



# wwPDB X-ray Structure Validation Summary Report

Nov 5, 2014 – 05:00 PM EST

PDB ID : 4MVR  
Title : Structural Basis for Ca<sup>2+</sup> Selectivity of a Voltage-gated Calcium Channel  
Authors : Tang, L.; Gamal El-Din, T.M.; Payandeh, J.; Gilbert, Q.M.; Heard, T.M.;  
Scheuer, T.; Zheng, N.; Catterall, W.A.  
Deposited on : 2013-09-24  
Resolution : 3.20 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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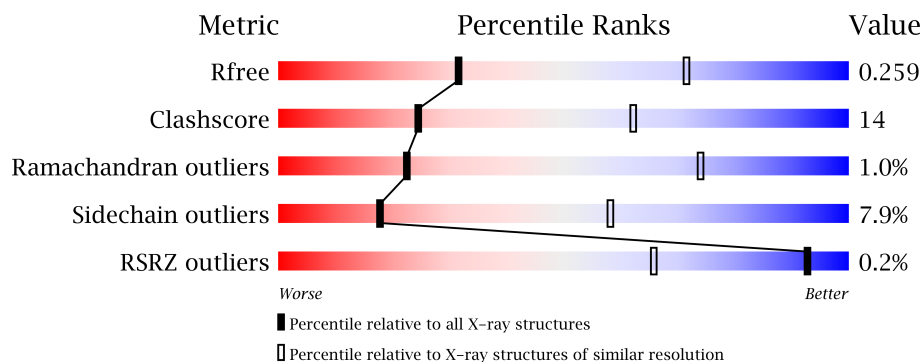
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable24103
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.1.3
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable24103

