Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 07:31 PM EDT

PDB ID	:	6C1P
Title	:	HypoPP mutant
Authors	:	Catterall, W.A.; Zheng, N.; Jiang, D.; Gamal El-Din, T.M.
Deposited on	:	2018-01-05
Resolution	:	2.90 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:

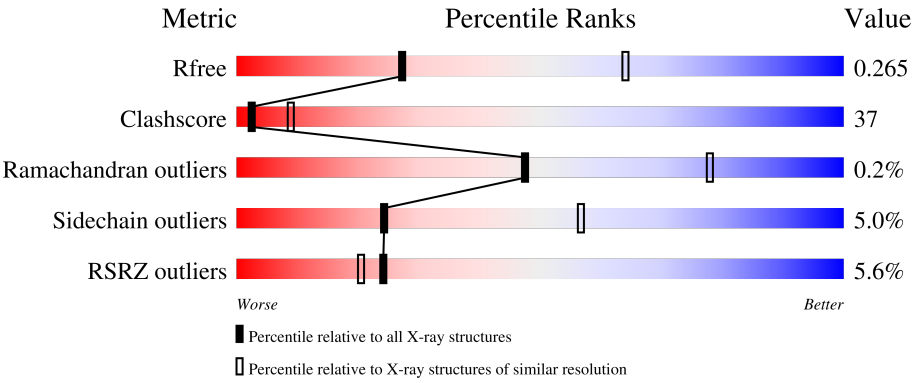
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	285	5% 35% 39% · 24%
1	B	285	4% 31% 42% · 24%
1	C	285	5% 33% 40% · 23%
1	D	285	4% 36% 39% · 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	D	1301	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7543 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	218	Total	C	N	O	S	0	0	0
			1785	1219	264	290	12			
1	B	217	Total	C	N	O	S	0	0	0
			1777	1213	263	289	12			
1	C	219	Total	C	N	O	S	0	0	0
			1790	1221	265	292	12			
1	D	218	Total	C	N	O	S	0	0	0
			1786	1219	264	291	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	initiating methionine	UNP A8EVM5
A	984	ASP	-	expression tag	UNP A8EVM5
A	985	TYR	-	expression tag	UNP A8EVM5
A	986	LYS	-	expression tag	UNP A8EVM5
A	987	ASP	-	expression tag	UNP A8EVM5
A	988	ASP	-	expression tag	UNP A8EVM5
A	989	ASP	-	expression tag	UNP A8EVM5
A	990	ASP	-	expression tag	UNP A8EVM5
A	991	LYS	-	expression tag	UNP A8EVM5
A	992	GLY	-	expression tag	UNP A8EVM5
A	993	SER	-	expression tag	UNP A8EVM5
A	994	LEU	-	expression tag	UNP A8EVM5
A	995	VAL	-	expression tag	UNP A8EVM5
A	996	PRO	-	expression tag	UNP A8EVM5
A	997	ARG	-	expression tag	UNP A8EVM5
A	998	GLY	-	expression tag	UNP A8EVM5
A	999	SER	-	expression tag	UNP A8EVM5
A	1000	HIS	-	expression tag	UNP A8EVM5
A	1102	GLY	ARG	engineered mutation	UNP A8EVM5
A	1217	CYS	ILE	engineered mutation	UNP A8EVM5
B	983	MET	-	initiating methionine	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1102	GLY	ARG	engineered mutation	UNP A8EVM5
B	1217	CYS	ILE	engineered mutation	UNP A8EVM5
C	983	MET	-	initiating methionine	UNP A8EVM5
C	984	ASP	-	expression tag	UNP A8EVM5
C	985	TYR	-	expression tag	UNP A8EVM5
C	986	LYS	-	expression tag	UNP A8EVM5
C	987	ASP	-	expression tag	UNP A8EVM5
C	988	ASP	-	expression tag	UNP A8EVM5
C	989	ASP	-	expression tag	UNP A8EVM5
C	990	ASP	-	expression tag	UNP A8EVM5
C	991	LYS	-	expression tag	UNP A8EVM5
C	992	GLY	-	expression tag	UNP A8EVM5
C	993	SER	-	expression tag	UNP A8EVM5
C	994	LEU	-	expression tag	UNP A8EVM5
C	995	VAL	-	expression tag	UNP A8EVM5
C	996	PRO	-	expression tag	UNP A8EVM5
C	997	ARG	-	expression tag	UNP A8EVM5
C	998	GLY	-	expression tag	UNP A8EVM5
C	999	SER	-	expression tag	UNP A8EVM5
C	1000	HIS	-	expression tag	UNP A8EVM5
C	1102	GLY	ARG	engineered mutation	UNP A8EVM5
C	1217	CYS	ILE	engineered mutation	UNP A8EVM5
D	983	MET	-	initiating methionine	UNP A8EVM5
D	984	ASP	-	expression tag	UNP A8EVM5
D	985	TYR	-	expression tag	UNP A8EVM5

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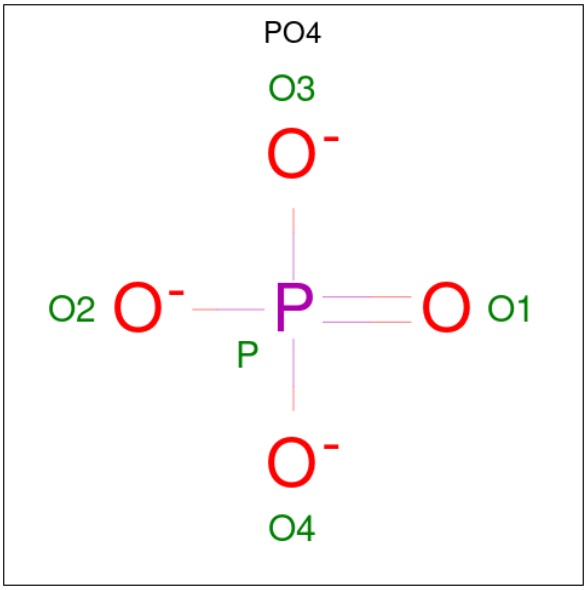
Chain	Residue	Modelled	Actual	Comment	Reference
D	986	LYS	-	expression tag	UNP A8EVM5
D	987	ASP	-	expression tag	UNP A8EVM5
D	988	ASP	-	expression tag	UNP A8EVM5
D	989	ASP	-	expression tag	UNP A8EVM5
D	990	ASP	-	expression tag	UNP A8EVM5
D	991	LYS	-	expression tag	UNP A8EVM5
D	992	GLY	-	expression tag	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	1102	GLY	ARG	engineered mutation	UNP A8EVM5
D	1217	CYS	ILE	engineered mutation	UNP A8EVM5

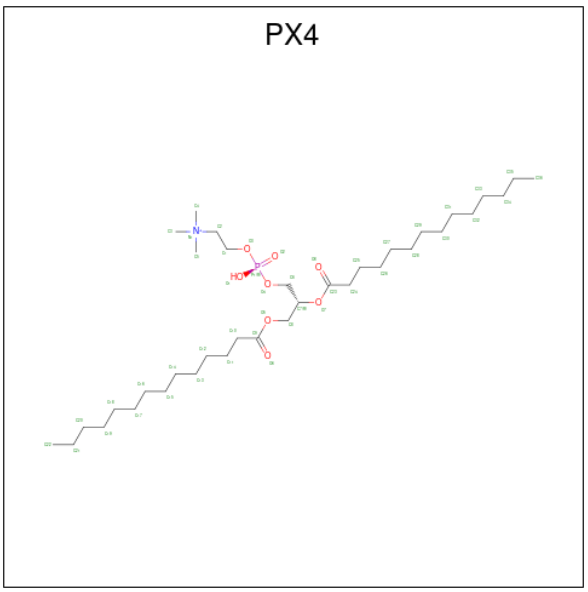
- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 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
3	A	1	Total C O P 21 12 8 1	0	0
3	A	1	Total C N O P 13 7 1 4 1	0	0
3	A	1	Total C N O P 36 26 1 8 1	0	0
3	B	1	Total C N O P 36 26 1 8 1	0	0
3	B	1	Total C N O P 23 14 1 7 1	0	0
3	B	1	Total C O P 19 10 8 1	0	0
3	B	1	Total C O P 15 7 7 1	0	0
3	B	1	Total C O P 29 20 8 1	0	0
3	B	1	Total C O P 22 15 6 1	0	0
3	C	1	Total C O P 8 3 4 1	0	0
3	C	1	Total C N O P 36 26 1 8 1	0	0
3	D	1	Total C N O P 36 26 1 8 1	0	0
3	D	1	Total C O P 30 21 8 1	0	0

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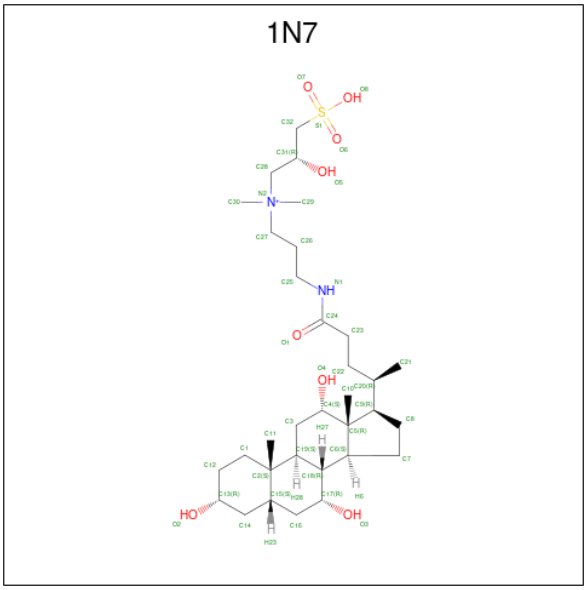
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C N O P 36 26 1 8 1	0	0
3	D	1	Total C O P 9 3 5 1	0	0

- Molecule 4 is CHAPSO (three-letter code: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



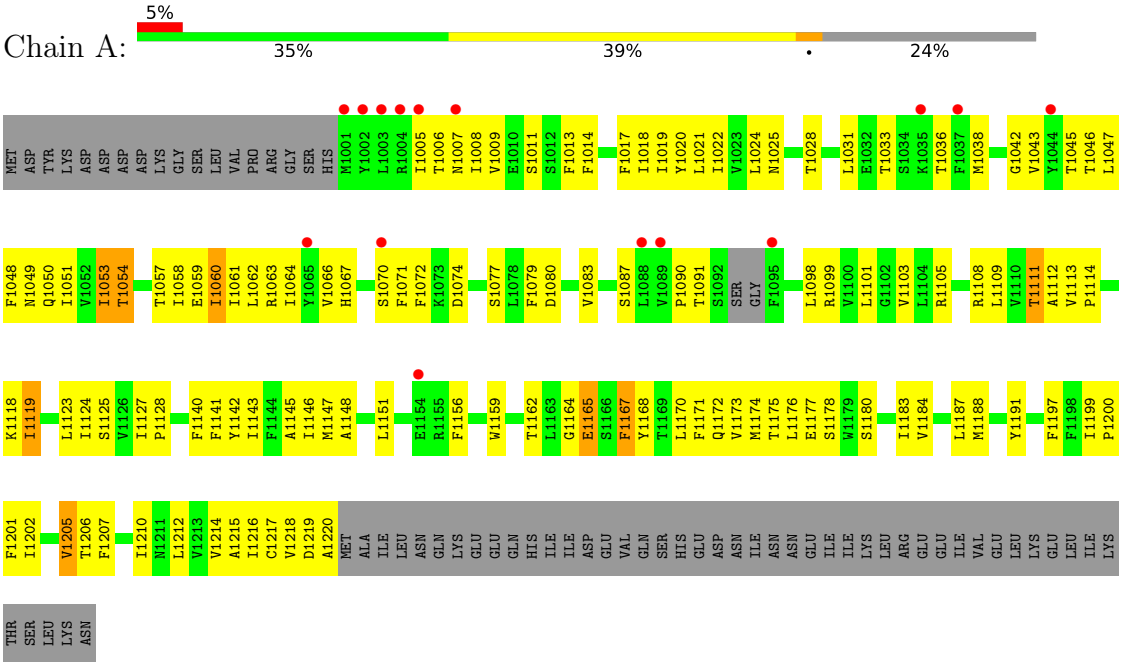
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 26 23 3	0	0

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.

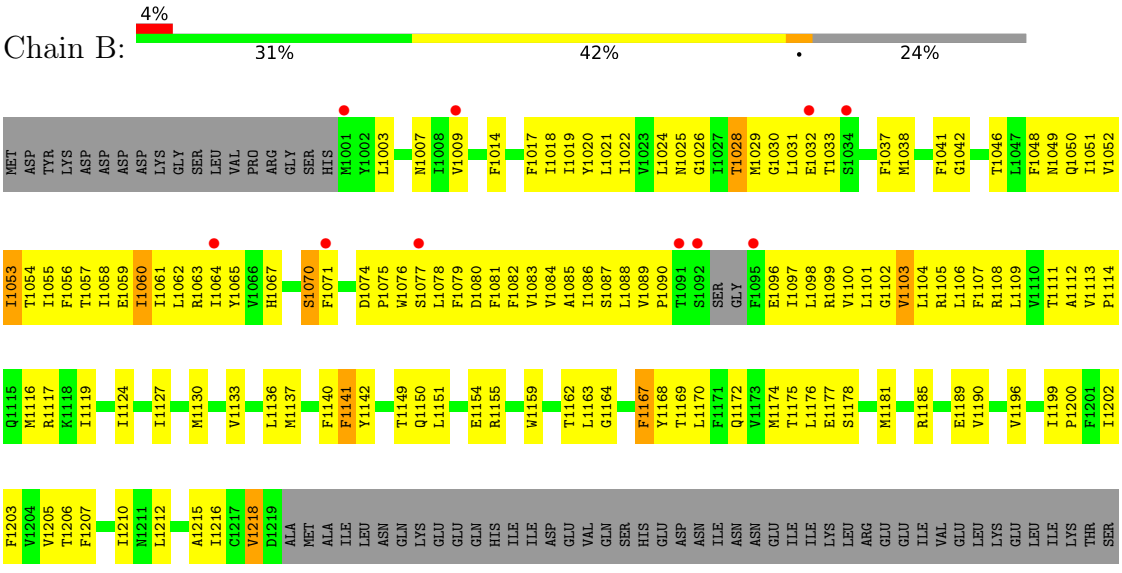
• Molecule 1: Ion transport protein

Chain A:



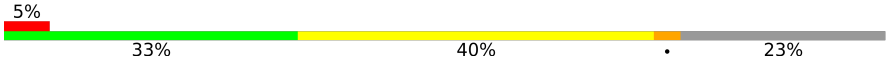
• Molecule 1: Ion transport protein

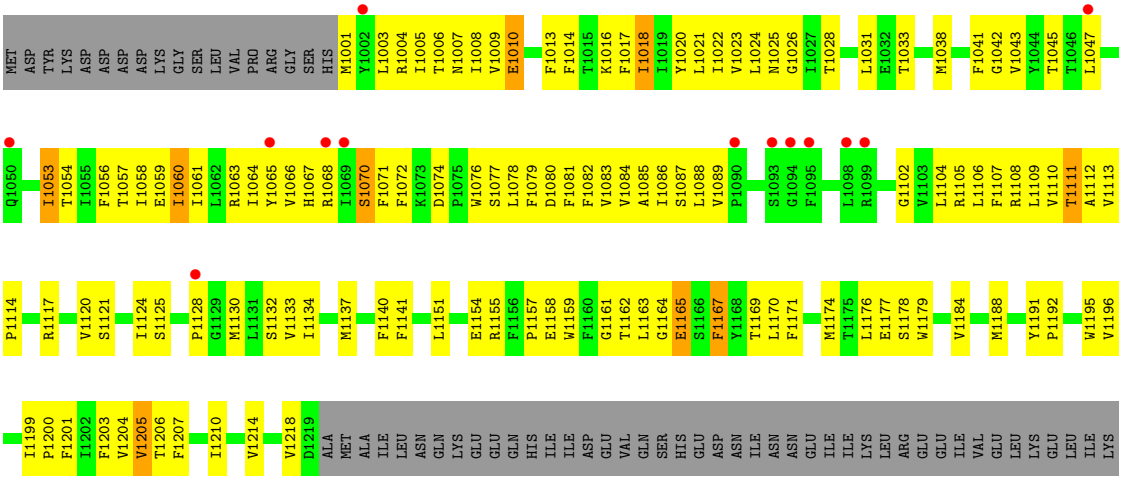
Chain B:



• Molecule 1: Ion transport protein

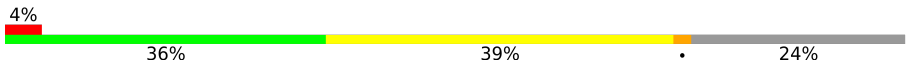
Chain C:

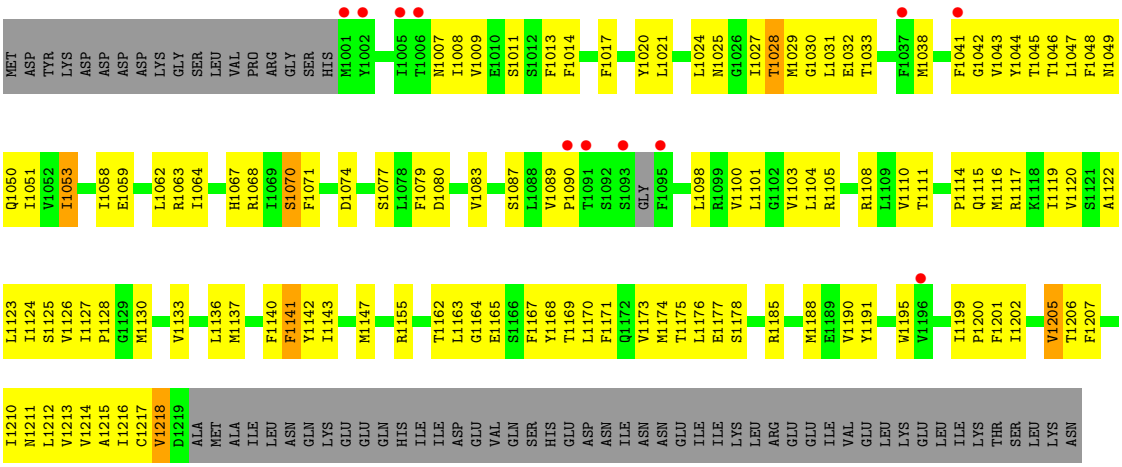




• Molecule 1: Ion transport protein

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	125.50Å 125.55Å 192.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.46 – 2.90 48.46 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.46-2.90) 97.6 (48.46-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.235 , 0.260 0.237 , 0.265	Depositor DCC
R_{free} test set	3725 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	78.9	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 91.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.449 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7543	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7481e-03.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1N7, PX4, PO4

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	0.60	0/1835	0.73	0/2496
1	B	0.64	0/1827	0.77	0/2485
1	C	0.56	0/1841	0.77	1/2505 (0.0%)
1	D	0.57	0/1836	0.83	3/2497 (0.1%)
All	All	0.59	0/7339	0.78	4/9983 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1114	PRO	N-CA-C	13.74	147.83	112.10
1	D	1115	GLN	N-CA-CB	-8.31	95.63	110.60
1	C	1114	PRO	N-CA-C	5.69	126.89	112.10
1	D	1114	PRO	CB-CA-C	-5.48	98.30	112.00

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	1785	0	1855	121	0
1	B	1777	0	1841	200	0
1	C	1790	0	1859	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1786	0	1855	101	0
2	A	5	0	0	0	0
2	D	5	0	0	0	0
3	A	70	0	79	16	0
3	B	144	0	147	8	0
3	C	44	0	51	7	0
3	D	111	0	134	16	0
4	C	26	0	35	5	0
All	All	7543	0	7856	574	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 37.

