



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 03:28 am BST

PDB ID : 6MVW  
Title : NavAb voltage-gated sodium channel, I217C/F203W  
Authors : Lenaeus, M.J.; Catterall, W.A.  
Deposited on : 2018-10-28  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

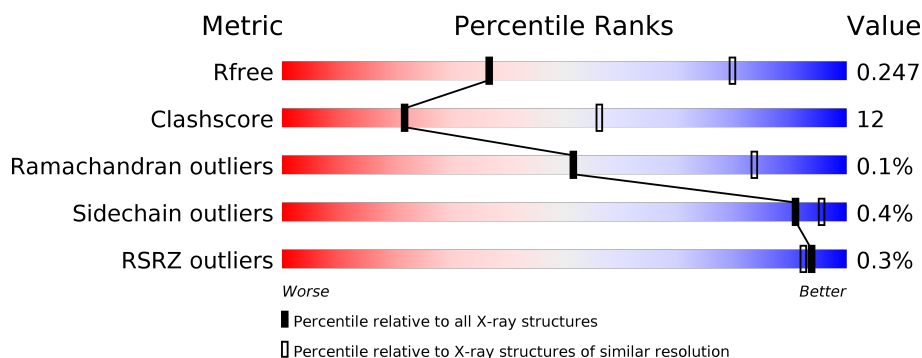
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div></div> <div>58%18%24%</div> </div>
1	B	285	<div> <div>%</div> <div>56%20%24%</div> </div>
1	C	285	<div> <div></div> <div>58%18%24%</div> </div>
1	D	285	<div> <div></div> <div>55%21%24%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7206 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	217	Total	C	N	O	S	0	0	0
			1700	1158	254	277	11			
1	B	218	Total	C	N	O	S	0	0	0
			1704	1156	257	280	11			
1	C	218	Total	C	N	O	S	0	0	0
			1725	1175	255	284	11			
1	D	217	Total	C	N	O	S	0	0	0
			1721	1175	254	280	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	initiating methionine	UNP A8EVM5
A	984	ASP	-	expression tag	UNP A8EVM5
A	985	TYR	-	expression tag	UNP A8EVM5
A	986	LYS	-	expression tag	UNP A8EVM5
A	987	ASP	-	expression tag	UNP A8EVM5
A	988	ASP	-	expression tag	UNP A8EVM5
A	989	ASP	-	expression tag	UNP A8EVM5
A	990	ASP	-	expression tag	UNP A8EVM5
A	991	LYS	-	expression tag	UNP A8EVM5
A	992	GLY	-	expression tag	UNP A8EVM5
A	993	SER	-	expression tag	UNP A8EVM5
A	994	LEU	-	expression tag	UNP A8EVM5
A	995	VAL	-	expression tag	UNP A8EVM5
A	996	PRO	-	expression tag	UNP A8EVM5
A	997	ARG	-	expression tag	UNP A8EVM5
A	998	GLY	-	expression tag	UNP A8EVM5
A	999	SER	-	expression tag	UNP A8EVM5
A	1000	HIS	-	expression tag	UNP A8EVM5
A	1203	TRP	PHE	engineered mutation	UNP A8EVM5
A	1217	CYS	ILE	engineered mutation	UNP A8EVM5
B	1983	MET	-	initiating methionine	UNP A8EVM5

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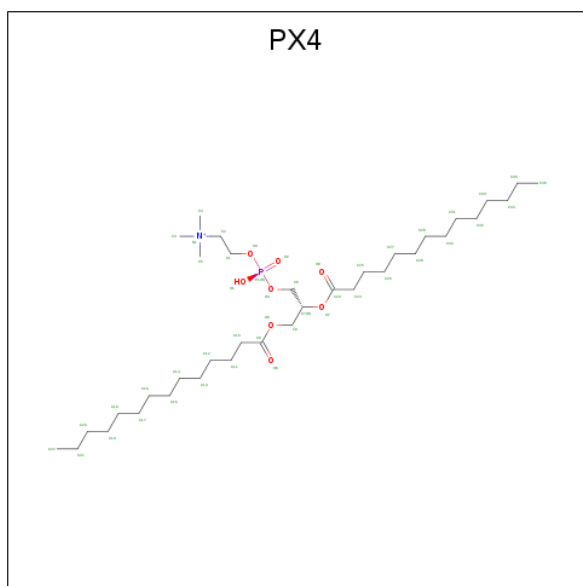
Chain	Residue	Modelled	Actual	Comment	Reference
B	1984	ASP	-	expression tag	UNP A8EVM5
B	1985	TYR	-	expression tag	UNP A8EVM5
B	1986	LYS	-	expression tag	UNP A8EVM5
B	1987	ASP	-	expression tag	UNP A8EVM5
B	1988	ASP	-	expression tag	UNP A8EVM5
B	1989	ASP	-	expression tag	UNP A8EVM5
B	1990	ASP	-	expression 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	2203	TRP	PHE	engineered mutation	UNP A8EVM5
B	2217	CYS	ILE	engineered mutation	UNP A8EVM5
C	983	MET	-	initiating methionine	UNP A8EVM5
C	984	ASP	-	expression tag	UNP A8EVM5
C	985	TYR	-	expression tag	UNP A8EVM5
C	986	LYS	-	expression tag	UNP A8EVM5
C	987	ASP	-	expression tag	UNP A8EVM5
C	988	ASP	-	expression tag	UNP A8EVM5
C	989	ASP	-	expression tag	UNP A8EVM5
C	990	ASP	-	expression tag	UNP A8EVM5
C	991	LYS	-	expression tag	UNP A8EVM5
C	992	GLY	-	expression tag	UNP A8EVM5
C	993	SER	-	expression tag	UNP A8EVM5
C	994	LEU	-	expression tag	UNP A8EVM5
C	995	VAL	-	expression tag	UNP A8EVM5
C	996	PRO	-	expression tag	UNP A8EVM5
C	997	ARG	-	expression tag	UNP A8EVM5
C	998	GLY	-	expression tag	UNP A8EVM5
C	999	SER	-	expression tag	UNP A8EVM5
C	1000	HIS	-	expression tag	UNP A8EVM5
C	1203	TRP	PHE	engineered mutation	UNP A8EVM5
C	1217	CYS	ILE	engineered mutation	UNP A8EVM5
D	1983	MET	-	initiating methionine	UNP A8EVM5
D	1984	ASP	-	expression tag	UNP A8EVM5
D	1985	TYR	-	expression tag	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1986	LYS	-	expression tag	UNP A8EVM5
D	1987	ASP	-	expression tag	UNP A8EVM5
D	1988	ASP	-	expression tag	UNP A8EVM5
D	1989	ASP	-	expression tag	UNP A8EVM5
D	1990	ASP	-	expression tag	UNP A8EVM5
D	1991	LYS	-	expression tag	UNP A8EVM5
D	1992	GLY	-	expression tag	UNP A8EVM5
D	1993	SER	-	expression tag	UNP A8EVM5
D	1994	LEU	-	expression tag	UNP A8EVM5
D	1995	VAL	-	expression tag	UNP A8EVM5
D	1996	PRO	-	expression tag	UNP A8EVM5
D	1997	ARG	-	expression tag	UNP A8EVM5
D	1998	GLY	-	expression tag	UNP A8EVM5
D	1999	SER	-	expression tag	UNP A8EVM5
D	2000	HIS	-	expression tag	UNP A8EVM5
D	2203	TRP	PHE	engineered mutation	UNP A8EVM5
D	2217	CYS	ILE	engineered mutation	UNP A8EVM5

- Molecule 2 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C<sub>36</sub>H<sub>73</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	17	1	8	1		
2	A	1	Total	C	O	P		0	0
			16	7	8	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			37	28	8	1		
2	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	B	1	Total	C	O	P	0	0
			22	13	8	1		
2	B	1	Total	C	N	O	P	0
			31	22	1	7	1	
2	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	D	1	Total	C	N	O	P	0
			31	22	1	7	1	
2	D	1	Total	C	N	O	P	0
			24	14	1	8	1	

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		


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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

These plots are drawn for all protein, RNA and DNA 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.

- Chain A:
- 
- Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows positions 1 to 100. A red dot is at position 9. A green bar at the top indicates 58% conservation, a yellow bar indicates 18%, and a grey bar indicates 24%.
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1        | GLU        | 0.02                       |
| 2        | GLN        | 0.02                       |
| 3        | HIS        | 0.02                       |
| 4        | ILE        | 0.02                       |
| 5        | ILE        | 0.02                       |
| 6        | ASP        | 0.02                       |
| 7        | GLU        | 0.02                       |
| 8        | VAL        | 0.02                       |
| 9        | GLN        | 0.25                       |
| 10       | GLN        | 0.02                       |
| 11       | ILE        | 0.02                       |
| 12       | ASN        | 0.02                       |
| 13       | GLU        | 0.02                       |
| 14       | ILE        | 0.02                       |
| 15       | ILE        | 0.02                       |
| 16       | LEU        | 0.02                       |
| 17       | ARG        | 0.02                       |
| 18       | GLU        | 0.02                       |
| 19       | GLU        | 0.02                       |
| 20       | GLU        | 0.02                       |
| 21       | VAL        | 0.02                       |
| 22       | VAL        | 0.02                       |
| 23       | LEU        | 0.02                       |
| 24       | LEU        | 0.02                       |
| 25       | LEU        | 0.02                       |
| 26       | LEU        | 0.02                       |
| 27       | LEU        | 0.02                       |
| 28       | LEU        | 0.02                       |
| 29       | LEU        | 0.02                       |
| 30       | LEU        | 0.02                       |
| 31       | LEU        | 0.02                       |
| 32       | LEU        | 0.02                       |
| 33       | LEU        | 0.02                       |
| 34       | LEU        | 0.02                       |
| 35       | LEU        | 0.02                       |
| 36       | LEU        | 0.02                       |
| 37       | LEU        | 0.02                       |
| 38       | LEU        | 0.02                       |
| 39       | LEU        | 0.02                       |
| 40       | LEU        | 0.02                       |
| 41       | LEU        | 0.02                       |
| 42       | LEU        | 0.02                       |
| 43       | LEU        | 0.02                       |
| 44       | LEU        | 0.02                       |
| 45       | LEU        | 0.02                       |
| 46       | LEU        | 0.02                       |
| 47       | LEU        | 0.02                       |
| 48       | LEU        | 0.02                       |
| 49       | LEU        | 0.02                       |
| 50       | LEU        | 0.02                       |
| 51       | LEU        | 0.02                       |
| 52       | LEU        | 0.02                       |
| 53       | LEU        | 0.02                       |
| 54       | LEU        | 0.02                       |
| 55       | LEU        | 0.02                       |
| 56       | LEU        | 0.02                       |
| 57       | LEU        | 0.02                       |
| 58       | LEU        | 0.02                       |
| 59       | LEU        | 0.02                       |
| 60       | LEU        | 0.02                       |
| 61       | LEU        | 0.02                       |
| 62       | LEU        | 0.02                       |
| 63       | LEU        | 0.02                       |
| 64       | LEU        | 0.02                       |
| 65       | LEU        | 0.02                       |
| 66       | LEU        | 0.02                       |
| 67       | LEU        | 0.02                       |
| 68       | LEU        | 0.02                       |
| 69       | LEU        | 0.02                       |
| 70       | LEU        | 0.02                       |
| 71       | LEU        | 0.02                       |
| 72       | LEU        | 0.02                       |
| 73       | LEU        | 0.02                       |
| 74       | LEU        | 0.02                       |
| 75       | LEU        | 0.02                       |
| 76       | LEU        | 0.02                       |
| 77       | LEU        | 0.02                       |
| 78       | LEU        | 0.02                       |
| 79       | LEU        | 0.02                       |
| 80       | LEU        | 0.02                       |
| 81       | LEU        | 0.02                       |
| 82       | LEU        | 0.02                       |
| 83       | LEU        | 0.02                       |
| 84       | LEU        | 0.02                       |
| 85       | LEU        | 0.02                       |
| 86       | LEU        | 0.02                       |
| 87       | LEU        | 0.02                       |
| 88       | LEU        | 0.02                       |
| 89       | LEU        | 0.02                       |
| 90       | LEU        | 0.02                       |
| 91       | LEU        | 0.02                       |
| 92       | LEU        | 0.02                       |
| 93       | LEU        | 0.02                       |
| 94       | LEU        | 0.02                       |
| 95       | LEU        | 0.02                       |
| 96       | LEU        | 0.02                       |
| 97       | LEU        | 0.02                       |
| 98       | LEU        | 0.02                       |
| 99       | LEU        | 0.02                       |
| 100      | LEU        | 0.02                       |