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	237	
1	B	237	
1	C	237	
1	D	237	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	PX4	A	1305	-	X
3	PX4	B	1302	-	X
3	PX4	D	1303	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7387 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			1798	1224	268	295	11			
1	B	219	Total	C	N	O	S	0	0	0
			1798	1224	268	295	11			
1	C	219	Total	C	N	O	S	0	0	0
			1798	1224	268	295	11			
1	D	219	Total	C	N	O	S	0	0	0
			1798	1224	268	295	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	EXPRESSION TAG	UNP A8EVM5
A	984	ASP	-	EXPRESSION TAG	UNP A8EVM5
A	985	TYR	-	EXPRESSION TAG	UNP A8EVM5
A	986	LYS	-	EXPRESSION TAG	UNP A8EVM5
A	987	ASP	-	EXPRESSION TAG	UNP A8EVM5
A	988	ASP	-	EXPRESSION TAG	UNP A8EVM5
A	989	ASP	-	EXPRESSION TAG	UNP A8EVM5
A	990	ASP	-	EXPRESSION TAG	UNP A8EVM5
A	991	LYS	-	EXPRESSION TAG	UNP A8EVM5
A	992	GLY	-	EXPRESSION TAG	UNP A8EVM5
A	993	SER	-	EXPRESSION TAG	UNP A8EVM5
A	994	LEU	-	EXPRESSION TAG	UNP A8EVM5
A	995	VAL	-	EXPRESSION TAG	UNP A8EVM5
A	996	PRO	-	EXPRESSION TAG	UNP A8EVM5
A	997	ARG	-	EXPRESSION TAG	UNP A8EVM5
A	998	GLY	-	EXPRESSION TAG	UNP A8EVM5
A	999	SER	-	EXPRESSION TAG	UNP A8EVM5
A	1000	HIS	-	EXPRESSION TAG	UNP A8EVM5
A	1177	ASP	GLU	CONFLICT	UNP A8EVM5
A	1178	ASP	SER	CONFLICT	UNP A8EVM5
A	1181	ASP	MET	CONFLICT	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1217	CYS	ILE	CONFLICT	UNP A8EVM5
B	983	MET	-	EXPRESSION TAG	UNP A8EVM5
B	984	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	985	TYR	-	EXPRESSION TAG	UNP A8EVM5
B	986	LYS	-	EXPRESSION TAG	UNP A8EVM5
B	987	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	988	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	989	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	990	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	991	LYS	-	EXPRESSION TAG	UNP A8EVM5
B	992	GLY	-	EXPRESSION TAG	UNP A8EVM5
B	993	SER	-	EXPRESSION TAG	UNP A8EVM5
B	994	LEU	-	EXPRESSION TAG	UNP A8EVM5
B	995	VAL	-	EXPRESSION TAG	UNP A8EVM5
B	996	PRO	-	EXPRESSION TAG	UNP A8EVM5
B	997	ARG	-	EXPRESSION TAG	UNP A8EVM5
B	998	GLY	-	EXPRESSION TAG	UNP A8EVM5
B	999	SER	-	EXPRESSION TAG	UNP A8EVM5
B	1000	HIS	-	EXPRESSION TAG	UNP A8EVM5
B	1177	ASP	GLU	CONFLICT	UNP A8EVM5
B	1178	ASP	SER	CONFLICT	UNP A8EVM5
B	1181	ASP	MET	CONFLICT	UNP A8EVM5
B	1217	CYS	ILE	CONFLICT	UNP A8EVM5
C	983	MET	-	EXPRESSION TAG	UNP A8EVM5
C	984	ASP	-	EXPRESSION TAG	UNP A8EVM5
C	985	TYR	-	EXPRESSION TAG	UNP A8EVM5
C	986	LYS	-	EXPRESSION TAG	UNP A8EVM5
C	987	ASP	-	EXPRESSION TAG	UNP A8EVM5
C	988	ASP	-	EXPRESSION TAG	UNP A8EVM5
C	989	ASP	-	EXPRESSION TAG	UNP A8EVM5
C	990	ASP	-	EXPRESSION TAG	UNP A8EVM5
C	991	LYS	-	EXPRESSION TAG	UNP A8EVM5
C	992	GLY	-	EXPRESSION TAG	UNP A8EVM5
C	993	SER	-	EXPRESSION TAG	UNP A8EVM5
C	994	LEU	-	EXPRESSION TAG	UNP A8EVM5
C	995	VAL	-	EXPRESSION TAG	UNP A8EVM5
C	996	PRO	-	EXPRESSION TAG	UNP A8EVM5
C	997	ARG	-	EXPRESSION TAG	UNP A8EVM5
C	998	GLY	-	EXPRESSION TAG	UNP A8EVM5
C	999	SER	-	EXPRESSION TAG	UNP A8EVM5
C	1000	HIS	-	EXPRESSION TAG	UNP A8EVM5
C	1177	ASP	GLU	CONFLICT	UNP A8EVM5

