



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:57 PM UTC

PDB ID : 3RVZ / pdb_00003rvz
Title : Crystal structure of the NavAb voltage-gated sodium channel (Ile217Cys, 2.8 Å)
Authors : Payandeh, J.; Scheuer, T.; Zheng, N.; Catterall, W.A.
Deposited on : 2011-05-06
Resolution : 2.80 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

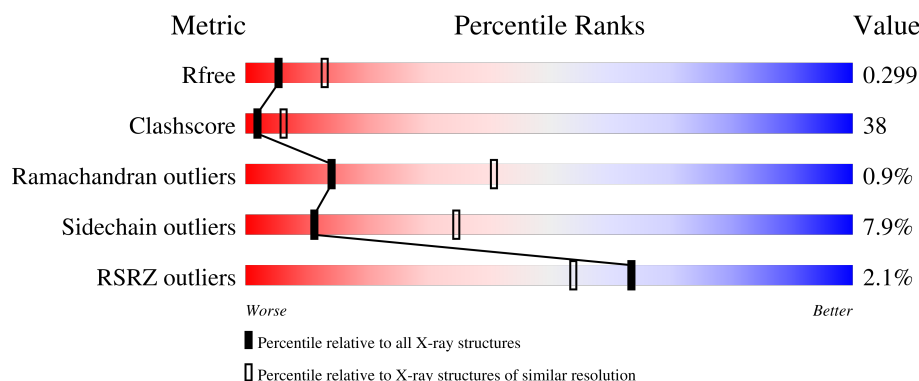
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	285	
1	B	285	

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	PX4	A	4004	-	X	-	-
2	PX4	A	4013	-	X	-	-
2	PX4	A	4014	-	X	-	-
2	PX4	B	4016	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3728 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
			1797	1225	268	292	12			
1	B	219	Total	C	N	O	S	0	0	0
			1797	1225	268	292	12			

There are 38 discrepancies between the modelled and reference sequences:

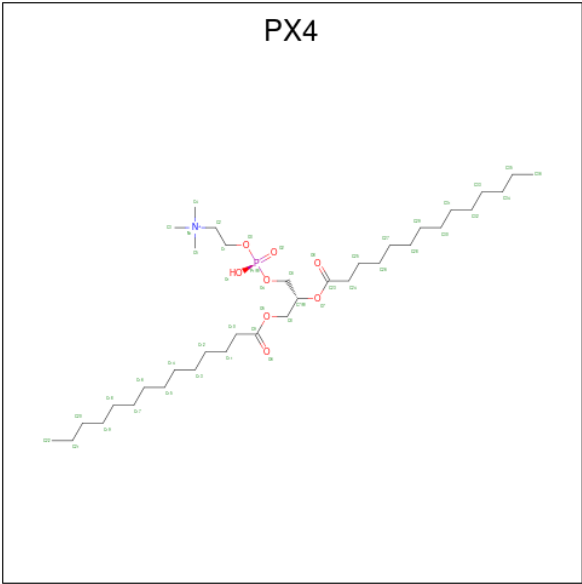
Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	expression tag	UNP A8EVM5
A	984	ASP	-	expression tag	UNP A8EVM5
A	985	TYR	-	expression tag	UNP A8EVM5
A	986	LYS	-	expression tag	UNP A8EVM5
A	987	ASP	-	expression tag	UNP A8EVM5
A	988	ASP	-	expression tag	UNP A8EVM5
A	989	ASP	-	expression tag	UNP A8EVM5
A	990	ASP	-	expression tag	UNP A8EVM5
A	991	LYS	-	expression tag	UNP A8EVM5
A	992	GLY	-	expression tag	UNP A8EVM5
A	993	SER	-	expression tag	UNP A8EVM5
A	994	LEU	-	expression tag	UNP A8EVM5
A	995	VAL	-	expression tag	UNP A8EVM5
A	996	PRO	-	expression tag	UNP A8EVM5
A	997	ARG	-	expression tag	UNP A8EVM5
A	998	GLY	-	expression tag	UNP A8EVM5
A	999	SER	-	expression tag	UNP A8EVM5
A	1000	HIS	-	expression tag	UNP A8EVM5
A	1217	CYS	ILE	engineered mutation	UNP A8EVM5
B	1983	MET	-	expression tag	UNP A8EVM5
B	1984	ASP	-	expression tag	UNP A8EVM5
B	1985	TYR	-	expression tag	UNP A8EVM5
B	1986	LYS	-	expression tag	UNP A8EVM5
B	1987	ASP	-	expression tag	UNP A8EVM5
B	1988	ASP	-	expression tag	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1989	ASP	-	expression tag	UNP A8EVM5
B	1990	ASP	-	expression tag	UNP A8EVM5
B	1991	LYS	-	expression tag	UNP A8EVM5
B	1992	GLY	-	expression tag	UNP A8EVM5
B	1993	SER	-	expression tag	UNP A8EVM5
B	1994	LEU	-	expression tag	UNP A8EVM5
B	1995	VAL	-	expression tag	UNP A8EVM5
B	1996	PRO	-	expression tag	UNP A8EVM5
B	1997	ARG	-	expression tag	UNP A8EVM5
B	1998	GLY	-	expression tag	UNP A8EVM5
B	1999	SER	-	expression tag	UNP A8EVM5
B	2000	HIS	-	expression tag	UNP A8EVM5
B	2217	CYS	ILE	engineered mutation	UNP A8EVM5

- Molecule 2 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PX4) (formula: C₃₆H₇₃NO₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			12	4	7	1		
2	A	1	Total	O	P		0	0
			5	4	1			
2	A	1	Total	C			0	0
			8	8				
2	A	1	Total	C	O	P	0	0
			11	5	5	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 6 6	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total C 6 6	0	0
2	B	1	Total C O P 21 13 7 1	0	0
2	B	1	Total C O P 10 3 6 1	0	0
2	B	1	Total C O P 22 14 7 1	0	0
2	B	1	Total C O P 10 3 6 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total C 6 6	0	0

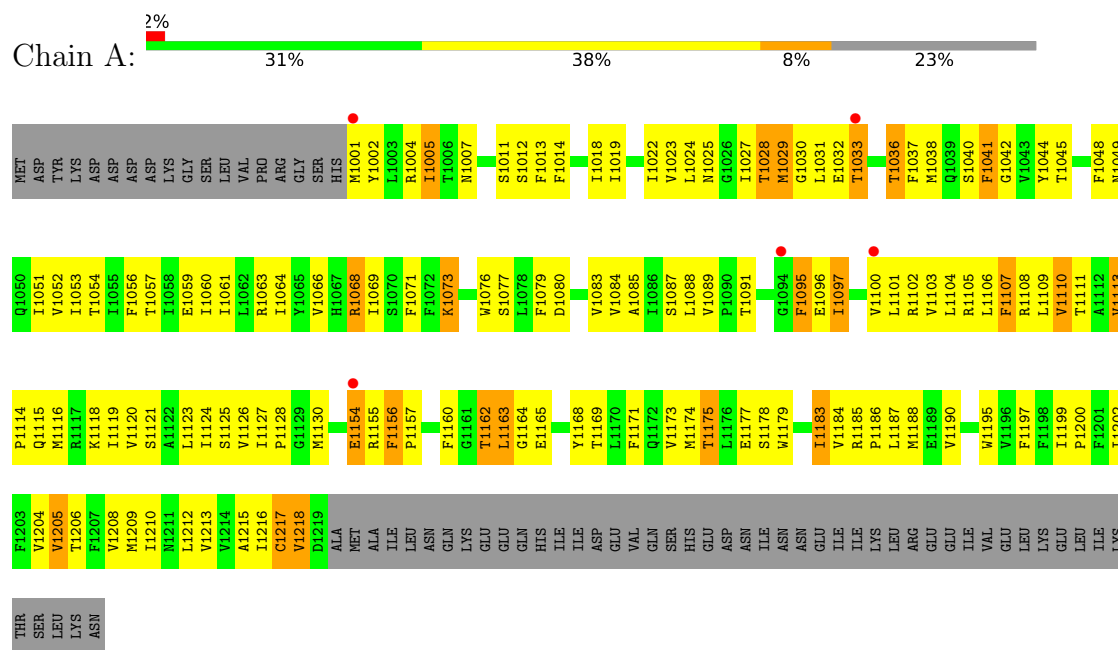
- Molecule 3 is water.

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

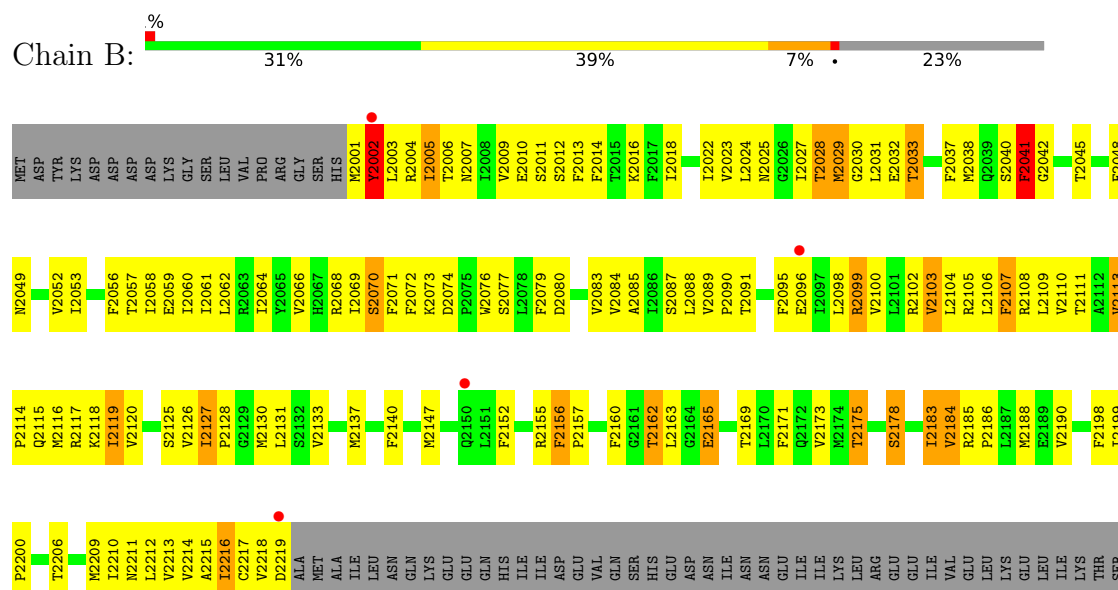
3 Residue-property plots

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



LEU
LYS
ASN

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.28Å 126.14Å 192.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.82	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 84.9 (50.00-2.82)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.267 , 0.292 0.279 , 0.299	Depositor DCC
R_{free} test set	1569 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 97.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.439 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3728	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/1848	1.01	10/2514 (0.4%)
1	B	0.61	1/1848 (0.1%)	1.06	13/2514 (0.5%)
All	All	0.57	1/3696 (0.0%)	1.03	23/5028 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2127	ILE	C-O	-5.89	1.17	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2183	ILE	N-CA-C	8.80	119.13	111.56
1	B	2113	VAL	N-CA-C	7.61	115.45	107.76
1	B	2116	MET	N-CA-C	-7.39	103.16	111.07
1	B	2184	VAL	N-CA-C	7.01	117.80	110.72
1	B	2107	PHE	N-CA-C	-7.00	104.72	113.18
1	B	2216	ILE	CB-CA-C	-6.23	103.62	112.22
1	B	2198	PHE	N-CA-C	6.20	119.31	111.69
1	A	1156	PHE	CA-C-N	6.05	125.53	119.24
1	A	1156	PHE	C-N-CA	6.05	125.53	119.24
1	B	2218	VAL	N-CA-CB	-6.00	105.63	111.57
1	A	1110	VAL	N-CA-C	-5.98	103.92	112.35
1	A	1068	ARG	CB-CA-C	-5.86	109.80	116.54
1	A	1097	ILE	N-CA-C	-5.85	104.14	110.23
1	A	1073	LYS	N-CA-C	-5.80	105.57	114.16
1	B	2165	GLU	N-CA-C	-5.73	104.94	111.07
1	A	1183	ILE	N-CA-C	5.73	116.15	111.62
1	A	1113	VAL	N-CA-C	5.72	116.75	107.71
1	B	2218	VAL	N-CA-C	5.62	116.76	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1116	MET	N-CA-C	-5.42	105.27	111.07
1	B	2175	THR	N-CA-C	-5.35	106.83	113.19
1	B	2156	PHE	CA-C-N	5.14	126.26	119.84
1	B	2156	PHE	C-N-CA	5.14	126.26	119.84
1	A	1175	THR	N-CA-C	-5.01	107.22	113.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1797	0	1869	150	0
1	B	1797	0	1869	153	0
2	A	58	0	43	2	0
2	B	74	0	59	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	3728	0	3840	291	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 38.