- Chain B: 

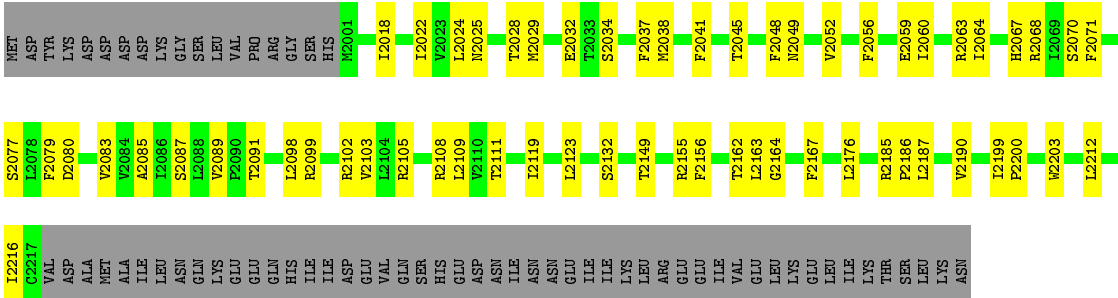
- Chain C:**

Amino Acid	Type	Percentage
MET	Grey	24%
ASP	Green	58%
TYR	Yellow	18%
LYS	Green	58%
ASP	Green	58%
ASP	Green	58%
ASP	Green	58%
LYS	Green	58%
GLY	Green	58%
SER	Green	58%
LEU	Green	58%
VAL	Green	58%
PRO	Green	58%
ARG	Green	58%
GLY	Green	58%
SER	Green	58%
HIS	Grey	24%
M1001	Green	58%
Y1002	Yellow	18%
L1003	Yellow	18%
M1007	Green	58%
I1008	Green	58%
V1009	Green	58%
I1019	Yellow	18%
I1022	Yellow	18%
V1023	Yellow	18%
L1024	Green	58%
N1025	Yellow	18%
G1026	Green	58%
I1027	Green	58%
T1028	Yellow	18%
M1029	Yellow	18%
E1032	Yellow	18%
T1033	Yellow	18%
M1038	Yellow	18%
T1046	Yellow	18%
N1049	Yellow	18%
I1053	Yellow	18%
I1058	Yellow	18%
E1059	Green	58%
I1060	Yellow	18%
I1061	Green	58%
L1062	Green	58%
R1063	Green	58%
Y1064	Yellow	18%
I1065	Yellow	18%
V1066	Yellow	18%
I1067	Green	58%
R1068	Yellow	18%
F1071	Yellow	18%
D1074	Yellow	18%
P1075	Green	58%
H1076	Green	58%
S1077	Yellow	18%
V1103	Yellow	18%
R1108	Yellow	18%
L1109	Yellow	18%
V1110	Yellow	18%
T1111	Yellow	18%
A1112	Yellow	18%
M1116	Yellow	18%
I1119	Yellow	18%
V1120	Yellow	18%
L1123	Yellow	18%
M1130	Yellow	18%
V1133	Yellow	18%
M1137	Yellow	18%
F1152	Yellow	18%
R1155	Yellow	18%
T1162	Yellow	18%
L1163	Yellow	18%
G1164	Yellow	18%
T1175	Yellow	18%
L1187	Yellow	18%
M1188	Yellow	18%
F1189	Yellow	18%
V1190	Yellow	18%
Y1191	Yellow	18%
I1202	Yellow	18%
T1206	Orange	-
L1212	Yellow	18%
V1213	Yellow	18%
V1214	Yellow	18%
V1215	Yellow	18%
ASP	Green	58%
ALA	Yellow	18%
MET	Grey	24%
ILE	Yellow	18%
ALA	Yellow	18%
LEU	Yellow	18%
LEU	Yellow	18%



GLN	LYS	GLU	GLN	HIS	ILE	ASP	GLU	VAL	GLN	SER	HIS	GLU	ASP	ASN	ILE	ASN	ASN	ASN	GLU	ILE	ILE	LYS	LEU	ARG	GLU	GLU	ILE	VAL	GLU	LEU	LYS	GLU	LEU	ILE	LYS	THR	SER	LEU	LYS	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 1: Ion transport protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.22Å 126.09Å 192.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.20 29.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.96-3.20) 92.6 (29.96-3.20)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.212 , 0.246 0.214 , 0.247	Depositor DCC
$R_{free}$ test set	2002 reflections (3.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.8	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 67.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.438 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7206	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4975e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, 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	0.26	0/1749	0.38	0/2393
1	B	0.25	0/1752	0.39	0/2397
1	C	0.26	0/1775	0.39	0/2428
1	D	0.26	0/1771	0.40	0/2421
All	All	0.26	0/7047	0.39	0/9639

There are no bond length outliers.

There are no bond angle outliers.

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	1700	0	1686	37	0
1	B	1704	0	1687	48	0
1	C	1725	0	1727	39	0
1	D	1721	0	1733	50	0
2	A	80	0	83	3	0
2	B	89	0	108	9	0
2	C	92	0	144	11	0
2	D	55	0	67	3	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	15	0	0	0	0
All	All	7206	0	7235	172	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 12.

