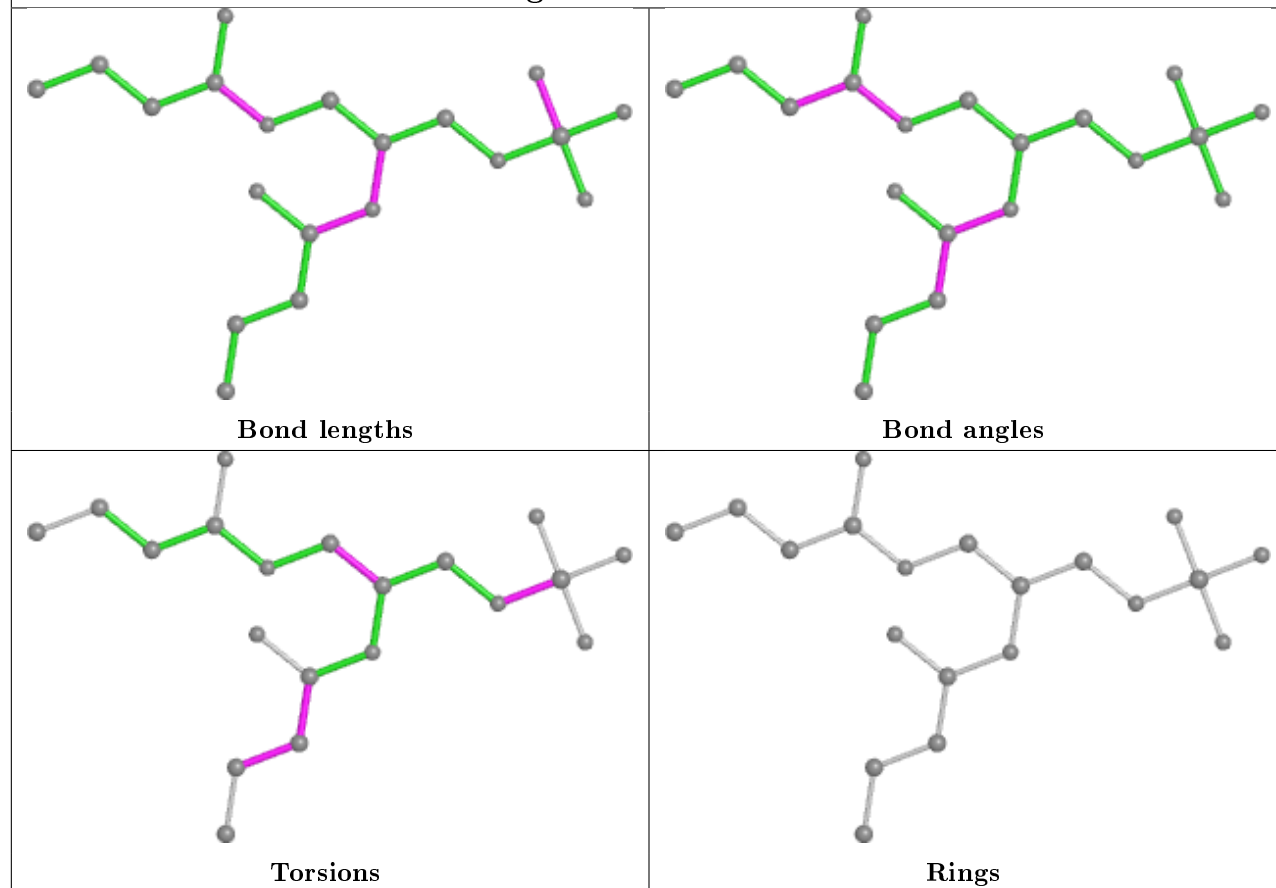




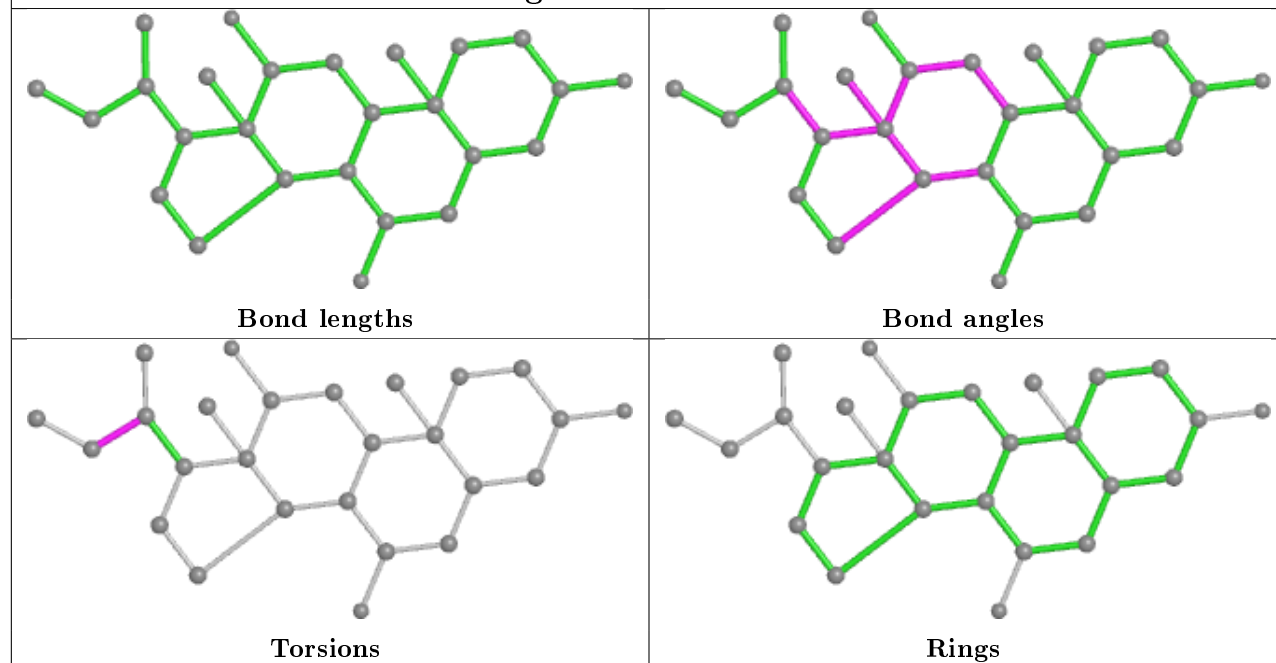


