Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 05:53 PM EDT

PDB ID	:	6MWG
Title	:	NavAb Voltage-gated Sodium Channel, residues 1-239, with mutation T206V
Authors	:	Lenaeus, M.J.; Catterall, W.A.
Deposited on	:	2018-10-29
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

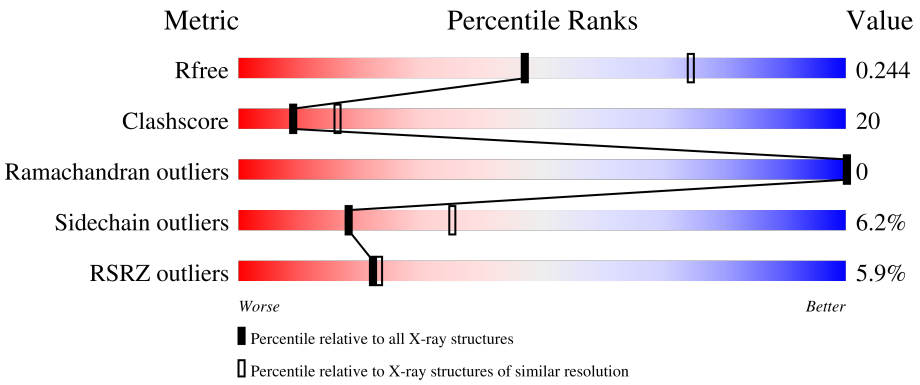
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	B	257	5% 67% 23% • 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CPS	B	2306	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2147 atoms, of which 75 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.

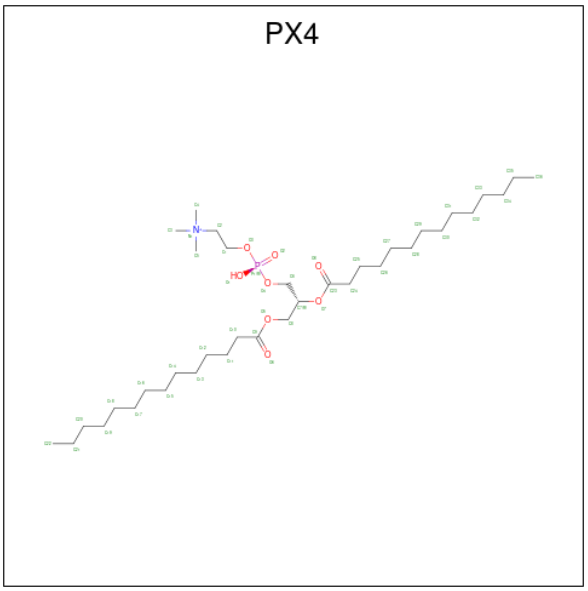
- Molecule 1 is a protein called Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	237	1843	1248	274	310	11	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

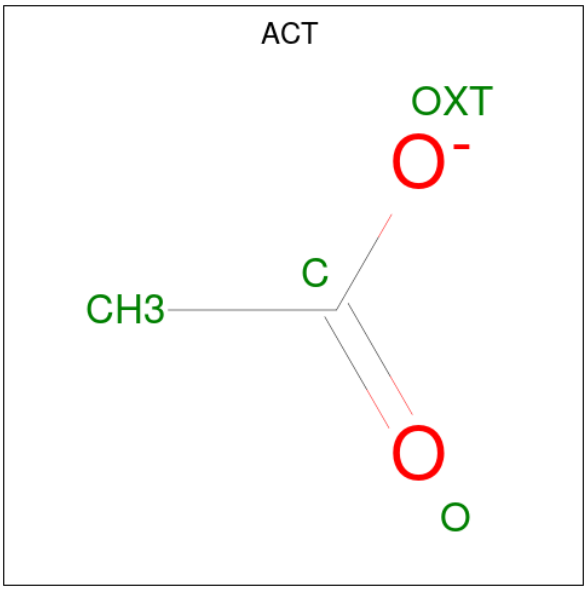
Chain	Residue	Modelled	Actual	Comment	Reference
B	1983	MET	-	initiating methionine	UNP A8EVM5
B	1984	ASP	-	expression tag	UNP A8EVM5
B	1985	TYR	-	expression tag	UNP A8EVM5
B	1986	LYS	-	expression tag	UNP A8EVM5
B	1987	ASP	-	expression tag	UNP A8EVM5
B	1988	ASP	-	expression tag	UNP A8EVM5
B	1989	ASP	-	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	VAL	THR	engineered mutation	UNP A8EVM5

- Molecule 2 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).



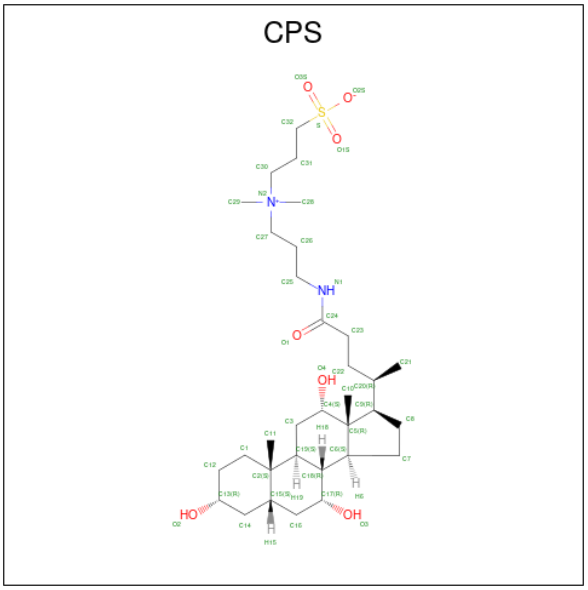
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O P 42 32 1 8 1	0	0
2	B	1	Total C O P 40 31 8 1	0	0
2	B	1	Total C N O P 46 36 1 8 1	0	0
2	B	1	Total C O P 19 12 6 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H N O 69 24 40 1 4	0	0
4	B	1	Total C H O 60 22 35 3	0	0

- Molecule 5 is water.

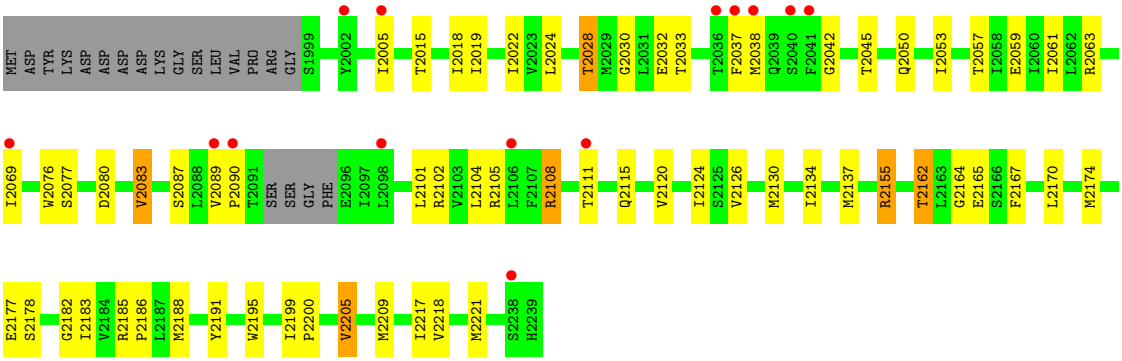
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	24	Total O 24 24	0	0

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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	124.17Å 124.17Å 189.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.50 29.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.77-2.50) 90.0 (29.77-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.220 , 0.239 0.222 , 0.244	Depositor DCC
R_{free} test set	1291 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	56.6	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 82.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2147	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CPS, PX4, ACT

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	B	0.37	0/1890	0.46	0/2584

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	B	1843	0	1824	67	0
2	B	147	0	210	9	0
3	B	4	0	3	0	0
4	B	54	75	70	12	0
5	B	24	0	0	0	0
All	All	2072	75	2107	84	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 20.