All (291) 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:2018:ILE:CD1	1:B:2059:GLU:OE1	1.89	1.20
1:A:1217:CYS:SG	1:B:2214:VAL:HG22	1.84	1.17
1:B:2018:ILE:HD12	1:B:2059:GLU:OE1	1.46	1.11
1:A:1018:ILE:HD12	1:A:1059:GLU:OE1	1.54	1.04
1:B:2002:TYR:CE1	1:B:2006:THR:OG1	2.13	1.01
1:B:2162:THR:HG22	1:B:2165:GLU:H	1.26	0.98
1:B:2002:TYR:HE1	1:B:2006:THR:OG1	1.47	0.97
1:B:2096:GLU:HG3	1:B:2099:ARG:HB3	1.45	0.96
1:A:1174:MET:HG3	1:A:1205:VAL:HG11	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2025:ASN:OD1	1:B:2105:ARG:NH1	1.99	0.96
1:A:1029:MET:HE3	1:A:1103:VAL:HA	1.47	0.95
1:A:1045:THR:O	1:A:1049:ASN:ND2	2.03	0.90
1:A:1059:GLU:OE2	1:A:1108:ARG:NH2	2.04	0.90
1:B:2001:MET:HG3	1:B:2004:ARG:HD3	1.54	0.87
1:A:1001:MET:HG3	1:A:1004:ARG:HD3	1.55	0.87
1:A:1059:GLU:O	1:A:1063:ARG:HG3	1.76	0.85
1:B:2029:MET:HE3	1:B:2103:VAL:HA	1.59	0.84
1:B:2053:ILE:HD11	1:B:2088:LEU:HD23	1.58	0.84
1:A:1018:ILE:CD1	1:A:1059:GLU:OE1	2.26	0.84
1:B:2118:LYS:HA	1:B:2118:LYS:HE2	1.59	0.84
1:B:2083:VAL:HG11	1:B:2105:ARG:HA	1.57	0.84
1:A:1174:MET:HG3	1:A:1205:VAL:CG1	2.08	0.83
1:B:2018:ILE:CG1	1:B:2059:GLU:OE1	2.25	0.83
1:B:2130:MET:HE3	1:B:2212:LEU:HD21	1.61	0.81
1:B:2059:GLU:OE2	1:B:2108:ARG:NH2	2.15	0.79
1:B:2002:TYR:C	1:B:2002:TYR:HD1	1.90	0.79
1:B:2100:VAL:O	1:B:2103:VAL:HG13	1.82	0.78
1:A:1048:PHE:O	1:A:1052:VAL:HG23	1.86	0.75
1:A:1085:ALA:HA	1:A:1088:LEU:HD12	1.69	0.75
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.67	0.75
1:B:2014:PHE:CZ	1:B:2059:GLU:HG3	2.24	0.73
1:A:1025:ASN:OD1	1:A:1105:ARG:HD2	1.88	0.72
1:A:1177:GLU:OE1	1:A:1178:SER:OG	2.05	0.72
1:B:2002:TYR:C	1:B:2002:TYR:CD1	2.63	0.72
1:B:2001:MET:O	1:B:2004:ARG:HB3	1.89	0.71
1:B:2057:THR:O	1:B:2060:ILE:HG22	1.90	0.71
1:B:2096:GLU:HG3	1:B:2099:ARG:CB	2.18	0.71
1:B:2025:ASN:OD1	1:B:2105:ARG:HD2	1.91	0.70
1:B:2080:ASP:O	1:B:2084:VAL:HG23	1.92	0.70
1:B:2018:ILE:HG13	1:B:2059:GLU:OE1	1.91	0.70
1:B:2032:GLU:HA	1:B:2038:MET:HE3	1.72	0.70
1:A:1032:GLU:HA	1:A:1038:MET:HE3	1.73	0.69
1:B:2045:THR:O	1:B:2049:ASN:ND2	2.24	0.69
1:A:1076:TRP:CZ2	2:A:4006:PX4:H46	2.27	0.69
1:A:1130:MET:HE3	1:A:1212:LEU:HD21	1.74	0.69
1:A:1022:ILE:HD12	1:A:1108:ARG:HB3	1.73	0.69
1:B:2074:ASP:HB3	1:B:2077:SER:OG	1.92	0.69
1:A:1217:CYS:SG	1:B:2214:VAL:CG2	2.76	0.68
1:B:2100:VAL:O	1:B:2103:VAL:CG1	2.42	0.68
1:A:1118:LYS:HE2	1:A:1118:LYS:HA	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:VAL:HG11	1:B:2147:MET:HG2	1.74	0.68
1:B:2028:THR:HG23	1:B:2045:THR:HG23	1.75	0.68
1:A:1130:MET:SD	1:A:1216:ILE:HD11	2.34	0.67
1:B:2185:ARG:HB2	1:B:2186:PRO:HD3	1.74	0.67
1:B:2027:ILE:O	1:B:2031:LEU:HD13	1.93	0.67
1:B:2199:ILE:HB	1:B:2200:PRO:HD3	1.75	0.67
1:B:2002:TYR:CD1	1:B:2006:THR:OG1	2.47	0.67
1:A:1080:ASP:O	1:A:1084:VAL:HG23	1.95	0.66
1:A:1123:LEU:HD22	1:B:2211:ASN:HD22	1.59	0.66
1:B:2048:PHE:O	1:B:2052:VAL:HG23	1.95	0.65
1:A:1169:THR:O	1:A:1173:VAL:HG23	1.97	0.65
1:A:1057:THR:O	1:A:1060:ILE:HG22	1.97	0.65
1:A:1002:TYR:O	1:A:1005:ILE:HG23	1.96	0.65
1:A:1100:VAL:O	1:A:1103:VAL:HG12	1.97	0.64
1:A:1185:ARG:HB2	1:A:1186:PRO:HD3	1.78	0.64
1:A:1038:MET:HA	1:A:1038:MET:HE2	1.81	0.63
1:A:1104:LEU:O	1:A:1107:PHE:HB2	1.99	0.63
1:B:2130:MET:SD	1:B:2216:ILE:HD11	2.39	0.62
1:B:2079:PHE:CE2	1:B:2083:VAL:HG21	2.34	0.62
1:B:2022:ILE:HG21	1:B:2109:LEU:HB2	1.81	0.62
1:A:1025:ASN:O	1:A:1028:THR:HG22	1.99	0.62
1:B:2127:ILE:HB	1:B:2128:PRO:HD3	1.82	0.61
1:A:1217:CYS:SG	1:B:2214:VAL:HA	2.40	0.61
1:A:1125:SER:O	1:A:1128:PRO:HD2	2.00	0.61
1:B:2160:PHE:CE2	1:B:2169:THR:HG21	2.35	0.61
1:A:1206:THR:O	1:A:1210:ILE:HG13	2.01	0.61
1:B:2209:MET:O	1:B:2213:VAL:HG23	2.01	0.61
1:A:1209:MET:O	1:A:1213:VAL:HG23	2.00	0.60
1:B:2018:ILE:O	1:B:2022:ILE:HG12	2.00	0.60
1:B:2071:PHE:CE1	1:B:2077:SER:HB2	2.36	0.60
1:A:1162:THR:HG22	1:A:1164:GLY:N	2.17	0.60
1:B:2128:PRO:HA	1:B:2131:LEU:CD1	2.31	0.60
1:B:2162:THR:HB	1:B:2165:GLU:HB2	1.84	0.60
1:B:2212:LEU:C	1:B:2212:LEU:HD23	2.27	0.60
1:A:1001:MET:O	1:A:1004:ARG:HB3	2.00	0.59
1:A:1120:VAL:HG12	1:A:1124:ILE:CD1	2.32	0.58
1:A:1057:THR:O	1:A:1061:ILE:HG13	2.03	0.58
1:A:1162:THR:HG22	1:A:1164:GLY:H	1.67	0.58
1:B:2155:ARG:HD2	1:B:2190:VAL:HG11	1.85	0.58
1:B:2126:VAL:HG11	1:B:2216:ILE:HG23	1.84	0.58
1:A:1033:THR:HG21	1:B:2163:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:VAL:HG12	1:A:1114:PRO:O	2.03	0.57
1:A:1126:VAL:HG11	1:A:1216:ILE:HG23	1.86	0.57
1:B:2114:PRO:O	1:B:2115:GLN:HB2	2.05	0.57
1:A:1071:PHE:CE1	1:A:1077:SER:HB3	2.39	0.57
1:A:1108:ARG:HG2	1:A:1108:ARG:HH11	1.70	0.56
1:B:2089:VAL:HG13	1:B:2090:PRO:HD2	1.86	0.56
1:A:1001:MET:O	1:A:1005:ILE:HG22	2.05	0.56
1:A:1068:ARG:HG3	1:A:1069:ILE:H	1.70	0.56
1:A:1029:MET:HE2	1:A:1106:LEU:HD21	1.87	0.56
1:A:1101:LEU:O	1:A:1104:LEU:HB2	2.04	0.56
1:B:2206:THR:O	1:B:2210:ILE:HG13	2.05	0.56
1:B:2022:ILE:HD11	1:B:2108:ARG:HG2	1.88	0.56
1:A:1154:GLU:OE1	1:A:1154:GLU:HA	2.05	0.56
1:A:1028:THR:HA	1:A:1031:LEU:HD12	1.87	0.56
1:A:1079:PHE:CE2	1:A:1083:VAL:HG21	2.41	0.56
1:B:2040:SER:C	1:B:2042:GLY:H	2.13	0.56
1:A:1018:ILE:O	1:A:1022:ILE:HG12	2.05	0.56
1:A:1114:PRO:O	1:A:1115:GLN:HB2	2.05	0.56
1:B:2002:TYR:HE1	1:B:2006:THR:HG1	0.67	0.55
1:B:2022:ILE:HD12	1:B:2108:ARG:HB3	1.88	0.55
1:B:2110:VAL:HG11	1:B:2120:VAL:HG21	1.88	0.55
1:B:2113:VAL:HG12	1:B:2114:PRO:O	2.06	0.55
1:A:1109:LEU:O	1:A:1109:LEU:HG	2.07	0.55
1:B:2053:ILE:HD11	1:B:2088:LEU:HA	1.86	0.55
1:B:2096:GLU:CG	1:B:2096:GLU:O	2.55	0.55
1:A:1023:VAL:O	1:A:1027:ILE:HG13	2.06	0.55
1:B:2162:THR:HG22	1:B:2165:GLU:N	2.08	0.55
1:B:2057:THR:O	1:B:2061:ILE:HG13	2.07	0.55
1:B:2080:ASP:OD1	1:B:2111:THR:HG21	2.07	0.55
1:A:1087:SER:OG	1:A:1105:ARG:NH2	2.40	0.54
1:B:2060:ILE:O	1:B:2064:ILE:HG13	2.08	0.54
1:A:1184:VAL:O	1:A:1188:MET:HG3	2.08	0.54
1:A:1027:ILE:O	1:A:1031:LEU:HD12	2.07	0.54
1:A:1041:PHE:CD1	1:A:1041:PHE:N	2.76	0.54
1:B:2066:VAL:HG12	1:B:2066:VAL:O	2.06	0.54
1:B:2171:PHE:O	1:B:2175:THR:HG23	2.08	0.53
1:B:2018:ILE:HD11	1:B:2059:GLU:OE1	2.00	0.53
1:A:1060:ILE:O	1:A:1064:ILE:HG13	2.09	0.53
1:A:1120:VAL:HG12	1:A:1124:ILE:HD12	1.90	0.52
1:A:1053:ILE:HD11	1:A:1088:LEU:HD23	1.90	0.52
1:B:2031:LEU:C	1:B:2033:THR:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2184:VAL:O	1:B:2188:MET:HG3	2.10	0.52
1:A:1130:MET:HE2	1:A:1212:LEU:HD11	1.92	0.52
1:B:2085:ALA:O	1:B:2088:LEU:HB2	2.09	0.52
1:A:1130:MET:CE	1:A:1216:ILE:HD11	2.39	0.52
1:A:1103:VAL:HG11	1:B:2147:MET:CG	2.40	0.51
1:A:1128:PRO:C	1:A:1130:MET:H	2.18	0.51
1:A:1155:ARG:HD2	1:A:1190:VAL:HG11	1.92	0.51
1:B:2156:PHE:N	1:B:2157:PRO:HD3	2.26	0.51
1:B:2184:VAL:HG12	1:B:2188:MET:HE2	1.92	0.51
1:B:2110:VAL:CG1	1:B:2120:VAL:HG21	2.40	0.51
1:B:2007:ASN:O	1:B:2011:SER:HB3	2.11	0.51
1:B:2032:GLU:HA	1:B:2038:MET:CE	2.38	0.51
1:B:2215:ALA:O	1:B:2219:ASP:N	2.44	0.51
1:A:1036:THR:HG22	1:A:1037:PHE:N	2.25	0.51
