



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:11 PM UTC

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

This is a 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 ⓘ symbol.

The types of validation reports are described at

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

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

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

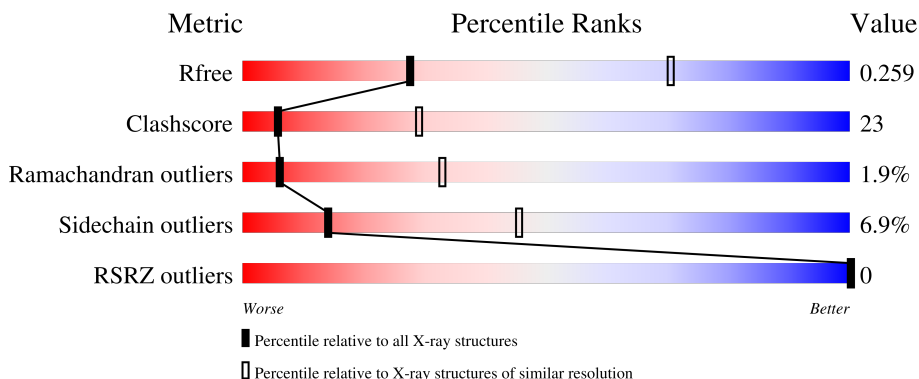
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	284	41% 29% 6% • 23%
1	B	284	44% 26% 7% 23%
1	C	284	44% 26% 6% 23%
1	D	284	44% 33% • 20%

2 Entry composition

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

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

- Molecule 1 is a protein called Ion transport protein.

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

There are 80 discrepancies between the modelled and reference sequences:

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

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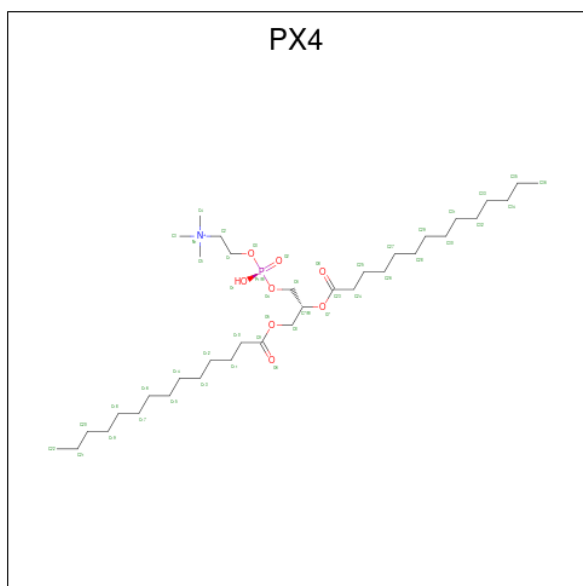
Chain	Residue	Modelled	Actual	Comment	Reference
B	985	TYR	-	expression tag	UNP A8EVM5
B	986	LYS	-	expression tag	UNP A8EVM5
B	987	ASP	-	expression tag	UNP A8EVM5
B	988	ASP	-	expression tag	UNP A8EVM5
B	989	ASP	-	expression tag	UNP A8EVM5
B	990	ASP	-	expression tag	UNP A8EVM5
B	991	LYS	-	expression tag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

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

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



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

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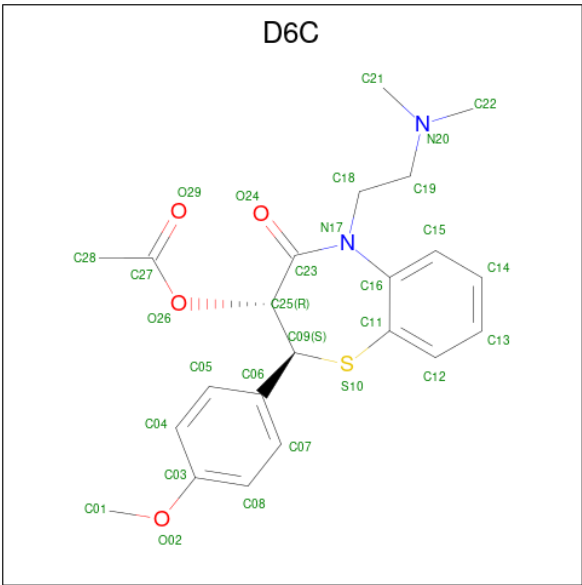
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 10 3 6 1	0	0
2	A	1	Total C O P 10 3 6 1	0	0
2	B	1	Total C O P 10 3 6 1	0	0
2	B	1	Total C O P 21 13 7 1	0	0
2	C	1	Total C O P 21 13 7 1	0	0
2	C	1	Total C O P 10 3 6 1	0	0
2	C	1	Total C O P 21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

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

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

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



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

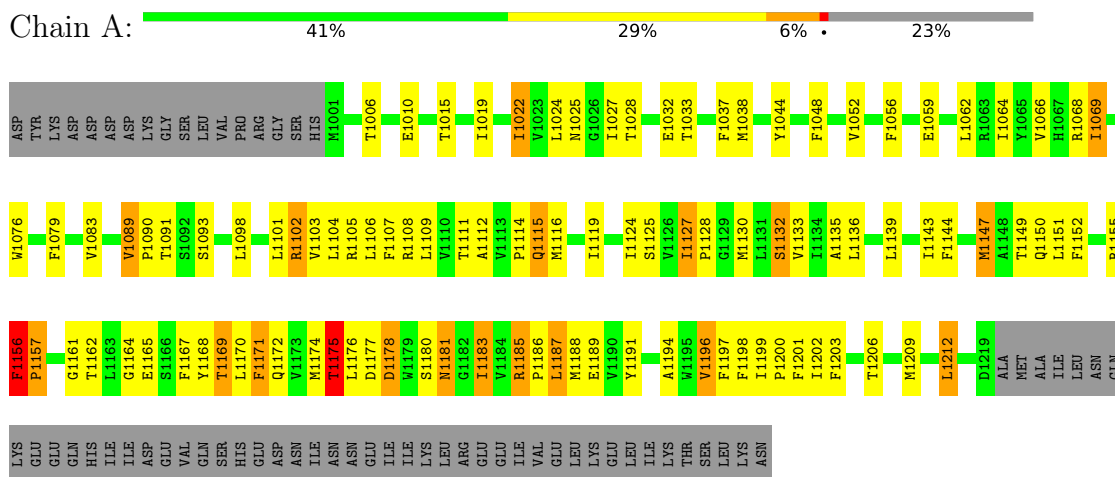
- Molecule 5 is water.

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

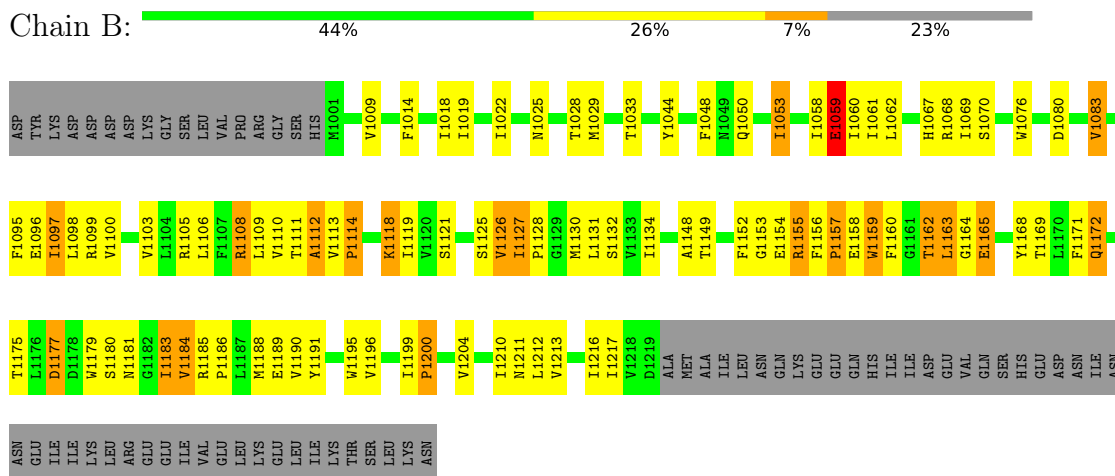
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ion transport protein



• Molecule 1: Ion transport protein



• Molecule 1: Ion transport protein



ASP	R1102	L1176	ILE
TTR	V1103	D1177	ILE
LYS	L1104	D1178	LYS
ASP	R1105	W1179	LEU
ASP	L1106	S1180	ARG
ASP	L1107	N1181	GLU
ASP	R1108	G1182	GLU
LYS	L1109	I1183	ILE
GLY	V1110	V1184	VAL
T1111	T1111	R1185	GLU
LEU	A1112	P1186	LEU
VAL	V1113	L1187	LYS
PRO	P1114	M1188	GLU
ARG	Q1115	W1195	LEU
GLY	M1116	V1196	ILE
SER	R1117	F1197	LYS
HIS	K1118	F1198	THR
HIS	I1119	I1199	SER
M1001	V1120	P1200	LEU
I1018	S1121	F1201	LYS
I1022	A1122	I1202	ASN
V1023	L1123	F1203	
L1024	I1124	V1204	
M1025	S1125	V1205	
		T1206	
T1028	L1131	F1207	
M1029	S1132	V1208	
	V1133	M1209	
	I1134		
E1032	A1135	I1217	
T1033	I1136	V1218	
	M1137	D1219	
F1048	F1140	ALA	ALA
N1049	F1144	MET	ALA
Q1050	A1145	ILE	LEU
I1053	I1146	LEU	ASN
T1054	M1147	GLN	LYS
T1057	A1148	LYS	GLU
I1058	T1149	GLU	GLU
E1059	Q1150	LYS	GLN
	I1151	GLN	HIS
R1063	F1152	ILE	ILE
		ASP	ASP
H1067	F1156	VAL	GLN
R1068	F1160	GLU	SER
I1069	G1161	GLU	HIS
S1070	T1162	VAL	GLU
	L1163	GLN	GLU
P1075	F1167	ASN	ASP
W1076	Y1168	ASN	ASN
		ILE	ILE
V1083	F1171	ASN	ASN
	Q1172	ASN	ASN
T1091	V1173	ASN	ASN
R1099	M1174	ASN	ASN
V1100	M1175	ASN	ASN
L1101		GLU	GLU

● Molecule 1: Ion transport protein



ASP	D1080	Y1168	VAL
TTR	W1083	L1169	GLN
LYS	T1091	L1170	SER
ASP	S1092	V1173	HIS
ASP	S1093	M1174	GLU
ASP	E1096	L1176	ASN
LYS	L1097	D1178	ASN
GLY	L1098	W1179	ASN
LEU	R1099	S1180	GLU
VAL	V1100	N1181	ILE
PRO	L1101	G1182	ILE
ARG	R1102	I1183	LYS
GLY	V1103	V1184	LEU
SER	L1106	R1185	ARG
HIS	F1107	P1186	GLU
M1001	L1108	L1187	GLU
Y1002	V1110	M1188	ILE
L1003	T1111	W1195	VAL
R1004	A1112	V1196	GLU
T1005	V1113	F1197	LEU
T1006	M1116	F1198	LEU
M1007	R1117	I1199	ILE
I1008	V1120	P1200	THR
W1009	I1124	F1201	SER
E1010	S1125	I1202	LEU
L1021	V1126	F1203	LYS
I1027	P1127	V1204	LEU
T1028	P1128	V1205	ASN
M1029	L1131	F1207	
	L1139		
G1042	L1143	I1210	
V1043	I1146	M1211	
Y1044	M1147	L1212	
T1045	A1148	V1213	
T1046	T1149	V1214	
L1047	F1152	A1215	
F1048	G1153	I1216	
	E1154	I1217	
I1051	R1155	V1218	
V1052	F1156	D1219	
I1055	P1157	A1220	
H1067	E1158	M1221	
R1068	W1159	I1223	
I1069	F1160	L1224	
S1070	G1161	E1228	
F1071	T1162	GLU	GLN
W1076	ASP	HIS	GLU
F1079	GLU	ILE	ILE
		ASP	ASP