All (84) 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:B:2217:ILE:HG22	1:B:2221:MET:HE2	1.36	1.07
1:B:2218:VAL:HA	1:B:2221:MET:HE3	1.33	1.06
1:B:2162:THR:HG22	1:B:2165:GLU:H	1.28	0.97
1:B:2038:MET:HA	1:B:2038:MET:HE2	1.51	0.91
1:B:2218:VAL:HA	1:B:2221:MET:CE	2.07	0.84
1:B:2137:MET:HE1	1:B:2205:VAL:HA	1.62	0.81
1:B:2089:VAL:HG13	1:B:2090:PRO:HD2	1.67	0.77
1:B:2089:VAL:CG1	1:B:2090:PRO:HD2	2.17	0.74
1:B:2199:ILE:HB	1:B:2200:PRO:HD3	1.71	0.72
1:B:2102:ARG:HH21	1:B:2102:ARG:CG	2.04	0.71
1:B:2102:ARG:HH21	1:B:2102:ARG:HG2	1.57	0.70
4:B:2307:CPS:H10B	4:B:2307:CPS:C22	2.21	0.70
1:B:2137:MET:CE	1:B:2205:VAL:HG22	2.21	0.69
4:B:2306:CPS:H10A	4:B:2306:CPS:C21	2.24	0.68
1:B:2137:MET:HE1	1:B:2205:VAL:HG22	1.76	0.67
1:B:2174:MET:HG3	1:B:2205:VAL:HG11	1.78	0.66
1:B:2083:VAL:HG11	1:B:2105:ARG:HA	1.77	0.66
1:B:2174:MET:HG3	1:B:2205:VAL:CG1	2.27	0.64
1:B:2038:MET:HA	1:B:2038:MET:CE	2.25	0.62
4:B:2306:CPS:H21A	4:B:2306:CPS:O4	2.03	0.59
1:B:2080:ASP:OD2	1:B:2111:THR:HG21	2.04	0.58
1:B:2028:THR:HG23	1:B:2045:THR:CG2	2.34	0.57
1:B:2037:PHE:HD2	1:B:2038:MET:HE3	1.68	0.57
1:B:2037:PHE:CD2	1:B:2038:MET:HE3	2.40	0.57
4:B:2306:CPS:H10A	4:B:2306:CPS:H21A	1.88	0.55
1:B:2083:VAL:CG1	1:B:2105:ARG:HA	2.36	0.54
4:B:2307:CPS:C22	4:B:2307:CPS:C10	2.86	0.54
4:B:2306:CPS:C21	4:B:2306:CPS:C24	2.85	0.54
2:B:2303:PX4:H26	2:B:2303:PX4:H56	1.92	0.52
1:B:2059:GLU:OE1	1:B:2108:ARG:NH2	2.43	0.52
1:B:2217:ILE:HG22	1:B:2221:MET:CE	2.24	0.51
1:B:2217:ILE:O	1:B:2221:MET:HG3	2.10	0.51
1:B:2137:MET:HE3	1:B:2205:VAL:HG22	1.92	0.51
1:B:2080:ASP:CG	1:B:2111:THR:HG21	2.31	0.51
1:B:2182:GLY:C	1:B:2183:ILE:HD12	2.31	0.51
1:B:2059:GLU:CD	1:B:2108:ARG:HH22	2.15	0.49
1:B:2032:GLU:HG3	1:B:2045:THR:HG21	1.93	0.49
2:B:2301:PX4:O3	2:B:2301:PX4:H6	2.10	0.49
1:B:2076:TRP:CZ2	2:B:2304:PX4:H18	2.48	0.49
1:B:2101:LEU:HD22	1:B:2104:LEU:HD11	1.94	0.49
1:B:2177:GLU:OE1	1:B:2178:SER:OG	2.11	0.48
1:B:2038:MET:CE	1:B:2042:GLY:HA2	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2080:ASP:OD1	1:B:2111:THR:HG21	2.14	0.48
2:B:2301:PX4:O3	2:B:2301:PX4:H10	2.14	0.47
1:B:2130:MET:HE2	1:B:2134:ILE:HD11	1.96	0.47
1:B:2030:GLY:O	1:B:2033:THR:HB	2.14	0.47
1:B:2188:MET:HA	1:B:2191:TYR:O	2.14	0.47
1:B:2217:ILE:C	1:B:2221:MET:HE2	2.36	0.46
1:B:2174:MET:CG	1:B:2205:VAL:HG11	2.44	0.46
4:B:2306:CPS:H21	4:B:2306:CPS:H23A	1.70	0.46
1:B:2102:ARG:CG	1:B:2102:ARG:NH2	2.72	0.45
1:B:2038:MET:HE2	1:B:2042:GLY:HA2	1.98	0.45
1:B:2170:LEU:HD23	1:B:2170:LEU:HA	1.76	0.45
1:B:2015:THR:O	1:B:2019:ILE:HG13	2.17	0.45
1:B:2105:ARG:O	1:B:2108:ARG:HB2	2.17	0.45
2:B:2302:PX4:H38	2:B:2302:PX4:H63	1.99	0.45
1:B:2185:ARG:HB2	1:B:2186:PRO:HD3	1.98	0.44
1:B:2195:TRP:O	1:B:2199:ILE:HG12	2.16	0.44
1:B:2018:ILE:O	1:B:2022:ILE:HG13	2.17	0.44
1:B:2155:ARG:HH11	1:B:2155:ARG:CG	2.29	0.44
1:B:2191:TYR:CD2	2:B:2303:PX4:H14	2.53	0.43
4:B:2306:CPS:O4	4:B:2306:CPS:H20	2.19	0.43
1:B:2063:ARG:NH2	1:B:2077:SER:HB3	2.34	0.43
1:B:2108:ARG:CG	1:B:2108:ARG:HH11	2.32	0.42
1:B:2032:GLU:CG	1:B:2045:THR:HG21	2.50	0.42
1:B:2120:VAL:O	1:B:2124:ILE:HG12	2.19	0.42
1:B:2162:THR:HG22	1:B:2165:GLU:N	2.12	0.42
2:B:2301:PX4:H46	2:B:2302:PX4:H28	2.01	0.42
4:B:2306:CPS:C24	4:B:2306:CPS:H21B	2.48	0.42
1:B:2076:TRP:CH2	2:B:2304:PX4:H18	2.55	0.41
1:B:2089:VAL:HG12	1:B:2090:PRO:HD2	1.97	0.41
1:B:2050:GLN:HA	1:B:2053:ILE:HG22	2.02	0.41
1:B:2057:THR:O	1:B:2061:ILE:HG13	2.20	0.41
1:B:2162:THR:HG23	1:B:2164:GLY:H	1.84	0.41
1:B:2050:GLN:O	1:B:2053:ILE:HG22	2.21	0.41
1:B:2126:VAL:HG12	4:B:2307:CPS:H16A	2.02	0.41
1:B:2137:MET:HE1	1:B:2205:VAL:CG2	2.49	0.41
1:B:2089:VAL:CG1	1:B:2090:PRO:CD	2.96	0.41
2:B:2301:PX4:H46	2:B:2302:PX4:H32	2.03	0.41
4:B:2306:CPS:O4	4:B:2306:CPS:C20	2.69	0.41
1:B:2087:SER:OG	1:B:2105:ARG:NH2	2.49	0.41
4:B:2306:CPS:H10B	4:B:2306:CPS:H3	1.72	0.40
1:B:2155:ARG:HH11	1:B:2155:ARG:HG3	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2218:VAL:CA	1:B:2221:MET:HE3	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	233/257 (91%)	230 (99%)	3 (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	B	193/236 (82%)	181 (94%)	12 (6%)	18 35