All (574) 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:1080:ASP:HA	1:B:1083:VAL:CG1	1.28	1.55
1:B:1080:ASP:CA	1:B:1083:VAL:CG1	2.07	1.31
1:B:1080:ASP:CA	1:B:1083:VAL:HG12	1.60	1.28
1:C:1079:PHE:CE2	1:C:1083:VAL:HG21	1.71	1.24
1:C:1079:PHE:CD2	1:C:1083:VAL:HG21	1.78	1.18
1:B:1083:VAL:CG2	1:B:1105:ARG:HA	1.81	1.09
1:B:1080:ASP:C	1:B:1083:VAL:HG12	1.73	1.07
1:C:1079:PHE:O	1:C:1083:VAL:HG23	1.57	1.01
1:A:1162:THR:HG22	1:A:1164:GLY:H	1.22	0.99
1:B:1080:ASP:HA	1:B:1083:VAL:HG11	0.98	0.97
1:B:1162:THR:HG22	1:B:1164:GLY:H	1.28	0.95
1:B:1080:ASP:O	1:B:1084:VAL:N	1.98	0.95
1:C:1083:VAL:HG11	1:C:1105:ARG:HA	1.46	0.95
1:C:1162:THR:HG22	1:C:1164:GLY:H	1.32	0.93
1:B:1081:PHE:O	1:B:1085:ALA:N	2.02	0.93
1:C:1003:LEU:O	1:C:1007:ASN:ND2	2.01	0.93
1:B:1026:GLY:HA2	1:B:1106:LEU:HD13	1.52	0.91
1:C:1082:PHE:O	1:C:1086:ILE:N	2.03	0.91
1:B:1083:VAL:HG22	1:B:1105:ARG:HA	1.50	0.91
1:B:1077:SER:O	1:B:1081:PHE:N	2.04	0.90
1:B:1080:ASP:O	1:B:1083:VAL:CG1	2.19	0.89
1:C:1026:GLY:HA2	1:C:1106:LEU:HD13	1.54	0.88
1:C:1060:ILE:HG13	1:C:1071:PHE:HZ	1.37	0.88
1:C:1083:VAL:O	1:C:1087:SER:OG	1.92	0.87
1:B:1059:GLU:OE2	1:B:1063:ARG:NH1	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:PHE:O	1:B:1086:ILE:N	2.08	0.87
1:A:1175:THR:HB	1:C:1176:LEU:HD13	1.57	0.85
1:D:1025:ASN:HA	1:D:1028:THR:HB	1.57	0.85
1:C:1083:VAL:CG1	1:C:1105:ARG:HA	2.08	0.84
1:B:1083:VAL:O	1:B:1087:SER:OG	1.94	0.83
1:B:1085:ALA:HA	1:B:1088:LEU:HB2	1.59	0.83
1:B:1083:VAL:HG11	1:B:1108:ARG:HG2	1.61	0.83
1:B:1021:LEU:HD22	1:B:1052:VAL:HG22	1.62	0.82
1:C:1134:ILE:HG12	3:C:1303:PX4:H70	1.62	0.82
1:B:1084:VAL:O	1:B:1088:LEU:N	2.12	0.81
1:C:1059:GLU:OE2	1:C:1063:ARG:NH1	2.13	0.81
1:C:1137:MET:HB3	3:C:1303:PX4:H62	1.62	0.81
1:C:1165:GLU:HG3	3:C:1303:PX4:H5	1.60	0.81
1:B:1083:VAL:HG21	1:B:1105:ARG:HA	1.61	0.81
1:D:1137:MET:HB3	3:D:1302:PX4:H62	1.62	0.79
1:B:1080:ASP:CA	1:B:1083:VAL:HG11	1.95	0.79
1:B:1029:MET:SD	1:B:1103:VAL:HA	2.22	0.78
1:B:1080:ASP:O	1:B:1083:VAL:HG13	1.82	0.78
1:B:1083:VAL:CG2	1:B:1105:ARG:CA	2.59	0.78
1:B:1057:THR:O	1:B:1061:ILE:N	2.17	0.77
1:B:1080:ASP:O	1:B:1083:VAL:HG12	1.81	0.77
1:B:1105:ARG:HA	1:B:1108:ARG:HG3	1.66	0.77
1:B:1162:THR:HG22	1:B:1164:GLY:N	2.00	0.76
1:C:1079:PHE:C	1:C:1083:VAL:HG23	2.05	0.75
1:D:1063:ARG:NH2	1:D:1080:ASP:OD2	2.18	0.75
1:B:1178:SER:HA	1:D:1177:GLU:OE2	1.87	0.75
1:C:1080:ASP:O	1:C:1084:VAL:N	2.16	0.74
1:A:1063:ARG:NH2	1:A:1080:ASP:OD2	2.20	0.74
1:A:1177:GLU:OE2	1:C:1178:SER:HA	1.87	0.74
1:C:1079:PHE:CZ	1:C:1083:VAL:HG21	2.21	0.73
1:B:1076:TRP:HB3	1:B:1111:THR:HG23	1.70	0.73
1:D:1098:LEU:HD23	1:D:1101:LEU:HD12	1.70	0.72
1:A:1013:PHE:O	1:A:1017:PHE:N	2.22	0.72
1:C:1083:VAL:CG1	1:C:1105:ARG:CA	2.67	0.72
1:B:1185:ARG:NH2	1:D:1169:THR:OG1	2.21	0.72
1:D:1074:ASP:HB3	1:D:1077:SER:HB2	1.71	0.72
1:B:1080:ASP:C	1:B:1083:VAL:CG1	2.42	0.72
1:D:1111:THR:O	1:D:1117:ARG:NE	2.18	0.71
1:C:1111:THR:O	1:C:1117:ARG:NE	2.23	0.71
1:B:1024:LEU:HB3	1:B:1048:PHE:HZ	1.55	0.71
1:C:1079:PHE:CD2	1:C:1083:VAL:CG2	2.65	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1060:ILE:HG13	1:C:1071:PHE:CZ	2.24	0.70
1:A:1074:ASP:HB3	1:A:1077:SER:HB2	1.73	0.70
3:A:1304:PX4:H50	1:C:1199:ILE:HG21	1.72	0.70
1:D:1162:THR:HG22	1:D:1164:GLY:H	1.56	0.70
1:C:1177:GLU:OE2	1:D:1178:SER:HA	1.92	0.70
1:C:1060:ILE:HD11	1:C:1080:ASP:HB3	1.73	0.70
1:C:1077:SER:O	1:C:1081:PHE:N	2.23	0.69
1:C:1081:PHE:O	1:C:1085:ALA:N	2.19	0.69
1:C:1080:ASP:OD2	1:C:1108:ARG:NH2	2.25	0.69
1:B:1097:ILE:O	1:B:1101:LEU:N	2.16	0.69
1:B:1098:LEU:O	1:B:1102:GLY:N	2.25	0.69
1:A:1021:LEU:HA	1:A:1024:LEU:HD22	1.74	0.69
1:B:1083:VAL:HG21	1:B:1108:ARG:HG3	1.74	0.69
1:B:1085:ALA:O	1:B:1089:VAL:N	2.24	0.68
1:B:1079:PHE:O	1:B:1083:VAL:HG12	1.94	0.68
1:B:1022:ILE:HG21	1:B:1109:LEU:HB2	1.74	0.68
1:A:1020:TYR:O	1:A:1024:LEU:HD13	1.93	0.68
1:C:1080:ASP:OD2	1:C:1111:THR:HG21	1.94	0.68
1:B:1003:LEU:O	1:B:1007:ASN:ND2	2.26	0.68
1:C:1060:ILE:HG12	1:C:1081:PHE:HA	1.75	0.68
1:C:1207:PHE:HA	1:C:1210:ILE:HD12	1.76	0.67
3:A:1304:PX4:H55	3:A:1304:PX4:H20	1.75	0.67
1:A:1017:PHE:O	1:A:1020:TYR:HB3	1.94	0.67
1:C:1071:PHE:CE1	1:C:1077:SER:HB3	2.29	0.67
1:A:1080:ASP:OD1	1:A:1111:THR:HG21	1.94	0.67
1:A:1067:HIS:HB3	1:A:1070:SER:HB3	1.77	0.67
1:A:1214:VAL:O	1:A:1218:VAL:HG23	1.95	0.67
1:B:1086:ILE:HG21	1:B:1101:LEU:HB2	1.77	0.66
1:A:1006:THR:HG23	1:A:1066:VAL:HG13	1.78	0.66
1:C:1085:ALA:HA	1:C:1088:LEU:HB2	1.77	0.66
1:B:1028:THR:O	1:B:1032:GLU:HG3	1.96	0.66
1:C:1064:ILE:O	1:C:1068:ARG:N	2.27	0.66
1:C:1191:TYR:HD1	4:C:1301:1N7:H16	1.59	0.66
1:C:1060:ILE:O	1:C:1064:ILE:HG13	1.96	0.66
1:B:1141:PHE:HB3	1:B:1167:PHE:CE1	2.30	0.66
1:C:1162:THR:HG22	1:C:1164:GLY:N	2.07	0.66
1:A:1207:PHE:HA	1:A:1210:ILE:HD12	1.78	0.65
1:D:1013:PHE:O	1:D:1017:PHE:N	2.27	0.65
1:B:1029:MET:HB2	1:B:1106:LEU:HD11	1.77	0.65
1:B:1060:ILE:HG12	1:B:1081:PHE:HA	1.78	0.65
1:B:1176:LEU:HD13	1:D:1175:THR:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1079:PHE:CE2	1:C:1083:VAL:CG2	2.66	0.65
1:B:1083:VAL:HG22	1:B:1105:ARG:CA	2.22	0.65
1:B:1172:GLN:O	1:B:1175:THR:OG1	2.12	0.65
1:C:1059:GLU:HG2	1:C:1063:ARG:HG3	1.79	0.65
1:B:1124:ILE:HG23	1:B:1127:ILE:HD12	1.78	0.65
1:D:1048:PHE:HA	1:D:1051:ILE:HD12	1.80	0.64
1:A:1184:VAL:HG12	1:A:1188:MET:HE2	1.80	0.64
1:C:1102:GLY:HA3	1:C:1105:ARG:HH21	1.62	0.64
1:B:1054:THR:O	1:B:1058:ILE:N	2.22	0.64
1:D:1064:ILE:O	1:D:1068:ARG:N	2.29	0.63
1:B:1053:ILE:HD11	1:B:1087:SER:HB2	1.79	0.63
1:D:1202:ILE:O	1:D:1206:THR:OG1	2.15	0.63
1:B:1056:PHE:HB3	1:B:1084:VAL:HG22	1.80	0.63
1:D:1079:PHE:CZ	1:D:1083:VAL:HG21	2.33	0.63
1:A:1143:ILE:HG23	1:B:1103:VAL:HG13	1.81	0.63
1:B:1056:PHE:O	1:B:1060:ILE:HB	1.97	0.63
1:B:1100:VAL:O	1:B:1103:VAL:N	2.27	0.62
1:A:1108:ARG:O	1:A:1112:ALA:N	2.27	0.62
1:C:1056:PHE:HB3	1:C:1084:VAL:HG22	1.82	0.62
1:D:1014:PHE:CE2	1:D:1059:GLU:HG3	2.34	0.62
1:D:1021:LEU:HD23	1:D:1024:LEU:HD22	1.82	0.62
1:C:1017:PHE:O	1:C:1020:TYR:HB3	1.99	0.62
1:D:1214:VAL:O	1:D:1218:VAL:N	2.33	0.62
1:A:1191:TYR:HD1	3:A:1303:PX4:H3	1.64	0.62
1:D:1067:HIS:HB2	1:D:1071:PHE:HB2	1.82	0.61
1:C:1057:THR:O	1:C:1061:ILE:N	2.34	0.61
1:C:1084:VAL:O	1:C:1088:LEU:N	2.33	0.61
1:B:1026:GLY:HA2	1:B:1106:LEU:CD1	2.27	0.61
1:B:1059:GLU:CD	1:B:1108:ARG:HH22	2.03	0.61
1:B:1142:TYR:OH	1:D:1030:GLY:HA3	2.01	0.61
1:C:1079:PHE:CG	1:C:1083:VAL:HG21	2.35	0.61
1:C:1104:LEU:O	1:C:1107:PHE:HB2	2.01	0.61
1:A:1014:PHE:CZ	1:A:1059:GLU:HG3	2.36	0.60
1:C:1060:ILE:HD11	1:C:1080:ASP:CB	2.31	0.60
1:D:1053:ILE:HD11	1:D:1087:SER:HB2	1.83	0.60
1:B:1021:LEU:HD13	1:B:1052:VAL:HA	1.82	0.60
1:B:1164:GLY:HA2	3:B:2001:PX4:H16	1.84	0.60
1:C:1200:PRO:O	1:C:1204:VAL:N	2.30	0.60
1:B:1104:LEU:O	1:B:1107:PHE:N	2.27	0.60
1:B:1149:THR:HG21	1:D:1033:THR:HG23	1.83	0.60
1:A:1048:PHE:HA	1:A:1051:ILE:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1207:PHE:HA	1:D:1210:ILE:HD12	1.84	0.59
3:D:1302:PX4:H56	3:D:1302:PX4:H22	1.83	0.59
1:A:1143:ILE:O	1:A:1147:MET:HG3	2.02	0.59
1:B:1057:THR:HG23	1:B:1088:LEU:HD11	1.83	0.59
1:A:1143:ILE:HG21	1:B:1107:PHE:CE2	2.38	0.59
1:C:1105:ARG:HA	1:C:1108:ARG:HG3	1.85	0.59
1:A:1140:PHE:CE2	1:A:1205:VAL:HG23	2.38	0.58
1:B:1167:PHE:HB3	3:B:2001:PX4:H47	1.85	0.58
1:A:1214:VAL:HG13	1:A:1218:VAL:CG2	2.32	0.58
1:B:1024:LEU:O	1:B:1028:THR:N	2.28	0.58
1:A:1022:ILE:HG21	1:A:1109:LEU:HB2	1.84	0.58
1:A:1214:VAL:CG1	1:A:1218:VAL:CG2	2.81	0.58
1:A:1060:ILE:HD11	1:A:1080:ASP:HB3	1.85	0.58
1:C:1014:PHE:CZ	1:C:1059:GLU:HG3	2.39	0.58
1:A:1168:TYR:HA	3:A:1304:PX4:H48	1.83	0.58
1:B:1101:LEU:HA	1:B:1104:LEU:HG	1.86	0.57
1:C:1056:PHE:O	1:C:1060:ILE:HB	2.03	0.57
1:D:1014:PHE:HE2	1:D:1059:GLU:HG3	1.69	0.57
1:D:1041:PHE:HB3	1:D:1044:TYR:HB2	1.86	0.57
1:D:1191:TYR:HE1	3:D:1304:PX4:H4	1.69	0.57
1:A:1167:PHE:HB3	3:A:1304:PX4:O8	2.04	0.57
1:D:1213:VAL:O	1:D:1217:CYS:N	2.32	0.57
1:B:1108:ARG:O	1:B:1112:ALA:N	2.32	0.57
1:C:1013:PHE:O	1:C:1017:PHE:N	2.37	0.57
1:D:1032:GLU:OE2	1:D:1049:ASN:ND2	2.37	0.57
1:C:1025:ASN:HA	1:C:1028:THR:HG22	1.87	0.57
1:C:1083:VAL:HG12	1:C:1105:ARG:CB	2.34	0.57
1:A:1007:ASN:O	1:A:1011:SER:HB3	2.05	0.57
1:C:1018:ILE:HG13	1:C:1059:GLU:CD	2.25	0.57
1:A:1217:CYS:HB2	1:C:1214:VAL:HG22	1.87	0.57
1:C:1054:THR:O	1:C:1058:ILE:HG12	2.05	0.57
1:A:1171:PHE:CD1	3:A:1304:PX4:H53	2.40	0.57
1:C:1079:PHE:O	1:C:1083:VAL:N	2.33	0.57
1:A:1064:ILE:HG12	1:A:1072:PHE:HE1	1.69	0.56
1:B:1202:ILE:O	1:B:1206:THR:OG1	2.07	0.56
1:A:1119:ILE:HD11	1:C:1133:VAL:HG22	1.88	0.56
1:B:1137:MET:HB3	3:B:2001:PX4:H68	1.88	0.56
1:B:1087:SER:OG	1:B:1102:GLY:HA2	2.05	0.56
1:C:1057:THR:O	1:C:1060:ILE:HG22	2.06	0.56
1:A:1214:VAL:CG1	1:A:1218:VAL:HG21	2.35	0.56
1:B:1021:LEU:HD11	1:B:1055:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1061:ILE:O	1:C:1064:ILE:HB	2.05	0.56
1:C:1191:TYR:CD1	4:C:1301:1N7:H16	2.40	0.56
1:A:1180:SER:HB3	1:B:1177:GLU:OE1	2.05	0.56
1:C:1067:HIS:HB3	1:C:1070:SER:HB3	1.88	0.56
1:A:1063:ARG:HE	1:A:1071:PHE:HE2	1.54	0.55
1:A:1214:VAL:HG13	1:A:1218:VAL:HG23	1.88	0.55
1:D:1108:ARG:O	1:D:1111:THR:HG22	2.05	0.55
1:D:1133:VAL:HG11	1:D:1212:LEU:HD12	1.88	0.55
1:A:1049:ASN:O	1:A:1053:ILE:HB	2.06	0.55
1:A:1214:VAL:O	1:A:1218:VAL:N	2.34	0.55
1:C:1005:ILE:HA	1:C:1008:ILE:HD12	1.88	0.55
1:C:1022:ILE:HD13	1:C:1108:ARG:C	2.27	0.55
1:A:1079:PHE:CZ	1:A:1083:VAL:HG21	2.41	0.55
1:A:1162:THR:HG22	1:A:1164:GLY:N	2.05	0.55
1:B:1174:MET:HG3	1:B:1205:VAL:HG11	1.88	0.55
1:C:1021:LEU:HD23	1:C:1024:LEU:HD22	1.89	0.55
1:D:1136:LEU:O	1:D:1140:PHE:N	2.27	0.55
1:C:1014:PHE:HZ	1:C:1059:GLU:HG3	1.72	0.55
1:D:1053:ILE:HD11	1:D:1087:SER:CB	2.36	0.55
1:B:1142:TYR:CE1	3:B:2006:PX4:H54	2.42	0.55
1:A:1019:ILE:HD13	1:A:1113:VAL:HG22	1.87	0.54
1:C:1206:THR:O	1:C:1210:ILE:HG13	2.07	0.54
1:D:1120:VAL:O	1:D:1124:ILE:HG13	2.07	0.54
1:B:1067:HIS:HB3	1:B:1070:SER:HB3	1.89	0.54
1:B:1087:SER:HB3	1:B:1105:ARG:NE	2.22	0.54
1:D:1067:HIS:HB3	1:D:1070:SER:HB3	1.87	0.54
1:A:1077:SER:O	1:A:1080:ASP:HB2	2.08	0.54
1:C:1176:LEU:HA	1:C:1179:TRP:CD1	2.42	0.54
1:B:1085:ALA:O	1:B:1089:VAL:HG23	2.07	0.54
1:C:1140:PHE:CE2	1:C:1205:VAL:HG23	2.43	0.54
1:D:1173:VAL:O	1:D:1176:LEU:HD23	2.07	0.54
1:D:1043:VAL:O	1:D:1047:LEU:HG	2.08	0.54
1:A:1173:VAL:O	1:A:1176:LEU:HD23	2.08	0.54
1:A:1125:SER:O	1:A:1128:PRO:HD2	2.08	0.54
1:B:1022:ILE:HD13	1:B:1108:ARG:C	2.28	0.54
1:B:1080:ASP:HB3	1:B:1108:ARG:HE	1.72	0.54
1:B:1056:PHE:CD2	1:B:1108:ARG:HD3	2.43	0.54
1:B:1113:VAL:HG12	1:B:1114:PRO:O	2.08	0.54
1:D:1029:MET:SD	1:D:1103:VAL:HA	2.48	0.54
1:B:1053:ILE:HG13	1:B:1087:SER:O	2.08	0.53
1:C:1079:PHE:O	1:C:1083:VAL:CG2	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1083:VAL:HG13	1:B:1084:VAL:N	2.23	0.53
1:C:1140:PHE:HE2	1:C:1205:VAL:HG23	1.73	0.53
1:D:1108:ARG:NH1	1:D:1108:ARG:HB3	2.24	0.53
1:C:1079:PHE:HZ	1:C:1107:PHE:HB2	1.73	0.53
1:A:1043:VAL:O	1:A:1047:LEU:HG	2.08	0.53
1:B:1056:PHE:HB3	1:B:1084:VAL:CG2	2.37	0.53
1:D:1025:ASN:O	1:D:1029:MET:N	2.39	0.53
1:B:1022:ILE:O	1:B:1026:GLY:N	2.40	0.53
1:C:1056:PHE:HB3	1:C:1084:VAL:CG2	2.37	0.53
1:A:1050:GLN:O	1:A:1054:THR:OG1	2.25	0.53
1:B:1037:PHE:CE1	1:B:1041:PHE:HB2	2.44	0.53
1:C:1080:ASP:CG	1:C:1111:THR:HG21	2.28	0.53
1:D:1080:ASP:OD1	1:D:1111:THR:HG21	2.08	0.53
1:A:1087:SER:HB3	1:A:1105:ARG:HH21	1.74	0.53
1:A:1148:ALA:HB2	1:A:1197:PHE:CZ	2.44	0.52
1:B:1022:ILE:CG2	1:B:1109:LEU:HB2	2.39	0.52
1:B:1154:GLU:HB3	1:B:1155:ARG:HG2	1.91	0.52
1:D:1007:ASN:O	1:D:1011:SER:HB3	2.09	0.52
1:A:1202:ILE:O	1:A:1206:THR:OG1	2.18	0.52
1:C:1053:ILE:HD11	1:C:1087:SER:HB2	1.92	0.52
1:D:1028:THR:HG23	1:D:1045:THR:HG23	1.91	0.52
1:A:1098:LEU:HD23	1:A:1101:LEU:HD12	1.91	0.52
1:B:1079:PHE:C	1:B:1083:VAL:HG12	2.29	0.52
1:B:1083:VAL:CG2	1:B:1108:ARG:HG3	2.39	0.52
1:B:1167:PHE:CZ	3:B:2001:PX4:H21	2.45	0.52
1:B:1014:PHE:CE2	1:B:1059:GLU:HG3	2.44	0.52
1:B:1133:VAL:O	1:B:1136:LEU:HB3	2.09	0.52
1:C:1063:ARG:O	1:C:1067:HIS:ND1	2.40	0.52
1:C:1079:PHE:CZ	1:C:1083:VAL:CG2	2.93	0.52
1:B:1181:MET:HG3	1:D:1178:SER:HB2	1.91	0.51
1:A:1142:TYR:CZ	1:A:1146:ILE:HD11	2.45	0.51
1:D:1130:MET:SD	1:D:1216:ILE:HD11	2.50	0.51
1:A:1021:LEU:HD23	1:A:1024:LEU:HD22	1.91	0.51
1:B:1019:ILE:HA	1:B:1022:ILE:HD12	1.92	0.51
1:B:1086:ILE:HG21	1:B:1101:LEU:CB	2.40	0.51
1:C:1083:VAL:HG11	1:C:1105:ARG:CA	2.27	0.51
1:D:1188:MET:SD	1:D:1195:TRP:HB3	2.51	0.51
1:B:1203:PHE:HZ	3:D:1302:PX4:H58	1.74	0.51
1:C:1125:SER:O	1:C:1128:PRO:HD2	2.11	0.51
1:D:1029:MET:HG2	1:D:1032:GLU:OE1	2.11	0.51
1:A:1214:VAL:HG12	1:A:1218:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1079:PHE:O	1:B:1083:VAL:N	2.35	0.51
1:A:1080:ASP:OD2	1:A:1108:ARG:NH2	2.44	0.51
1:B:1101:LEU:HD22	1:B:1104:LEU:HD11	1.92	0.51
1:B:1185:ARG:O	1:B:1189:GLU:HG2	2.11	0.51
1:C:1004:ARG:O	1:C:1008:ILE:HG13	2.11	0.51
1:C:1026:GLY:HA2	1:C:1106:LEU:CD1	2.36	0.51
1:C:1108:ARG:HA	1:C:1111:THR:HB	1.93	0.51
1:B:1080:ASP:N	1:B:1083:VAL:HG12	2.20	0.50
1:D:1164:GLY:HA3	3:D:1302:PX4:O2	2.11	0.50
1:D:1201:PHE:O	1:D:1205:VAL:HB	2.11	0.50
1:A:1053:ILE:HD11	1:A:1087:SER:HB2	1.92	0.50
1:A:1147:MET:CG	1:B:1103:VAL:HG11	2.41	0.50
1:C:1158:GLU:O	1:C:1165:GLU:HG2	2.11	0.50
1:A:1167:PHE:CD1	3:A:1304:PX4:H56	2.46	0.50
1:A:1171:PHE:HE1	1:C:1203:PHE:CE1	2.29	0.50
1:C:1137:MET:HE2	3:C:1303:PX4:H66	1.93	0.50
1:D:1028:THR:O	1:D:1032:GLU:HG3	2.10	0.50
1:D:1122:ALA:O	1:D:1126:VAL:HG23	2.12	0.50
1:A:1009:VAL:HG13	1:A:1063:ARG:HG2	1.94	0.50
