



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:09 PM UTC

PDB ID : 6KEB / pdb_00006keb
Title : Structure basis for Diltiazem block of a voltage-gated calcium channel
Authors : Tang, L.
Deposited on : 2019-07-04
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

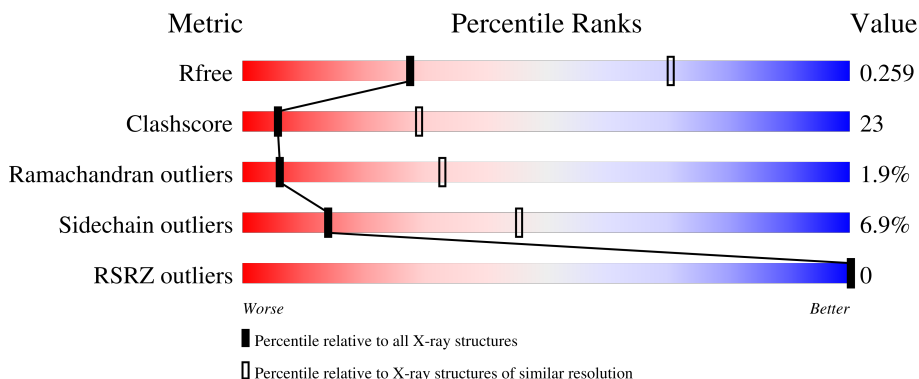
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	284	
1	B	284	
1	C	284	
1	D	284	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7469 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1800	1227	269	294	10			
1	B	219	Total	C	N	O	S	0	0	0
			1800	1227	269	294	10			
1	C	219	Total	C	N	O	S	0	0	0
			1800	1227	269	294	10			
1	D	228	Total	C	N	O	S	0	0	0
			1869	1270	281	307	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	984	ASP	-	expression tag	UNP A8EVM5
A	985	TYR	-	expression tag	UNP A8EVM5
A	986	LYS	-	expression tag	UNP A8EVM5
A	987	ASP	-	expression tag	UNP A8EVM5
A	988	ASP	-	expression tag	UNP A8EVM5
A	989	ASP	-	expression tag	UNP A8EVM5
A	990	ASP	-	expression tag	UNP A8EVM5
A	991	LYS	-	expression tag	UNP A8EVM5
A	992	GLY	-	expression tag	UNP A8EVM5
A	993	SER	-	expression tag	UNP A8EVM5
A	994	LEU	-	expression tag	UNP A8EVM5
A	995	VAL	-	expression tag	UNP A8EVM5
A	996	PRO	-	expression tag	UNP A8EVM5
A	997	ARG	-	expression tag	UNP A8EVM5
A	998	GLY	-	expression tag	UNP A8EVM5
A	999	SER	-	expression tag	UNP A8EVM5
A	1000	HIS	-	expression tag	UNP A8EVM5
A	1177	ASP	GLU	conflict	UNP A8EVM5
A	1178	ASP	SER	conflict	UNP A8EVM5
A	1181	ASN	MET	conflict	UNP A8EVM5
B	984	ASP	-	expression tag	UNP A8EVM5

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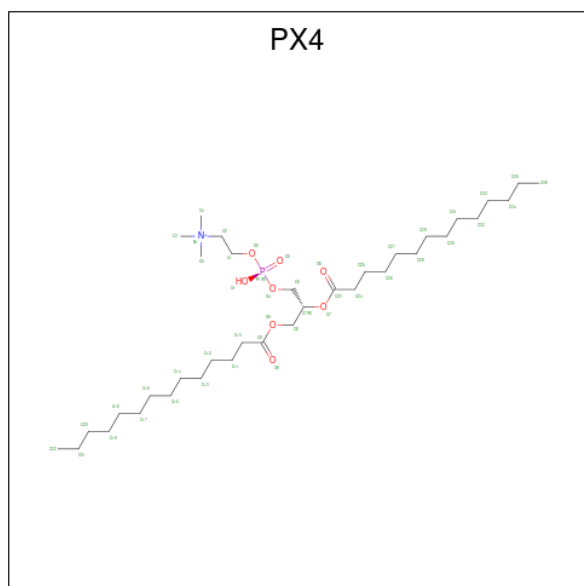
Chain	Residue	Modelled	Actual	Comment	Reference
B	985	TYR	-	expression tag	UNP A8EVM5
B	986	LYS	-	expression tag	UNP A8EVM5
B	987	ASP	-	expression tag	UNP A8EVM5
B	988	ASP	-	expression tag	UNP A8EVM5
B	989	ASP	-	expression tag	UNP A8EVM5
B	990	ASP	-	expression tag	UNP A8EVM5
B	991	LYS	-	expression tag	UNP A8EVM5
B	992	GLY	-	expression tag	UNP A8EVM5
B	993	SER	-	expression tag	UNP A8EVM5
B	994	LEU	-	expression tag	UNP A8EVM5
B	995	VAL	-	expression tag	UNP A8EVM5
B	996	PRO	-	expression tag	UNP A8EVM5
B	997	ARG	-	expression tag	UNP A8EVM5
B	998	GLY	-	expression tag	UNP A8EVM5
B	999	SER	-	expression tag	UNP A8EVM5
B	1000	HIS	-	expression tag	UNP A8EVM5
B	1177	ASP	GLU	conflict	UNP A8EVM5
B	1178	ASP	SER	conflict	UNP A8EVM5
B	1181	ASN	MET	conflict	UNP A8EVM5
C	984	ASP	-	expression tag	UNP A8EVM5
C	985	TYR	-	expression tag	UNP A8EVM5
C	986	LYS	-	expression tag	UNP A8EVM5
C	987	ASP	-	expression tag	UNP A8EVM5
C	988	ASP	-	expression tag	UNP A8EVM5
C	989	ASP	-	expression tag	UNP A8EVM5
C	990	ASP	-	expression tag	UNP A8EVM5
C	991	LYS	-	expression tag	UNP A8EVM5
C	992	GLY	-	expression tag	UNP A8EVM5
C	993	SER	-	expression tag	UNP A8EVM5
C	994	LEU	-	expression tag	UNP A8EVM5
C	995	VAL	-	expression tag	UNP A8EVM5
C	996	PRO	-	expression tag	UNP A8EVM5
C	997	ARG	-	expression tag	UNP A8EVM5
C	998	GLY	-	expression tag	UNP A8EVM5
C	999	SER	-	expression tag	UNP A8EVM5
C	1000	HIS	-	expression tag	UNP A8EVM5
C	1177	ASP	GLU	conflict	UNP A8EVM5
C	1178	ASP	SER	conflict	UNP A8EVM5
C	1181	ASN	MET	conflict	UNP A8EVM5
D	984	ASP	-	expression tag	UNP A8EVM5
D	985	TYR	-	expression tag	UNP A8EVM5
D	986	LYS	-	expression tag	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	987	ASP	-	expression tag	UNP A8EVM5
D	988	ASP	-	expression tag	UNP A8EVM5
D	989	ASP	-	expression tag	UNP A8EVM5
D	990	ASP	-	expression tag	UNP A8EVM5
D	991	LYS	-	expression tag	UNP A8EVM5
D	992	GLY	-	expression tag	UNP A8EVM5
D	993	SER	-	expression tag	UNP A8EVM5
D	994	LEU	-	expression tag	UNP A8EVM5
D	995	VAL	-	expression tag	UNP A8EVM5
D	996	PRO	-	expression tag	UNP A8EVM5
D	997	ARG	-	expression tag	UNP A8EVM5
D	998	GLY	-	expression tag	UNP A8EVM5
D	999	SER	-	expression tag	UNP A8EVM5
D	1000	HIS	-	expression tag	UNP A8EVM5
D	1177	ASP	GLU	conflict	UNP A8EVM5
D	1178	ASP	SER	conflict	UNP A8EVM5
D	1181	ASN	MET	conflict	UNP A8EVM5

- Molecule 2 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PX4) (formula: C₃₆H₇₃NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	A	1	Total	C	O	P	0	0
			21	13	7	1		

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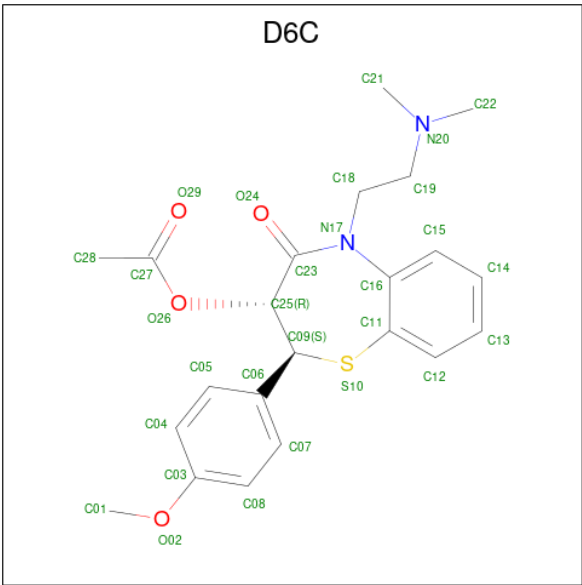
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 10 3 6 1	0	0
2	A	1	Total C O P 10 3 6 1	0	0
2	B	1	Total C O P 10 3 6 1	0	0
2	B	1	Total C O P 21 13 7 1	0	0
2	C	1	Total C O P 21 13 7 1	0	0
2	C	1	Total C O P 10 3 6 1	0	0
2	C	1	Total C O P 21 13 7 1	0	0
2	D	1	Total C O P 10 3 6 1	0	0
2	D	1	Total C O P 10 3 6 1	0	0
2	D	1	Total C O P 10 3 6 1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is [(2 {S},3 {R})-5-[2-(dimethylamino)ethyl]-2-(4-methoxyphenyl)-4-oxidanylide ne-2,3-dihydro-1,5-benzothiazepin-3-yl] ethanoate (CCD ID: D6C) (formula: C₂₂H₂₆N₂O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			29	22	2	4	1		

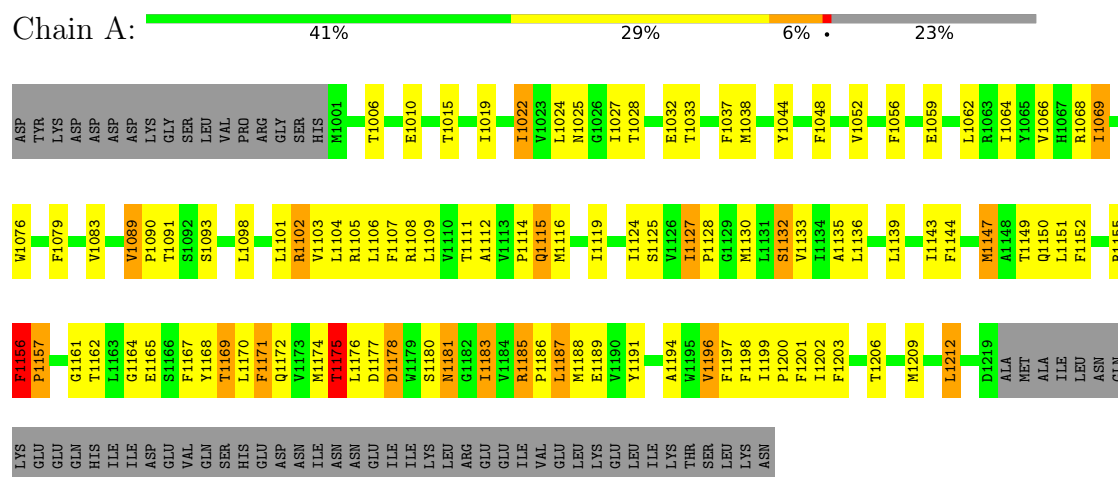
- Molecule 5 is water.