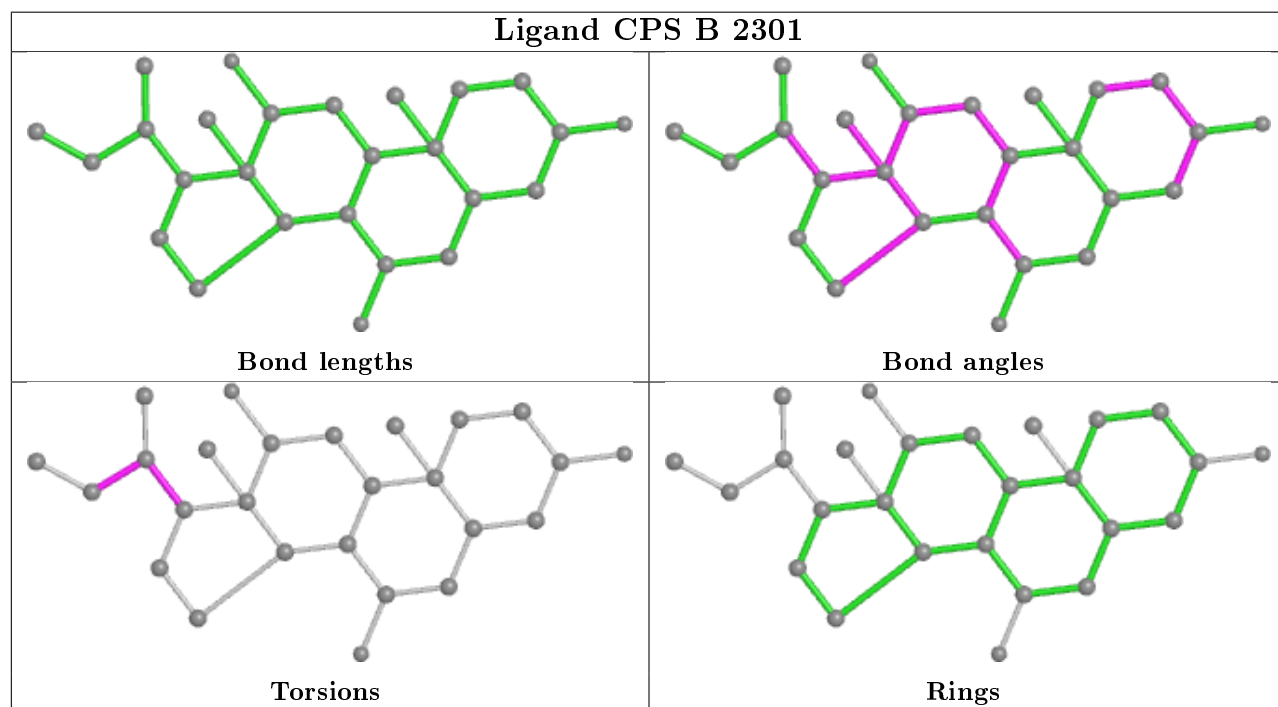
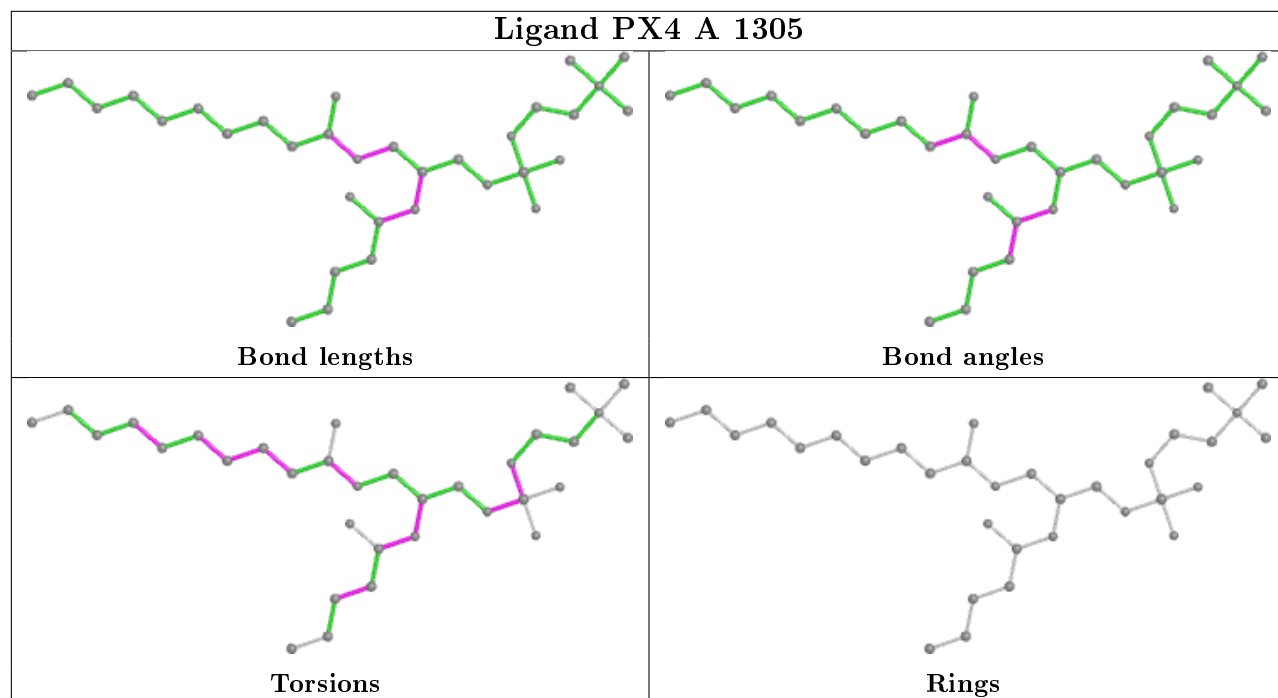