1:B:1059:GLU:OE1	1:B:1108:ARG:NH2	2.44	0.50
1:C:1053:ILE:HD11	1:C:1084:VAL:O	2.12	0.50
1:A:1119:ILE:HG13	1:C:1132:SER:HB3	1.94	0.50
1:B:1031:LEU:C	1:B:1033:THR:H	2.15	0.50
1:B:1071:PHE:CE2	1:B:1077:SER:HB3	2.46	0.50
3:D:1302:PX4:H17	3:D:1302:PX4:H47	1.94	0.50
1:B:1055:ILE:O	1:B:1059:GLU:N	2.26	0.50
1:C:1137:MET:HG3	3:C:1303:PX4:H71	1.93	0.50
1:C:1141:PHE:HB3	1:C:1167:PHE:CE1	2.46	0.50
1:D:1199:ILE:HB	1:D:1200:PRO:HD3	1.94	0.50
1:A:1168:TYR:HB2	3:A:1304:PX4:H46	1.93	0.50
1:B:1076:TRP:O	1:B:1079:PHE:HB3	2.12	0.50
1:A:1031:LEU:C	1:A:1033:THR:H	2.14	0.49
1:B:1021:LEU:HB3	1:B:1052:VAL:HG13	1.93	0.49
1:D:1211:ASN:O	1:D:1215:ALA:N	2.26	0.49
1:B:1060:ILE:HD13	1:B:1084:VAL:HG21	1.94	0.49
1:C:1079:PHE:CZ	1:C:1107:PHE:HB2	2.48	0.49
1:B:1080:ASP:OD1	1:B:1108:ARG:HG2	2.12	0.49
1:C:1174:MET:HE3	1:C:1205:VAL:HG13	1.93	0.49
1:B:1141:PHE:HB3	1:B:1167:PHE:HE1	1.77	0.49
1:A:1091:THR:OG1	1:A:1099:ARG:NH2	2.46	0.49
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1022:ILE:HG21	1:C:1109:LEU:N	2.27	0.49
1:C:1061:ILE:HA	1:C:1064:ILE:HD12	1.95	0.49
1:C:1083:VAL:HG12	1:C:1105:ARG:CA	2.40	0.49
1:D:1074:ASP:HB3	1:D:1077:SER:CB	2.42	0.49
1:B:1052:VAL:O	1:B:1056:PHE:N	2.40	0.49
1:B:1212:LEU:O	1:B:1215:ALA:HB3	2.13	0.49
1:D:1041:PHE:O	1:D:1044:TYR:HB2	2.13	0.49
1:B:1049:ASN:O	1:B:1053:ILE:HB	2.12	0.49
1:B:1054:THR:O	1:B:1058:ILE:HG12	2.13	0.49
1:C:1102:GLY:HA3	1:C:1105:ARG:NH2	2.28	0.49
1:D:1188:MET:HA	1:D:1191:TYR:O	2.12	0.49
1:A:1216:ILE:HG22	1:C:1214:VAL:HG11	1.94	0.49
1:C:1023:VAL:HG22	3:D:1303:PX4:H70	1.93	0.49
1:D:1038:MET:O	1:D:1042:GLY:HA3	2.13	0.49
1:A:1212:LEU:O	1:A:1215:ALA:HB3	2.13	0.48
1:C:1006:THR:HG23	1:C:1066:VAL:HG13	1.94	0.48
1:A:1184:VAL:O	1:A:1188:MET:HG3	2.13	0.48
1:B:1104:LEU:O	1:B:1107:PHE:HB2	2.14	0.48
1:C:1063:ARG:HH21	1:C:1077:SER:HA	1.79	0.48
1:C:1107:PHE:CE2	1:D:1143:ILE:HG21	2.49	0.48
1:D:1125:SER:O	1:D:1128:PRO:HD2	2.13	0.48
1:A:1214:VAL:CG1	1:A:1218:VAL:HG23	2.44	0.48
1:B:1022:ILE:HD13	1:B:1109:LEU:N	2.28	0.48
1:B:1087:SER:HB3	1:B:1105:ARG:NH2	2.29	0.48
1:B:1196:VAL:O	1:B:1200:PRO:HG2	2.14	0.48
1:A:1064:ILE:HG12	1:A:1072:PHE:CE1	2.49	0.48
1:D:1185:ARG:HA	1:D:1188:MET:HE2	1.96	0.48
1:B:1085:ALA:CA	1:B:1088:LEU:HB2	2.37	0.48
1:C:1071:PHE:CZ	1:C:1077:SER:HB3	2.48	0.48
1:A:1113:VAL:HG12	1:A:1114:PRO:O	2.14	0.48
1:B:1216:ILE:C	1:B:1218:VAL:H	2.17	0.48
1:C:1082:PHE:HA	1:C:1085:ALA:HB3	1.96	0.48
1:A:1008:ILE:O	1:A:1014:PHE:HB2	2.14	0.48
1:B:1155:ARG:HG3	1:B:1190:VAL:HG11	1.95	0.48
1:A:1020:TYR:CE1	1:A:1024:LEU:HD11	2.49	0.47
1:A:1119:ILE:O	1:A:1123:LEU:HG	2.14	0.47
1:B:1086:ILE:CG2	1:B:1101:LEU:HB2	2.44	0.47
1:C:1043:VAL:O	1:C:1047:LEU:HG	2.13	0.47
1:C:1105:ARG:O	1:C:1108:ARG:HB2	2.14	0.47
1:D:1191:TYR:HD1	3:D:1304:PX4:H14	1.79	0.47
1:B:1018:ILE:O	1:B:1022:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1059:GLU:OE1	1:C:1108:ARG:NH2	2.47	0.47
1:D:1058:ILE:O	1:D:1062:LEU:HG	2.13	0.47
1:B:1083:VAL:O	1:B:1087:SER:CB	2.62	0.47
1:A:1141:PHE:O	1:A:1145:ALA:N	2.31	0.47
1:D:1119:ILE:O	1:D:1123:LEU:HG	2.15	0.47
1:A:1053:ILE:HD11	1:A:1087:SER:CB	2.45	0.47
1:B:1079:PHE:HZ	1:B:1107:PHE:HB2	1.79	0.47
3:A:1304:PX4:H61	3:A:1304:PX4:H66	1.64	0.47
1:B:1199:ILE:HB	1:B:1200:PRO:HD3	1.97	0.47
1:B:1206:THR:O	1:B:1210:ILE:HG13	2.15	0.47
1:C:1009:VAL:HG21	1:C:1066:VAL:HG21	1.97	0.47
1:C:1064:ILE:HG12	1:C:1072:PHE:CE2	2.50	0.47
1:D:1029:MET:HA	1:D:1032:GLU:HB2	1.96	0.47
1:A:1021:LEU:O	1:A:1024:LEU:HB2	2.14	0.46
1:B:1057:THR:O	1:B:1061:ILE:HG13	2.15	0.46
1:B:1150:GLN:HE21	1:D:1100:VAL:HG13	1.80	0.46
1:A:1206:THR:O	1:A:1210:ILE:HG13	2.15	0.46
1:D:1170:LEU:O	1:D:1174:MET:N	2.39	0.46
3:A:1304:PX4:H50	1:C:1199:ILE:HG13	1.98	0.46
1:C:1171:PHE:O	1:C:1174:MET:HB3	2.15	0.46
1:D:1089:VAL:HA	1:D:1090:PRO:HD2	1.68	0.46
1:A:1033:THR:HG21	1:C:1163:LEU:HB2	1.96	0.46
1:A:1059:GLU:OE2	1:A:1063:ARG:NH1	2.49	0.46
1:B:1168:TYR:CD1	1:B:1168:TYR:C	2.89	0.46
1:D:1009:VAL:HG13	1:D:1063:ARG:HG2	1.96	0.46
1:A:1005:ILE:HG13	1:A:1066:VAL:HG22	1.97	0.46
1:B:1022:ILE:HG21	1:B:1109:LEU:CB	2.43	0.46
1:A:1215:ALA:O	1:A:1219:ASP:N	2.41	0.46
1:B:1083:VAL:CG1	1:B:1108:ARG:HG2	2.39	0.46
3:B:2006:PX4:H62	1:D:1027:ILE:HG12	1.96	0.46
1:A:1009:VAL:HA	1:A:1014:PHE:CD1	2.50	0.46
1:C:1079:PHE:CG	1:C:1083:VAL:CG2	2.96	0.46
1:B:1087:SER:HB3	1:B:1105:ARG:CZ	2.46	0.46
1:D:1143:ILE:O	1:D:1147:MET:HG3	2.16	0.46
1:B:1114:PRO:O	1:B:1116:MET:N	2.43	0.46
1:A:1038:MET:HE1	1:A:1042:GLY:HA2	1.98	0.45
1:A:1108:ARG:HA	1:A:1111:THR:HB	1.98	0.45
1:B:1022:ILE:HG13	1:B:1056:PHE:CZ	2.51	0.45
1:B:1038:MET:CE	1:B:1042:GLY:HA2	2.46	0.45
1:B:1083:VAL:HG23	1:B:1104:LEU:C	2.36	0.45
1:C:1083:VAL:CG1	1:C:1105:ARG:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1165:GLU:OE1	3:C:1303:PX4:H11	2.16	0.45
1:C:1200:PRO:HA	1:C:1203:PHE:HB2	1.97	0.45
1:C:1082:PHE:O	1:C:1085:ALA:N	2.49	0.45
1:C:1155:ARG:HH22	4:C:1301:1N7:H32	1.80	0.45
1:D:1165:GLU:HG3	3:D:1302:PX4:H5	1.97	0.45
1:A:1018:ILE:HG13	1:A:1059:GLU:CD	2.37	0.45
1:A:1058:ILE:O	1:A:1062:LEU:HG	2.17	0.45
1:D:1032:GLU:HA	1:D:1038:MET:HE3	1.98	0.45
1:A:1067:HIS:HB2	1:A:1071:PHE:HB2	1.99	0.45
1:A:1142:TYR:OH	1:B:1030:GLY:HA3	2.16	0.45
1:C:1080:ASP:HB3	1:C:1108:ARG:HE	1.81	0.45
1:D:1141:PHE:CZ	1:D:1201:PHE:HZ	2.35	0.45
1:D:1212:LEU:O	1:D:1216:ILE:HG13	2.16	0.45
1:B:1014:PHE:O	1:B:1017:PHE:HB3	2.17	0.45
1:B:1212:LEU:O	1:B:1216:ILE:HG13	2.15	0.45
1:B:1215:ALA:O	1:B:1218:VAL:HB	2.16	0.45
1:D:1049:ASN:O	1:D:1053:ILE:HB	2.17	0.45
4:C:1301:1N7:H10	4:C:1301:1N7:H34	1.71	0.45
1:A:1071:PHE:CE2	1:A:1077:SER:HB3	2.51	0.45
1:B:1017:PHE:O	1:B:1020:TYR:HB3	2.16	0.45
1:B:1024:LEU:HA	1:B:1024:LEU:HD12	1.43	0.45
1:B:1050:GLN:O	1:B:1054:THR:N	2.49	0.45
1:A:1147:MET:HG3	1:B:1103:VAL:HG11	1.99	0.45
1:B:1087:SER:HB3	1:B:1105:ARG:HE	1.81	0.45
1:C:1201:PHE:O	1:C:1205:VAL:HB	2.17	0.45
1:D:1049:ASN:O	1:D:1053:ILE:N	2.42	0.45
3:A:1304:PX4:H9	3:A:1304:PX4:H1	1.59	0.45
1:B:1018:ILE:HG13	1:B:1059:GLU:HG3	1.99	0.44
1:C:1159:TRP:O	1:C:1169:THR:OG1	2.35	0.44
1:D:1050:GLN:HA	1:D:1053:ILE:HB	1.99	0.44
1:A:1171:PHE:HE1	1:C:1203:PHE:CZ	2.35	0.44
1:A:1171:PHE:O	1:A:1174:MET:HB3	2.17	0.44
1:B:1111:THR:O	1:B:1117:ARG:NH2	2.44	0.44
1:C:1199:ILE:HB	1:C:1200:PRO:HD3	1.99	0.44
1:A:1214:VAL:HG12	1:A:1218:VAL:CG2	2.47	0.44
1:B:1163:LEU:HB2	1:D:1033:THR:HG21	1.98	0.44
1:B:1054:THR:O	1:B:1057:THR:HB	2.17	0.44
1:C:1013:PHE:HD1	1:C:1016:LYS:HE3	1.82	0.44
1:C:1041:PHE:O	1:C:1045:THR:OG1	2.20	0.44
1:C:1063:ARG:NH2	1:C:1077:SER:OG	2.50	0.44
1:C:1162:THR:O	1:C:1165:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1009:VAL:O	1:B:1014:PHE:CD2	2.70	0.44
1:B:1170:LEU:HD23	1:B:1170:LEU:HA	1.66	0.44
1:C:1001:MET:O	1:C:1004:ARG:HB3	2.17	0.44
1:B:1022:ILE:HG21	1:B:1109:LEU:CA	2.48	0.44
1:C:1130:MET:O	1:C:1133:VAL:N	2.49	0.44
3:D:1302:PX4:H2	3:D:1302:PX4:H12	1.61	0.44
1:A:1168:TYR:CD1	1:A:1168:TYR:C	2.90	0.44
1:A:1036:THR:OG1	3:A:1302:PX4:O2	2.34	0.44
1:B:1048:PHE:O	1:B:1052:VAL:HG23	2.18	0.44
1:B:1025:ASN:HB2	1:B:1052:VAL:HG21	1.99	0.43
1:B:1080:ASP:OD1	1:B:1108:ARG:HA	2.18	0.43
1:B:1207:PHE:HA	1:B:1210:ILE:HD12	2.00	0.43
1:C:1031:LEU:C	1:C:1033:THR:H	2.20	0.43
1:C:1110:VAL:CG1	1:C:1120:VAL:HG21	2.48	0.43
1:B:1018:ILE:HG21	1:B:1059:GLU:OE2	2.18	0.43
1:B:1021:LEU:HD11	1:B:1055:ILE:CD1	2.48	0.43
1:C:1113:VAL:O	1:C:1117:ARG:HG3	2.17	0.43
1:D:1032:GLU:HG2	1:D:1038:MET:HE3	2.00	0.43
1:B:1078:LEU:HA	1:B:1081:PHE:HB3	2.00	0.43
1:C:1080:ASP:CB	1:C:1108:ARG:HE	2.30	0.43
1:C:1121:SER:HA	1:C:1124:ILE:HD12	2.01	0.43
3:A:1304:PX4:H47	1:C:1195:TRP:CE3	2.54	0.43
1:C:1111:THR:HG22	1:C:1112:ALA:N	2.34	0.43
1:D:1077:SER:O	1:D:1080:ASP:HB2	2.17	0.43
1:A:1140:PHE:HE2	1:A:1205:VAL:HG23	1.84	0.43
1:A:1201:PHE:CZ	1:A:1205:VAL:HG21	2.53	0.43
1:D:1110:VAL:HG13	1:D:1116:MET:HB3	2.00	0.43
1:D:1155:ARG:HG3	1:D:1190:VAL:HG11	1.99	0.43
1:B:1031:LEU:C	1:B:1033:THR:N	2.71	0.43
1:B:1086:ILE:HA	1:B:1089:VAL:HG23	2.01	0.43
1:B:1140:PHE:HE2	1:B:1205:VAL:HG23	1.84	0.43
1:C:1038:MET:O	1:C:1042:GLY:N	2.51	0.43
1:C:1056:PHE:CE2	1:C:1108:ARG:HD3	2.54	0.43
1:A:1218:VAL:C	1:A:1220:ALA:H	2.22	0.43
1:A:1151:LEU:HA	1:A:1151:LEU:HD23	1.80	0.43
1:A:1159:TRP:O	1:A:1165:GLU:HB3	2.19	0.43
1:B:1024:LEU:HB3	1:B:1048:PHE:CZ	2.44	0.43
1:B:1028:THR:HG23	1:B:1049:ASN:HD21	1.84	0.43
1:D:1008:ILE:HG22	1:D:1014:PHE:CD1	2.54	0.43
1:A:1045:THR:HG22	1:A:1046:THR:N	2.34	0.43
1:A:1124:ILE:HG23	1:A:1127:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1178:SER:HA	1:B:1177:GLU:OE2	2.17	0.43
3:C:1303:PX4:H19	3:C:1303:PX4:H17	1.77	0.43
1:C:1087:SER:OG	1:C:1102:GLY:HA2	2.19	0.43
1:C:1038:MET:HA	1:C:1038:MET:HE2	2.00	0.42
1:C:1108:ARG:HB3	1:C:1108:ARG:NH1	2.34	0.42
1:D:1098:LEU:HD23	1:D:1098:LEU:HA	1.76	0.42
3:D:1302:PX4:H17	3:D:1302:PX4:H19	1.85	0.42
1:A:1170:LEU:HA	1:A:1170:LEU:HD23	1.82	0.42
3:A:1303:PX4:H12	3:A:1303:PX4:H2	1.61	0.42
1:B:1100:VAL:O	1:B:1103:VAL:HG12	2.20	0.42
1:C:1085:ALA:HA	1:C:1088:LEU:HD12	2.02	0.42
1:C:1157:PRO:HA	1:C:1161:GLY:CA	2.49	0.42
1:C:1195:TRP:CZ2	1:C:1196:VAL:HG22	2.54	0.42
1:A:1009:VAL:HA	1:A:1014:PHE:CE1	2.54	0.42
1:B:1087:SER:CB	1:B:1105:ARG:HE	2.31	0.42
1:C:1154:GLU:HB3	1:C:1155:ARG:HG2	2.01	0.42
1:D:1021:LEU:HD23	1:D:1021:LEU:HA	1.78	0.42
1:C:1151:LEU:HD23	1:C:1151:LEU:HA	1.79	0.42
1:C:1184:VAL:O	1:C:1188:MET:HG3	2.20	0.42
1:A:1156:PHE:CZ	1:A:1187:LEU:HA	2.54	0.42
1:B:1083:VAL:CG2	1:B:1105:ARG:N	2.83	0.42
1:B:1114:PRO:C	1:B:1116:MET:H	2.20	0.42
1:B:1084:VAL:HG23	1:B:1108:ARG:HE	1.84	0.42
1:C:1085:ALA:O	1:C:1089:VAL:HG23	2.19	0.42
3:D:1302:PX4:H58	3:D:1302:PX4:H65	1.75	0.42
1:B:1105:ARG:O	1:B:1108:ARG:HB2	2.20	0.42
1:B:1151:LEU:HD23	1:B:1151:LEU:HA	1.89	0.42
1:B:1203:PHE:HZ	3:D:1302:PX4:H65	1.84	0.42
1:C:1074:ASP:O	1:C:1078:LEU:HB2	2.19	0.42
1:B:1083:VAL:CG1	1:B:1084:VAL:N	2.83	0.42
1:C:1001:MET:O	1:C:1001:MET:HG2	2.20	0.42
1:D:1031:LEU:HA	1:D:1031:LEU:HD23	1.77	0.42
3:B:2001:PX4:H13	3:B:2001:PX4:H1	1.84	0.42
1:C:1110:VAL:HG13	1:C:1120:VAL:HG21	2.01	0.42
1:A:1071:PHE:CZ	1:A:1077:SER:HB3	2.54	0.42
1:B:1061:ILE:O	1:B:1064:ILE:HB	2.19	0.42
1:D:1025:ASN:OD1	1:D:1105:ARG:NH1	2.52	0.42
1:B:1021:LEU:HD23	1:B:1021:LEU:HA	1.84	0.41
1:B:1058:ILE:O	1:B:1062:LEU:HG	2.20	0.41
1:C:1018:ILE:HD13	1:C:1018:ILE:HA	1.68	0.41
1:C:1080:ASP:OD1	1:C:1111:THR:HG21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:LEU:C	1:A:1033:THR:N	2.73	0.41
1:D:1126:VAL:HG11	1:D:1216:ILE:HG23	2.01	0.41
1:A:1019:ILE:CD1	1:A:1113:VAL:HG22	2.50	0.41
1:A:1021:LEU:HD23	1:A:1024:LEU:CD2	2.50	0.41
1:B:1048:PHE:O	1:B:1051:ILE:HB	2.20	0.41
1:B:1074:ASP:OD1	1:B:1075:PRO:HD2	2.20	0.41
1:B:1178:SER:HA	1:D:1177:GLU:CD	2.41	0.41
1:C:1025:ASN:OD1	1:C:1105:ARG:NH1	2.53	0.41
1:C:1083:VAL:HG12	1:C:1105:ARG:HB3	2.01	0.41
1:C:1191:TYR:HA	1:C:1192:PRO:HD2	1.87	0.41
1:D:1168:TYR:N	3:D:1302:PX4:O8	2.54	0.41
1:B:1159:TRP:O	1:B:1169:THR:OG1	2.33	0.41
1:C:1009:VAL:HG12	1:C:1010:GLU:OE1	2.20	0.41
1:D:1053:ILE:HA	1:D:1053:ILE:HD13	1.75	0.41
1:D:1142:TYR:HE1	3:D:1303:PX4:H55	1.85	0.41
1:A:1057:THR:O	1:A:1061:ILE:HG13	2.20	0.41
1:B:1084:VAL:HG23	1:B:1108:ARG:NE	2.36	0.41
1:B:1096:GLU:OE1	1:B:1099:ARG:NH2	2.54	0.41
1:A:1047:LEU:O	1:A:1051:ILE:HG13	2.21	0.41
1:B:1104:LEU:C	1:B:1106:LEU:N	2.71	0.41
1:C:1013:PHE:HA	1:C:1016:LYS:HB2	2.02	0.41
4:C:1301:1N7:C17	4:C:1301:1N7:H15	2.50	0.41
1:D:1079:PHE:CE1	1:D:1083:VAL:HG21	2.55	0.41
1:A:1025:ASN:HA	1:A:1028:THR:OG1	2.21	0.41
1:A:1172:GLN:HA	1:C:1179:TRP:HZ2	1.86	0.41
1:A:1183:ILE:O	1:A:1187:LEU:HB2	2.20	0.41
1:A:1216:ILE:HG22	1:C:1214:VAL:HG21	2.02	0.41
1:B:1078:LEU:HA	1:B:1078:LEU:HD23	1.86	0.41
1:B:1108:ARG:NH1	1:B:1108:ARG:HB3	2.35	0.41
1:B:1203:PHE:CE1	1:D:1171:PHE:HE1	2.39	0.41
1:C:1053:ILE:HG13	1:C:1087:SER:O	2.21	0.41
1:C:1170:LEU:HA	1:C:1170:LEU:HD23	1.67	0.41
1:D:1155:ARG:HE	3:D:1304:PX4:H6	1.86	0.41
1:A:1183:ILE:O	1:A:1187:LEU:HD13	2.20	0.40
1:B:1048:PHE:HA	1:B:1051:ILE:HB	2.03	0.40
1:B:1074:ASP:OD1	1:B:1076:TRP:HD1	2.04	0.40
1:B:1103:VAL:O	1:B:1106:LEU:HG	2.20	0.40
1:D:1032:GLU:CD	1:D:1049:ASN:HD21	2.24	0.40
1:A:1167:PHE:CE1	3:A:1304:PX4:H56	2.57	0.40
1:B:1130:MET:HG2	1:B:1212:LEU:HG	2.02	0.40
1:D:1025:ASN:CA	1:D:1028:THR:HB	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1127:ILE:O	1:D:1130:MET:HB2	2.21	0.40
1:A:1156:PHE:CE1	1:A:1187:LEU:HD12	2.56	0.40
1:B:1163:LEU:O	1:B:1167:PHE:HB2	2.21	0.40
3:B:2001:PX4:H72	3:B:2001:PX4:H65	1.90	0.40
1:C:1031:LEU:HD23	1:C:1031:LEU:HA	1.78	0.40
1:C:1195:TRP:CE2	1:C:1196:VAL:HG22	2.57	0.40
1:D:1020:TYR:CZ	1:D:1024:LEU:HD11	2.57	0.40
3:A:1304:PX4:H58	1:C:1203:PHE:HZ	1.85	0.40
1:B:1022:ILE:HG13	1:B:1056:PHE:HZ	1.85	0.40
1:B:1059:GLU:CD	1:B:1108:ARG:NH2	2.72	0.40
1:D:1048:PHE:O	1:D:1051:ILE:HB	2.22	0.40
1:D:1104:LEU:HD23	1:D:1104:LEU:HA	1.75	0.40
1:B:1014:PHE:HE2	1:B:1059:GLU:HG3	1.87	0.40
1:B:1140:PHE:CE2	1:B:1205:VAL:HG23	2.57	0.40
1:C:1065:TYR:HD1	1:C:1065:TYR:HA	1.70	0.40
1:C:1076:TRP:O	1:C:1079:PHE:HB3	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	214/285 (75%)	199 (93%)	14 (6%)	1 (0%)	29 61
1	B	213/285 (75%)	195 (92%)	17 (8%)	1 (0%)	29 61
1	C	217/285 (76%)	200 (92%)	17 (8%)	0	100 100
1	D	214/285 (75%)	201 (94%)	13 (6%)	0	100 100
All	All	858/1140 (75%)	795 (93%)	61 (7%)	2 (0%)	47 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1090	PRO
1	B	1090	PRO