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2005	ILE
1	B	2024	LEU
1	B	2028	THR
1	B	2069	ILE
1	B	2083	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2108	ARG
1	B	2115	GLN
1	B	2155	ARG
1	B	2162	THR
1	B	2167	PHE
1	B	2205	VAL
1	B	2209	MET

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PX4	B	2303	-	45,45,45	1.04	4 (8%)	51,53,53	1.05	3 (5%)
3	ACT	B	2305	-	3,3,3	0.79	0	3,3,3	1.37	0
4	CPS	B	2306	-	32,32,45	2.61	9 (28%)	51,51,70	2.88	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PX4	B	2301	-	41,41,45	1.08	4 (9%)	47,49,53	1.17	2 (4%)
4	CPS	B	2307	-	28,28,45	3.20	14 (50%)	46,46,70	3.53	19 (41%)
2	PX4	B	2302	-	39,39,45	1.03	5 (12%)	43,44,53	1.19	3 (6%)
2	PX4	B	2304	-	18,18,45	1.17	2 (11%)	21,21,53	1.09	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PX4	B	2303	-	-	19/49/49/49	-
4	CPS	B	2306	-	1/1/12/15	5/9/74/90	0/4/4/4
2	PX4	B	2301	-	-	20/45/45/49	-
4	CPS	B	2307	-	-	0/4/69/90	0/4/4/4
2	PX4	B	2302	-	-	18/41/41/49	-
2	PX4	B	2304	-	-	11/17/17/49	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2307	CPS	C10-C5	10.03	1.70	1.54
4	B	2306	CPS	O4-C4	-6.86	1.32	1.43
4	B	2307	CPS	O4-C4	-6.16	1.33	1.43
4	B	2306	CPS	C3-C4	6.12	1.63	1.53
4	B	2307	CPS	C5-C4	-5.75	1.45	1.54
4	B	2307	CPS	C5-C6	-5.44	1.46	1.55
4	B	2306	CPS	C10-C5	5.21	1.62	1.54
4	B	2306	CPS	C20-C9	4.90	1.63	1.54
4	B	2307	CPS	C5-C9	-3.95	1.48	1.55
4	B	2306	CPS	C18-C6	3.84	1.61	1.53
4	B	2306	CPS	C24-N1	3.60	1.44	1.32
4	B	2307	CPS	O3-C17	-3.46	1.36	1.43
4	B	2306	CPS	C21-C20	3.24	1.61	1.53
4	B	2306	CPS	O3-C17	-2.74	1.37	1.43
2	B	2302	PX4	P1-O3	2.72	1.65	1.54
2	B	2304	PX4	P1-O3	2.71	1.65	1.54
4	B	2307	CPS	C3-C4	2.64	1.57	1.53
4	B	2307	CPS	C1-C12	-2.59	1.47	1.53
4	B	2307	CPS	C2-C15	-2.57	1.51	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2301	PX4	O5-C9	2.49	1.40	1.33
2	B	2301	PX4	O5-C8	-2.46	1.39	1.45
2	B	2303	PX4	O7-C23	2.44	1.41	1.34
2	B	2302	PX4	O7-C23	2.44	1.41	1.34
2	B	2304	PX4	O5-C9	2.42	1.40	1.33
2	B	2303	PX4	O5-C9	2.41	1.40	1.33
4	B	2307	CPS	C22-C20	-2.41	1.44	1.52
2	B	2301	PX4	O7-C23	2.39	1.41	1.34
4	B	2307	CPS	C21-C20	2.37	1.60	1.52
4	B	2307	CPS	C18-C6	2.37	1.58	1.53
2	B	2303	PX4	O7-C7	-2.36	1.40	1.46
2	B	2302	PX4	O7-C7	-2.33	1.40	1.46
2	B	2301	PX4	O7-C7	-2.31	1.40	1.46
4	B	2306	CPS	C2-C15	-2.25	1.51	1.55
2	B	2302	PX4	O5-C8	-2.24	1.40	1.45
2	B	2302	PX4	O5-C9	2.20	1.39	1.33
4	B	2307	CPS	C14-C15	-2.20	1.50	1.53
2	B	2303	PX4	O5-C8	-2.15	1.40	1.45
4	B	2307	CPS	C9-C20	2.03	1.59	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2307	CPS	C9-C5-C6	11.54	111.73	100.09
4	B	2306	CPS	C8-C9-C5	-8.15	95.56	103.55
4	B	2307	CPS	C6-C5-C4	7.96	114.82	107.40
4	B	2307	CPS	C8-C9-C5	-7.78	95.92	103.55
4	B	2307	CPS	C10-C5-C4	-7.75	101.18	109.07
4	B	2306	CPS	C3-C4-C5	-7.25	103.80	111.24
4	B	2306	CPS	C9-C5-C6	7.17	107.32	100.09
4	B	2306	CPS	C8-C9-C20	6.97	122.94	112.15
4	B	2307	CPS	C10-C5-C9	-5.78	102.16	111.21
4	B	2307	CPS	C10-C5-C6	-5.50	102.61	111.21
4	B	2306	CPS	C21-C20-C9	5.44	121.25	112.92
4	B	2307	CPS	C16-C15-C2	-5.34	106.99	112.66
4	B	2306	CPS	C9-C5-C4	-5.06	113.05	117.67
4	B	2307	CPS	C8-C9-C20	4.80	123.72	113.66
2	B	2301	PX4	O7-C23-C24	4.65	121.53	111.50
4	B	2306	CPS	C7-C6-C18	-4.38	112.22	118.33
4	B	2306	CPS	C16-C15-C2	-4.34	108.05	112.66
4	B	2307	CPS	C7-C6-C18	-4.33	112.28	118.33
2	B	2302	PX4	O7-C23-C24	4.08	120.29	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2307	CPS	O4-C4-C5	-4.03	104.22	111.03
4	B	2306	CPS	C3-C19-C2	3.96	117.81	113.73
2	B	2303	PX4	O7-C23-C24	3.84	119.78	111.50
4	B	2306	CPS	C10-C5-C6	3.59	116.83	111.21
4	B	2307	CPS	C9-C5-C4	3.51	120.87	117.67
4	B	2307	CPS	C7-C6-C5	-3.27	100.34	103.55
2	B	2304	PX4	O5-C9-C10	3.23	122.05	111.91
4	B	2307	CPS	C14-C13-C12	-3.20	106.73	110.55
4	B	2306	CPS	C10-C5-C4	-3.10	105.91	109.07
2	B	2301	PX4	O5-C9-C10	3.01	121.35	111.91
4	B	2307	CPS	C7-C8-C9	2.92	110.91	105.13
4	B	2306	CPS	C14-C13-C12	-2.73	107.30	110.55
4	B	2307	CPS	C3-C4-C5	-2.60	108.58	111.24
4	B	2306	CPS	O4-C4-C3	2.56	114.34	109.12
4	B	2307	CPS	O3-C17-C18	-2.52	103.79	109.43
4	B	2306	CPS	C3-C19-C18	-2.50	107.22	110.88
4	B	2306	CPS	C22-C20-C9	2.50	115.44	110.28
4	B	2306	CPS	C1-C2-C19	-2.48	107.45	111.35
4	B	2306	CPS	C10-C5-C9	-2.47	107.35	111.21
2	B	2302	PX4	O5-C9-C10	2.44	119.57	111.91
2	B	2303	PX4	O5-C9-C10	2.44	119.56	111.91
2	B	2303	PX4	C8-C7-C6	-2.37	106.17	111.79
4	B	2306	CPS	C16-C17-C18	2.28	113.91	111.48
4	B	2307	CPS	C3-C19-C2	2.25	116.05	113.73
4	B	2307	CPS	C19-C18-C17	-2.23	109.20	111.88
2	B	2302	PX4	C8-C7-C6	-2.20	106.59	111.79
2	B	2304	PX4	O5-C9-O6	-2.13	118.22	123.59
4	B	2306	CPS	C7-C8-C9	2.08	109.25	105.13
4	B	2307	CPS	C5-C6-C18	2.07	117.38	114.74