1:A:1083:VAL:HG11	1:A:1105:ARG:HA	1.91	0.51
1:A:1064:ILE:O	1:A:1068:ARG:N	2.34	0.51
1:A:1130:MET:CE	1:A:1212:LEU:HD21	2.40	0.51
1:B:2115:GLN:O	1:B:2119:ILE:HG12	2.11	0.50
1:A:1213:VAL:O	1:A:1217:CYS:HB2	2.11	0.50
1:B:2022:ILE:CD1	1:B:2108:ARG:HG2	2.40	0.50
1:A:1076:TRP:CE2	2:A:4006:PX4:H46	2.46	0.50
1:A:1108:ARG:HG2	1:A:1108:ARG:NH1	2.26	0.50
1:B:2068:ARG:HG3	1:B:2069:ILE:N	2.26	0.50
1:A:1105:ARG:O	1:A:1108:ARG:HB2	2.11	0.50
1:B:2130:MET:HE3	1:B:2212:LEU:CD2	2.37	0.50
1:A:1130:MET:HE3	1:A:1212:LEU:CD2	2.42	0.50
1:B:2002:TYR:O	1:B:2005:ILE:HG23	2.12	0.50
1:B:2169:THR:O	1:B:2173:VAL:HG23	2.12	0.50
1:B:2128:PRO:HA	1:B:2131:LEU:HD11	1.94	0.50
1:B:2038:MET:HA	1:B:2038:MET:HE2	1.92	0.49
1:B:2053:ILE:CD1	1:B:2088:LEU:HD23	2.38	0.49
1:A:1156:PHE:N	1:A:1157:PRO:HD3	2.27	0.49
1:B:2068:ARG:HG3	1:B:2069:ILE:H	1.77	0.49
1:B:2018:ILE:HG13	1:B:2059:GLU:CD	2.36	0.49
1:A:1019:ILE:HD13	1:A:1113:VAL:HG22	1.94	0.49
1:A:1029:MET:HE2	1:A:1106:LEU:CG	2.42	0.49
1:A:1056:PHE:HE2	1:A:1108:ARG:HD3	1.77	0.49
1:A:1157:PRO:O	1:A:1165:GLU:OE2	2.30	0.49
1:A:1162:THR:CG2	1:A:1164:GLY:H	2.26	0.49
1:B:2104:LEU:O	1:B:2107:PHE:HB2	2.13	0.49
1:A:1130:MET:CE	1:A:1212:LEU:HD11	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2062:LEU:O	1:B:2066:VAL:HG23	2.12	0.48
1:A:1029:MET:HE2	1:A:1106:LEU:CD2	2.43	0.48
1:B:2031:LEU:C	1:B:2033:THR:N	2.71	0.48
1:B:2109:LEU:O	1:B:2109:LEU:HG	2.13	0.48
1:A:1014:PHE:CZ	1:A:1059:GLU:HG3	2.49	0.48
1:A:1068:ARG:HG3	1:A:1069:ILE:N	2.27	0.48
1:A:1160:PHE:CZ	1:A:1169:THR:HG21	2.49	0.48
1:A:1168:TYR:CZ	1:B:2188:MET:HE1	2.48	0.48
1:A:1007:ASN:O	1:A:1011:SER:HB3	2.14	0.48
1:A:1162:THR:HG22	1:A:1165:GLU:H	1.79	0.48
1:A:1028:THR:HA	1:A:1031:LEU:CD1	2.44	0.47
1:A:1110:VAL:CG1	1:A:1120:VAL:HG21	2.44	0.47
1:B:2001:MET:CG	1:B:2004:ARG:HD3	2.37	0.47
1:B:2091:THR:HA	1:B:2102:ARG:HH22	1.80	0.47
1:B:2185:ARG:N	1:B:2186:PRO:CD	2.78	0.47
1:A:1041:PHE:N	1:A:1041:PHE:HD1	2.12	0.47
1:A:1110:VAL:HG11	1:A:1120:VAL:HG21	1.96	0.47
1:B:2118:LYS:HE2	1:B:2118:LYS:CA	2.40	0.47
1:A:1022:ILE:HG21	1:A:1109:LEU:HB2	1.97	0.47
1:A:1029:MET:HE2	1:A:1106:LEU:HG	1.96	0.47
1:B:2083:VAL:CG1	1:B:2105:ARG:HA	2.37	0.46
1:A:1114:PRO:O	1:A:1115:GLN:CB	2.62	0.46
1:A:1162:THR:CG2	1:A:1163:LEU:N	2.79	0.46
1:B:2103:VAL:O	1:B:2103:VAL:HG23	2.15	0.46
1:B:2114:PRO:O	1:B:2115:GLN:CB	2.62	0.46
1:A:1195:TRP:O	1:A:1199:ILE:HG12	2.15	0.46
1:B:2076:TRP:CZ3	1:B:2117:ARG:HG2	2.51	0.46
1:B:2152:PHE:HB2	1:B:2160:PHE:CD1	2.51	0.46
1:A:1080:ASP:OD1	1:A:1111:THR:HG21	2.15	0.45
1:A:1105:ARG:C	1:A:1107:PHE:N	2.74	0.45
1:B:2029:MET:HE2	1:B:2106:LEU:HD21	1.97	0.45
1:B:2003:LEU:HA	1:B:2006:THR:HB	1.98	0.45
1:A:1031:LEU:C	1:A:1033:THR:H	2.25	0.45
1:A:1184:VAL:HG12	1:A:1188:MET:HE2	1.98	0.45
1:A:1066:VAL:HG12	1:A:1066:VAL:O	2.17	0.45
1:A:1120:VAL:HG12	1:A:1124:ILE:HD11	1.97	0.45
1:A:1031:LEU:C	1:A:1033:THR:N	2.72	0.45
1:A:1084:VAL:O	1:A:1088:LEU:HG	2.17	0.45
1:A:1012:SER:O	1:A:1013:PHE:C	2.60	0.45
1:A:1031:LEU:HD22	1:A:1037:PHE:CE1	2.51	0.45
1:B:2137:MET:HE2	1:B:2209:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2012:SER:O	1:B:2013:PHE:C	2.60	0.45
1:A:1119:ILE:O	1:A:1123:LEU:HG	2.17	0.44
1:B:2037:PHE:HE2	1:B:2045:THR:OG1	2.00	0.44
1:B:2041:PHE:CD1	1:B:2041:PHE:N	2.85	0.44
1:B:2119:ILE:N	1:B:2119:ILE:HD13	2.33	0.44
1:A:1071:PHE:C	1:A:1073:LYS:H	2.25	0.44
1:A:1187:LEU:HD12	1:A:1187:LEU:HA	1.87	0.44
1:B:2137:MET:CE	1:B:2209:MET:HE3	2.48	0.44
1:A:1105:ARG:HG3	1:A:1106:LEU:N	2.33	0.44
1:A:1119:ILE:O	1:A:1120:VAL:C	2.61	0.44
1:B:2137:MET:O	1:B:2140:PHE:HB3	2.18	0.44
1:A:1095:PHE:CE1	1:A:1097:ILE:HD12	2.53	0.44
1:B:2102:ARG:C	1:B:2104:LEU:N	2.76	0.44
1:B:2130:MET:CE	1:B:2212:LEU:HD11	2.48	0.43
1:A:1041:PHE:HD1	1:A:1041:PHE:H	1.65	0.43
1:A:1076:TRP:HZ2	1:A:1121:SER:OG	2.02	0.43
1:A:1120:VAL:CG1	1:A:1124:ILE:HD11	2.49	0.43
1:B:2012:SER:OG	1:B:2016:LYS:HE3	2.18	0.43
1:B:2037:PHE:HD2	1:B:2038:MET:CE	2.32	0.43
1:B:2108:ARG:HG3	1:B:2108:ARG:HH11	1.82	0.43
1:A:1030:GLY:O	1:A:1033:THR:HB	2.18	0.43
1:A:1171:PHE:O	1:A:1175:THR:HG23	2.19	0.43
1:B:2023:VAL:O	1:B:2027:ILE:HG13	2.19	0.43
1:A:1156:PHE:CE1	1:A:1187:LEU:HD12	2.54	0.43
1:A:1185:ARG:N	1:A:1186:PRO:CD	2.82	0.43
1:B:2069:ILE:HG23	1:B:2070:SER:N	2.33	0.43
1:A:1217:CYS:CB	1:B:2214:VAL:HG22	2.47	0.43
1:B:2127:ILE:N	1:B:2128:PRO:HD2	2.34	0.42
1:B:2119:ILE:O	1:B:2120:VAL:C	2.61	0.42
1:B:2087:SER:HA	1:B:2102:ARG:HG2	2.01	0.42
1:A:1040:SER:C	1:A:1042:GLY:H	2.27	0.42
1:B:2105:ARG:O	1:B:2108:ARG:HB2	2.20	0.42
1:A:1127:ILE:HB	1:A:1128:PRO:HD3	2.02	0.42
1:B:2064:ILE:HG12	1:B:2071:PHE:CD2	2.54	0.42
1:B:2211:ASN:O	1:B:2214:VAL:HB	2.19	0.42
1:A:1105:ARG:C	1:A:1107:PHE:H	2.27	0.42
1:B:2080:ASP:CG	1:B:2111:THR:HG21	2.45	0.42
1:A:1060:ILE:HD11	1:A:1071:PHE:HZ	1.85	0.42
1:B:2080:ASP:OD2	1:B:2108:ARG:NH1	2.52	0.42
1:B:2102:ARG:C	1:B:2104:LEU:H	2.27	0.42
1:B:2125:SER:O	1:B:2128:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:ASP:OD2	1:A:1108:ARG:CZ	2.68	0.41
1:A:1085:ALA:O	1:A:1088:LEU:HB2	2.20	0.41
1:A:1087:SER:HA	1:A:1102:ARG:HG2	2.02	0.41
1:A:1183:ILE:O	1:A:1187:LEU:HB2	2.19	0.41
1:B:2006:THR:O	1:B:2010:GLU:HB2	2.20	0.41
1:B:2030:GLY:O	1:B:2033:THR:HB	2.20	0.41
1:A:1102:ARG:C	1:A:1104:LEU:N	2.78	0.41
1:A:1217:CYS:O	1:A:1218:VAL:HG23	2.21	0.41
1:A:1130:MET:HE3	1:A:1216:ILE:HD11	2.01	0.41
1:A:1217:CYS:HA	1:B:2214:VAL:HG13	2.02	0.41
1:B:2209:MET:HE2	1:B:2209:MET:HA	2.02	0.41
1:A:1204:VAL:O	1:A:1208:VAL:HG23	2.21	0.41
1:B:2001:MET:O	1:B:2002:TYR:C	2.64	0.41
1:A:1044:TYR:N	1:A:1044:TYR:CD1	2.88	0.41
1:A:1057:THR:C	1:A:1060:ILE:HG22	2.46	0.41
1:A:1091:THR:HA	1:A:1102:ARG:HH22	1.85	0.41
1:B:2058:ILE:O	1:B:2062:LEU:HG	2.21	0.41
1:B:2009:VAL:HA	1:B:2014:PHE:CD2	2.55	0.41
1:B:2064:ILE:O	1:B:2068:ARG:N	2.44	0.41
1:B:2089:VAL:HG11	1:B:2098:LEU:HD13	2.02	0.41
1:A:1168:TYR:CZ	1:B:2188:MET:CE	3.04	0.41
1:A:1177:GLU:OE1	1:B:2178:SER:HA	2.20	0.41
1:A:1051:ILE:O	1:A:1054:THR:HB	2.21	0.41
1:B:2006:THR:O	1:B:2006:THR:HG22	2.21	0.41
1:B:2162:THR:CB	1:B:2165:GLU:HB2	2.50	0.41
1:B:2052:VAL:HG12	1:B:2056:PHE:CD1	2.57	0.40
1:B:2066:VAL:O	1:B:2066:VAL:CG1	2.69	0.40
1:B:2040:SER:C	1:B:2042:GLY:N	2.78	0.40
1:A:1037:PHE:CZ	1:A:1041:PHE:HB2	2.57	0.40
1:A:1179:TRP:O	1:A:1184:VAL:HG23	2.21	0.40
1:B:2064:ILE:HD13	1:B:2072:PHE:CZ	2.56	0.40
1:A:1202:ILE:O	1:A:1206:THR:OG1	2.38	0.40
1:B:2002:TYR:CD1	1:B:2003:LEU:N	2.90	0.40
1:B:2071:PHE:C	1:B:2073:LYS:H	2.29	0.40
1:A:1088:LEU:O	1:A:1089:VAL:C	2.64	0.40
1:A:1197:PHE:CD2	1:A:1197:PHE:C	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/285 (76%)	175 (81%)	40 (18%)	2 (1%)	14	41
1	B	217/285 (76%)	182 (84%)	33 (15%)	2 (1%)	14	41
All	All	434/570 (76%)	357 (82%)	73 (17%)	4 (1%)	14	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1218	VAL
1	A	1215	ALA
1	B	2002	TYR
1	B	2041	PHE

