Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2024 – 09:49 AM EST

PDB ID	:	4MVO
Title	:	Structural Basis for Ca2+ Selectivity of a Voltage-gated Calcium Channel
Authors	:	Tang, L.; Gamal El-Din, T.M.; Payandeh, J.; Martinez, G.Q.; Heard, T.M.; Scheuer, T.; Zheng, N.; Catterall, W.A.
Deposited on	:	2013-09-24
Resolution	:	3.30 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:

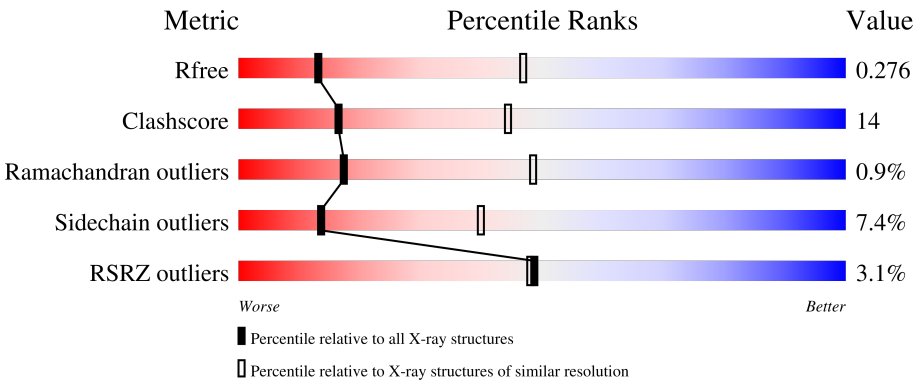
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	A	237	2% 56% 33% • 8%
1	B	237	4% 55% 35% • 8%
1	C	237	3% 54% 36% • 8%
1	D	237	3% 60% 30% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7391 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
			Total	C	N	O	S			
1	A	219	1798	1224	269	294	11	0	0	0
1	B	219	1798	1224	269	294	11	0	0	0
1	C	219	1798	1224	269	294	11	0	0	0
1	D	219	1798	1224	269	294	11	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	expression tag	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	1177	ASP	GLU	conflict	UNP A8EVM5
A	1178	ASP	SER	conflict	UNP A8EVM5
A	1181	ASN	MET	conflict	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1217	CYS	ILE	conflict	UNP A8EVM5
B	983	MET	-	expression tag	UNP A8EVM5
B	984	ASP	-	expression tag	UNP A8EVM5
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
B	1217	CYS	ILE	conflict	UNP A8EVM5
C	983	MET	-	expression tag	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

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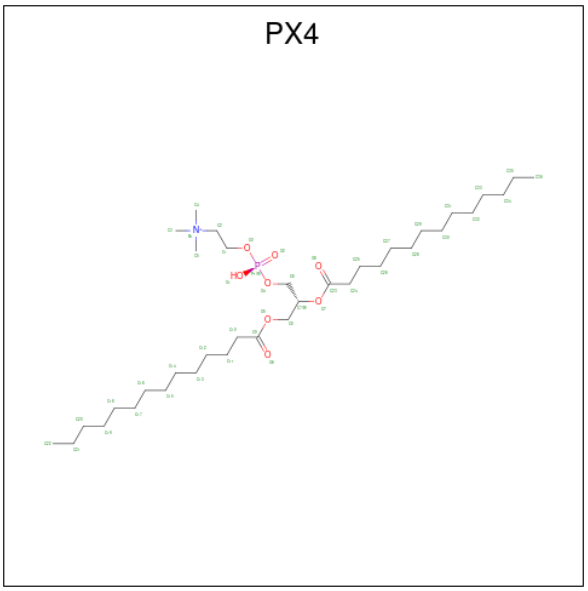
Chain	Residue	Modelled	Actual	Comment	Reference
C	1178	ASP	SER	conflict	UNP A8EVM5
C	1181	ASN	MET	conflict	UNP A8EVM5
C	1217	CYS	ILE	conflict	UNP A8EVM5
D	983	MET	-	expression tag	UNP A8EVM5
D	984	ASP	-	expression tag	UNP A8EVM5
D	985	TYR	-	expression tag	UNP A8EVM5
D	986	LYS	-	expression tag	UNP A8EVM5
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
D	1217	CYS	ILE	conflict	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
			Total	C	O	P		
2	A	1	10	3	6	1	0	0
			Total	C	O	P		
2	A	1	10	3	6	1	0	0
			Total	C	O	P		
2	A	1	21	13	7	1	0	0
			Total	C	O	P		
2	A	1	21	13	7	1	0	0
			Total	C				
2	A	1	6	6			0	0
			Total	C	O	P		
2	A	1	10	3	6	1	0	0
			Total	C	O	P		
2	B	1	10	3	6	1	0	0
			Total	C				
2	B	1	6	6			0	0
			Total	C	O	P		
2	B	1	10	3	6	1	0	0
			Total	C	O	P		
2	C	1	21	13	7	1	0	0
			Total	C				
2	C	1	6	6			0	0
			Total	C	O	P		
2	C	1	10	3	6	1	0	0
			Total	C	O	P		
2	C	1	10	3	6	1	0	0
			Total	C	O	P		
2	D	1	21	13	7	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C 6 6	0	0
2	D	1	Total C O P 10 3 6 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is water.

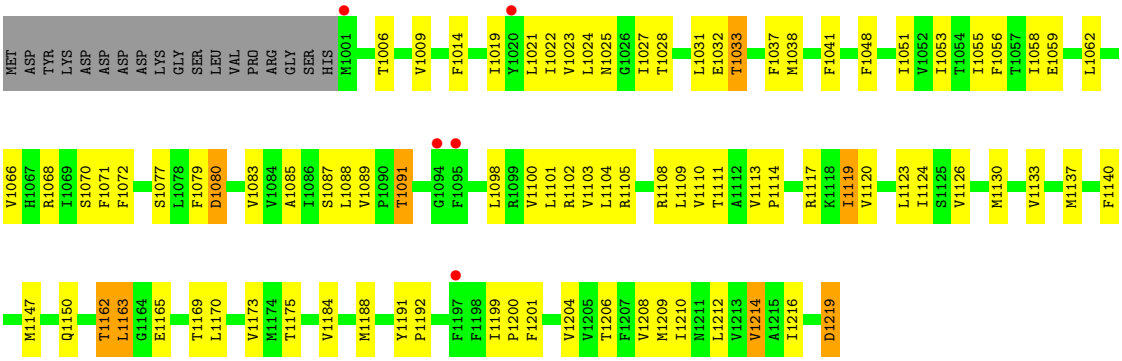
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0
4	D	2	Total O 2 2	0	0

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.

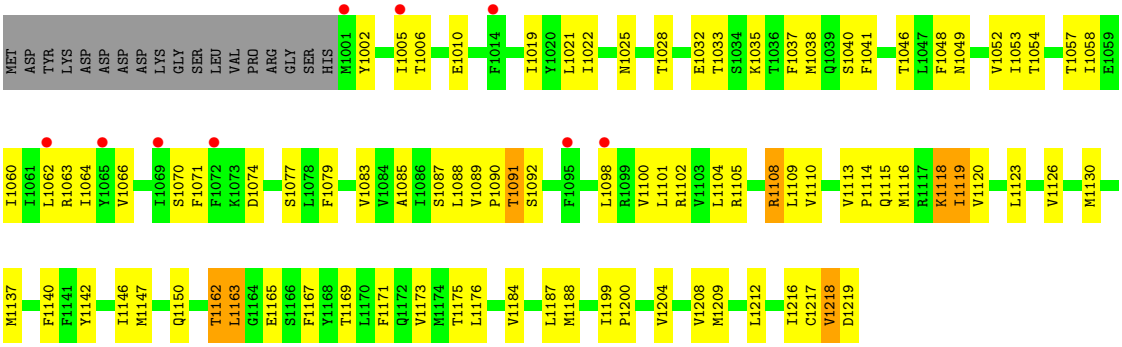
• Molecule 1: Ion transport protein

Chain A:



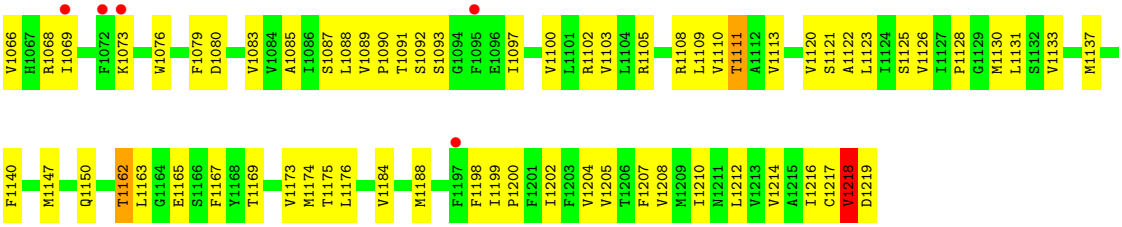
• Molecule 1: Ion transport protein

Chain B:



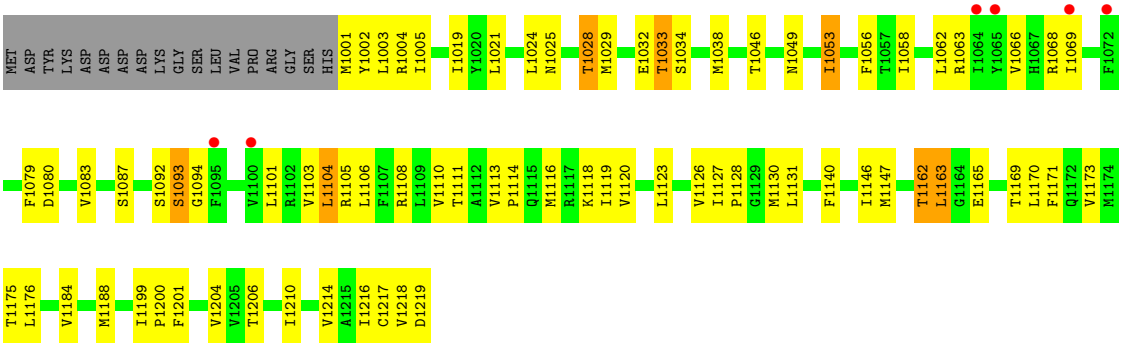
• Molecule 1: Ion transport protein

Chain C:



- Molecule 1: Ion transport protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	177.47Å 177.48Å 130.96Å 90.00° 132.63° 90.00°	Depositor
Resolution (Å)	29.85 – 3.30 29.84 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.85-3.30) 93.8 (29.84-3.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.260 , 0.279 0.257 , 0.276	Depositor DCC
R_{free} test set	2133 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	102.9	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.449 for k,h,-1/2*h-1/2*k-l 0.458 for -k,-h,-1/2*h+1/2*k-l 0.448 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7391	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: CA, 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	0.62	0/1849	0.74	0/2517
1	B	0.62	0/1849	0.74	0/2517
1	C	0.63	0/1849	0.76	0/2517
1	D	0.62	0/1849	0.76	1/2517 (0.0%)
All	All	0.62	0/7396	0.75	1/10068 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1104	LEU	CB-CG-CD2	-5.31	101.97	111.00

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	1798	0	1863	63	0
1	B	1798	0	1863	54	0
1	C	1798	0	1863	61	0
1	D	1798	0	1863	52	0
2	A	78	0	64	1	0
2	B	26	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	47	0	40	1	0
2	D	37	0	35	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
All	All	7391	0	7612	215	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 14.