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	2306	CPS	C5

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2301	PX4	O8-C23-O7-C7
2	B	2301	PX4	C24-C23-O7-C7
2	B	2302	PX4	C6-O4-P1-O1
2	B	2302	PX4	C6-O4-P1-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2302	PX4	C6-O4-P1-O3
2	B	2303	PX4	O3-C1-C2-N1
2	B	2304	PX4	C6-O4-P1-O1
2	B	2304	PX4	C6-O4-P1-O2
2	B	2304	PX4	C6-O4-P1-O3
2	B	2301	PX4	O6-C9-O5-C8
2	B	2302	PX4	O8-C23-O7-C7
2	B	2301	PX4	C10-C9-O5-C8
2	B	2302	PX4	C24-C23-O7-C7
4	B	2306	CPS	C21-C20-C22-C23
2	B	2304	PX4	C6-C7-C8-O5
2	B	2301	PX4	C9-C10-C11-C12
2	B	2302	PX4	C9-C10-C11-C12
4	B	2306	CPS	C21-C20-C9-C5
2	B	2301	PX4	C6-O4-P1-O3
2	B	2303	PX4	C1-O3-P1-O4
2	B	2302	PX4	C26-C27-C28-C29
2	B	2301	PX4	C15-C16-C17-C18
2	B	2303	PX4	C17-C18-C19-C20
2	B	2301	PX4	C28-C29-C30-C31
2	B	2303	PX4	C12-C13-C14-C15
2	B	2303	PX4	C24-C25-C26-C27
2	B	2303	PX4	C14-C15-C16-C17
2	B	2303	PX4	C11-C12-C13-C14
2	B	2303	PX4	C16-C17-C18-C19
2	B	2302	PX4	C29-C30-C31-C32
2	B	2301	PX4	C14-C15-C16-C17
2	B	2301	PX4	C25-C26-C27-C28
2	B	2302	PX4	C31-C32-C33-C34
2	B	2303	PX4	C29-C30-C31-C32
2	B	2304	PX4	C12-C13-C14-C15
2	B	2303	PX4	C23-C24-C25-C26
2	B	2303	PX4	C15-C16-C17-C18
2	B	2304	PX4	C13-C14-C15-C16
2	B	2301	PX4	C29-C30-C31-C32
4	B	2306	CPS	C21-C20-C9-C8
2	B	2302	PX4	C28-C29-C30-C31
2	B	2304	PX4	C14-C15-C16-C17
2	B	2301	PX4	C12-C13-C14-C15
2	B	2301	PX4	C6-C7-C8-O5
2	B	2303	PX4	C32-C33-C34-C35
2	B	2303	PX4	C7-C6-O4-P1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2304	PX4	C10-C9-O5-C8
2	B	2302	PX4	O4-C6-C7-O7
2	B	2301	PX4	O7-C7-C8-O5
2	B	2301	PX4	C6-O4-P1-O1
2	B	2303	PX4	C1-O3-P1-O1
2	B	2303	PX4	C1-O3-P1-O2
2	B	2303	PX4	C6-O4-P1-O1
2	B	2302	PX4	O4-C6-C7-C8
2	B	2304	PX4	O6-C9-O5-C8
2	B	2302	PX4	C15-C16-C17-C18
2	B	2302	PX4	C19-C20-C21-C22
2	B	2301	PX4	C1-C2-N1-C3
2	B	2302	PX4	C18-C19-C20-C21
2	B	2301	PX4	C11-C12-C13-C14
2	B	2303	PX4	C6-O4-P1-O3
2	B	2301	PX4	C17-C18-C19-C20
2	B	2304	PX4	O4-C6-C7-C8
2	B	2304	PX4	C11-C10-C9-O5
2	B	2301	PX4	C1-C2-N1-C5
2	B	2303	PX4	O4-C6-C7-O7
2	B	2301	PX4	C1-C2-N1-C4
2	B	2302	PX4	C11-C10-C9-O5
4	B	2306	CPS	C22-C23-C24-N1
2	B	2302	PX4	C11-C10-C9-O6
2	B	2302	PX4	C10-C11-C12-C13
4	B	2306	CPS	C22-C23-C24-O1
2	B	2303	PX4	C33-C34-C35-C36

There are no ring outliers.

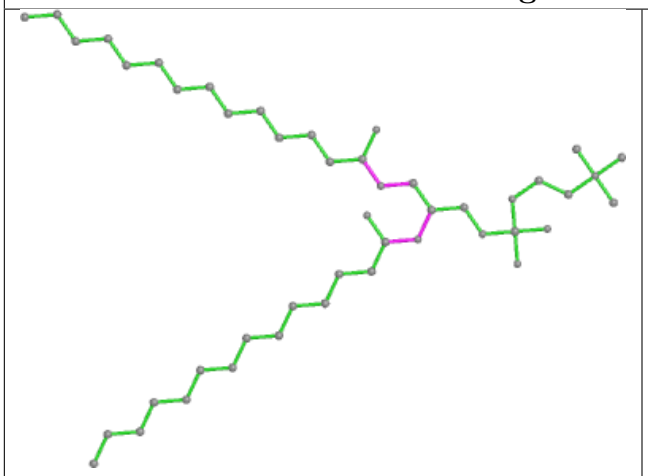
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2303	PX4	2	0
4	B	2306	CPS	9	0
2	B	2301	PX4	4	0
4	B	2307	CPS	3	0
2	B	2302	PX4	3	0
2	B	2304	PX4	2	0

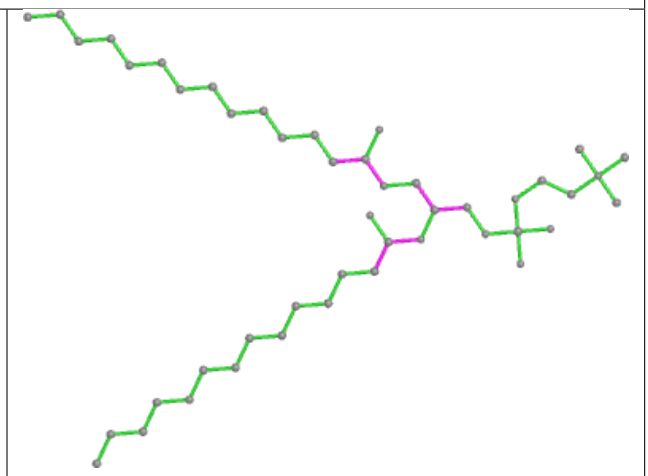
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