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	202/264 (76%)	187 (93%)	15 (7%)	13	37
1	B	202/264 (76%)	185 (92%)	17 (8%)	10	32
All	All	404/528 (76%)	372 (92%)	32 (8%)	11	35

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1005	ILE
1	A	1024	LEU

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Mol	Chain	Res	Type
1	A	1028	THR
1	A	1029	MET
1	A	1033	THR
1	A	1036	THR
1	A	1041	PHE
1	A	1095	PHE
1	A	1096	GLU
1	A	1107	PHE
1	A	1154	GLU
1	A	1162	THR
1	A	1163	LEU
1	A	1205	VAL
1	A	1217	CYS
1	B	2002	TYR
1	B	2005	ILE
1	B	2024	LEU
1	B	2028	THR
1	B	2029	MET
1	B	2033	THR
1	B	2041	PHE
1	B	2070	SER
1	B	2095	PHE
1	B	2099	ARG
1	B	2103	VAL
1	B	2119	ILE
1	B	2133	VAL
1	B	2162	THR
1	B	2178	SER
1	B	2183	ILE
1	B	2217	CYS

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	2211	ASN

5.3.3 RNA ⓘ

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](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PX4	A	4004	-	4,4,45	2.41	2 (50%)	6,6,53	1.54	2 (33%)
2	PX4	A	4005	-	7,7,45	0.45	0	6,6,53	0.34	0
2	PX4	B	4011	-	21,21,45	1.02	1 (4%)	23,25,53	0.91	0
2	PX4	A	4007	-	5,5,45	0.48	0	4,4,53	0.28	0
2	PX4	B	4016	-	4,4,45	2.54	2 (50%)	6,6,53	1.49	2 (33%)
2	PX4	A	4006	-	10,10,45	1.13	1 (10%)	12,12,53	1.13	2 (16%)
2	PX4	B	4001	-	20,20,45	0.97	1 (5%)	22,24,53	0.90	0
2	PX4	A	4014	-	4,4,45	2.42	2 (50%)	6,6,53	1.53	2 (33%)
2	PX4	A	4003	-	11,11,45	1.10	1 (9%)	11,14,53	1.04	1 (9%)
2	PX4	B	4012	-	9,9,45	1.11	1 (11%)	10,12,53	1.11	2 (20%)
2	PX4	A	4013	-	4,4,45	2.63	2 (50%)	6,6,53	1.50	2 (33%)
2	PX4	B	4002	-	9,9,45	1.11	1 (11%)	10,12,53	1.14	2 (20%)
2	PX4	B	4017	-	5,5,45	0.52	0	4,4,53	0.33	0
2	PX4	A	4015	-	5,5,45	0.42	0	4,4,53	0.25	0

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	A	4005	-	-	0/5/5/49	-
2	PX4	B	4011	-	-	4/24/24/49	-
2	PX4	A	4007	-	-	0/3/3/49	-
2	PX4	A	4006	-	-	1/8/8/49	-
2	PX4	B	4001	-	-	3/22/22/49	-
2	PX4	B	4012	-	-	2/8/8/49	-
2	PX4	A	4003	-	-	2/10/10/49	-
2	PX4	B	4017	-	-	0/3/3/49	-
2	PX4	B	4002	-	-	2/8/8/49	-
2	PX4	A	4015	-	-	0/3/3/49	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4013	PX4	P1-O4	3.86	1.65	1.54
2	B	4016	PX4	P1-O4	3.57	1.65	1.54
2	A	4004	PX4	P1-O4	3.45	1.64	1.54
2	A	4013	PX4	P1-O3	3.42	1.64	1.54
2	B	4016	PX4	P1-O3	3.42	1.64	1.54
2	B	4001	PX4	P1-O3	3.37	1.69	1.58
2	A	4014	PX4	P1-O4	3.36	1.64	1.54
2	A	4014	PX4	P1-O3	3.29	1.64	1.54
2	A	4004	PX4	P1-O3	3.27	1.64	1.54
2	B	4011	PX4	P1-O3	3.22	1.69	1.58
2	B	4012	PX4	P1-O3	2.62	1.64	1.54
2	A	4006	PX4	P1-O3	2.62	1.64	1.54
2	B	4002	PX4	P1-O3	2.58	1.64	1.54
2	A	4003	PX4	P1-O3	2.56	1.64	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4013	PX4	O1-P1-O2	2.66	120.36	110.95
2	B	4002	PX4	O1-P1-O2	2.63	121.09	110.83
2	A	4004	PX4	O1-P1-O2	2.58	120.07	110.95
2	A	4014	PX4	O1-P1-O2	2.58	120.06	110.95
2	B	4016	PX4	O1-P1-O2	2.55	119.96	110.95
2	A	4004	PX4	O4-P1-O3	-2.49	100.17	107.91
2	B	4012	PX4	O1-P1-O2	2.47	120.47	110.83
2	B	4016	PX4	O4-P1-O3	-2.43	100.36	107.91
2	A	4014	PX4	O4-P1-O3	-2.42	100.38	107.91
2	A	4006	PX4	O3-P1-O4	-2.38	100.46	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4006	PX4	O1-P1-O2	2.37	120.06	110.83
2	A	4013	PX4	O4-P1-O3	-2.35	100.60	107.91
2	A	4003	PX4	O1-P1-O2	2.30	119.80	110.83
2	B	4002	PX4	O3-P1-O4	-2.15	101.05	106.67
2	B	4012	PX4	O3-P1-O4	-2.11	101.17	106.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4001	PX4	O4-C6-C7-O7
2	B	4002	PX4	O4-C6-C7-O7
2	B	4011	PX4	O4-C6-C7-O7
2	B	4011	PX4	C6-C7-O7-C23
2	A	4003	PX4	O4-C6-C7-O7
2	B	4012	PX4	O4-C6-C7-O7
2	B	4002	PX4	O4-C6-C7-C8
2	B	4001	PX4	O4-C6-C7-C8
2	B	4001	PX4	C1-O3-P1-O2
2	B	4011	PX4	O4-C6-C7-C8
2	B	4012	PX4	O4-C6-C7-C8
2	A	4003	PX4	O4-C6-C7-C8
2	B	4011	PX4	C8-C7-O7-C23
2	A	4006	PX4	C6-C7-O7-C23

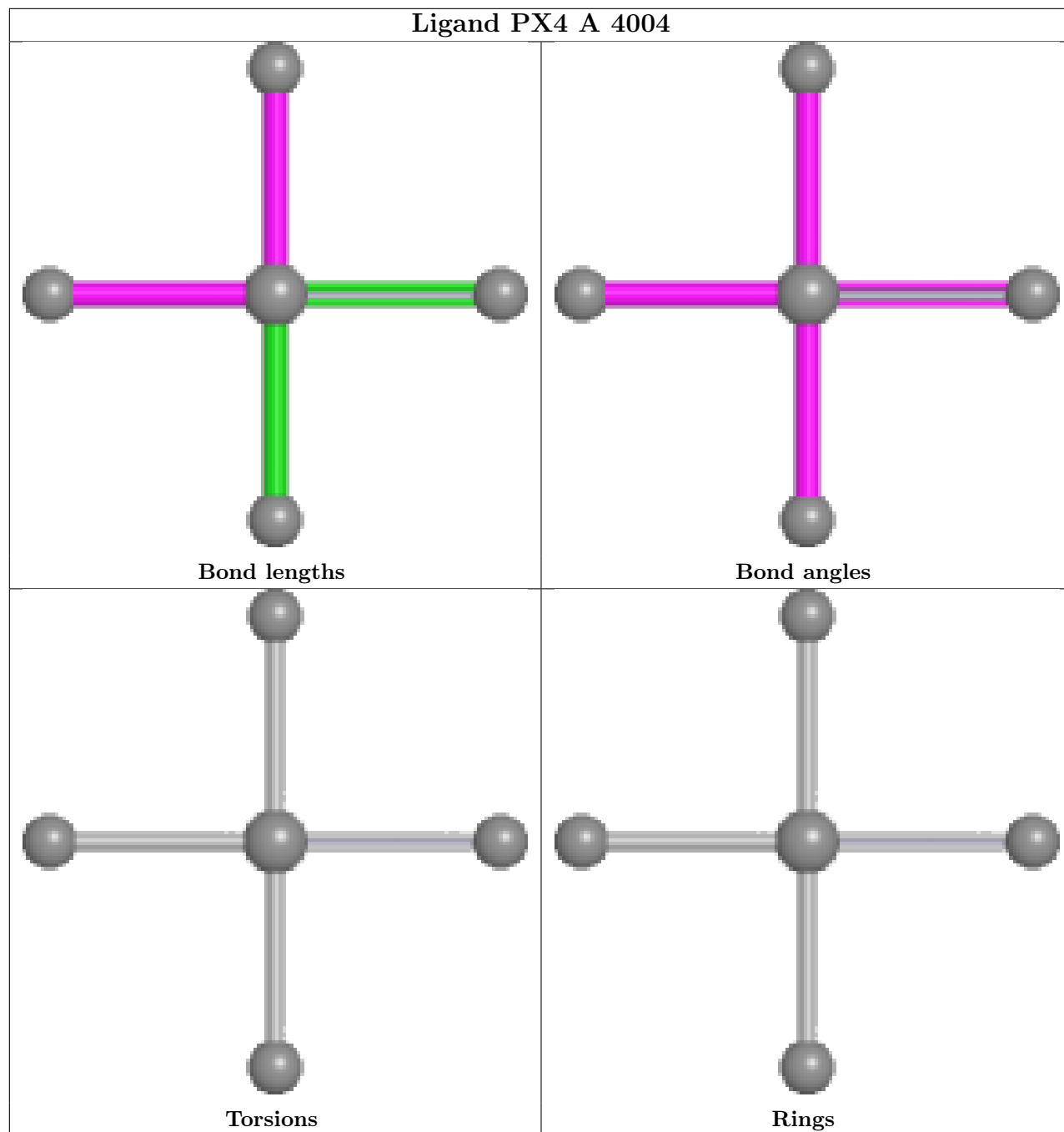
There are no ring outliers.