All (215) 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:1162:THR:HG22	1:B:1165:GLU:H	1.37	0.90
1:D:1162:THR:HG22	1:D:1165:GLU:H	1.46	0.81
1:C:1162:THR:HG22	1:C:1165:GLU:H	1.47	0.80
1:B:1163:LEU:HB2	1:D:1033:THR:HG21	1.65	0.78
1:A:1162:THR:HG22	1:A:1165:GLU:H	1.48	0.77
1:B:1126:VAL:HG11	1:B:1216:ILE:HG23	1.66	0.77
1:B:1089:VAL:O	1:B:1102:ARG:NH2	2.20	0.75
1:C:1019:ILE:HD13	1:C:1113:VAL:HG22	1.70	0.74
1:A:1033:THR:HG21	1:C:1163:LEU:HB2	1.71	0.71
1:C:1103:VAL:HG11	1:D:1147:MET:HG2	1.75	0.69
1:A:1140:PHE:CZ	1:A:1204:VAL:HG11	2.30	0.66
1:B:1032:GLU:HG2	1:B:1038:MET:HE3	1.78	0.65
1:B:1147:MET:HG2	1:D:1103:VAL:HG11	1.79	0.65
1:A:1103:VAL:HG11	1:C:1147:MET:HG3	1.79	0.65
1:C:1184:VAL:O	1:C:1188:MET:HG3	1.97	0.64
1:A:1130:MET:SD	1:A:1216:ILE:HD11	2.38	0.64
1:A:1089:VAL:HG11	1:A:1098:LEU:HD13	1.80	0.64
1:D:1025:ASN:OD1	1:D:1105:ARG:HD2	1.98	0.64
1:D:1140:PHE:CZ	1:D:1204:VAL:HG11	2.32	0.64
1:C:1040:SER:C	1:C:1041:PHE:HD1	2.01	0.63
1:A:1006:THR:HG23	1:A:1066:VAL:HG13	1.80	0.63
1:C:1130:MET:SD	1:C:1216:ILE:HD11	2.39	0.63
1:C:1140:PHE:CZ	1:C:1204:VAL:HG11	2.34	0.62
1:C:1217:CYS:HB2	1:D:1214:VAL:HG22	1.81	0.62
1:B:1087:SER:HB3	1:B:1105:ARG:HH21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1128:PRO:HA	1:D:1131:LEU:HD12	1.83	0.61
1:D:1019:ILE:HD13	1:D:1113:VAL:HG22	1.82	0.61
1:C:1063:ARG:HH12	1:C:1108:ARG:HH22	1.46	0.61
1:B:1140:PHE:CZ	1:B:1204:VAL:HG11	2.36	0.61
1:D:1032:GLU:HA	1:D:1038:MET:HE3	1.83	0.61
1:C:1090:PRO:O	1:C:1092:SER:N	2.29	0.60
1:C:1085:ALA:HA	1:C:1088:LEU:HD12	1.83	0.60
1:C:1090:PRO:C	1:C:1092:SER:H	2.05	0.60
1:B:1019:ILE:HD13	1:B:1113:VAL:HG22	1.83	0.60
1:A:1137:MET:SD	1:A:1208:VAL:HG11	2.41	0.60
1:D:1184:VAL:HG12	1:D:1188:MET:HE2	1.82	0.60
1:A:1114:PRO:HA	1:A:1117:ARG:HB2	1.85	0.59
1:A:1056:PHE:HE2	1:A:1108:ARG:HD3	1.68	0.59
1:D:1130:MET:SD	1:D:1216:ILE:HD11	2.42	0.59
1:D:1025:ASN:O	1:D:1028:THR:HG22	2.03	0.58
2:A:1303:PX4:H24	2:A:1303:PX4:O6	2.04	0.58
1:C:1175:THR:HB	1:D:1176:LEU:HD13	1.86	0.58
1:C:1025:ASN:OD1	1:C:1105:ARG:HD2	2.04	0.57
1:A:1089:VAL:O	1:A:1102:ARG:NH2	2.38	0.57
1:A:1126:VAL:HG11	1:A:1216:ILE:HG23	1.87	0.57
1:A:1206:THR:O	1:A:1210:ILE:HG13	2.05	0.57
1:B:1087:SER:HA	1:B:1102:ARG:HG2	1.86	0.57
1:A:1184:VAL:O	1:A:1188:MET:HG3	2.05	0.57
1:D:1101:LEU:HD22	1:D:1104:LEU:HD11	1.85	0.57
1:D:1034:SER:HB2	2:D:1303:PX4:H14	1.86	0.56
1:B:1184:VAL:O	1:B:1188:MET:HG3	2.05	0.56
1:A:1025:ASN:OD1	1:A:1105:ARG:HD2	2.05	0.56
1:A:1032:GLU:HG2	1:A:1038:MET:HE3	1.87	0.56
1:A:1133:VAL:HG11	1:A:1212:LEU:HD12	1.87	0.55
1:B:1025:ASN:OD1	1:B:1105:ARG:HD2	2.06	0.55
1:D:1001:MET:HG3	1:D:1004:ARG:HD3	1.88	0.55
1:B:1176:LEU:HD13	1:D:1175:THR:HB	1.89	0.54
1:C:1089:VAL:O	1:C:1102:ARG:NH2	2.39	0.54
1:C:1169:THR:O	1:C:1173:VAL:HG23	2.07	0.54
1:D:1206:THR:O	1:D:1210:ILE:HG13	2.08	0.54
1:D:1173:VAL:O	1:D:1176:LEU:HD23	2.08	0.54
1:B:1090:PRO:O	1:B:1092:SER:N	2.37	0.53
1:C:1006:THR:HG23	1:C:1066:VAL:HG13	1.89	0.53
1:D:1083:VAL:HG11	1:D:1105:ARG:HA	1.89	0.53
1:C:1137:MET:SD	1:C:1208:VAL:HG11	2.49	0.53
1:B:1098:LEU:HD23	1:B:1101:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1053:ILE:HD11	1:D:1087:SER:HB2	1.91	0.53
1:D:1113:VAL:HG12	1:D:1114:PRO:O	2.09	0.53
1:D:1128:PRO:HA	1:D:1131:LEU:CD1	2.39	0.53
1:A:1019:ILE:HD13	1:A:1113:VAL:HG22	1.92	0.52
1:B:1006:THR:HG23	1:B:1066:VAL:HG13	1.90	0.52
1:D:1199:ILE:HB	1:D:1200:PRO:HD3	1.92	0.52
1:C:1218:VAL:HG12	1:C:1219:ASP:OD1	2.10	0.52
1:B:1058:ILE:O	1:B:1062:LEU:HG	2.09	0.51
1:A:1071:PHE:HD2	1:A:1072:PHE:CD2	2.28	0.51
1:A:1184:VAL:HG12	1:A:1188:MET:HE2	1.91	0.51
1:A:1024:LEU:HD23	1:A:1048:PHE:CZ	2.45	0.51
1:A:1214:VAL:HG22	1:B:1217:CYS:HB2	1.92	0.51
1:C:1080:ASP:OD1	1:C:1111:THR:HG21	2.10	0.51
1:C:1133:VAL:HG11	1:C:1212:LEU:HD12	1.93	0.51
1:D:1171:PHE:O	1:D:1175:THR:HG23	2.11	0.51
1:A:1022:ILE:HG21	1:A:1109:LEU:HB2	1.93	0.51
1:B:1079:PHE:CE2	1:B:1083:VAL:HG21	2.46	0.51
1:D:1002:TYR:HD1	1:D:1003:LEU:HG	1.76	0.51
1:B:1079:PHE:O	1:B:1083:VAL:HG23	2.11	0.51
1:C:1022:ILE:HG21	1:C:1109:LEU:HB2	1.93	0.51
1:B:1110:VAL:CG1	1:B:1120:VAL:HG21	2.41	0.51
1:A:1079:PHE:CE2	1:A:1083:VAL:HG21	2.46	0.50
1:C:1083:VAL:HG11	1:C:1105:ARG:HA	1.92	0.50
1:C:1033:THR:HG21	1:D:1163:LEU:HB2	1.94	0.50
1:D:1019:ILE:HD13	1:D:1113:VAL:CG2	2.41	0.50
1:B:1032:GLU:HA	1:B:1038:MET:HE3	1.94	0.50
1:A:1085:ALA:HA	1:A:1088:LEU:HD12	1.94	0.50
1:A:1032:GLU:HA	1:A:1038:MET:HE3	1.94	0.49
1:C:1048:PHE:O	1:C:1052:VAL:HG23	2.11	0.49
1:B:1037:PHE:CE1	1:B:1041:PHE:HD2	2.29	0.49
1:B:1212:LEU:O	1:B:1216:ILE:HG13	2.13	0.49
1:A:1130:MET:HE2	1:A:1212:LEU:HD11	1.94	0.49
1:B:1063:ARG:HH12	1:B:1108:ARG:HH22	1.59	0.49
1:C:1032:GLU:HA	1:C:1038:MET:HE3	1.95	0.49
1:B:1173:VAL:O	1:B:1176:LEU:HD23	2.13	0.49
1:A:1079:PHE:O	1:A:1083:VAL:HG23	2.13	0.48
1:B:1169:THR:O	1:B:1173:VAL:HG23	2.13	0.48
1:D:1063:ARG:HH12	1:D:1108:ARG:NH2	2.10	0.48
1:C:1207:PHE:HA	1:C:1210:ILE:HD12	1.95	0.48
1:B:1171:PHE:O	1:B:1175:THR:HG23	2.14	0.48
1:A:1058:ILE:O	1:A:1062:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1113:VAL:HG12	1:B:1114:PRO:O	2.13	0.48
1:C:1001:MET:HG3	1:C:1004:ARG:HD3	1.96	0.48
1:C:1100:VAL:HG12	1:D:1147:MET:HE3	1.96	0.48
1:D:1127:ILE:HA	1:D:1130:MET:HE2	1.96	0.48
1:A:1169:THR:O	1:A:1173:VAL:HG23	2.14	0.48
1:A:1133:VAL:CG1	1:A:1212:LEU:HD12	2.43	0.48
1:D:1169:THR:O	1:D:1173:VAL:HG23	2.13	0.48
1:C:1199:ILE:HB	1:C:1200:PRO:HD3	1.95	0.47
1:C:1022:ILE:HD11	1:C:1108:ARG:HB3	1.96	0.47
1:A:1100:VAL:HG22	1:C:1150:GLN:HG3	1.96	0.47
1:A:1071:PHE:CE1	1:A:1077:SER:HB3	2.49	0.47
1:C:1076:TRP:HZ2	1:C:1121:SER:OG	1.97	0.47
1:C:1056:PHE:HE2	1:C:1108:ARG:HD3	1.79	0.47
1:C:1198:PHE:O	1:C:1202:ILE:HG13	2.15	0.47
1:D:1063:ARG:HH12	1:D:1108:ARG:HH22	1.62	0.47
1:C:1079:PHE:O	1:C:1083:VAL:HG23	2.14	0.46
1:A:1087:SER:HA	1:A:1102:ARG:HG2	1.96	0.46
1:B:1130:MET:SD	1:B:1216:ILE:HD11	2.56	0.46
1:A:1051:ILE:O	1:A:1055:ILE:HG13	2.15	0.46
1:B:1199:ILE:HB	1:B:1200:PRO:HD3	1.97	0.46
1:D:1216:ILE:C	1:D:1218:VAL:H	2.19	0.46
1:A:1170:LEU:HD22	1:A:1201:PHE:CE2	2.51	0.46
1:B:1040:SER:HB3	1:B:1041:PHE:CE1	2.50	0.46
1:A:1009:VAL:HA	1:A:1014:PHE:CD2	2.51	0.46
1:C:1087:SER:HA	1:C:1102:ARG:HG2	1.98	0.46
1:B:1218:VAL:HG13	1:B:1219:ASP:OD1	2.15	0.45
1:C:1025:ASN:O	1:C:1028:THR:HG22	2.17	0.45
2:C:1301:PX4:H16	2:C:1301:PX4:O6	2.17	0.45
1:B:1126:VAL:HG11	1:B:1216:ILE:CG2	2.42	0.45
1:D:1080:ASP:OD2	1:D:1108:ARG:NH2	2.49	0.45
1:B:1022:ILE:HG21	1:B:1109:LEU:HB2	1.98	0.45
1:A:1212:LEU:O	1:A:1216:ILE:HG13	2.16	0.45
1:A:1175:THR:HB	1:C:1176:LEU:HD13	1.98	0.45
1:C:1128:PRO:HA	1:C:1131:LEU:HG	1.99	0.45
1:D:1170:LEU:HD22	1:D:1201:PHE:CE2	2.52	0.45
1:D:1184:VAL:O	1:D:1188:MET:HG3	2.17	0.45
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.98	0.45
1:A:1219:ASP:N	1:A:1219:ASP:OD1	2.49	0.44
1:D:1110:VAL:CG1	1:D:1120:VAL:HG21	2.48	0.44
1:A:1163:LEU:HB2	1:B:1033:THR:HG21	1.99	0.44
1:C:1110:VAL:HG11	1:C:1120:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1085:ALA:O	1:C:1088:LEU:HB2	2.18	0.44
1:C:1069:ILE:O	1:C:1073:LYS:HG3	2.18	0.44
1:A:1110:VAL:CG1	1:A:1120:VAL:HG21	2.48	0.44
1:A:1103:VAL:CG1	1:C:1147:MET:HG3	2.46	0.43
1:B:1048:PHE:O	1:B:1052:VAL:HG23	2.18	0.43
1:B:1101:LEU:HD22	1:B:1104:LEU:HD11	2.00	0.43
1:B:1064:ILE:HG12	1:B:1071:PHE:CD2	2.54	0.43
1:B:1074:ASP:HB3	1:B:1077:SER:HB2	2.01	0.43
1:D:1002:TYR:O	1:D:1005:ILE:HG12	2.19	0.43
1:D:1123:LEU:O	1:D:1126:VAL:HG23	2.18	0.43
1:C:1047:LEU:O	1:C:1051:ILE:HG13	2.18	0.43
1:A:1087:SER:CB	1:A:1105:ARG:HH21	2.32	0.43
1:C:1090:PRO:C	1:C:1092:SER:N	2.72	0.43
1:D:1021:LEU:HD23	1:D:1021:LEU:HA	1.73	0.43
1:A:1023:VAL:O	1:A:1027:ILE:HG13	2.19	0.43
1:B:1115:GLN:HA	1:B:1118:LYS:HB3	2.00	0.43
1:C:1097:ILE:H	1:C:1097:ILE:HG13	1.65	0.43
1:C:1174:MET:C	1:C:1176:LEU:H	2.22	0.43
1:B:1110:VAL:HG11	1:B:1120:VAL:HG21	2.00	0.42
1:B:1085:ALA:O	1:B:1088:LEU:HB2	2.19	0.42
1:C:1100:VAL:O	1:C:1103:VAL:HG12	2.19	0.42
1:D:1056:PHE:HE2	1:D:1108:ARG:HH11	1.66	0.42
1:A:1031:LEU:HD23	1:A:1031:LEU:HA	1.77	0.42
1:A:1056:PHE:CE2	1:A:1108:ARG:HD3	2.52	0.42
1:A:1101:LEU:HD22	1:A:1104:LEU:HD11	2.01	0.42
1:C:1123:LEU:O	1:C:1126:VAL:HG23	2.20	0.42
1:A:1087:SER:HB3	1:A:1105:ARG:HH21	1.84	0.42
1:C:1174:MET:HB2	1:C:1205:VAL:HG11	2.01	0.42
1:D:1092:SER:O	1:D:1093:SER:HB2	2.19	0.42
1:A:1037:PHE:HD2	1:A:1038:MET:HE2	1.84	0.42
1:D:1079:PHE:CE2	1:D:1083:VAL:HG21	2.55	0.42
1:A:1110:VAL:HG11	1:A:1120:VAL:HG21	2.02	0.41
1:A:1216:ILE:O	1:C:1214:VAL:HG11	2.19	0.41
1:C:1058:ILE:O	1:C:1062:LEU:HG	2.20	0.41
1:A:1024:LEU:HD23	1:A:1048:PHE:HZ	1.85	0.41
1:B:1002:TYR:O	1:B:1005:ILE:HG12	2.20	0.41
1:B:1022:ILE:HD11	1:B:1108:ARG:HB3	2.02	0.41
1:B:1116:MET:O	1:B:1119:ILE:HG22	2.20	0.41
1:C:1133:VAL:CG1	1:C:1212:LEU:HD12	2.51	0.41
1:D:1058:ILE:HD13	1:D:1058:ILE:HA	1.91	0.41
1:D:1062:LEU:O	1:D:1066:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1040:SER:C	1:C:1041:PHE:CD1	2.87	0.41
1:A:1021:LEU:HA	1:A:1021:LEU:HD23	1.68	0.41
1:A:1120:VAL:O	1:A:1124:ILE:HG13	2.20	0.41
1:B:1089:VAL:HA	1:B:1090:PRO:HD3	1.87	0.41
1:D:1110:VAL:HG11	1:D:1120:VAL:HG21	2.02	0.41
1:A:1014:PHE:CE2	1:A:1059:GLU:HG3	2.55	0.41
1:D:1029:MET:SD	1:D:1106:LEU:HD21	2.61	0.41
1:A:1037:PHE:CE1	1:A:1041:PHE:HD2	2.37	0.41
1:B:1057:THR:HA	1:B:1060:ILE:HG22	2.03	0.41
1:B:1087:SER:CB	1:B:1105:ARG:HH21	2.32	0.41
1:C:1038:MET:HA	1:C:1038:MET:HE2	2.03	0.41
1:A:1080:ASP:OD1	1:A:1080:ASP:N	2.53	0.41
1:A:1188:MET:HA	1:A:1191:TYR:O	2.21	0.41
1:B:1123:LEU:O	1:B:1126:VAL:HG23	2.20	0.41
1:C:1063:ARG:HH12	1:C:1108:ARG:NH2	2.16	0.41
1:D:1114:PRO:O	1:D:1116:MET:N	2.52	0.41
1:D:1146:ILE:HG12	1:D:1163:LEU:HD21	2.03	0.41
1:B:1021:LEU:HD23	1:B:1021:LEU:HA	1.69	0.41
1:D:1101:LEU:HD23	1:D:1101:LEU:HA	1.90	0.41
1:A:1123:LEU:O	1:A:1126:VAL:HG23	2.21	0.41
1:B:1137:MET:SD	1:B:1208:VAL:HG11	2.61	0.41
1:C:1110:VAL:CG1	1:C:1120:VAL:HG21	2.52	0.40
1:C:1122:ALA:O	1:C:1125:SER:OG	2.38	0.40
1:A:1119:ILE:O	1:A:1123:LEU:HG	2.22	0.40
1:A:1150:GLN:HG3	1:B:1100:VAL:HG22	2.03	0.40
1:B:1142:TYR:O	1:B:1146:ILE:HG13	2.22	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	A	217/237 (92%)	197 (91%)	19 (9%)	1 (0%)	29	61
1	B	217/237 (92%)	198 (91%)	18 (8%)	1 (0%)	29	61
1	C	217/237 (92%)	196 (90%)	18 (8%)	3 (1%)	11	38
1	D	217/237 (92%)	200 (92%)	14 (6%)	3 (1%)	11	38
All	All	868/948 (92%)	791 (91%)	69 (8%)	8 (1%)	17	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1091	THR
1	C	1093	SER
1	B	1091	THR
1	D	1093	SER
1	D	1094	GLY
1	D	1217	CYS
1	A	1091	THR
1	C	1218	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/218 (93%)	186 (92%)	16 (8%)	12	37
1	B	202/218 (93%)	183 (91%)	19 (9%)	8	30
1	C	202/218 (93%)	191 (95%)	11 (5%)	22	53
1	D	202/218 (93%)	188 (93%)	14 (7%)	15	44
All	All	808/872 (93%)	748 (93%)	60 (7%)	13	40