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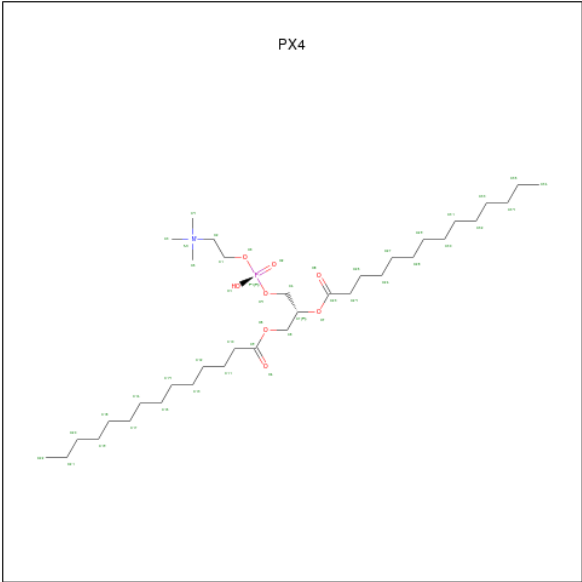
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1178	ASP	SER	CONFLICT	UNP A8EVM5
C	1181	ASP	MET	CONFLICT	UNP A8EVM5
C	1217	CYS	ILE	CONFLICT	UNP A8EVM5
D	983	MET	-	EXPRESSION TAG	UNP A8EVM5
D	984	ASP	-	EXPRESSION TAG	UNP A8EVM5
D	985	TYR	-	EXPRESSION TAG	UNP A8EVM5
D	986	LYS	-	EXPRESSION TAG	UNP A8EVM5
D	987	ASP	-	EXPRESSION TAG	UNP A8EVM5
D	988	ASP	-	EXPRESSION TAG	UNP A8EVM5
D	989	ASP	-	EXPRESSION TAG	UNP A8EVM5
D	990	ASP	-	EXPRESSION TAG	UNP A8EVM5
D	991	LYS	-	EXPRESSION TAG	UNP A8EVM5
D	992	GLY	-	EXPRESSION TAG	UNP A8EVM5
D	993	SER	-	EXPRESSION TAG	UNP A8EVM5
D	994	LEU	-	EXPRESSION TAG	UNP A8EVM5
D	995	VAL	-	EXPRESSION TAG	UNP A8EVM5
D	996	PRO	-	EXPRESSION TAG	UNP A8EVM5
D	997	ARG	-	EXPRESSION TAG	UNP A8EVM5
D	998	GLY	-	EXPRESSION TAG	UNP A8EVM5
D	999	SER	-	EXPRESSION TAG	UNP A8EVM5
D	1000	HIS	-	EXPRESSION TAG	UNP A8EVM5
D	1177	ASP	GLU	CONFLICT	UNP A8EVM5
D	1178	ASP	SER	CONFLICT	UNP A8EVM5
D	1181	ASP	MET	CONFLICT	UNP A8EVM5
D	1217	CYS	ILE	CONFLICT	UNP A8EVM5

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0

- Molecule 3 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
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	A	1	Total	C	O	P	0	0
			21	13	7	1		
3	A	1	Total	C	O	P	0	0
			21	13	7	1		
3	A	1	Total	C			0	0
			6	6				
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C			0	0
			6	6				
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			21	13	7	1		
3	C	1	Total	C			0	0
			6	6				
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			21	13	7	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		

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

- Molecule 4 is water.

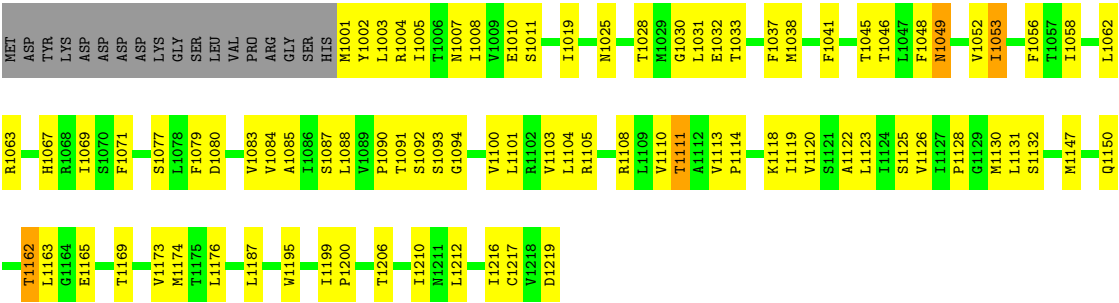
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			1	1		
4	C	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		





● Molecule 1: Ion transport protein

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.44Å 177.53Å 130.78Å 90.00° 132.70° 90.00°	Depositor
Resolution (Å)	35.05 – 3.20 35.03 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (35.05-3.20) 94.7 (35.03-3.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.239 , 0.262 0.240 , 0.259	Depositor DCC
$R_{free}$ test set	2367 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	92.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 51.3	EDS
Estimated twinning fraction	0.448 for k,h,-1/2*h-1/2*k-l 0.437 for -k,-h,-1/2*h+1/2*k-l 0.437 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 46607 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	0.68	0/1849	0.78	0/2517
1	B	0.67	0/1849	0.77	0/2517
1	C	0.68	0/1849	0.76	0/2517
1	D	0.65	0/1849	0.75	0/2517
All	All	0.67	0/7396	0.77	0/10068