All (172) 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:1033:THR:HG21	1:B:2163:LEU:HB2	1.56	0.87
1:D:2087:SER:HA	1:D:2102:ARG:HG2	1.57	0.86
1:B:2087:SER:HA	1:B:2102:ARG:HG2	1.61	0.82
1:C:1033:THR:HG21	1:D:2163:LEU:HB2	1.64	0.80
1:C:1029:MET:HG2	1:C:1103:VAL:HG23	1.66	0.78
1:D:2029:MET:HG2	1:D:2103:VAL:HG23	1.68	0.75
1:A:1033:THR:HG23	1:B:2149:THR:HG21	1.68	0.75
1:D:2032:GLU:OE2	1:D:2049:ASN:ND2	2.20	0.73
1:B:2029:MET:HG2	1:B:2103:VAL:HG23	1.70	0.73
1:D:2091:THR:OG1	1:D:2099:ARG:NH2	2.21	0.73
1:B:2091:THR:OG1	1:B:2099:ARG:NH2	2.21	0.72
1:B:2025:ASN:HB2	1:B:2052:VAL:HG21	1.72	0.72
1:A:1029:MET:HG2	1:A:1103:VAL:HG23	1.72	0.71
1:D:2167:PHE:HB3	2:D:2301:PX4:H47	1.73	0.70
1:C:1064:ILE:O	1:C:1068:ARG:N	2.26	0.68
1:B:2089:VAL:HG11	1:B:2098:LEU:HD13	1.75	0.68
1:C:1022:ILE:HG21	1:C:1109:LEU:HB2	1.76	0.67
1:D:2155:ARG:HD2	1:D:2190:VAL:HG11	1.75	0.66
1:A:1022:ILE:HG21	1:A:1109:LEU:HB2	1.77	0.65
2:C:1302:PX4:H57	2:C:1302:PX4:H30	1.78	0.65
1:A:1029:MET:HE3	1:A:1103:VAL:HA	1.78	0.64
2:C:1302:PX4:H66	2:C:1302:PX4:H42	1.79	0.64
1:A:1025:ASN:HA	1:A:1028:THR:HB	1.79	0.64
1:D:2162:THR:HG22	1:D:2164:GLY:H	1.61	0.64
1:C:1033:THR:HG23	1:D:2149:THR:HG21	1.81	0.63
1:D:2089:VAL:O	1:D:2102:ARG:NH2	2.29	0.62
1:D:2059:GLU:OE1	1:D:2108:ARG:NH2	2.32	0.62
1:A:1091:THR:O	1:A:1099:ARG:NH2	2.32	0.62
1:C:1116:MET:HA	1:C:1119:ILE:HD12	1.82	0.62
1:B:2003:LEU:O	1:B:2007:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2024:LEU:HB3	1:B:2048:PHE:HZ	1.64	0.62
1:C:1137:MET:HG2	2:C:1302:PX4:H38	1.82	0.62
1:D:2064:ILE:O	1:D:2068:ARG:N	2.32	0.61
1:D:2025:ASN:HA	1:D:2028:THR:HB	1.83	0.60
1:C:1162:THR:HG22	1:C:1164:GLY:H	1.66	0.60
1:C:1032:GLU:OE2	1:C:1049:ASN:ND2	2.35	0.60
1:A:1162:THR:HG22	1:A:1164:GLY:H	1.66	0.60
1:C:1023:VAL:HA	2:C:1301:PX4:H44	1.84	0.59
1:A:1165:GLU:HG3	2:B:2303:PX4:H3	1.85	0.59
1:B:2006:THR:HG23	1:B:2066:VAL:HG13	1.86	0.58
1:B:2025:ASN:ND2	1:B:2049:ASN:OD1	2.29	0.57
1:A:1216:ILE:HG22	1:B:2214:VAL:HG11	1.86	0.56
1:B:2033:THR:HG21	1:C:1163:LEU:HB2	1.87	0.56
2:C:1301:PX4:H21	2:C:1301:PX4:H50	1.88	0.56
1:B:2162:THR:HG22	1:B:2164:GLY:H	1.71	0.56
1:C:1027:ILE:HG12	2:C:1301:PX4:H33	1.88	0.56
1:A:1032:GLU:OE2	1:A:1049:ASN:ND2	2.39	0.55
1:A:1217:CYS:HA	1:B:2214:VAL:HG13	1.89	0.55
1:B:2087:SER:OG	1:B:2105:ARG:NH2	2.36	0.55
1:D:2098:LEU:O	1:D:2102:ARG:HG3	2.08	0.54
1:B:2064:ILE:O	1:B:2068:ARG:N	2.37	0.54
1:D:2022:ILE:HG21	1:D:2109:LEU:HB2	1.89	0.54
1:A:1174:MET:HE3	2:B:2303:PX4:H67	1.90	0.53
1:B:2199:ILE:HG21	2:B:2303:PX4:H51	1.89	0.53
2:C:1302:PX4:H36	2:C:1302:PX4:H61	1.90	0.53
1:C:1202:ILE:O	1:C:1206:THR:OG1	2.20	0.53
1:C:1110:VAL:HG11	1:C:1120:VAL:HG21	1.91	0.53
1:C:1076:TRP:HB3	1:C:1111:THR:HG23	1.89	0.53
1:C:1175:THR:HB	1:D:2176:LEU:HD13	1.90	0.53
1:D:2087:SER:OG	1:D:2105:ARG:NH2	2.37	0.53
1:A:1064:ILE:O	1:A:1068:ARG:N	2.40	0.52
1:B:2091:THR:O	1:B:2099:ARG:NH1	2.38	0.52
1:A:1175:THR:HB	1:B:2176:LEU:HD13	1.89	0.52
1:C:1060:ILE:HD13	1:C:1108:ARG:HH21	1.75	0.52
1:A:1076:TRP:HB3	1:A:1111:THR:HG23	1.91	0.52
1:B:2024:LEU:HB3	1:B:2048:PHE:CZ	2.43	0.52
1:D:2089:VAL:HG11	1:D:2098:LEU:HD13	1.91	0.52
1:B:2038:MET:HA	1:B:2038:MET:HE2	1.92	0.51
1:B:2162:THR:HB	1:B:2165:GLU:HB2	1.91	0.51
1:B:2216:ILE:HG22	1:C:1214:VAL:HG21	1.93	0.51
1:A:1038:MET:HE2	1:A:1038:MET:HA	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1019:ILE:HG12	1:C:1112:ALA:HB1	1.93	0.50
1:B:2202:ILE:O	1:B:2206:THR:OG1	2.25	0.50
1:D:2025:ASN:HB2	1:D:2052:VAL:HG21	1.92	0.50
1:A:1025:ASN:OD1	1:A:1105:ARG:NH1	2.37	0.50
1:B:2025:ASN:OD1	1:B:2105:ARG:NH1	2.38	0.49
1:A:1087:SER:OG	1:A:1105:ARG:NH2	2.35	0.49
1:C:1137:MET:HG2	2:C:1302:PX4:H33	1.94	0.49
1:C:1130:MET:HG2	1:C:1212:LEU:HD22	1.94	0.48
1:B:2022:ILE:HG21	1:B:2109:LEU:HB2	1.95	0.48
1:D:2071:PHE:CE2	1:D:2077:SER:HB3	2.49	0.48
1:D:2038:MET:HE2	1:D:2038:MET:HA	1.96	0.48
1:A:1130:MET:HG2	1:A:1212:LEU:HD22	1.96	0.48
1:B:2014:PHE:CE2	1:B:2018:ILE:HD11	2.49	0.48
1:B:2203:TRP:CH2	2:B:2303:PX4:H64	2.49	0.48
1:D:2024:LEU:HB3	1:D:2048:PHE:CZ	2.49	0.48
1:A:1110:VAL:HG11	1:A:1120:VAL:HG21	1.96	0.48
1:B:2032:GLU:OE2	1:B:2049:ASN:ND2	2.46	0.48
1:D:2041:PHE:O	1:D:2045:THR:OG1	2.27	0.47
1:C:1119:ILE:HD13	1:D:2132:SER:O	2.14	0.47
1:C:1155:ARG:HD2	1:C:1190:VAL:HG11	1.95	0.47
1:C:1009:VAL:HG21	1:C:1066:VAL:HG21	1.96	0.47
1:C:1188:MET:HA	1:C:1191:TYR:O	2.15	0.47
1:A:1185:ARG:O	1:A:1189:GLU:HG2	2.15	0.47
1:C:1119:ILE:O	1:C:1123:LEU:HG	2.15	0.47
2:C:1301:PX4:H24	2:C:1301:PX4:H29	1.47	0.47
2:C:1302:PX4:H2	2:C:1302:PX4:H7	1.68	0.47
1:C:1003:LEU:O	1:C:1007:ASN:ND2	2.48	0.46
1:B:2199:ILE:HB	1:B:2200:PRO:HD3	1.97	0.46
1:C:1025:ASN:HA	1:C:1028:THR:HB	1.97	0.46
1:A:1056:PHE:HE2	1:A:1108:ARG:HD3	1.80	0.46
1:A:1188:MET:HA	1:A:1191:TYR:O	2.15	0.46
2:A:1301:PX4:H2	2:A:1301:PX4:H12	1.69	0.46
1:D:2200:PRO:HA	1:D:2203:TRP:HB2	1.98	0.46
1:C:1029:MET:HE3	1:C:1103:VAL:HA	1.98	0.46
1:A:1067:HIS:HB2	1:A:1071:PHE:HB2	1.98	0.46
1:C:1038:MET:HA	1:C:1038:MET:HE2	1.97	0.46
1:A:1137:MET:HG2	2:B:2303:PX4:H66	1.98	0.45
1:D:2185:ARG:HB2	1:D:2186:PRO:HD3	1.98	0.45
1:A:1133:VAL:HG22	1:D:2119:ILE:HD12	1.98	0.45
1:B:2137:MET:HG2	2:B:2301:PX4:H35	1.98	0.45
1:A:1050:GLN:HA	1:A:1053:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2085:ALA:O	1:D:2089:VAL:HG23	2.17	0.45
1:B:2097:ILE:H	1:B:2097:ILE:HG13	1.62	0.45
1:C:1058:ILE:O	1:C:1062:LEU:HG	2.16	0.45
1:C:1212:LEU:HD23	1:C:1212:LEU:HA	1.79	0.44
1:D:2119:ILE:O	1:D:2123:LEU:HG	2.17	0.44
1:C:1152:PHE:HB3	1:C:1187:LEU:HD21	2.00	0.44
1:D:2079:PHE:CZ	1:D:2083:VAL:HG21	2.53	0.44
2:A:1303:PX4:H49	2:A:1303:PX4:H54	1.71	0.44
1:D:2080:ASP:OD2	1:D:2111:THR:HG21	2.18	0.44
1:D:2091:THR:HB	1:D:2102:ARG:HH12	1.82	0.44
1:D:2025:ASN:OD1	1:D:2105:ARG:HD2	2.18	0.44
1:D:2162:THR:HG22	1:D:2164:GLY:N	2.31	0.44
1:A:1047:LEU:O	1:A:1051:ILE:N	2.36	0.44
1:A:1212:LEU:HD23	1:A:1212:LEU:HA	1.89	0.44
1:B:2064:ILE:HG12	1:B:2071:PHE:CD1	2.53	0.44
1:D:2024:LEU:HB3	1:D:2048:PHE:HZ	1.81	0.44
1:B:2080:ASP:OD2	1:B:2111:THR:HG21	2.18	0.43
1:B:2203:TRP:HZ2	2:B:2303:PX4:H59	1.82	0.43
1:C:1133:VAL:HB	1:C:1212:LEU:HD21	2.01	0.43
1:D:2083:VAL:HG12	1:D:2105:ARG:HA	2.00	0.43
1:A:1079:PHE:CZ	1:A:1083:VAL:HG21	2.53	0.43
1:D:2067:HIS:HB3	1:D:2070:SER:HB2	2.01	0.43
1:C:1060:ILE:HA	1:C:1060:ILE:HD12	1.93	0.43
1:B:2010:GLU:OE1	1:B:2010:GLU:N	2.52	0.43
1:B:2193:TYR:O	2:B:2302:PX4:H22	2.19	0.43
1:B:2185:ARG:HB2	1:B:2186:PRO:HD3	2.00	0.42
1:A:1124:ILE:HG23	1:A:1127:ILE:HD12	2.01	0.42
1:B:2049:ASN:O	1:B:2053:ILE:HG23	2.19	0.42
1:B:2155:ARG:HD2	1:B:2190:VAL:HG11	2.02	0.42
1:D:2164:GLY:HA2	2:D:2301:PX4:H17	1.99	0.42
1:D:2199:ILE:HB	1:D:2200:PRO:HD3	2.01	0.42
1:B:2098:LEU:O	1:B:2102:ARG:HG3	2.18	0.42
1:D:2212:LEU:O	1:D:2216:ILE:HG13	2.19	0.42
1:A:1155:ARG:HD2	1:A:1190:VAL:HG11	2.01	0.42
1:B:2162:THR:HG22	1:B:2164:GLY:N	2.34	0.42
2:D:2301:PX4:H58	2:D:2301:PX4:H65	1.68	0.42
1:A:1063:ARG:HE	1:A:1071:PHE:HE1	1.68	0.42
1:D:2080:ASP:OD2	1:D:2108:ARG:NH1	2.53	0.42
1:B:2080:ASP:OD2	1:B:2108:ARG:NH1	2.53	0.41
1:C:1071:PHE:CE2	1:C:1077:SER:HB3	2.56	0.41
1:C:1074:ASP:HB3	1:C:1077:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2060:ILE:HA	1:B:2060:ILE:HD12	1.95	0.41
1:B:2188:MET:HA	1:B:2191:TYR:O	2.21	0.41
1:D:2060:ILE:HD12	1:D:2060:ILE:HA	1.81	0.41
1:A:1056:PHE:CE2	1:A:1108:ARG:HD3	2.56	0.41
1:C:1049:ASN:O	1:C:1053:ILE:HG23	2.21	0.41
1:D:2018:ILE:HG23	1:D:2056:PHE:CE2	2.56	0.41
1:D:2156:PHE:CE1	1:D:2187:LEU:HD23	2.56	0.41
1:D:2060:ILE:HD12	1:D:2063:ARG:HD3	2.03	0.41
1:C:1023:VAL:HG13	2:C:1301:PX4:H40	2.03	0.41
1:A:1193:TYR:HD2	2:A:1301:PX4:H18	1.87	0.40
1:D:2022:ILE:CD1	1:D:2108:ARG:HB3	2.52	0.40
2:B:2301:PX4:H9	2:B:2301:PX4:H2	1.91	0.40
1:B:2057:THR:OG1	1:B:2088:LEU:HD21	2.22	0.40
1:D:2034:SER:HB3	1:D:2037:PHE:HB3	2.03	0.40
1:D:2059:GLU:O	1:D:2063:ARG:HG3	2.22	0.40
1:A:1080:ASP:OD2	1:A:1111:THR:HG21	2.22	0.40
1:B:2024:LEU:HD23	1:B:2024:LEU:HA	1.92	0.40
1:D:2091:THR:O	1:D:2099:ARG:NH1	2.54	0.40
1:D:2025:ASN:OD1	1:D:2105:ARG:NH1	2.38	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	215/285 (75%)	210 (98%)	5 (2%)	0	100	100
1	B	216/285 (76%)	209 (97%)	6 (3%)	1 (0%)	29	67
1	C	216/285 (76%)	211 (98%)	5 (2%)	0	100	100
1	D	215/285 (75%)	206 (96%)	9 (4%)	0	100	100
All	All	862/1140 (76%)	836 (97%)	25 (3%)	1 (0%)	51	83



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2093	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/264 (67%)	177 (100%)	0	100	100
1	B	178/264 (67%)	177 (99%)	1 (1%)	86	94
1	C	184/264 (70%)	182 (99%)	2 (1%)	73	88
1	D	184/264 (70%)	184 (100%)	0	100	100
All	All	723/1056 (68%)	720 (100%)	3 (0%)	91	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2206	THR
1	C	1046	THR
1	C	1206	THR

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

Mol	Chain	Res	Type
1	B	2007	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	A	1304	-	4,4,4	0.92	0	6,6,6	0.44	0
3	PO4	B	2305	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PX4	A	1303	-	36,36,45	1.11	2 (5%)	40,41,53	1.14	2 (5%)
3	PO4	D	2304	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PX4	A	1301	-	26,26,45	1.27	3 (11%)	32,34,53	1.09	1 (3%)
2	PX4	C	1302	-	45,45,45	1.16	3 (6%)	51,53,53	1.04	2 (3%)
2	PX4	A	1302	-	15,15,45	1.40	2 (13%)	19,20,53	1.44	1 (5%)
2	PX4	B	2302	-	21,21,45	1.44	3 (14%)	25,26,53	1.31	2 (8%)
3	PO4	C	1303	-	4,4,4	0.91	0	6,6,6	0.43	0
3	PO4	D	2303	-	4,4,4	0.92	0	6,6,6	0.44	0
3	PO4	C	1304	-	4,4,4	0.91	0	6,6,6	0.43	0
2	PX4	D	2301	-	30,30,45	1.08	2 (6%)	35,37,53	1.09	1 (2%)
3	PO4	B	2304	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PX4	C	1301	-	45,45,45	1.16	3 (6%)	51,53,53	1.08	2 (3%)
2	PX4	D	2302	-	23,23,45	1.54	3 (13%)	29,31,53	1.24	3 (10%)
2	PX4	B	2301	-	35,35,45	1.29	3 (8%)	41,43,53	1.17	2 (4%)
2	PX4	B	2303	-	30,30,45	1.07	2 (6%)	35,37,53	1.08	1 (2%)
3	PO4	D	2305	-	4,4,4	0.94	0	6,6,6	0.44	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	D	2301	-	-	20/33/33/49	-
2	PX4	A	1303	-	-	14/38/38/49	-
2	PX4	B	2303	-	-	22/33/33/49	-
2	PX4	C	1302	-	-	28/49/49/49	-
2	PX4	A	1302	-	-	5/15/15/49	-
2	PX4	B	2302	-	-	11/23/23/49	-
2	PX4	A	1301	-	-	14/29/29/49	-
2	PX4	C	1301	-	-	23/49/49/49	-
2	PX4	D	2302	-	-	13/26/26/49	-
2	PX4	B	2301	-	-	24/39/39/49	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2302	PX4	O5-C9	3.85	1.44	1.33
2	B	2301	PX4	O5-C9	3.83	1.44	1.33
2	C	1302	PX4	O5-C9	3.82	1.44	1.33
2	B	2302	PX4	O5-C9	3.79	1.44	1.33
2	A	1303	PX4	O5-C9	3.77	1.44	1.33
2	C	1301	PX4	O5-C9	3.77	1.44	1.33
2	A	1302	PX4	O7-C23	3.72	1.43	1.35
2	D	2302	PX4	O7-C23	3.53	1.43	1.35
2	B	2301	PX4	O7-C23	3.35	1.43	1.34
2	C	1301	PX4	O7-C23	3.33	1.43	1.34
2	A	1301	PX4	O7-C23	3.29	1.43	1.34
2	D	2301	PX4	O7-C23	3.27	1.43	1.34
2	B	2303	PX4	O7-C23	3.27	1.43	1.34
2	A	1303	PX4	O7-C23	3.21	1.43	1.34
2	C	1302	PX4	O7-C23	3.20	1.43	1.34
2	B	2302	PX4	O7-C23	3.17	1.43	1.34
2	C	1302	PX4	C4-N1	-2.83	1.41	1.50
2	A	1301	PX4	C4-N1	-2.80	1.41	1.50
2	D	2302	PX4	C4-N1	-2.80	1.41	1.50
2	D	2301	PX4	C4-N1	-2.80	1.41	1.50
2	C	1301	PX4	C4-N1	-2.79	1.41	1.50
2	B	2301	PX4	C4-N1	-2.77	1.41	1.50
2	B	2303	PX4	C4-N1	-2.71	1.42	1.50
2	B	2302	PX4	P1-O2	2.57	1.58	1.50
2	A	1302	PX4	O5-C9	2.25	1.44	1.33
2	A	1301	PX4	O5-C9	2.23	1.44	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2301	PX4	O7-C23-C24	4.95	122.17	111.50
2	A	1302	PX4	O7-C23-C24	4.77	119.86	111.09
2	D	2302	PX4	O7-C23-C24	4.40	119.18	111.09
2	D	2301	PX4	O7-C23-C24	4.29	120.74	111.50
2	B	2303	PX4	O7-C23-C24	4.26	120.67	111.50
2	C	1301	PX4	O7-C23-C24	4.23	120.62	111.50
2	A	1301	PX4	O7-C23-C24	4.16	120.48	111.50
2	B	2302	PX4	O7-C23-C24	4.04	120.21	111.50
2	C	1302	PX4	O7-C23-C24	4.01	120.14	111.50
2	A	1303	PX4	O7-C23-C24	3.77	119.62	111.50
2	D	2302	PX4	O5-C9-C10	2.79	120.67	111.91
2	B	2301	PX4	O5-C9-C10	2.67	120.28	111.91
2	A	1303	PX4	O5-C9-C10	2.63	120.17	111.91
2	C	1302	PX4	O5-C9-C10	2.56	119.95	111.91
2	B	2302	PX4	O5-C9-C10	2.50	119.75	111.91
2	C	1301	PX4	O5-C9-C10	2.37	119.34	111.91
2	D	2302	PX4	C7-O7-C23	-2.10	113.98	117.90