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1028	THR
1	A	1033	THR
1	A	1053	ILE

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Mol	Chain	Res	Type
1	A	1068	ARG
1	A	1070	SER
1	A	1080	ASP
1	A	1091	THR
1	A	1111	THR
1	A	1119	ILE
1	A	1147	MET
1	A	1162	THR
1	A	1163	LEU
1	A	1192	PRO
1	A	1209	MET
1	A	1214	VAL
1	A	1219	ASP
1	B	1010	GLU
1	B	1028	THR
1	B	1035	LYS
1	B	1046	THR
1	B	1049	ASN
1	B	1053	ILE
1	B	1054	THR
1	B	1070	SER
1	B	1091	THR
1	B	1108	ARG
1	B	1118	LYS
1	B	1119	ILE
1	B	1150	GLN
1	B	1162	THR
1	B	1163	LEU
1	B	1167	PHE
1	B	1187	LEU
1	B	1209	MET
1	B	1218	VAL
1	C	1010	GLU
1	C	1024	LEU
1	C	1028	THR
1	C	1035	LYS
1	C	1041	PHE
1	C	1053	ILE
1	C	1068	ARG
1	C	1111	THR
1	C	1162	THR
1	C	1167	PHE

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Mol	Chain	Res	Type
1	C	1218	VAL
1	D	1024	LEU
1	D	1028	THR
1	D	1033	THR
1	D	1046	THR
1	D	1049	ASN
1	D	1053	ILE
1	D	1068	ARG
1	D	1069	ILE
1	D	1111	THR
1	D	1118	LYS
1	D	1119	ILE
1	D	1162	THR
1	D	1163	LEU
1	D	1219	ASP

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)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	-	5,5,45	0.31	0	4,4,53	0.31	0
2	PX4	A	1306	-	9,9,45	0.56	0	11,12,53	1.36	1 (9%)
2	PX4	A	1303	-	20,20,45	1.47	2 (10%)	22,24,53	1.88	2 (9%)
2	PX4	D	1303	-	9,9,45	0.65	0	11,12,53	1.28	1 (9%)
2	PX4	A	1304	-	20,20,45	1.43	2 (10%)	22,24,53	1.88	2 (9%)
2	PX4	C	1302	-	5,5,45	0.23	0	4,4,53	0.14	0
2	PX4	A	1302	-	9,9,45	0.56	0	11,12,53	1.37	2 (18%)
2	PX4	B	1301	-	9,9,45	0.51	0	11,12,53	1.12	2 (18%)
2	PX4	C	1303	-	9,9,45	0.45	0	11,12,53	1.26	1 (9%)
2	PX4	C	1304	-	9,9,45	0.72	0	11,12,53	1.49	2 (18%)
2	PX4	A	1305	-	5,5,45	0.26	0	4,4,53	0.33	0
2	PX4	B	1302	-	5,5,45	0.28	0	4,4,53	0.33	0
2	PX4	D	1301	-	20,20,45	1.45	2 (10%)	22,24,53	1.69	3 (13%)
2	PX4	B	1303	-	9,9,45	0.81	0	11,12,53	1.56	2 (18%)
2	PX4	A	1301	-	9,9,45	0.52	0	11,12,53	1.23	2 (18%)
2	PX4	C	1301	-	20,20,45	1.39	2 (10%)	22,24,53	1.92	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	D	1302	-	-	3/3/3/49	-
2	PX4	A	1306	-	-	7/8/8/49	-
2	PX4	A	1303	-	-	11/22/22/49	-
2	PX4	D	1303	-	-	5/8/8/49	-
2	PX4	A	1304	-	-	6/22/22/49	-
2	PX4	C	1302	-	-	2/3/3/49	-
2	PX4	A	1302	-	-	5/8/8/49	-
2	PX4	B	1301	-	-	7/8/8/49	-
2	PX4	C	1303	-	-	5/8/8/49	-
2	PX4	C	1304	-	-	6/8/8/49	-
2	PX4	A	1305	-	-	1/3/3/49	-
2	PX4	B	1302	-	-	1/3/3/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PX4	D	1301	-	-	11/22/22/49	-
2	PX4	B	1303	-	-	6/8/8/49	-
2	PX4	A	1301	-	-	5/8/8/49	-
2	PX4	C	1301	-	-	18/22/22/49	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1303	PX4	O6-C9	5.16	1.37	1.22
2	D	1301	PX4	O6-C9	5.15	1.37	1.22
2	C	1301	PX4	O6-C9	5.13	1.37	1.22
2	A	1304	PX4	O6-C9	4.98	1.37	1.22
2	D	1301	PX4	O5-C9	2.74	1.41	1.33
2	A	1303	PX4	O5-C9	2.54	1.40	1.33
2	A	1304	PX4	O5-C9	2.40	1.40	1.33
2	C	1301	PX4	O5-C9	2.06	1.39	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1301	PX4	O5-C9-O6	-7.48	104.72	123.59
2	A	1304	PX4	O5-C9-O6	-7.22	105.38	123.59
2	A	1303	PX4	O5-C9-O6	-6.57	107.00	123.59
2	D	1301	PX4	O5-C9-O6	-5.62	109.40	123.59
2	A	1303	PX4	O6-C9-C10	-4.99	104.26	123.73
2	D	1301	PX4	O6-C9-C10	-4.52	106.10	123.73
2	A	1304	PX4	O6-C9-C10	-4.38	106.65	123.73
2	C	1301	PX4	O6-C9-C10	-3.86	108.66	123.73
2	C	1303	PX4	O3-P1-O4	2.80	114.18	106.73
2	D	1303	PX4	O1-P1-O4	2.56	113.53	106.73
2	B	1303	PX4	O3-P1-O4	2.51	113.41	106.73
2	A	1302	PX4	O4-P1-O2	2.44	113.32	106.47
2	A	1302	PX4	O1-P1-O4	2.36	113.02	106.73
2	A	1306	PX4	O3-P1-O4	2.19	112.55	106.73
2	D	1301	PX4	C8-C7-C6	-2.18	106.38	112.79
2	C	1304	PX4	O1-P1-O4	2.17	112.51	106.73
2	A	1301	PX4	O4-P1-O2	2.16	112.53	106.47
2	A	1301	PX4	P1-O4-C6	2.14	124.18	118.30
2	C	1304	PX4	O4-P1-O2	2.11	112.38	106.47
2	B	1301	PX4	O1-P1-O4	2.08	112.28	106.73
2	B	1303	PX4	O5-C8-C7	2.08	120.18	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1301	PX4	O3-P1-O4	2.06	112.22	106.73

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	PX4	C6-O4-P1-O1
2	A	1301	PX4	C6-O4-P1-O2
2	A	1301	PX4	C6-O4-P1-O3
2	A	1302	PX4	C6-O4-P1-O1
2	A	1302	PX4	C6-O4-P1-O3
2	A	1302	PX4	C6-C7-C8-O5
2	A	1303	PX4	C6-O4-P1-O1
2	A	1303	PX4	C6-O4-P1-O2
2	A	1303	PX4	C6-C7-C8-O5
2	A	1306	PX4	C6-O4-P1-O1
2	A	1306	PX4	C6-O4-P1-O2
2	A	1306	PX4	C6-O4-P1-O3
2	A	1306	PX4	C6-C7-C8-O5
2	B	1301	PX4	C6-O4-P1-O1
2	B	1301	PX4	C6-O4-P1-O3
2	B	1301	PX4	C6-C7-C8-O5
2	B	1303	PX4	C6-O4-P1-O1
2	B	1303	PX4	C6-O4-P1-O2
2	B	1303	PX4	C6-O4-P1-O3
2	B	1303	PX4	O4-C6-C7-C8
2	C	1301	PX4	C1-O3-P1-O1
2	C	1301	PX4	C1-O3-P1-O2
2	C	1301	PX4	C6-O4-P1-O1
2	C	1301	PX4	O4-C6-C7-C8
2	C	1301	PX4	C6-C7-C8-O5
2	C	1303	PX4	C6-O4-P1-O1
2	C	1303	PX4	C6-O4-P1-O2
2	C	1303	PX4	C6-O4-P1-O3
2	C	1303	PX4	C6-C7-C8-O5
2	C	1304	PX4	C6-O4-P1-O1
2	C	1304	PX4	C6-O4-P1-O3
2	C	1304	PX4	O4-C6-C7-C8
2	D	1301	PX4	C6-O4-P1-O1
2	D	1301	PX4	C6-C7-C8-O5
2	D	1301	PX4	O7-C7-C8-O5
2	D	1303	PX4	C6-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
2	D	1303	PX4	O7-C7-C8-O5
2	A	1303	PX4	O4-C6-C7-O7
2	B	1303	PX4	O4-C6-C7-O7
2	C	1301	PX4	O4-C6-C7-O7
2	C	1304	PX4	O4-C6-C7-O7
2	D	1303	PX4	O4-C6-C7-O7
2	A	1303	PX4	O7-C7-C8-O5
2	A	1303	PX4	O4-C6-C7-C8
2	D	1303	PX4	O4-C6-C7-C8
2	C	1301	PX4	O6-C9-O5-C8
2	C	1301	PX4	C9-C10-C11-C12
2	C	1301	PX4	O7-C7-C8-O5
2	A	1304	PX4	C9-C10-C11-C12
2	A	1303	PX4	O6-C9-O5-C8
2	A	1304	PX4	O6-C9-O5-C8
2	A	1302	PX4	O7-C7-C8-O5
2	A	1306	PX4	O4-C6-C7-O7
2	C	1301	PX4	C6-O4-P1-O3
2	D	1301	PX4	C6-O4-P1-O3
2	C	1301	PX4	C13-C14-C15-C16
2	A	1303	PX4	C1-O3-P1-O2
2	C	1301	PX4	C12-C13-C14-C15
2	C	1302	PX4	C32-C33-C34-C35
2	A	1301	PX4	C6-C7-C8-O5
2	B	1303	PX4	C6-C7-C8-O5
2	A	1304	PX4	C12-C13-C14-C15
2	A	1304	PX4	C13-C14-C15-C16
2	A	1301	PX4	O7-C7-C8-O5
2	A	1306	PX4	O7-C7-C8-O5
2	B	1301	PX4	O7-C7-C8-O5
2	C	1303	PX4	O7-C7-C8-O5
2	D	1301	PX4	O6-C9-O5-C8
2	B	1301	PX4	O4-C6-C7-O7
2	A	1306	PX4	O4-C6-C7-C8
2	D	1301	PX4	C10-C11-C12-C13
2	D	1301	PX4	C13-C14-C15-C16
2	A	1303	PX4	C6-O4-P1-O3
2	D	1301	PX4	C12-C13-C14-C15
2	A	1302	PX4	C6-O4-P1-O2
2	B	1301	PX4	C6-O4-P1-O2
2	C	1304	PX4	C6-O4-P1-O2
2	D	1302	PX4	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	A	1304	PX4	O4-C6-C7-O7
2	C	1301	PX4	C1-O3-P1-O4
2	A	1303	PX4	C14-C15-C16-C17
2	C	1302	PX4	C31-C32-C33-C34
2	C	1301	PX4	C6-O4-P1-O2
2	D	1301	PX4	C6-O4-P1-O2
2	A	1305	PX4	C33-C34-C35-C36
2	B	1301	PX4	O4-C6-C7-C8
2	B	1302	PX4	C33-C34-C35-C36
2	A	1304	PX4	O4-C6-C7-C8
2	C	1301	PX4	C10-C11-C12-C13
2	C	1301	PX4	C11-C12-C13-C14
2	D	1303	PX4	C6-O4-P1-O3
2	C	1301	PX4	C11-C10-C9-O6
2	A	1303	PX4	C11-C12-C13-C14
2	D	1302	PX4	C33-C34-C35-C36
2	C	1304	PX4	C6-C7-C8-O5
2	D	1301	PX4	C11-C10-C9-O6
2	D	1302	PX4	C32-C33-C34-C35
2	C	1301	PX4	C14-C15-C16-C17
2	D	1301	PX4	O4-C6-C7-C8