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

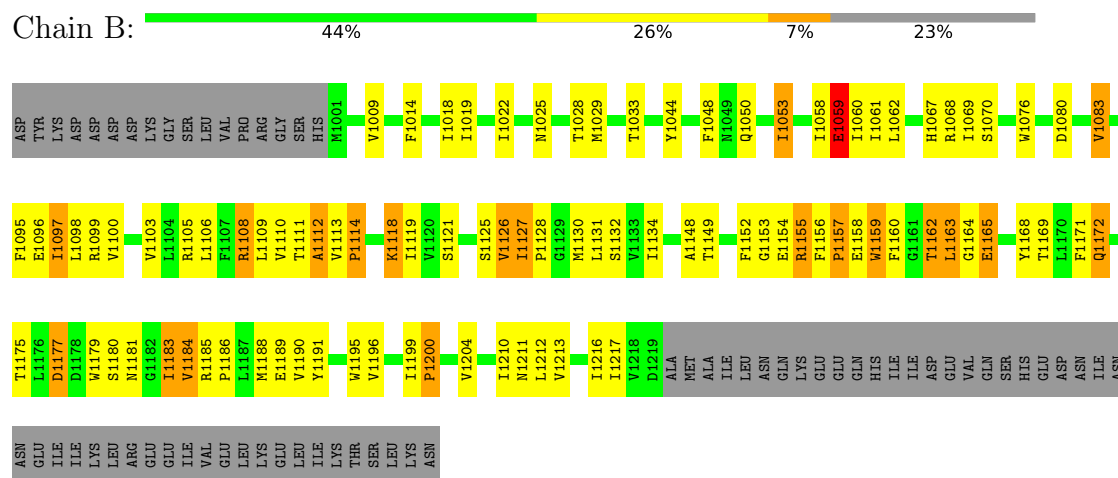
3 Residue-property plots

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

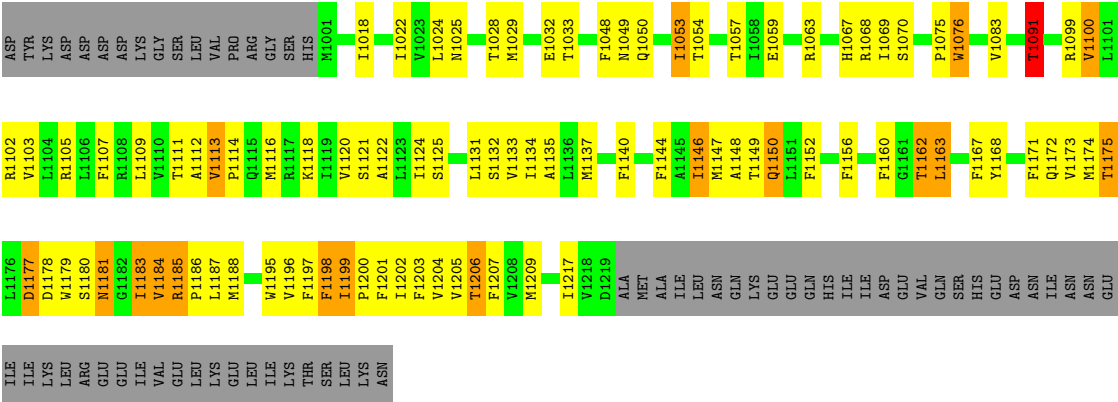


• Molecule 1: Ion transport protein

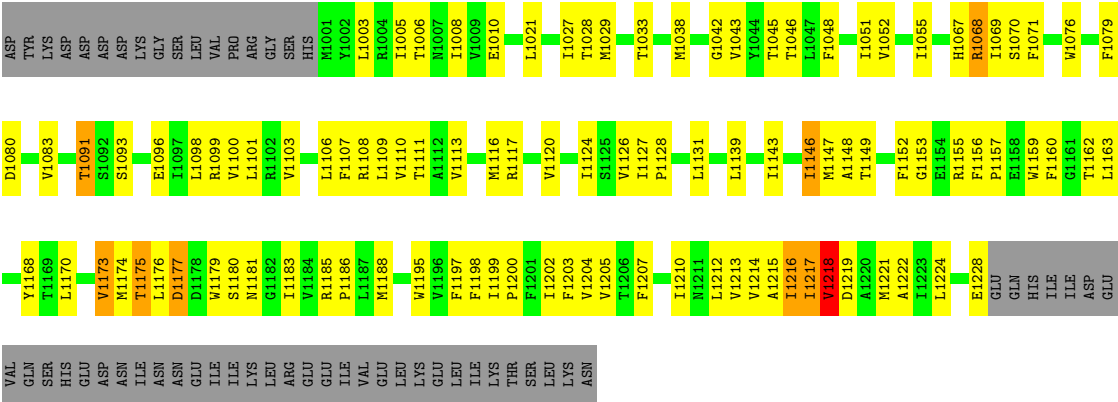


• Molecule 1: Ion transport protein





● Molecule 1: Ion transport protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.60Å 125.63Å 191.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 3.20 29.85 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.9 (29.85-3.20) 89.9 (29.85-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.243 , 0.277 0.226 , 0.259	Depositor DCC
R_{free} test set	2296 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.440 for k,h,-l	Xtriage
Reported twinning fraction	0.528 for H, K, L 0.472 for K, H, -L	Depositor
Outliers	0 of 45638 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7469	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PX4, D6C

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	1.06	9/1851 (0.5%)	1.05	5/2520 (0.2%)
1	B	1.06	2/1851 (0.1%)	1.17	14/2520 (0.6%)
1	C	1.14	6/1851 (0.3%)	1.15	14/2520 (0.6%)
1	D	1.00	2/1920 (0.1%)	1.05	7/2612 (0.3%)
All	All	1.06	19/7473 (0.3%)	1.11	40/10172 (0.4%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1181	ASN	C-O	-7.00	1.16	1.24
1	A	1183	ILE	C-O	-6.99	1.14	1.24
1	B	1181	ASN	C-O	-6.66	1.16	1.24
1	A	1187	LEU	C-O	-6.48	1.16	1.24
1	C	1113	VAL	CA-C	-6.42	1.48	1.53

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1183	ILE	N-CA-C	12.97	121.87	111.62
1	C	1116	MET	N-CA-C	-12.83	95.86	112.93
1	C	1181	ASN	N-CA-C	-10.80	99.48	111.14
1	B	1159	TRP	N-CA-C	10.54	122.85	111.36
1	B	1127	ILE	N-CA-C	9.60	123.88	112.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1800	0	1869	100	0
1	B	1800	0	1869	98	0
1	C	1800	0	1869	80	0
1	D	1869	0	1943	116	0
2	A	51	0	34	0	0
2	B	31	0	24	0	0
2	C	52	0	43	3	0
2	D	30	0	15	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	D	29	0	0	2	0
5	B	2	0	0	0	0
5	C	3	0	0	3	0
All	All	7469	0	7666	349	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 23.

The worst 5 of 349 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:VAL:HG12	1:A:1090:PRO:CD	1.67	1.22
1:A:1089:VAL:CG1	1:A:1090:PRO:HD2	1.77	1.12
1:B:1168:TYR:HE2	1:D:1185:ARG:NE	1.48	1.10
1:D:1180:SER:O	1:D:1185:ARG:HG2	1.59	1.02
1:B:1217:ILE:HD12	1:D:1217:ILE:HG12	1.47	0.95

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	217/284 (76%)	181 (83%)	29 (13%)	7 (3%)	3	21
1	B	217/284 (76%)	186 (86%)	26 (12%)	5 (2%)	5	29
1	C	217/284 (76%)	193 (89%)	21 (10%)	3 (1%)	9	39
1	D	226/284 (80%)	188 (83%)	36 (16%)	2 (1%)	14	47
All	All	877/1136 (77%)	748 (85%)	112 (13%)	17 (2%)	6	33

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1102	ARG
1	B	1153	GLY
1	B	1177	ASP
1	C	1132	SER
1	A	1175	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/263 (77%)	186 (92%)	16 (8%)	11	40
1	B	202/263 (77%)	184 (91%)	18 (9%)	9	34
1	C	202/263 (77%)	191 (95%)	11 (5%)	20	53
1	D	209/263 (80%)	198 (95%)	11 (5%)	20	53
All	All	815/1052 (78%)	759 (93%)	56 (7%)	14	45

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1165	GLU
1	D	1228	GLU

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Mol	Chain	Res	Type
1	C	1053	ILE
1	D	1218	VAL
1	D	1106	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1050	GLN
1	C	1150	GLN
1	D	1211	ASN
1	D	1067	HIS
1	B	1007	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PX4	D	1302	-	9,9,45	1.30	1 (11%)	10,12,53	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PX4	C	1303	-	9,9,45	1.42	2 (22%)	10,12,53	1.26	0
2	PX4	A	1301	-	9,9,45	1.59	2 (22%)	10,12,53	0.94	0
2	PX4	A	1303	-	9,9,45	1.79	2 (22%)	10,12,53	1.03	1 (10%)
2	PX4	B	1303	-	20,20,45	2.01	3 (15%)	22,24,53	1.48	2 (9%)
2	PX4	C	1304	-	20,20,45	2.01	3 (15%)	22,24,53	1.40	2 (9%)
2	PX4	B	1302	-	9,9,45	1.41	1 (11%)	10,12,53	0.94	0
4	D6C	D	1304	-	31,31,31	2.06	7 (22%)	43,43,43	3.30	12 (27%)
2	PX4	D	1303	-	9,9,45	1.97	2 (22%)	10,12,53	1.35	2 (20%)
2	PX4	C	1302	-	20,20,45	1.81	5 (25%)	22,24,53	1.66	2 (9%)
2	PX4	A	1304	-	9,9,45	1.58	2 (22%)	10,12,53	1.21	0
2	PX4	D	1301	-	9,9,45	1.73	2 (22%)	10,12,53	1.37	2 (20%)
2	PX4	A	1302	-	20,20,45	2.07	3 (15%)	22,24,53	1.63	3 (13%)