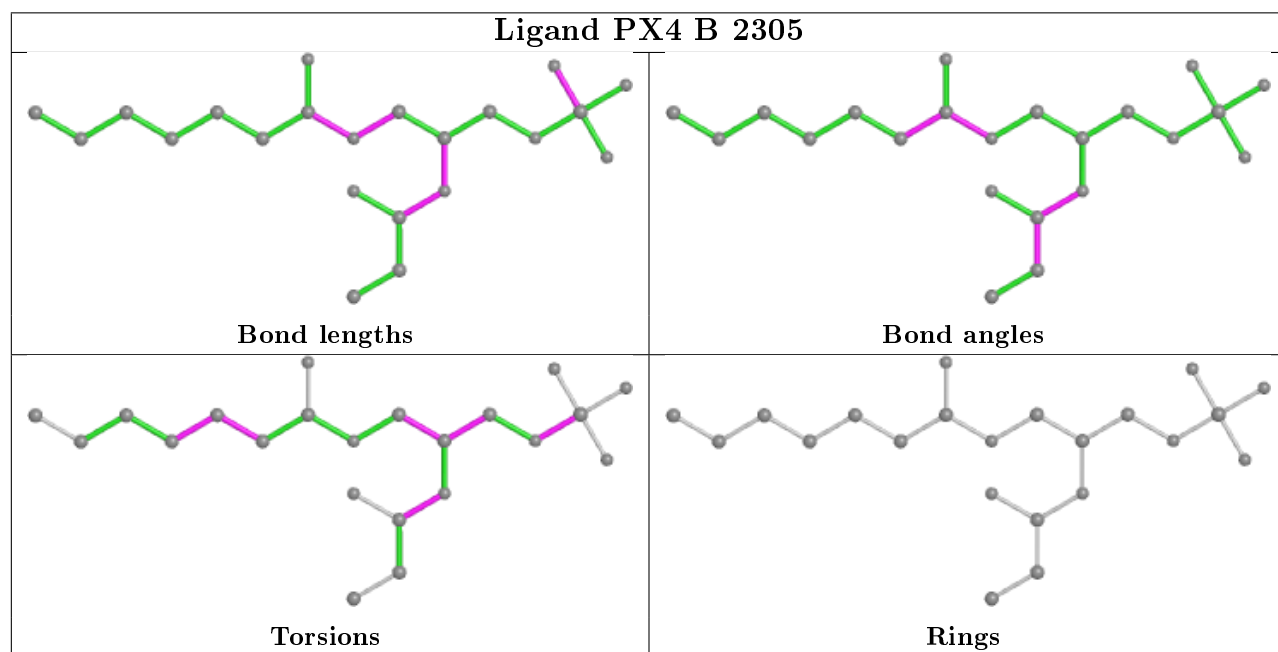
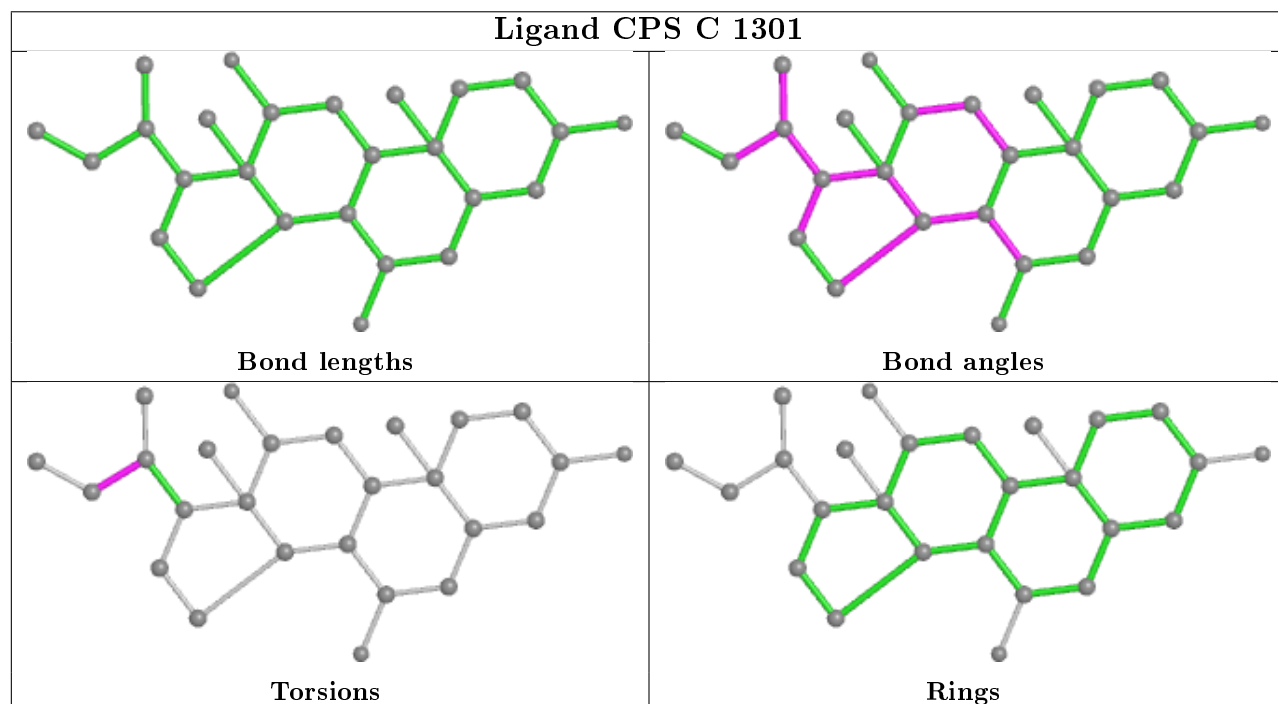
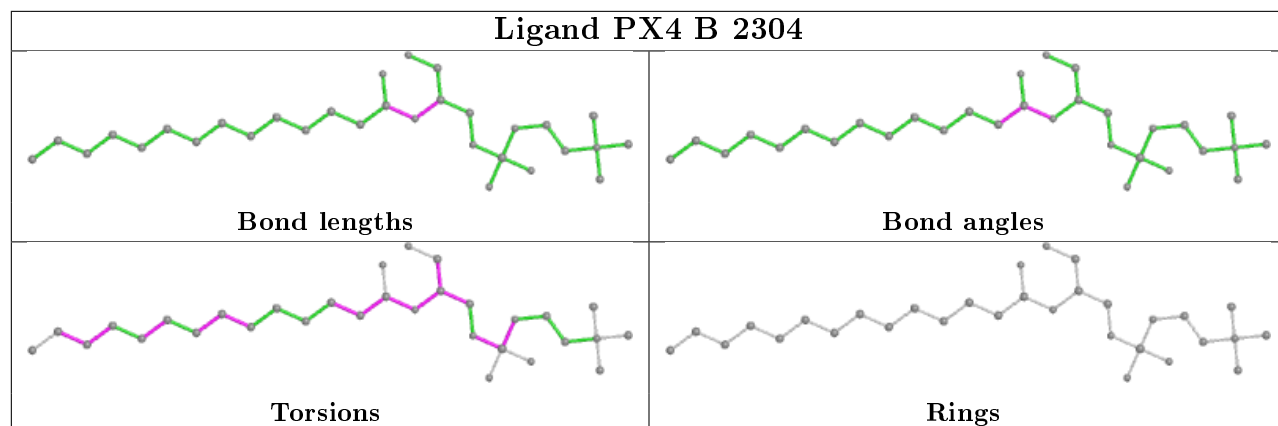
## Ligand PX4 C 1303



## Ligand CPS C 1302







## 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

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	262/285 (91%)	-0.11	6 (2%) 60 47	52, 96, 174, 231	0
1	B	259/285 (90%)	-0.04	4 (1%) 73 61	50, 108, 187, 230	0
1	C	261/285 (91%)	-0.09	7 (2%) 54 39	55, 107, 177, 210	0
1	D	268/285 (94%)	-0.14	3 (1%) 80 69	59, 97, 173, 200	0
All	All	1050/1140 (92%)	-0.09	20 (1%) 66 53	50, 100, 179, 231	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1264	SER	4.5
1	A	1263	THR	4.1
1	C	1263	THR	4.0
1	B	2255	VAL	3.0
1	A	1001	MET	2.8
1	B	2044	TYR	2.6
1	C	1039	GLN	2.4
1	C	1041	PHE	2.3
1	D	2039	GLN	2.3
1	B	2070	SER	2.2
1	C	1040	SER	2.2
1	D	2020	TYR	2.2
1	A	1041	PHE	2.2
1	C	1262	LYS	2.2
1	C	1245	ASN	2.1
1	A	1000	HIS	2.1
1	A	1036	THR	2.1
1	B	2036	THR	2.1
1	C	1036	THR	2.1
1	D	1995	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.