There are no chirality outliers.

All (174) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2301	PX4	C1-O3-P1-O1
2	D	2301	PX4	C1-O3-P1-O2
2	D	2301	PX4	C1-O3-P1-O4
2	D	2301	PX4	O3-C1-C2-N1
2	D	2301	PX4	C6-C7-C8-O5
2	D	2301	PX4	O7-C7-C8-O5
2	D	2301	PX4	C24-C23-O7-C7
2	B	2303	PX4	C1-O3-P1-O1
2	B	2303	PX4	C1-O3-P1-O2
2	B	2303	PX4	C6-C7-C8-O5
2	B	2303	PX4	O7-C7-C8-O5
2	B	2303	PX4	C24-C23-O7-C7
2	C	1302	PX4	C1-O3-P1-O1
2	C	1302	PX4	C1-O3-P1-O2
2	C	1302	PX4	C1-O3-P1-O4
2	A	1302	PX4	C6-O4-P1-O1
2	A	1302	PX4	C6-O4-P1-O3
2	A	1302	PX4	O7-C7-C8-O5
2	A	1301	PX4	C1-O3-P1-O2

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Mol	Chain	Res	Type	Atoms
2	A	1301	PX4	O3-C1-C2-N1
2	A	1301	PX4	O4-C6-C7-O7
2	A	1301	PX4	O8-C23-O7-C7
2	A	1301	PX4	C24-C23-O7-C7
2	C	1301	PX4	C6-O4-P1-O2
2	C	1301	PX4	C6-O4-P1-O3
2	C	1301	PX4	C24-C23-O7-C7
2	D	2302	PX4	C1-O3-P1-O1
2	D	2302	PX4	C1-O3-P1-O2
2	D	2302	PX4	C6-O4-P1-O2
2	D	2302	PX4	O3-C1-C2-N1
2	B	2301	PX4	C1-O3-P1-O1
2	B	2301	PX4	O3-C1-C2-N1
2	B	2301	PX4	C24-C23-O7-C7
2	D	2302	PX4	O6-C9-O5-C8
2	B	2301	PX4	O6-C9-O5-C8
2	D	2301	PX4	O8-C23-O7-C7
2	B	2303	PX4	O8-C23-O7-C7
2	C	1301	PX4	O8-C23-O7-C7
2	B	2301	PX4	C10-C9-O5-C8
2	D	2302	PX4	C10-C9-O5-C8
2	B	2301	PX4	O8-C23-O7-C7
2	A	1301	PX4	O6-C9-O5-C8
2	A	1301	PX4	C10-C9-O5-C8
2	A	1303	PX4	C24-C23-O7-C7
2	A	1303	PX4	O8-C23-O7-C7
2	C	1302	PX4	O7-C7-C8-O5
2	B	2302	PX4	O7-C7-C8-O5
2	C	1301	PX4	C14-C15-C16-C17
2	C	1301	PX4	C12-C13-C14-C15
2	D	2301	PX4	C23-C24-C25-C26
2	A	1301	PX4	C23-C24-C25-C26
2	C	1302	PX4	C9-C10-C11-C12
2	B	2303	PX4	C1-O3-P1-O4
2	C	1302	PX4	C6-O4-P1-O3
2	D	2302	PX4	C1-O3-P1-O4
2	B	2301	PX4	C1-O3-P1-O4
2	C	1301	PX4	C10-C9-O5-C8
2	C	1301	PX4	C9-C10-C11-C12
2	B	2301	PX4	C13-C14-C15-C16
2	B	2303	PX4	C30-C31-C32-C33
2	C	1301	PX4	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	D	2301	PX4	C29-C30-C31-C32
2	A	1303	PX4	C25-C26-C27-C28
2	C	1302	PX4	C14-C15-C16-C17
2	D	2301	PX4	C30-C31-C32-C33
2	C	1302	PX4	C25-C26-C27-C28
2	B	2302	PX4	C24-C23-O7-C7
2	B	2303	PX4	C26-C27-C28-C29
2	C	1302	PX4	C13-C14-C15-C16
2	B	2301	PX4	C23-C24-C25-C26
2	B	2303	PX4	C27-C28-C29-C30
2	C	1302	PX4	C16-C17-C18-C19
2	C	1301	PX4	O6-C9-O5-C8
2	B	2301	PX4	C10-C11-C12-C13
2	C	1301	PX4	C25-C26-C27-C28
2	D	2301	PX4	C32-C33-C34-C35
2	C	1302	PX4	C12-C13-C14-C15
2	B	2302	PX4	O8-C23-O7-C7
2	C	1302	PX4	C27-C28-C29-C30
2	A	1303	PX4	C30-C31-C32-C33
2	A	1301	PX4	C25-C26-C27-C28
2	D	2301	PX4	C24-C25-C26-C27
2	B	2301	PX4	C14-C15-C16-C17
2	C	1301	PX4	C28-C29-C30-C31
2	A	1303	PX4	C23-C24-C25-C26
2	C	1301	PX4	C23-C24-C25-C26
2	C	1301	PX4	C11-C12-C13-C14
2	D	2302	PX4	C6-O4-P1-O3
2	C	1301	PX4	C16-C17-C18-C19
2	A	1301	PX4	O4-C6-C7-C8
2	C	1302	PX4	C6-C7-C8-O5
2	B	2302	PX4	C6-C7-C8-O5
2	C	1302	PX4	C26-C27-C28-C29
2	D	2301	PX4	C26-C27-C28-C29
2	B	2302	PX4	C9-C10-C11-C12
2	B	2301	PX4	C24-C25-C26-C27
2	B	2303	PX4	C25-C26-C27-C28
2	A	1302	PX4	C6-O4-P1-O2
2	B	2303	PX4	O4-C6-C7-O7
2	C	1301	PX4	O4-C6-C7-O7
2	B	2301	PX4	C16-C17-C18-C19
2	D	2301	PX4	C25-C26-C27-C28
2	D	2301	PX4	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
2	B	2303	PX4	O4-C6-C7-C8
2	D	2302	PX4	O4-C6-C7-C8
2	B	2303	PX4	C23-C24-C25-C26
2	B	2301	PX4	C25-C26-C27-C28
2	D	2301	PX4	C28-C29-C30-C31
2	A	1303	PX4	C6-C7-C8-O5
2	A	1302	PX4	C6-C7-C8-O5
2	A	1301	PX4	C6-C7-C8-O5
2	C	1302	PX4	O4-C6-C7-O7
2	B	2302	PX4	O4-C6-C7-O7
2	D	2302	PX4	O4-C6-C7-O7
2	B	2301	PX4	O4-C6-C7-O7
2	B	2302	PX4	C23-C24-C25-C26
2	A	1301	PX4	O7-C7-C8-O5
2	B	2301	PX4	O7-C7-C8-O5
2	C	1302	PX4	C10-C11-C12-C13
2	D	2301	PX4	C7-C6-O4-P1
2	B	2302	PX4	C7-C6-O4-P1
2	B	2303	PX4	C28-C29-C30-C31
2	B	2302	PX4	O4-C6-C7-C8
2	C	1302	PX4	C32-C33-C34-C35
2	C	1301	PX4	C6-C7-C8-O5
2	B	2301	PX4	C6-C7-C8-O5
2	A	1303	PX4	O7-C7-C8-O5
2	C	1302	PX4	C33-C34-C35-C36
2	C	1301	PX4	C17-C18-C19-C20
2	A	1301	PX4	C1-O3-P1-O4
2	B	2303	PX4	C7-C6-O4-P1
2	B	2303	PX4	C6-O4-P1-O1
2	C	1302	PX4	C6-O4-P1-O2
2	D	2302	PX4	C6-O4-P1-O1
2	B	2301	PX4	C1-O3-P1-O2
2	B	2303	PX4	C24-C25-C26-C27
2	C	1302	PX4	O4-C6-C7-C8
2	C	1301	PX4	O4-C6-C7-C8
2	B	2301	PX4	O4-C6-C7-C8
2	C	1302	PX4	C2-C1-O3-P1
2	A	1301	PX4	C2-C1-O3-P1
2	B	2301	PX4	C2-C1-O3-P1
2	C	1301	PX4	C18-C19-C20-C21
2	C	1301	PX4	C24-C25-C26-C27
2	A	1303	PX4	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
2	C	1301	PX4	O3-C1-C2-N1
2	A	1303	PX4	C28-C29-C30-C31
2	D	2301	PX4	C6-O4-P1-O3
2	C	1301	PX4	C7-C6-O4-P1
2	C	1302	PX4	C18-C19-C20-C21
2	C	1302	PX4	C17-C18-C19-C20
2	B	2303	PX4	C33-C34-C35-C36
2	A	1303	PX4	C11-C12-C13-C14
2	A	1303	PX4	C6-O4-P1-O1
2	B	2301	PX4	C11-C10-C9-O5
2	B	2303	PX4	C1-C2-N1-C4
2	D	2302	PX4	C11-C10-C9-O5
2	C	1302	PX4	C31-C32-C33-C34
2	A	1303	PX4	O4-C6-C7-O7
2	C	1302	PX4	C11-C10-C9-O5
2	C	1302	PX4	O7-C23-C24-C25
2	B	2301	PX4	C11-C10-C9-O6
2	B	2301	PX4	C15-C16-C17-C18
2	B	2302	PX4	C11-C10-C9-O5
2	A	1303	PX4	C12-C13-C14-C15
2	C	1302	PX4	C11-C10-C9-O6
2	B	2301	PX4	C11-C12-C13-C14
2	D	2302	PX4	C11-C10-C9-O6
2	D	2301	PX4	C6-O4-P1-O2
2	B	2303	PX4	C1-C2-N1-C5
2	C	1302	PX4	O8-C23-C24-C25
2	B	2302	PX4	C11-C10-C9-O6
2	A	1303	PX4	C8-C7-O7-C23
2	B	2303	PX4	C29-C30-C31-C32