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	200/263 (76%)	190 (95%)	10 (5%)	24	57
1	B	199/263 (76%)	188 (94%)	11 (6%)	21	53
1	C	201/263 (76%)	191 (95%)	10 (5%)	24	57
1	D	201/263 (76%)	192 (96%)	9 (4%)	27	61
All	All	801/1052 (76%)	761 (95%)	40 (5%)	24	57

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1053	ILE
1	A	1054	THR
1	A	1060	ILE
1	A	1103	VAL
1	A	1111	THR
1	A	1118	LYS
1	A	1119	ILE
1	A	1165	GLU
1	A	1167	PHE
1	A	1205	VAL
1	B	1028	THR
1	B	1046	THR
1	B	1053	ILE
1	B	1060	ILE
1	B	1065	TYR
1	B	1070	SER
1	B	1103	VAL
1	B	1119	ILE
1	B	1141	PHE
1	B	1167	PHE

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Mol	Chain	Res	Type
1	B	1218	VAL
1	C	1010	GLU
1	C	1018	ILE
1	C	1053	ILE
1	C	1060	ILE
1	C	1070	SER
1	C	1111	THR
1	C	1165	GLU
1	C	1167	PHE
1	C	1205	VAL
1	C	1218	VAL
1	D	1028	THR
1	D	1046	THR
1	D	1053	ILE
1	D	1070	SER
1	D	1141	PHE
1	D	1163	LEU
1	D	1167	PHE
1	D	1205	VAL
1	D	1218	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1150	GLN

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)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PX4	D	1304	-	35,35,45	1.35	3 (8%)	41,43,53	1.04	3 (7%)
3	PX4	C	1302	-	7,7,45	0.53	0	8,9,53	0.52	0
3	PX4	D	1305	-	8,8,45	0.53	0	9,10,53	0.44	0
3	PX4	A	1303	-	12,12,45	1.16	1 (8%)	16,17,53	0.63	1 (6%)
4	1N7	C	1301	-	29,29,46	3.35	11 (37%)	47,47,72	7.81	25 (53%)
3	PX4	B	2006	-	21,21,45	1.01	1 (4%)	23,24,53	0.89	1 (4%)
3	PX4	B	2005	-	28,28,45	1.28	2 (7%)	32,33,53	1.23	4 (12%)
2	PO4	A	1301	-	4,4,4	0.93	0	6,6,6	0.52	0
3	PX4	A	1304	-	35,35,45	1.28	3 (8%)	41,43,53	1.17	2 (4%)
2	PO4	D	1301	-	4,4,4	0.90	0	6,6,6	0.35	0
3	PX4	D	1302	-	35,35,45	1.33	3 (8%)	41,43,53	1.35	5 (12%)
3	PX4	C	1303	-	35,35,45	1.28	4 (11%)	41,43,53	1.11	2 (4%)
3	PX4	D	1303	-	29,29,45	1.26	2 (6%)	32,34,53	1.26	3 (9%)
3	PX4	B	2004	-	14,14,45	1.33	1 (7%)	16,18,53	1.04	1 (6%)
3	PX4	A	1302	-	20,20,45	1.43	3 (15%)	24,25,53	1.42	3 (12%)
3	PX4	B	2002	-	22,22,45	1.35	3 (13%)	27,29,53	0.75	1 (3%)
3	PX4	B	2001	-	35,35,45	1.28	3 (8%)	41,43,53	1.28	2 (4%)
3	PX4	B	2003	-	18,18,45	1.45	2 (11%)	21,23,53	1.23	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
3	PX4	D	1304	-	-	20/39/39/49	-
3	PX4	C	1302	-	-	2/7/7/49	-
3	PX4	D	1305	-	-	3/8/8/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	A	1303	-	-	5/12/12/49	-
4	1N7	C	1301	-	-	1/6/71/92	0/4/4/4
3	PX4	B	2006	-	-	10/22/22/49	-
3	PX4	B	2005	-	-	12/30/30/49	-
3	PX4	A	1304	-	-	24/39/39/49	-
3	PX4	D	1302	-	-	15/39/39/49	-
3	PX4	C	1303	-	-	21/39/39/49	-
3	PX4	D	1303	-	-	20/33/33/49	-
3	PX4	B	2004	-	-	9/16/16/49	-
3	PX4	A	1302	-	-	13/22/22/49	-
3	PX4	B	2002	-	-	13/24/24/49	-
3	PX4	B	2001	-	-	13/39/39/49	-
3	PX4	B	2003	-	-	12/22/22/49	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1301	1N7	C3-C4	9.17	1.68	1.53
4	C	1301	1N7	C8-C7	6.52	1.71	1.54
4	C	1301	1N7	C18-C19	5.85	1.65	1.53
4	C	1301	1N7	C16-C15	5.38	1.62	1.53
4	C	1301	1N7	C20-C9	-5.12	1.45	1.54
4	C	1301	1N7	C5-C9	5.06	1.64	1.55
4	C	1301	1N7	C7-C6	4.64	1.64	1.54
4	C	1301	1N7	C16-C17	4.49	1.60	1.52
3	B	2004	PX4	O5-C9	4.27	1.45	1.33
3	D	1302	PX4	O5-C9	4.20	1.45	1.33
4	C	1301	1N7	O4-C4	-4.19	1.36	1.43
3	D	1304	PX4	O5-C9	4.15	1.45	1.33
3	D	1303	PX4	O5-C9	4.12	1.45	1.33
3	B	2001	PX4	O5-C9	4.08	1.45	1.33
3	C	1303	PX4	O5-C9	4.03	1.45	1.33
3	B	2005	PX4	O5-C9	4.03	1.45	1.33
3	A	1304	PX4	O5-C9	4.01	1.45	1.33
3	B	2003	PX4	O5-C9	4.01	1.45	1.33
3	A	1302	PX4	O5-C9	3.99	1.45	1.33
3	B	2002	PX4	O5-C9	3.84	1.44	1.33
3	B	2006	PX4	O7-C23	3.69	1.44	1.33
3	D	1302	PX4	O7-C23	3.51	1.44	1.34
3	A	1304	PX4	O7-C23	3.49	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2003	PX4	O7-C23	3.44	1.44	1.34
3	D	1303	PX4	O7-C23	3.38	1.43	1.34
3	B	2005	PX4	O7-C23	3.33	1.43	1.34
3	B	2001	PX4	O7-C23	3.24	1.43	1.34
3	C	1303	PX4	O7-C23	3.23	1.43	1.34
3	A	1302	PX4	O7-C23	3.19	1.43	1.34
3	D	1304	PX4	O7-C23	3.09	1.43	1.34
3	D	1302	PX4	C4-N1	-2.86	1.41	1.50
3	D	1304	PX4	C4-N1	-2.83	1.41	1.50
3	A	1304	PX4	C4-N1	-2.79	1.41	1.50
3	B	2002	PX4	C4-N1	-2.78	1.41	1.50
4	C	1301	1N7	C5-C6	2.75	1.60	1.55
3	B	2001	PX4	C4-N1	-2.72	1.42	1.50
3	A	1303	PX4	C4-N1	-2.65	1.42	1.50
3	C	1303	PX4	C4-N1	-2.63	1.42	1.50
4	C	1301	1N7	C3-C19	-2.31	1.49	1.53
3	C	1303	PX4	C10-C9	2.21	1.57	1.50
3	B	2002	PX4	C10-C9	2.09	1.56	1.50
3	A	1302	PX4	C10-C9	2.08	1.56	1.50

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1301	1N7	C11-C2-C19	-26.32	74.91	111.18
4	C	1301	1N7	C10-C5-C9	-21.22	78.00	111.21
4	C	1301	1N7	C10-C5-C4	-18.40	90.33	109.07
4	C	1301	1N7	C10-C5-C6	-14.12	89.11	111.21
4	C	1301	1N7	C11-C2-C1	-13.00	87.30	108.26
4	C	1301	1N7	C6-C5-C4	12.03	118.60	107.40
4	C	1301	1N7	C9-C5-C4	11.95	128.57	117.67
4	C	1301	1N7	C9-C5-C6	11.00	111.19	100.09
4	C	1301	1N7	C11-C2-C15	-10.63	92.33	110.36
4	C	1301	1N7	C19-C2-C15	10.01	122.64	108.58
4	C	1301	1N7	C15-C16-C17	7.87	123.14	114.46
4	C	1301	1N7	C2-C19-C18	6.71	119.03	111.82
4	C	1301	1N7	C16-C17-C18	6.58	118.50	111.48
4	C	1301	1N7	C1-C12-C13	6.00	118.17	110.47
4	C	1301	1N7	C1-C2-C15	5.36	115.70	107.77
3	B	2001	PX4	O7-C23-C24	5.26	122.83	111.50
3	D	1302	PX4	O7-C23-C24	5.22	122.75	111.50
4	C	1301	1N7	C1-C2-C19	4.93	119.10	111.35
4	C	1301	1N7	C3-C4-C5	4.83	116.20	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1303	PX4	O5-C9-C10	4.31	122.69	111.38
4	C	1301	1N7	C19-C18-C17	4.27	116.98	111.88
3	A	1302	PX4	O7-C23-C24	4.11	120.36	111.50
4	C	1301	1N7	C7-C6-C18	4.00	123.93	118.33
4	C	1301	1N7	C5-C9-C20	-4.00	114.72	119.50
3	C	1303	PX4	O7-C23-C24	3.98	120.08	111.50
3	A	1304	PX4	O7-C23-C24	3.75	119.58	111.50
3	B	2003	PX4	O7-C23-C24	3.56	120.74	110.80
4	C	1301	1N7	C12-C1-C2	3.48	118.75	112.78
4	C	1301	1N7	C15-C14-C13	3.48	117.86	112.76
3	D	1304	PX4	O7-C23-C24	3.44	118.92	111.50
3	B	2005	PX4	O7-C23-C24	3.36	120.16	110.80
3	D	1303	PX4	O7-C23-C24	3.33	118.67	111.50
3	B	2005	PX4	O5-C9-C10	3.25	122.11	111.91
3	A	1302	PX4	O5-C9-C10	3.20	121.94	111.91
3	B	2004	PX4	O5-C9-C10	3.14	119.61	111.38
3	B	2001	PX4	O5-C9-C10	3.10	121.65	111.91
3	B	2003	PX4	O5-C9-C10	2.96	119.15	111.38
3	D	1304	PX4	O5-C9-C10	2.96	121.19	111.91
3	D	1302	PX4	O5-C9-C10	2.81	120.71	111.91
3	A	1304	PX4	O5-C9-C10	2.79	120.67	111.91
3	C	1303	PX4	O5-C9-C10	2.71	120.41	111.91
4	C	1301	1N7	C7-C6-C5	-2.68	100.93	103.55
4	C	1301	1N7	C14-C15-C2	2.58	115.39	112.66
3	B	2002	PX4	O5-C9-C10	2.35	119.29	111.91
3	D	1302	PX4	C8-C7-C6	-2.31	106.33	111.79
3	B	2006	PX4	O7-C23-C24	2.29	119.11	111.91
4	C	1301	1N7	C19-C18-C6	-2.23	106.65	109.71
3	A	1302	PX4	O5-C9-O6	-2.22	118.00	123.59
3	D	1302	PX4	C1-C2-N1	-2.20	108.44	115.78
3	D	1303	PX4	O5-C8-C7	2.12	114.60	108.43
3	A	1303	PX4	C1-C2-N1	-2.11	108.74	115.78
3	D	1302	PX4	O7-C23-O8	-2.08	118.68	123.70
3	B	2005	PX4	O5-C8-C7	2.07	114.45	108.43
3	B	2005	PX4	C7-O7-C23	-2.03	112.79	117.79
3	D	1304	PX4	C7-O7-C23	-2.02	112.81	117.79

There are no chirality outliers.

All (193) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1302	PX4	C6-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
3	A	1302	PX4	C6-O4-P1-O3
3	A	1302	PX4	O6-C9-O5-C8
3	A	1302	PX4	C10-C9-O5-C8
3	A	1303	PX4	O3-C1-C2-N1
3	A	1304	PX4	C6-O4-P1-O2
3	A	1304	PX4	O3-C1-C2-N1
3	A	1304	PX4	O4-C6-C7-O7
3	B	2001	PX4	O3-C1-C2-N1
3	B	2001	PX4	C24-C23-O7-C7
3	B	2002	PX4	C6-O4-P1-O1
3	B	2002	PX4	C6-O4-P1-O2
3	B	2003	PX4	O7-C7-C8-O5
3	B	2004	PX4	C6-O4-P1-O1
3	B	2004	PX4	C6-C7-C8-O5
3	B	2004	PX4	O7-C7-C8-O5
3	B	2006	PX4	C1-O3-P1-O1
3	B	2006	PX4	C1-O3-P1-O2
3	B	2006	PX4	C6-O4-P1-O2
3	C	1302	PX4	C1-O3-P1-O1
3	C	1303	PX4	C1-O3-P1-O2
3	C	1303	PX4	C6-O4-P1-O1
3	C	1303	PX4	C6-O4-P1-O2
3	C	1303	PX4	C6-O4-P1-O3
3	C	1303	PX4	O6-C9-O5-C8
3	C	1303	PX4	C10-C9-O5-C8
3	D	1302	PX4	O3-C1-C2-N1
3	D	1302	PX4	O6-C9-O5-C8
3	D	1302	PX4	C10-C9-O5-C8
3	D	1302	PX4	C24-C23-O7-C7
3	D	1303	PX4	C1-O3-P1-O1
3	D	1303	PX4	C6-O4-P1-O1
3	D	1303	PX4	C6-O4-P1-O2
3	D	1304	PX4	O3-C1-C2-N1
3	D	1304	PX4	O8-C23-O7-C7
3	D	1304	PX4	C24-C23-O7-C7
3	B	2002	PX4	O6-C9-O5-C8
3	D	1303	PX4	O6-C9-O5-C8
3	D	1304	PX4	O6-C9-O5-C8
3	A	1302	PX4	O8-C23-O7-C7
3	B	2001	PX4	O8-C23-O7-C7
3	D	1302	PX4	O8-C23-O7-C7
3	B	2002	PX4	C10-C9-O5-C8