4 Data and refinement statistics

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

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.06	9/1851 (0.5%)	1.05	5/2520 (0.2%)
1	B	1.06	2/1851 (0.1%)	1.17	14/2520 (0.6%)
1	C	1.14	6/1851 (0.3%)	1.15	14/2520 (0.6%)
1	D	1.00	2/1920 (0.1%)	1.05	7/2612 (0.3%)
All	All	1.06	19/7473 (0.3%)	1.11	40/10172 (0.4%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1181	ASN	C-O	-7.00	1.16	1.24
1	A	1183	ILE	C-O	-6.99	1.14	1.24
1	B	1181	ASN	C-O	-6.66	1.16	1.24
1	A	1187	LEU	C-O	-6.48	1.16	1.24
1	C	1113	VAL	CA-C	-6.42	1.48	1.53
1	C	1177	ASP	CA-C	-6.27	1.44	1.52
1	C	1113	VAL	N-CA	-6.24	1.42	1.46
1	C	1180	SER	CA-C	-6.17	1.44	1.52
1	A	1157	PRO	C-O	-6.14	1.15	1.24
1	A	1187	LEU	CA-C	-5.92	1.45	1.52
1	A	1189	GLU	CA-C	5.64	1.59	1.52
1	D	1173	VAL	CA-C	5.55	1.59	1.52
1	C	1184	VAL	CA-C	-5.37	1.47	1.52
1	B	1156	PHE	C-O	-5.23	1.18	1.24
1	C	1185	ARG	C-O	-5.22	1.19	1.24
1	A	1169	THR	CA-C	5.21	1.58	1.53
1	A	1157	PRO	N-CA	-5.11	1.41	1.47
1	D	1177	ASP	C-O	-5.01	1.18	1.24
1	A	1185	ARG	C-O	-5.00	1.20	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1183	ILE	N-CA-C	12.97	121.87	111.62
1	C	1116	MET	N-CA-C	-12.83	95.86	112.93
1	C	1181	ASN	N-CA-C	-10.80	99.48	111.14
1	B	1159	TRP	N-CA-C	10.54	122.85	111.36
1	B	1127	ILE	N-CA-C	9.60	123.88	112.35
1	B	1127	ILE	CB-CA-C	-8.28	103.16	114.00
1	C	1183	ILE	CA-C-N	-8.17	114.73	122.66
1	C	1183	ILE	C-N-CA	-8.17	114.73	122.66
1	C	1100	VAL	N-CA-C	-7.43	105.88	111.90
1	A	1183	ILE	N-CA-CB	-7.29	105.66	111.64
1	D	1218	VAL	N-CA-C	7.13	117.24	110.53
1	B	1183	ILE	N-CA-C	6.99	123.88	109.34
1	B	1108	ARG	N-CA-C	-6.91	103.67	111.07
1	A	1196	VAL	CB-CA-C	-6.89	103.15	111.97
1	B	1113	VAL	N-CA-C	6.73	113.69	107.56
1	C	1113	VAL	N-CA-C	6.62	113.58	107.56
1	A	1156	PHE	CA-C-N	6.48	125.71	118.97
1	A	1156	PHE	C-N-CA	6.48	125.71	118.97
1	C	1146	ILE	CB-CA-C	-6.30	103.77	112.02
1	C	1198	PHE	CA-C-O	-6.08	113.98	120.42
1	B	1157	PRO	CA-C-N	-6.01	112.42	120.54
1	B	1157	PRO	C-N-CA	-6.01	112.42	120.54
1	C	1179	TRP	N-CA-C	-6.01	104.65	111.14
1	D	1152	PHE	N-CA-C	5.99	117.61	111.14
1	D	1216	ILE	N-CA-C	-5.69	104.96	110.42
1	B	1112	ALA	CA-C-N	-5.63	118.77	122.60
1	B	1112	ALA	C-N-CA	-5.63	118.77	122.60
1	D	1224	LEU	N-CA-C	5.63	117.09	111.07
1	B	1126	VAL	N-CA-C	5.60	119.96	111.89
1	C	1199	ILE	CA-C-N	5.55	125.21	119.05
1	C	1199	ILE	C-N-CA	5.55	125.21	119.05
1	B	1155	ARG	N-CA-C	5.54	117.40	111.36
1	B	1059	GLU	N-CA-C	-5.47	105.31	111.28
1	B	1119	ILE	N-CA-C	5.42	116.19	110.72
1	D	1146	ILE	N-CA-C	-5.42	105.05	110.30
1	C	1091	THR	N-CA-C	5.31	117.82	111.71
1	C	1204	VAL	CB-CA-C	-5.29	105.11	111.88
1	D	1159	TRP	N-CA-C	5.12	116.94	111.36
1	C	1203	PHE	CB-CA-C	-5.10	103.11	110.96
1	D	1068	ARG	CB-CA-C	-5.08	110.31	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1800	0	1869	100	0
1	B	1800	0	1869	98	0
1	C	1800	0	1869	80	0
1	D	1869	0	1943	116	0
2	A	51	0	34	0	0
2	B	31	0	24	0	0
2	C	52	0	43	3	0
2	D	30	0	15	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	D	29	0	0	2	0
5	B	2	0	0	0	0
5	C	3	0	0	3	0
All	All	7469	0	7666	349	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (349) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:VAL:HG12	1:A:1090:PRO:CD	1.67	1.22
1:A:1089:VAL:CG1	1:A:1090:PRO:HD2	1.77	1.12
1:B:1168:TYR:HE2	1:D:1185:ARG:NE	1.48	1.10
1:D:1180:SER:O	1:D:1185:ARG:HG2	1.59	1.02
1:B:1217:ILE:HD12	1:D:1217:ILE:HG12	1.47	0.95
1:B:1127:ILE:HB	1:B:1128:PRO:HD3	1.48	0.94
1:B:1168:TYR:CE2	1:D:1185:ARG:NE	2.40	0.89
1:A:1089:VAL:HG12	1:A:1090:PRO:HD2	0.92	0.89
1:B:1217:ILE:CD1	1:D:1217:ILE:HG12	2.03	0.88
1:D:1126:VAL:HG11	1:D:1216:ILE:HG23	1.56	0.88
1:C:1196:VAL:O	1:C:1200:PRO:HG2	1.74	0.86
1:B:1095:PHE:HB2	1:B:1097:ILE:HG13	1.57	0.86
1:B:1018:ILE:HG21	1:B:1059:GLU:OE1	1.76	0.85
1:C:1160:PHE:HB2	5:C:1401:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1198:PHE:O	1:C:1202:ILE:HG13	1.77	0.84
1:A:1162:THR:HG23	1:A:1165:GLU:H	1.43	0.83
1:A:1090:PRO:O	1:A:1091:THR:HG22	1.79	0.82
1:B:1105:ARG:O	1:B:1108:ARG:HB3	1.80	0.81
1:B:1096:GLU:OE2	1:B:1099:ARG:CZ	2.30	0.80
1:A:1091:THR:HB	1:A:1102:ARG:NH2	1.97	0.79
1:C:1068:ARG:HG3	1:C:1069:ILE:N	1.96	0.79
1:A:1155:ARG:O	1:A:1157:PRO:HD2	1.82	0.78
1:C:1076:TRP:HB3	1:C:1111:THR:HG23	1.66	0.77
1:A:1032:GLU:HA	1:A:1038:MET:HE3	1.68	0.76
1:B:1155:ARG:HB3	1:B:1155:ARG:NH1	2.00	0.75
1:A:1090:PRO:O	1:A:1091:THR:CG2	2.35	0.75
1:D:1111:THR:O	1:D:1117:ARG:HD2	1.86	0.75
1:B:1080:ASP:OD1	1:B:1111:THR:HG21	1.86	0.74
1:D:1173:VAL:O	1:D:1176:LEU:HD23	1.88	0.74
1:B:1152:PHE:O	1:B:1154:GLU:N	2.22	0.72
1:D:1185:ARG:N	1:D:1186:PRO:CD	2.52	0.71
1:C:1146:ILE:HD12	1:D:1103:VAL:HG21	1.72	0.71
1:D:1174:MET:HG3	1:D:1205:VAL:HG11	1.72	0.71
1:C:1091:THR:O	1:C:1099:ARG:NH2	2.22	0.71
1:A:1079:PHE:CE1	1:A:1083:VAL:HG21	2.26	0.71
1:B:1155:ARG:HB3	1:B:1155:ARG:HH11	1.54	0.70
1:D:1213:VAL:HA	1:D:1216:ILE:HG13	1.72	0.70
1:A:1172:GLN:OE1	1:A:1183:ILE:HG13	1.92	0.70
1:A:1149:THR:HG21	1:C:1033:THR:HG23	1.74	0.69
1:C:1197:PHE:O	1:C:1200:PRO:HD2	1.93	0.69
1:B:1157:PRO:O	1:B:1158:GLU:C	2.33	0.68
1:D:1214:VAL:HA	1:D:1217:ILE:CG2	2.24	0.67
1:C:1195:TRP:CH2	2:C:1304:PX4:H16	2.28	0.67
1:D:1215:ALA:O	1:D:1219:ASP:N	2.24	0.67
1:A:1155:ARG:O	1:A:1157:PRO:CD	2.42	0.67
1:D:1218:VAL:HG22	1:D:1221:MET:CE	2.24	0.67
1:D:1185:ARG:HB2	1:D:1186:PRO:HD3	1.77	0.67
1:B:1022:ILE:CG2	1:B:1109:LEU:HB2	2.25	0.66
1:C:1025:ASN:HA	1:C:1028:THR:HG22	1.78	0.66
1:A:1089:VAL:CG1	1:A:1090:PRO:CD	2.55	0.66
1:A:1155:ARG:C	1:A:1157:PRO:CD	2.69	0.66
1:B:1177:ASP:OD2	1:D:1180:SER:N	2.28	0.66
1:C:1188:MET:CE	1:D:1168:TYR:CZ	2.79	0.65
1:D:1126:VAL:CG1	1:D:1216:ILE:HG23	2.24	0.65
1:D:1218:VAL:CG2	1:D:1221:MET:CE	2.74	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1106:LEU:HB2	1:D:1143:ILE:HG12	1.79	0.65
1:B:1169:THR:O	1:B:1172:GLN:HB3	1.97	0.65
1:A:1155:ARG:C	1:A:1157:PRO:HD3	2.22	0.64
1:D:1068:ARG:HG3	1:D:1069:ILE:H	1.63	0.64
1:C:1156:PHE:HB2	5:C:1401:HOH:O	1.98	0.64
1:B:1112:ALA:O	1:B:1114:PRO:HD3	1.97	0.64
1:A:1006:THR:HG23	1:A:1066:VAL:HG13	1.80	0.64
1:D:1170:LEU:HD21	1:D:1197:PHE:HE1	1.61	0.64
1:B:1168:TYR:CE2	1:D:1185:ARG:CZ	2.81	0.64
1:B:1095:PHE:HB2	1:B:1097:ILE:CG1	2.27	0.63
1:C:1199:ILE:O	1:C:1202:ILE:HB	1.98	0.63
1:C:1083:VAL:HG11	1:C:1105:ARG:HA	1.81	0.63
1:C:1167:PHE:HB3	2:C:1302:PX4:O6	1.99	0.63
1:A:1177:ASP:OD2	1:B:1180:SER:N	2.32	0.62
1:C:1068:ARG:CG	1:C:1069:ILE:H	2.11	0.62
1:A:1172:GLN:NE2	1:B:1180:SER:OG	2.31	0.62
1:B:1022:ILE:HG21	1:B:1109:LEU:HB2	1.80	0.62
1:C:1068:ARG:HG3	1:C:1069:ILE:H	1.62	0.62
1:D:1068:ARG:HG3	1:D:1069:ILE:N	2.15	0.61
1:D:1048:PHE:HA	1:D:1051:ILE:HD12	1.82	0.61
1:D:1185:ARG:N	1:D:1186:PRO:HD2	2.15	0.61
1:C:1147:MET:HE3	1:D:1100:VAL:O	2.00	0.61
1:A:1172:GLN:OE1	1:A:1183:ILE:CG1	2.49	0.60
1:B:1096:GLU:O	1:B:1099:ARG:N	2.34	0.59
1:D:1079:PHE:CZ	1:D:1083:VAL:HG21	2.37	0.59
1:A:1116:MET:HA	1:A:1119:ILE:HG22	1.84	0.59
1:A:1164:GLY:O	1:A:1167:PHE:N	2.36	0.59
1:B:1022:ILE:HD11	1:B:1108:ARG:HG3	1.83	0.59
1:B:1159:TRP:O	1:B:1165:GLU:O	2.21	0.59
1:B:1168:TYR:HE2	1:D:1185:ARG:CZ	2.11	0.59
1:B:1160:PHE:CZ	1:B:1169:THR:HG21	2.38	0.58
1:C:1150:GLN:HE21	1:D:1100:VAL:HG13	1.69	0.58
1:C:1195:TRP:CZ3	2:C:1304:PX4:H16	2.38	0.58
1:B:1110:VAL:HG23	1:D:1139:LEU:CD2	2.33	0.58
1:C:1188:MET:HE2	1:D:1168:TYR:CZ	2.38	0.57
1:D:1180:SER:C	1:D:1185:ARG:HG2	2.28	0.57
1:D:1217:ILE:HG13	1:D:1217:ILE:O	2.01	0.57
1:A:1068:ARG:HG3	1:A:1069:ILE:H	1.70	0.56
1:C:1067:HIS:HB3	1:C:1070:SER:HB2	1.87	0.56
1:C:1121:SER:HA	1:C:1124:ILE:HD12	1.87	0.56
1:A:1194:ALA:O	1:A:1198:PHE:HD1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1196:VAL:O	1:B:1200:PRO:HG2	2.05	0.56
1:D:1155:ARG:O	1:D:1157:PRO:HD3	2.06	0.56
1:A:1033:THR:HG21	1:B:1163:LEU:HB2	1.86	0.56
1:A:1124:ILE:O	1:A:1127:ILE:HB	2.06	0.56
1:A:1089:VAL:HG12	1:A:1090:PRO:HD3	1.79	0.56
1:C:1183:ILE:O	1:C:1187:LEU:HD13	2.06	0.56
1:A:1076:TRP:H	1:A:1076:TRP:CD1	2.23	0.56
1:A:1090:PRO:C	1:A:1091:THR:HG22	2.31	0.55
1:A:1068:ARG:HG3	1:A:1069:ILE:N	2.22	0.55
1:B:1105:ARG:HG3	1:B:1106:LEU:HD23	1.87	0.55
1:A:1089:VAL:CB	1:A:1090:PRO:HD2	2.34	0.55
1:B:1050:GLN:HA	1:B:1053:ILE:HG22	1.89	0.55
1:A:1091:THR:HB	1:A:1102:ARG:HH21	1.71	0.54
1:B:1100:VAL:HG12	1:D:1147:MET:HG2	1.88	0.54
1:D:1212:LEU:O	1:D:1216:ILE:HG13	2.07	0.54
1:A:1171:PHE:HE1	1:A:1175:THR:HG23	1.73	0.54
1:B:1022:ILE:CD1	1:B:1108:ARG:HG3	2.38	0.54
1:B:1168:TYR:HE2	1:D:1185:ARG:CD	2.21	0.54
1:C:1112:ALA:O	1:C:1114:PRO:HD3	2.08	0.53
1:D:1147:MET:HB3	1:D:1197:PHE:HE2	1.74	0.53
1:D:1176:LEU:HD23	1:D:1176:LEU:N	2.23	0.53
1:D:1174:MET:C	1:D:1176:LEU:H	2.15	0.53
1:D:1148:ALA:HB1	1:D:1160:PHE:CD1	2.44	0.53
1:A:1168:TYR:OH	1:B:1184:VAL:HB	2.07	0.53
1:B:1172:GLN:NE2	1:D:1180:SER:HB3	2.24	0.53
1:D:1218:VAL:HG22	1:D:1221:MET:HE3	1.90	0.53
1:B:1058:ILE:HD13	1:B:1061:ILE:HD12	1.91	0.53
1:B:1118:LYS:HD3	1:B:1118:LYS:N	2.23	0.53
1:D:1043:VAL:HA	1:D:1046:THR:OG1	2.09	0.53
1:D:1218:VAL:HG23	1:D:1221:MET:CE	2.39	0.53
1:A:1064:ILE:O	1:A:1068:ARG:N	2.42	0.52
1:A:1197:PHE:CD1	1:A:1197:PHE:C	2.87	0.52
1:D:1124:ILE:HG23	1:D:1127:ILE:HD12	1.90	0.52
1:A:1104:LEU:O	1:A:1107:PHE:HB2	2.09	0.52
1:B:1162:THR:HG22	1:B:1164:GLY:N	2.24	0.52
1:A:1198:PHE:O	1:A:1201:PHE:HB3	2.09	0.52
1:A:1025:ASN:O	1:A:1028:THR:HG22	2.09	0.52
1:D:1029:MET:SD	1:D:1103:VAL:HG23	2.49	0.52
1:D:1214:VAL:HA	1:D:1217:ILE:HG23	1.90	0.52
1:C:1025:ASN:HA	1:C:1028:THR:CG2	2.40	0.52
1:C:1188:MET:HE1	1:D:1168:TYR:CZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1106:LEU:HD23	1:B:1106:LEU:N	2.25	0.52
1:B:1210:ILE:C	1:B:1212:LEU:H	2.18	0.52
1:A:1178:ASP:HA	1:C:1177:ASP:OD1	2.10	0.52