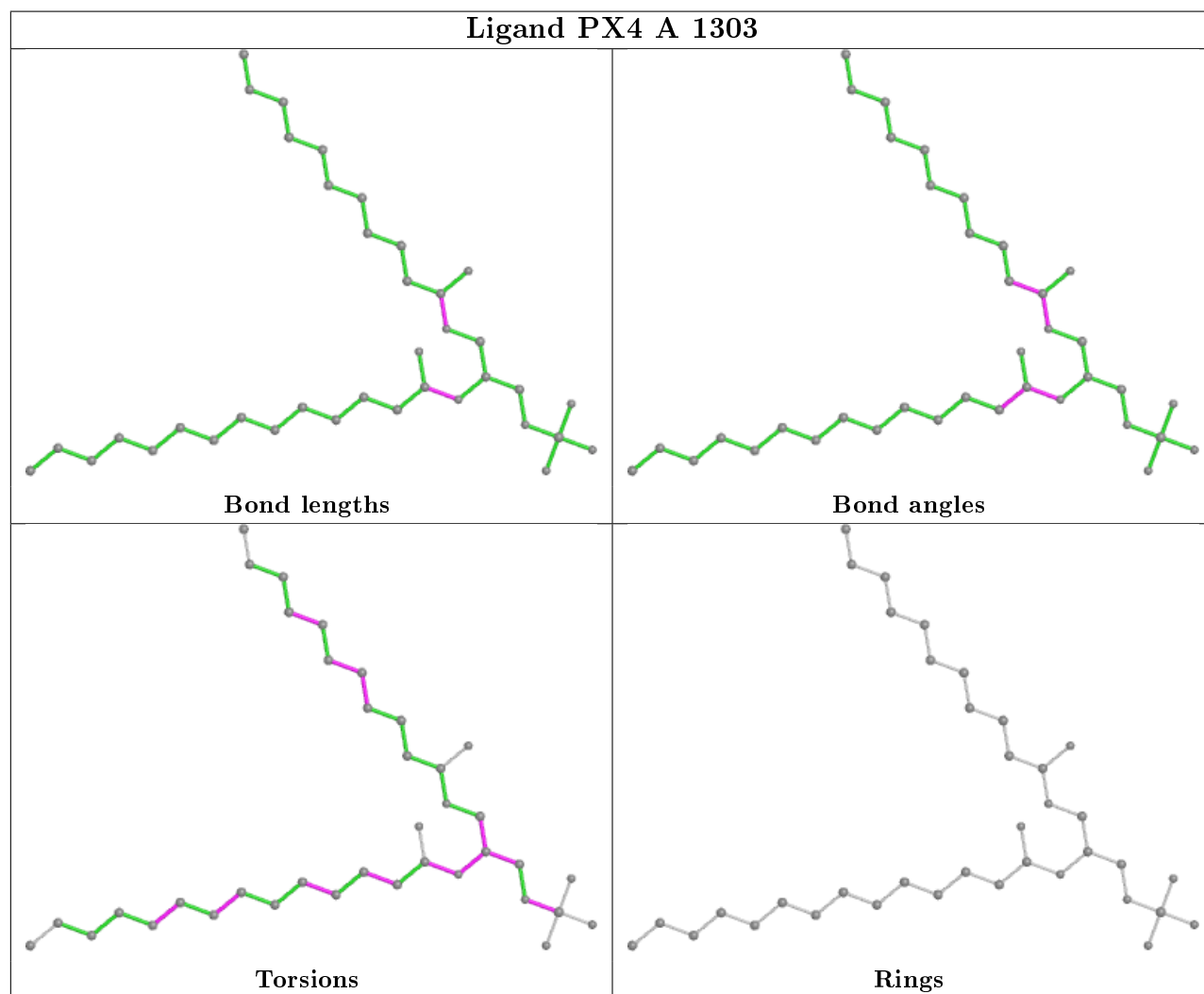
There are no ring outliers.

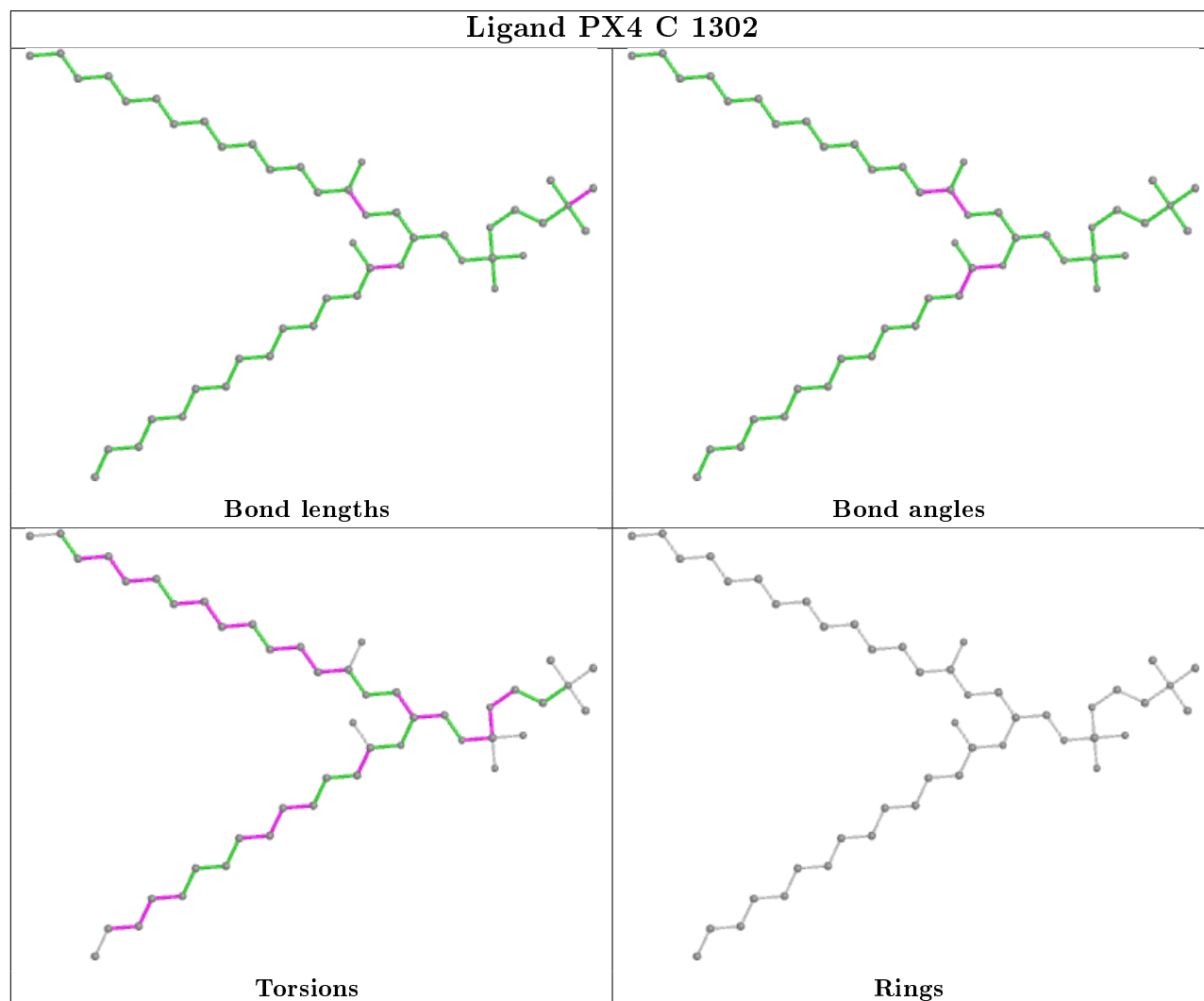
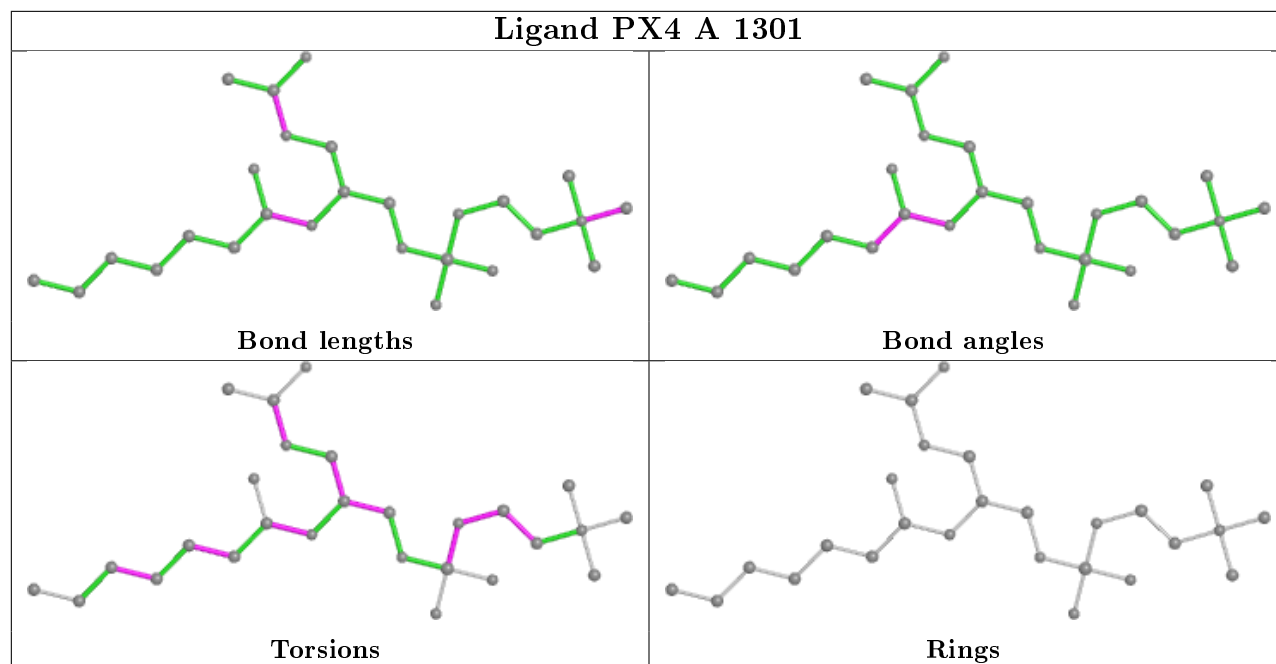
8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1303	PX4	1	0
2	A	1301	PX4	2	0
2	C	1302	PX4	6	0
2	B	2302	PX4	1	0
2	D	2301	PX4	3	0
2	C	1301	PX4	5	0
2	B	2301	PX4	2	0
2	B	2303	PX4	6	0