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	D	1302	-	-	6/8/8/49	-
2	PX4	C	1303	-	-	3/8/8/49	-
2	PX4	A	1301	-	-	3/8/8/49	-
2	PX4	A	1303	-	-	5/8/8/49	-
2	PX4	B	1303	-	-	12/22/22/49	-
2	PX4	C	1304	-	-	7/22/22/49	-
2	PX4	B	1302	-	-	3/8/8/49	-
4	D6C	D	1304	-	-	5/15/35/35	0/3/3/3
2	PX4	D	1303	-	-	3/8/8/49	-
2	PX4	C	1302	-	-	12/22/22/49	-
2	PX4	A	1304	-	-	4/8/8/49	-
2	PX4	D	1301	-	-	3/8/8/49	-
2	PX4	A	1302	-	-	12/22/22/49	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1302	PX4	O6-C9	7.12	1.43	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1303	PX4	O6-C9	6.38	1.41	1.22
2	C	1304	PX4	O6-C9	6.15	1.40	1.22
4	D	1304	D6C	C09-S10	-5.58	1.79	1.84
4	D	1304	D6C	C16-N17	5.54	1.48	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1304	D6C	C25-C09-S10	9.74	118.76	109.10
4	D	1304	D6C	C25-C23-N17	8.19	124.16	115.49
4	D	1304	D6C	C11-S10-C09	7.47	113.10	102.57
4	D	1304	D6C	C16-N17-C23	7.39	134.79	122.98
4	D	1304	D6C	C09-C25-C23	7.11	120.32	113.99

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	PX4	C6-C7-C8-O5
2	A	1302	PX4	C6-O4-P1-O1
2	A	1302	PX4	C6-O4-P1-O2
2	A	1302	PX4	C6-O4-P1-O3
2	A	1303	PX4	C6-O4-P1-O1

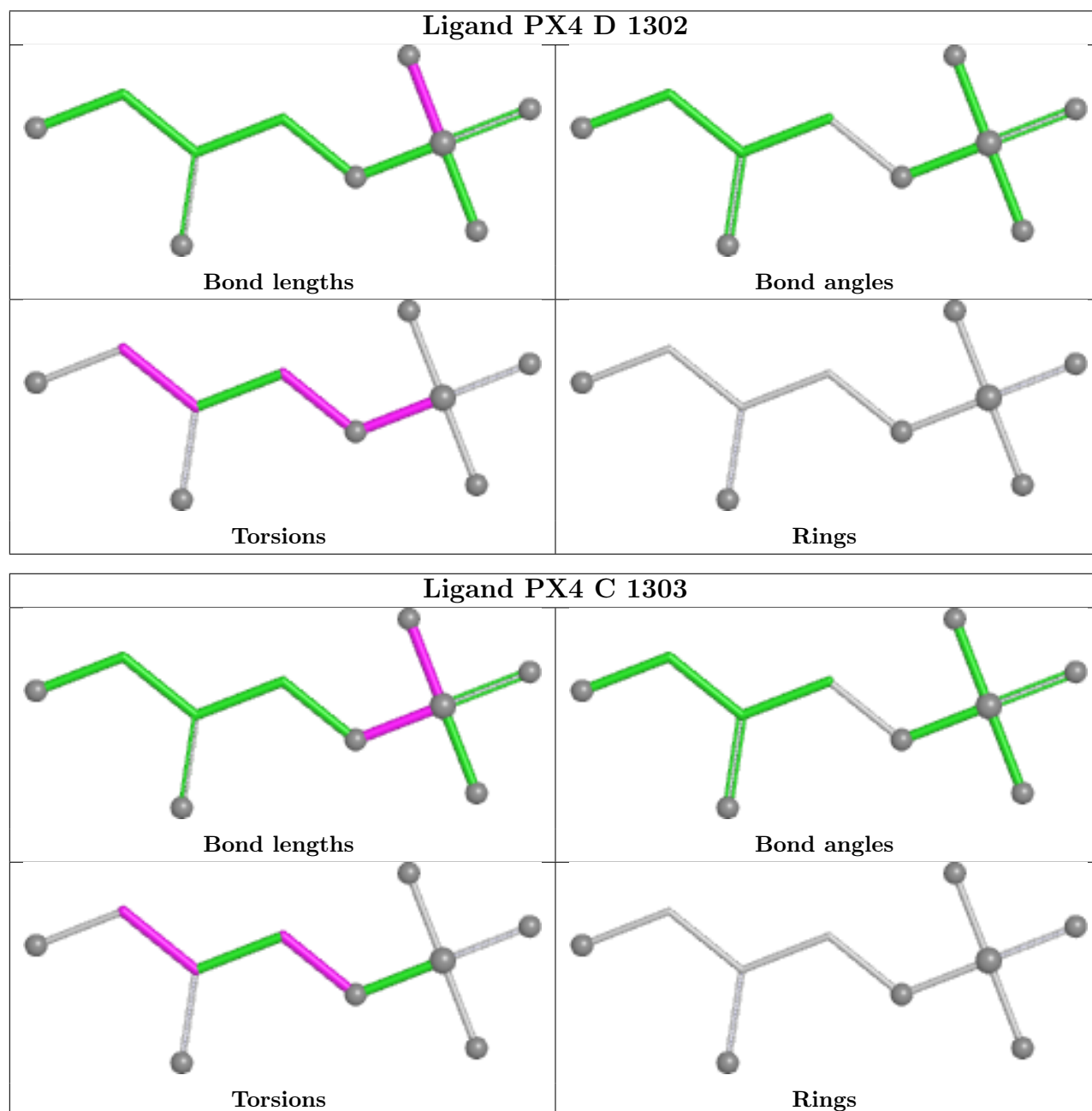
There are no ring outliers.

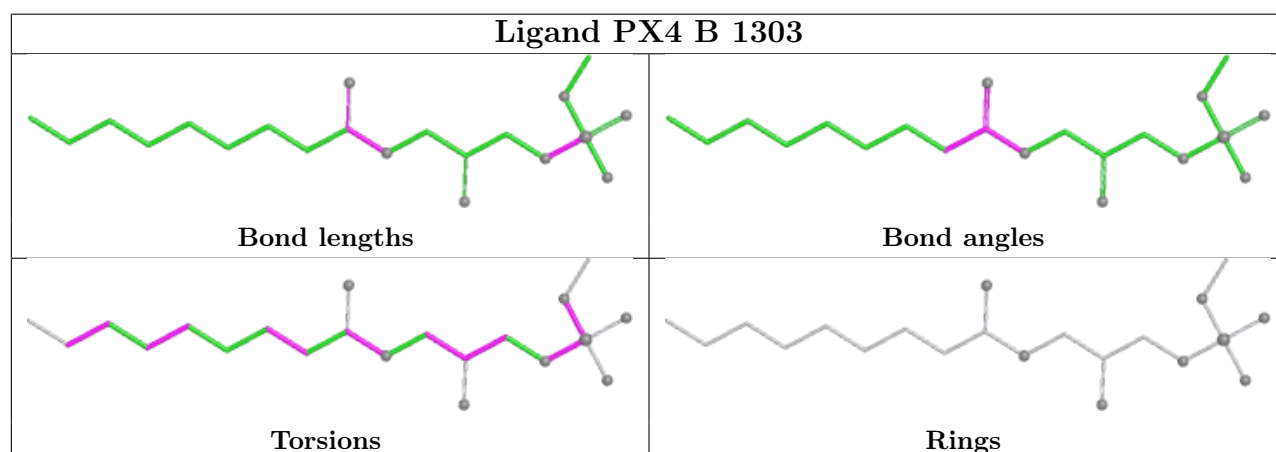
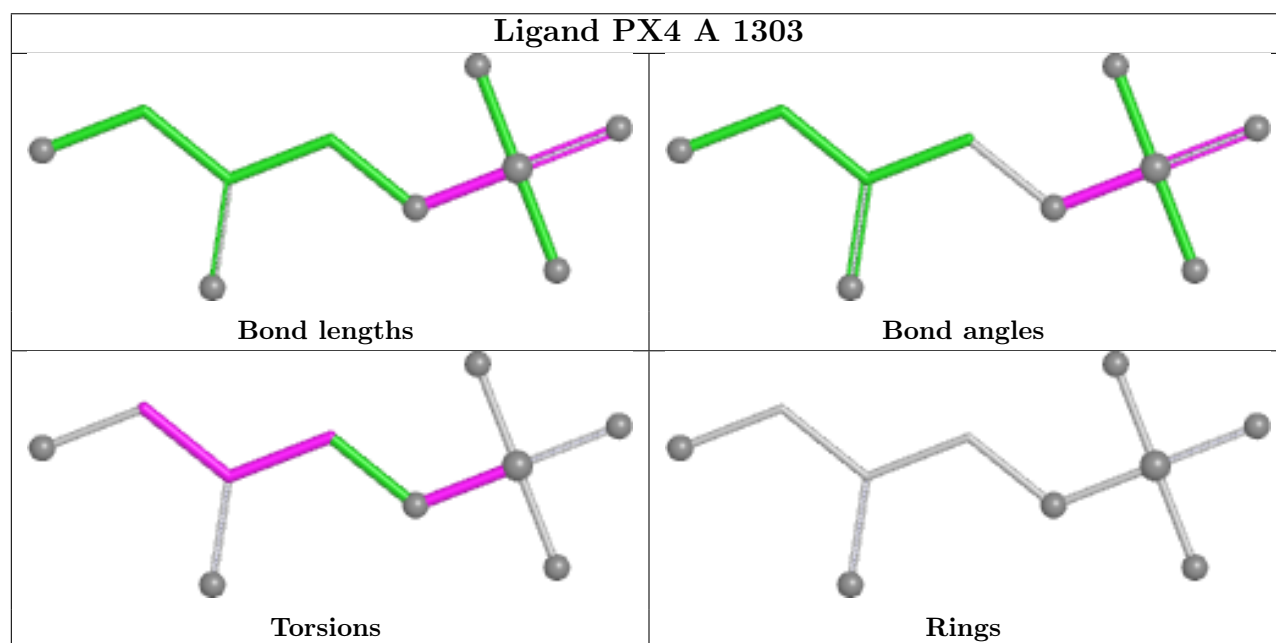
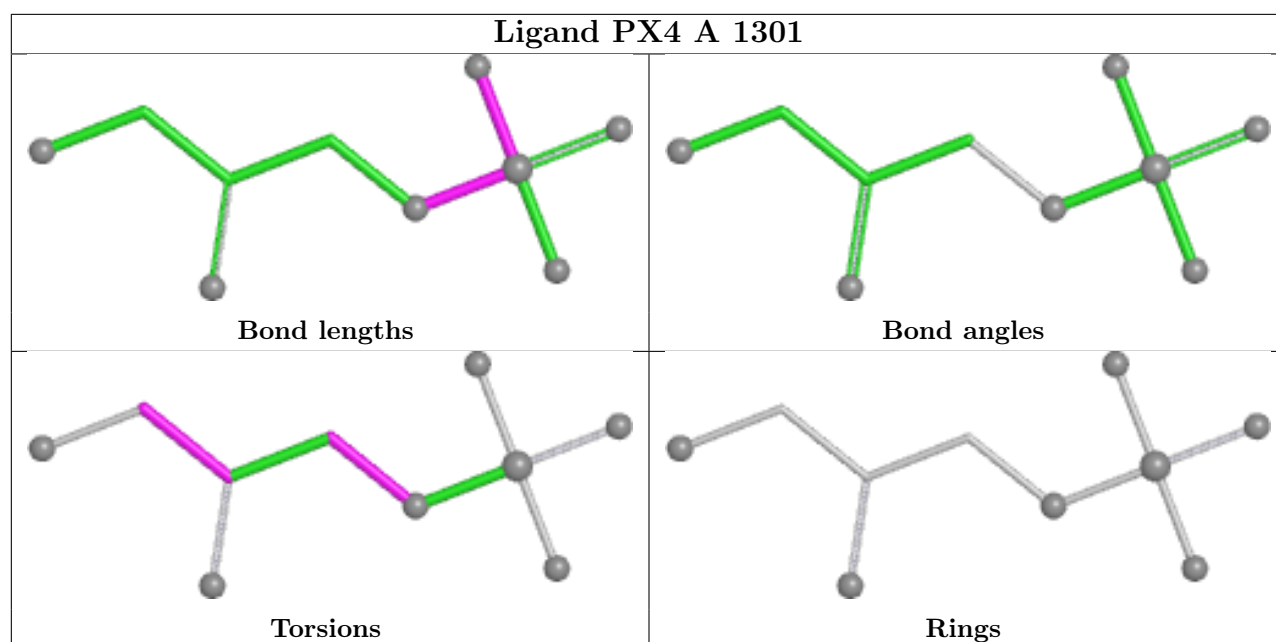
3 monomers are involved in 5 short contacts:

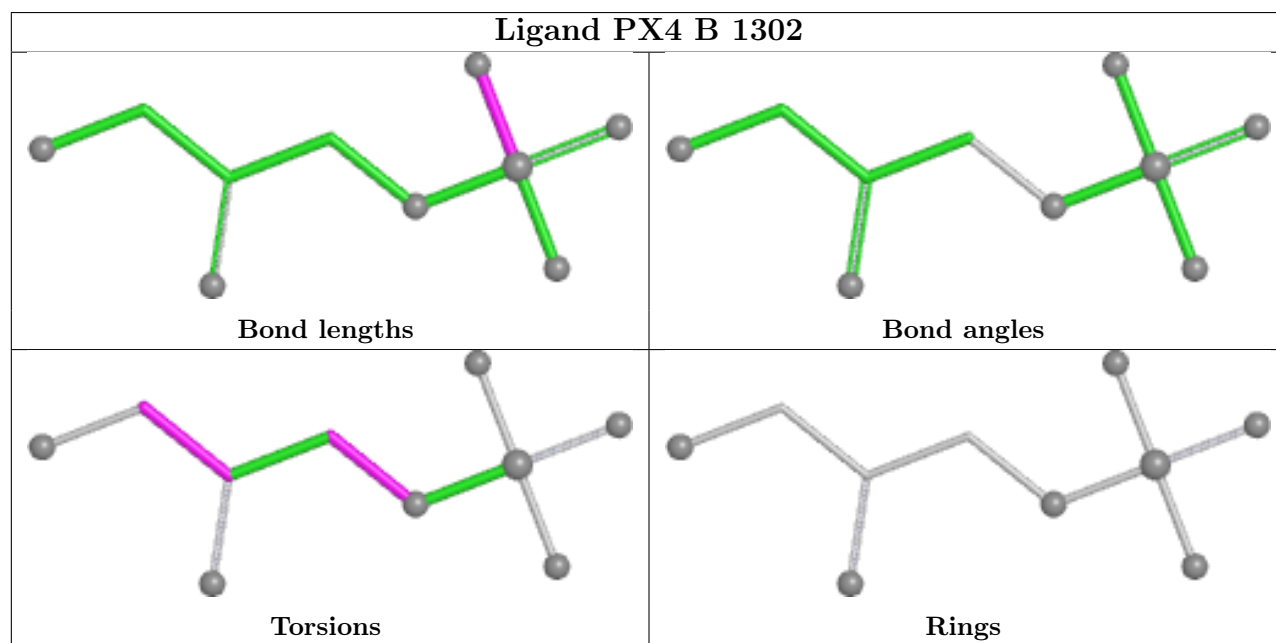
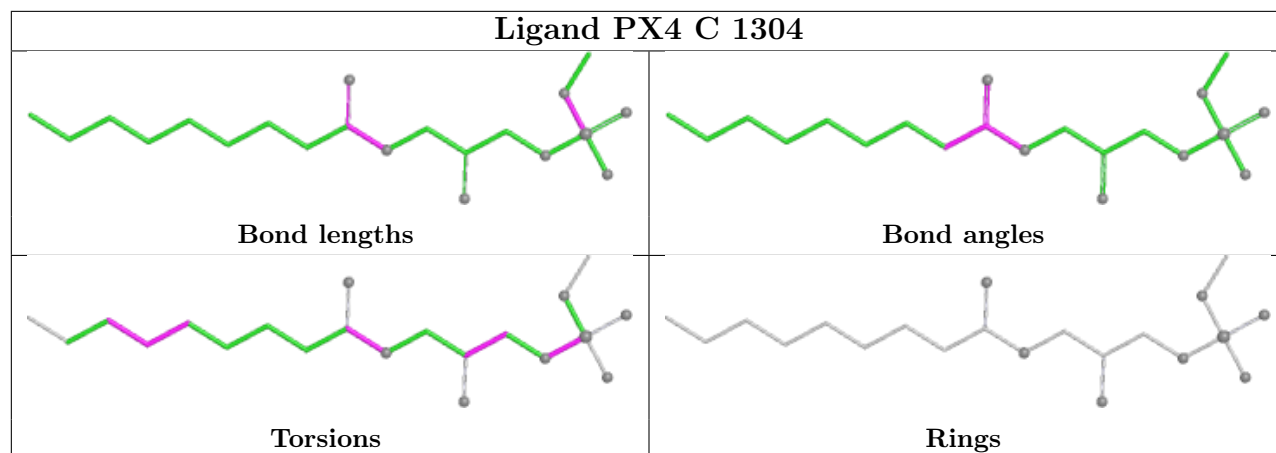
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1304	PX4	2	0
4	D	1304	D6C	2	0
2	C	1302	PX4	1	0

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.

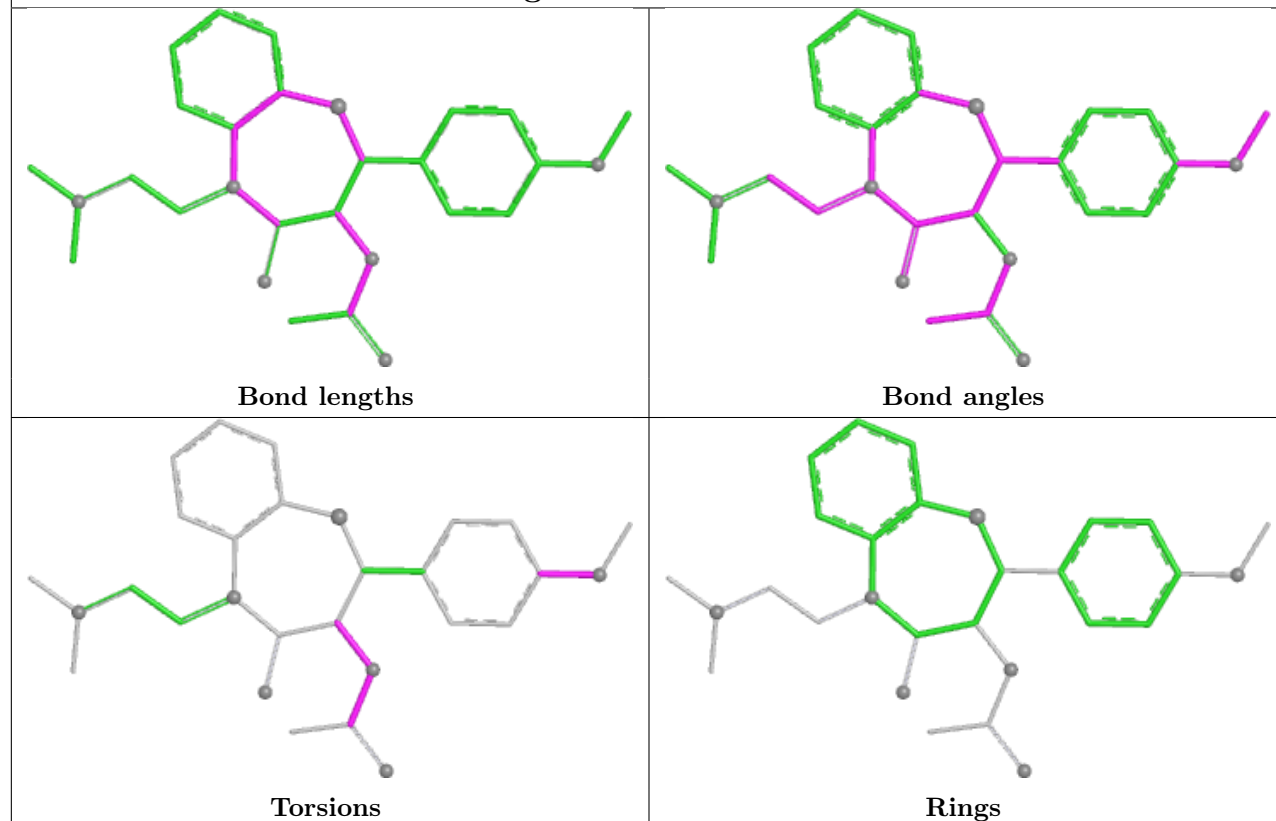
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