1:B:1067:HIS:HB3	1:B:1070:SER:HB3	1.92	0.52
1:B:1158:GLU:O	1:B:1165:GLU:HG2	2.10	0.51
1:D:1003:LEU:HA	1:D:1006:THR:HB	1.92	0.51
1:B:1162:THR:HB	1:B:1165:GLU:HB2	1.91	0.51
1:C:1198:PHE:O	1:C:1202:ILE:CG1	2.56	0.51
1:D:1174:MET:HG3	1:D:1205:VAL:CG1	2.39	0.51
1:D:1203:PHE:O	1:D:1207:PHE:N	2.43	0.51
1:A:1171:PHE:CE2	1:B:1199:ILE:HG23	2.46	0.51
1:B:1022:ILE:HD11	1:B:1108:ARG:CG	2.41	0.51
1:D:1214:VAL:O	1:D:1218:VAL:HB	2.10	0.51
1:C:1188:MET:HE1	1:D:1168:TYR:CE1	2.46	0.51
1:B:1127:ILE:HB	1:B:1128:PRO:CD	2.32	0.50
1:A:1024:LEU:HB3	1:A:1048:PHE:HZ	1.76	0.50
1:B:1025:ASN:OD1	1:B:1105:ARG:HD2	2.10	0.50
1:A:1185:ARG:N	1:A:1186:PRO:CD	2.74	0.50
1:D:1127:ILE:HB	1:D:1128:PRO:HD3	1.92	0.50
1:B:1083:VAL:HG11	1:B:1105:ARG:HA	1.93	0.50
1:C:1174:MET:SD	1:C:1209:MET:HE3	2.51	0.50
1:D:1076:TRP:CH2	1:D:1117:ARG:O	2.65	0.50
1:D:1080:ASP:OD1	1:D:1108:ARG:HG2	2.11	0.50
1:D:1218:VAL:O	1:D:1222:ALA:N	2.41	0.50
1:C:1137:MET:O	1:C:1140:PHE:N	2.44	0.50
1:A:1024:LEU:HB3	1:A:1048:PHE:CZ	2.47	0.50
1:A:1147:MET:HA	1:A:1150:GLN:HG2	1.94	0.50
1:D:1111:THR:O	1:D:1117:ARG:CD	2.57	0.50
1:C:1059:GLU:OE2	1:C:1063:ARG:NH1	2.45	0.49
1:D:1107:PHE:O	1:D:1110:VAL:HB	2.12	0.49
1:C:1018:ILE:HG13	1:C:1059:GLU:OE2	2.12	0.49
1:B:1185:ARG:N	1:B:1186:PRO:CD	2.76	0.49
1:C:1122:ALA:O	1:C:1125:SER:OG	2.31	0.49
1:D:1052:VAL:HA	1:D:1055:ILE:HD12	1.95	0.48
1:A:1147:MET:HG3	1:C:1103:VAL:HG11	1.95	0.48
1:C:1102:ARG:O	1:C:1105:ARG:HG2	2.13	0.48
1:A:1162:THR:CG2	1:A:1165:GLU:H	2.21	0.48
1:D:1218:VAL:HA	1:D:1221:MET:HE2	1.95	0.48
1:A:1124:ILE:HA	1:A:1127:ILE:HD12	1.96	0.48
1:B:1127:ILE:CB	1:B:1128:PRO:HD3	2.31	0.48
1:A:1144:PHE:O	1:A:1147:MET:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1079:PHE:CE2	1:D:1083:VAL:HG21	2.49	0.48
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.95	0.48
1:B:1105:ARG:O	1:B:1108:ARG:CB	2.55	0.48
1:B:1110:VAL:HG23	1:D:1139:LEU:HD22	1.96	0.48
1:A:1174:MET:C	1:A:1176:LEU:H	2.22	0.48
1:C:1050:GLN:O	1:C:1054:THR:OG1	2.28	0.48
1:C:1083:VAL:CG1	1:C:1105:ARG:HA	2.42	0.48
1:D:1091:THR:O	1:D:1099:ARG:NH2	2.43	0.48
1:D:1218:VAL:CG2	1:D:1221:MET:HE2	2.44	0.48
1:D:1128:PRO:HA	1:D:1131:LEU:HB2	1.96	0.47
1:A:1185:ARG:HA	1:A:1188:MET:HE2	1.97	0.47
1:C:1172:GLN:O	1:C:1175:THR:N	2.42	0.47
1:D:1038:MET:HA	1:D:1042:GLY:HA2	1.95	0.47
1:A:1115:GLN:N	1:A:1115:GLN:OE1	2.48	0.47
1:A:1133:VAL:HB	1:A:1212:LEU:HD12	1.97	0.47
1:C:1181:ASN:O	1:C:1186:PRO:CD	2.63	0.47
1:A:1162:THR:HG22	1:A:1165:GLU:HG3	1.96	0.47
1:A:1177:ASP:OD2	1:B:1179:TRP:CD1	2.68	0.47
1:D:1126:VAL:HG11	1:D:1216:ILE:CG2	2.38	0.47
1:B:1131:LEU:HA	1:B:1134:ILE:HB	1.96	0.47
1:C:1197:PHE:C	1:C:1200:PRO:HD2	2.39	0.47
1:D:1098:LEU:HA	1:D:1101:LEU:HD12	1.97	0.47
4:D:1304:D6C:C15	4:D:1304:D6C:C19	2.92	0.47
1:A:1200:PRO:O	1:A:1203:PHE:N	2.44	0.47
1:C:1152:PHE:C	5:C:1401:HOH:O	2.58	0.47
1:A:1143:ILE:HD12	1:C:1107:PHE:CE1	2.50	0.47
1:C:1199:ILE:N	1:C:1200:PRO:CD	2.78	0.47
1:A:1091:THR:HB	1:A:1102:ARG:HH22	1.76	0.46
1:A:1180:SER:HG	1:C:1168:TYR:HE1	1.61	0.46
1:A:1169:THR:O	1:A:1172:GLN:N	2.48	0.46
1:D:1146:ILE:O	1:D:1147:MET:C	2.58	0.46
1:C:1024:LEU:HD23	1:C:1048:PHE:CZ	2.50	0.46
1:C:1162:THR:HG22	1:C:1163:LEU:H	1.80	0.46
1:C:1199:ILE:HB	1:C:1200:PRO:HD3	1.96	0.46
1:A:1091:THR:O	1:A:1091:THR:OG1	2.33	0.46
1:A:1171:PHE:CE1	1:A:1175:THR:HG23	2.48	0.46
1:B:1177:ASP:OD2	1:D:1180:SER:CB	2.63	0.46
1:A:1136:LEU:O	1:A:1139:LEU:HB3	2.16	0.46
1:C:1134:ILE:O	1:C:1135:ALA:C	2.56	0.46
1:C:1197:PHE:C	1:C:1197:PHE:CD1	2.93	0.46
1:D:1109:LEU:O	1:D:1113:VAL:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1110:VAL:O	1:D:1117:ARG:HG3	2.16	0.46
1:A:1147:MET:HG2	1:C:1100:VAL:CG1	2.45	0.46
1:D:1181:ASN:O	1:D:1186:PRO:HD3	2.16	0.46
1:D:1188:MET:SD	1:D:1195:TRP:HD1	2.39	0.46
1:B:1171:PHE:O	1:B:1175:THR:HG23	2.16	0.46
1:C:1149:THR:HG23	1:C:1162:THR:O	2.16	0.46
1:B:1213:VAL:O	1:B:1217:ILE:HG22	2.15	0.45
1:D:1028:THR:HG23	1:D:1045:THR:HG23	1.97	0.45
1:A:1076:TRP:HB3	1:A:1111:THR:HG23	1.98	0.45
1:A:1098:LEU:HA	1:A:1101:LEU:HD12	1.98	0.45
1:C:1120:VAL:HG12	1:C:1124:ILE:HD11	1.97	0.45
1:B:1029:MET:SD	1:B:1103:VAL:HG23	2.56	0.45
1:B:1213:VAL:HA	1:B:1216:ILE:HB	1.98	0.45
1:D:1210:ILE:O	1:D:1214:VAL:HG23	2.17	0.45
1:A:1206:THR:HA	1:A:1209:MET:HB2	1.98	0.45
1:D:1071:PHE:CD1	1:D:1071:PHE:C	2.95	0.45
1:A:1052:VAL:HG13	1:A:1056:PHE:CE1	2.52	0.45
1:B:1162:THR:HG22	1:B:1164:GLY:H	1.80	0.45
1:D:1176:LEU:HD12	4:D:1304:D6C:C07	2.46	0.45
1:B:1168:TYR:HE2	1:D:1185:ARG:HE	1.49	0.45
1:D:1005:ILE:HA	1:D:1008:ILE:HG13	1.98	0.45
1:D:1213:VAL:O	1:D:1217:ILE:HG22	2.16	0.45
1:B:1168:TYR:CE2	1:D:1185:ARG:CD	2.98	0.45
1:C:1147:MET:CE	1:D:1100:VAL:O	2.65	0.45
1:C:1149:THR:CG2	1:C:1162:THR:O	2.64	0.45
1:C:1174:MET:SD	1:C:1205:VAL:CG1	3.05	0.45
1:C:1195:TRP:H	1:C:1195:TRP:CD1	2.33	0.45
1:A:1180:SER:O	1:A:1185:ARG:N	2.40	0.45
1:B:1159:TRP:CD1	1:B:1159:TRP:N	2.78	0.45
1:C:1120:VAL:CG1	1:C:1124:ILE:HD11	2.47	0.45
1:B:1155:ARG:NH2	1:B:1190:VAL:CG2	2.80	0.45
1:B:1109:LEU:O	1:B:1109:LEU:HD12	2.17	0.44
1:D:1174:MET:C	1:D:1176:LEU:N	2.72	0.44
1:D:1183:ILE:C	1:D:1186:PRO:HD2	2.42	0.44
1:C:1053:ILE:O	1:C:1057:THR:OG1	2.30	0.44
1:D:1153:GLY:HA3	1:D:1160:PHE:O	2.17	0.44
1:A:1091:THR:CB	1:A:1102:ARG:HH22	2.31	0.44
1:A:1149:THR:CG2	1:C:1033:THR:HG23	2.44	0.44
1:B:1044:TYR:O	1:B:1048:PHE:HB2	2.17	0.44
1:B:1103:VAL:HG11	1:D:1147:MET:HG3	2.00	0.44
1:B:1217:ILE:HD11	1:D:1217:ILE:HG12	1.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1169:THR:O	1:B:1172:GLN:N	2.51	0.44
1:D:1116:MET:O	1:D:1120:VAL:HG23	2.18	0.44
1:A:1105:ARG:HG3	1:A:1106:LEU:HD23	2.00	0.44
1:A:1101:LEU:O	1:A:1103:VAL:N	2.51	0.43
1:A:1105:ARG:HG3	1:A:1106:LEU:N	2.33	0.43
1:A:1177:ASP:C	1:A:1177:ASP:OD1	2.61	0.43
1:B:1148:ALA:HB1	1:B:1160:PHE:CD1	2.52	0.43
1:C:1147:MET:O	1:C:1148:ALA:C	2.57	0.43
1:B:1009:VAL:HA	1:B:1014:PHE:CD2	2.53	0.43
1:B:1158:GLU:HG2	1:B:1159:TRP:CD1	2.53	0.43
1:D:1076:TRP:CE3	1:D:1117:ARG:HG2	2.52	0.43
1:B:1009:VAL:CG2	1:B:1062:LEU:HB3	2.49	0.43
1:A:1172:GLN:HG3	1:A:1177:ASP:HB3	2.01	0.43
1:C:1184:VAL:O	1:C:1185:ARG:C	2.60	0.43
1:D:1067:HIS:HB3	1:D:1070:SER:HB3	2.00	0.43
1:C:1188:MET:CE	1:D:1168:TYR:CE1	3.01	0.43
1:C:1206:THR:O	1:C:1207:PHE:C	2.62	0.43
1:C:1167:PHE:O	1:C:1171:PHE:N	2.40	0.43
1:D:1096:GLU:HA	1:D:1096:GLU:OE1	2.19	0.43
1:A:1130:MET:HE3	1:A:1212:LEU:HD21	2.00	0.43
1:A:1132:SER:O	1:A:1135:ALA:HB3	2.19	0.43
1:B:1022:ILE:HG21	1:B:1109:LEU:CB	2.49	0.43
1:B:1188:MET:HA	1:B:1191:TYR:O	2.19	0.43
1:A:1076:TRP:CD1	1:A:1076:TRP:N	2.85	0.43
1:B:1130:MET:HE2	1:B:1134:ILE:HD11	2.01	0.43
1:D:1163:LEU:HA	1:D:1163:LEU:HD23	1.78	0.43
1:D:1199:ILE:O	1:D:1202:ILE:HB	2.18	0.43
1:B:1025:ASN:HA	1:B:1028:THR:HG22	2.01	0.42
1:C:1173:VAL:HG12	1:C:1202:ILE:HG12	2.00	0.42
1:C:1184:VAL:O	1:C:1187:LEU:N	2.50	0.42
1:D:1177:ASP:C	1:D:1179:TRP:N	2.75	0.42
1:D:1200:PRO:C	1:D:1202:ILE:N	2.76	0.42
1:A:1059:GLU:OE1	1:A:1108:ARG:NH2	2.52	0.42
1:B:1148:ALA:O	1:B:1149:THR:C	2.61	0.42
1:C:1112:ALA:O	1:C:1114:PRO:CD	2.66	0.42
1:A:1019:ILE:HD11	1:A:1112:ALA:O	2.19	0.42
1:A:1174:MET:C	1:A:1176:LEU:N	2.77	0.42
1:B:1033:THR:HG23	1:D:1149:THR:HG21	2.01	0.42
1:C:1131:LEU:C	1:C:1133:VAL:H	2.27	0.42
1:D:1006:THR:O	1:D:1006:THR:HG22	2.20	0.42
1:D:1197:PHE:CD1	1:D:1197:PHE:O	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:GLY:HA3	1:A:1165:GLU:OE2	2.19	0.42
1:A:1181:ASN:OD1	1:C:1178:ASP:OD2	2.37	0.42
1:B:1059:GLU:HG2	1:B:1060:ILE:HD12	2.02	0.42
1:C:1144:PHE:CE2	1:C:1201:PHE:HB2	2.54	0.42
1:A:1156:PHE:CZ	1:A:1187:LEU:HA	2.55	0.42
1:B:1096:GLU:O	1:B:1098:LEU:N	2.52	0.42
1:B:1155:ARG:NH2	1:B:1190:VAL:HG22	2.35	0.42
1:D:1068:ARG:CG	1:D:1069:ILE:H	2.22	0.42
1:D:1021:LEU:HD11	1:D:1055:ILE:HD13	2.01	0.42
1:A:1188:MET:HA	1:A:1191:TYR:O	2.19	0.42
1:B:1160:PHE:CE2	1:B:1169:THR:HG21	2.55	0.42
1:B:1025:ASN:O	1:B:1028:THR:HG22	2.19	0.42
1:B:1106:LEU:CB	1:D:1143:ILE:HG12	2.49	0.42
1:C:1113:VAL:HG12	1:C:1114:PRO:O	2.19	0.42
1:C:1029:MET:HA	1:C:1032:GLU:HB2	2.02	0.41
1:D:1173:VAL:O	1:D:1176:LEU:CD2	2.64	0.41
1:B:1076:TRP:CD1	1:B:1076:TRP:H	2.36	0.41
1:B:1080:ASP:CG	1:B:1111:THR:HG21	2.42	0.41
1:A:1152:PHE:O	1:A:1156:PHE:HB2	2.20	0.41
1:D:1096:GLU:N	1:D:1096:GLU:CD	2.78	0.41
1:A:1090:PRO:O	1:A:1091:THR:HG23	2.19	0.41
1:A:1172:GLN:HA	1:A:1175:THR:OG1	2.20	0.41
1:C:1024:LEU:O	1:C:1028:THR:N	2.39	0.41
1:A:1147:MET:O	1:A:1151:LEU:N	2.53	0.41
1:C:1199:ILE:N	1:C:1200:PRO:HD3	2.34	0.41
1:A:1181:ASN:O	1:A:1186:PRO:HD3	2.20	0.41
1:B:1109:LEU:HD23	1:D:1139:LEU:HD13	2.02	0.41
1:D:1181:ASN:HA	1:D:1185:ARG:HG3	2.03	0.41
1:A:1062:LEU:O	1:A:1066:VAL:HG23	2.21	0.41
1:A:1105:ARG:O	1:A:1107:PHE:N	2.54	0.41
1:A:1196:VAL:O	1:A:1200:PRO:HD2	2.20	0.41
1:B:1022:ILE:HG21	1:B:1109:LEU:CA	2.50	0.41
1:C:1099:ARG:O	1:C:1099:ARG:HG2	2.20	0.41
1:A:1168:TYR:HE2	1:B:1185:ARG:HG2	1.86	0.41
1:B:1068:ARG:O	1:B:1069:ILE:C	2.64	0.41
1:C:1032:GLU:OE1	1:C:1049:ASN:ND2	2.54	0.41
1:D:1076:TRP:HB3	1:D:1111:THR:HG23	2.01	0.41
1:D:1217:ILE:O	1:D:1221:MET:HB2	2.21	0.41
1:B:1168:TYR:CD2	1:D:1185:ARG:CZ	3.04	0.40
1:A:1104:LEU:HD23	1:A:1104:LEU:HA	1.83	0.40
1:A:1125:SER:O	1:A:1128:PRO:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1197:PHE:HB3	1:D:1198:PHE:CD2	2.56	0.40
1:D:1175:THR:OG1	1:D:1177:ASP:HB2	2.21	0.40
1:B:1106:LEU:O	1:B:1109:LEU:HB3	2.21	0.40
1:B:1195:TRP:CD1	1:B:1195:TRP:H	2.38	0.40
1:C:1100:VAL:C	1:C:1102:ARG:N	2.79	0.40
1:A:1037:PHE:O	1:A:1038:MET:HE2	2.22	0.40
1:A:1169:THR:O	1:A:1170:LEU:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1102	ARG
1	B	1153	GLY
1	B	1177	ASP
1	C	1132	SER
1	A	1175	THR
1	C	1075	PRO
1	C	1076	TRP
1	A	1022	ILE