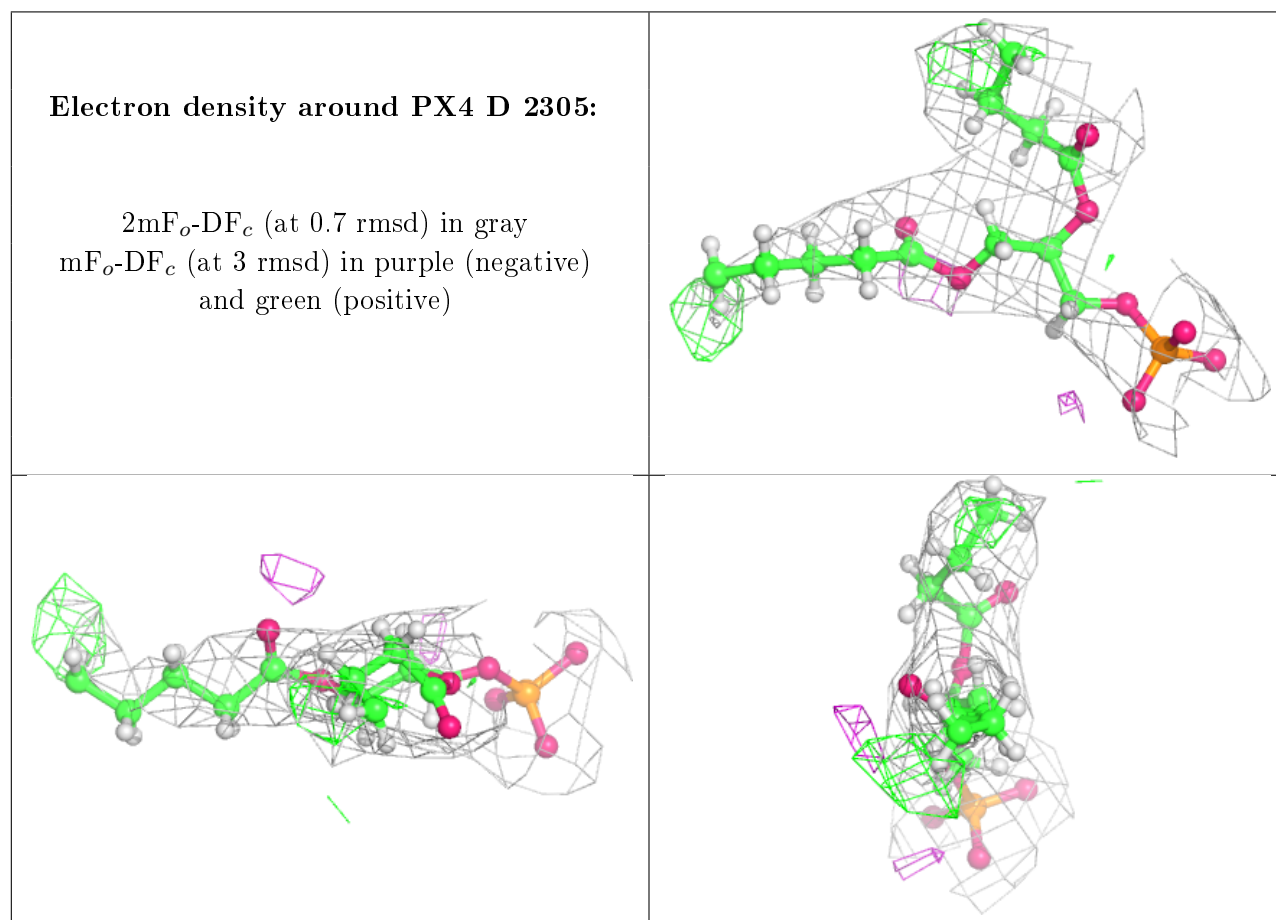
## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	D	2306	5/5	0.60	0.29	214,214,215,218	0
4	PO4	B	2307	5/5	0.73	0.21	202,203,203,205	0
4	PO4	A	1306	5/5	0.73	0.27	185,185,185,188	0
4	PO4	C	1306	5/5	0.74	0.27	192,193,193,195	0
3	PX4	D	2305	21/46	0.76	0.32	107,141,181,193	0
3	PX4	B	2305	22/46	0.80	0.32	99,124,152,160	0
3	PX4	B	2303	28/46	0.80	0.43	89,119,174,176	0
3	PX4	D	2304	27/46	0.81	0.50	109,133,159,161	0
3	PX4	A	1305	33/46	0.82	0.39	94,118,162,163	0
3	PX4	D	2303	19/46	0.83	0.30	97,118,146,157	0
3	PX4	C	1303	20/46	0.83	0.26	102,127,152,160	0
3	PX4	C	1305	36/46	0.84	0.40	95,118,166,166	0
3	PX4	A	1304	25/46	0.85	0.30	80,124,171,171	0
3	PX4	C	1304	27/46	0.87	0.27	89,111,145,146	0
5	CL	C	1307	1/1	0.90	0.18	80,80,80,80	0
3	PX4	B	2304	31/46	0.90	0.25	80,107,135,135	0
3	PX4	A	1303	26/46	0.91	0.27	80,110,137,137	0
3	PX4	B	2306	26/46	0.91	0.21	80,108,144,144	0
2	CPS	D	2302	26/42	0.91	0.27	80,96,101,101	0
2	CPS	A	1301	26/42	0.92	0.21	80,96,97,99	0
2	CPS	B	2302	26/42	0.92	0.31	86,104,107,109	0
2	CPS	A	1302	26/42	0.92	0.33	80,96,97,100	0
2	CPS	C	1301	26/42	0.93	0.28	80,96,107,107	0
2	CPS	C	1302	26/42	0.94	0.32	84,103,115,116	0
2	CPS	D	2301	26/42	0.95	0.25	80,96,108,110	0
2	CPS	B	2301	26/42	0.96	0.28	88,108,120,120	0

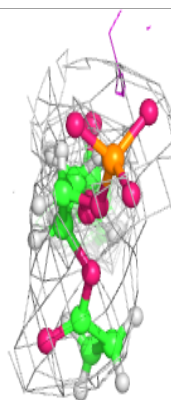
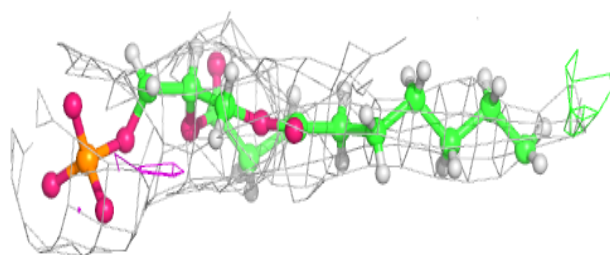
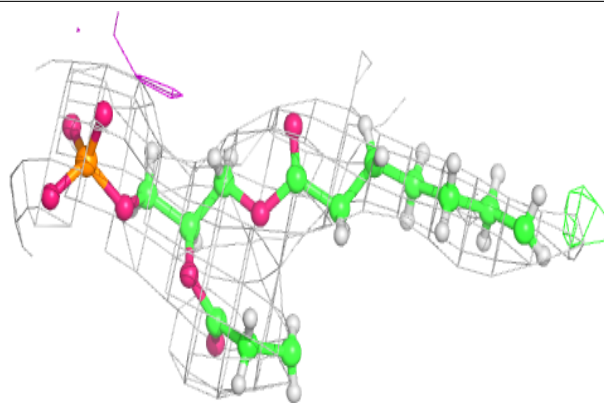


The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

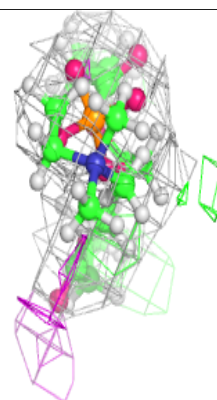
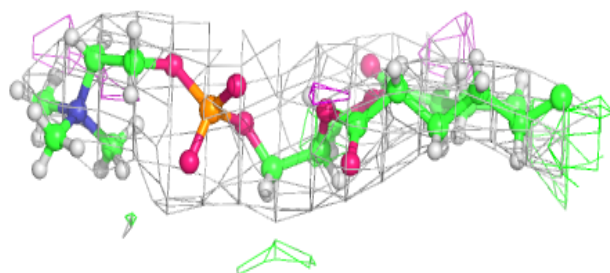
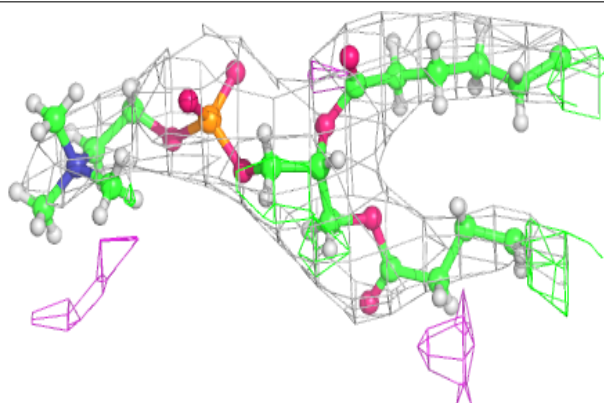