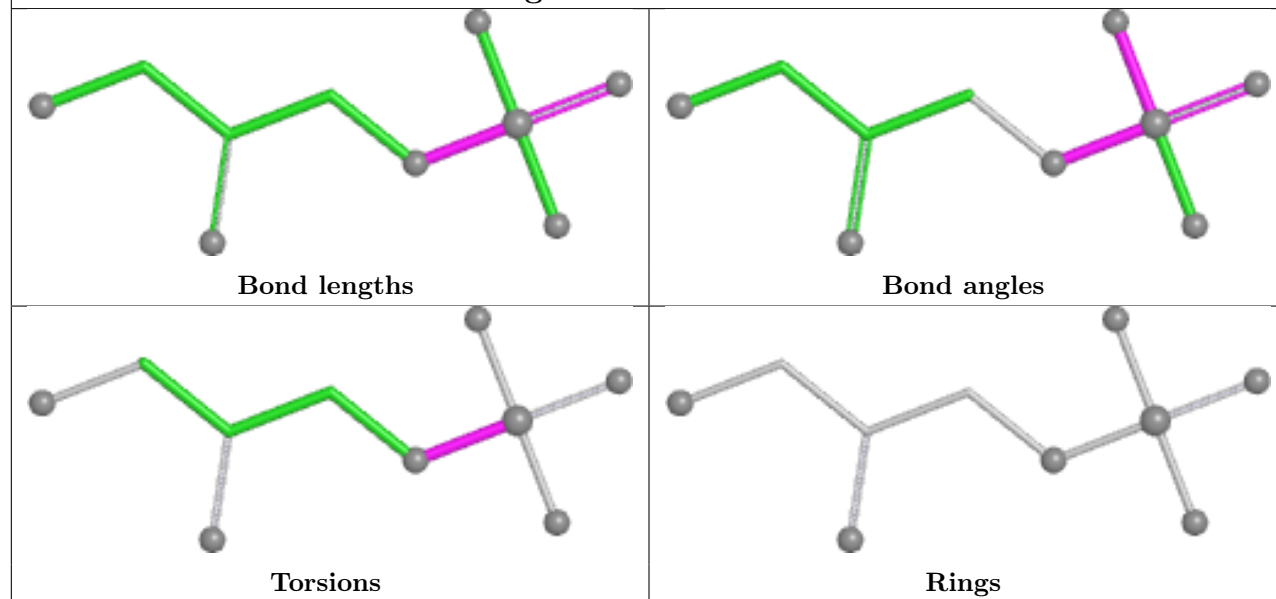


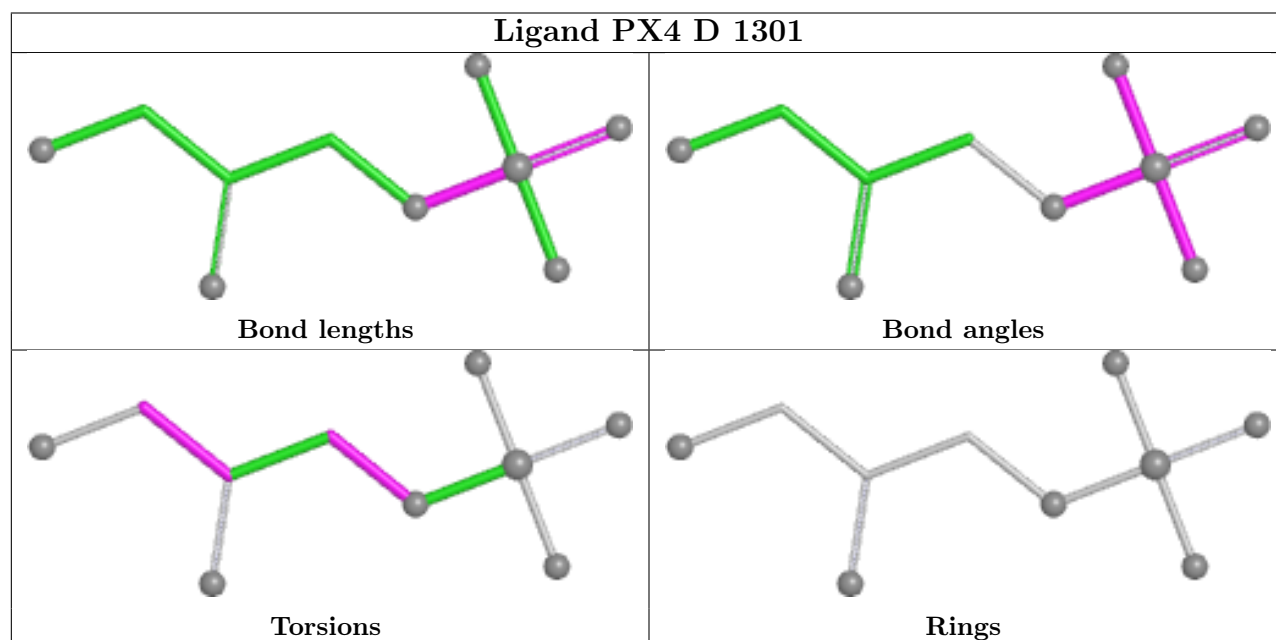
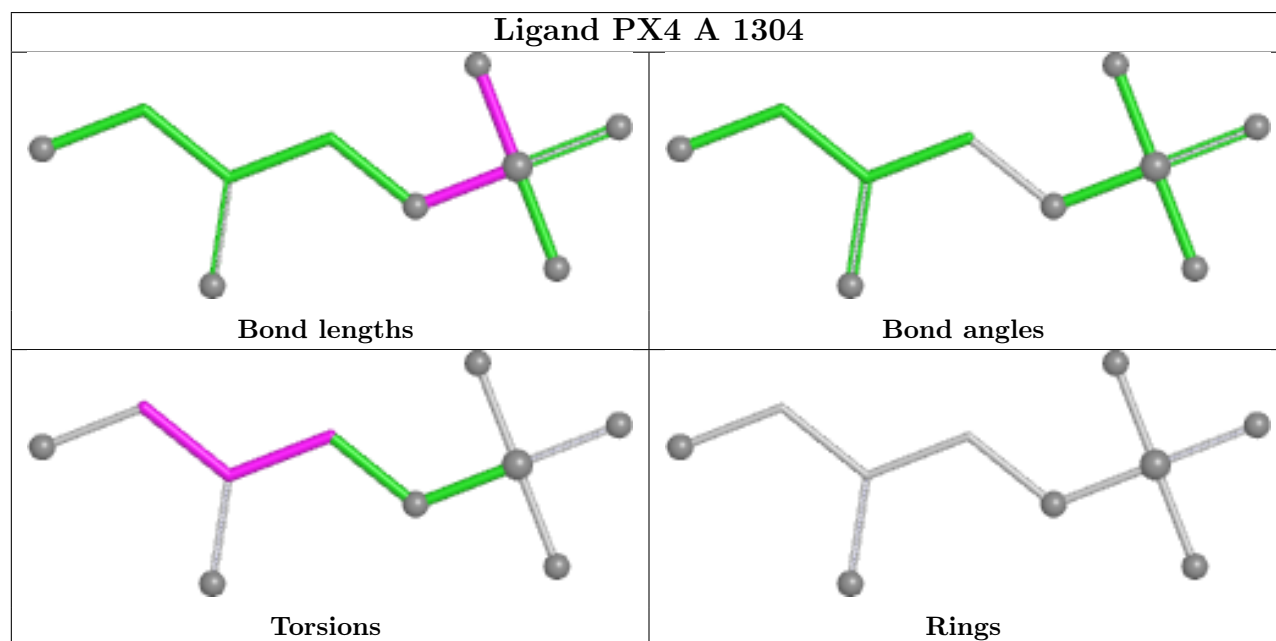
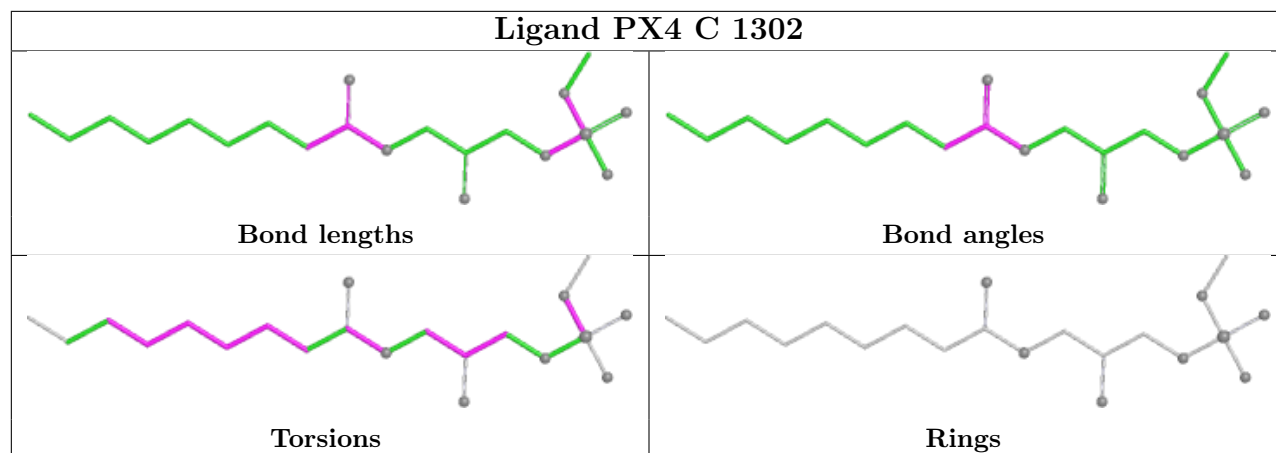


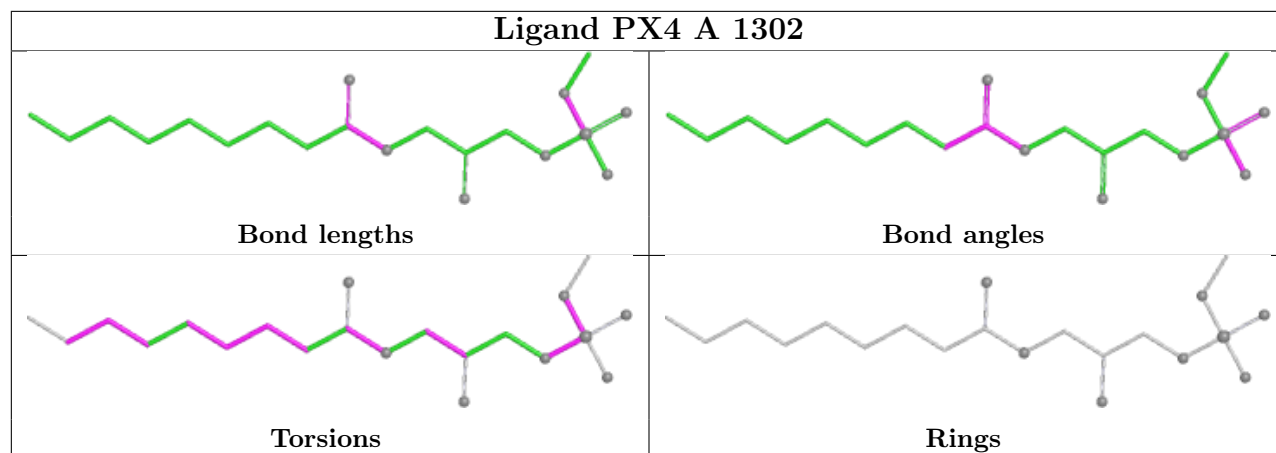
Ligand D6C D 1304



Ligand PX4 D 1303







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/284 (77%)	-1.08	0 100 100	28, 89, 129, 156	0
1	B	219/284 (77%)	-1.12	0 100 100	34, 91, 125, 149	0
1	C	219/284 (77%)	-1.15	0 100 100	27, 91, 127, 145	0
1	D	228/284 (80%)	-1.08	0 100 100	30, 87, 131, 162	0
All	All	885/1136 (77%)	-1.11	0 100 100	27, 89, 128, 162	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