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Mol	Chain	Res	Type
1	A	1109	LEU
1	A	1127	ILE
1	A	1156	PHE
1	A	1178	ASP
1	B	1189	GLU
1	D	1156	PHE
1	B	1097	ILE
1	B	1211	ASN
1	D	1027	ILE

5.3.2 Protein sidechains ⓘ

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

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

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

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1010	GLU
1	A	1015	THR
1	A	1022	ILE
1	A	1027	ILE
1	A	1044	TYR
1	A	1069	ILE
1	A	1089	VAL
1	A	1093	SER
1	A	1114	PRO
1	A	1115	GLN
1	A	1132	SER
1	A	1147	MET

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Mol	Chain	Res	Type
1	A	1171	PHE
1	A	1175	THR
1	A	1202	ILE
1	A	1212	LEU
1	B	1019	ILE
1	B	1053	ILE
1	B	1059	GLU
1	B	1083	VAL
1	B	1114	PRO
1	B	1118	LYS
1	B	1121	SER
1	B	1125	SER
1	B	1126	VAL
1	B	1132	SER
1	B	1162	THR
1	B	1163	LEU
1	B	1165	GLU
1	B	1172	GLN
1	B	1183	ILE
1	B	1184	VAL
1	B	1200	PRO
1	B	1204	VAL
1	C	1022	ILE
1	C	1053	ILE
1	C	1091	THR
1	C	1109	LEU
1	C	1118	LYS
1	C	1150	GLN
1	C	1162	THR
1	C	1163	LEU
1	C	1175	THR
1	C	1206	THR
1	C	1217	ILE
1	D	1010	GLU
1	D	1033	THR
1	D	1091	THR
1	D	1093	SER
1	D	1106	LEU
1	D	1162	THR
1	D	1175	THR
1	D	1204	VAL
1	D	1217	ILE

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Mol	Chain	Res	Type
1	D	1218	VAL
1	D	1228	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1181	ASN
1	A	1211	ASN
1	B	1007	ASN
1	B	1050	GLN
1	C	1150	GLN
1	D	1067	HIS
1	D	1211	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PX4	D	1302	-	9,9,45	1.30	1 (11%)	10,12,53	0.76	0
2	PX4	C	1303	-	9,9,45	1.42	2 (22%)	10,12,53	1.26	0
2	PX4	A	1301	-	9,9,45	1.59	2 (22%)	10,12,53	0.94	0
2	PX4	A	1303	-	9,9,45	1.79	2 (22%)	10,12,53	1.03	1 (10%)
2	PX4	B	1303	-	20,20,45	2.01	3 (15%)	22,24,53	1.48	2 (9%)
2	PX4	C	1304	-	20,20,45	2.01	3 (15%)	22,24,53	1.40	2 (9%)
2	PX4	B	1302	-	9,9,45	1.41	1 (11%)	10,12,53	0.94	0
4	D6C	D	1304	-	31,31,31	2.06	7 (22%)	43,43,43	3.30	12 (27%)
2	PX4	D	1303	-	9,9,45	1.97	2 (22%)	10,12,53	1.35	2 (20%)
2	PX4	C	1302	-	20,20,45	1.81	5 (25%)	22,24,53	1.66	2 (9%)
2	PX4	A	1304	-	9,9,45	1.58	2 (22%)	10,12,53	1.21	0
2	PX4	D	1301	-	9,9,45	1.73	2 (22%)	10,12,53	1.37	2 (20%)
2	PX4	A	1302	-	20,20,45	2.07	3 (15%)	22,24,53	1.63	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PX4	D	1302	-	-	6/8/8/49	-
2	PX4	C	1303	-	-	3/8/8/49	-
2	PX4	A	1301	-	-	3/8/8/49	-
2	PX4	A	1303	-	-	5/8/8/49	-
2	PX4	B	1303	-	-	12/22/22/49	-
2	PX4	C	1304	-	-	7/22/22/49	-
2	PX4	B	1302	-	-	3/8/8/49	-
4	D6C	D	1304	-	-	5/15/35/35	0/3/3/3
2	PX4	D	1303	-	-	3/8/8/49	-
2	PX4	C	1302	-	-	12/22/22/49	-
2	PX4	A	1304	-	-	4/8/8/49	-
2	PX4	D	1301	-	-	3/8/8/49	-
2	PX4	A	1302	-	-	12/22/22/49	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1302	PX4	O6-C9	7.12	1.43	1.22
2	B	1303	PX4	O6-C9	6.38	1.41	1.22
2	C	1304	PX4	O6-C9	6.15	1.40	1.22
4	D	1304	D6C	C09-S10	-5.58	1.79	1.84
4	D	1304	D6C	C16-N17	5.54	1.48	1.43
2	C	1302	PX4	O6-C9	5.45	1.38	1.22
4	D	1304	D6C	C23-N17	5.37	1.47	1.37
2	D	1303	PX4	P1-O2	4.76	1.65	1.50
2	A	1303	PX4	P1-O2	4.57	1.64	1.50
2	D	1301	PX4	P1-O2	4.39	1.64	1.50
2	B	1303	PX4	O5-C9	4.31	1.45	1.33
2	C	1304	PX4	O5-C9	4.02	1.45	1.33
2	C	1304	PX4	P1-O3	3.61	1.70	1.58
4	D	1304	D6C	C16-C11	-3.56	1.36	1.40
2	C	1303	PX4	P1-O3	3.41	1.67	1.54
2	B	1302	PX4	P1-O3	3.26	1.66	1.54
2	A	1302	PX4	O5-C9	3.15	1.42	1.33
2	A	1304	PX4	P1-O3	3.14	1.66	1.54
2	D	1303	PX4	P1-O4	3.05	1.69	1.60
2	A	1301	PX4	P1-O3	3.00	1.65	1.54
2	A	1304	PX4	P1-O4	2.75	1.69	1.60
2	C	1302	PX4	P1-O4	2.71	1.70	1.59
2	A	1302	PX4	P1-O3	2.69	1.67	1.58
2	C	1302	PX4	P1-O3	2.66	1.67	1.58
2	B	1303	PX4	P1-O4	2.54	1.69	1.59
2	D	1302	PX4	P1-O3	2.51	1.64	1.54
2	A	1301	PX4	P1-O4	2.38	1.67	1.60
2	C	1302	PX4	O5-C9	2.36	1.40	1.33
2	C	1302	PX4	C10-C9	2.26	1.57	1.50
4	D	1304	D6C	O26-C27	2.25	1.40	1.35
4	D	1304	D6C	C11-S10	2.09	1.79	1.77
4	D	1304	D6C	O26-C25	-2.07	1.40	1.44
2	A	1303	PX4	P1-O4	2.06	1.66	1.60
2	C	1303	PX4	P1-O4	2.05	1.66	1.60
2	D	1301	PX4	P1-O4	2.01	1.66	1.60

All (26) bond angle outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1304	D6C	C09-C25-C23	7.11	120.32	113.99
4	D	1304	D6C	O26-C27-C28	5.77	121.38	111.09
2	C	1302	PX4	O5-C9-O6	-5.66	109.46	123.63
4	D	1304	D6C	C06-C09-C25	-5.31	105.66	116.69
2	B	1303	PX4	O5-C9-O6	-4.58	112.18	123.63
2	C	1304	PX4	O6-C9-C10	-4.54	106.03	123.78
2	C	1302	PX4	O6-C9-C10	-4.33	106.85	123.78
2	A	1302	PX4	O6-C9-C10	-4.17	107.48	123.78
2	B	1303	PX4	O6-C9-C10	-4.12	107.68	123.78
2	A	1302	PX4	O5-C9-O6	-3.97	113.69	123.63
4	D	1304	D6C	O24-C23-C25	-3.92	115.33	121.25
4	D	1304	D6C	C18-N17-C16	-3.84	110.84	118.09
2	D	1301	PX4	O4-P1-O2	3.17	115.00	106.44
2	D	1303	PX4	O4-P1-O2	2.64	113.58	106.44
4	D	1304	D6C	C18-N17-C23	-2.51	114.30	117.90
4	D	1304	D6C	C01-O02-C03	-2.44	112.26	117.50
2	C	1304	PX4	O5-C9-O6	-2.42	117.56	123.63
2	A	1302	PX4	O1-P1-O2	-2.41	101.22	112.44
4	D	1304	D6C	C19-C18-N17	-2.16	107.63	111.55
2	D	1301	PX4	O3-P1-O1	2.08	115.62	107.80
2	D	1303	PX4	O3-P1-O4	2.03	111.95	106.67
2	A	1303	PX4	O4-P1-O2	2.01	111.88	106.44

There are no chirality outliers.

All (78) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	C	1304	PX4	C6-O4-P1-O3
2	D	1301	PX4	C6-C7-C8-O5
2	D	1302	PX4	C6-O4-P1-O1
2	D	1302	PX4	C6-O4-P1-O3
2	D	1303	PX4	C6-O4-P1-O3
4	D	1304	D6C	C28-C27-O26-C25
4	D	1304	D6C	O29-C27-O26-C25
4	D	1304	D6C	C04-C03-O02-C01
2	B	1303	PX4	O4-C6-C7-O7
4	D	1304	D6C	C08-C03-O02-C01
2	A	1302	PX4	O7-C7-C8-O5
2	B	1303	PX4	O6-C9-O5-C8
2	C	1302	PX4	O4-C6-C7-C8
2	A	1302	PX4	O6-C9-O5-C8
2	B	1303	PX4	C9-C10-C11-C12
2	A	1303	PX4	O4-C6-C7-O7
2	A	1304	PX4	O4-C6-C7-O7
2	C	1302	PX4	O7-C7-C8-O5
2	A	1303	PX4	O4-C6-C7-C8
2	A	1304	PX4	O4-C6-C7-C8
2	C	1302	PX4	C6-C7-C8-O5
2	C	1304	PX4	O4-C6-C7-O7
2	A	1304	PX4	C6-C7-C8-O5
2	B	1302	PX4	C6-C7-C8-O5
2	C	1302	PX4	C1-O3-P1-O2
2	C	1302	PX4	C11-C12-C13-C14
2	A	1301	PX4	O7-C7-C8-O5
2	D	1301	PX4	O7-C7-C8-O5
2	C	1304	PX4	C10-C9-O5-C8
2	B	1303	PX4	C6-C7-C8-O5
2	C	1304	PX4	C12-C13-C14-C15
2	C	1302	PX4	C9-C10-C11-C12
2	B	1303	PX4	C12-C13-C14-C15
2	D	1302	PX4	C6-O4-P1-O2
2	D	1303	PX4	C6-O4-P1-O2
2	A	1302	PX4	C10-C11-C12-C13
2	C	1302	PX4	C10-C9-O5-C8
2	A	1302	PX4	C14-C15-C16-C17
2	C	1302	PX4	C10-C11-C12-C13
2	C	1302	PX4	C12-C13-C14-C15
2	D	1302	PX4	C7-C6-O4-P1
2	A	1302	PX4	C9-C10-C11-C12

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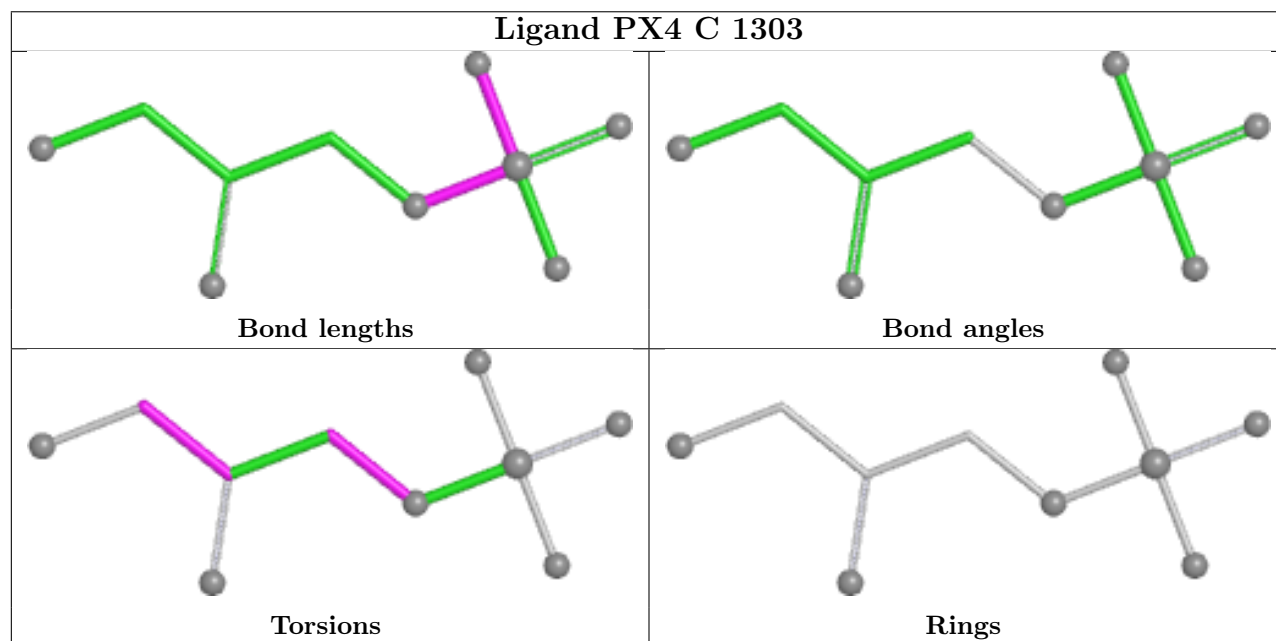
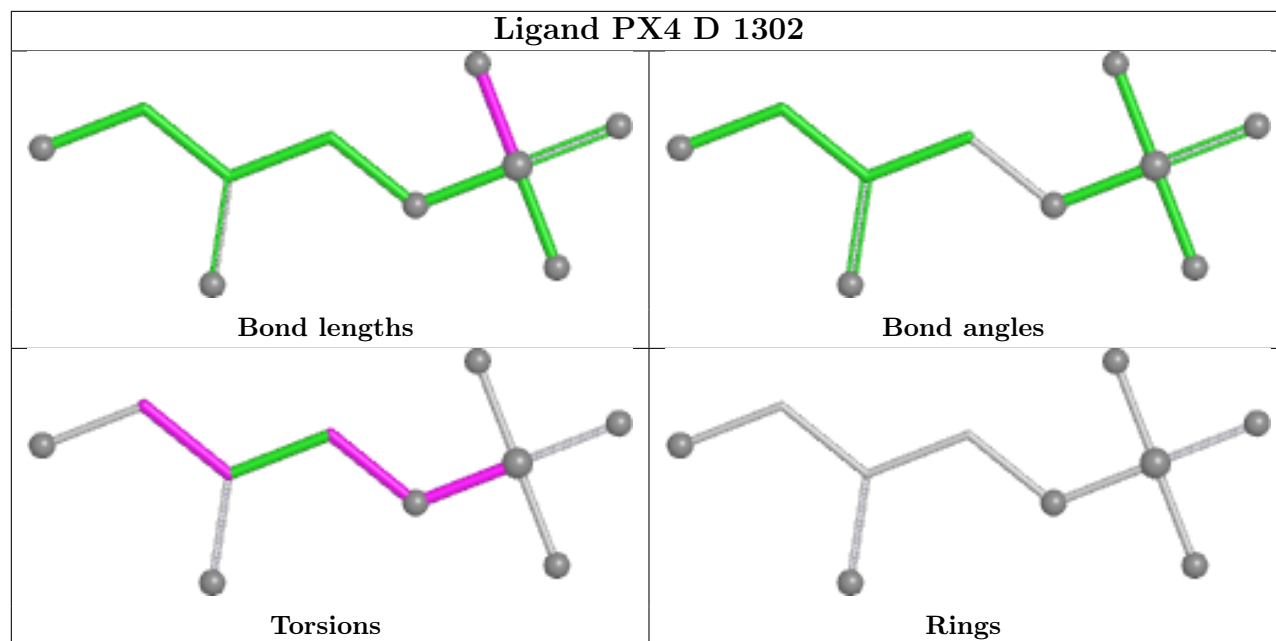
Mol	Chain	Res	Type	Atoms
2	A	1304	PX4	O7-C7-C8-O5
2	A	1302	PX4	C11-C12-C13-C14
2	D	1303	PX4	C6-O4-P1-O1
2	C	1304	PX4	C13-C14-C15-C16
2	A	1302	PX4	C1-O3-P1-O2
2	D	1302	PX4	C6-C7-C8-O5
2	C	1302	PX4	O6-C9-O5-C8
4	D	1304	D6C	C23-C25-O26-C27
2	B	1303	PX4	C14-C15-C16-C17
2	B	1302	PX4	O7-C7-C8-O5
2	A	1301	PX4	C7-C6-O4-P1
2	B	1303	PX4	C6-O4-P1-O2
2	B	1303	PX4	C6-O4-P1-O3
2	D	1301	PX4	C7-C6-O4-P1
2	A	1302	PX4	C13-C14-C15-C16
2	B	1303	PX4	C1-O3-P1-O1
2	C	1303	PX4	C7-C6-O4-P1
2	C	1302	PX4	C13-C14-C15-C16
2	A	1302	PX4	C6-C7-C8-O5
2	D	1302	PX4	O7-C7-C8-O5
2	B	1302	PX4	C7-C6-O4-P1