**Electron density around PX4 B 2305:**

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

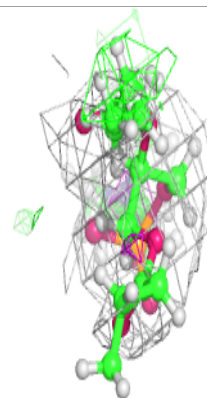
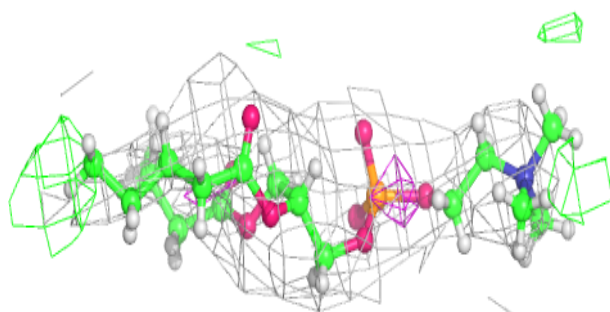
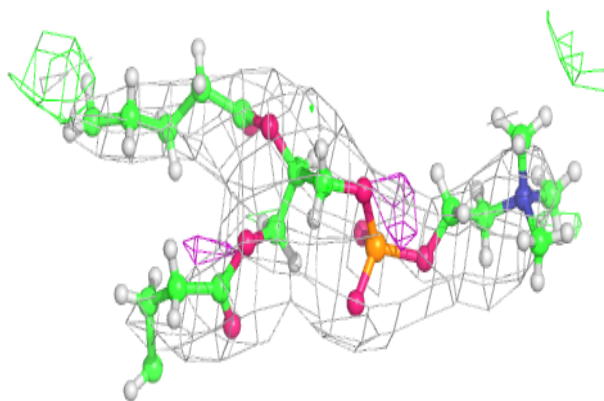
**Electron density around PX4 B 2303:**

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

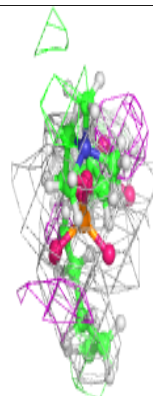
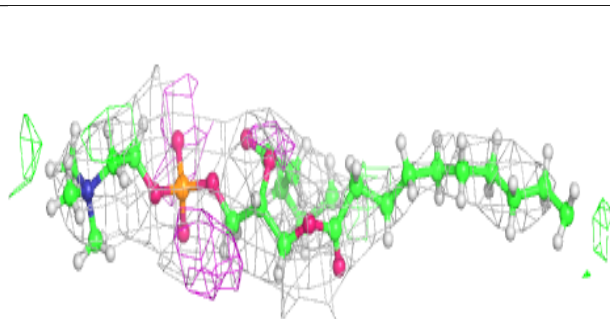
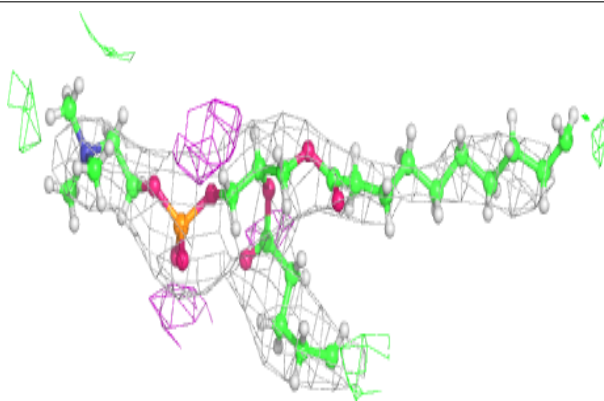


**Electron density around PX4 D 2304:**

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

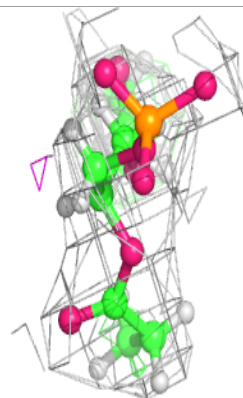
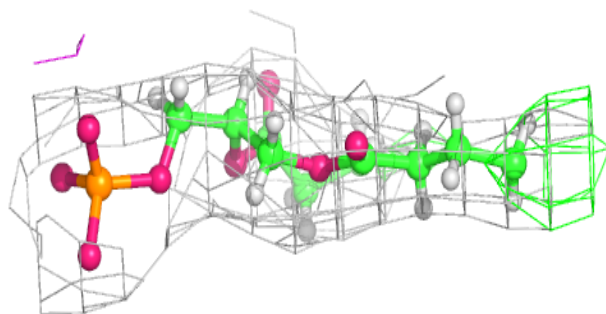
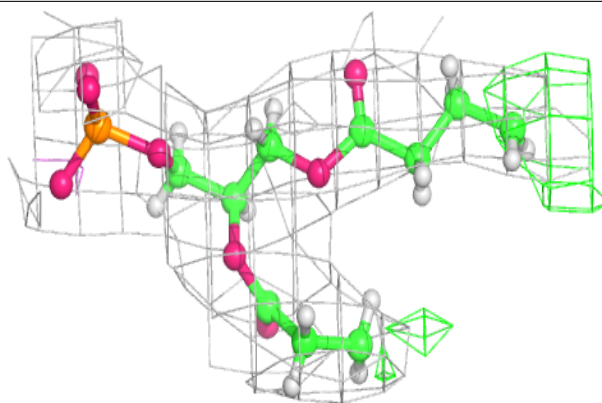
**Electron density around PX4 A 1305:**

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

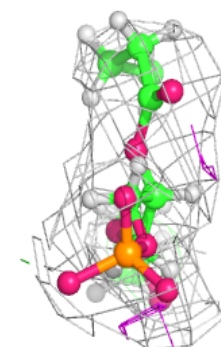
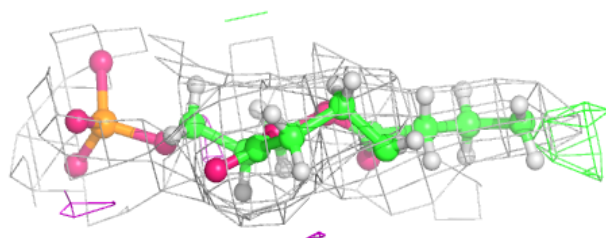
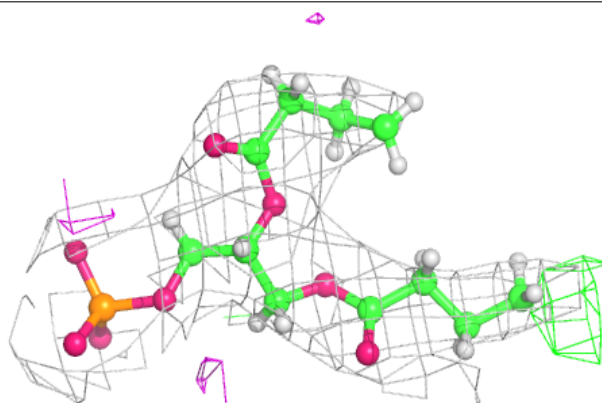


**Electron density around PX4 D 2303:**

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

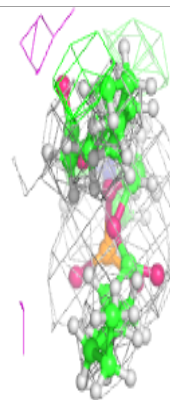
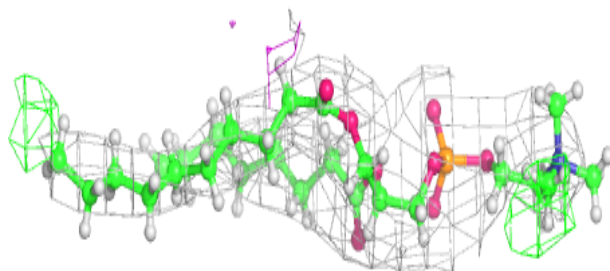
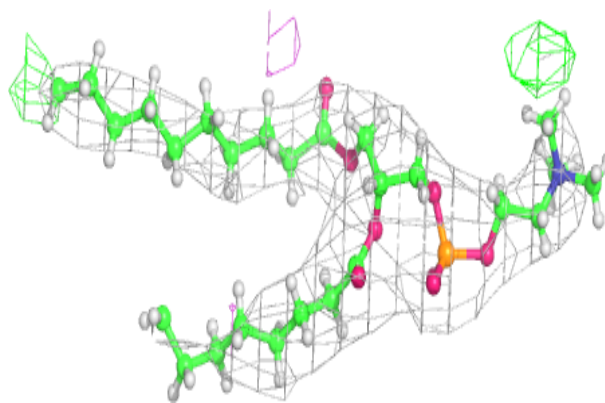
**Electron density around PX4 C 1303:**