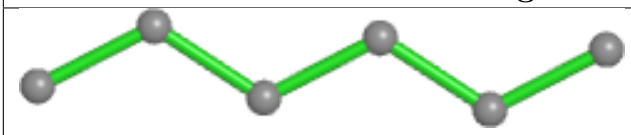
There are no ring outliers.

3 monomers are involved in 3 short contacts:

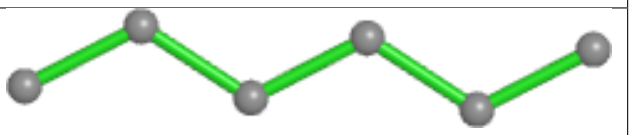
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1303	PX4	1	0
2	D	1303	PX4	1	0
2	C	1301	PX4	1	0

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 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.

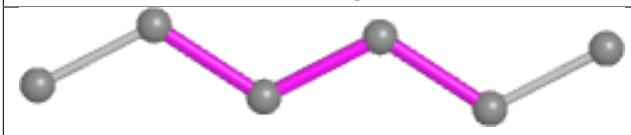
Ligand PX4 D 1302



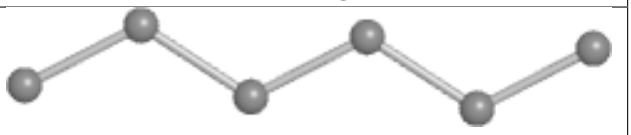
Bond lengths



Bond angles

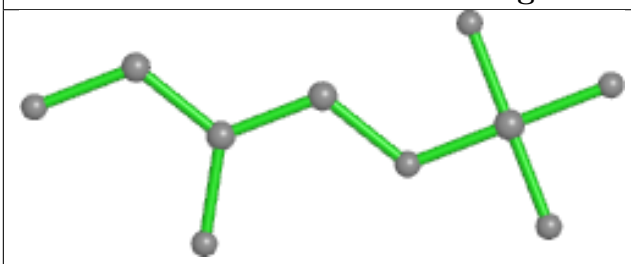


Torsions



Rings

Ligand PX4 A 1306



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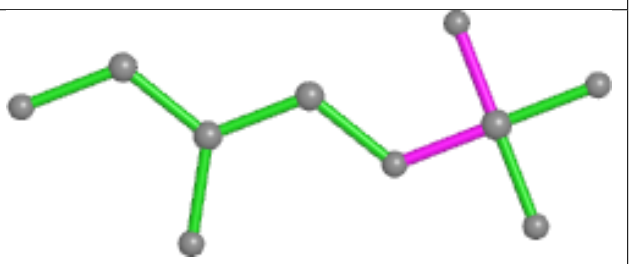

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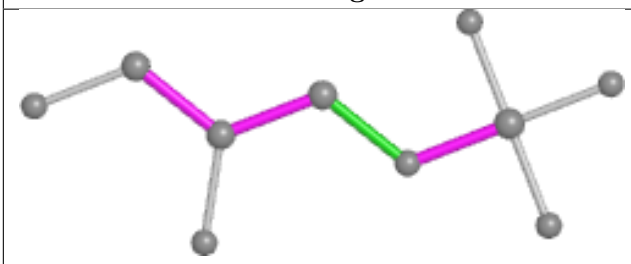

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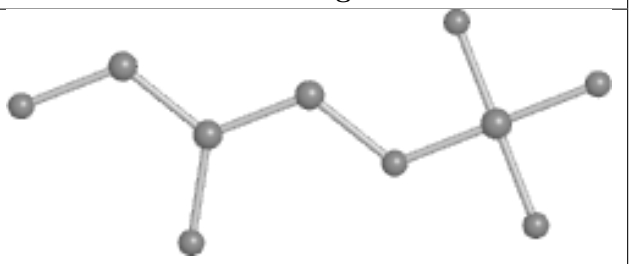
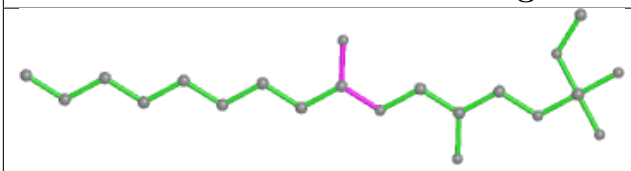


Rings

Ligand PX4 A 1303



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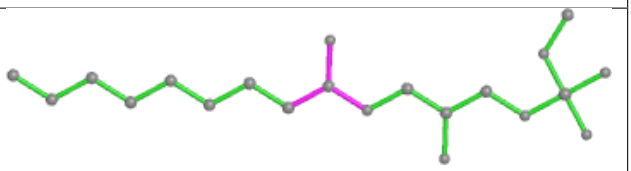
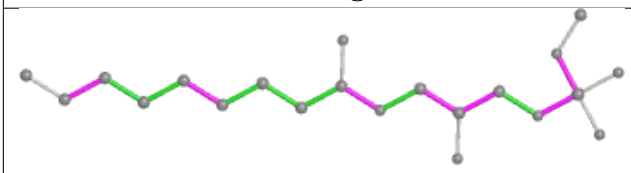


Bond angles



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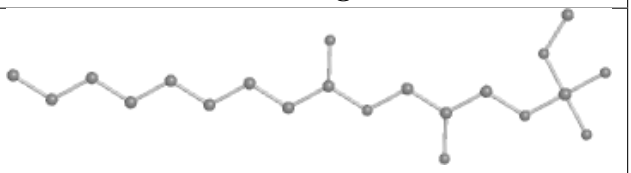
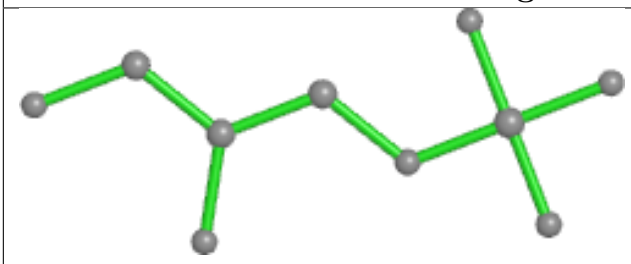


Rings

Ligand PX4 D 1303



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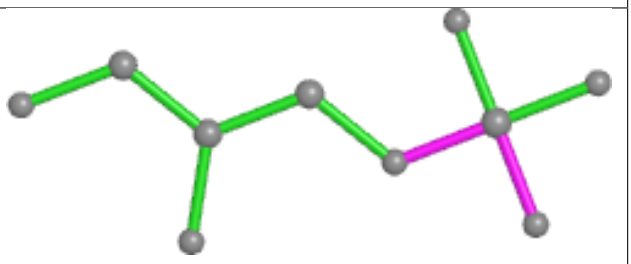
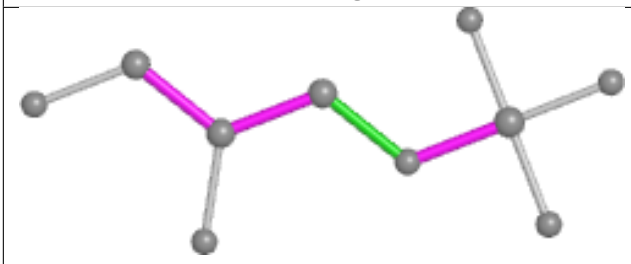
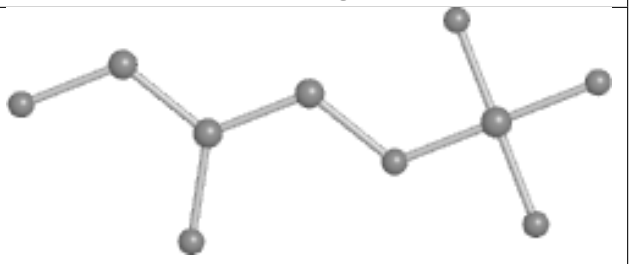


Bond angles

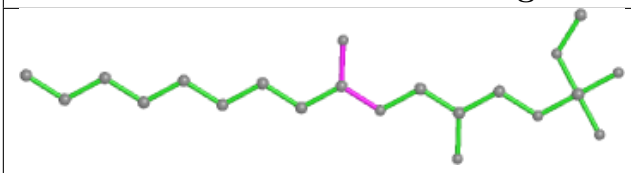


Torsions



Rings

Ligand PX4 A 1304



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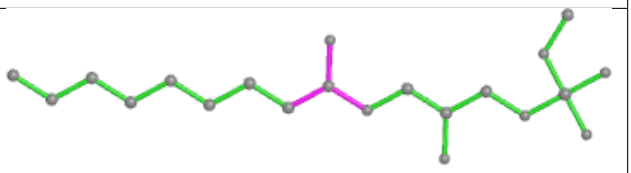
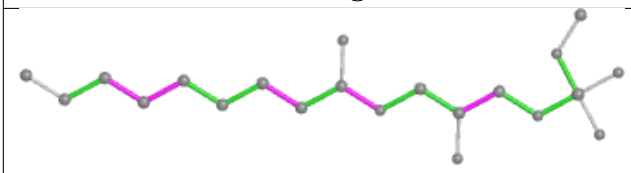


Bond angles



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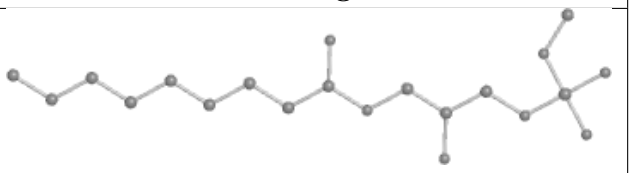
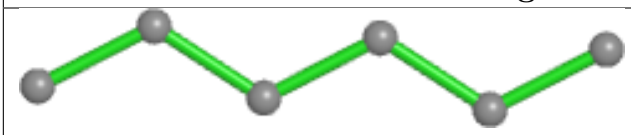


Rings

Ligand PX4 C 1302



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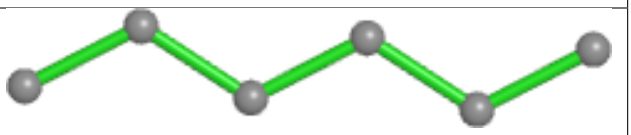
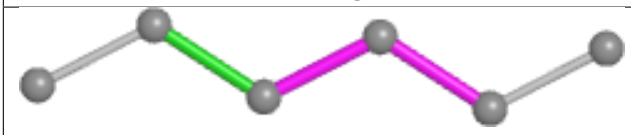


Bond angles



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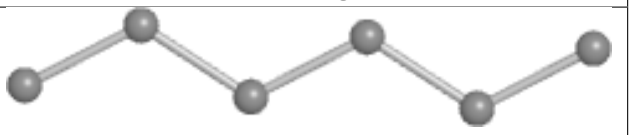
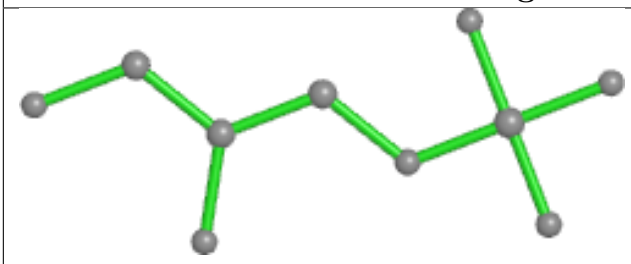