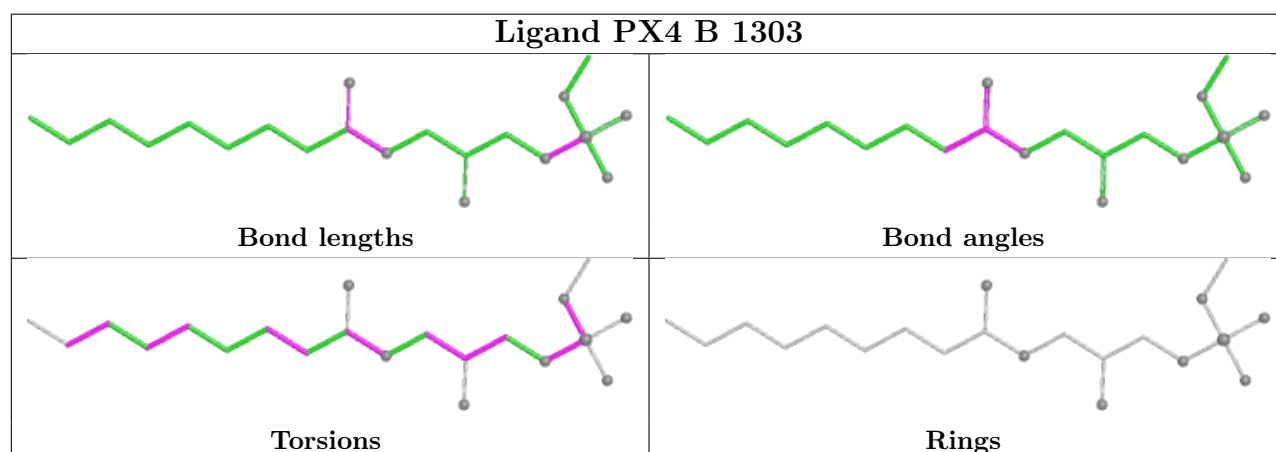
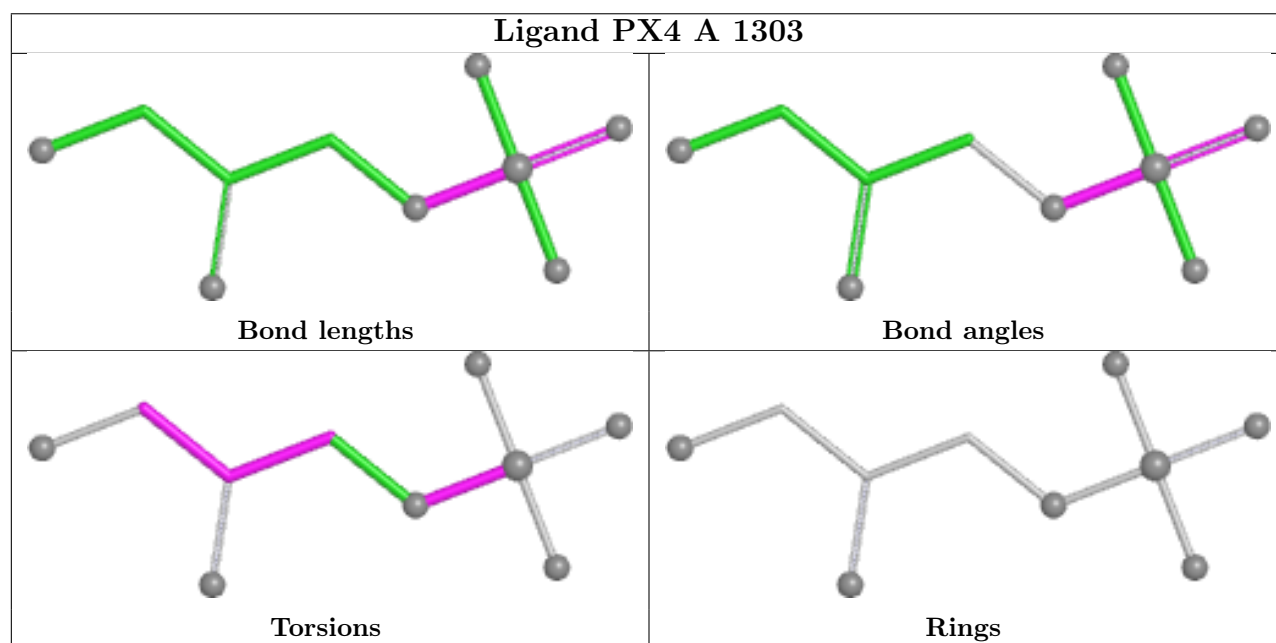
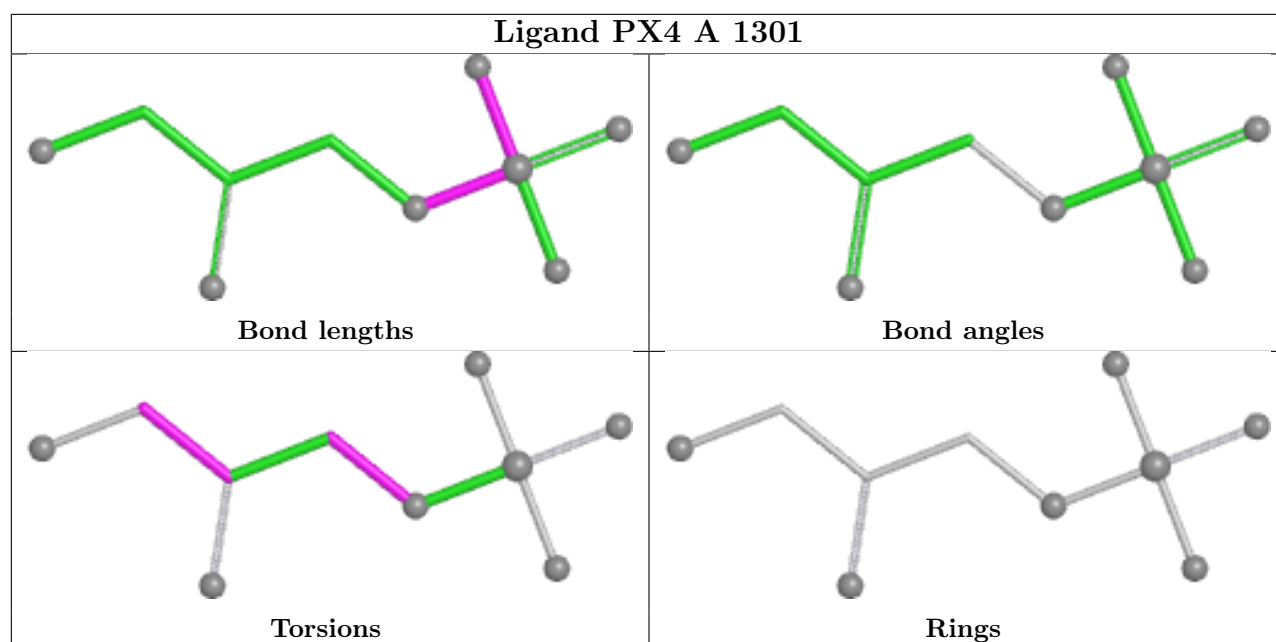
There are no ring outliers.

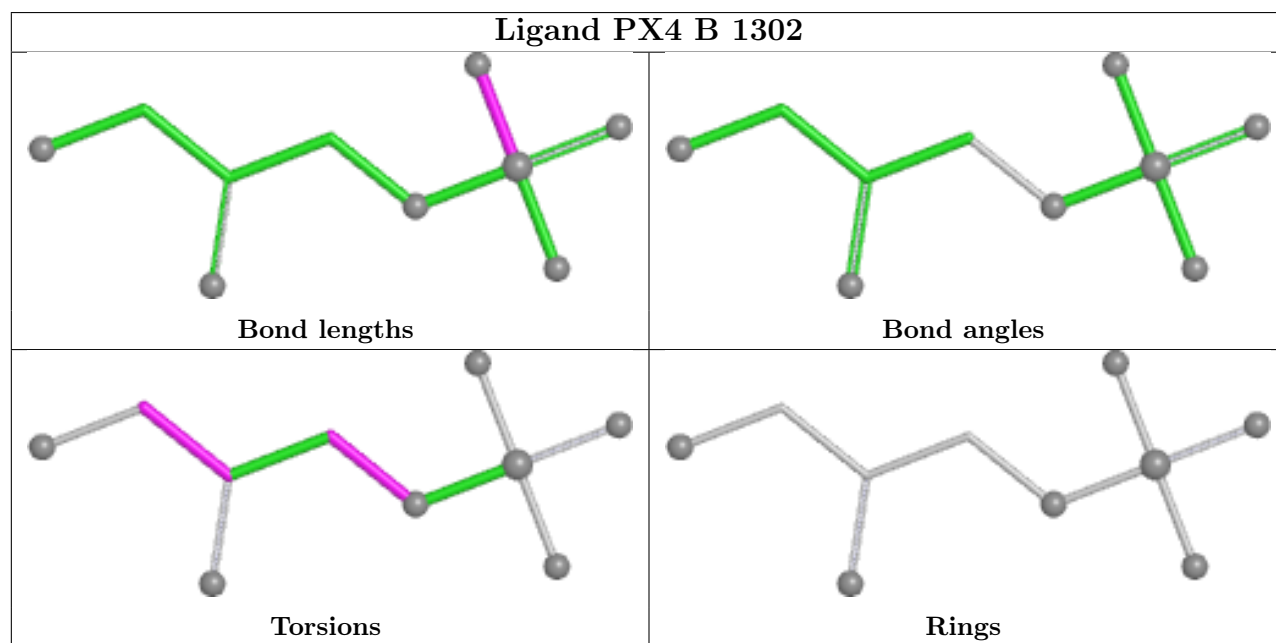
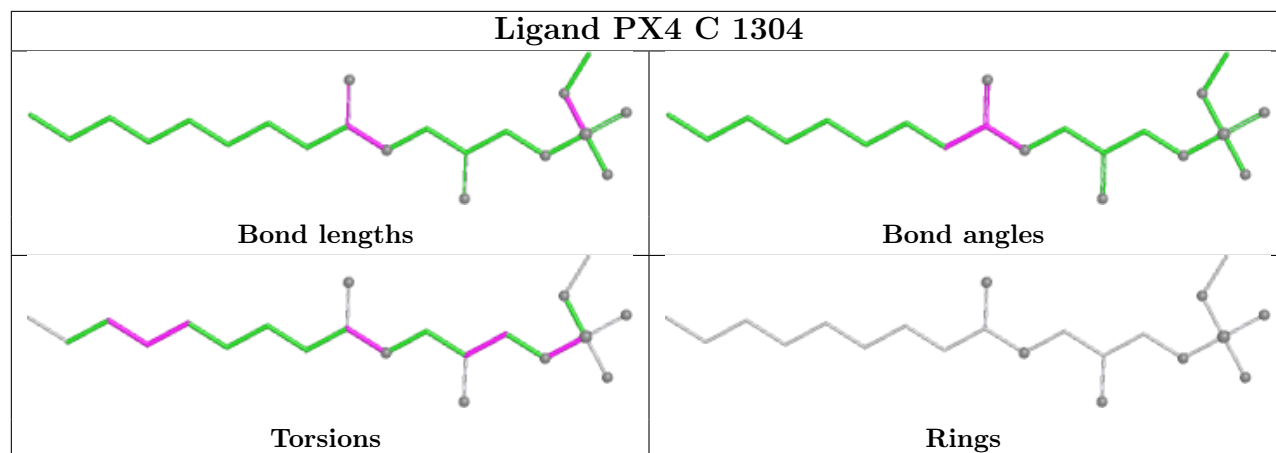
3 monomers are involved in 5 short contacts:

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

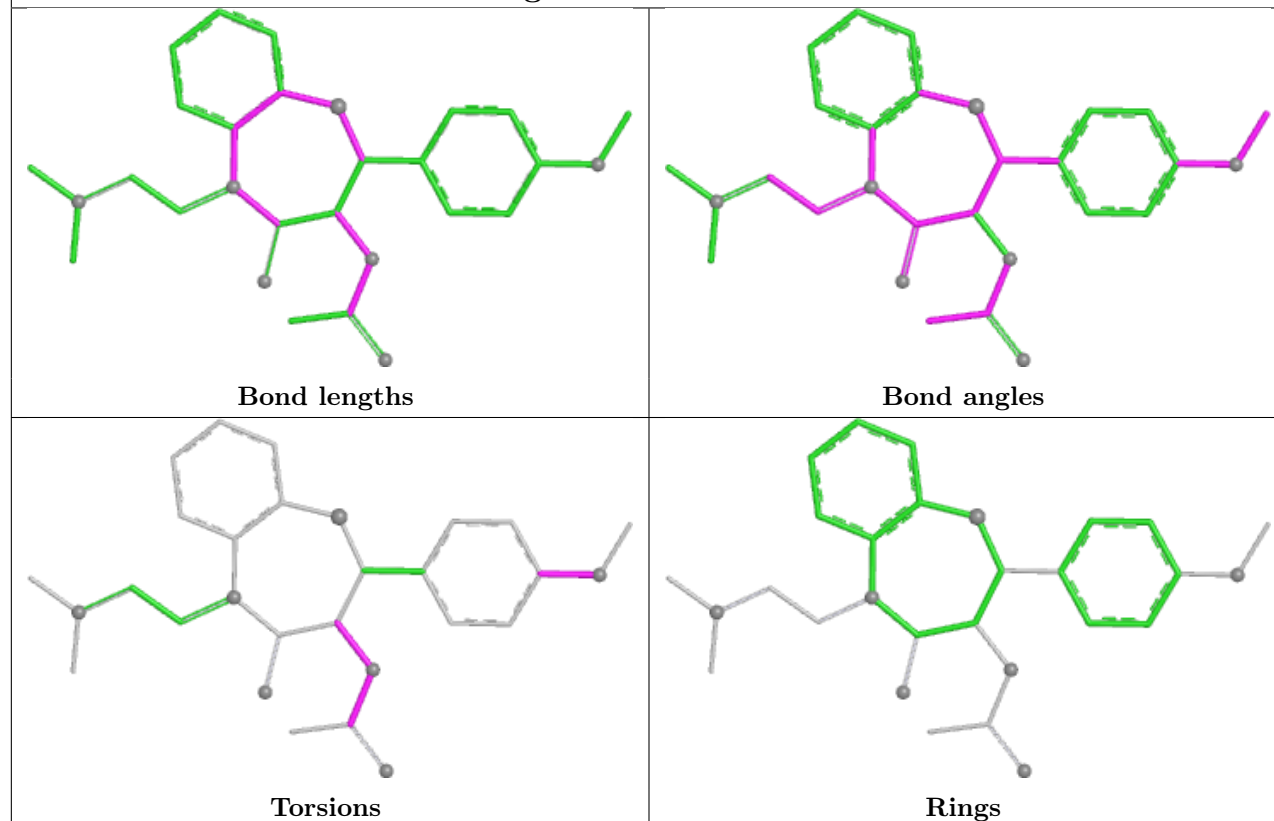
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



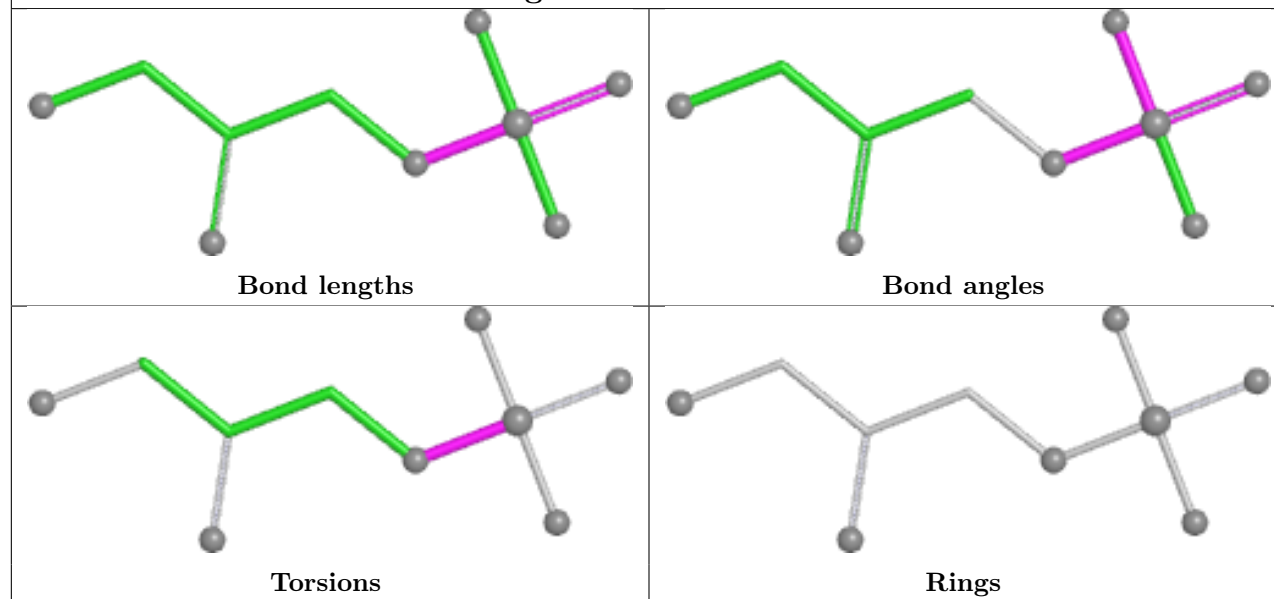


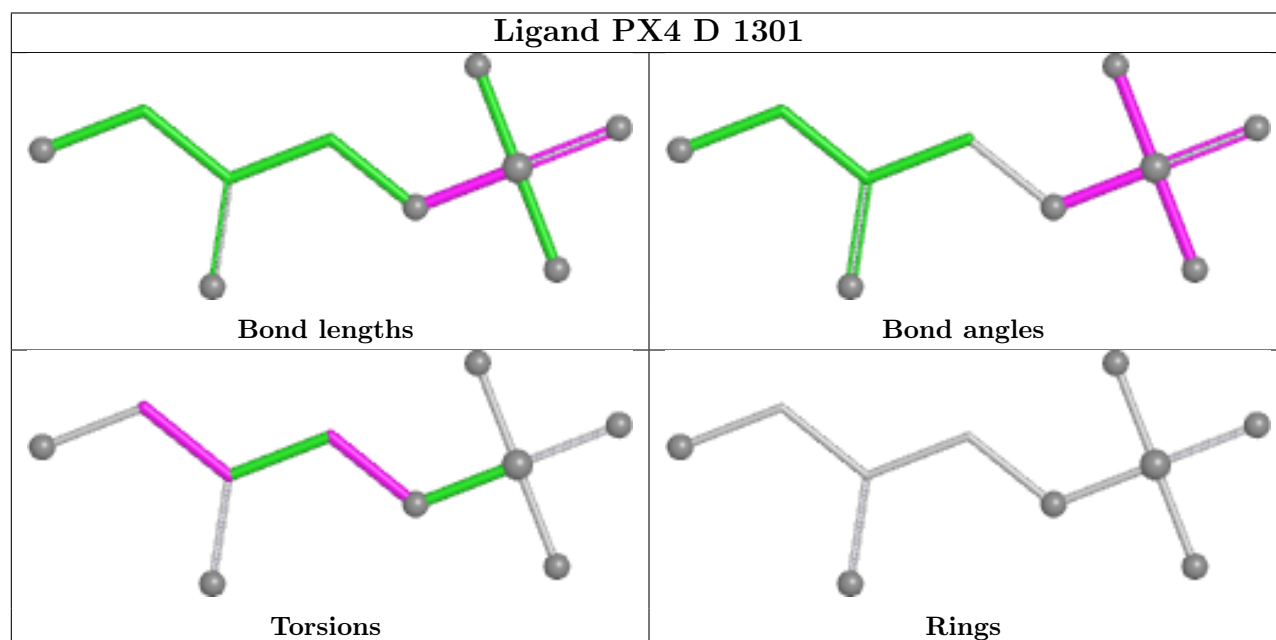
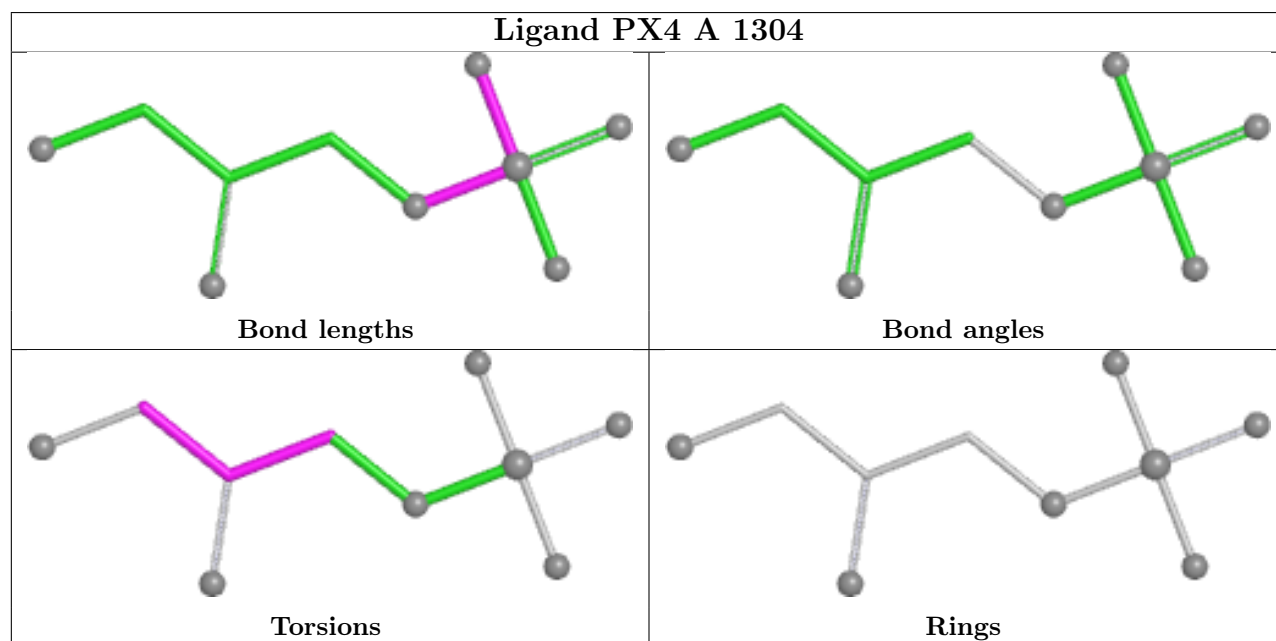
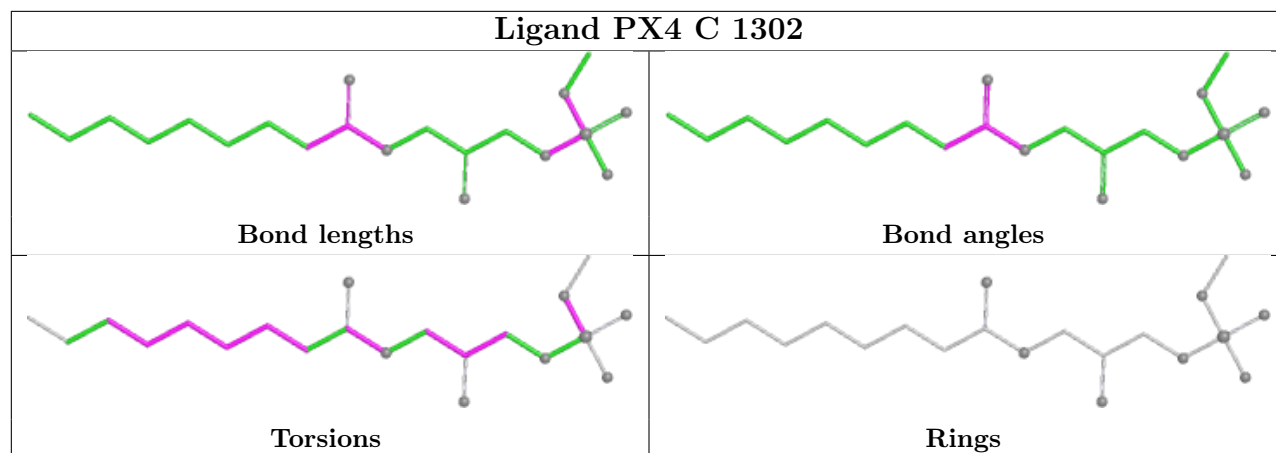