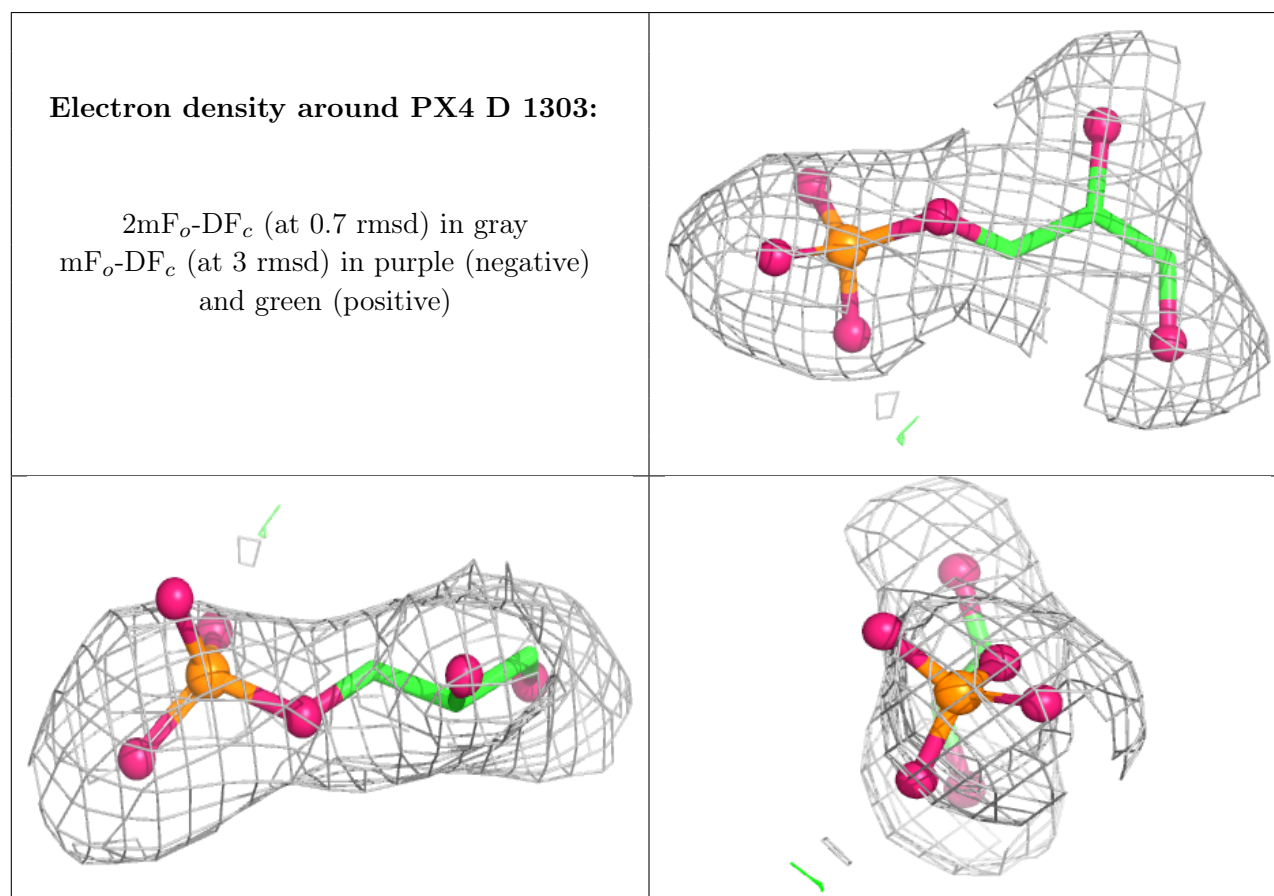
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PX4	D	1303	10/46	0.97	0.08	66,85,111,115	0
2	PX4	B	1302	10/46	0.98	0.06	80,101,114,126	0
2	PX4	C	1302	21/46	0.98	0.07	49,63,73,75	0
2	PX4	C	1303	10/46	0.98	0.06	60,72,85,89	0

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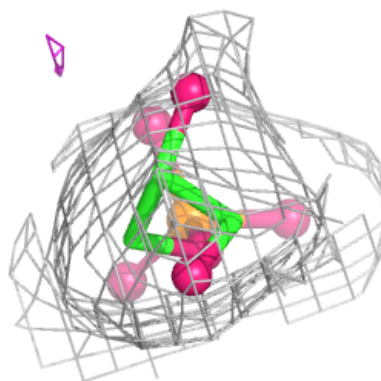
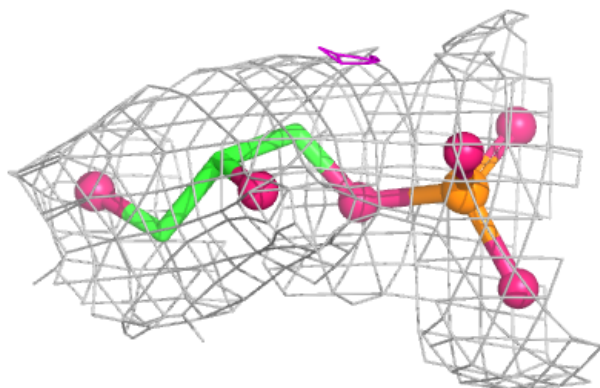
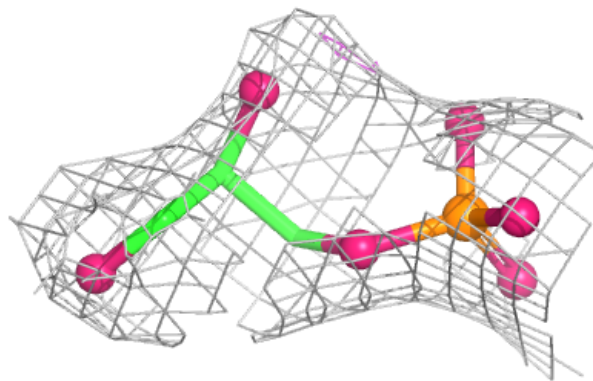
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PX4	C	1304	21/46	0.98	0.08	57,68,81,87	0
2	PX4	A	1304	10/46	0.98	0.06	79,92,107,109	0
4	D6C	D	1304	29/29	0.98	0.07	68,85,100,107	0
2	PX4	A	1301	10/46	0.99	0.08	62,77,88,92	0
2	PX4	A	1302	21/46	0.99	0.05	52,67,84,92	0
2	PX4	D	1301	10/46	0.99	0.07	62,84,96,98	0
2	PX4	D	1302	10/46	0.99	0.04	51,77,94,102	0
2	PX4	B	1303	21/46	0.99	0.05	53,66,71,76	0
3	CA	C	1301	1/1	0.99	0.03	62,62,62,62	0
2	PX4	A	1303	10/46	0.99	0.04	67,88,100,104	0
3	CA	B	1301	1/1	1.00	0.02	52,52,52,52	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.

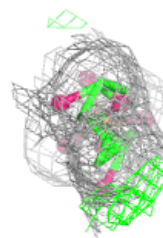
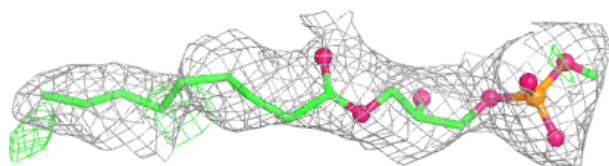
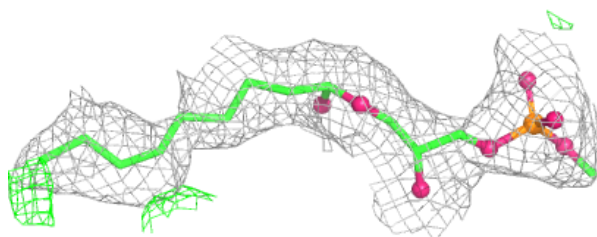


Electron density around PX4 B 1302:

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

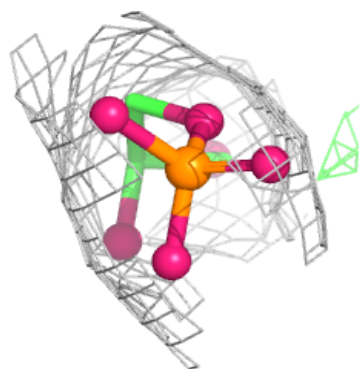
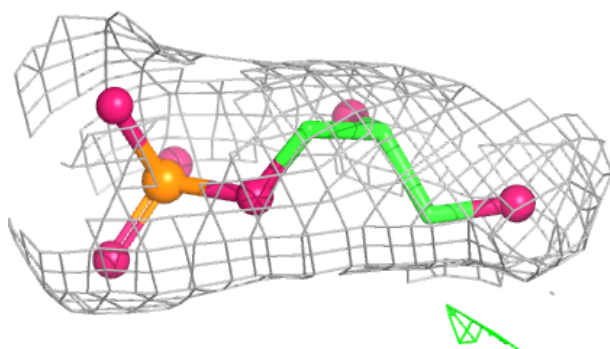
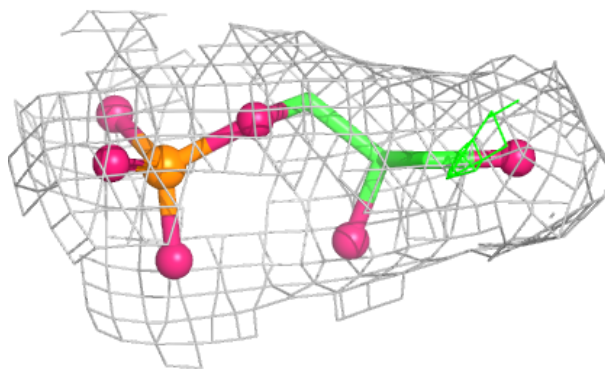
**Electron density around PX4 C 1302:**

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

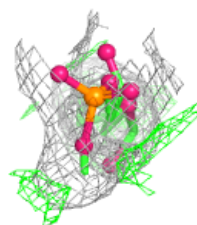
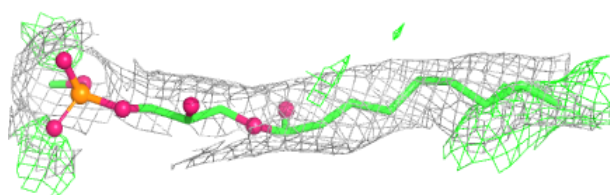
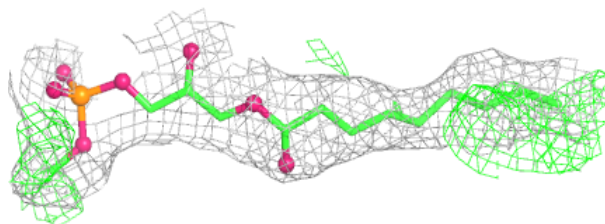