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1798	0	1861	53	0
1	B	1798	0	1861	61	0
1	C	1798	0	1861	51	0
1	D	1798	0	1861	55	0
2	A	1	0	0	0	0
3	A	68	0	59	8	0
3	B	26	0	21	0	0
3	C	47	0	40	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	47	0	40	2	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
All	All	7387	0	7604	210	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 210 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1162:THR:HG22	1:D:1165:GLU:H	1.42	0.85
1:C:1162:THR:HG22	1:C:1165:GLU:H	1.43	0.82
1:C:1133:VAL:HG11	1:C:1212:LEU:HD12	1.64	0.80
1:B:1162:THR:HG22	1:B:1165:GLU:H	1.46	0.79
1:C:1114:PRO:O	1:C:1115:GLN:HB2	1.86	0.76

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	217/237 (92%)	200 (92%)	17 (8%)	0	100	100
1	B	217/237 (92%)	201 (93%)	15 (7%)	1 (0%)	38	85
1	C	217/237 (92%)	201 (93%)	12 (6%)	4 (2%)	13	60
1	D	217/237 (92%)	195 (90%)	18 (8%)	4 (2%)	13	60
All	All	868/948 (92%)	797 (92%)	62 (7%)	9 (1%)	22	74

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1091	THR
1	D	1094	GLY
1	D	1091	THR
1	D	1093	SER
1	D	1217	CYS

### 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	202/218 (93%)	188 (93%)	14 (7%)	22	65
1	B	202/218 (93%)	183 (91%)	19 (9%)	13	45
1	C	202/218 (93%)	186 (92%)	16 (8%)	18	58
1	D	202/218 (93%)	187 (93%)	15 (7%)	20	62
All	All	808/872 (93%)	744 (92%)	64 (8%)	18	58

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1163	LEU
1	C	1028	THR
1	D	1132	SER
1	B	1187	LEU
1	B	1218	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	PX4	A	1302	-	9,9,45	0.76	0	12,12,53	7.99	3 (25%)
3	PX4	A	1303	-	19,20,45	1.41	2 (10%)	23,24,53	6.69	6 (26%)
3	PX4	A	1304	-	19,20,45	1.75	3 (15%)	23,24,53	8.74	5 (21%)
3	PX4	A	1305	-	5,5,45	1.95	1 (20%)	4,4,53	0.61	0
3	PX4	A	1306	-	9,9,45	1.04	0	12,12,53	9.65	5 (41%)
3	PX4	B	1301	-	9,9,45	0.96	0	12,12,53	7.30	4 (33%)
3	PX4	B	1302	-	5,5,45	0.92	0	4,4,53	0.96	0
3	PX4	B	1303	-	9,9,45	1.02	0	12,12,53	8.50	7 (58%)
3	PX4	C	1301	-	9,9,45	0.78	0	12,12,53	7.73	4 (33%)
3	PX4	C	1302	-	19,20,45	1.42	2 (10%)	23,24,53	8.06	4 (17%)
3	PX4	C	1303	-	5,5,45	0.85	0	4,4,53	1.04	0
3	PX4	C	1304	-	9,9,45	0.77	0	12,12,53	12.30	6 (50%)
3	PX4	D	1301	-	19,20,45	1.35	1 (5%)	23,24,53	8.42	5 (21%)
3	PX4	D	1302	-	9,9,45	0.88	0	12,12,53	8.02	4 (33%)
3	PX4	D	1303	-	5,5,45	1.45	1 (20%)	4,4,53	1.54	1 (25%)
3	PX4	D	1304	-	9,9,45	0.73	0	12,12,53	10.91	4 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	A	1302	-	-	0/8/8/49	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	A	1303	-	-	0/22/22/49	0/0/0/0
3	PX4	A	1304	-	-	0/22/22/49	0/0/0/0
3	PX4	A	1305	-	-	0/3/3/49	0/0/0/0
3	PX4	A	1306	-	-	0/8/8/49	0/0/0/0
3	PX4	B	1301	-	-	0/8/8/49	0/0/0/0
3	PX4	B	1302	-	-	0/3/3/49	0/0/0/0
3	PX4	B	1303	-	-	0/8/8/49	0/0/0/0
3	PX4	C	1301	-	-	0/8/8/49	0/0/0/0
3	PX4	C	1302	-	-	0/22/22/49	0/0/0/0
3	PX4	C	1303	-	-	0/3/3/49	0/0/0/0
3	PX4	C	1304	-	-	0/8/8/49	0/0/0/0
3	PX4	D	1301	-	-	0/22/22/49	0/0/0/0
3	PX4	D	1302	-	-	0/8/8/49	0/0/0/0
3	PX4	D	1303	-	-	0/3/3/49	0/0/0/0
3	PX4	D	1304	-	-	0/8/8/49	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1304	PX4	O6-C9	5.20	1.38	1.22
3	D	1301	PX4	O6-C9	4.94	1.37	1.22
3	A	1303	PX4	O6-C9	4.75	1.36	1.22
3	C	1302	PX4	O6-C9	4.65	1.36	1.22
3	A	1305	PX4	C31-C32	-4.28	1.53	1.55