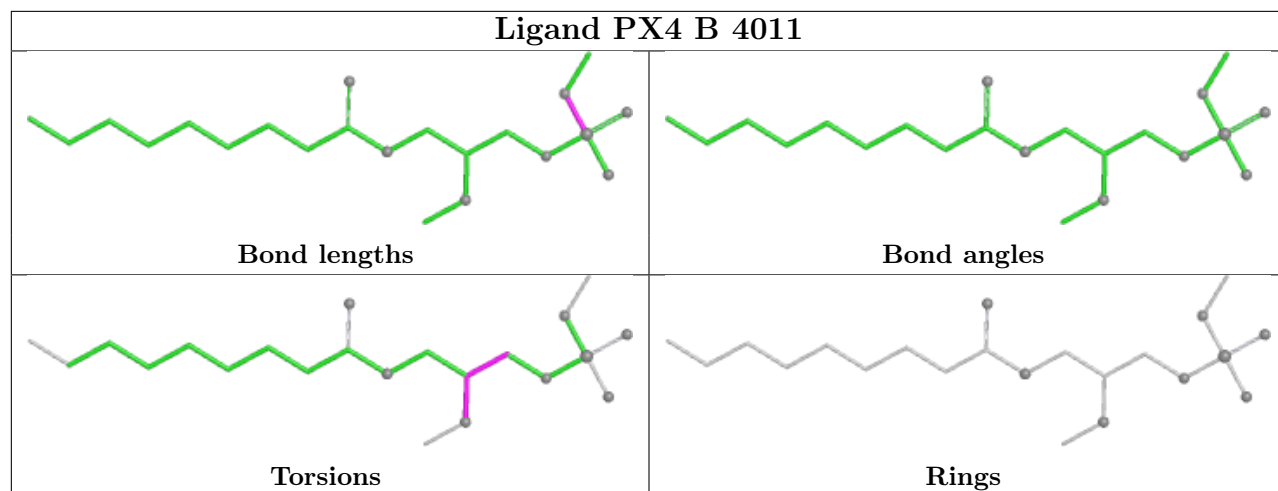
1 monomer is involved in 2 short contacts:

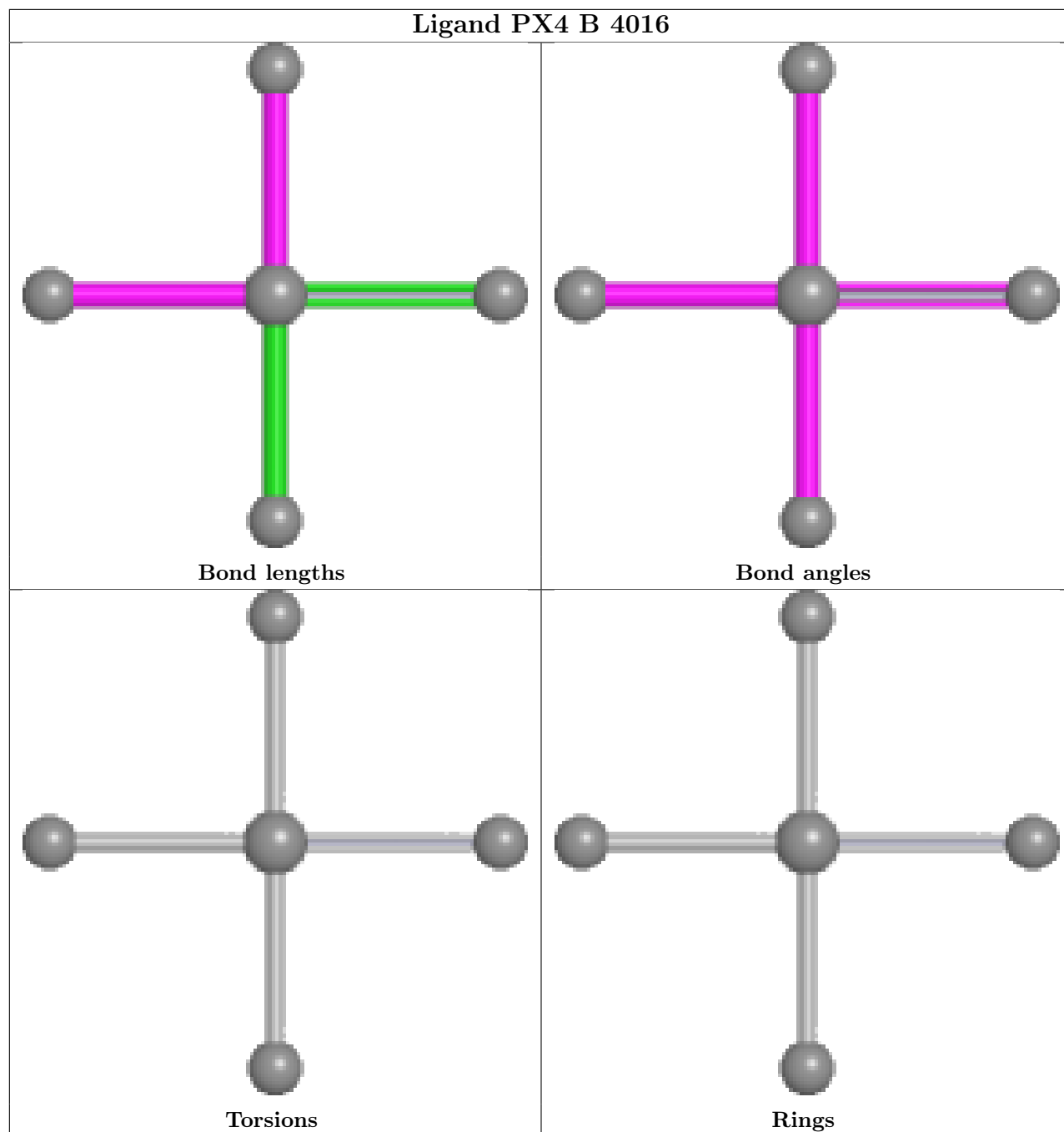
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4006	PX4	2	0

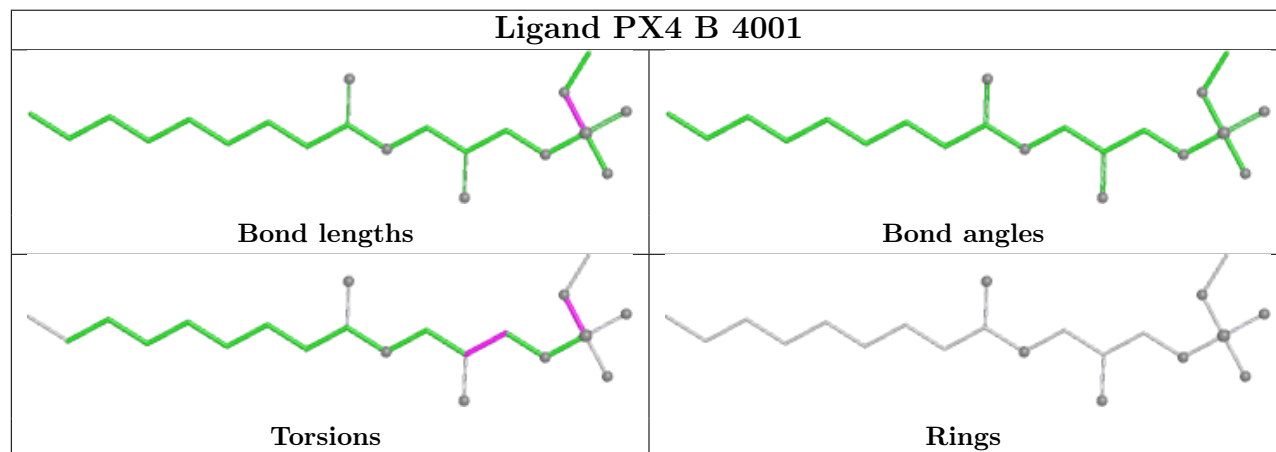
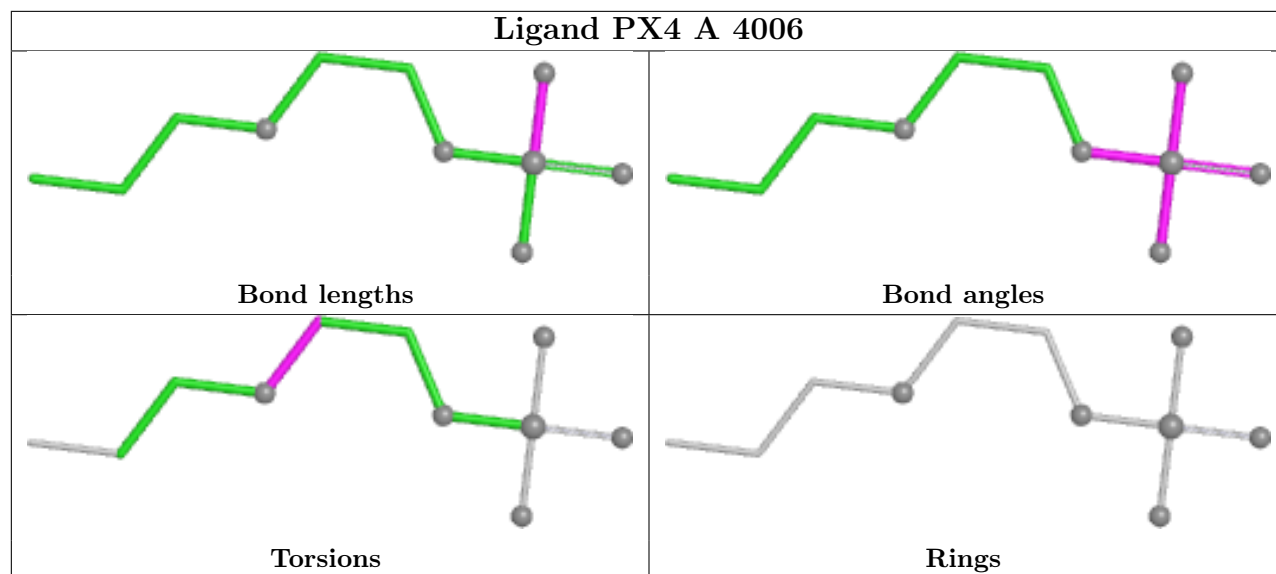
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