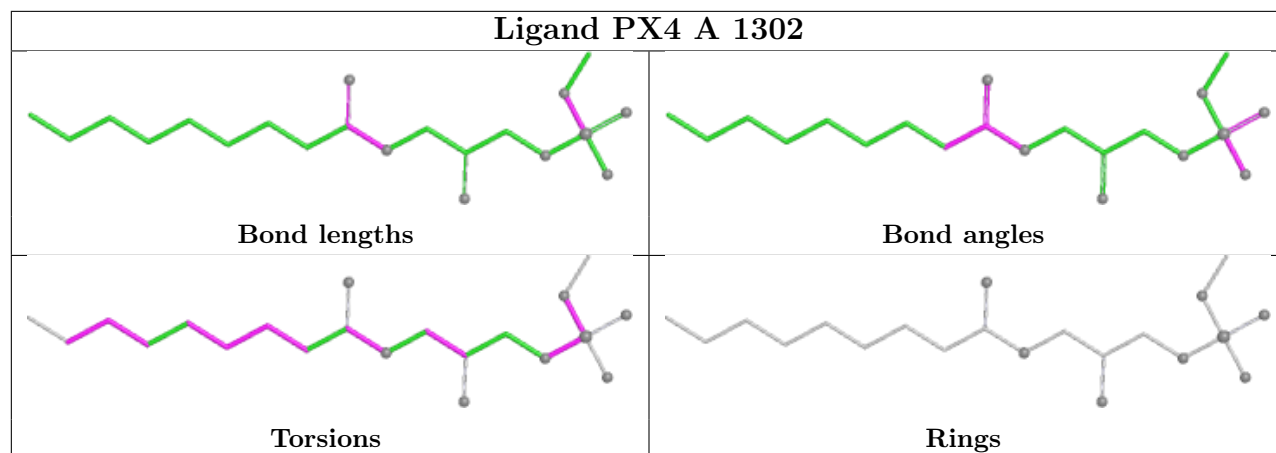
Ligand D6C D 1304



Ligand PX4 D 1303







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

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

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

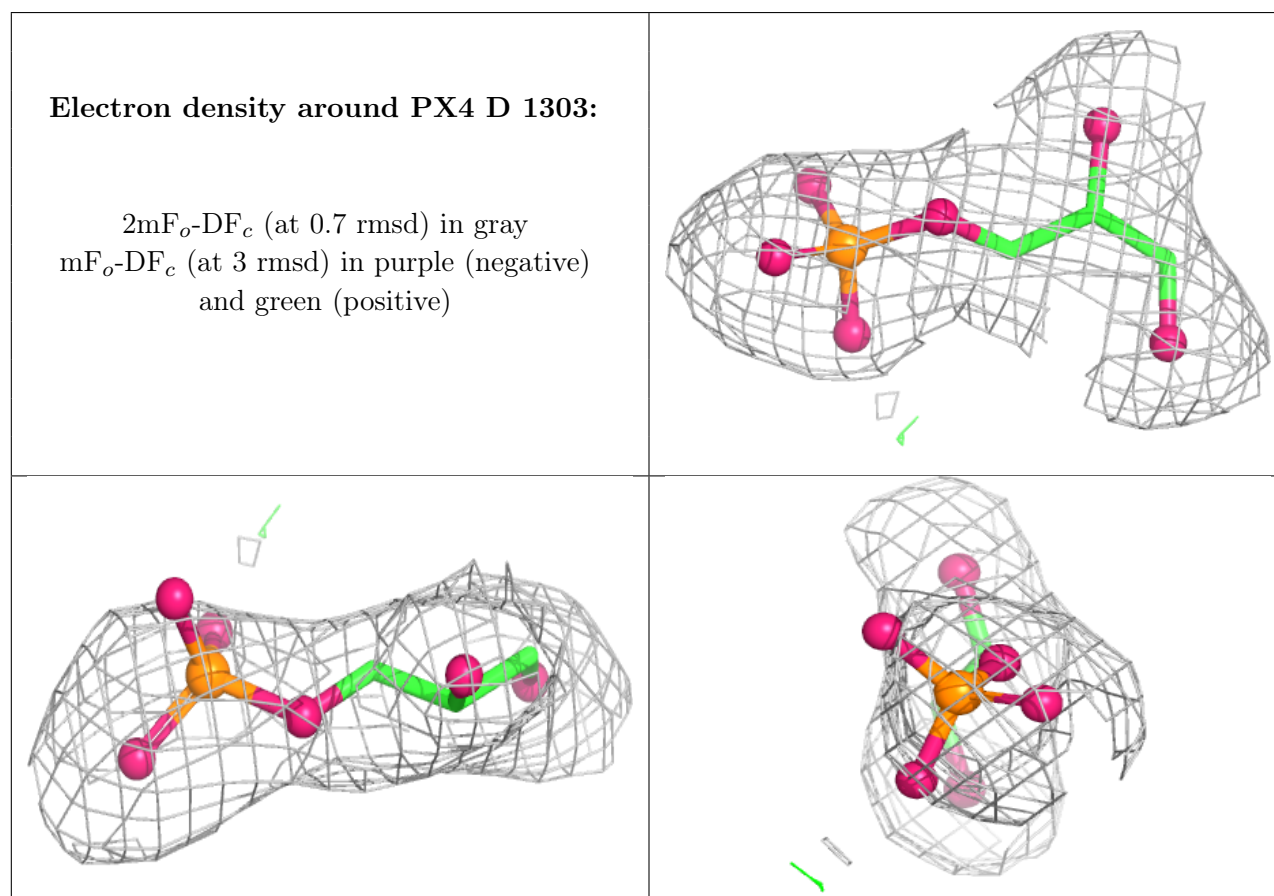
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PX4	D	1303	10/46	0.97	0.08	66,85,111,115	0
2	PX4	B	1302	10/46	0.98	0.06	80,101,114,126	0
2	PX4	C	1302	21/46	0.98	0.07	49,63,73,75	0
2	PX4	C	1303	10/46	0.98	0.06	60,72,85,89	0

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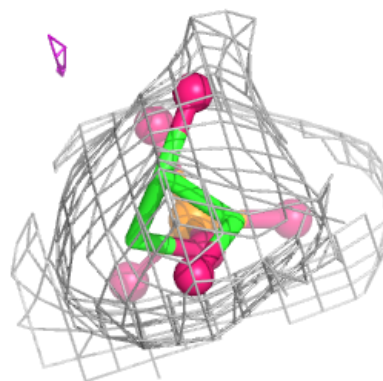
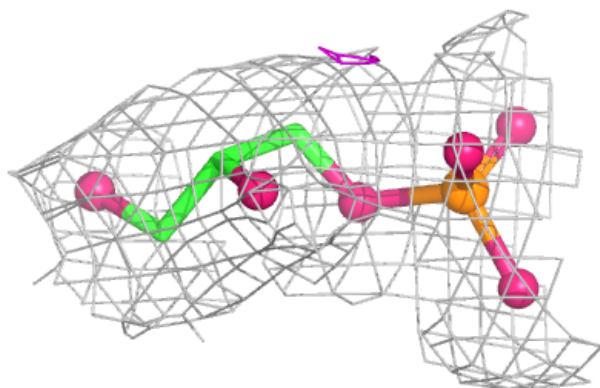
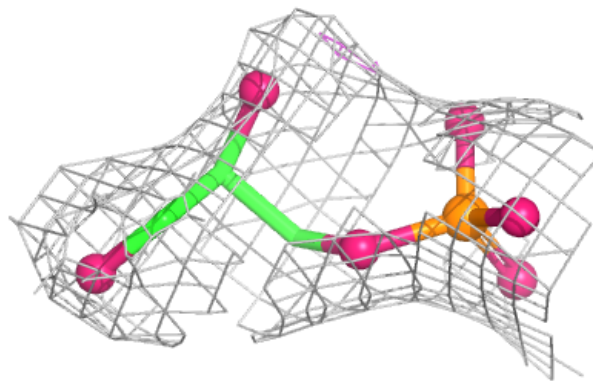
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PX4	C	1304	21/46	0.98	0.08	57,68,81,87	0
2	PX4	A	1304	10/46	0.98	0.06	79,92,107,109	0
4	D6C	D	1304	29/29	0.98	0.07	68,85,100,107	0
2	PX4	A	1301	10/46	0.99	0.08	62,77,88,92	0
2	PX4	A	1302	21/46	0.99	0.05	52,67,84,92	0
2	PX4	D	1301	10/46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

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

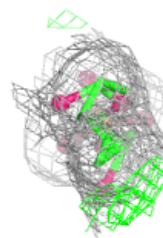
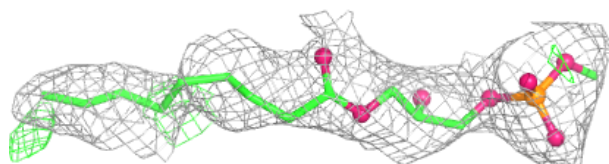
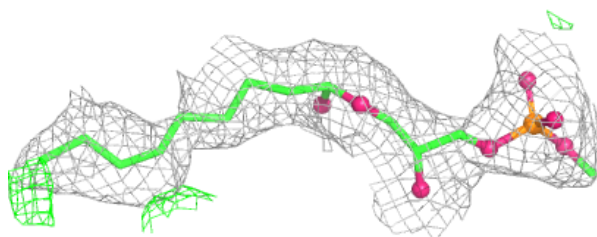


Electron density around PX4 B 1302:

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

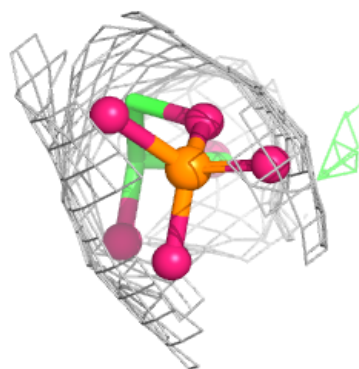
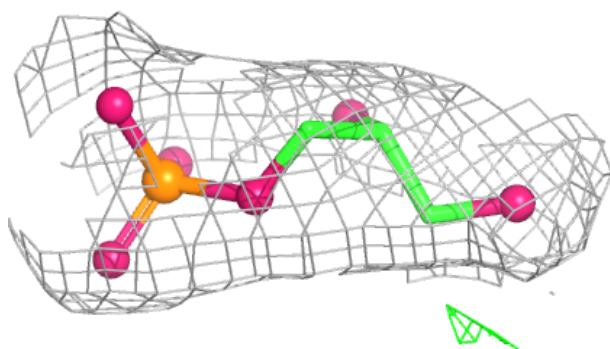
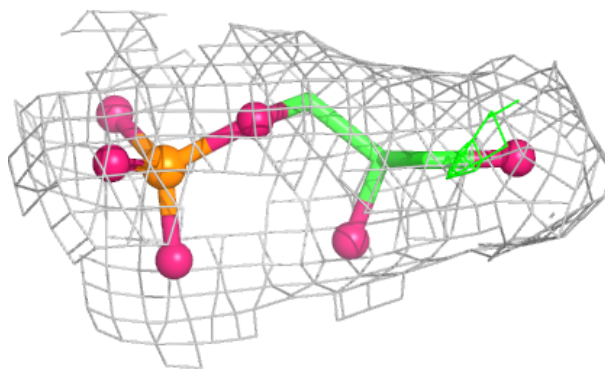
**Electron density around PX4 C 1302:**

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

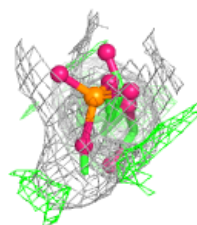
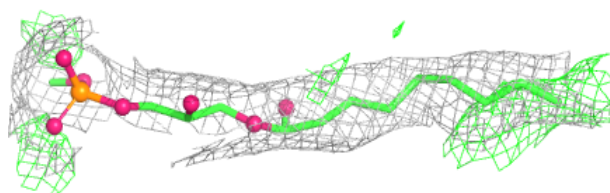
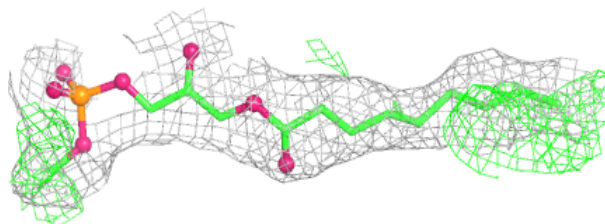


Electron density around PX4 C 1303:

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

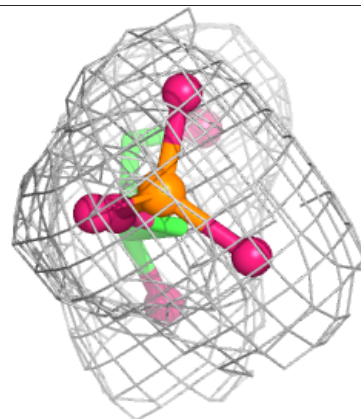
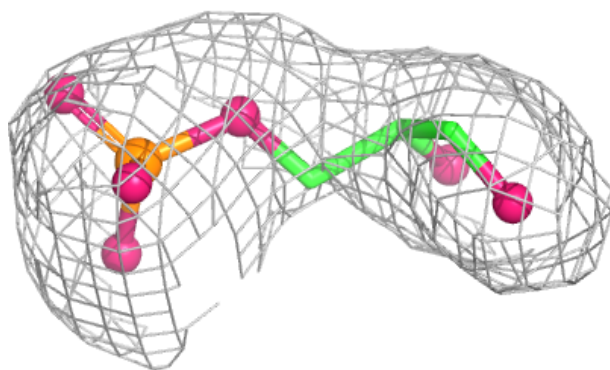
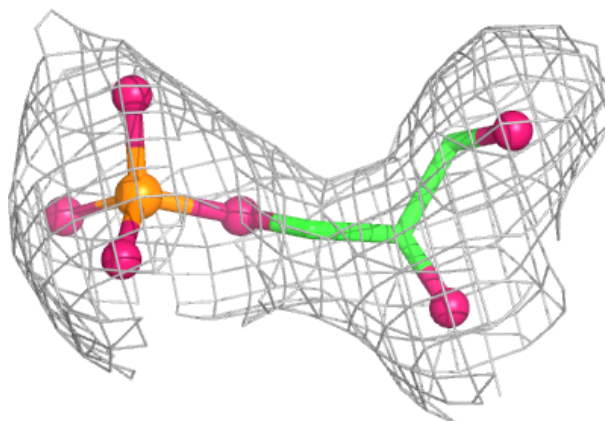
**Electron density around PX4 C 1304:**

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



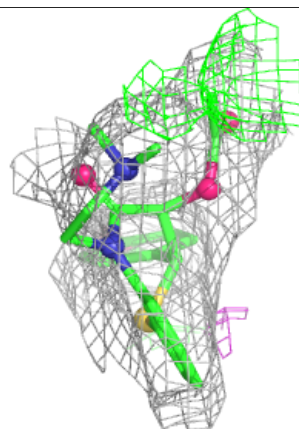
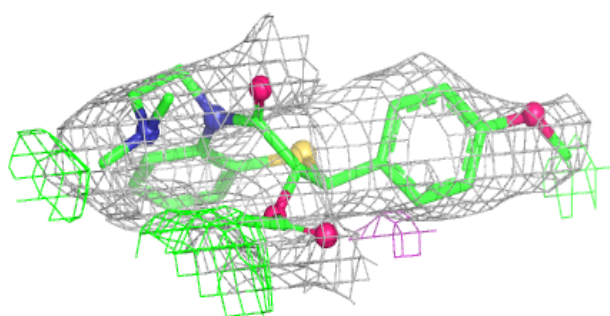
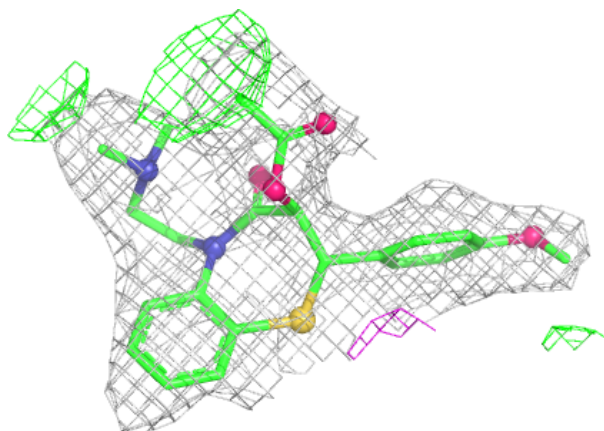
Electron density around PX4 A 1304:

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

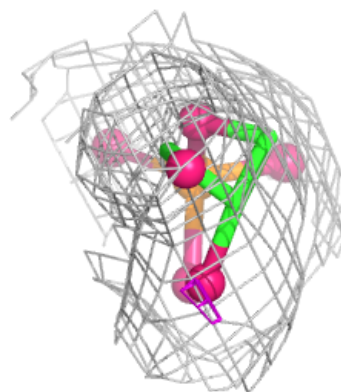
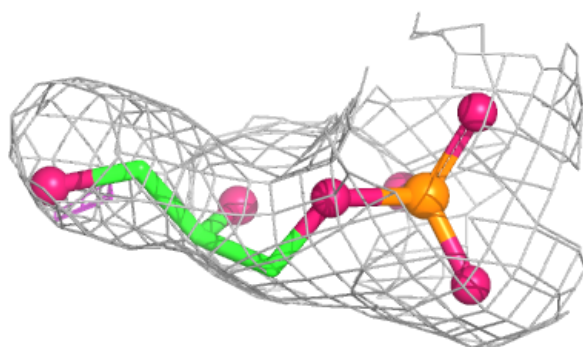
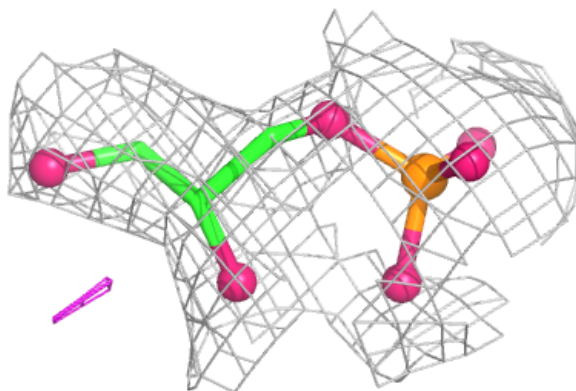


Electron density around D6C D 1304:

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

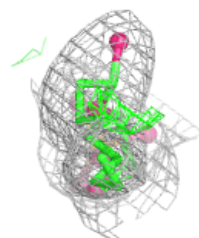
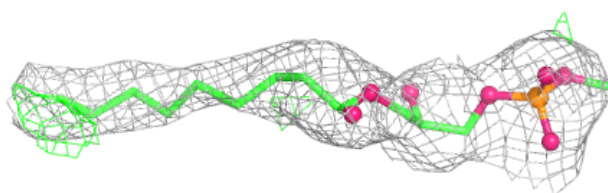
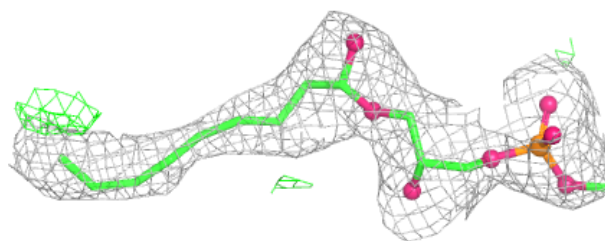
**Electron density around PX4 A 1301:**

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

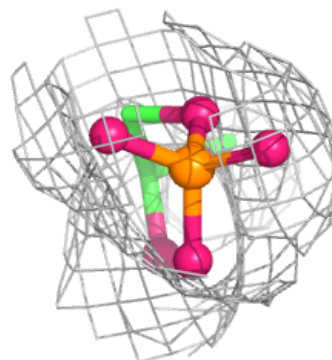
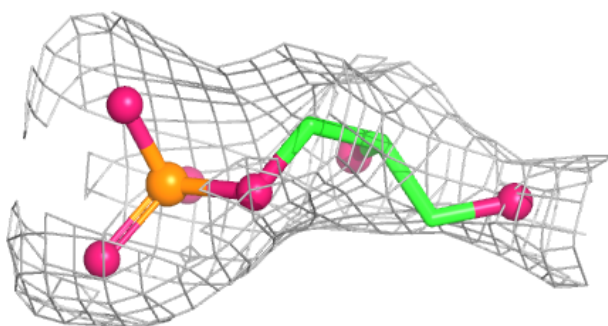


Electron density around PX4 A 1302:

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

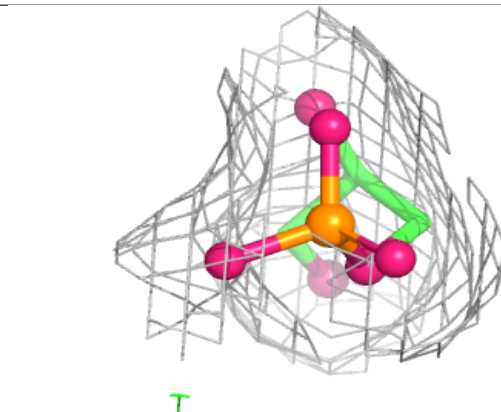
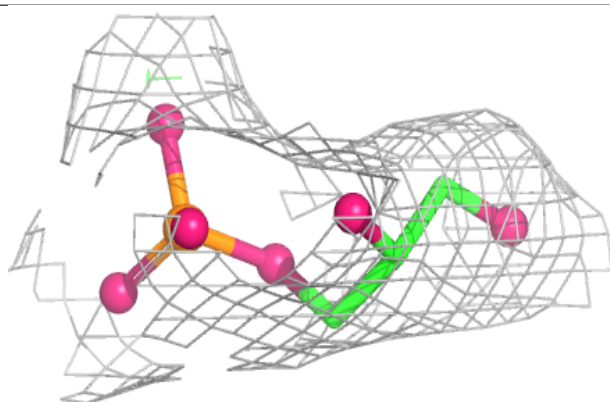
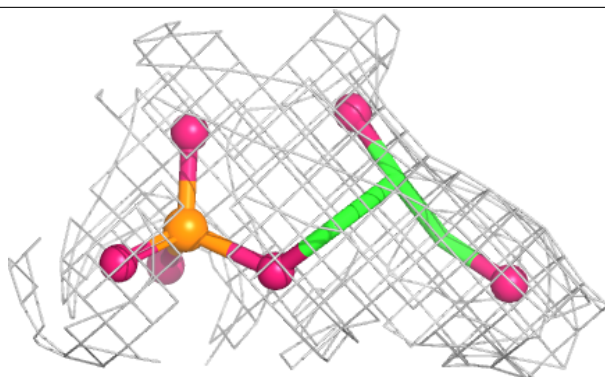
**Electron density around PX4 D 1301:**

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

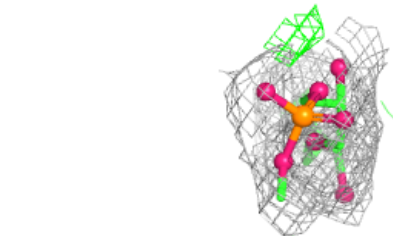
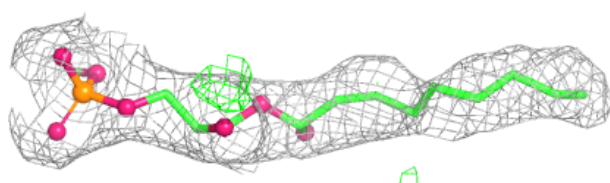
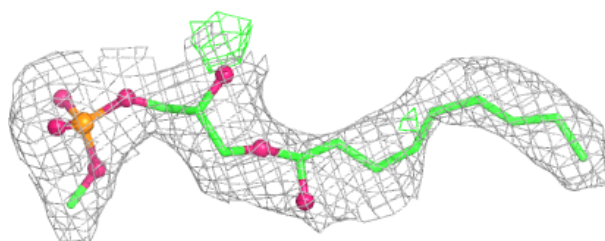


Electron density around PX4 D 1302:

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

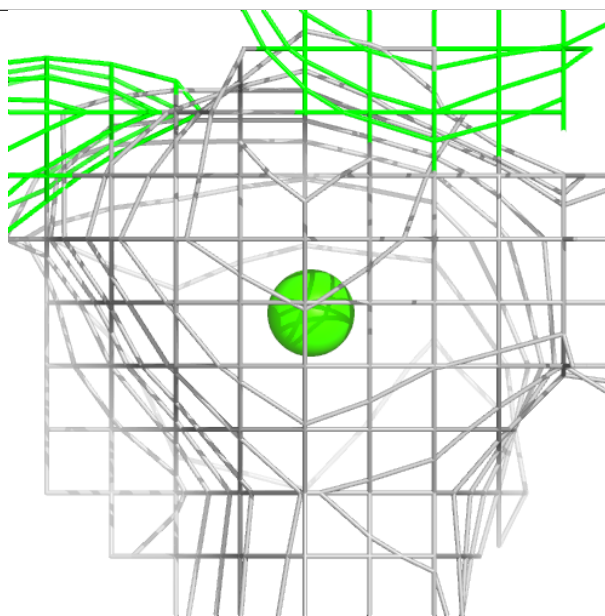
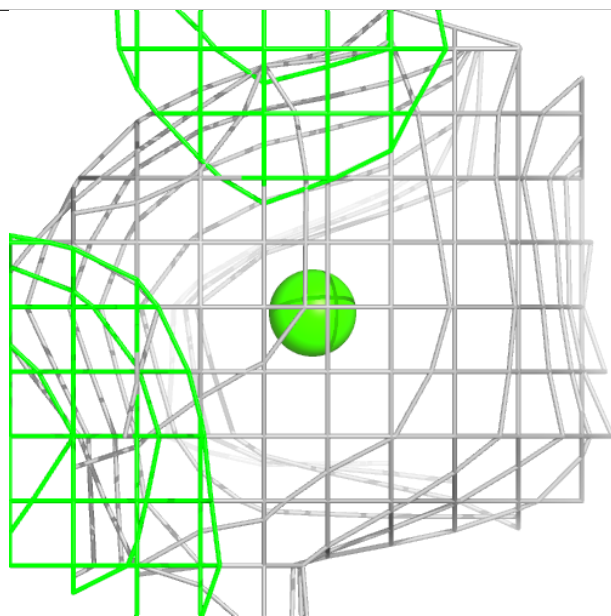
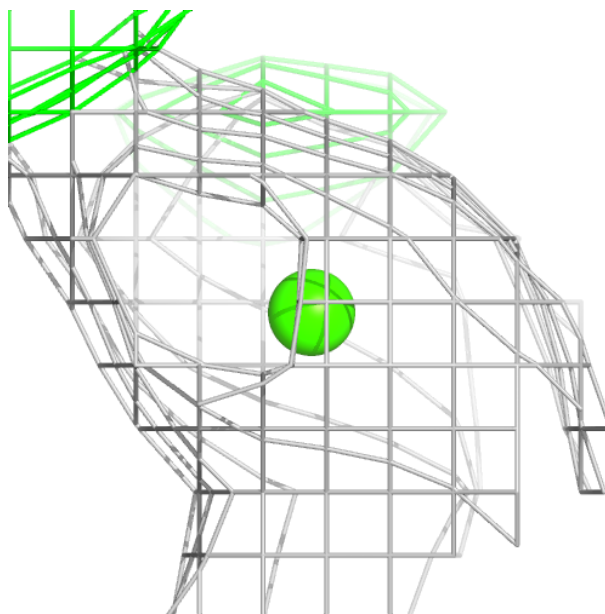
**Electron density around PX4 B 1303:**

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



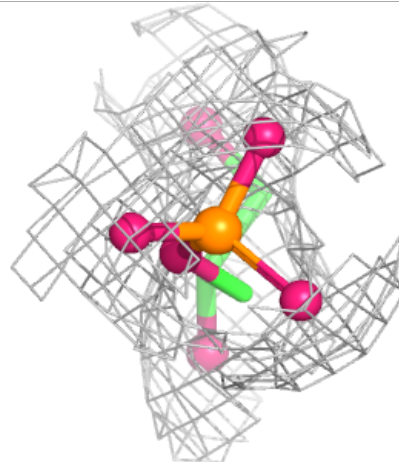
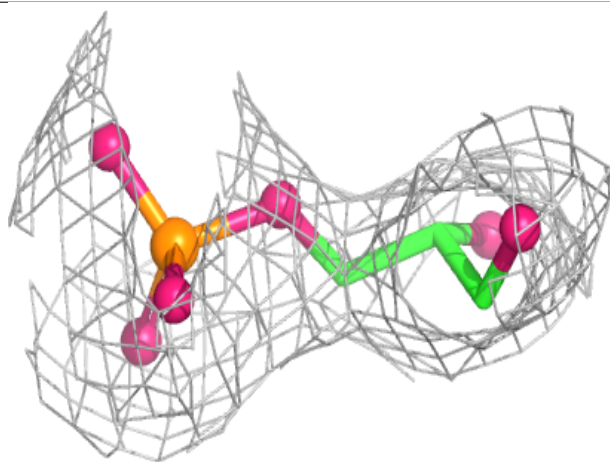
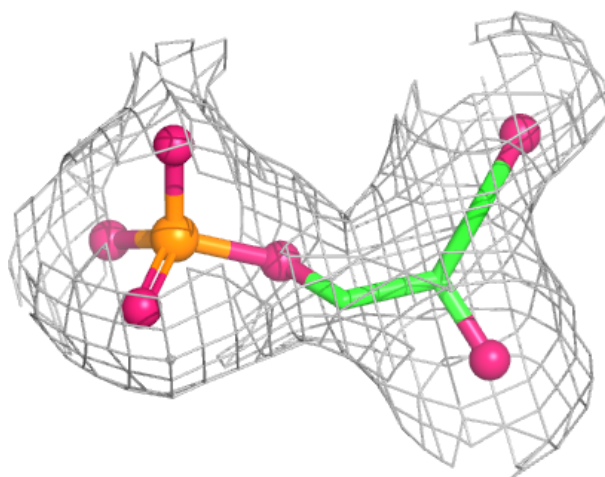
Electron density around CA C 1301:

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



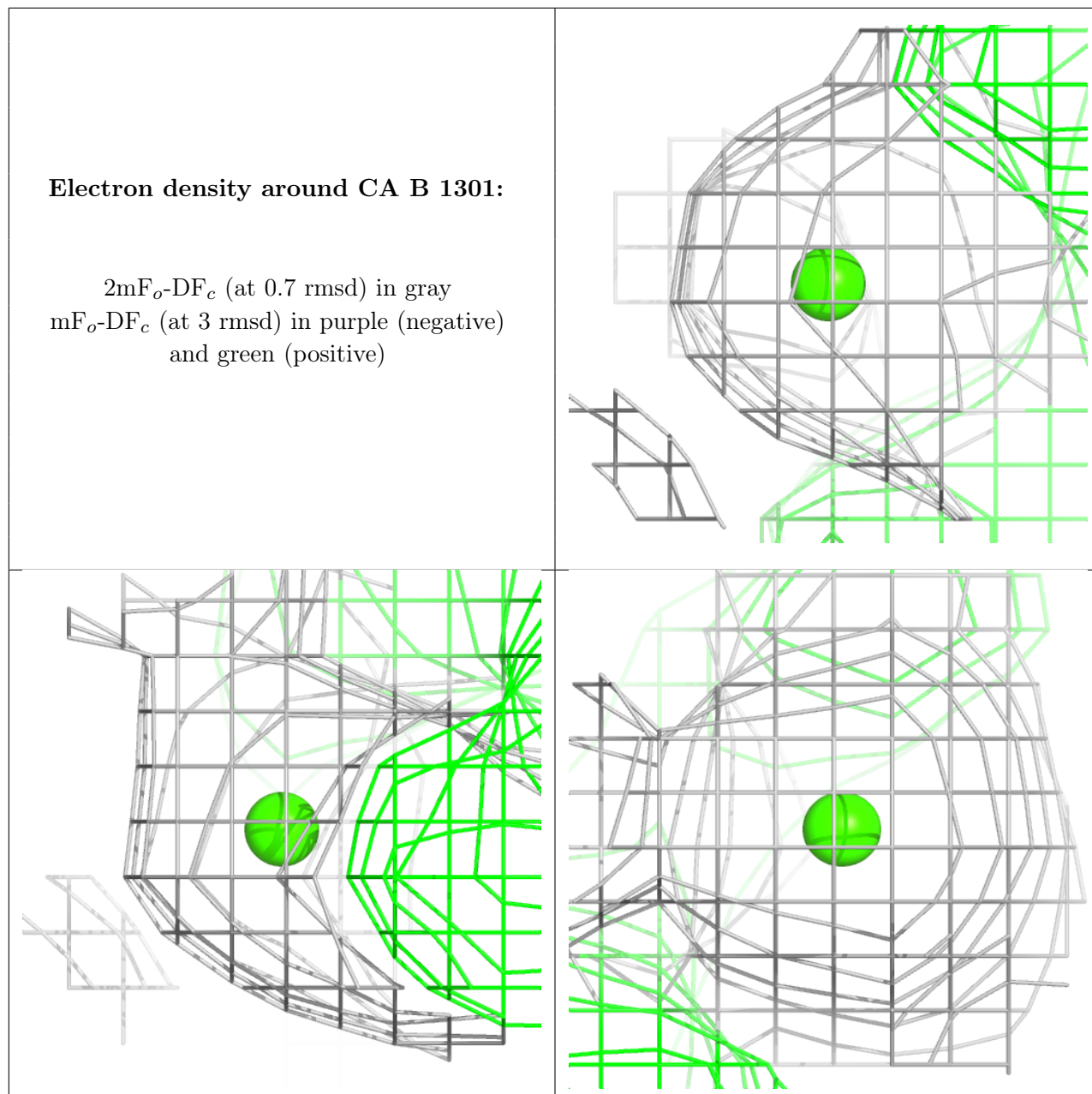
Electron density around PX4 A 1303:

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



Electron density around CA B 1301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.