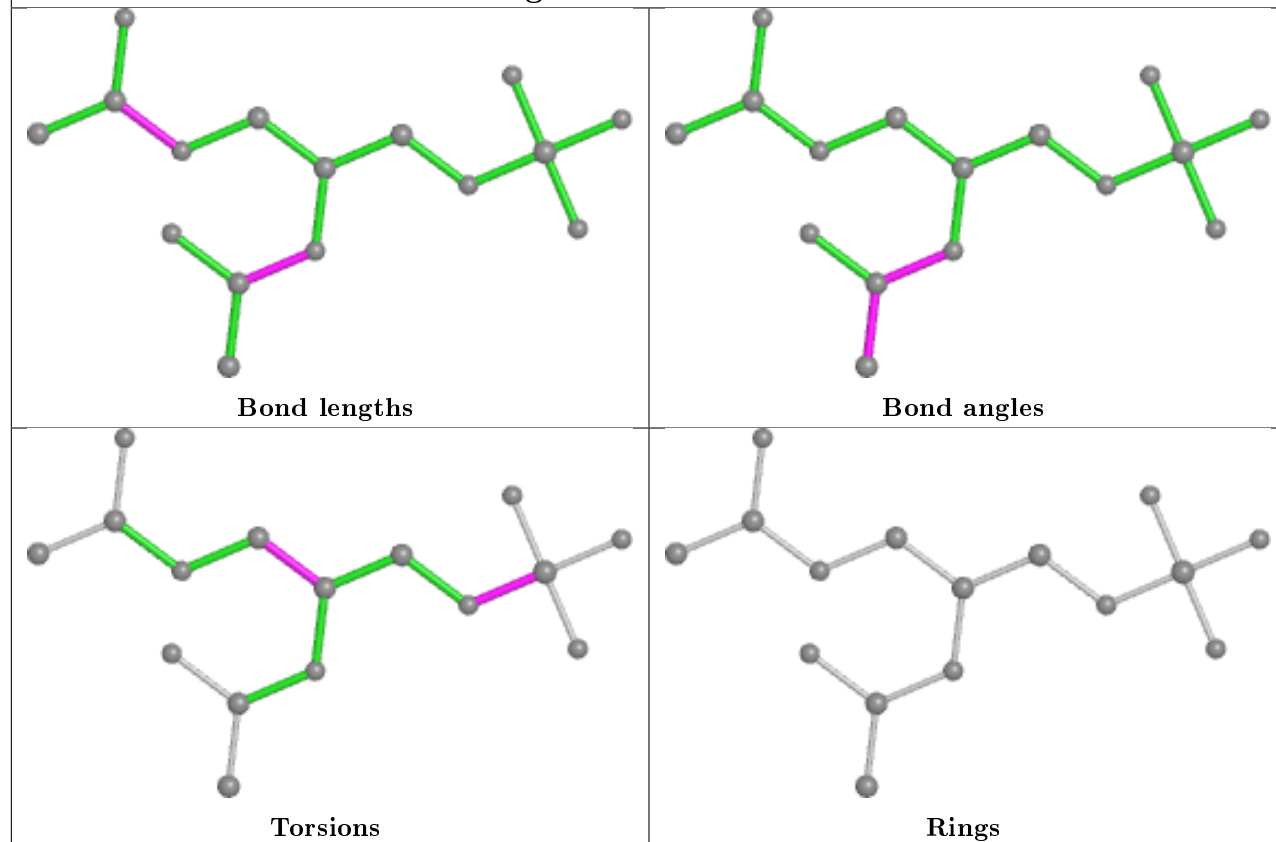


The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

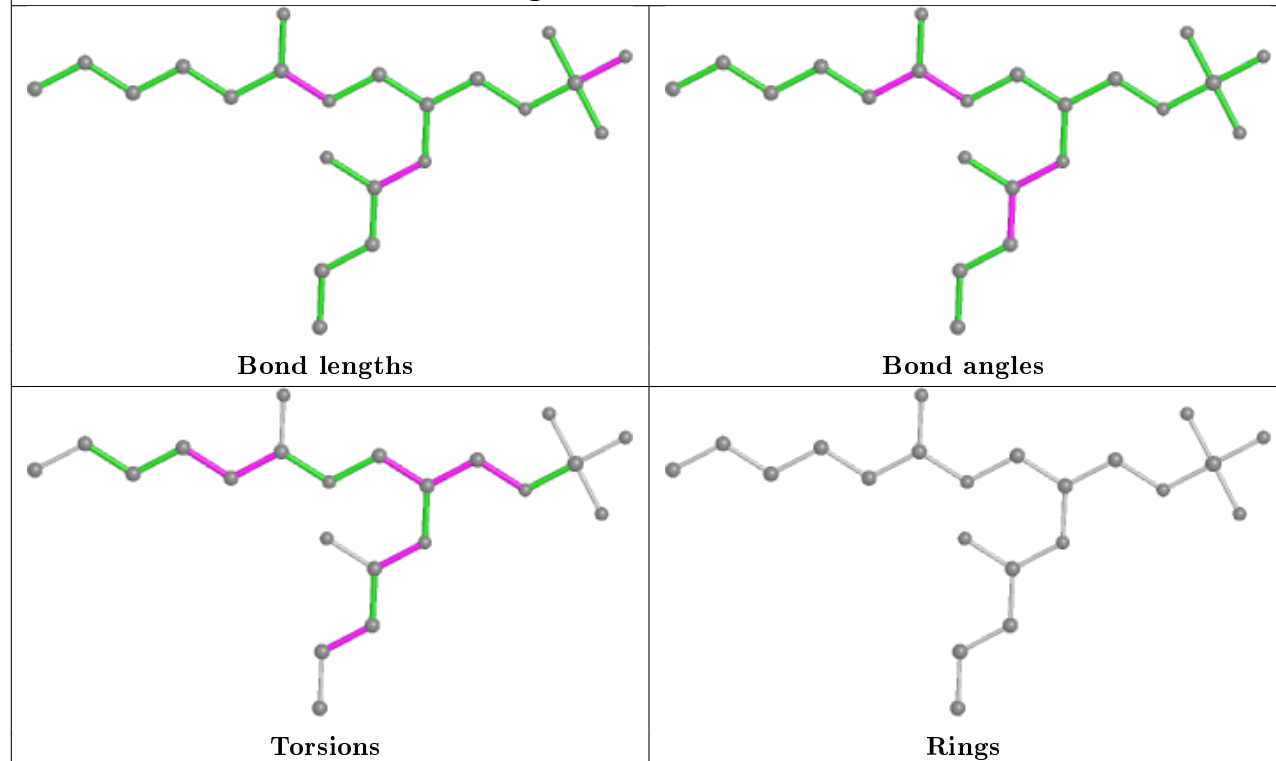


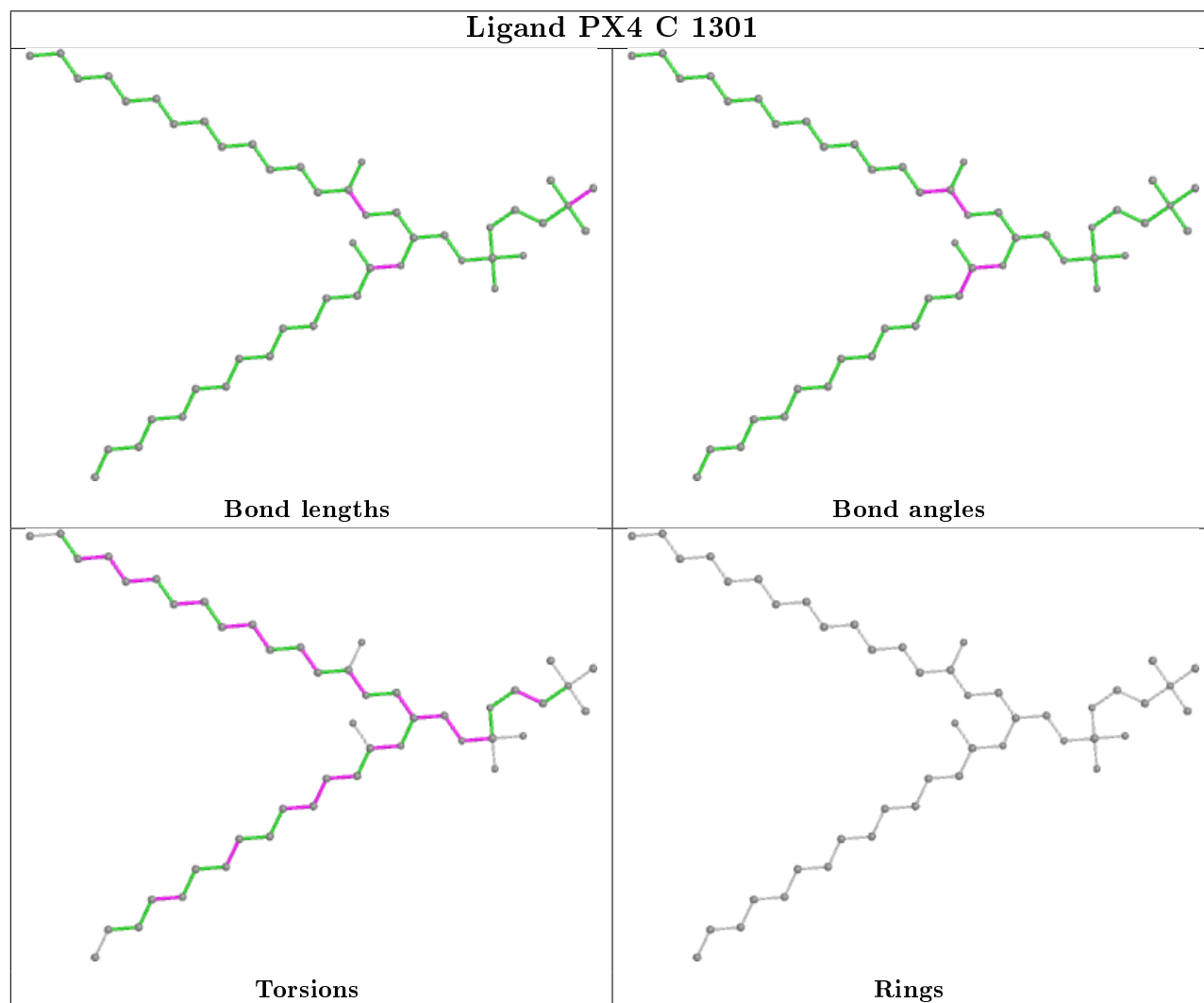
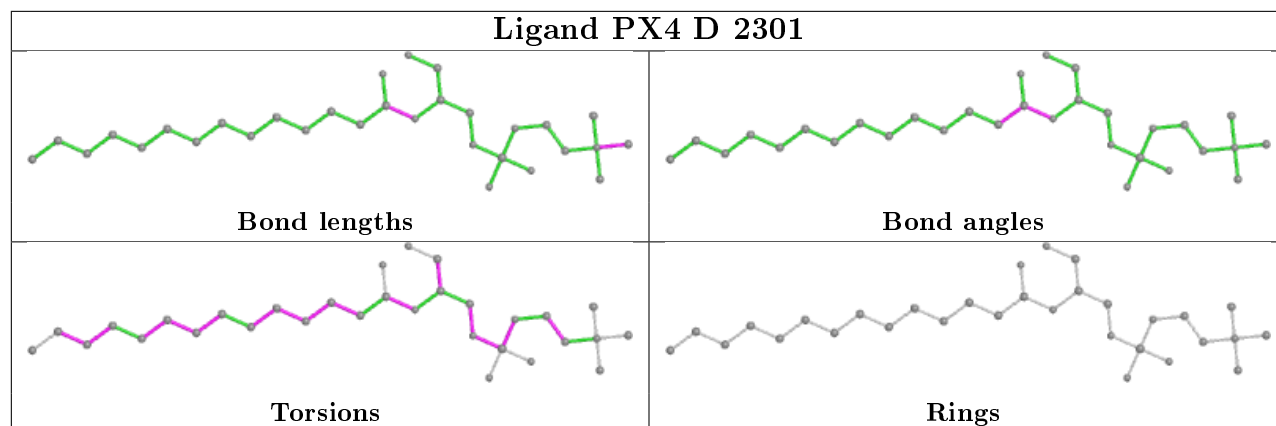