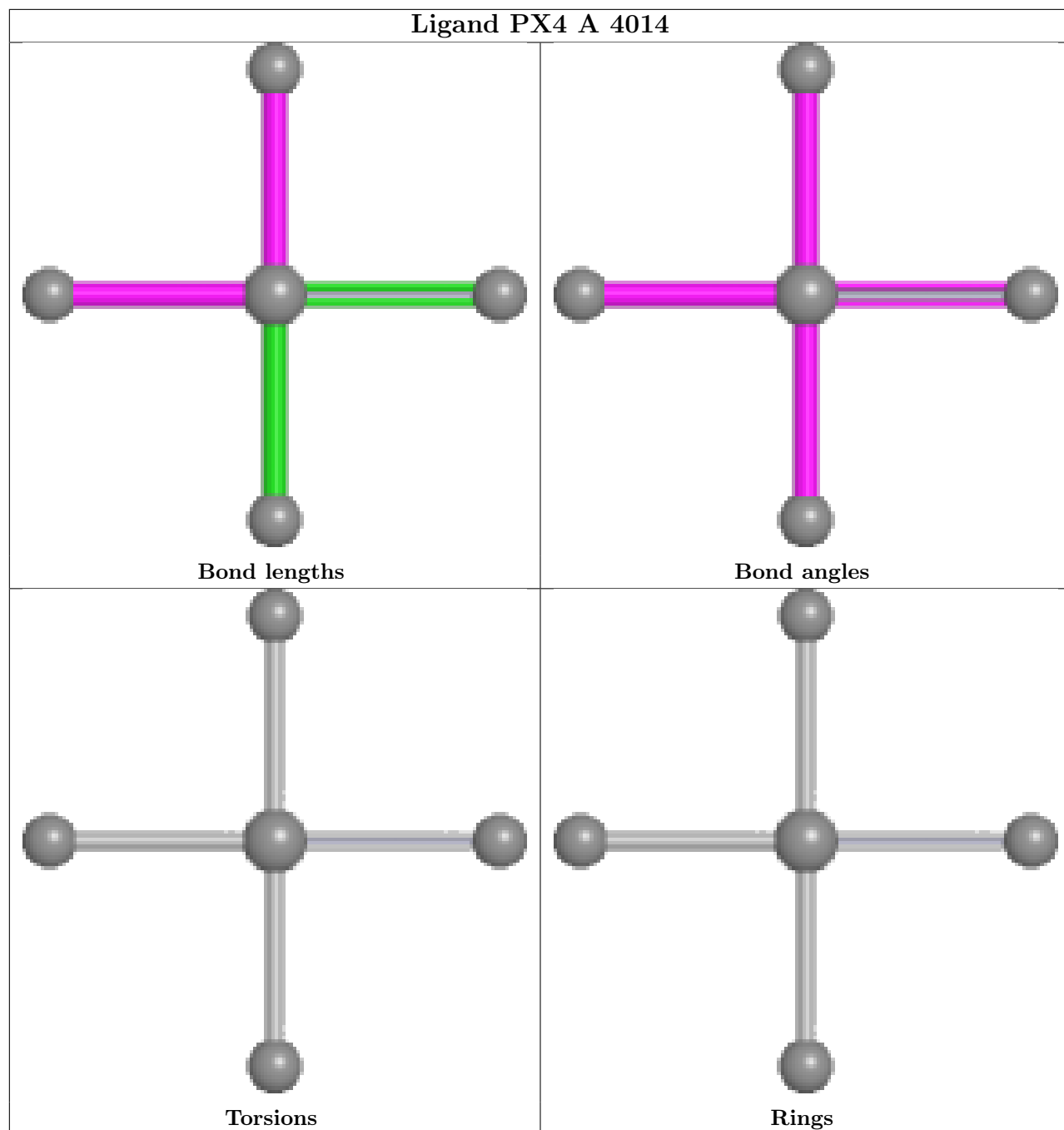
equivalents in the CSD to analyse the geometry.

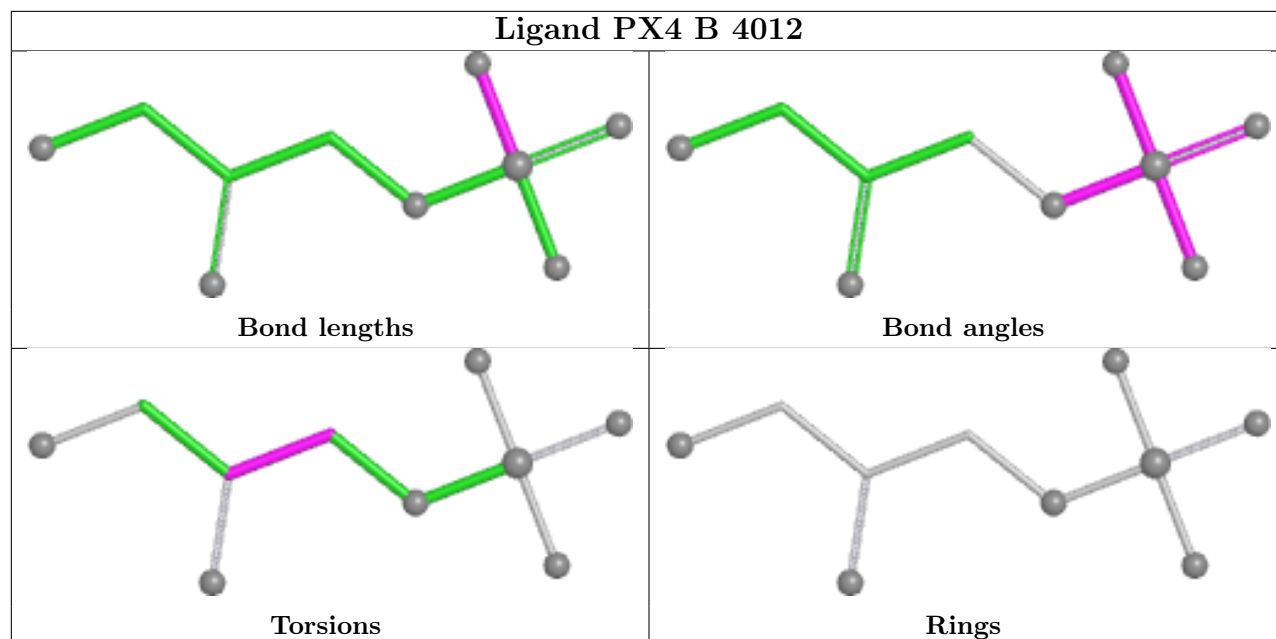
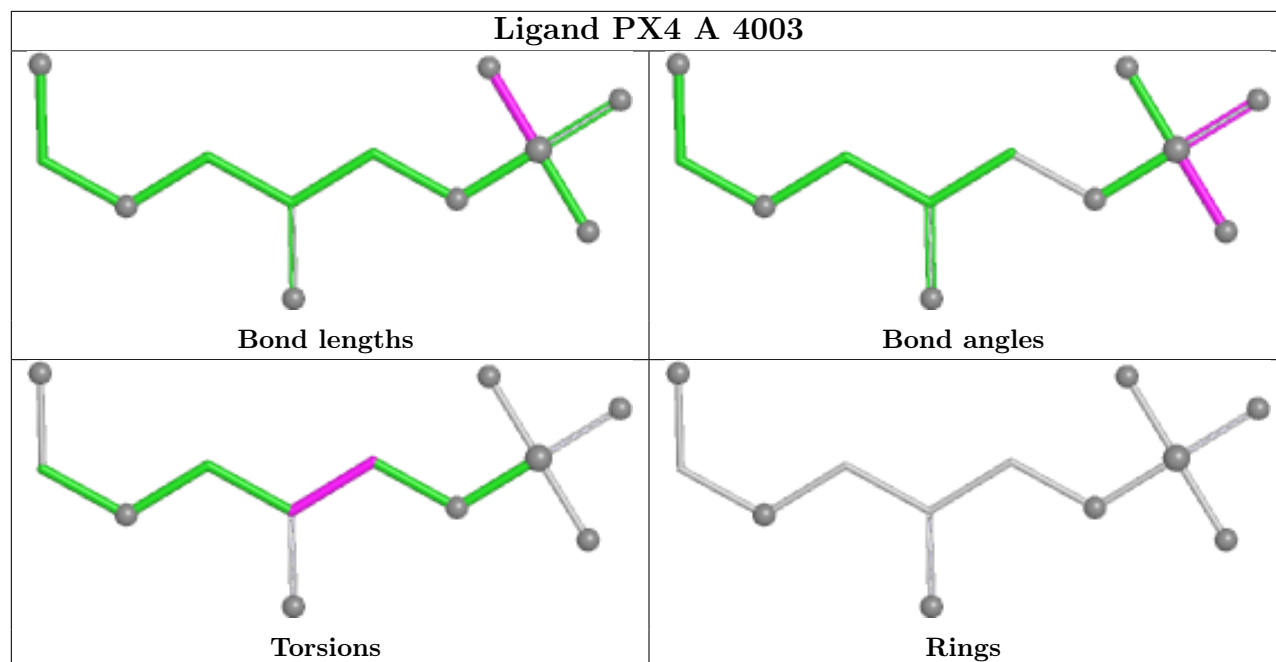