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Mol	Chain	Res	Type	Atoms
3	D	1303	PX4	C10-C9-O5-C8
3	D	1304	PX4	C10-C9-O5-C8
3	A	1302	PX4	C24-C23-O7-C7
3	B	2006	PX4	C24-C23-O7-C7
3	B	2002	PX4	O7-C7-C8-O5
3	B	2005	PX4	C24-C23-O7-C7
3	B	2005	PX4	O8-C23-O7-C7
3	B	2006	PX4	O8-C23-O7-C7
3	B	2002	PX4	O4-C6-C7-C8
3	B	2004	PX4	O4-C6-C7-O7
3	D	1304	PX4	C9-C10-C11-C12
3	B	2004	PX4	C7-C6-O4-P1
3	B	2003	PX4	C24-C23-O7-C7
3	B	2002	PX4	O4-C6-C7-O7
3	A	1303	PX4	C1-O3-P1-O4
3	A	1303	PX4	C6-O4-P1-O3
3	A	1304	PX4	C1-O3-P1-O4
3	A	1304	PX4	C6-O4-P1-O3
3	B	2002	PX4	C1-O3-P1-O4
3	B	2002	PX4	C6-O4-P1-O3
3	B	2004	PX4	C6-O4-P1-O3
3	C	1303	PX4	C1-O3-P1-O4
3	D	1303	PX4	C6-O4-P1-O3
3	D	1304	PX4	C6-O4-P1-O3
3	B	2004	PX4	O4-C6-C7-C8
3	B	2003	PX4	O8-C23-O7-C7
3	A	1304	PX4	C32-C33-C34-C35
3	C	1303	PX4	C30-C31-C32-C33
3	D	1302	PX4	C28-C29-C30-C31
3	B	2002	PX4	C10-C11-C12-C13
3	B	2006	PX4	C24-C25-C26-C27
3	D	1302	PX4	C32-C33-C34-C35
3	C	1303	PX4	C31-C32-C33-C34
3	D	1303	PX4	C27-C28-C29-C30
3	B	2001	PX4	C25-C26-C27-C28
3	D	1302	PX4	C27-C28-C29-C30
3	D	1302	PX4	C23-C24-C25-C26
3	B	2001	PX4	C30-C31-C32-C33
3	B	2005	PX4	C10-C11-C12-C13
3	B	2005	PX4	C14-C15-C16-C17
3	D	1304	PX4	C11-C12-C13-C14
3	B	2006	PX4	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
3	A	1304	PX4	C24-C25-C26-C27
3	B	2001	PX4	C26-C27-C28-C29
3	D	1302	PX4	C29-C30-C31-C32
3	D	1304	PX4	C16-C17-C18-C19
3	B	2001	PX4	C32-C33-C34-C35
3	D	1304	PX4	C10-C11-C12-C13
3	C	1303	PX4	C29-C30-C31-C32
3	A	1304	PX4	C10-C9-O5-C8
3	B	2006	PX4	C25-C26-C27-C28
3	D	1304	PX4	C23-C24-C25-C26
3	D	1304	PX4	C15-C16-C17-C18
3	B	2005	PX4	C10-C9-O5-C8
3	B	2006	PX4	C31-C32-C33-C34
3	D	1304	PX4	C13-C14-C15-C16
3	A	1304	PX4	O6-C9-O5-C8
3	D	1303	PX4	C32-C33-C34-C35
3	A	1302	PX4	C9-C10-C11-C12
3	D	1303	PX4	C24-C23-O7-C7
3	D	1304	PX4	C12-C13-C14-C15
3	D	1303	PX4	O8-C23-O7-C7
3	B	2005	PX4	O6-C9-O5-C8
3	C	1303	PX4	C28-C29-C30-C31
3	D	1303	PX4	C28-C29-C30-C31
3	B	2001	PX4	C6-C7-C8-O5
3	D	1302	PX4	C33-C34-C35-C36
3	B	2005	PX4	C17-C18-C19-C20
3	C	1303	PX4	C23-C24-C25-C26
3	D	1303	PX4	C31-C32-C33-C34
3	A	1302	PX4	C10-C11-C12-C13
3	A	1304	PX4	C27-C28-C29-C30
3	A	1302	PX4	C6-O4-P1-O2
3	B	2003	PX4	C1-O3-P1-O2
3	C	1302	PX4	C1-O3-P1-O2
3	D	1303	PX4	C24-C25-C26-C27
3	D	1303	PX4	C29-C30-C31-C32
3	D	1303	PX4	O4-C6-C7-C8
3	B	2003	PX4	C6-C7-C8-O5
3	C	1303	PX4	C6-C7-C8-O5
3	D	1302	PX4	C6-C7-C8-O5
3	B	2006	PX4	C30-C31-C32-C33
3	B	2005	PX4	C18-C19-C20-C21
3	A	1302	PX4	O7-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
3	A	1304	PX4	C23-C24-C25-C26
3	A	1304	PX4	O4-C6-C7-C8
3	D	1302	PX4	C25-C26-C27-C28
3	C	1303	PX4	O7-C7-C8-O5
3	D	1302	PX4	O7-C7-C8-O5
3	C	1303	PX4	C25-C26-C27-C28
3	B	2003	PX4	C6-O4-P1-O3
3	B	2005	PX4	C7-C6-O4-P1
3	A	1303	PX4	C1-O3-P1-O2
3	A	1303	PX4	C6-O4-P1-O1
3	A	1304	PX4	C1-O3-P1-O1
3	A	1304	PX4	C6-O4-P1-O1
3	B	2002	PX4	C1-O3-P1-O2
3	B	2003	PX4	C6-O4-P1-O2
3	B	2004	PX4	C6-O4-P1-O2
3	D	1304	PX4	C6-O4-P1-O2
3	B	2002	PX4	C6-C7-C8-O5
3	A	1304	PX4	C26-C27-C28-C29
3	C	1303	PX4	C1-C2-N1-C5
3	B	2002	PX4	O3-C1-C2-N1
3	B	2005	PX4	O7-C7-C8-O5
3	C	1303	PX4	C32-C33-C34-C35
4	C	1301	1N7	C21-C20-C9-C5
3	D	1303	PX4	O4-C6-C7-O7
3	B	2001	PX4	C31-C32-C33-C34
3	B	2001	PX4	O7-C7-C8-O5
3	B	2004	PX4	C1-O3-P1-O2
3	A	1302	PX4	C6-C7-C8-O5
3	B	2005	PX4	C6-C7-C8-O5
3	B	2003	PX4	C7-C6-O4-P1
3	A	1304	PX4	O8-C23-O7-C7
3	A	1304	PX4	C28-C29-C30-C31
3	A	1304	PX4	C31-C32-C33-C34
3	C	1303	PX4	C1-C2-N1-C4
3	D	1303	PX4	C1-O3-P1-O4
3	B	2003	PX4	C1-O3-P1-O1
3	D	1303	PX4	C8-C7-O7-C23
3	B	2001	PX4	C29-C30-C31-C32
3	D	1304	PX4	C14-C15-C16-C17
3	A	1304	PX4	C1-C2-N1-C4
3	C	1303	PX4	C1-C2-N1-C3
3	B	2003	PX4	O4-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	D	1305	PX4	C7-C6-O4-P1
3	D	1305	PX4	C1-O3-P1-O2
3	A	1302	PX4	O7-C23-C24-C25
3	B	2001	PX4	C24-C25-C26-C27
3	D	1304	PX4	C1-C2-N1-C3
3	B	2001	PX4	C9-C10-C11-C12
3	A	1304	PX4	C24-C23-O7-C7
3	C	1303	PX4	C11-C10-C9-O5
3	B	2005	PX4	C11-C12-C13-C14
3	D	1302	PX4	C24-C25-C26-C27
3	A	1304	PX4	C1-C2-N1-C5
3	D	1303	PX4	C30-C31-C32-C33
3	D	1303	PX4	C33-C34-C35-C36
3	D	1304	PX4	C1-C2-N1-C5
3	A	1302	PX4	C7-C6-O4-P1
3	B	2003	PX4	O7-C23-C24-C25
3	C	1303	PX4	C11-C10-C9-O6
3	A	1304	PX4	C29-C30-C31-C32
3	A	1304	PX4	C1-O3-P1-O2
3	A	1304	PX4	C1-C2-N1-C3
3	B	2003	PX4	C6-O4-P1-O1
3	D	1304	PX4	C6-O4-P1-O1
3	D	1305	PX4	C6-O4-P1-O2
3	D	1304	PX4	C1-C2-N1-C4

There are no ring outliers.

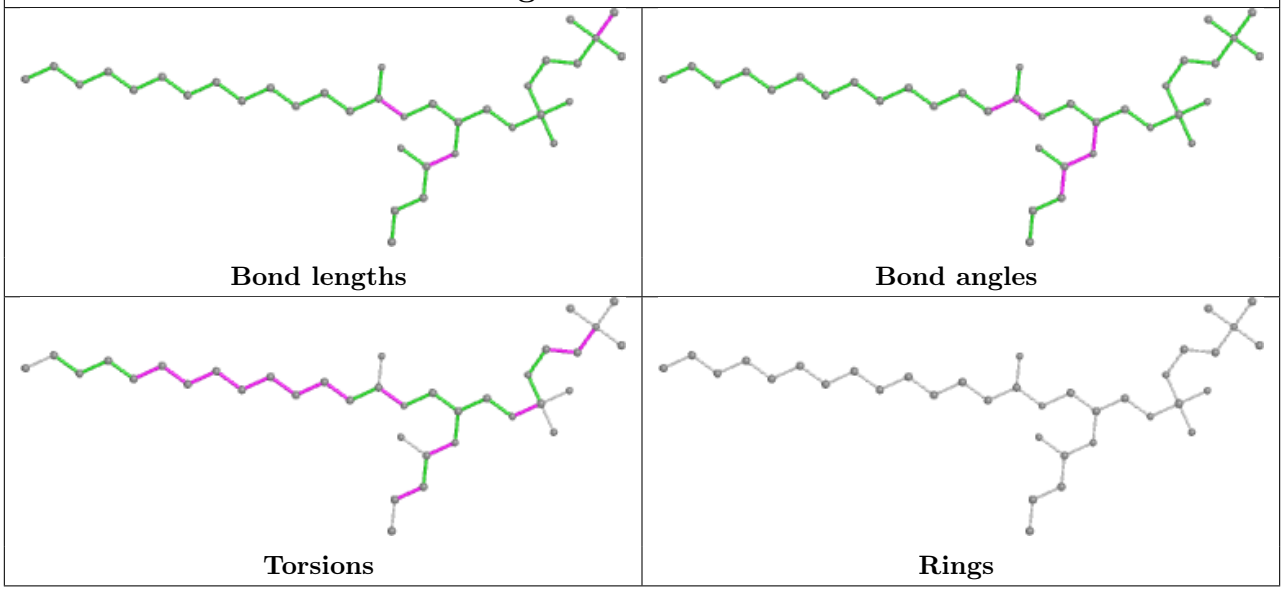
10 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1304	PX4	3	0
3	A	1303	PX4	2	0
4	C	1301	1N7	5	0
3	B	2006	PX4	2	0
3	A	1304	PX4	13	0
3	D	1302	PX4	11	0
3	C	1303	PX4	7	0
3	D	1303	PX4	2	0
3	A	1302	PX4	1	0
3	B	2001	PX4	6	0

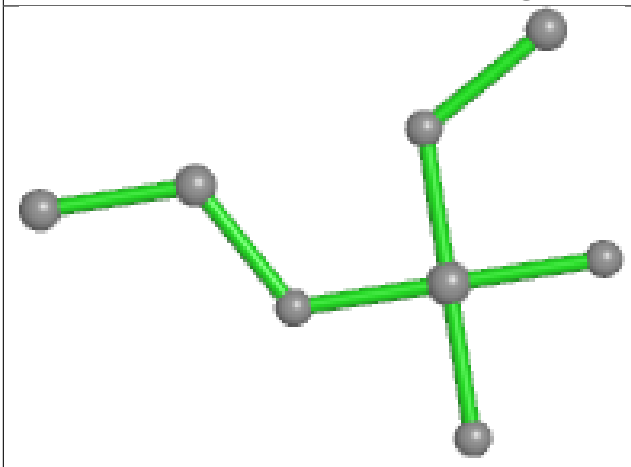
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