Rings

Ligand PX4 A 1302



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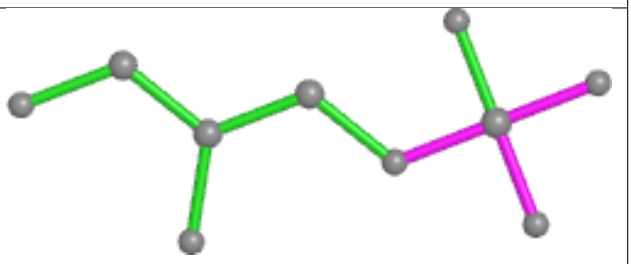
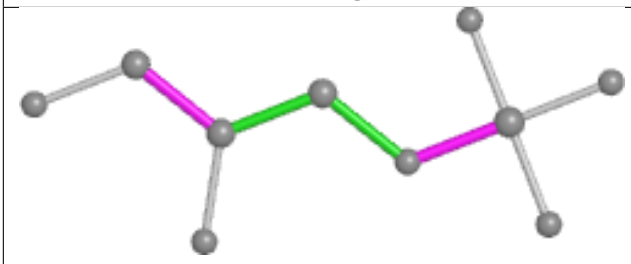
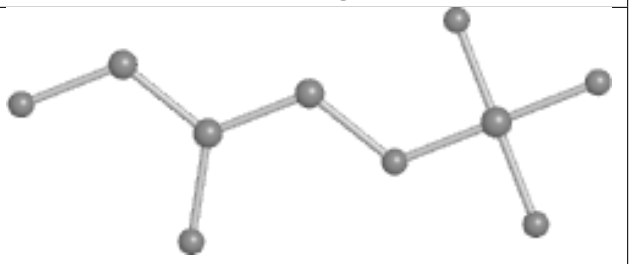


Bond angles

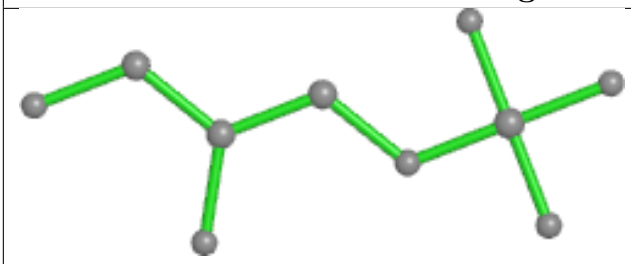


Torsions

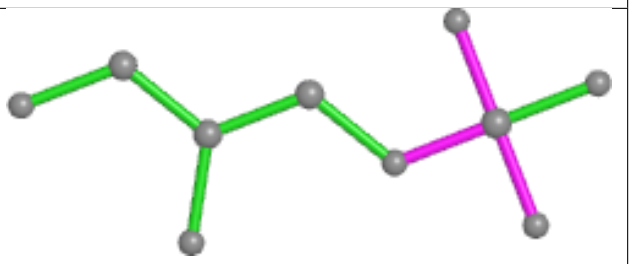


Rings

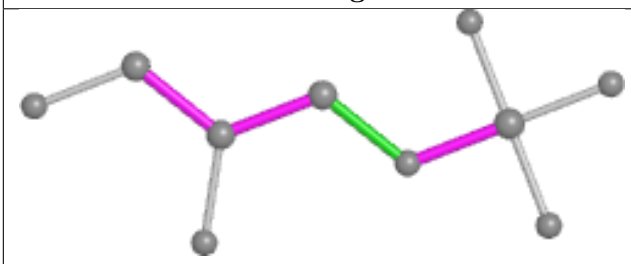
Ligand PX4 B 1301



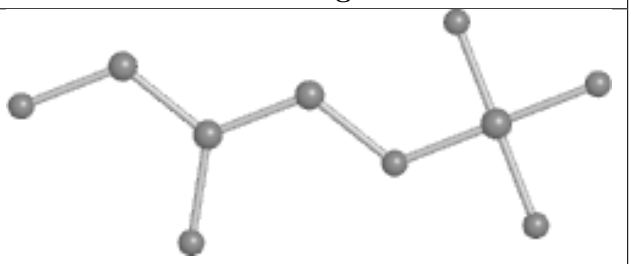
Bond lengths



Bond angles

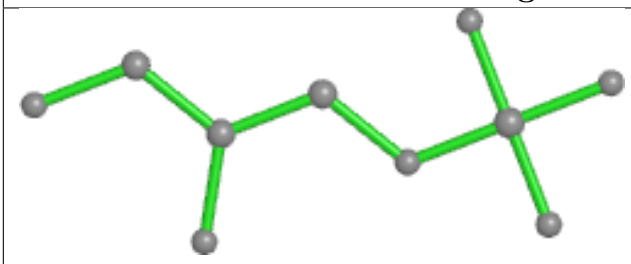


Torsions

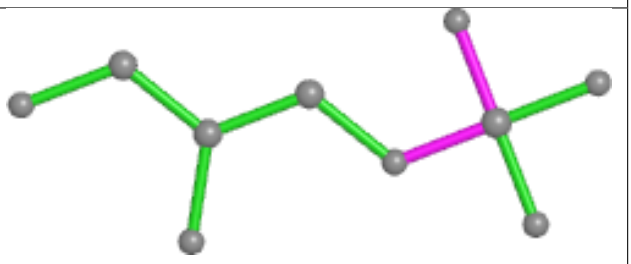


Rings

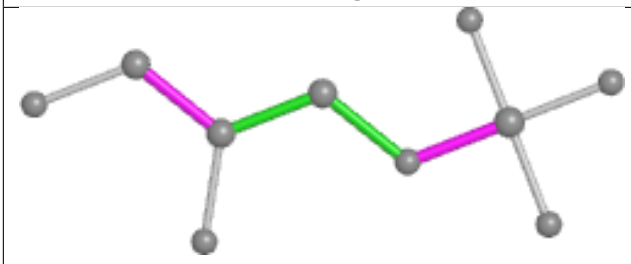
Ligand PX4 C 1303



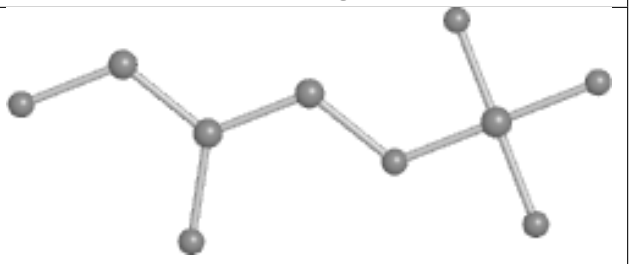
Bond lengths



Bond angles

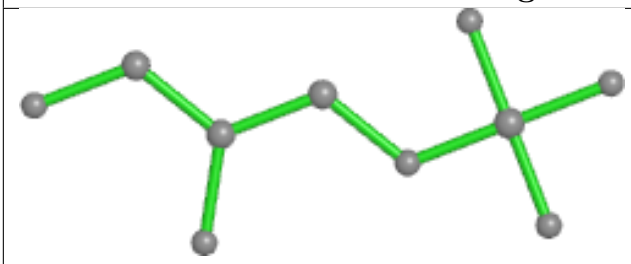


Torsions

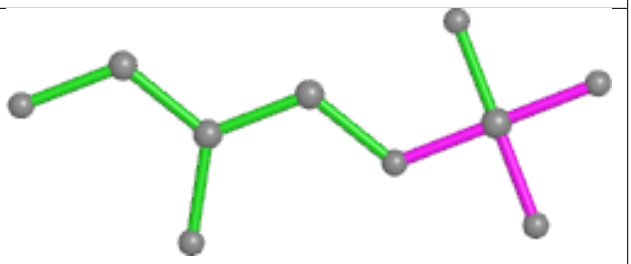


Rings

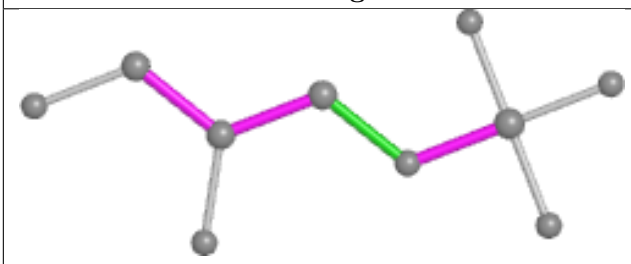
Ligand PX4 C 1304



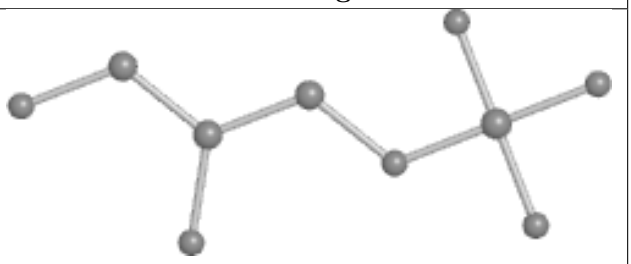
Bond lengths



Bond angles

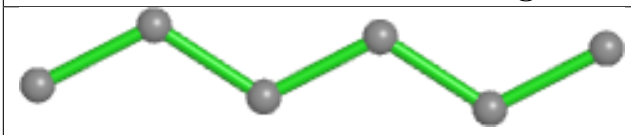


Torsions

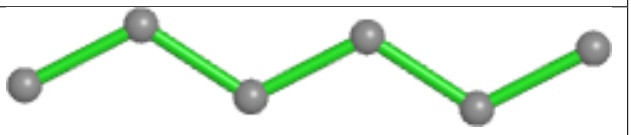


Rings

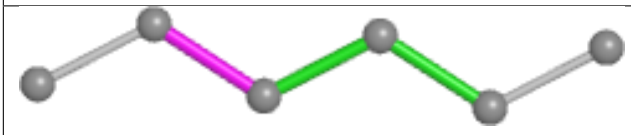
Ligand PX4 A 1305



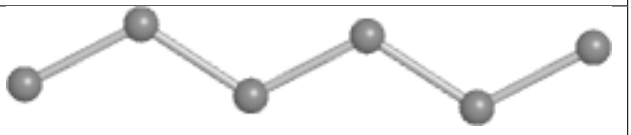
Bond lengths



Bond angles

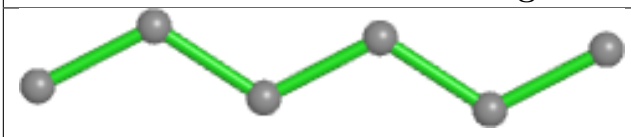


Torsions

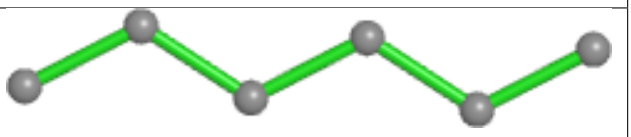


Rings

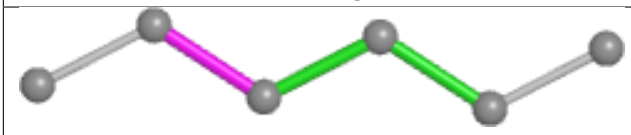
Ligand PX4 B 1302



Bond lengths



Bond angles



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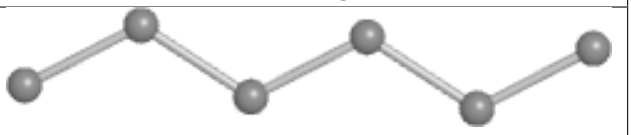
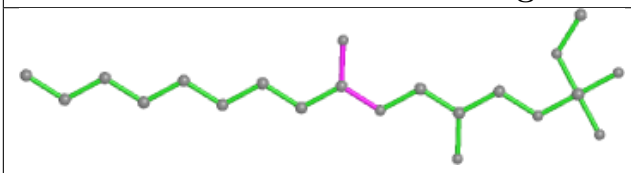
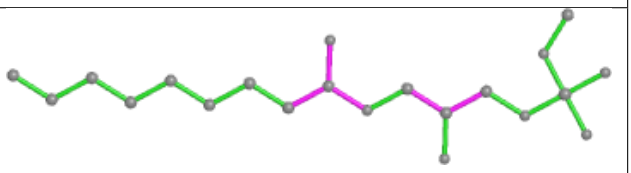