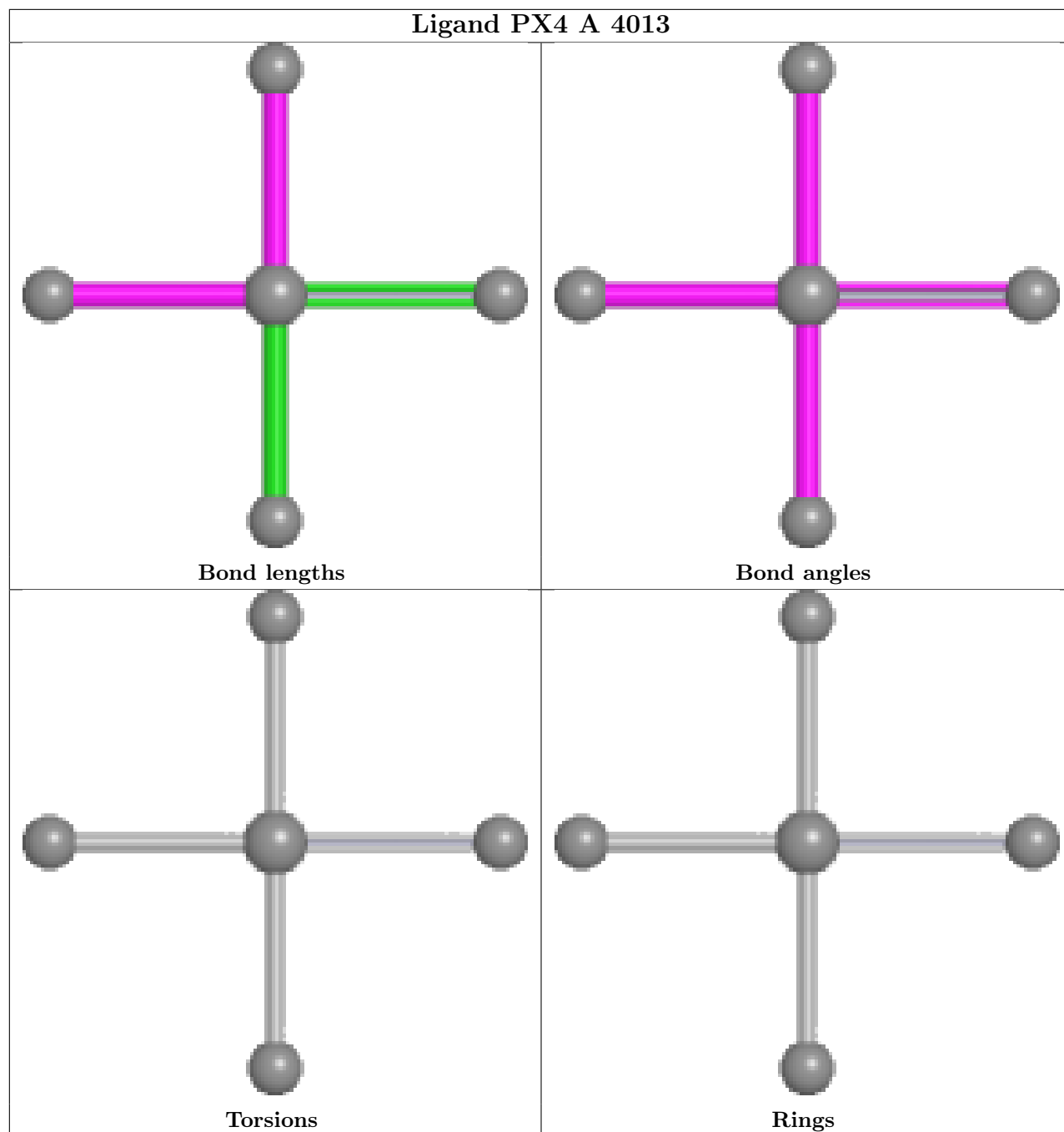


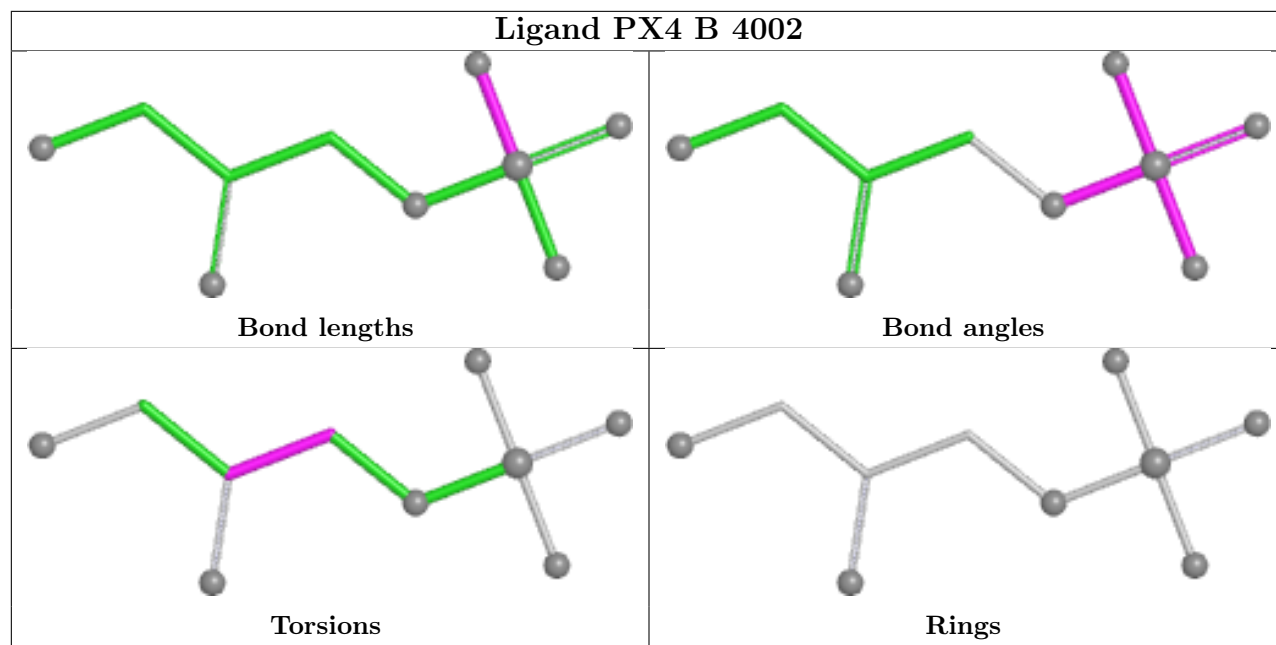












5.7 Other polymers [i](#)

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	219/285 (76%)	-0.37	5 (2%) 61 51	42, 91, 159, 205	0
1	B	219/285 (76%)	-0.40	4 (1%) 67 58	45, 91, 157, 220	0
All	All	438/570 (76%)	-0.38	9 (2%) 63 54	42, 91, 159, 220	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1001	MET	3.1
1	B	2219	ASP	2.7
1	B	2002	TYR	2.6
1	A	1094	GLY	2.4
1	A	1154	GLU	2.2
1	A	1033	THR	2.1
1	B	2150	GLN	2.1
1	B	2096	GLU	2.1
1	A	1100	VAL	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 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,

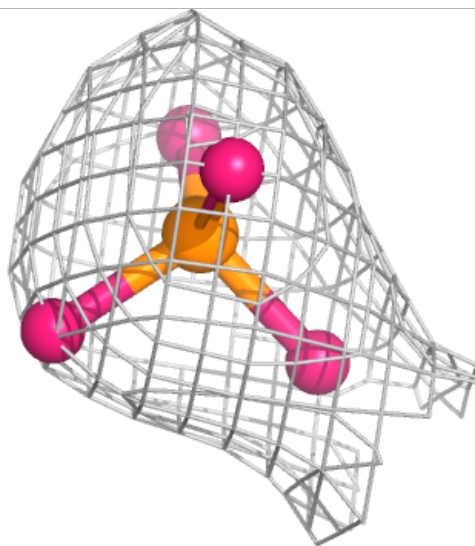
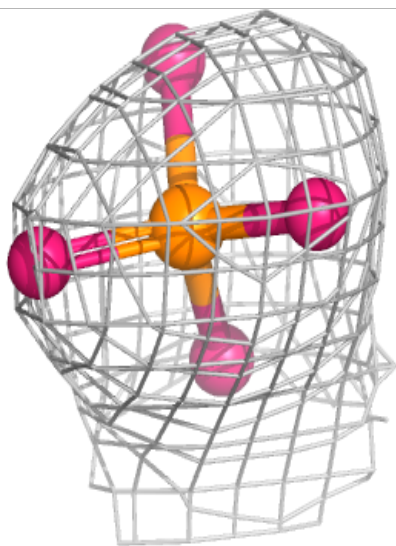
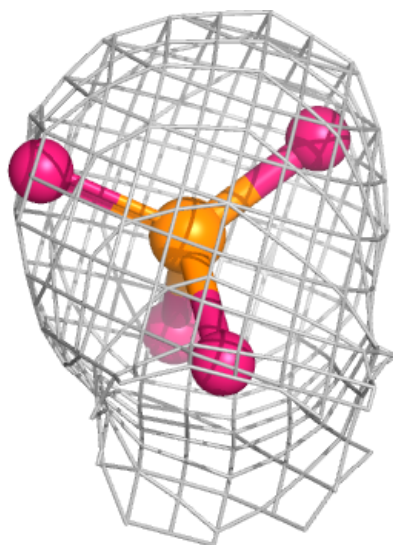
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PX4	B	4016	5/46	0.90	0.10	163,163,163,163	0
2	PX4	A	4015	6/46	0.96	0.21	95,95,95,95	0
2	PX4	A	4006	11/46	0.96	0.13	137,137,137,137	0
2	PX4	A	4003	12/46	0.97	0.08	64,128,128,128	0
2	PX4	A	4007	6/46	0.97	0.13	62,62,62,62	0
2	PX4	A	4013	5/46	0.97	0.07	121,121,121,121	0
2	PX4	A	4004	5/46	0.97	0.09	147,147,147,147	0
2	PX4	B	4001	21/46	0.97	0.09	48,96,96,96	0
2	PX4	B	4002	10/46	0.97	0.10	119,119,119,119	0
2	PX4	B	4011	22/46	0.97	0.10	48,100,100,100	0
2	PX4	A	4005	8/46	0.97	0.13	96,96,96,96	0
2	PX4	B	4017	6/46	0.97	0.18	67,67,67,67	0
2	PX4	A	4014	5/46	0.98	0.12	159,159,159,159	0
2	PX4	B	4012	10/46	0.98	0.08	120,120,120,120	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.

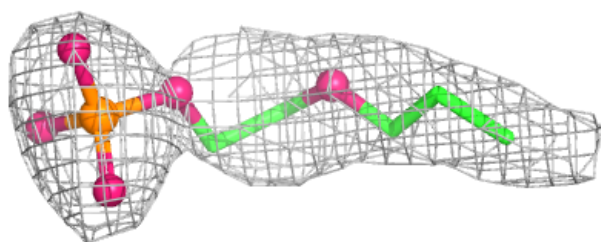
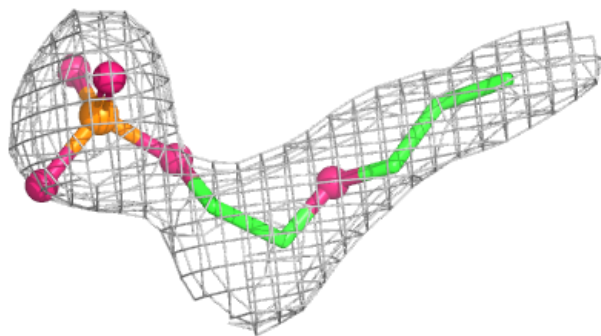
Electron density around PX4 B 4016:

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

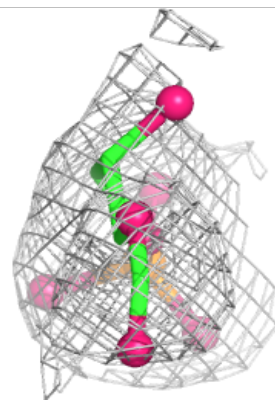
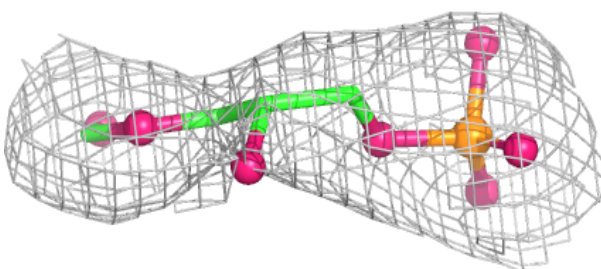
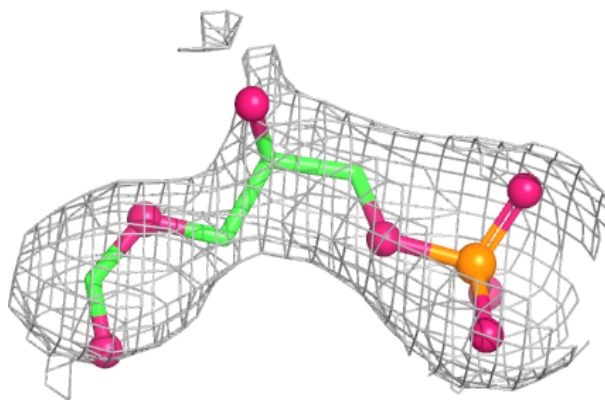


Electron density around PX4 A 4006:

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

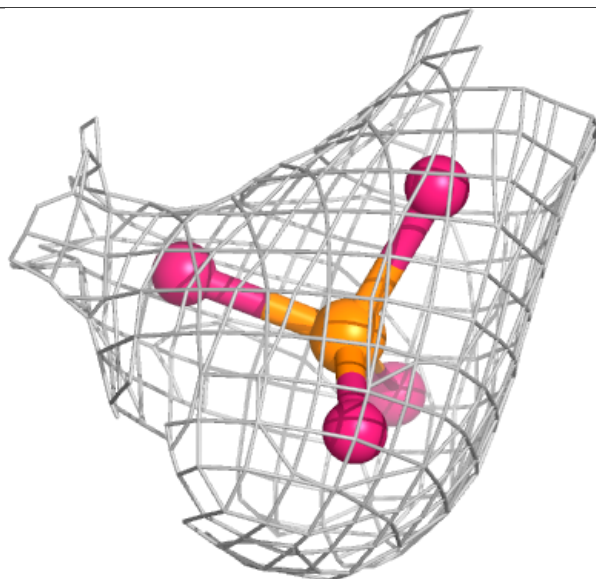
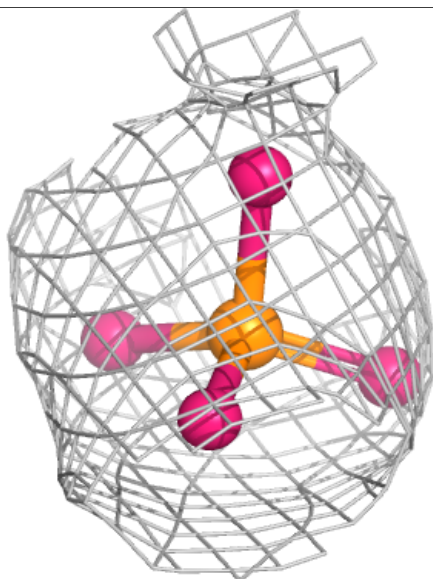
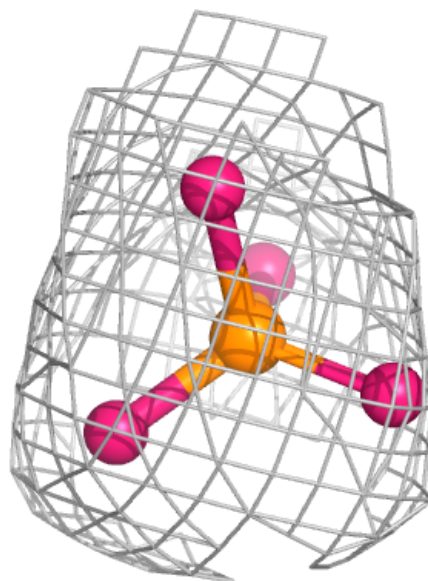
**Electron density around PX4 A 4003:**