Electron density around PX4 C 1303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

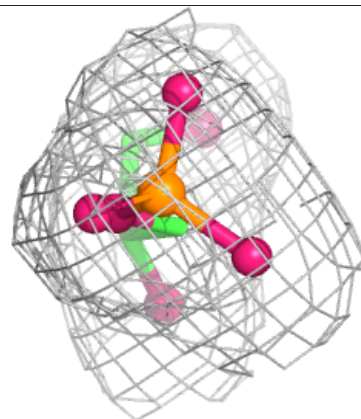
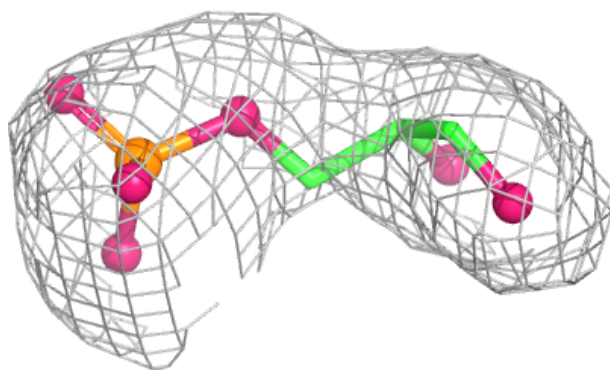
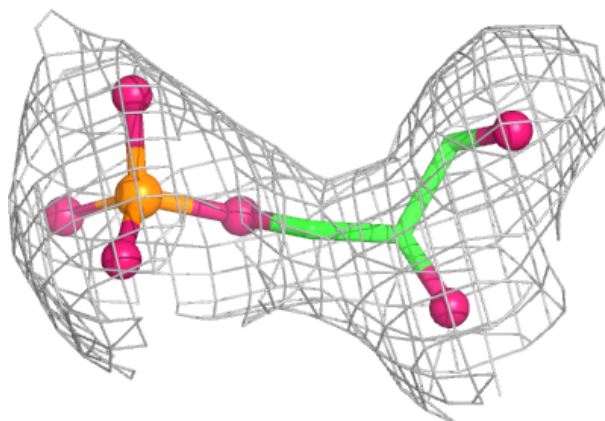
**Electron density around PX4 C 1304:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



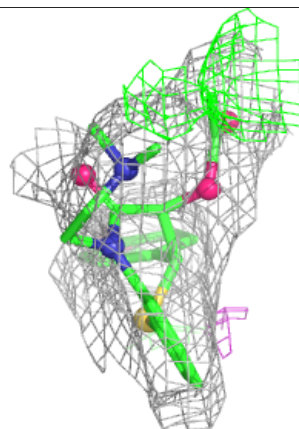
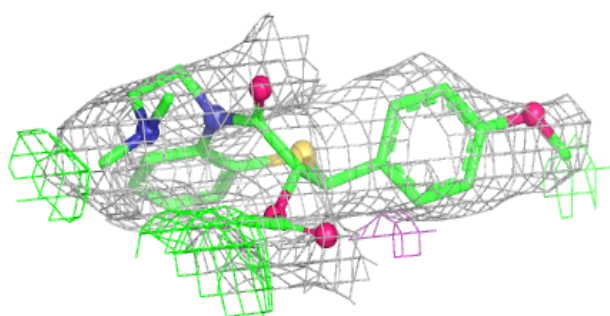
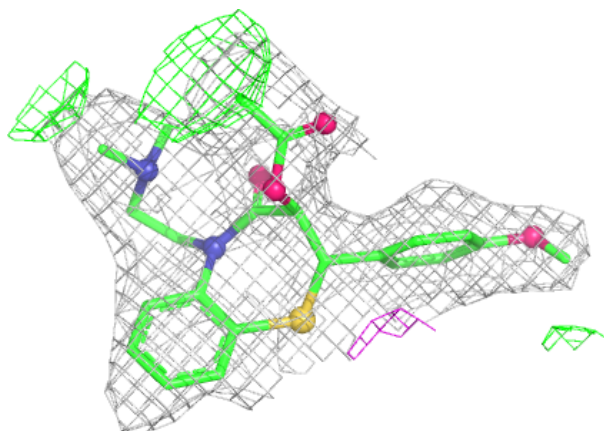
Electron density around PX4 A 1304:

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and green (positive)

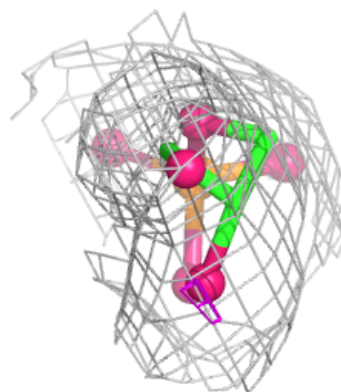
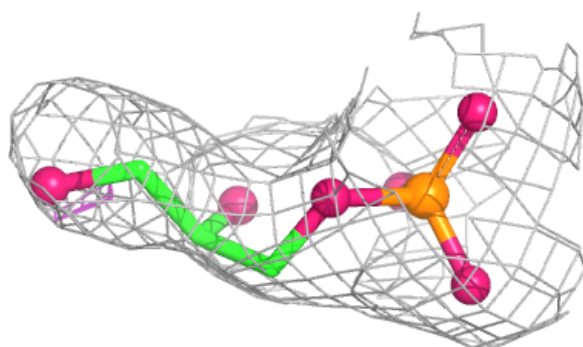
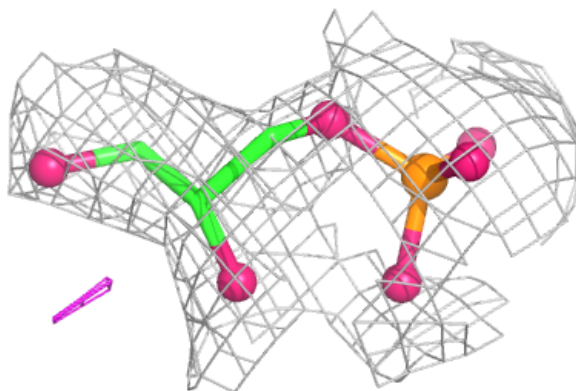


Electron density around D6C D 1304:

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and green (positive)

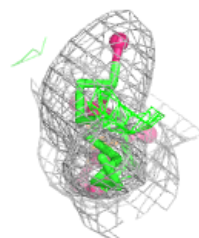
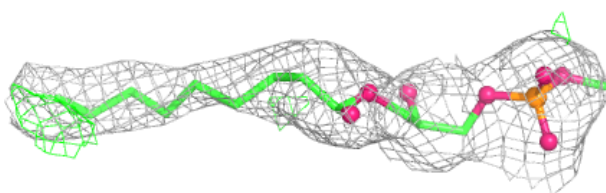
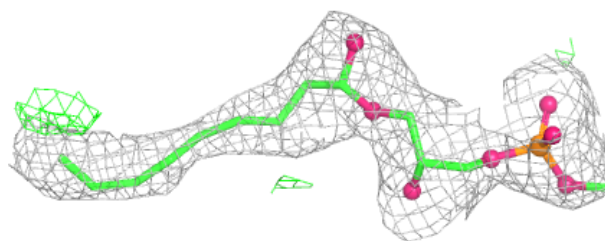
**Electron density around PX4 A 1301:**

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and green (positive)

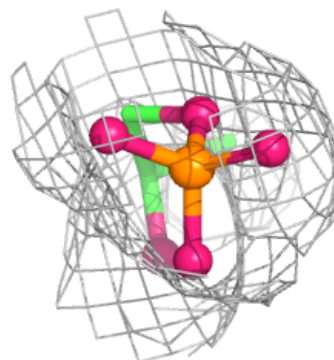
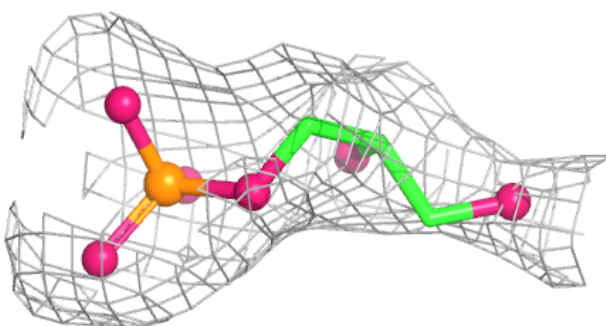


Electron density around PX4 A 1302:

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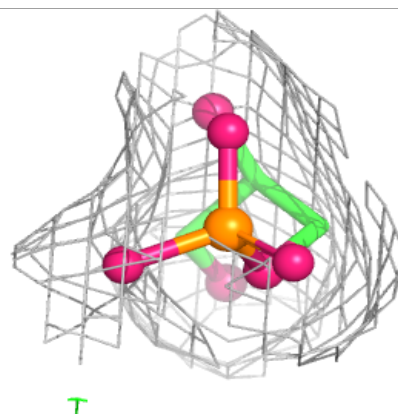
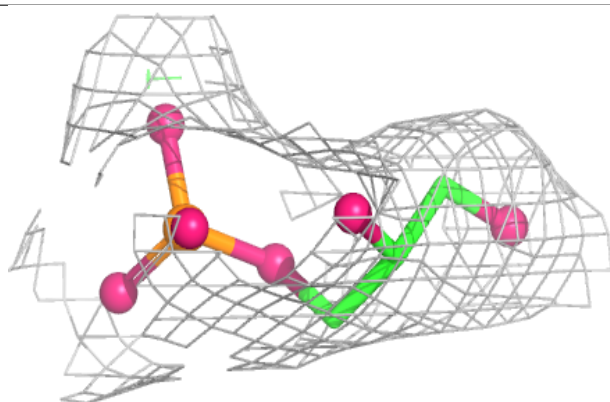
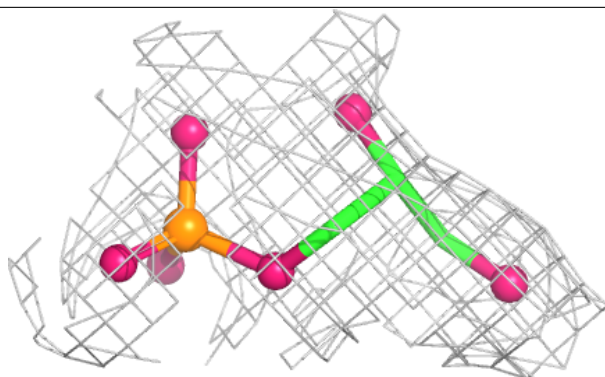
**Electron density around PX4 D 1301:**