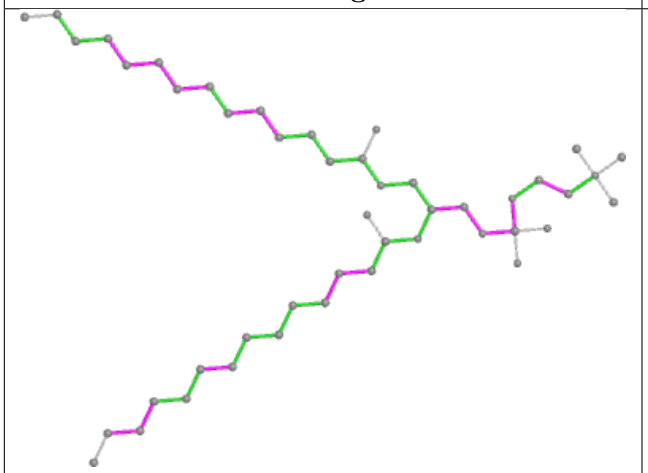
Ligand PX4 B 2303



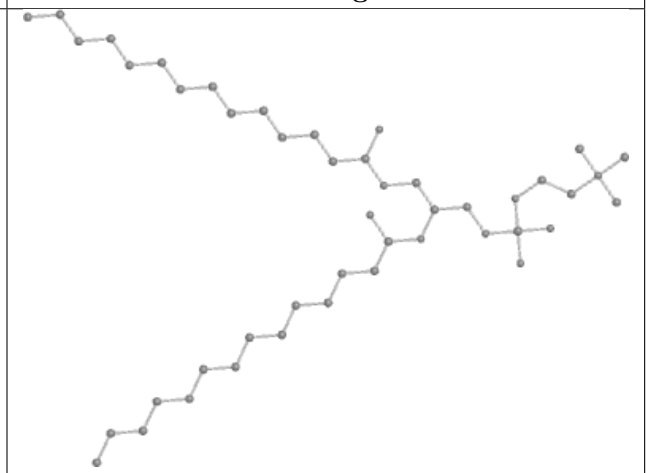
Bond lengths



Bond angles

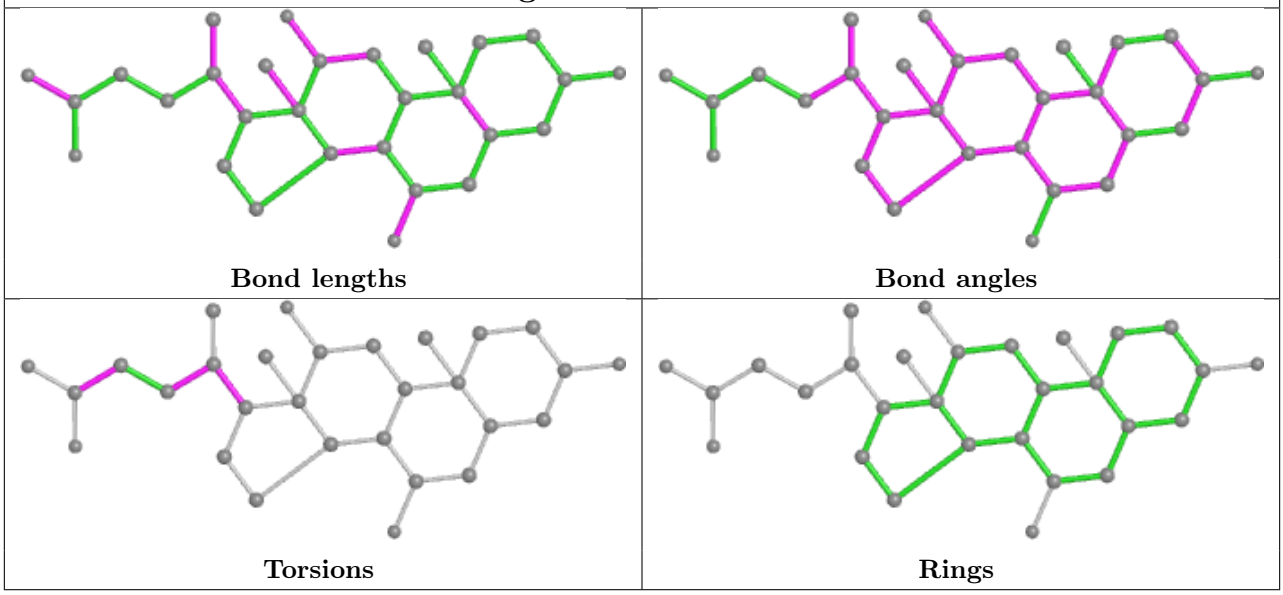


Torsions

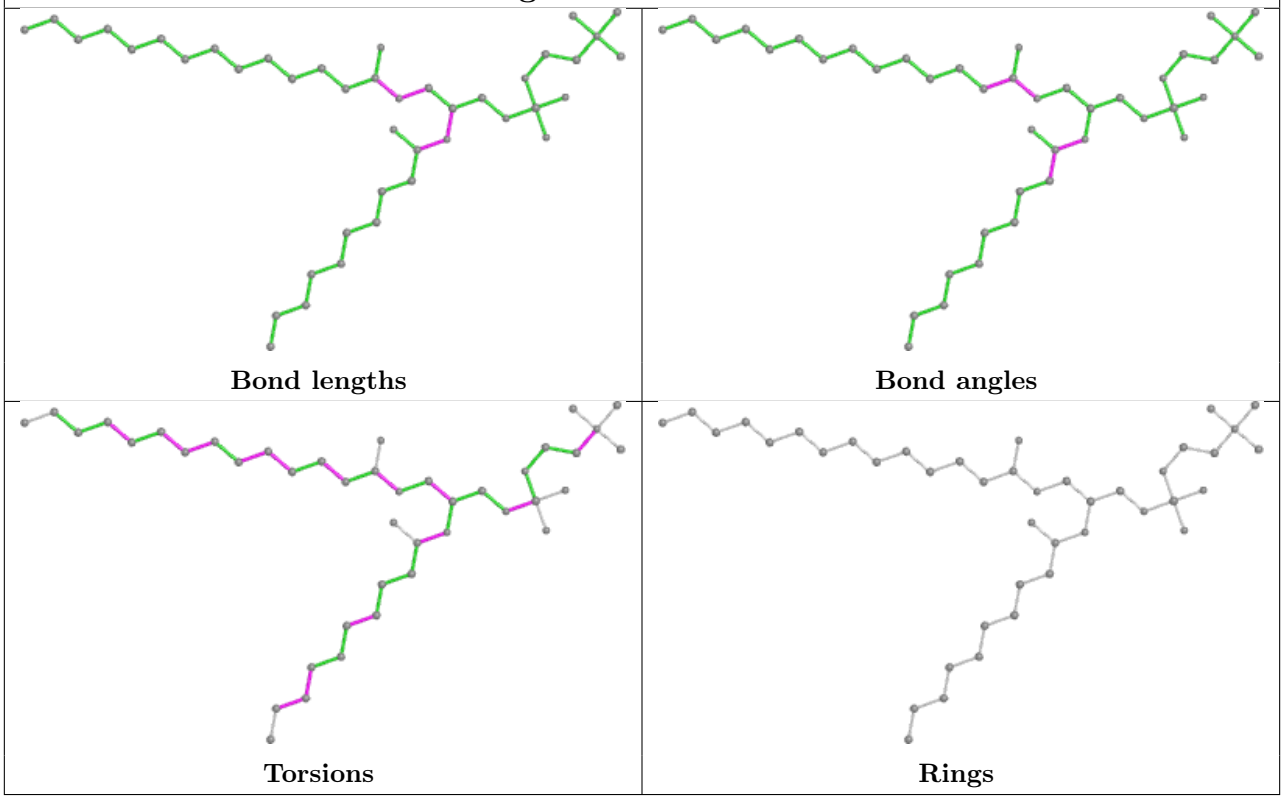


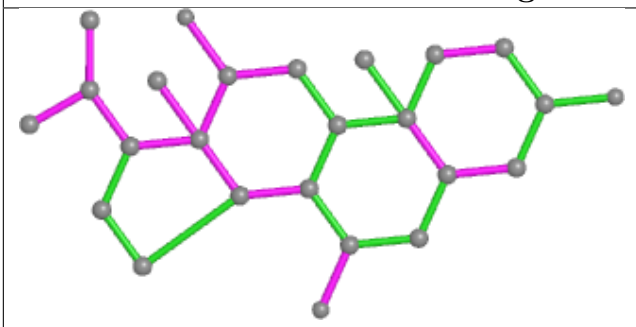
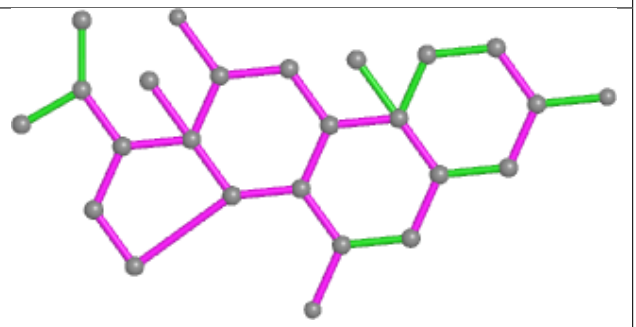
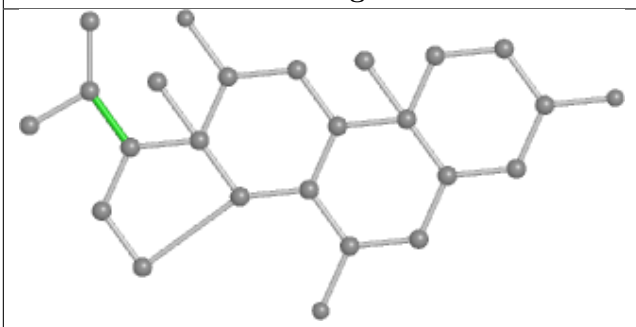
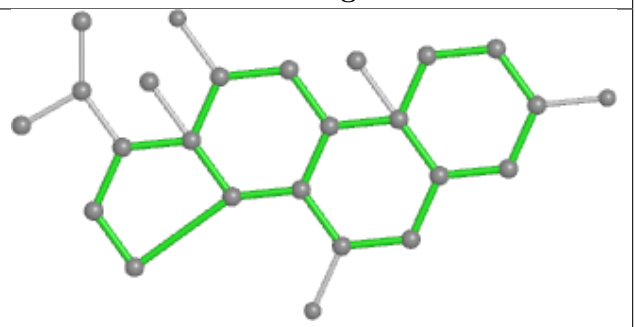
Rings