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



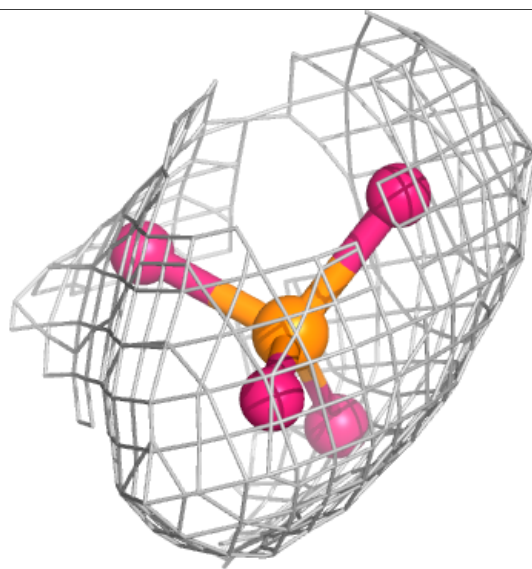
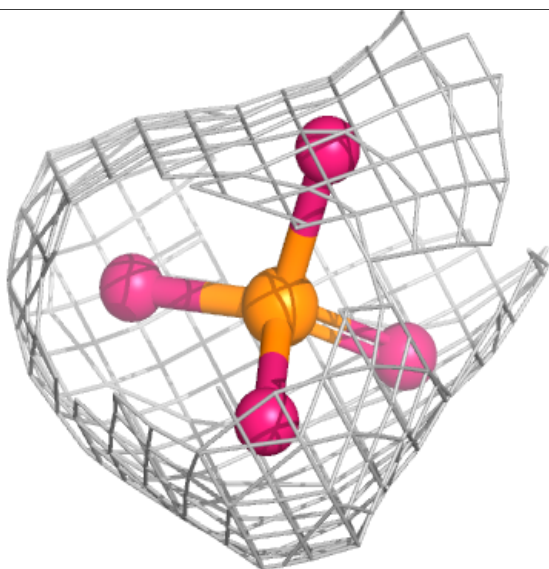
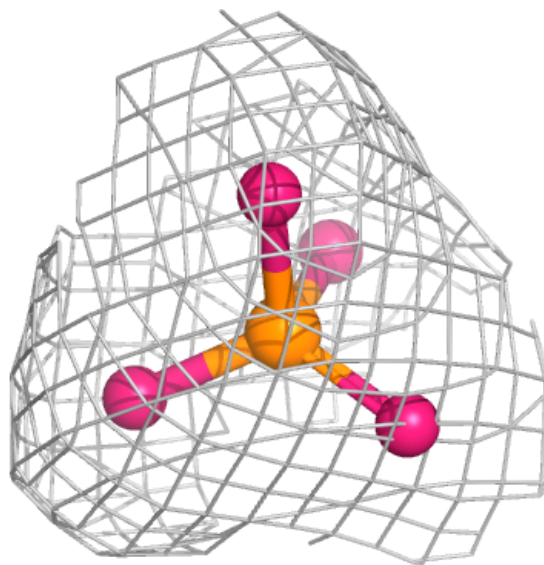
Electron density around PX4 A 4013:

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



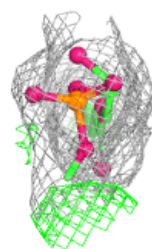
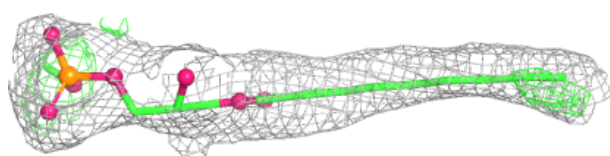
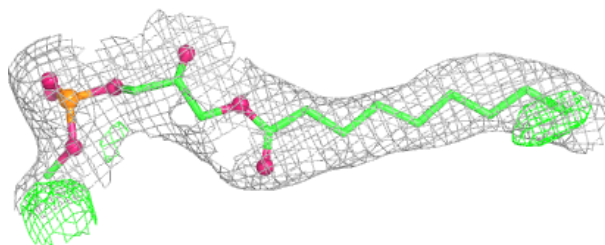
Electron density around PX4 A 4004:

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

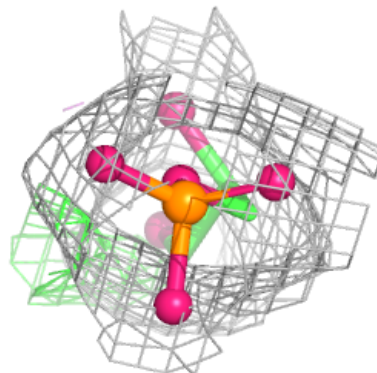
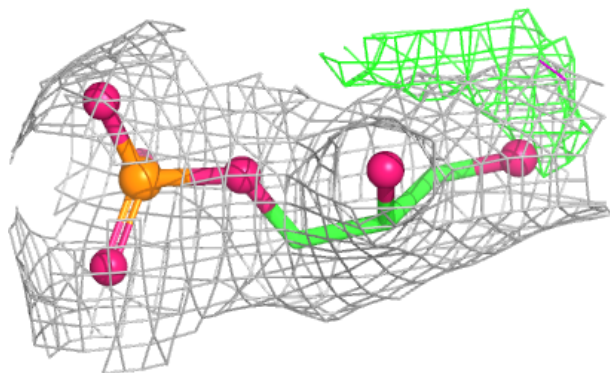
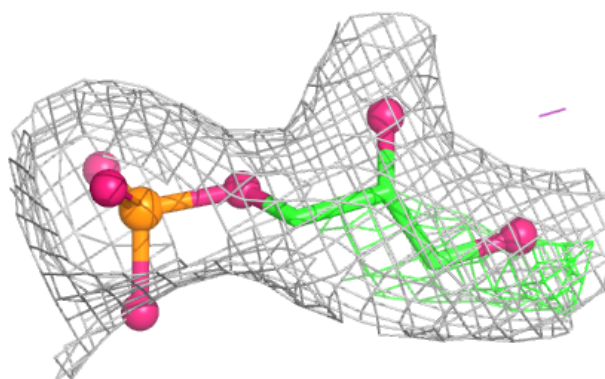


Electron density around PX4 B 4001:

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

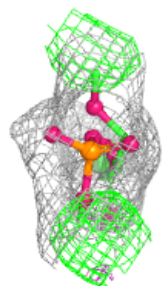
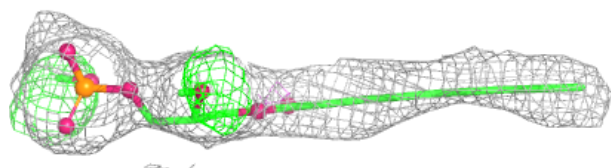
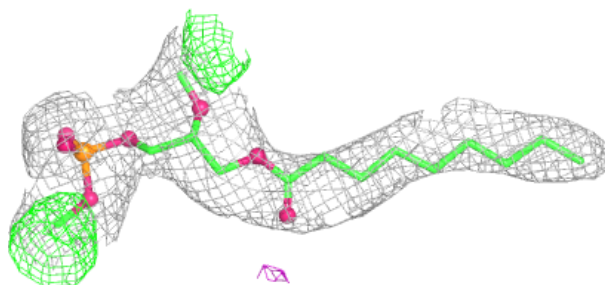
**Electron density around PX4 B 4002:**

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



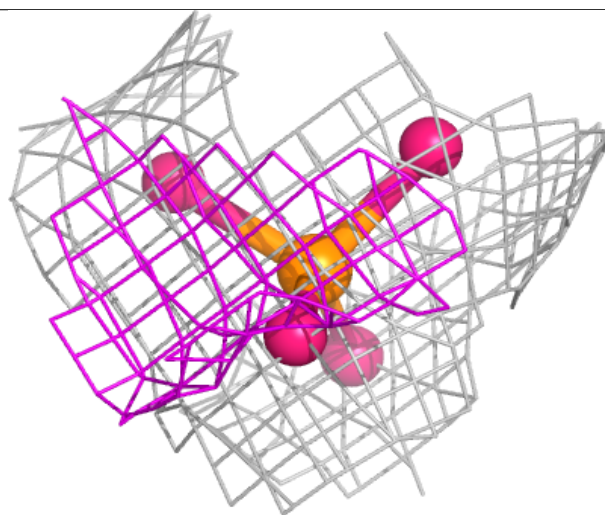
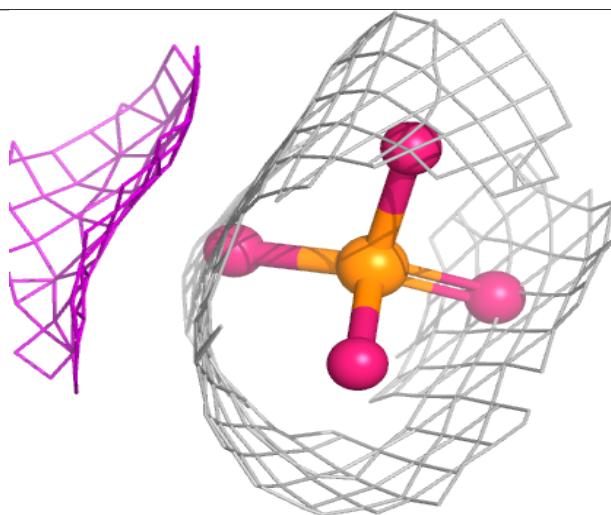
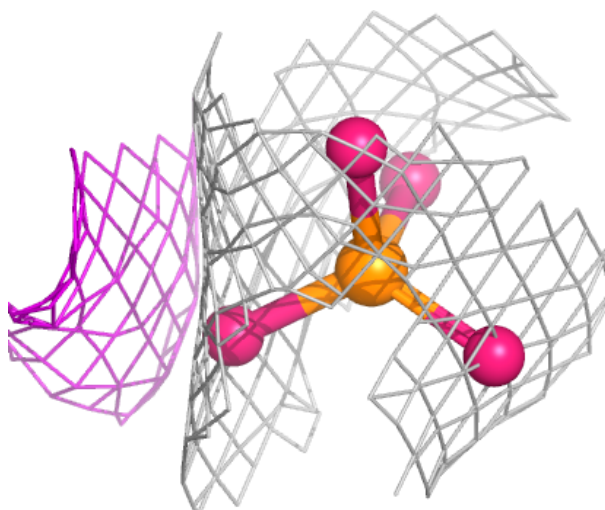
Electron density around PX4 B 4011:

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



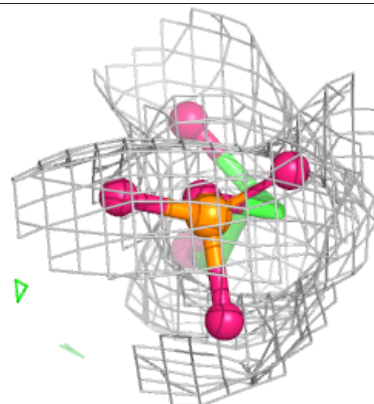
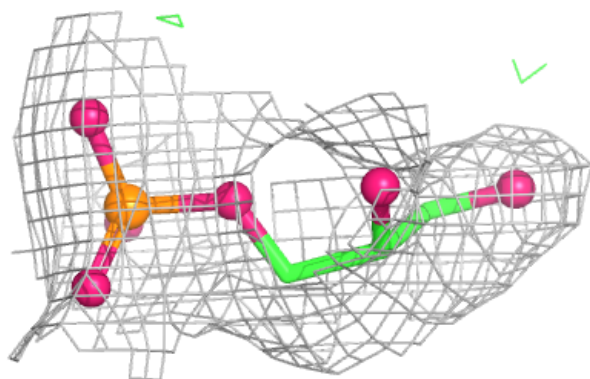
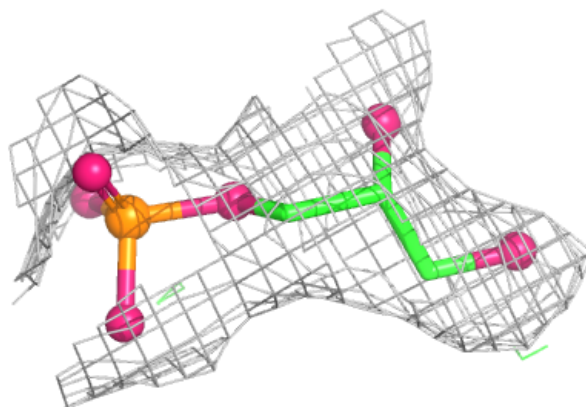
Electron density around PX4 A 4014:

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



Electron density around PX4 B 4012:

$2mF_o-DF_c$ (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.