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

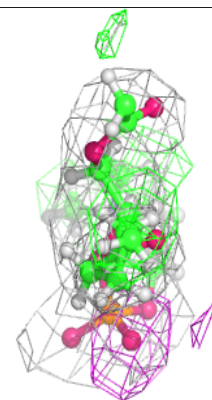
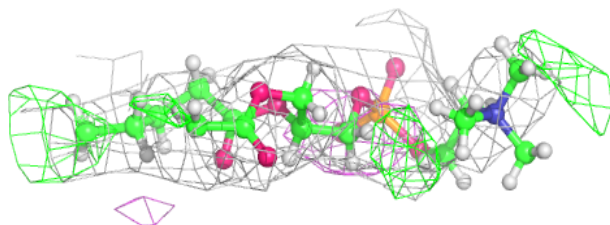
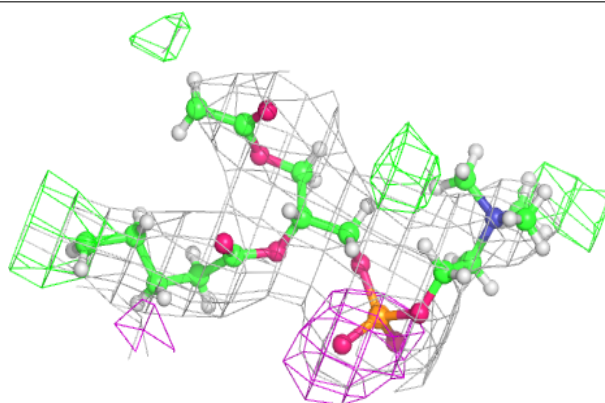


**Electron density around PX4 C 1305:**

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

**Electron density around PX4 A 1304:**

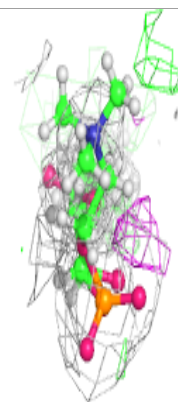
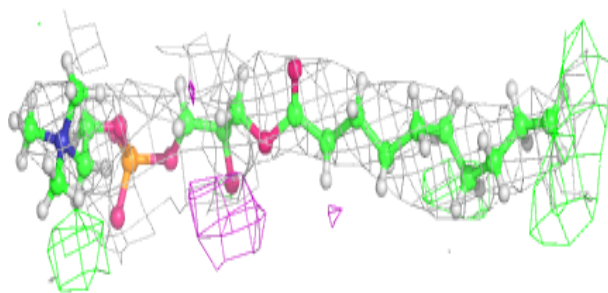
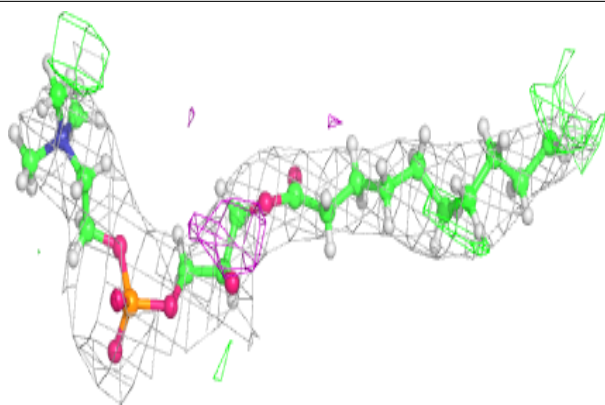
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



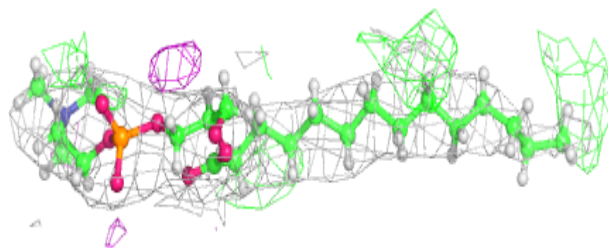
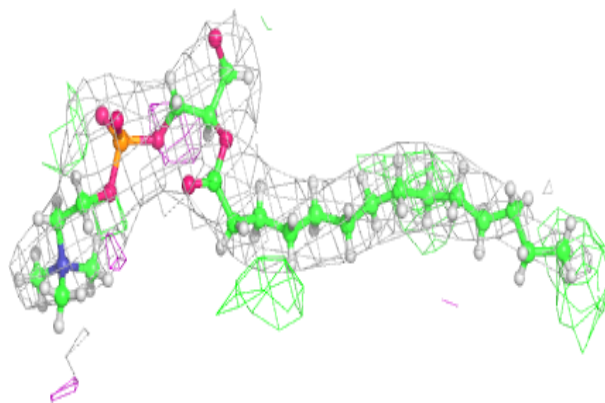


**Electron density around PX4 C 1304:**

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

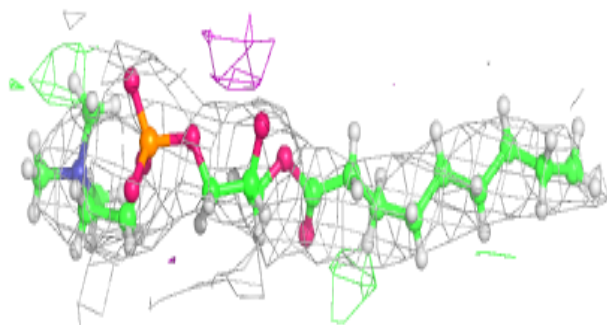
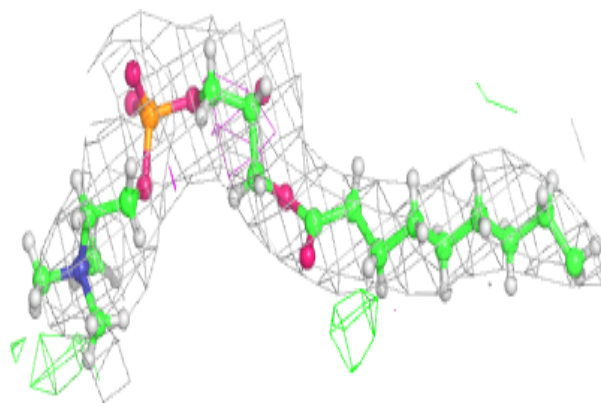
**Electron density around PX4 B 2304:**

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

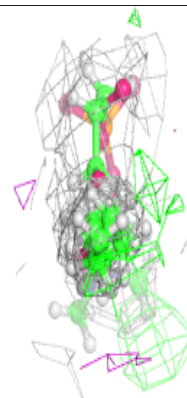
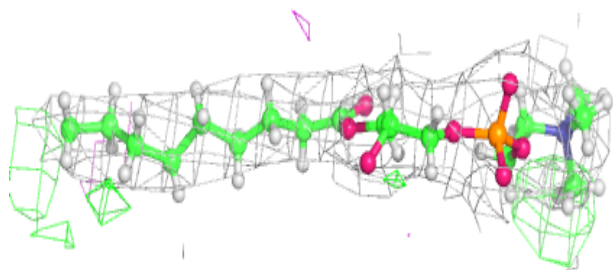
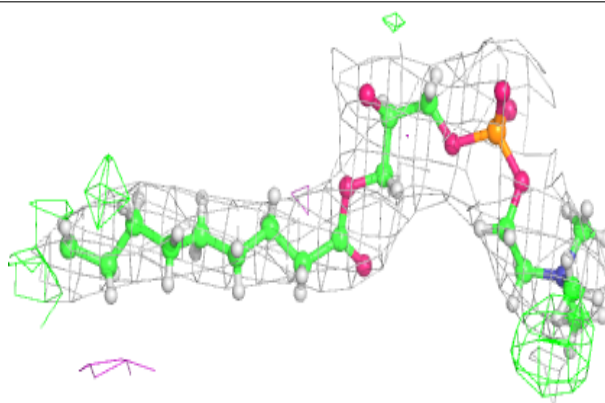