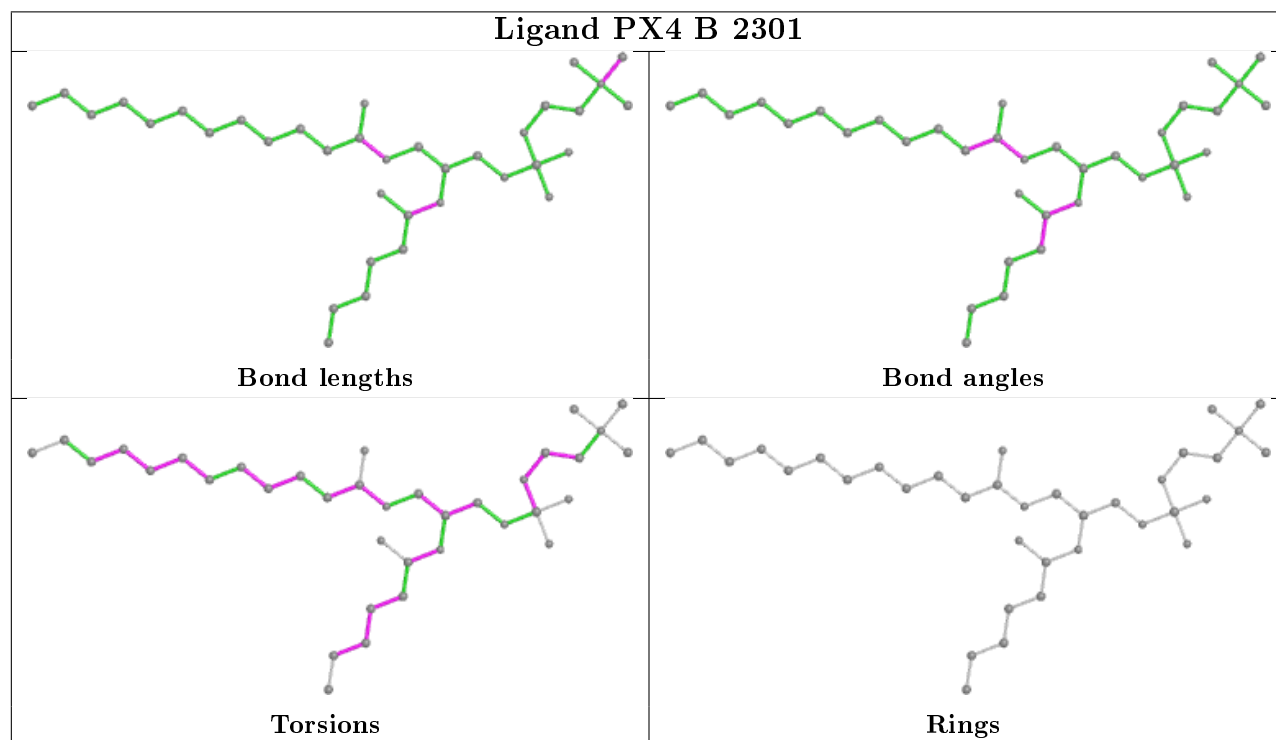
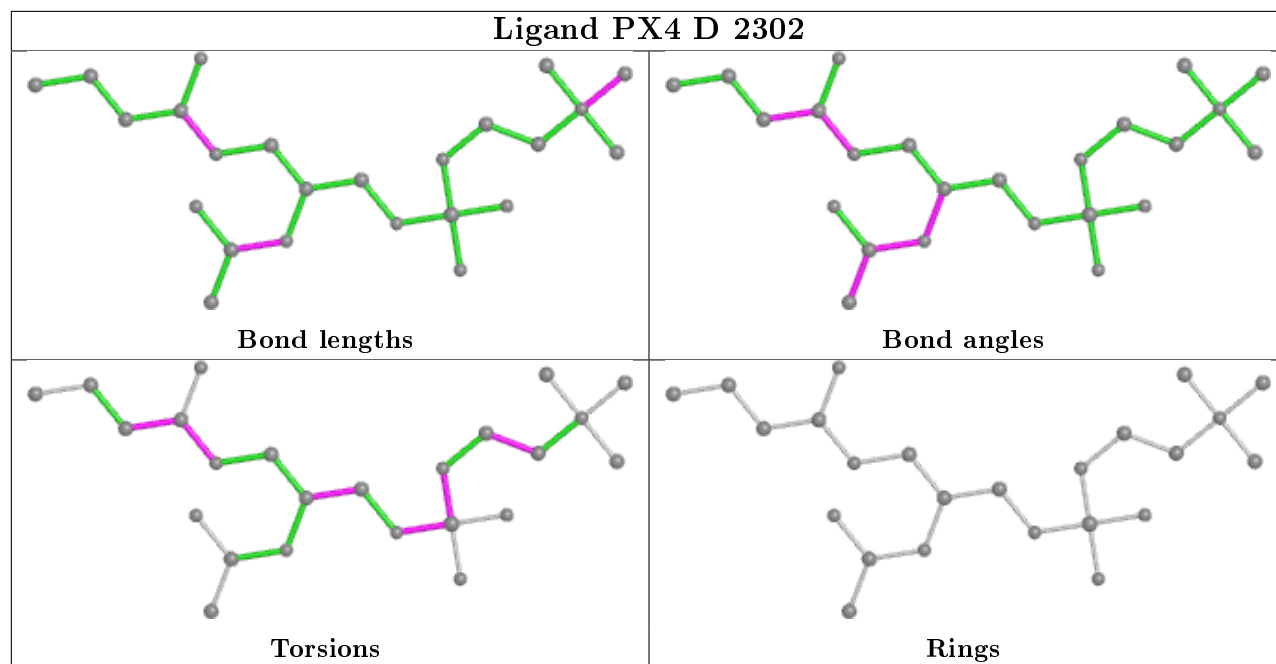
## Ligand PX4 A 1302

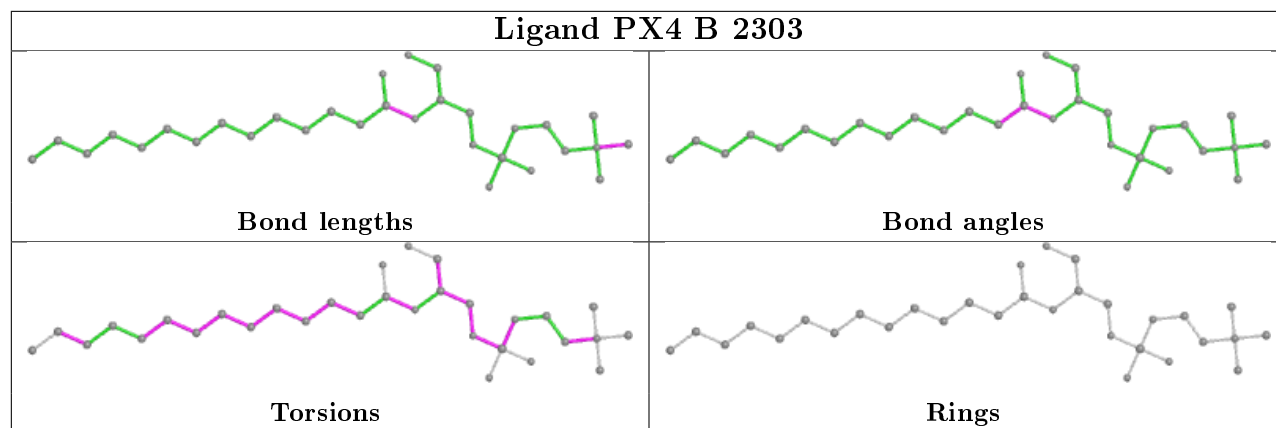


## Ligand PX4 B 2302









## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	217/285 (76%)	-0.02	1 (0%) 91 86	40, 91, 154, 172	0
1	B	218/285 (76%)	-0.11	2 (0%) 84 75	36, 93, 153, 193	0
1	C	218/285 (76%)	-0.07	0 100 100	39, 88, 140, 192	0
1	D	217/285 (76%)	-0.09	0 100 100	40, 87, 134, 184	0
All	All	870/1140 (76%)	-0.07	3 (0%) 94 92	36, 89, 148, 193	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1098	LEU	2.7
1	B	2093	SER	2.4
1	B	2092	SER	2.2

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

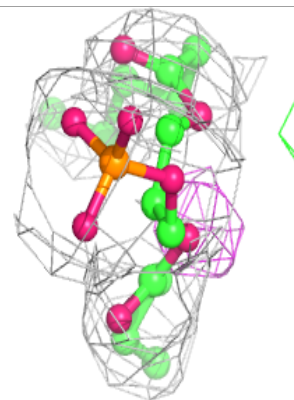
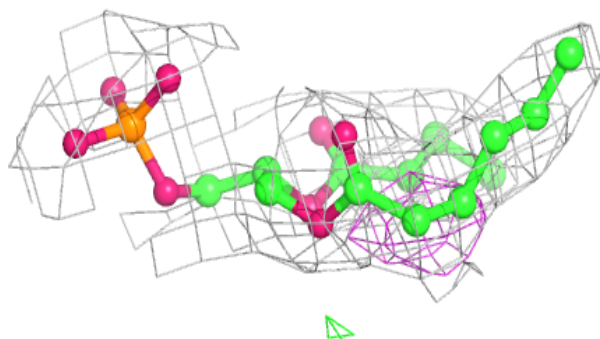
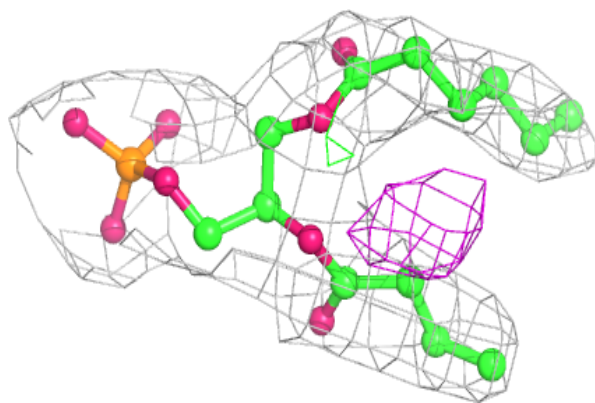
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	C	1303	5/5	0.68	0.21	178,179,180,183	0
3	PO4	D	2304	5/5	0.75	0.14	173,178,182,184	0
3	PO4	D	2305	5/5	0.83	0.26	104,113,120,121	0
3	PO4	C	1304	5/5	0.89	0.11	138,141,147,155	0
2	PX4	B	2302	22/46	0.89	0.28	26,91,137,142	0
2	PX4	A	1301	27/46	0.90	0.35	50,115,168,174	0
3	PO4	B	2305	5/5	0.90	0.14	151,156,165,167	0
3	PO4	D	2303	5/5	0.92	0.17	109,117,129,139	0
2	PX4	A	1303	37/46	0.92	0.38	40,96,128,145	0
3	PO4	A	1304	5/5	0.92	0.15	115,118,123,125	0
3	PO4	B	2304	5/5	0.94	0.12	96,96,104,107	0
2	PX4	D	2302	24/46	0.94	0.26	2,78,139,150	0
2	PX4	C	1302	46/46	0.94	0.31	36,84,106,117	0
2	PX4	B	2301	36/46	0.95	0.26	29,72,103,111	0
2	PX4	C	1301	46/46	0.95	0.29	33,84,119,128	0
2	PX4	A	1302	16/46	0.96	0.19	60,91,104,108	0
2	PX4	B	2303	31/46	0.96	0.28	39,58,102,107	0
2	PX4	D	2301	31/46	0.96	0.32	39,82,99,104	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.

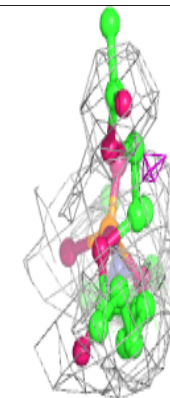
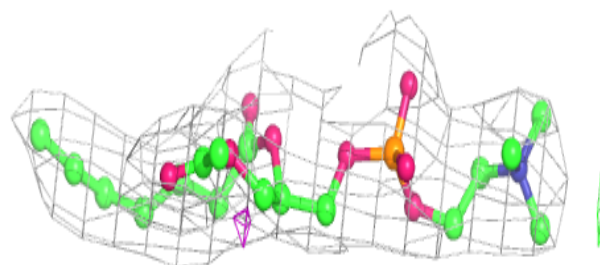
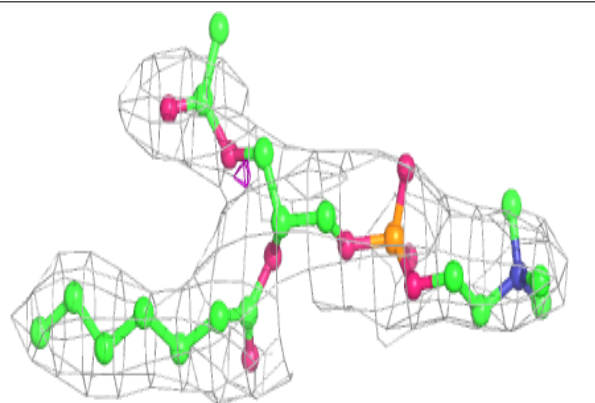


**Electron density around PX4 B 2302:**

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

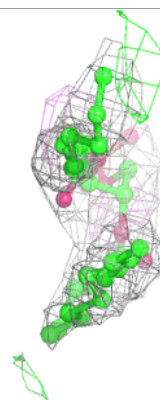
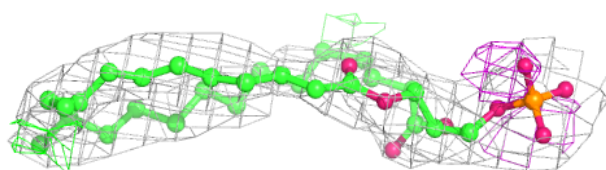
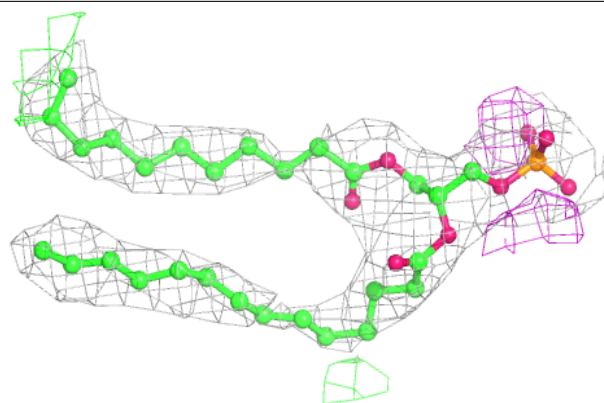
**Electron density around PX4 A 1301:**