Ligand CPS B 2306

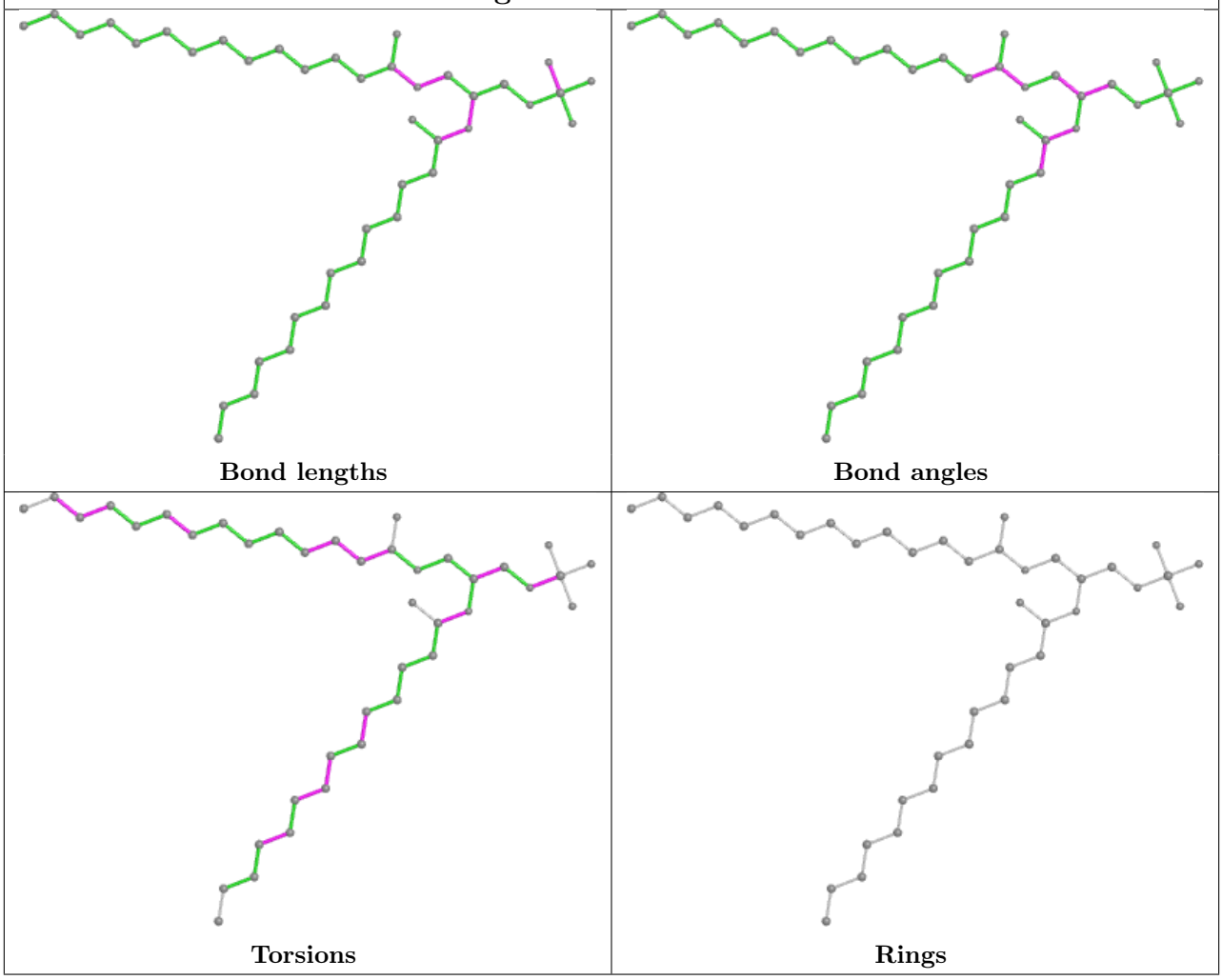


Ligand PX4 B 2301

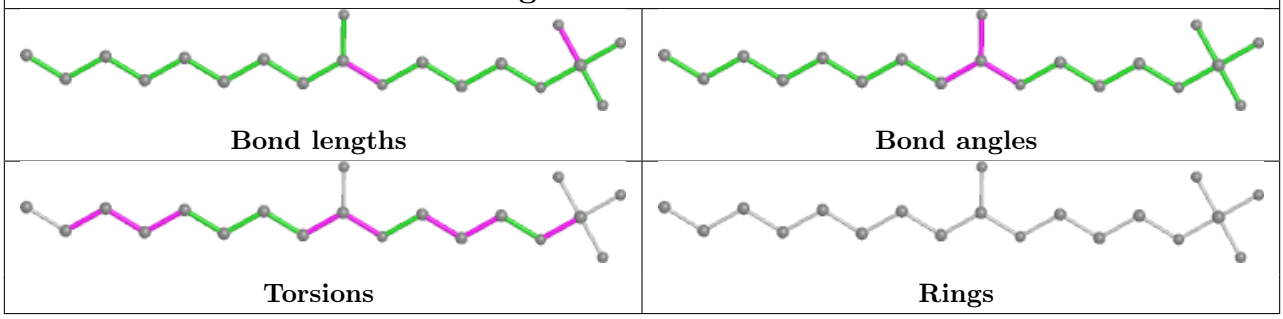


Ligand CPS B 2307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PX4 B 2302



Ligand PX4 B 2304



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	237/257 (92%)	0.16	14 (5%) 22 23	44, 79, 119, 164	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2041	PHE	4.0
1	B	2002	TYR	3.9
1	B	2089	VAL	3.5
1	B	2038	MET	3.4
1	B	2090	PRO	3.2
1	B	2040	SER	3.1
1	B	2069	ILE	2.9
1	B	2238	SER	2.6
1	B	2037	PHE	2.4
1	B	2036	THR	2.3
1	B	2106	LEU	2.1
1	B	2111	THR	2.1
1	B	2005	ILE	2.1
1	B	2098	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