**Electron density around PX4 A 1303:**

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

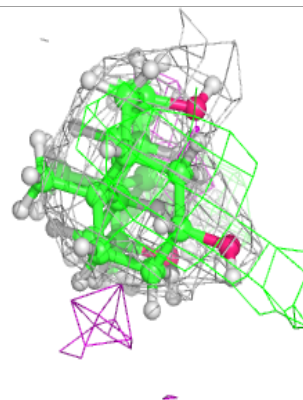
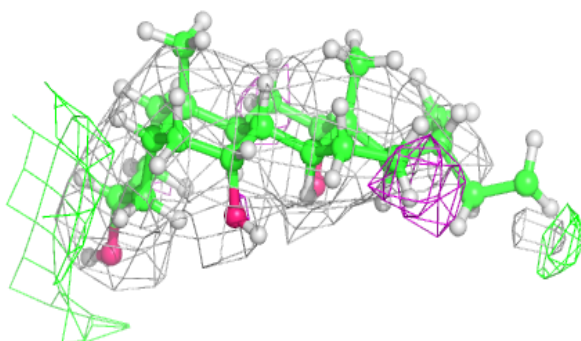
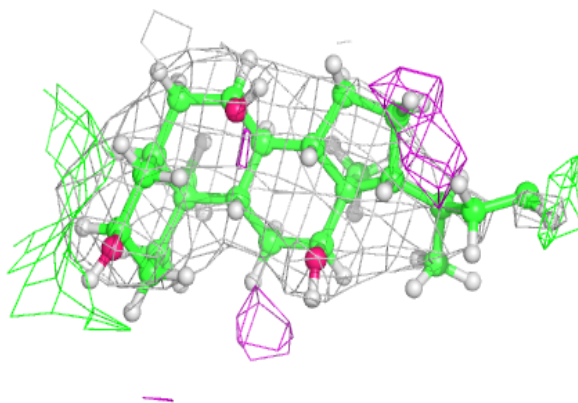
**Electron density around PX4 B 2306:**

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

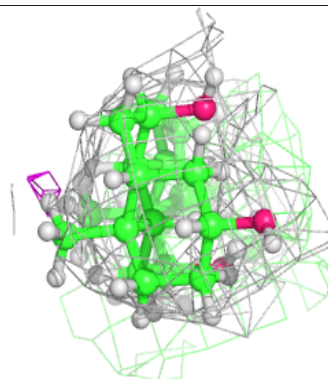
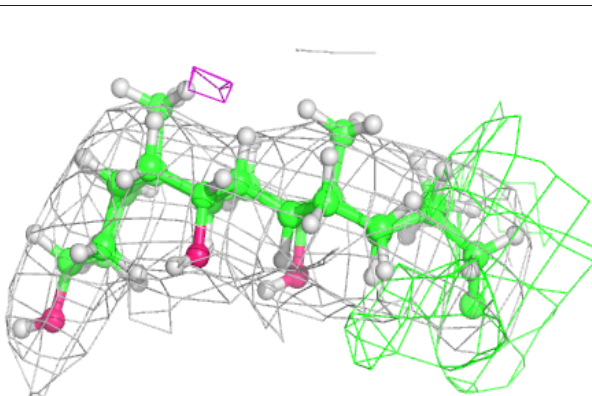
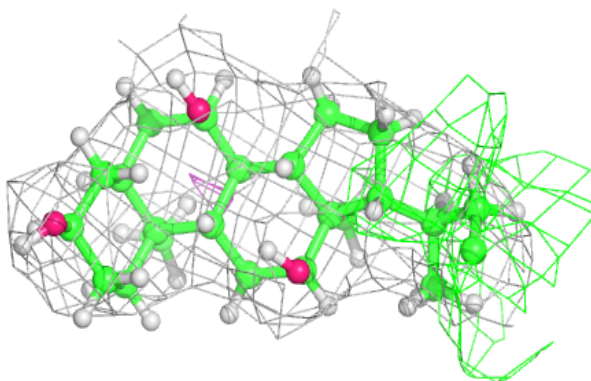


**Electron density around CPS D 2302:**

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

**Electron density around CPS A 1301:**

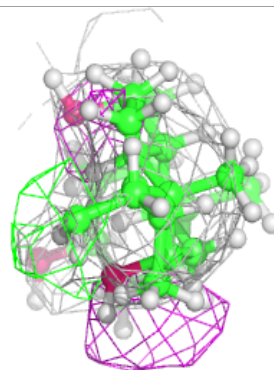
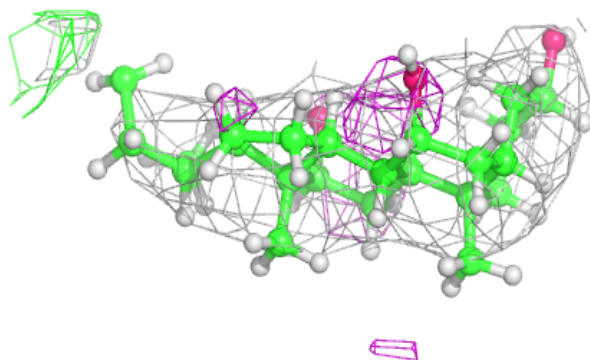
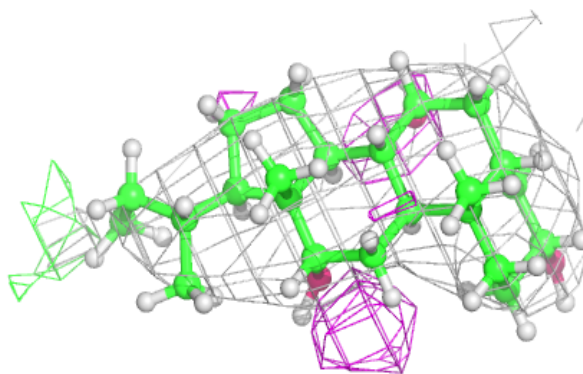
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



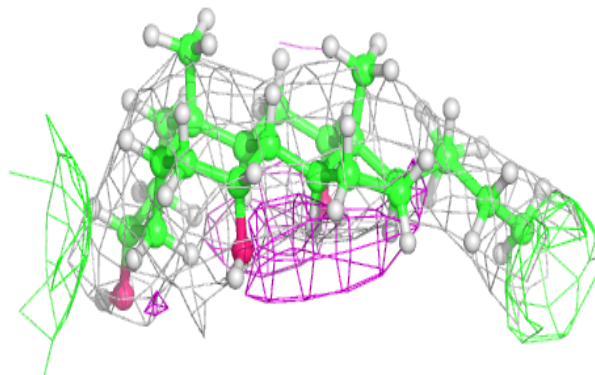
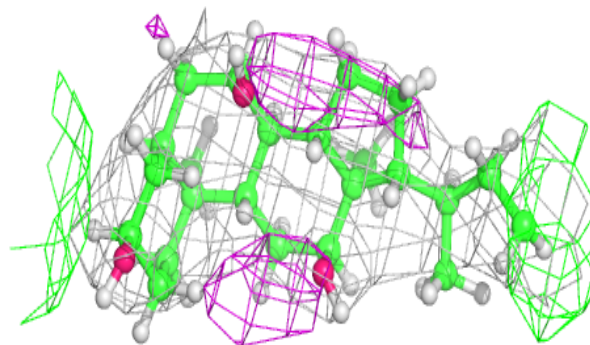