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

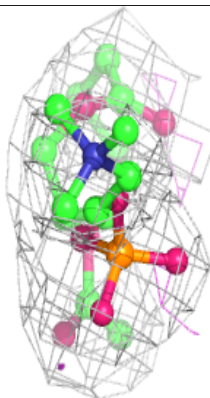
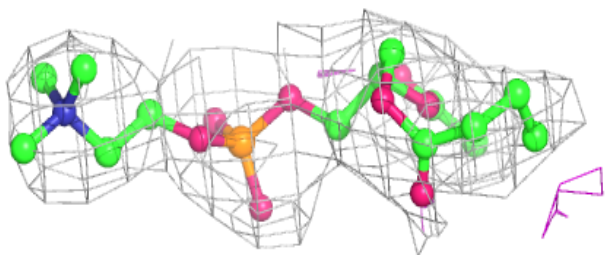
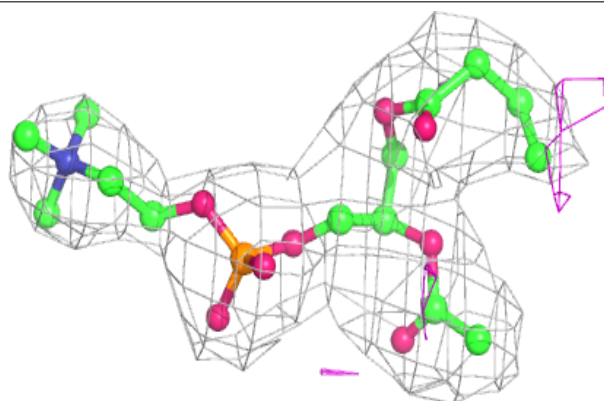


**Electron density around PX4 A 1303:**

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

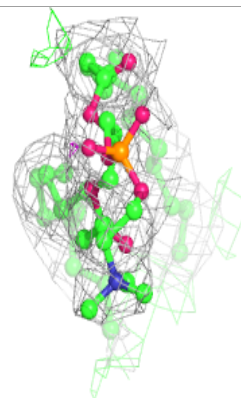
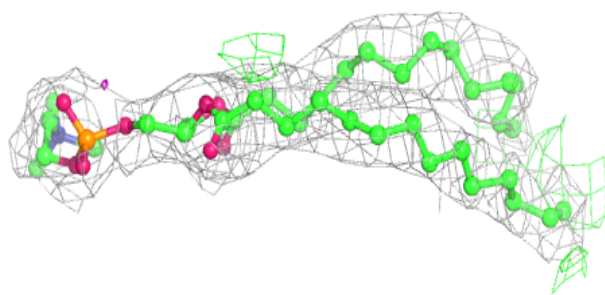
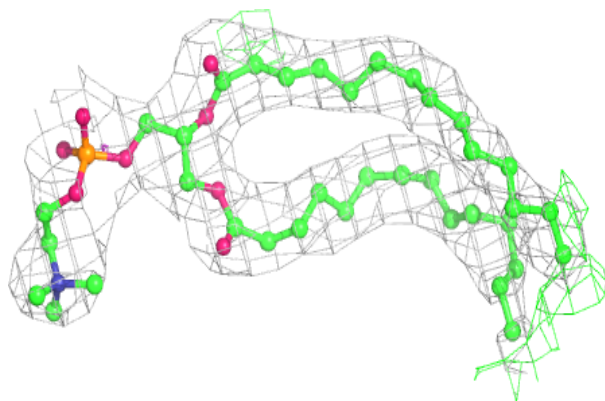
**Electron density around PX4 D 2302:**

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

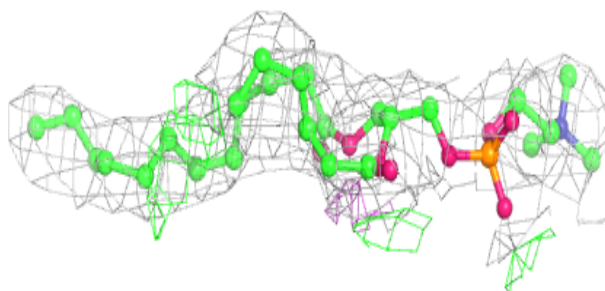
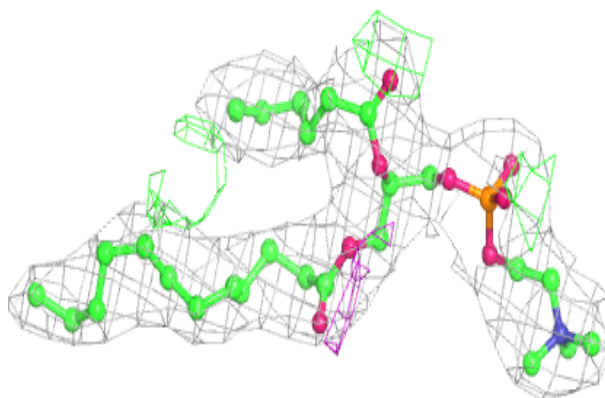


**Electron density around PX4 C 1302:**

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

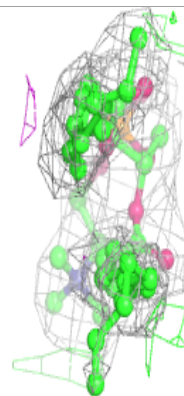
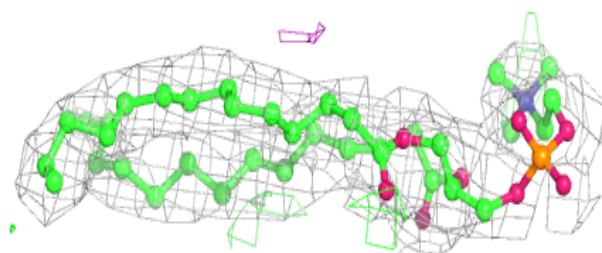
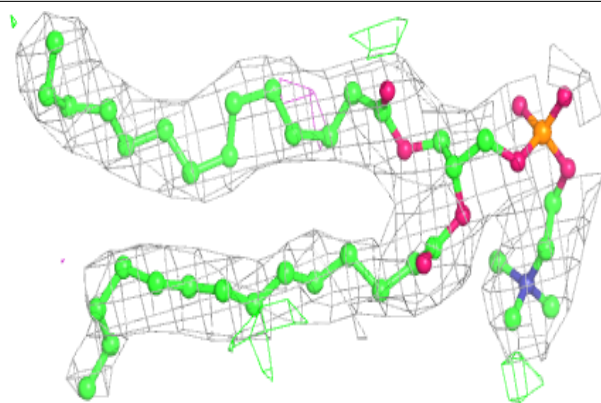
**Electron density around PX4 B 2301:**

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



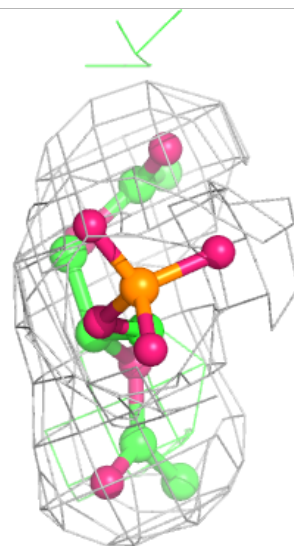
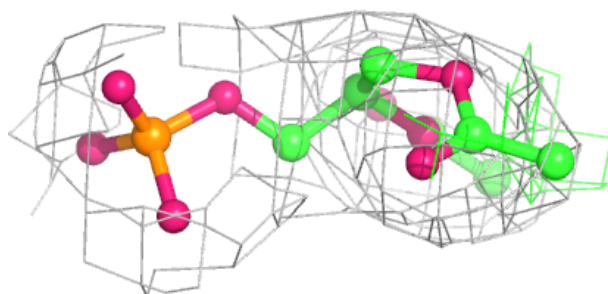
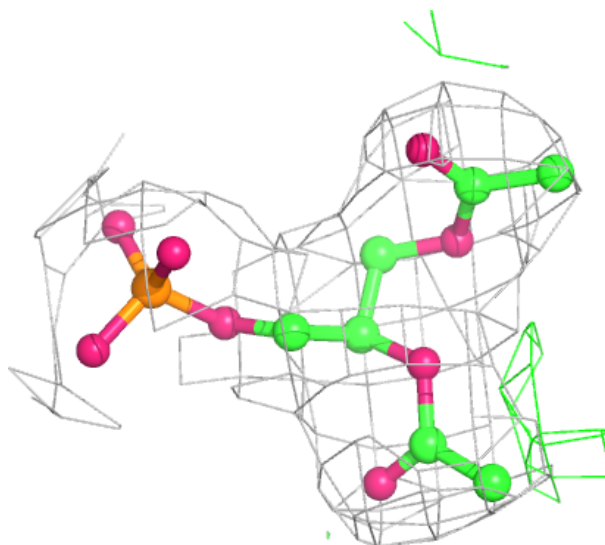
**Electron density around PX4 C 1301:**

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



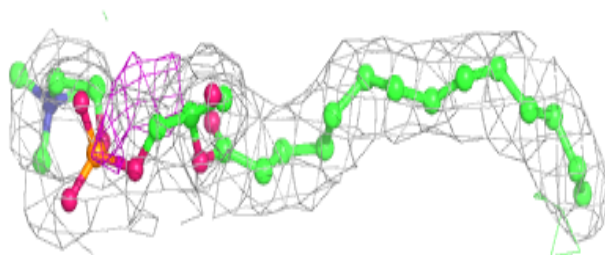
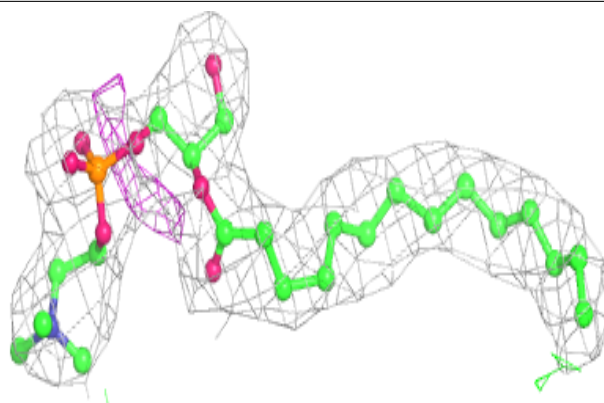
**Electron density around PX4 A 1302:**

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

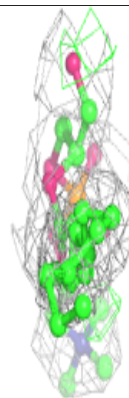
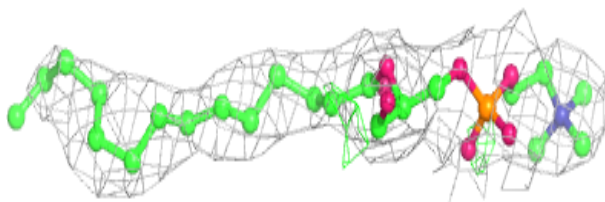
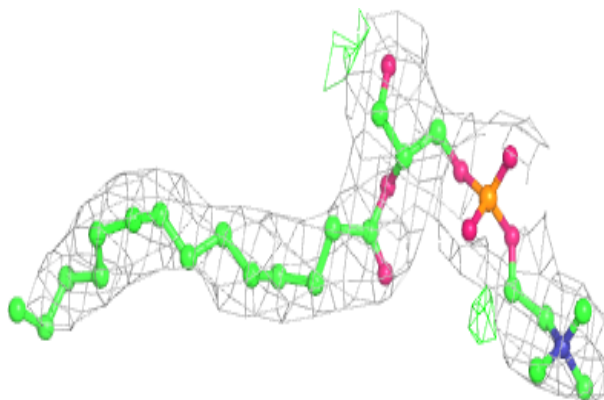


**Electron density around PX4 B 2303:**

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

**Electron density around PX4 D 2301:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.