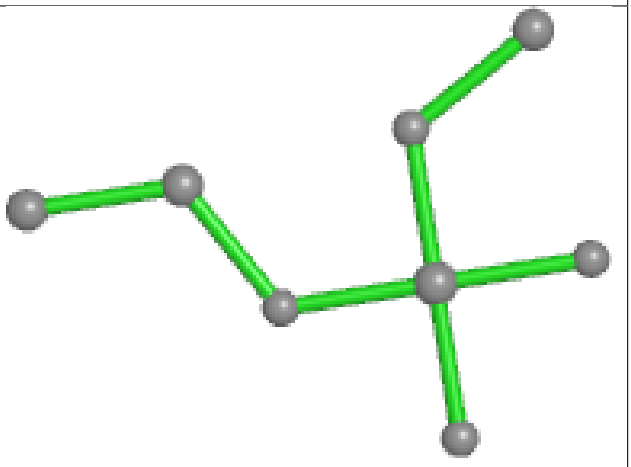
Ligand PX4 D 1304



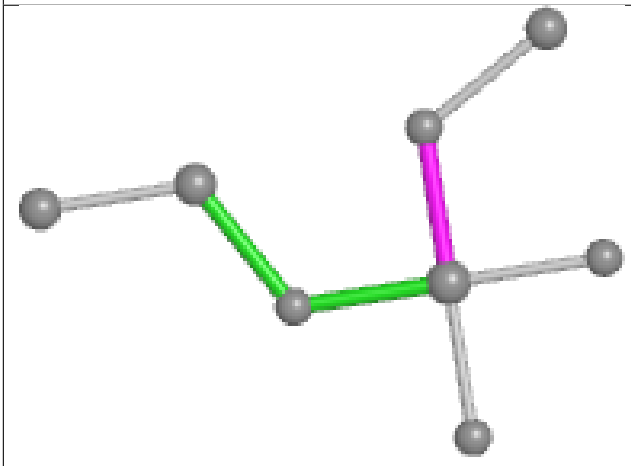
Ligand PX4 C 1302



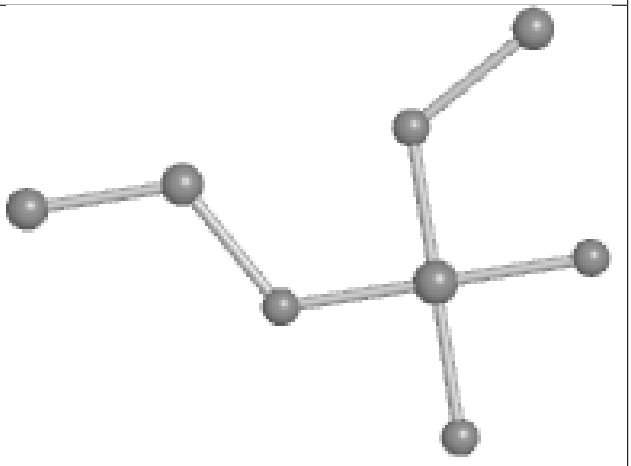
Bond lengths



Bond angles

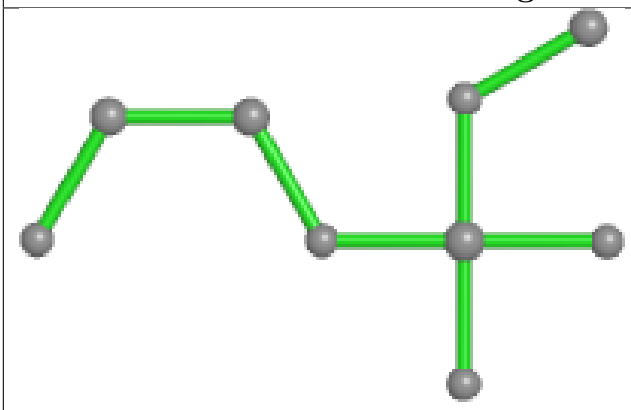


Torsions

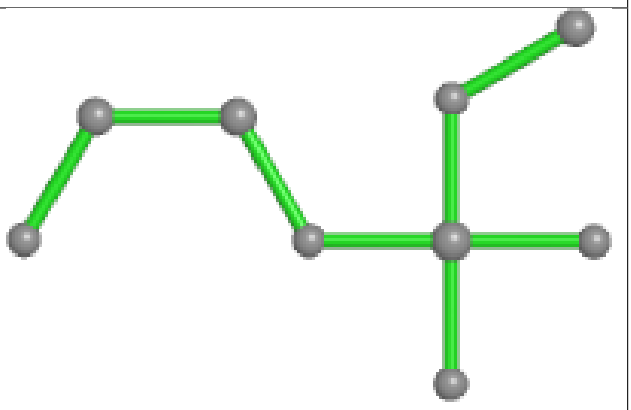


Rings

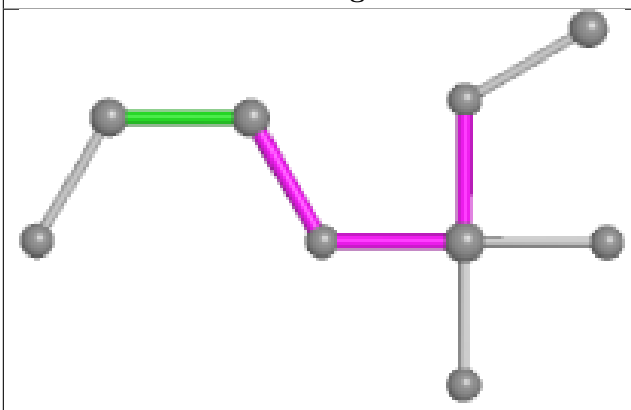
Ligand PX4 D 1305



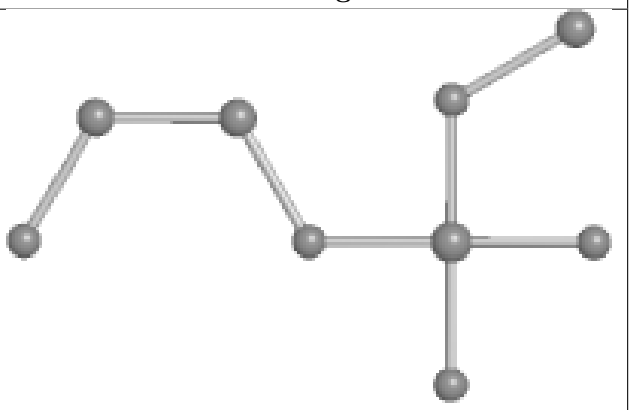
Bond lengths



Bond angles

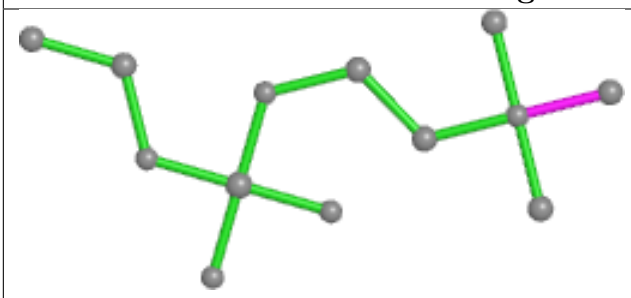


Torsions

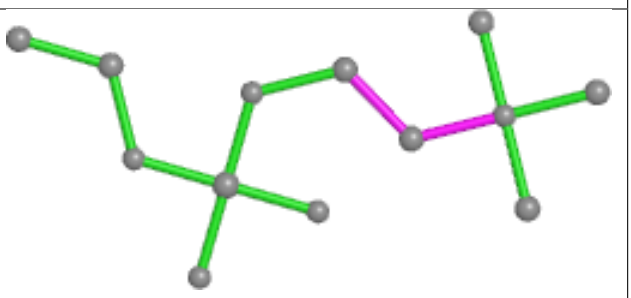


Rings

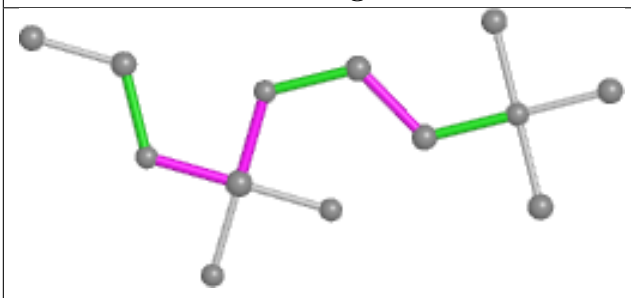
Ligand PX4 A 1303



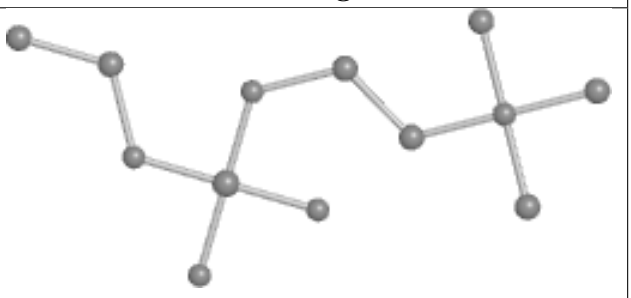
Bond lengths



Bond angles

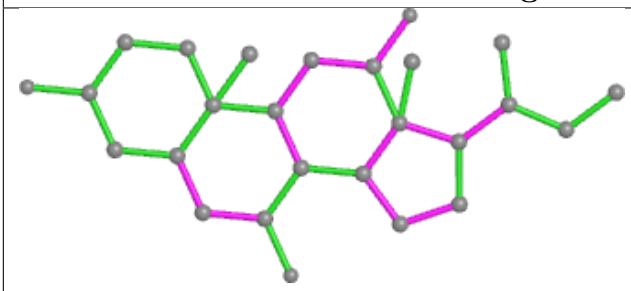


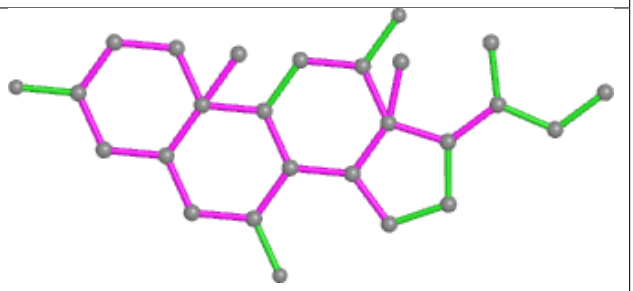
Torsions

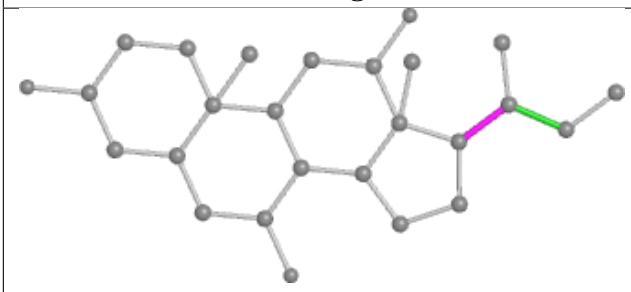


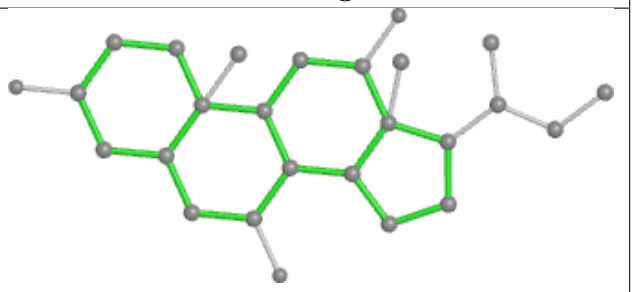
Rings

Ligand 1N7 C 1301

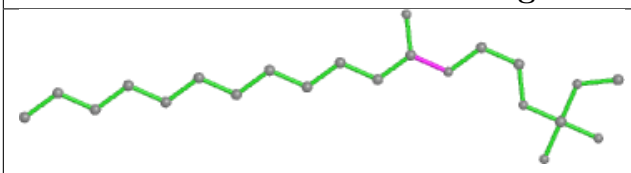

Bond lengths

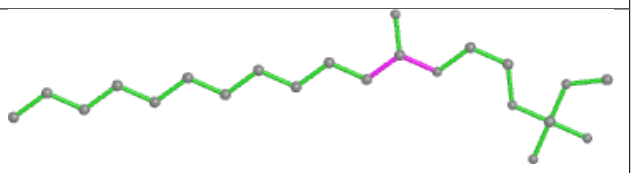

Bond angles

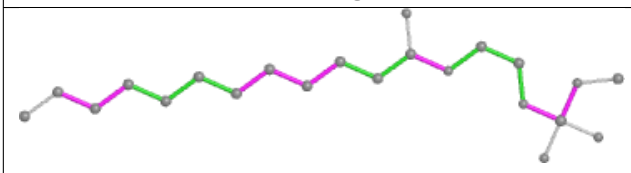

Torsions

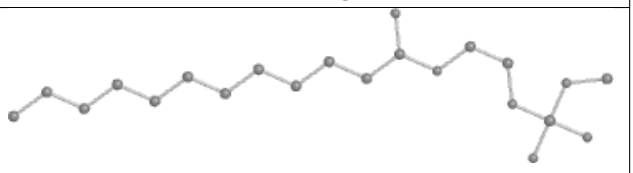

Rings

Ligand PX4 B 2006

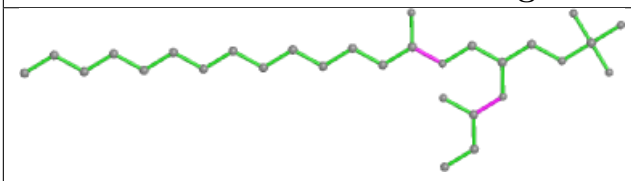

Bond lengths

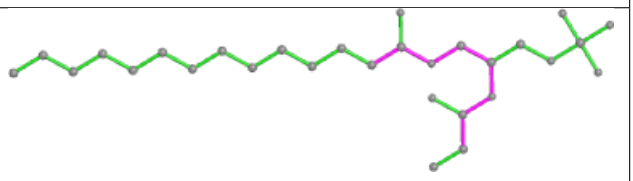

Bond angles

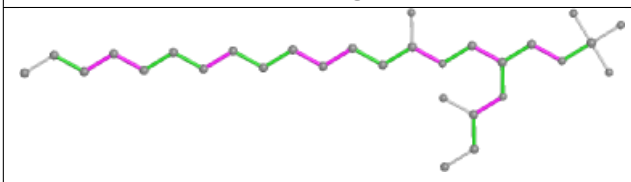

Torsions

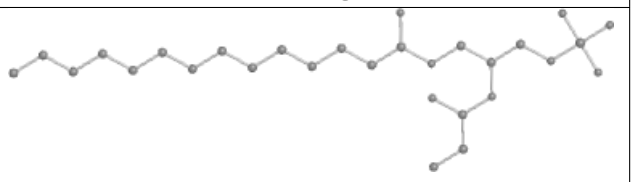

Rings

Ligand PX4 B 2005

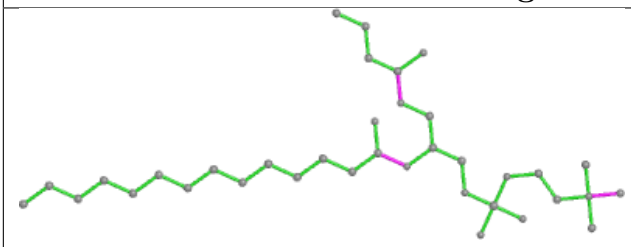

Bond lengths


Bond angles


Torsions


Rings

Ligand PX4 A 1304



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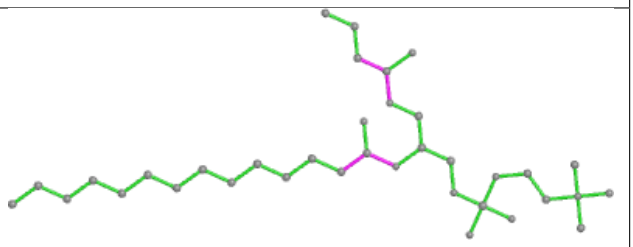
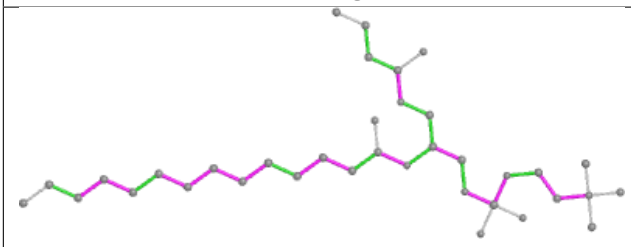
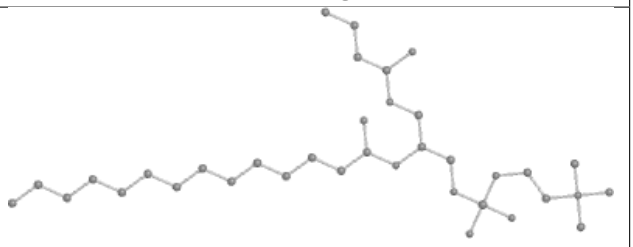


Bond angles

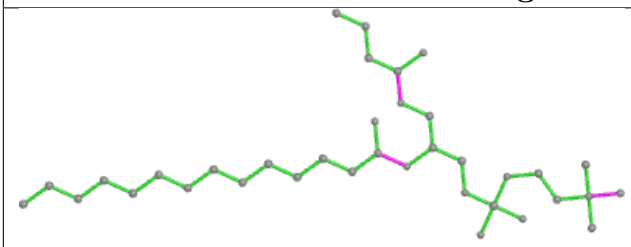


Torsions

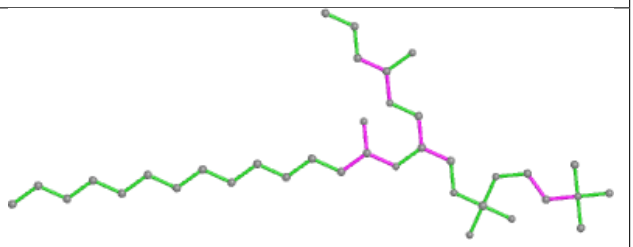


Rings

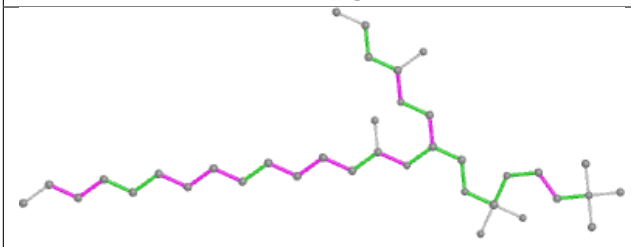
Ligand PX4 D 1302



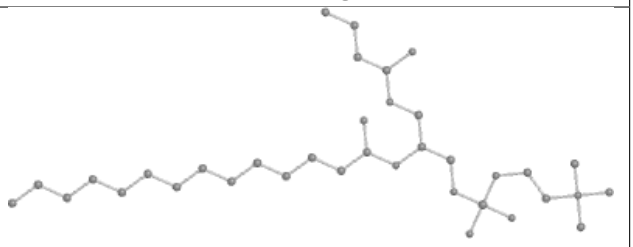
Bond lengths



Bond angles

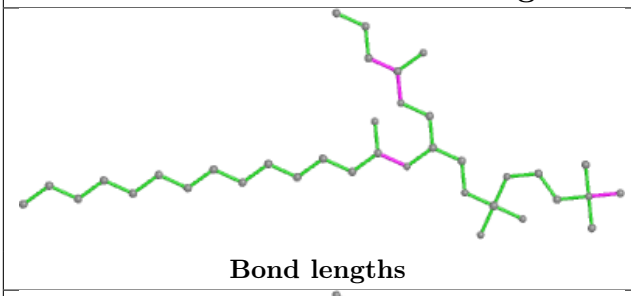


Torsions

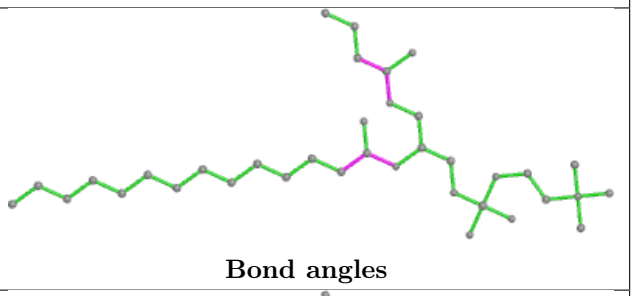


Rings

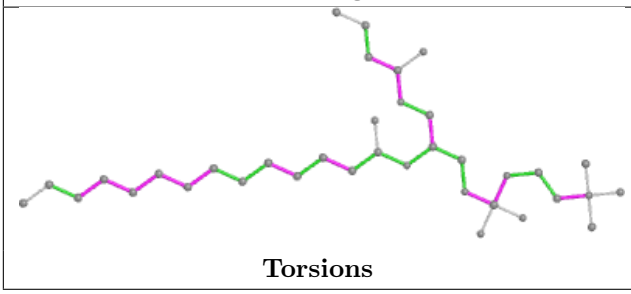
Ligand PX4 C 1303



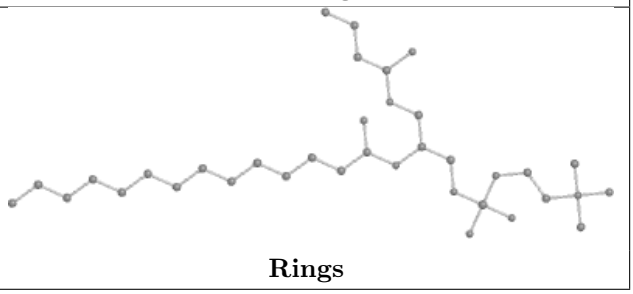
Bond lengths



Bond angles

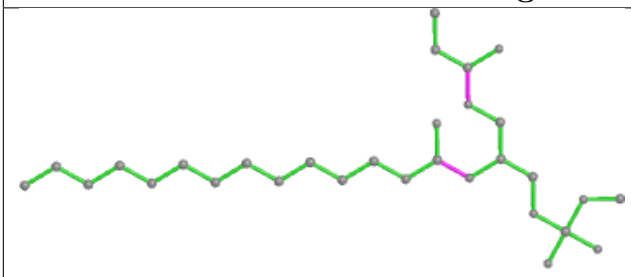


Torsions

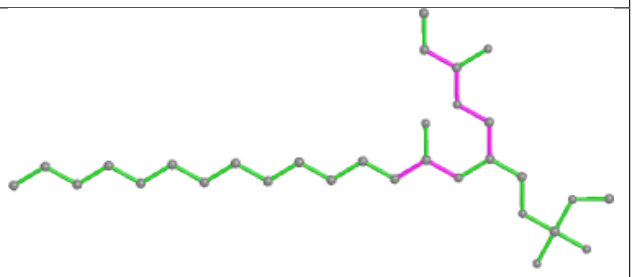


Rings

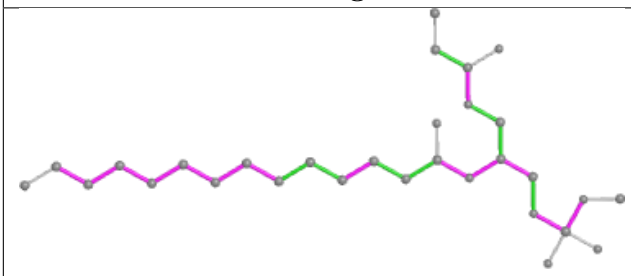
Ligand PX4 D 1303



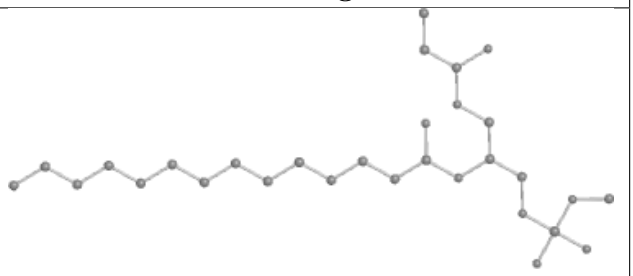
Bond lengths



Bond angles

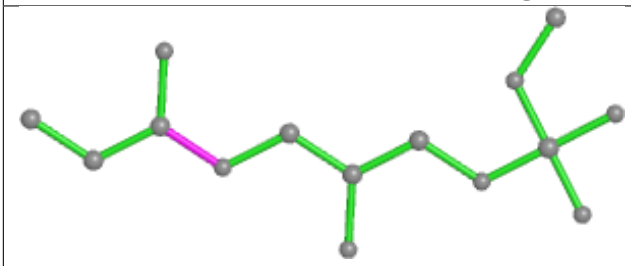


Torsions



Rings

Ligand PX4 B 2004



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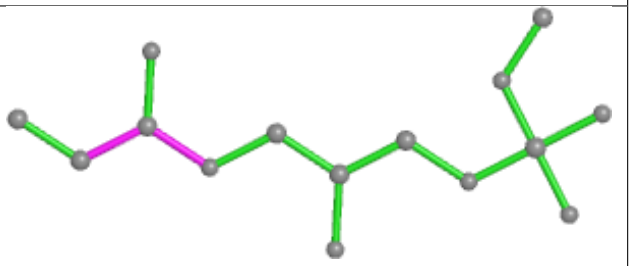
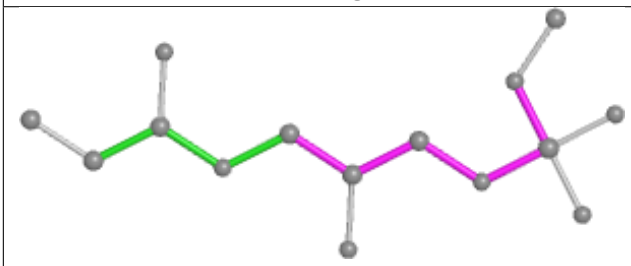
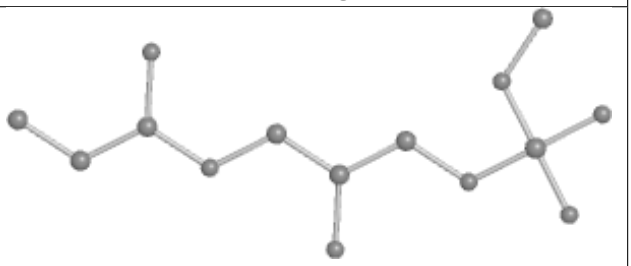