**Electron density around CPS B 2302:**

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

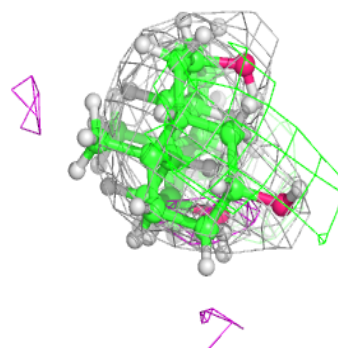
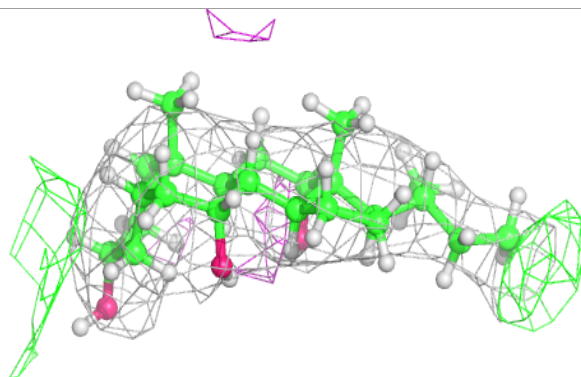
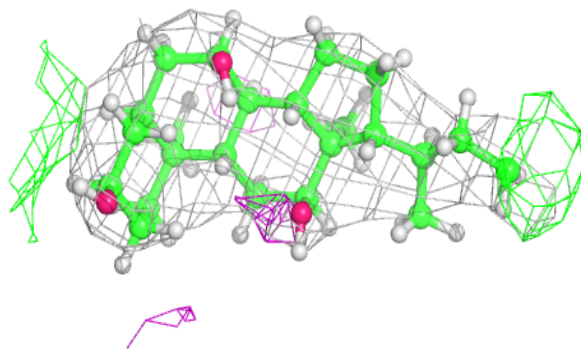
**Electron density around CPS A 1302:**

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

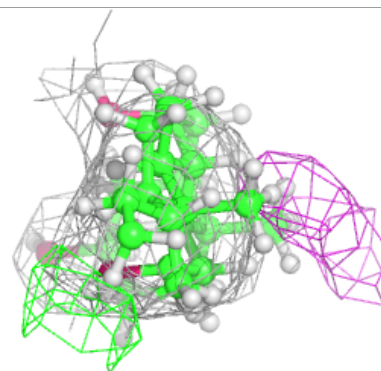
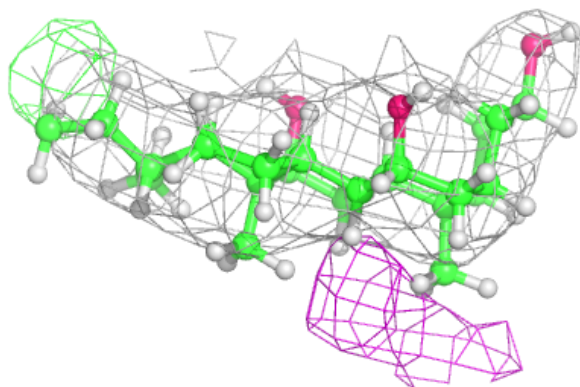
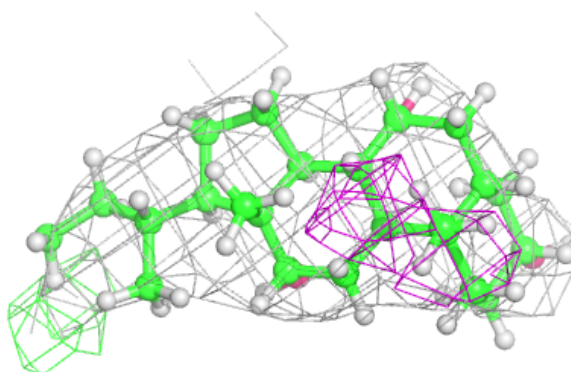


**Electron density around CPS C 1301:**

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

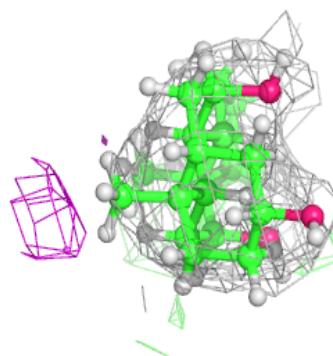
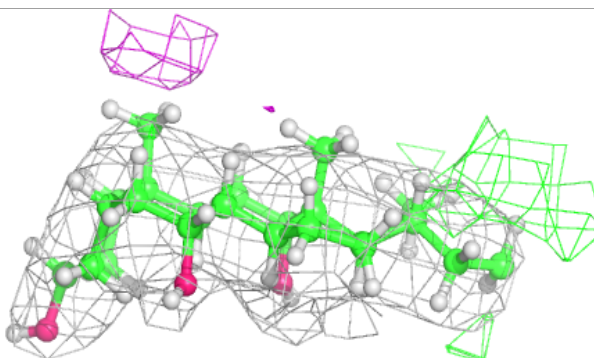
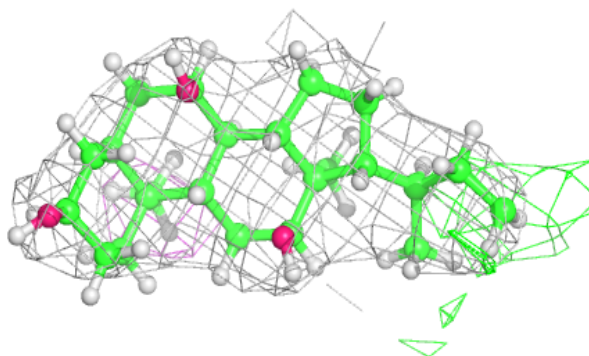
**Electron density around CPS C 1302:**

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

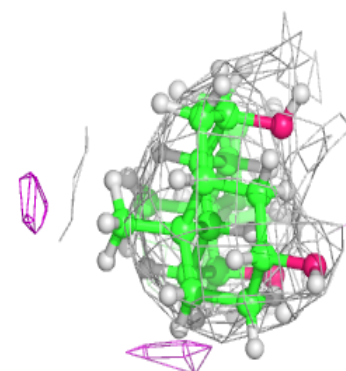
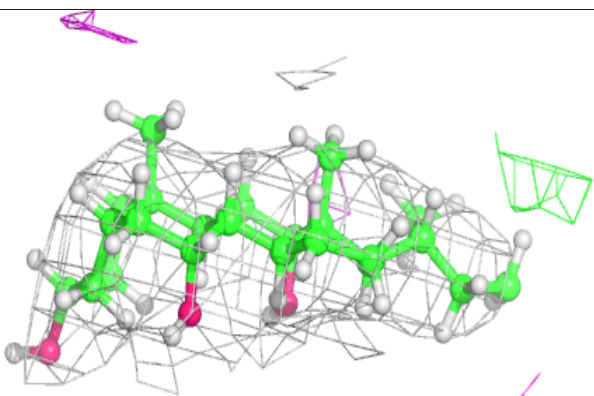
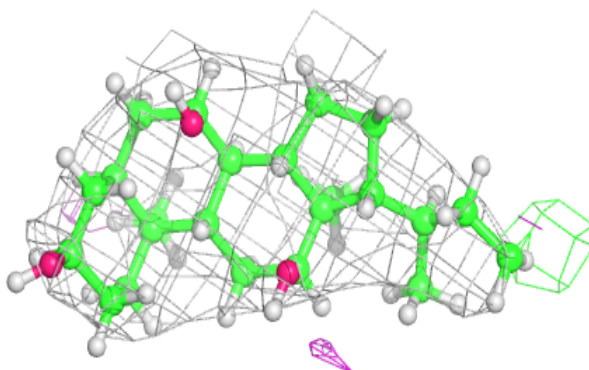


**Electron density around CPS D 2301:**

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

**Electron density around CPS B 2301:**

$2mF_o-DF_c$  (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.