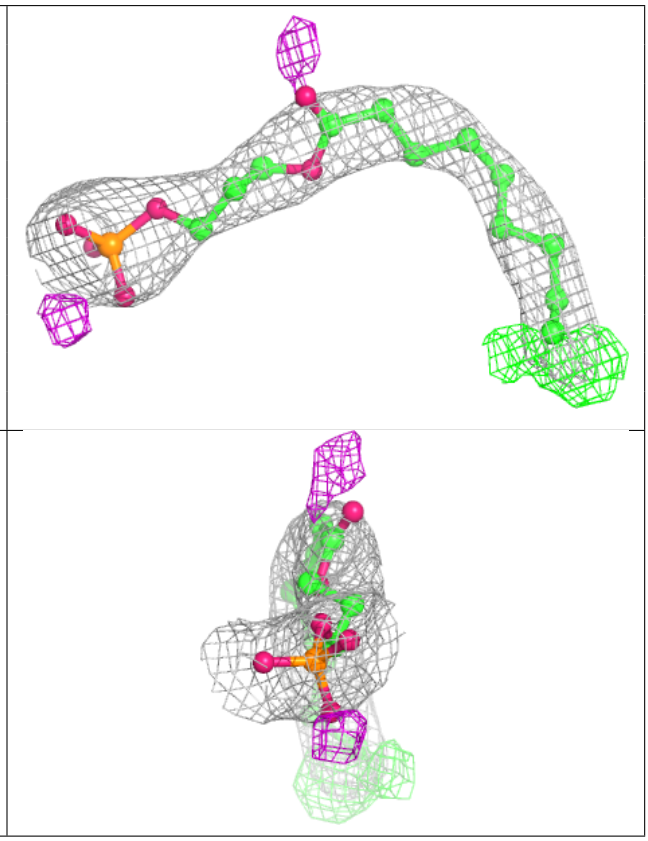
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PX4	B	2304	19/46	0.74	0.29	79,104,146,147	0
3	ACT	B	2305	4/4	0.77	0.32	89,103,105,106	0
2	PX4	B	2303	46/46	0.81	0.32	76,101,122,126	0
2	PX4	B	2302	40/46	0.86	0.19	74,90,118,122	0
4	CPS	B	2306	29/42	0.90	0.23	63,86,106,120	0
2	PX4	B	2301	42/46	0.94	0.16	71,87,107,125	0
4	CPS	B	2307	25/42	0.95	0.14	47,77,100,125	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.

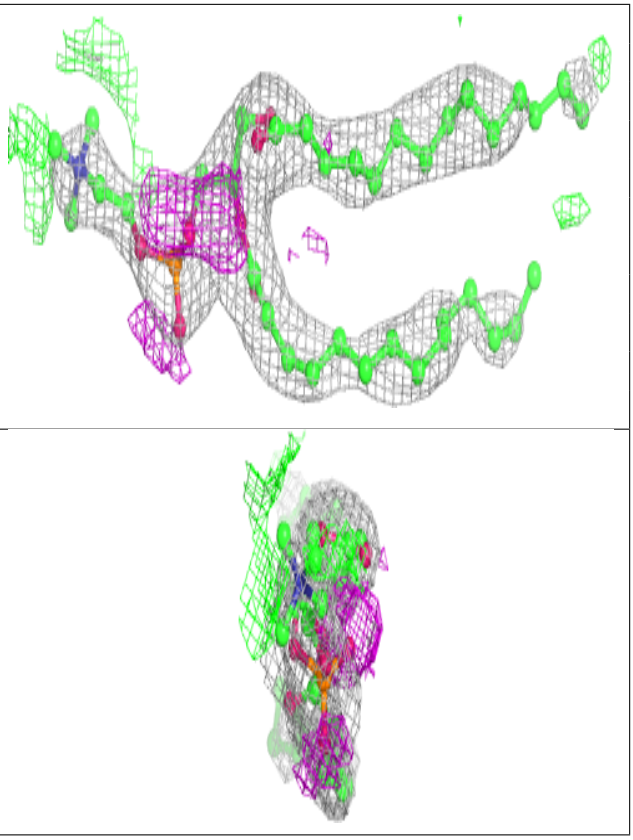
Electron density around PX4 B 2304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



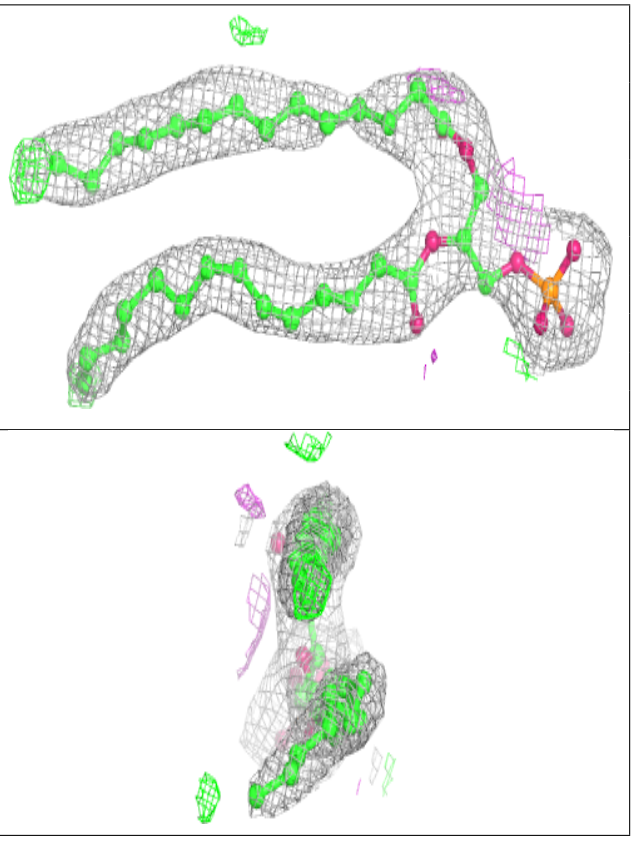
Electron density around PX4 B 2303:

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



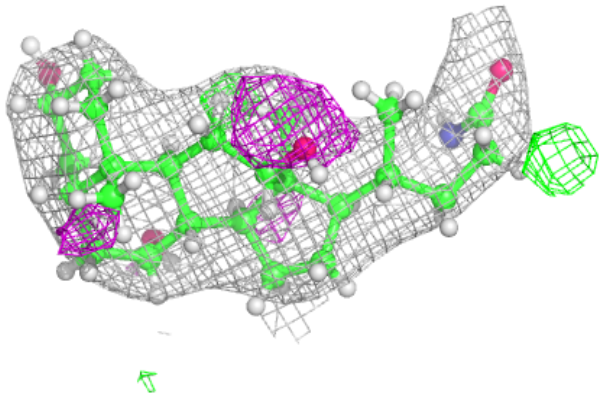
Electron density around PX4 B 2302:

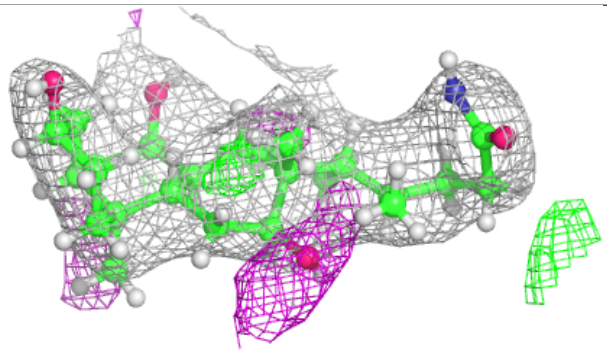
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

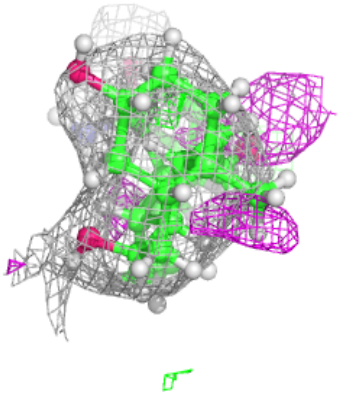


Electron density around CPS B 2306:

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

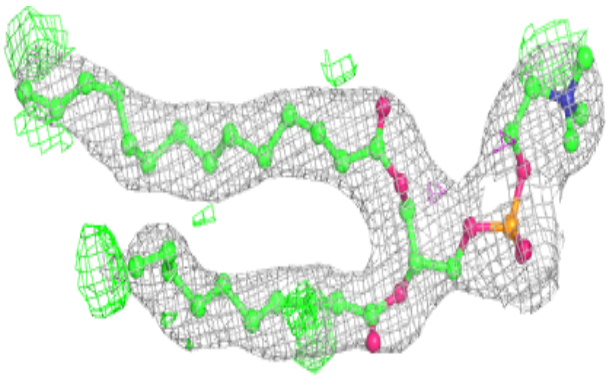


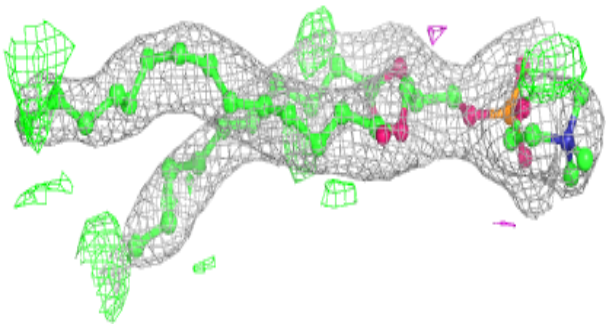


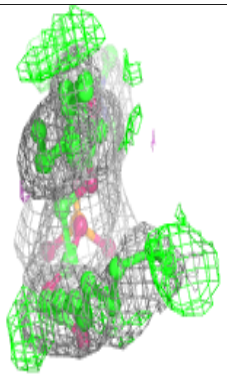


Electron density around PX4 B 2301:

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

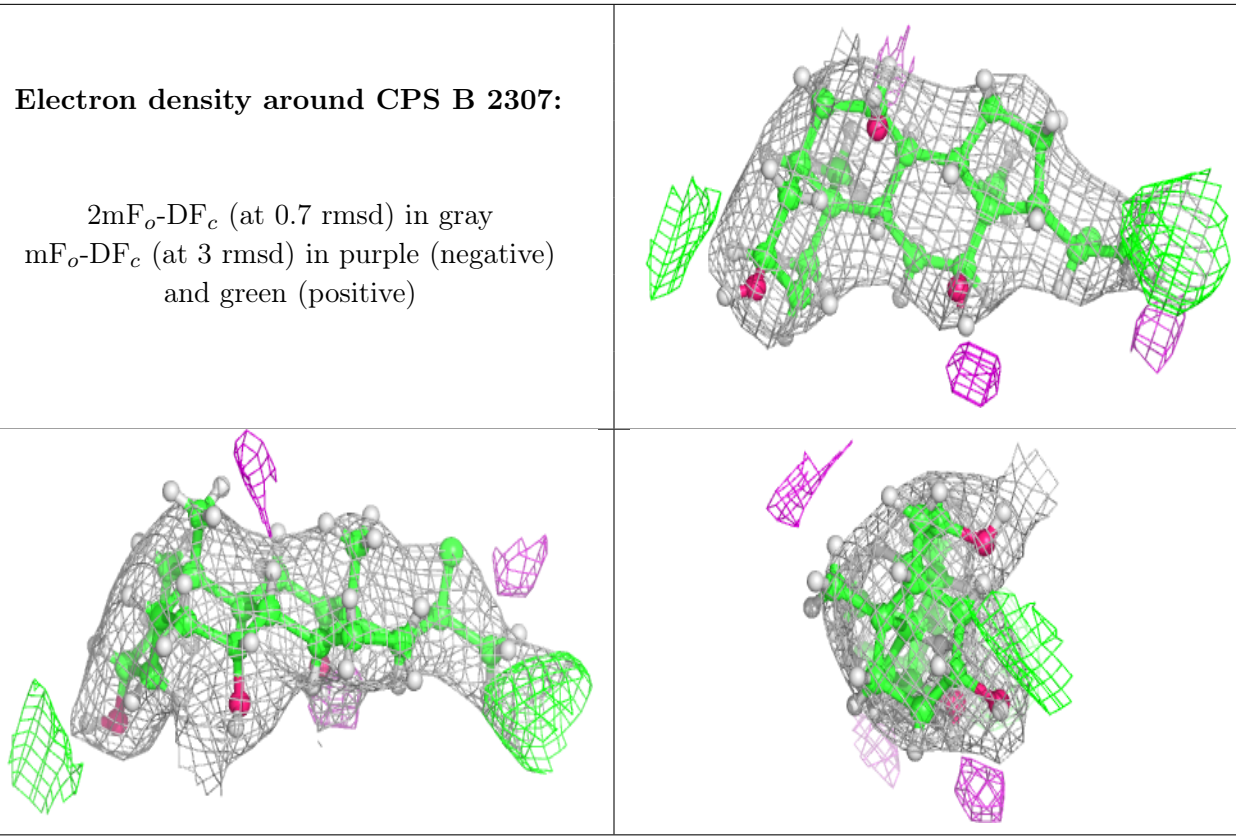






Electron density around CPS B 2307:

$2mF_o$-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.