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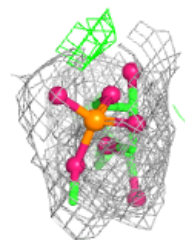
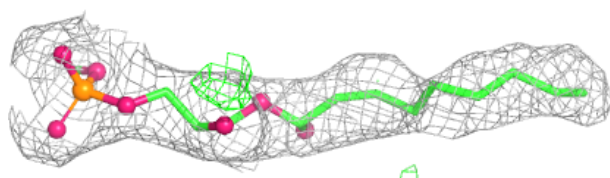
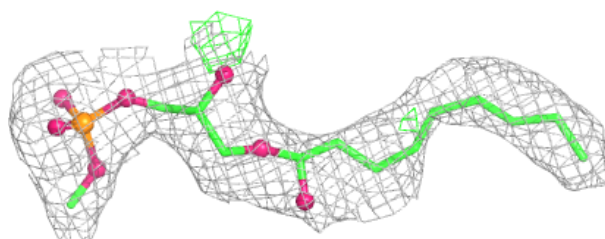


Electron density around PX4 D 1302:

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and green (positive)

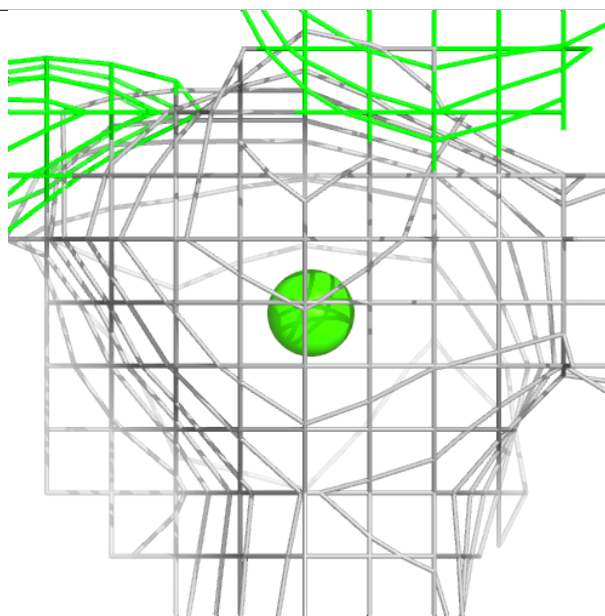
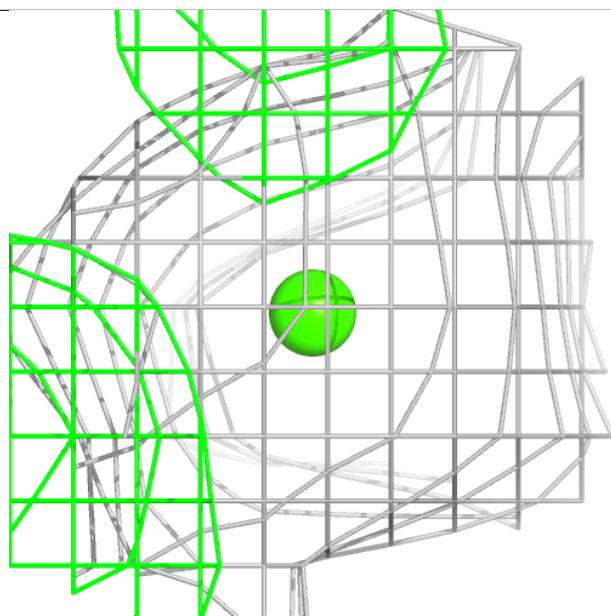
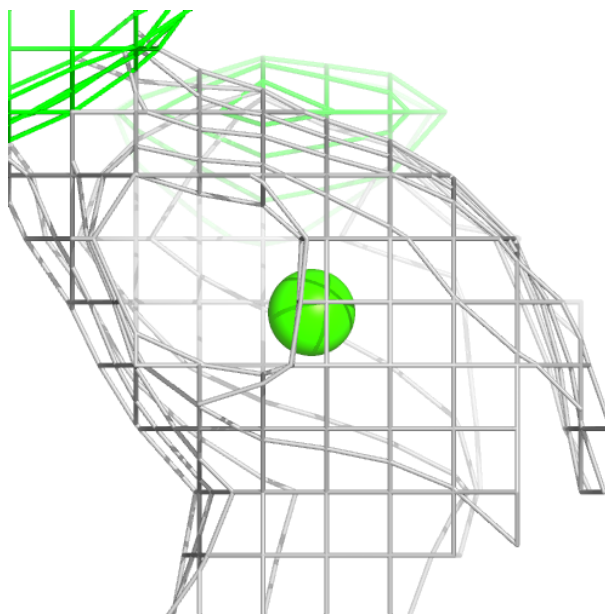
**Electron density around PX4 B 1303:**

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and green (positive)



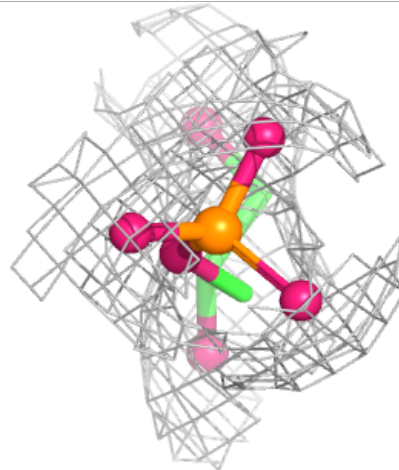
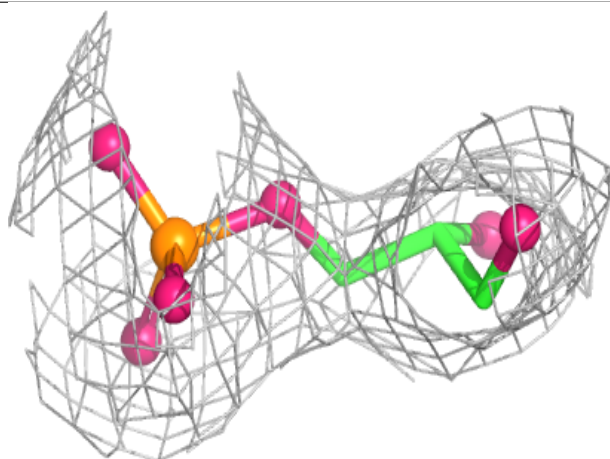
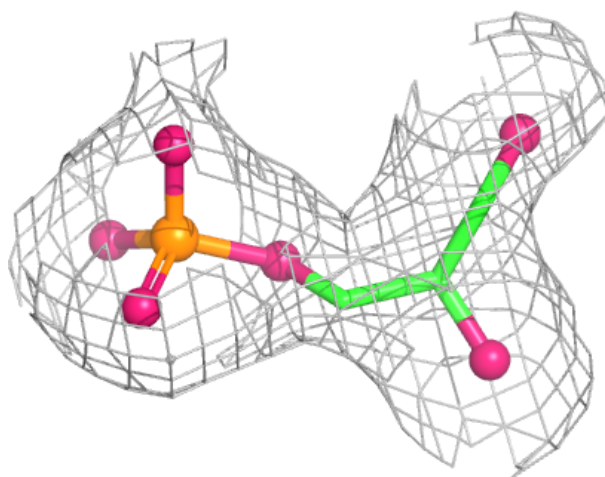
Electron density around CA C 1301:

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and green (positive)



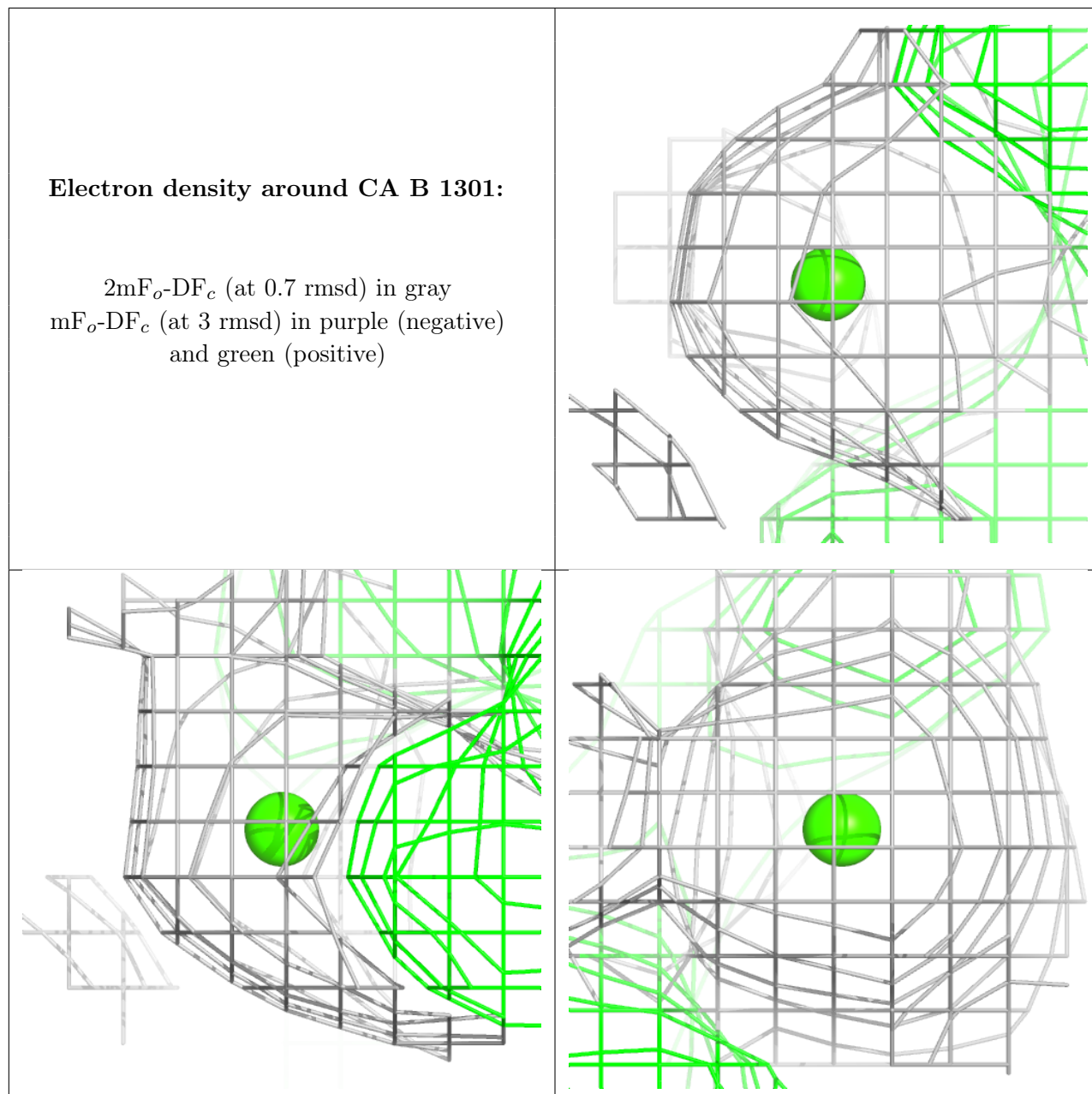
Electron density around PX4 A 1303:

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and green (positive)



Electron density around CA B 1301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.