Rings

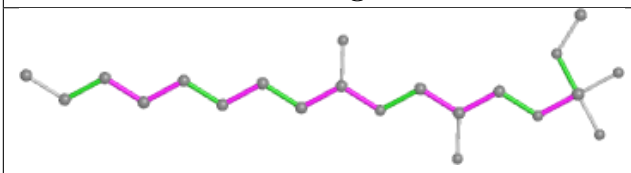
Ligand PX4 D 1301



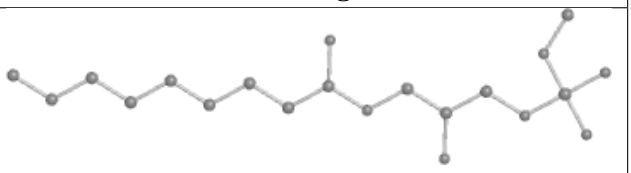
Bond lengths



Bond angles

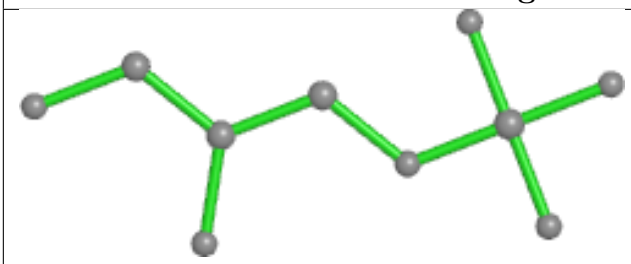


Torsions

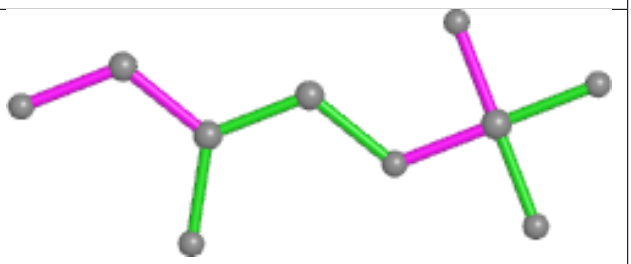


Rings

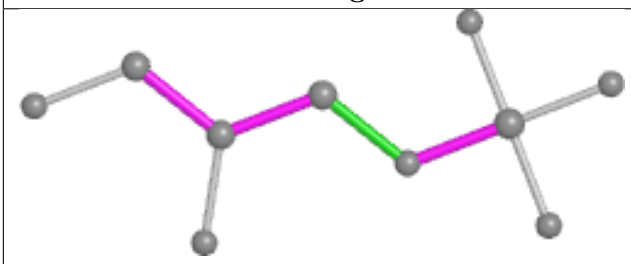
Ligand PX4 B 1303



Bond lengths



Bond angles



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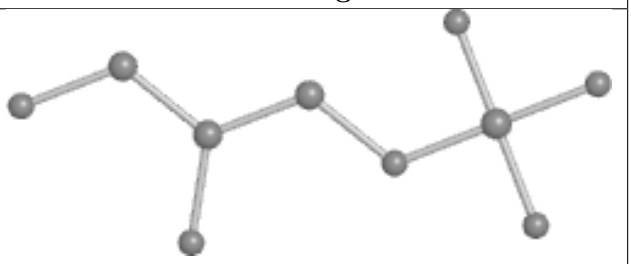
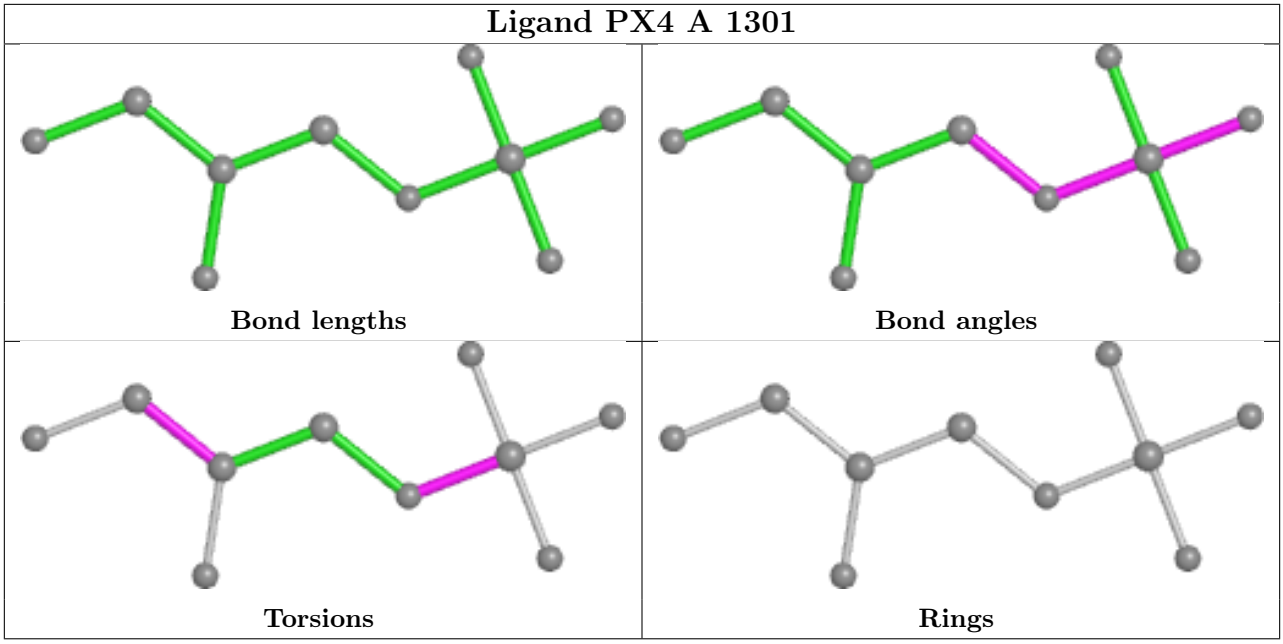
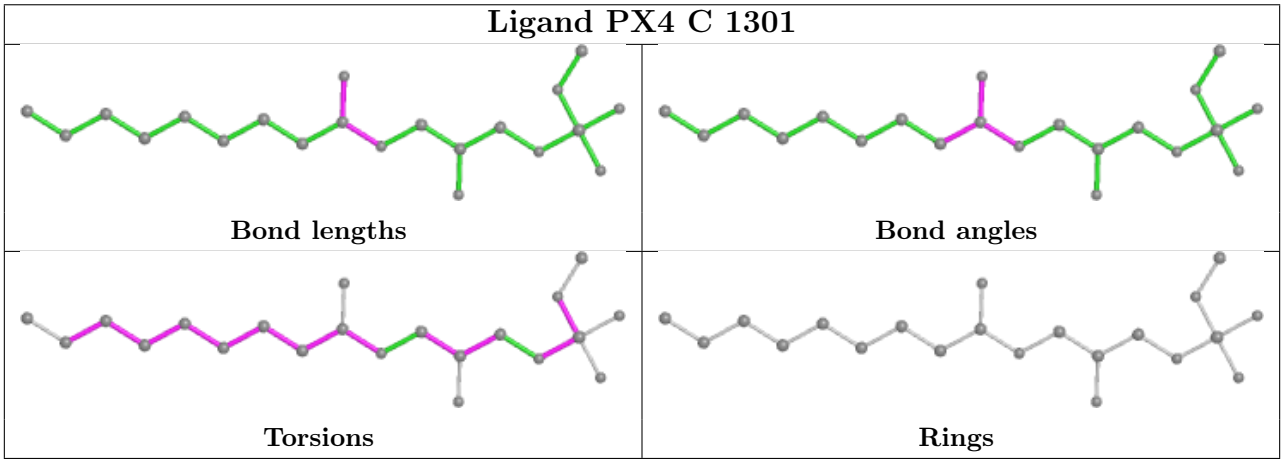


Rings





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	219/237 (92%)	0.36	5 (2%)	60	59	35, 98, 133, 158	0
1	B	219/237 (92%)	0.37	9 (4%)	37	35	35, 98, 135, 158	0
1	C	219/237 (92%)	0.37	7 (3%)	47	46	37, 97, 135, 165	0
1	D	219/237 (92%)	0.32	6 (2%)	54	52	35, 97, 134, 163	0
All	All	876/948 (92%)	0.35	27 (3%)	49	48	35, 98, 135, 165	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1065	TYR	4.8
1	C	1065	TYR	4.3
1	B	1065	TYR	4.0
1	A	1095	PHE	3.8
1	A	1094	GLY	3.6
1	A	1001	MET	3.5
1	B	1001	MET	3.4
1	B	1095	PHE	3.3
1	C	1069	ILE	3.3
1	D	1072	PHE	2.8
1	B	1069	ILE	2.8
1	B	1062	LEU	2.7
1	D	1069	ILE	2.6
1	D	1100	VAL	2.6
1	C	1072	PHE	2.5
1	B	1072	PHE	2.5
1	C	1001	MET	2.5
1	A	1020	TYR	2.4
1	B	1014	PHE	2.3
1	C	1073	LYS	2.3
1	C	1095	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1098	LEU	2.2
1	A	1197	PHE	2.2
1	D	1064	ILE	2.1
1	D	1095	PHE	2.1
1	B	1005	ILE	2.1
1	C	1197	PHE	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	A	1302	10/46	0.81	0.18	56,84,116,130	0
3	CA	A	1308	1/1	0.81	0.07	55,55,55,55	0
2	PX4	B	1303	10/46	0.83	0.19	70,89,114,118	0
2	PX4	C	1304	10/46	0.84	0.21	76,90,106,114	0
2	PX4	D	1303	10/46	0.85	0.18	76,95,113,116	0
2	PX4	D	1301	21/46	0.85	0.28	55,62,80,93	0
2	PX4	B	1301	10/46	0.86	0.18	61,83,109,125	0
2	PX4	A	1301	10/46	0.87	0.18	55,78,110,124	0
2	PX4	C	1303	10/46	0.87	0.17	58,84,110,127	0
2	PX4	C	1301	21/46	0.88	0.26	52,61,74,89	0
3	CA	A	1307	1/1	0.88	0.14	90,90,90,90	0
2	PX4	A	1304	21/46	0.88	0.24	51,65,89,94	0
2	PX4	A	1303	21/46	0.89	0.26	51,62,82,94	0
2	PX4	A	1305	6/46	0.90	0.28	42,43,53,53	0
2	PX4	C	1302	6/46	0.90	0.26	40,44,45,47	0
2	PX4	B	1302	6/46	0.90	0.30	44,46,53,54	0
2	PX4	A	1306	10/46	0.90	0.19	76,90,108,110	0

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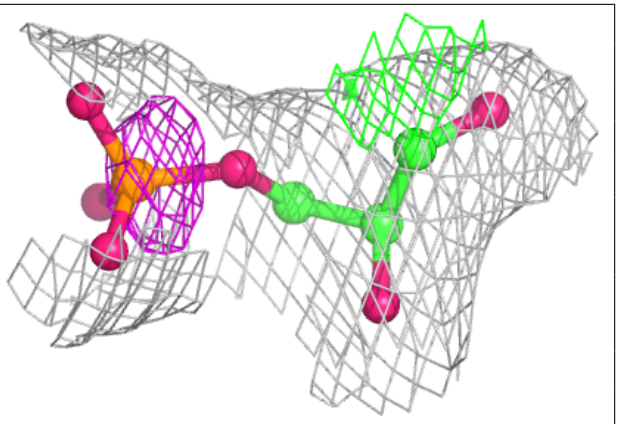
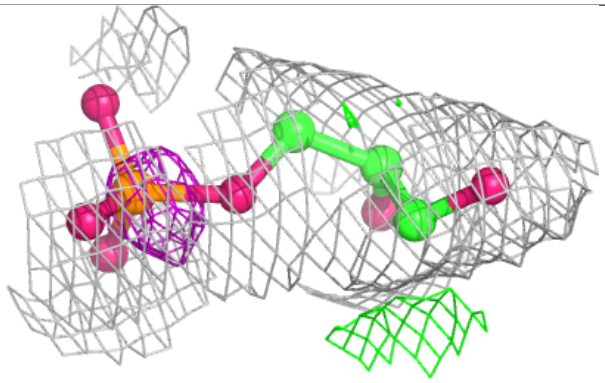
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PX4	D	1302	6/46	0.92	0.29	41,45,51,55	0
3	CA	B	1304	1/1	0.94	0.28	66,66,66,66	0

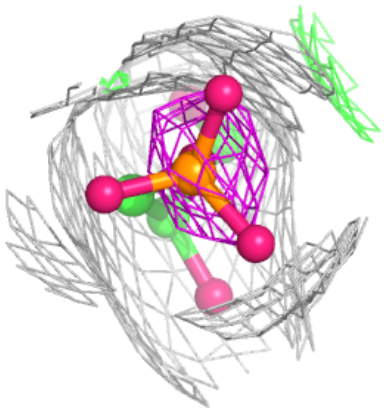
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PX4 A 1302:

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

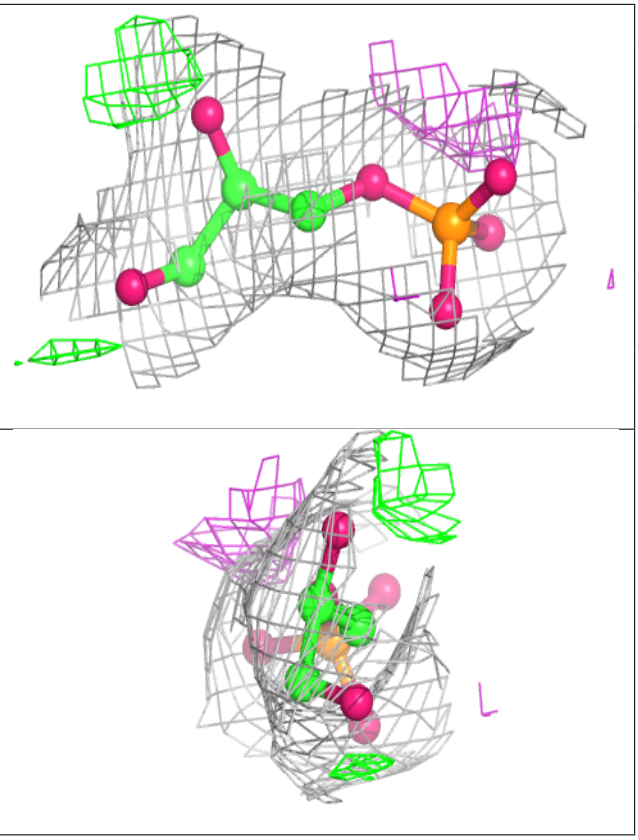






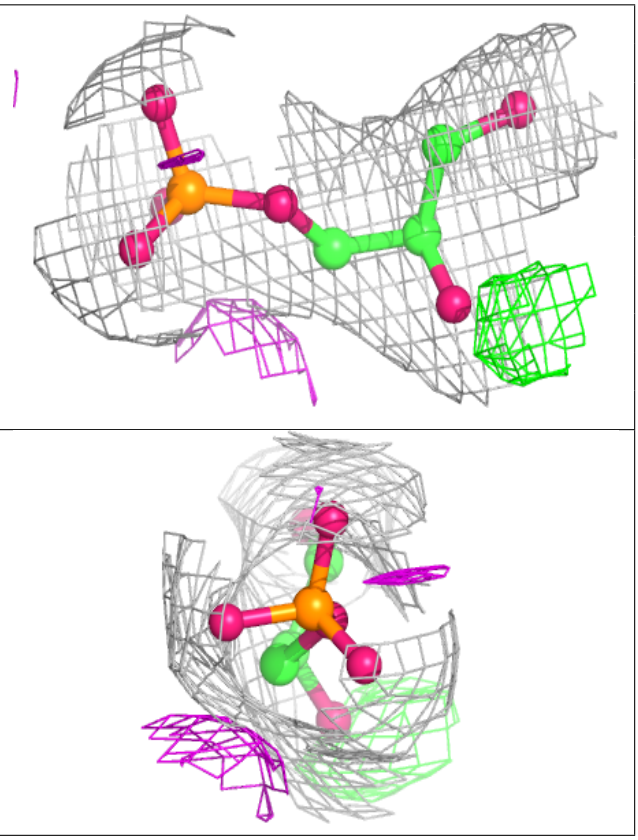
Electron density around PX4 B 1303:

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



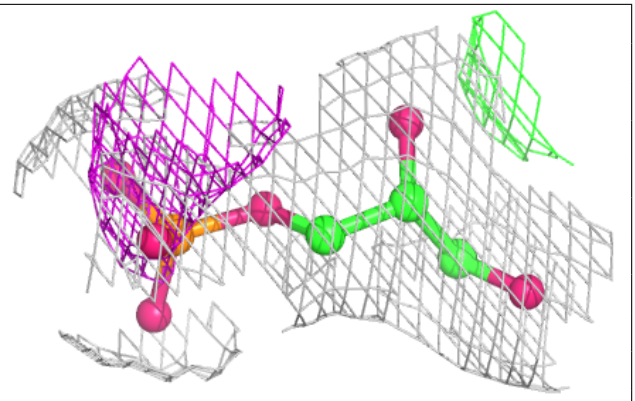
Electron density around PX4 C 1304:

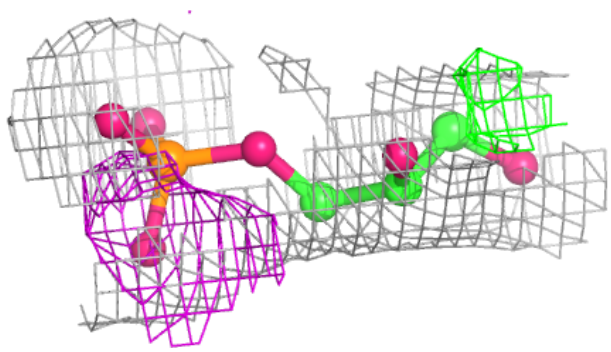
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

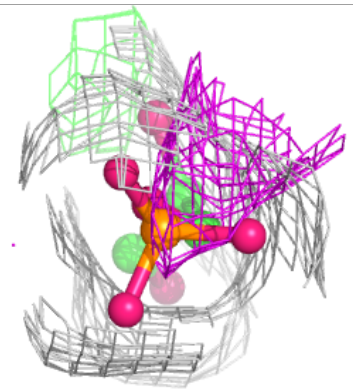


Electron density around PX4 D 1303:

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

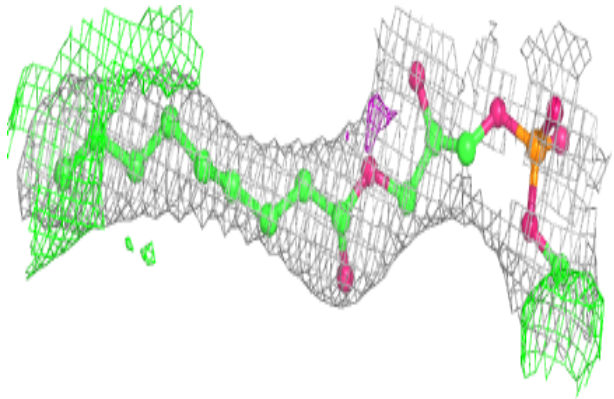


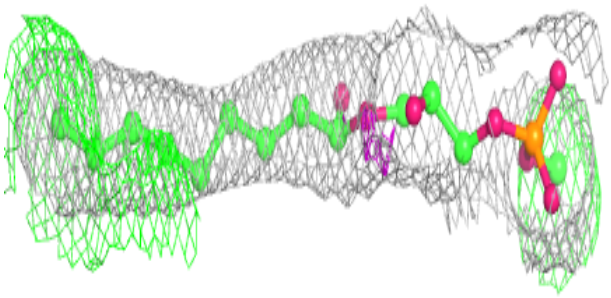


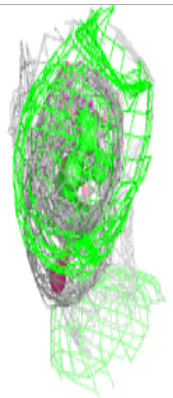


Electron density around PX4 D 1301:

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

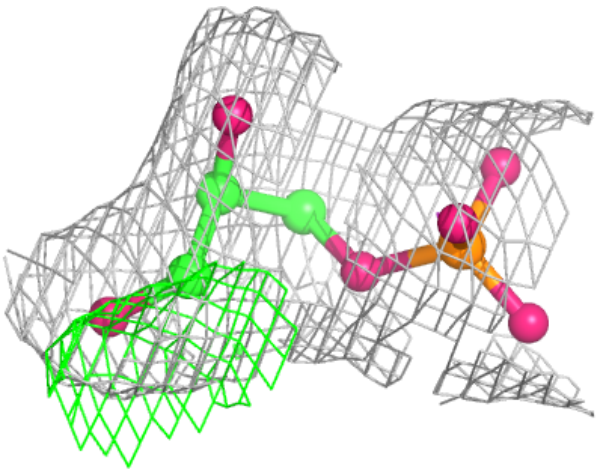


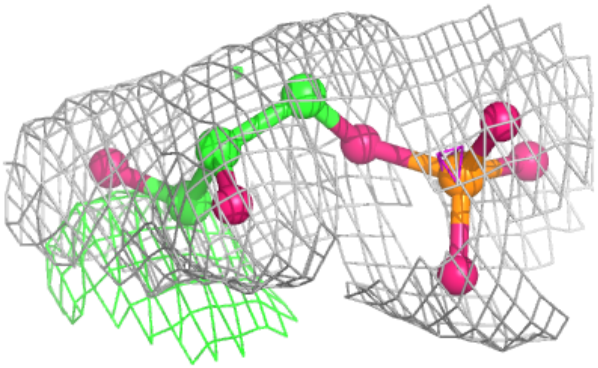


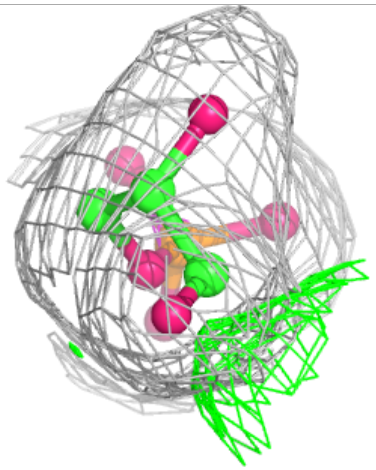


Electron density around PX4 B 1301:

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

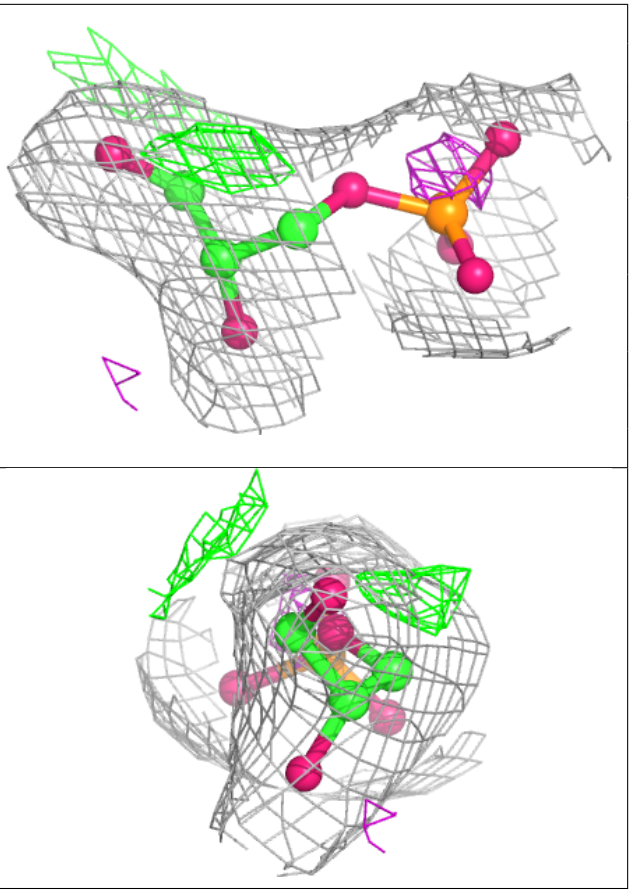


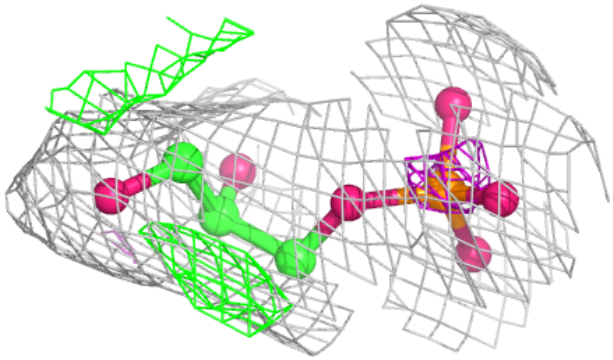




Electron density around PX4 A 1301:

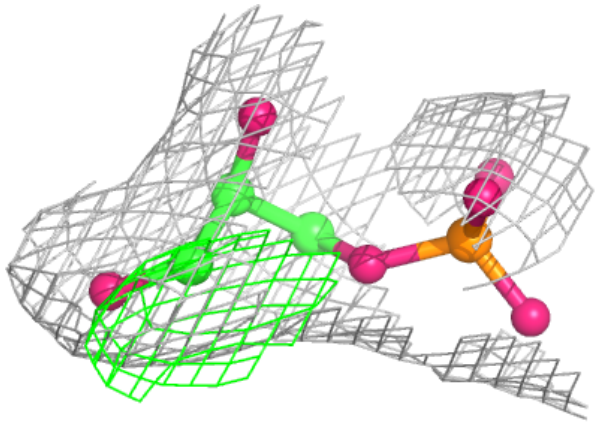
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

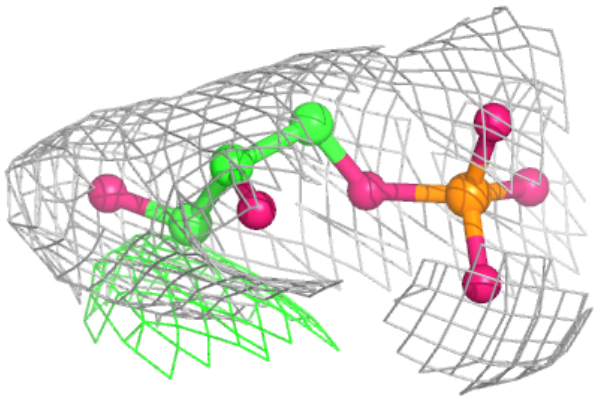


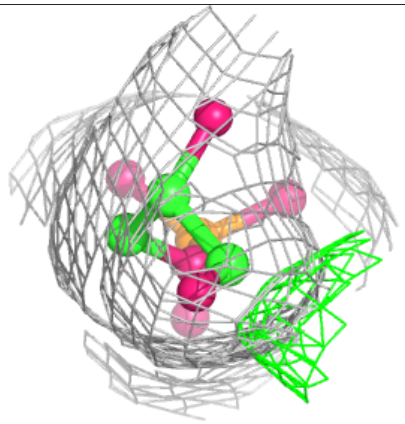


Electron density around PX4 C 1303:

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

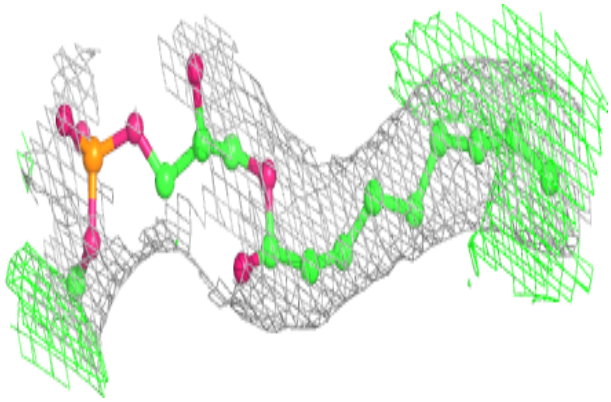


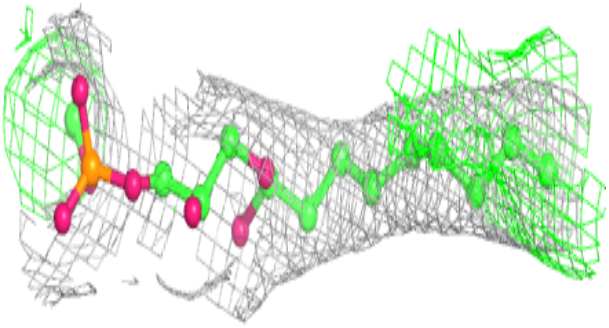


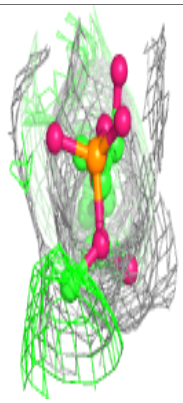


Electron density around PX4 C 1301:

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

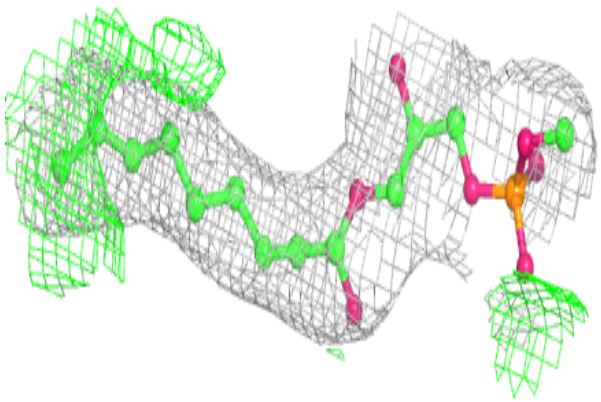


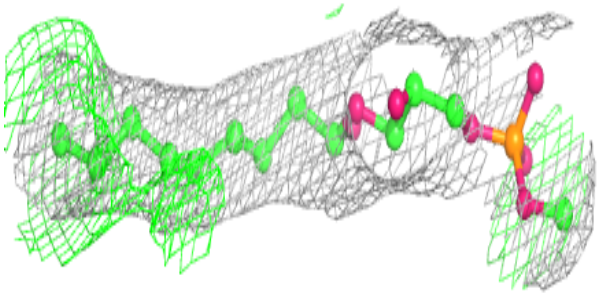


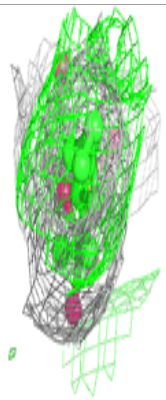


Electron density around PX4 A 1304:

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

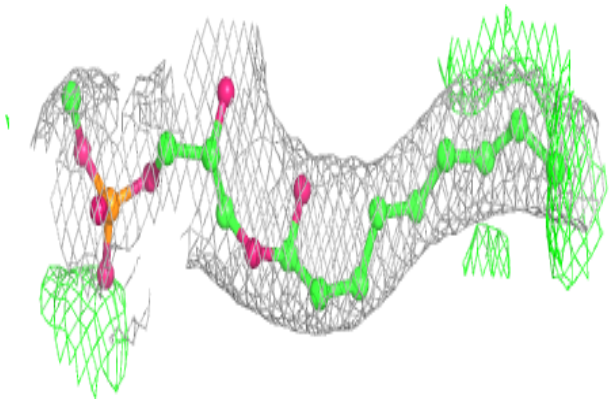


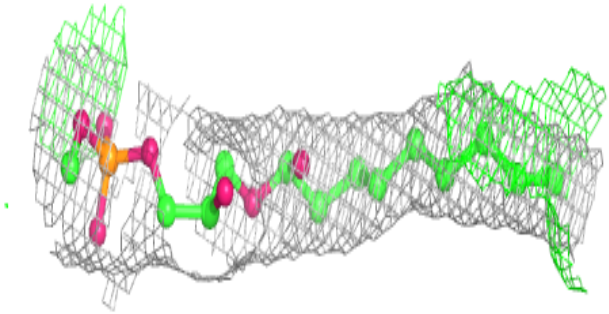


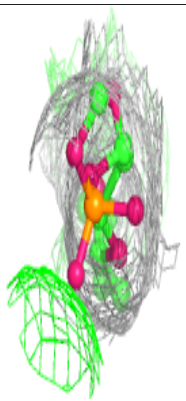


Electron density around PX4 A 1303:

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

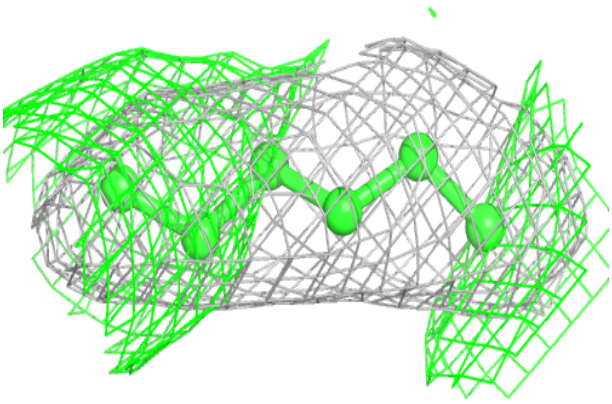


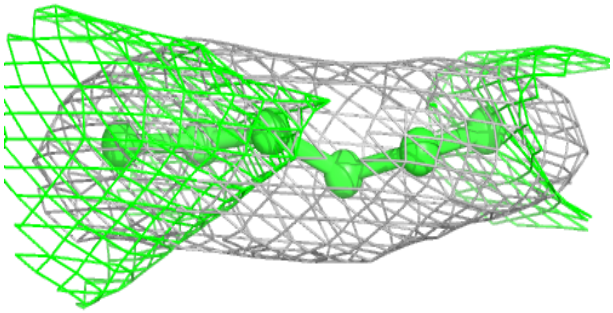


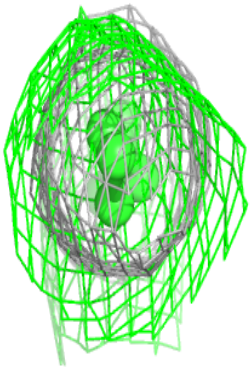


Electron density around PX4 A 1305:

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

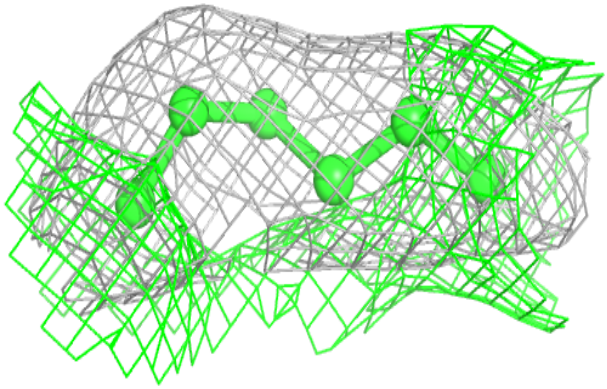


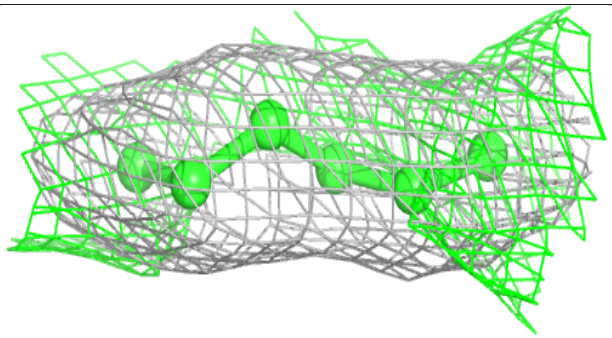


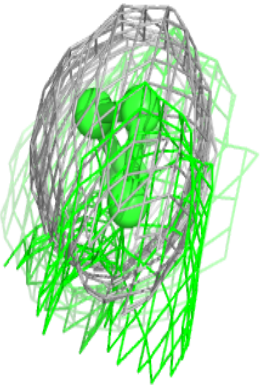


Electron density around PX4 C 1302:

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

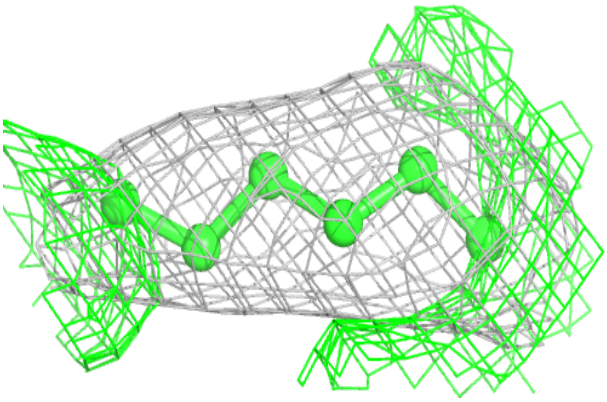


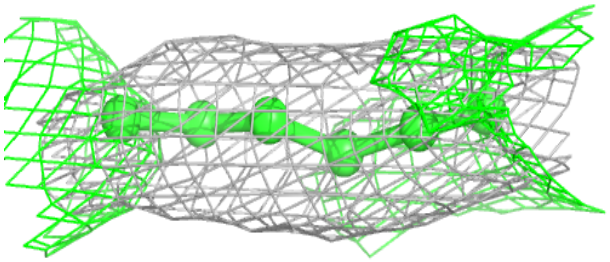


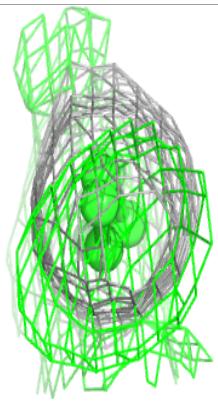


Electron density around PX4 B 1302:

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

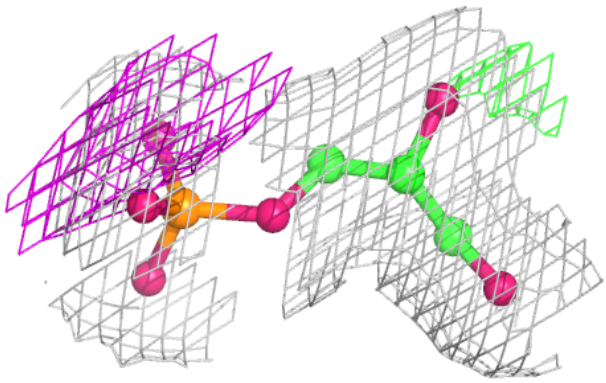


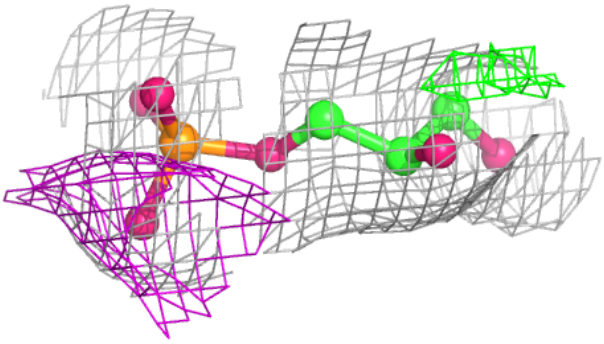


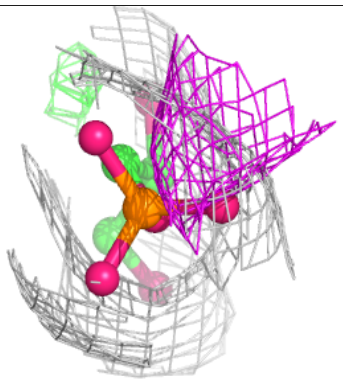


Electron density around PX4 A 1306:

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

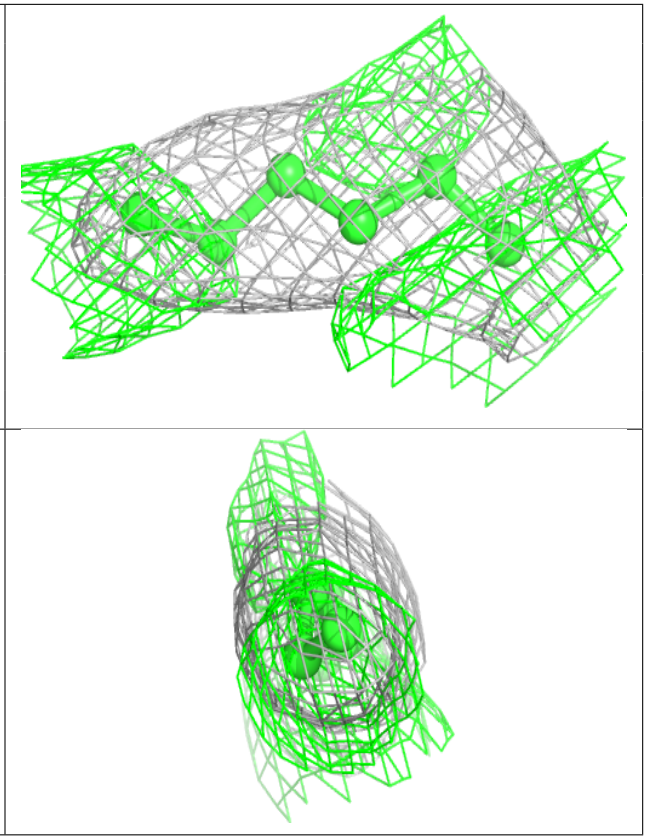






Electron density around PX4 D 1302:

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



6.5 Other polymers (i)

There are no such residues in this entry.