Bond angles

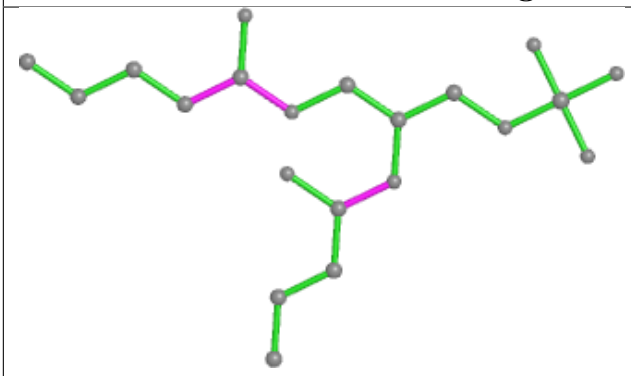


Torsions

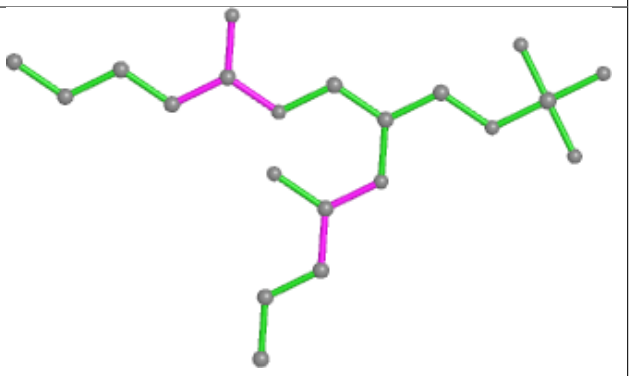


Rings

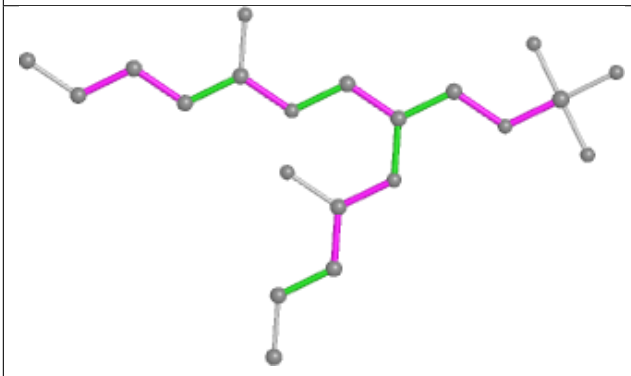
Ligand PX4 A 1302



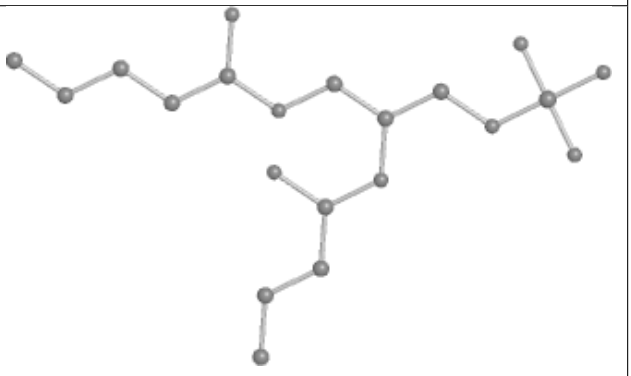
Bond lengths



Bond angles

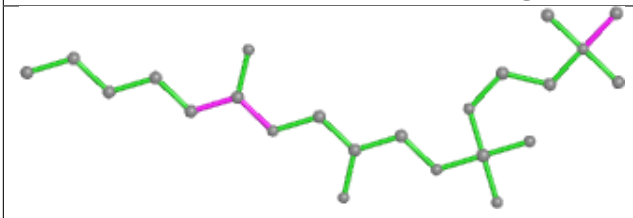


Torsions

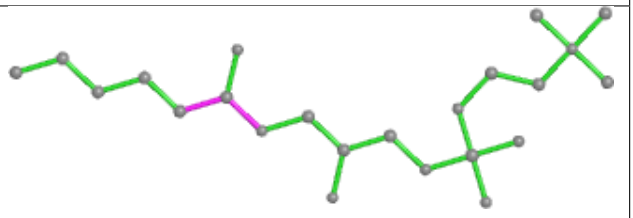


Rings

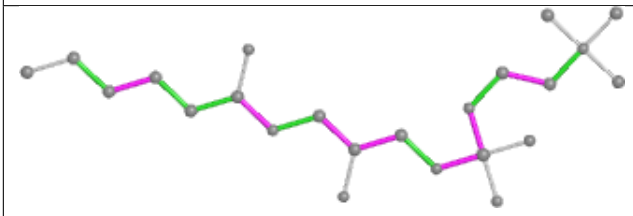
Ligand PX4 B 2002



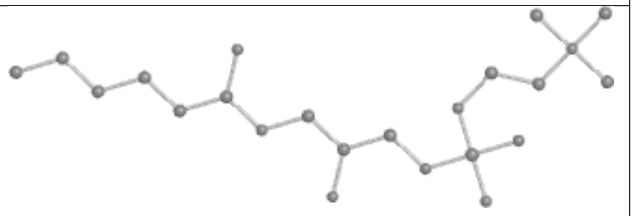
Bond lengths



Bond angles

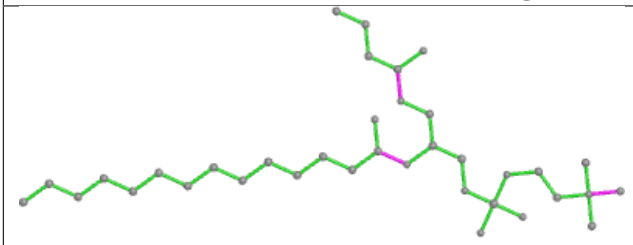


Torsions

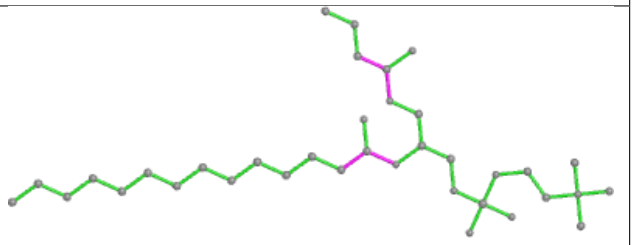


Rings

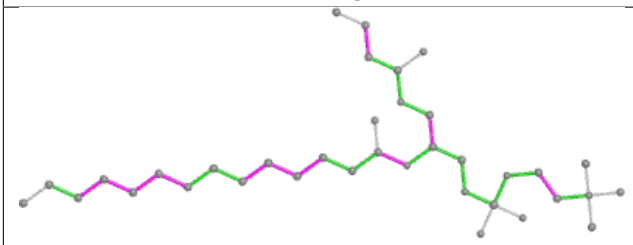
Ligand PX4 B 2001



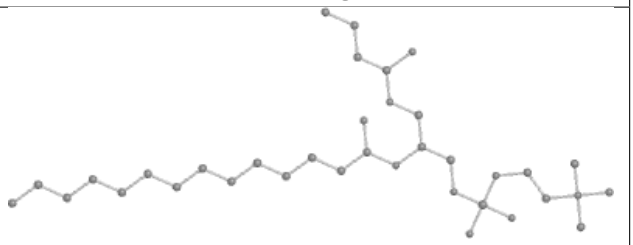
Bond lengths



Bond angles

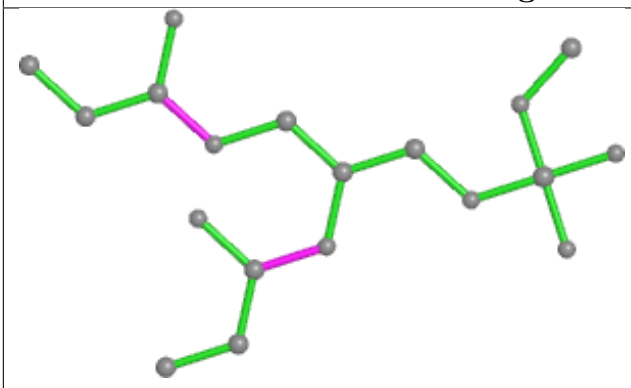


Torsions

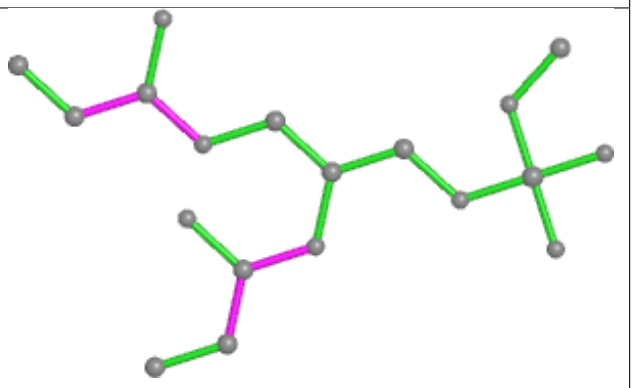


Rings

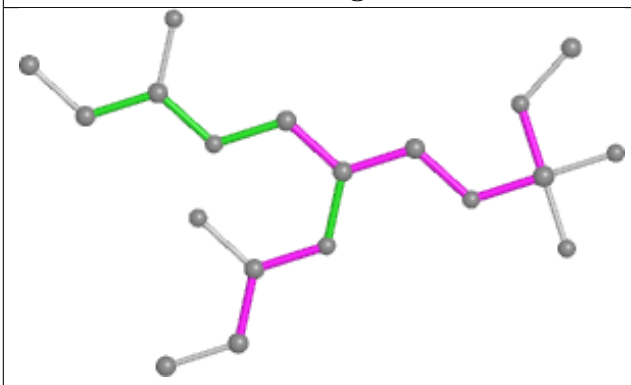
Ligand PX4 B 2003



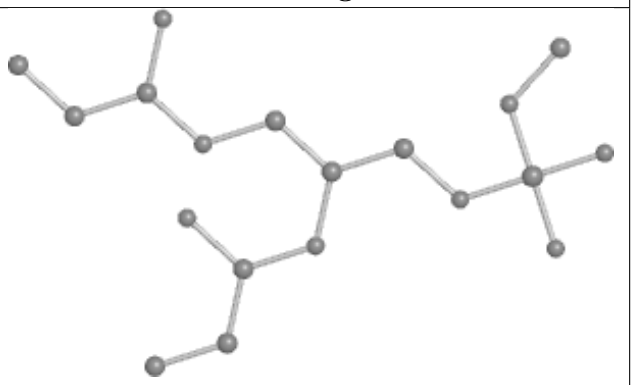
Bond lengths



Bond angles



Torsions



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	218/285 (76%)	0.33	15 (6%)	16	13	46, 109, 184, 366	0
1	B	217/285 (76%)	0.22	10 (4%)	32	29	42, 98, 180, 345	0
1	C	219/285 (76%)	0.53	13 (5%)	22	18	51, 105, 204, 404	0
1	D	218/285 (76%)	0.39	11 (5%)	28	25	51, 102, 193, 387	0
All	All	872/1140 (76%)	0.37	49 (5%)	24	20	42, 103, 191, 404	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1093	SER	44.6
1	D	1005	ILE	15.8
1	B	1009	VAL	10.4
1	C	1098	LEU	10.0
1	C	1002	TYR	9.7
1	D	1001	MET	8.7
1	C	1099	ARG	8.5
1	D	1093	SER	8.1
1	C	1094	GLY	7.7
1	D	1002	TYR	7.2
1	B	1091	THR	6.9
1	A	1005	ILE	6.8
1	D	1037	PHE	6.2
1	B	1095	PHE	5.7
1	C	1095	PHE	5.7
1	D	1041	PHE	5.5
1	A	1035	LYS	5.4
1	C	1047	LEU	5.2
1	B	1001	MET	4.9
1	D	1090	PRO	4.8
1	D	1196	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1065	TYR	4.0
1	A	1002	TYR	3.9
1	A	1004	ARG	3.4
1	D	1091	THR	3.4
1	C	1128	PRO	3.4
1	C	1065	TYR	3.3
1	B	1032	GLU	3.0
1	B	1077	SER	3.0
1	B	1092	SER	2.9
1	B	1034	SER	2.9
1	C	1068	ARG	2.9
1	C	1090	PRO	2.8
1	A	1037	PHE	2.7
1	D	1006	THR	2.7
1	A	1007	ASN	2.6
1	A	1088	LEU	2.6
1	A	1089	VAL	2.6
1	C	1069	ILE	2.6
1	A	1003	LEU	2.4
1	B	1064	ILE	2.4
1	C	1050	GLN	2.3
1	A	1001	MET	2.3
1	A	1070	SER	2.2
1	B	1071	PHE	2.2
1	A	1095	PHE	2.1
1	A	1044	TYR	2.1
1	A	1154	GLU	2.0
1	D	1095	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,

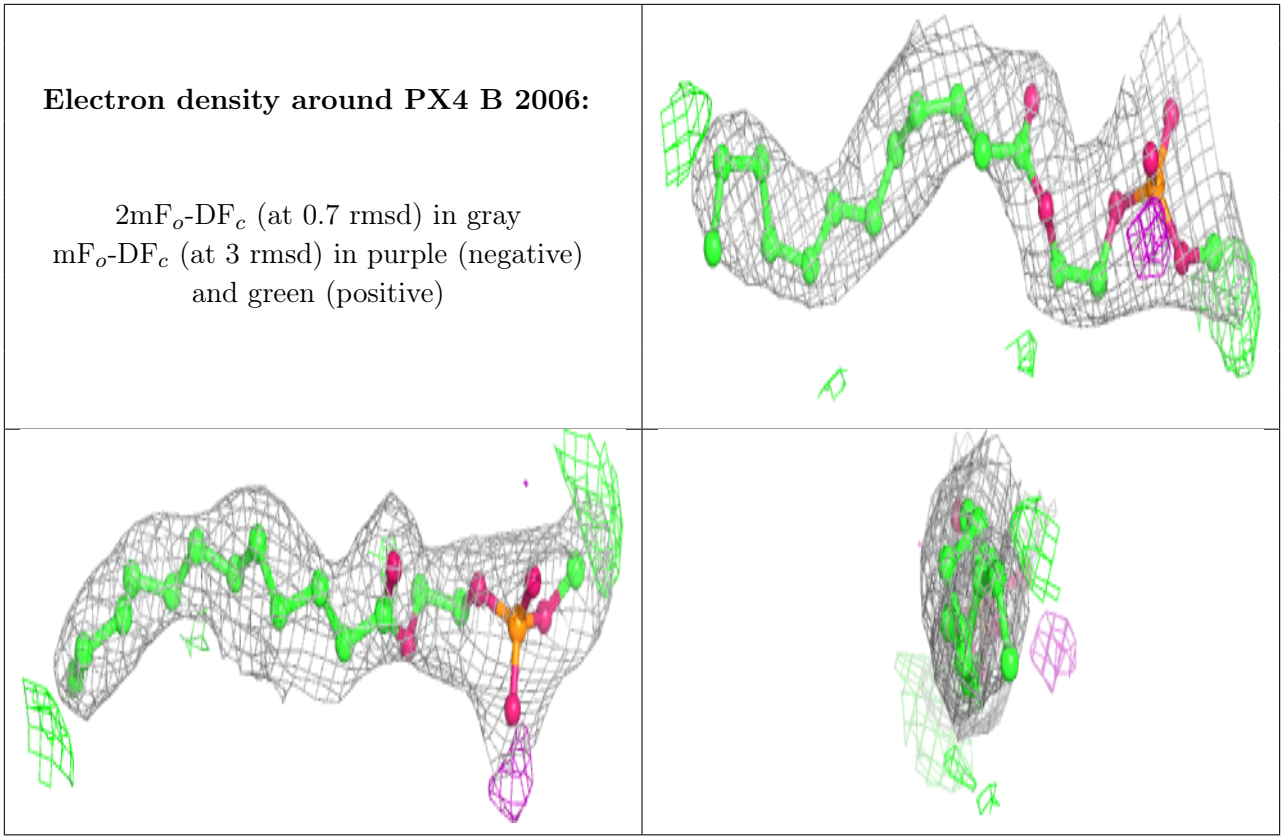
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	D	1301	5/5	-0.04	0.60	338,339,342,369	0
2	PO4	A	1301	5/5	0.78	0.31	329,338,347,364	0
3	PX4	B	2006	22/46	0.83	0.32	56,110,192,196	0
3	PX4	C	1302	8/46	0.85	0.25	94,143,232,233	0
3	PX4	A	1302	21/46	0.86	0.19	59,133,229,233	0
4	1N7	C	1301	26/43	0.87	0.33	83,121,175,206	0
3	PX4	B	2005	29/46	0.88	0.26	52,79,224,225	0
3	PX4	D	1304	36/46	0.89	0.39	60,102,242,245	0
3	PX4	A	1303	13/46	0.90	0.24	67,114,141,144	0
3	PX4	D	1303	30/46	0.90	0.31	45,108,180,184	0
3	PX4	B	2002	23/46	0.91	0.18	64,107,273,278	0
3	PX4	C	1303	36/46	0.92	0.25	37,97,222,223	0
3	PX4	B	2001	36/46	0.92	0.25	60,92,153,157	0
3	PX4	D	1305	9/46	0.93	0.11	109,113,211,211	0
3	PX4	A	1304	36/46	0.93	0.24	46,81,214,219	0
3	PX4	B	2004	15/46	0.94	0.17	72,88,217,217	0
3	PX4	B	2003	19/46	0.95	0.24	80,93,179,180	0
3	PX4	D	1302	36/46	0.95	0.29	50,83,177,182	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.

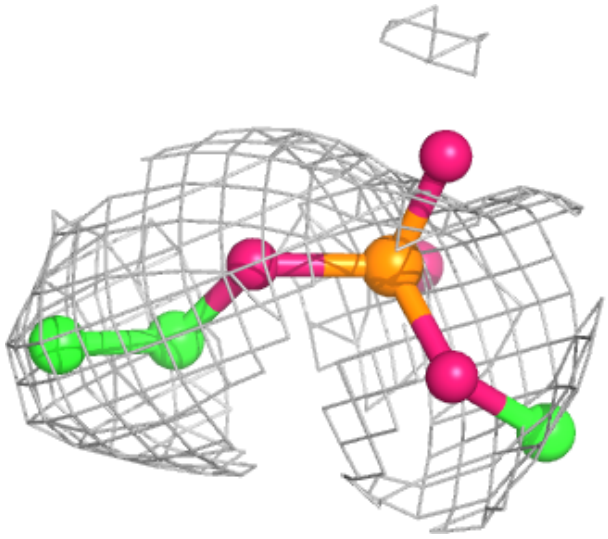
Electron density around PX4 B 2006:

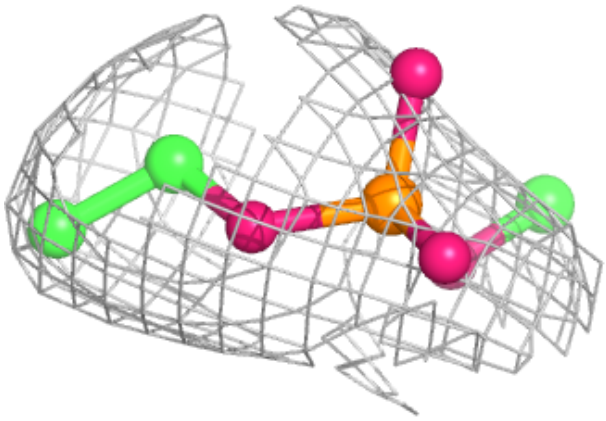
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

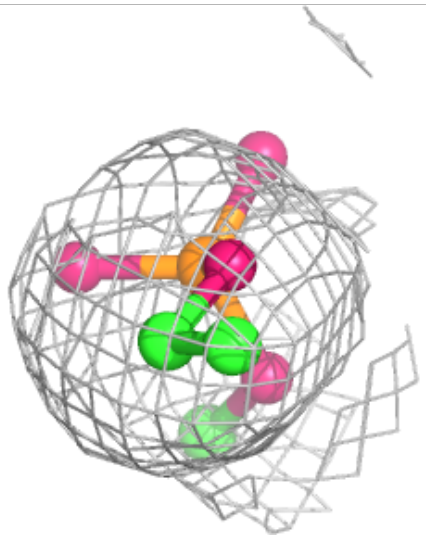


Electron density around PX4 C 1302:

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

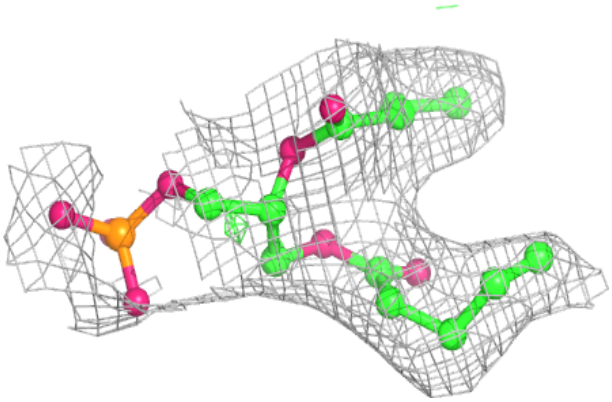


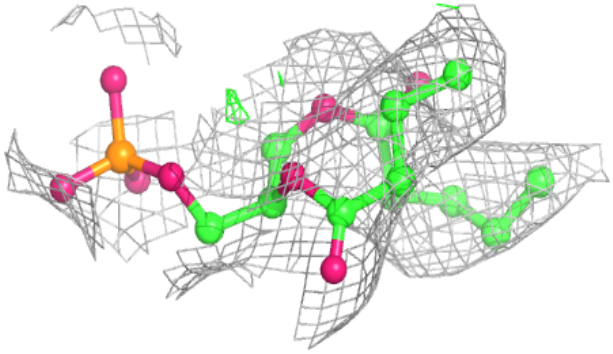


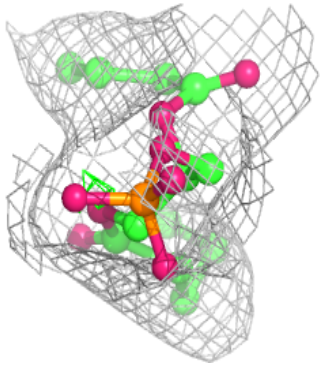


Electron density around PX4 A 1302:

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

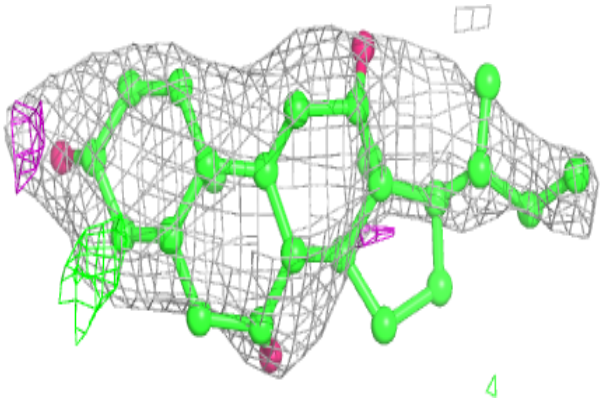


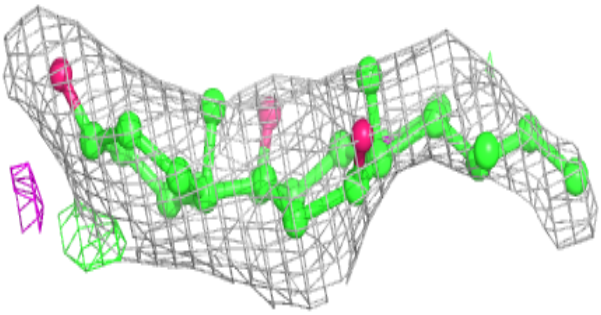


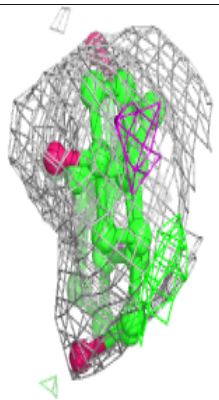


Electron density around 1N7 C 1301:

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

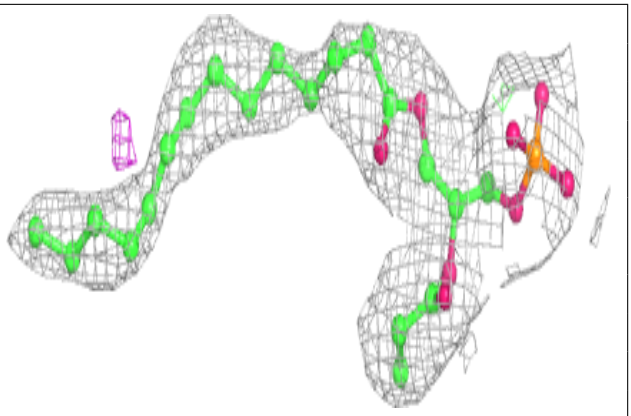


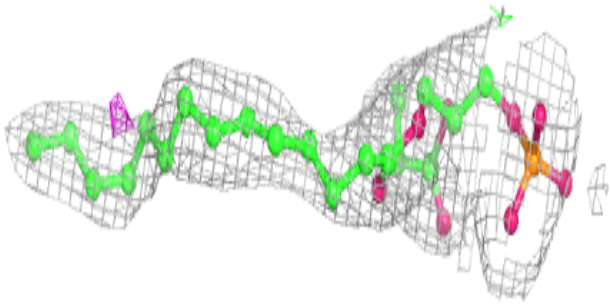


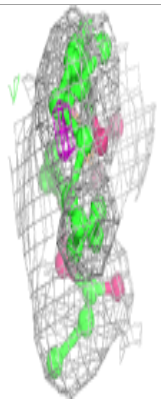


Electron density around PX4 B 2005:

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

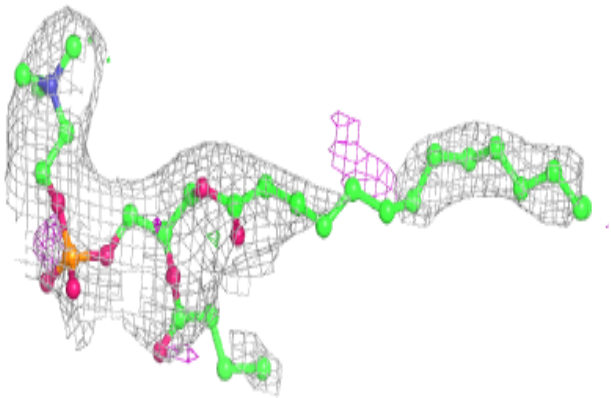


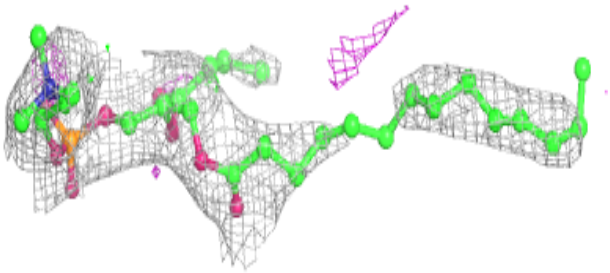


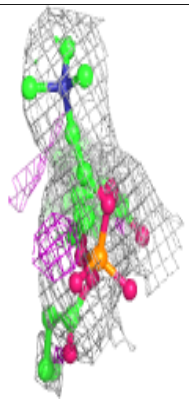


Electron density around PX4 D 1304:

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

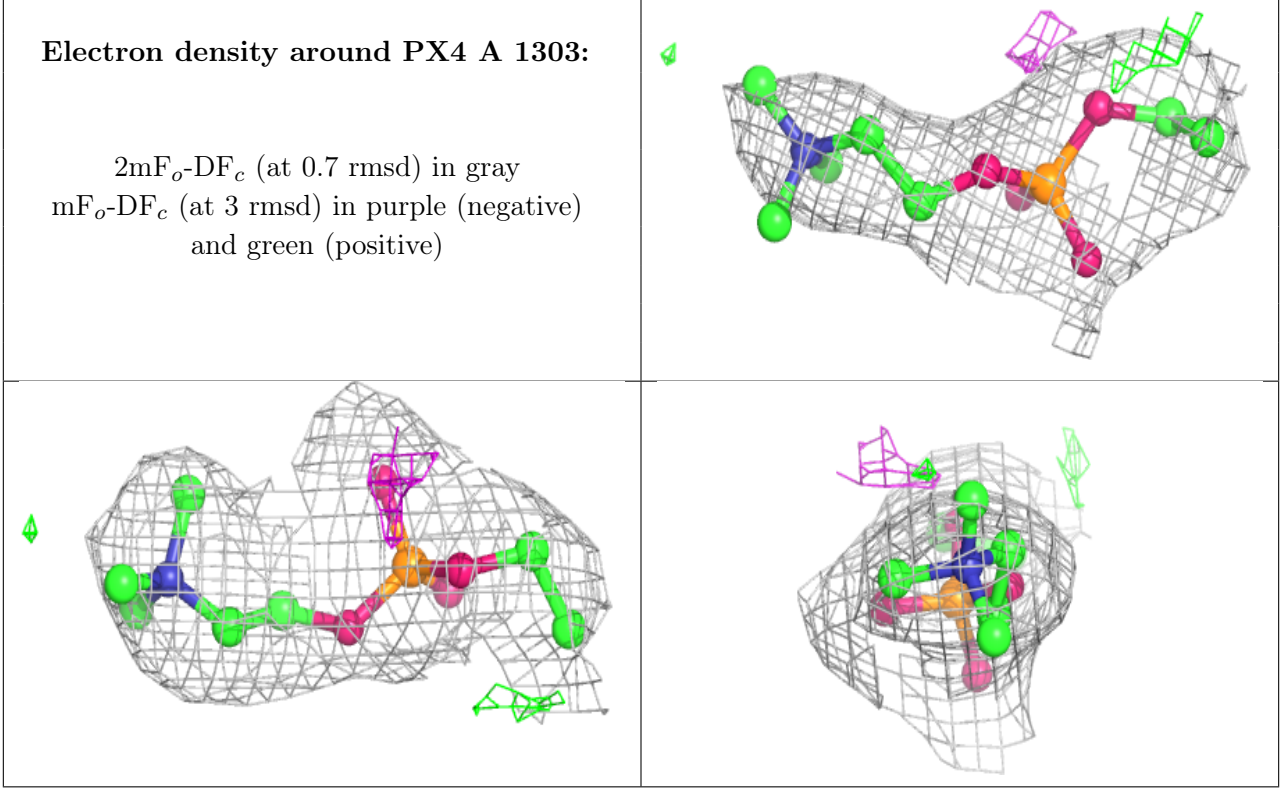






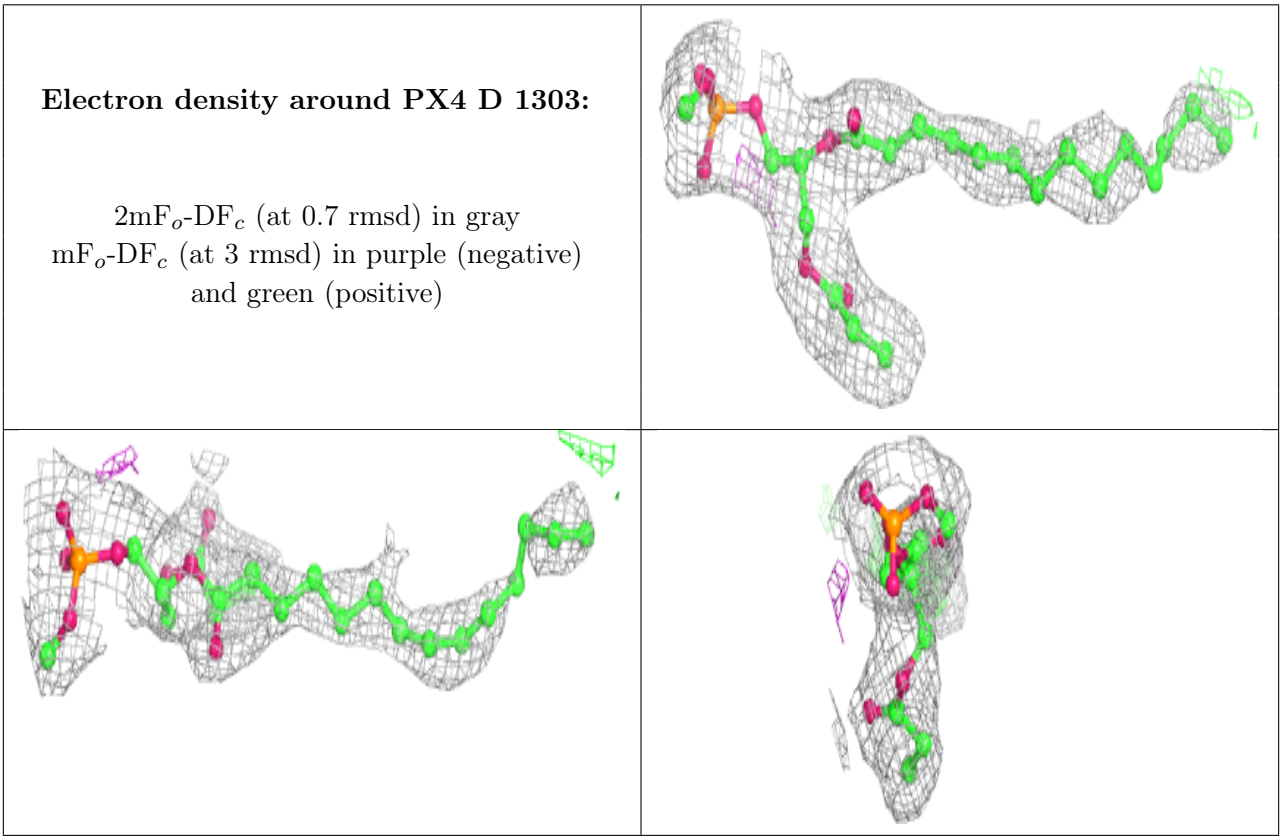
Electron density around PX4 A 1303:

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



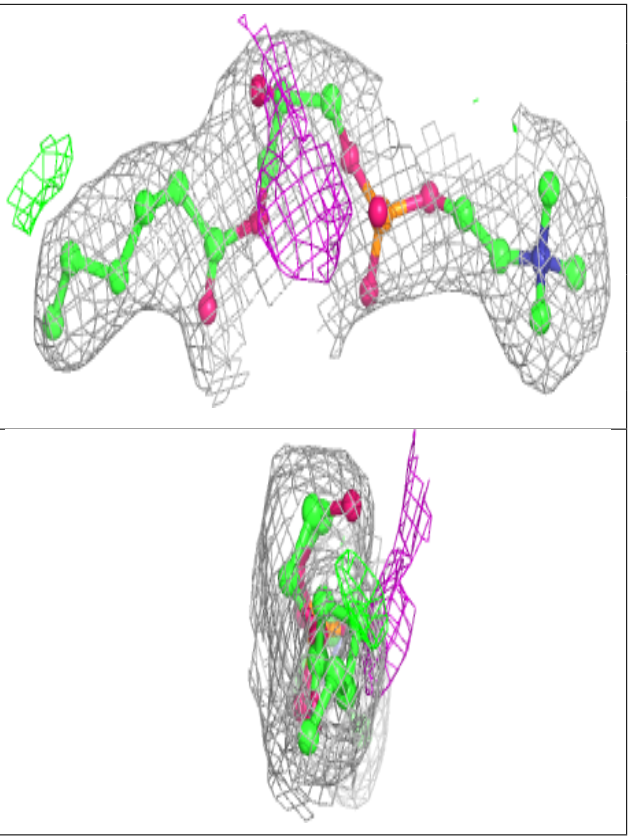
Electron density around PX4 D 1303:

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



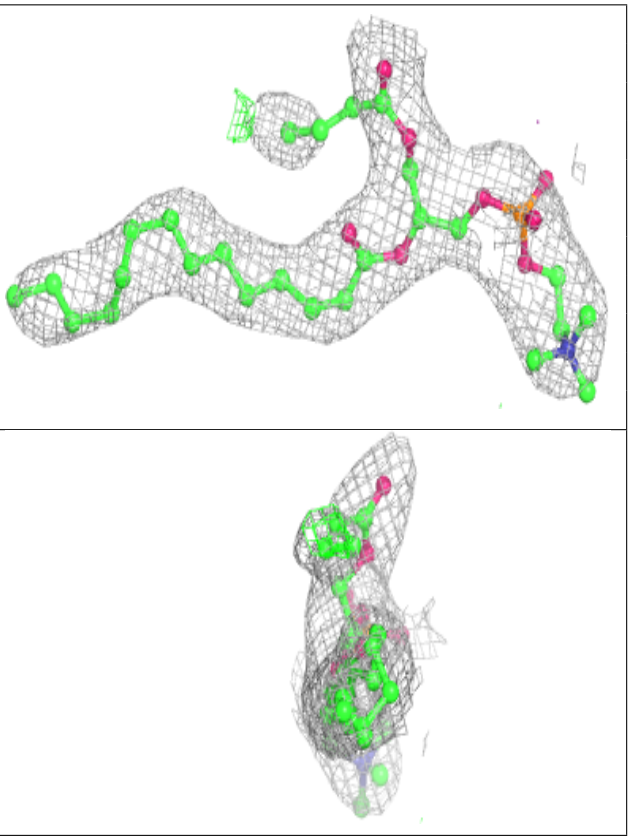
Electron density around PX4 B 2002:

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



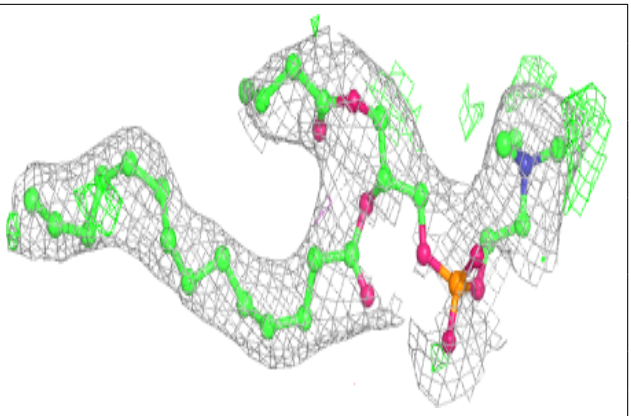
Electron density around PX4 C 1303:

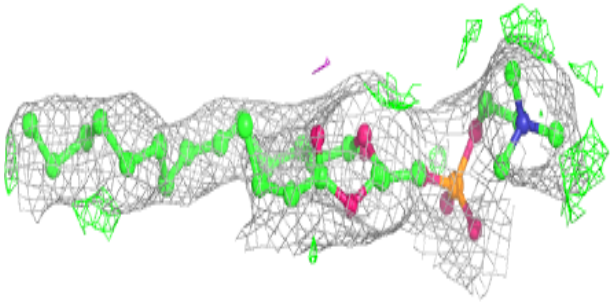
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

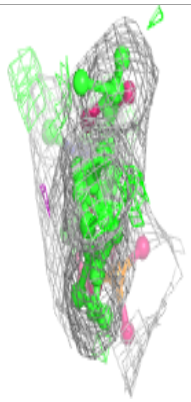


Electron density around PX4 B 2001:

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

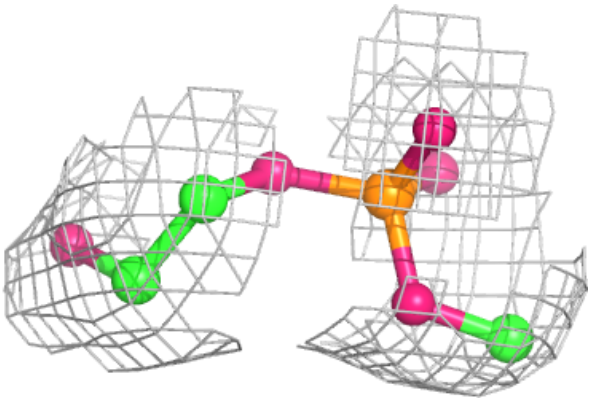


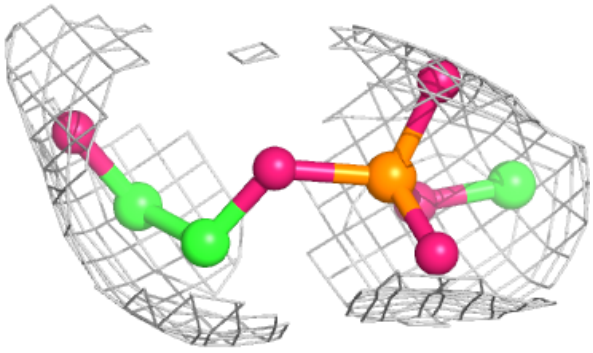


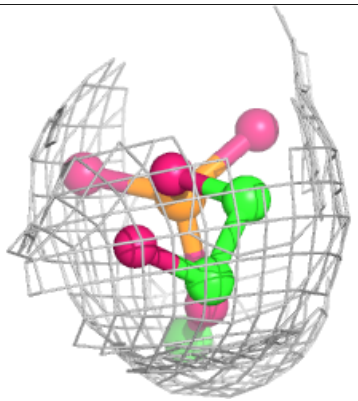


Electron density around PX4 D 1305:

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

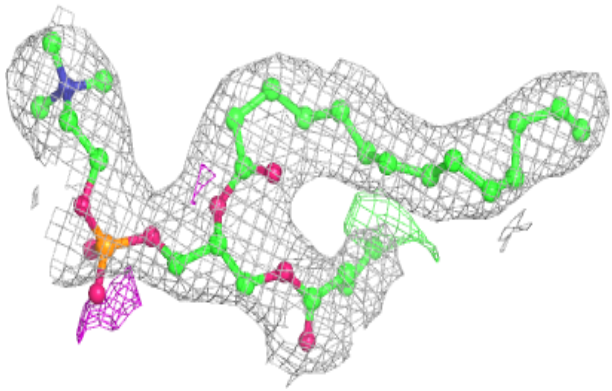


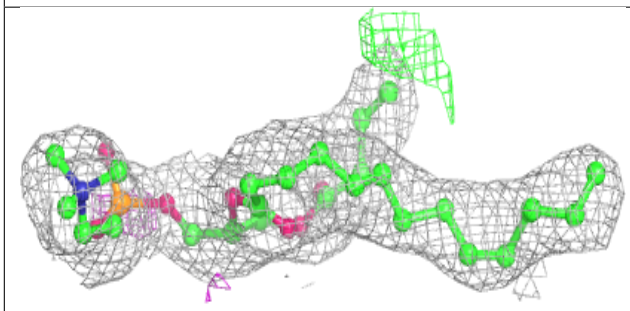


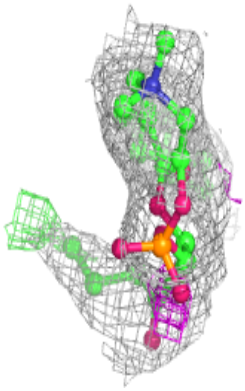


Electron density around PX4 A 1304:

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

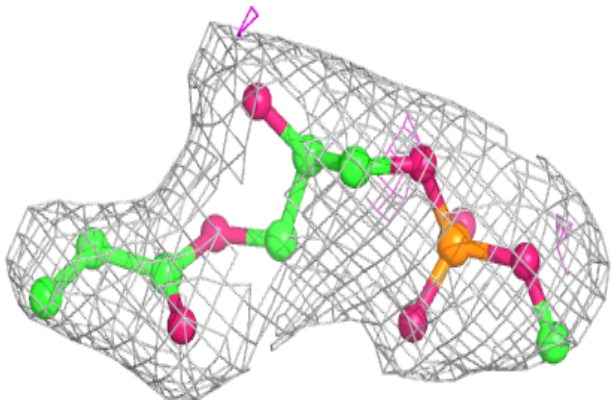


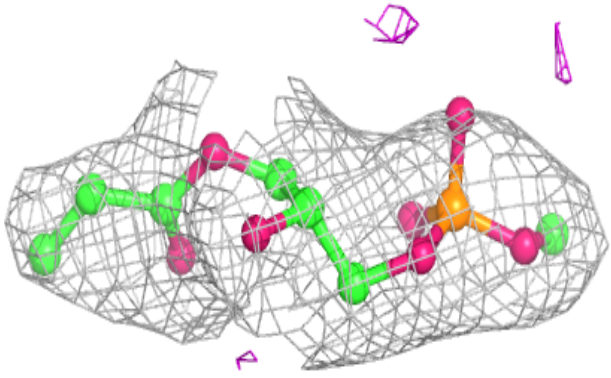


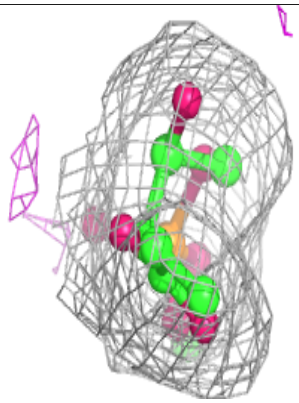


Electron density around PX4 B 2004:

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

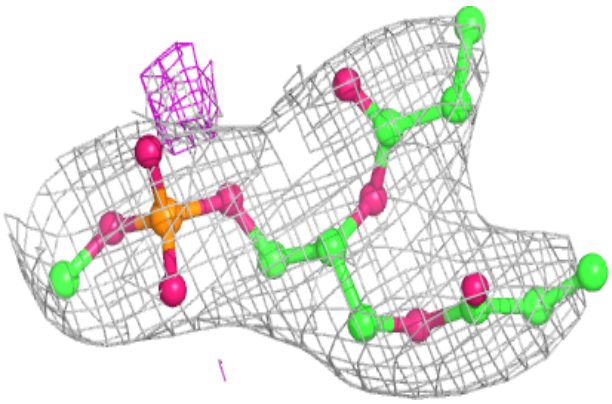


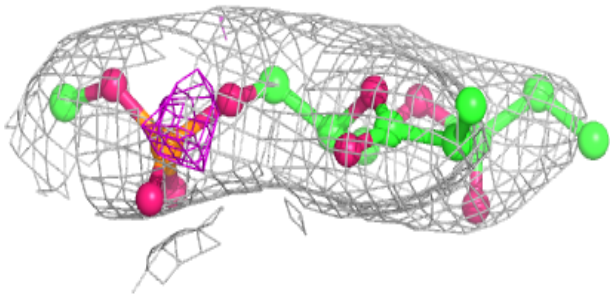


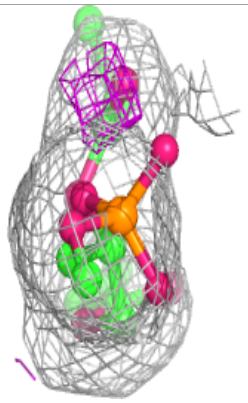


Electron density around PX4 B 2003:

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

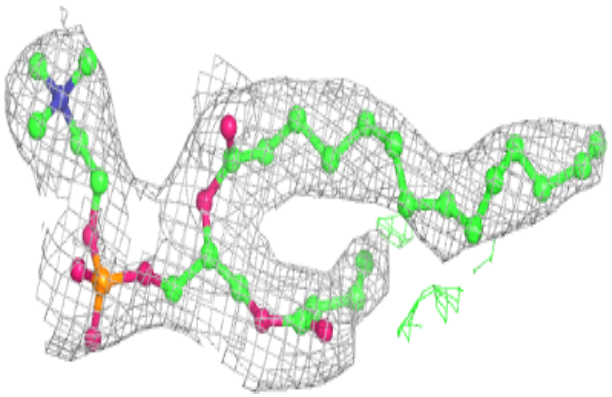


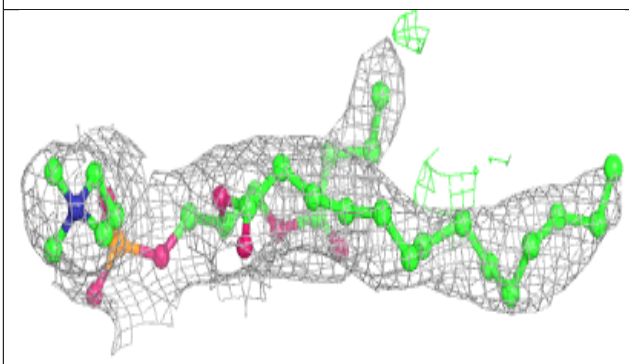


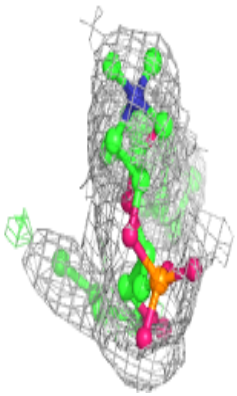


Electron density around PX4 D 1302:

$2mF_o$-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.