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1304	PX4	O7-C7-C8	-33.32	107.09	119.54
3	C	1304	PX4	O7-C7-C6	-33.19	107.14	119.54
3	C	1302	PX4	O7-C7-C8	-30.38	108.19	119.54
3	D	1301	PX4	O7-C7-C8	-30.07	108.31	119.54
3	D	1304	PX4	O7-C7-C8	-27.10	109.42	119.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	219/237 (92%)	-0.12	0 <span>100</span> <span>100</span>	35, 91, 144, 163	0
1	B	219/237 (92%)	-0.12	1 (0%) <span>88</span> <span>46</span>	32, 91, 147, 167	0
1	C	219/237 (92%)	-0.11	1 (0%) <span>88</span> <span>46</span>	37, 93, 145, 169	0
1	D	219/237 (92%)	-0.11	0 <span>100</span> <span>100</span>	35, 93, 147, 163	0
All	All	876/948 (92%)	-0.12	2 (0%) <span>93</span> <span>66</span>	32, 92, 145, 169	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1001	MET	2.1
1	B	1001	MET	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PX4	B	1302	6/46	0.31	2.77	57,61,63,73	0
3	PX4	A	1305	6/46	0.27	2.63	54,55,62,63	0
3	PX4	D	1303	6/46	0.29	2.37	45,49,56,64	0
3	PX4	C	1303	6/46	0.25	1.64	52,54,57,65	0
3	PX4	D	1301	21/46	0.22	0.13	75,83,99,106	0
3	PX4	C	1302	21/46	0.22	0.13	72,85,97,103	0
3	PX4	A	1306	10/46	0.21	-0.20	83,105,123,131	0
3	PX4	A	1303	21/46	0.21	-0.22	65,78,95,100	0
3	PX4	A	1304	21/46	0.20	-0.46	65,78,96,100	0
3	PX4	B	1303	10/46	0.16	-1.00	76,100,118,136	0
3	PX4	D	1304	10/46	0.15	-1.09	84,99,120,129	0
3	PX4	C	1301	10/46	0.20	-1.10	60,77,128,135	0
3	PX4	C	1304	10/46	0.14	-1.14	72,95,129,133	0
3	PX4	D	1302	10/46	0.21	-1.26	71,88,129,143	0
3	PX4	B	1301	10/46	0.17	-1.86	63,88,127,133	0
2	MN	A	1301	1/1	0.15	-2.19	100,100,100,100	0
3	PX4	A	1302	10/46	0.15	-2.66	70,95,136,137	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.