Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:50 PM GMT

PDB ID	:	4MVZ
Title	:	Structural Basis for Ca2+ Selectivity of a Voltage-gated Calcium Channel
Authors	:	Tang, L.; Gamal El-Din, T.M.; Payandeh, J.; Martinez, G.Q.; Heard, T.M.; Scheuer, T.; Zheng, N.; Catterall, W.A.
Deposited on	:	2013-09-24
Resolution	:	3.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

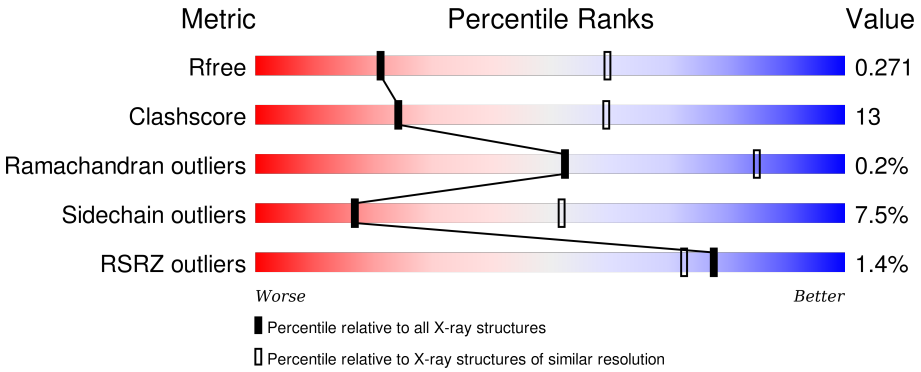
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	57% 33% • 8%
1	B	237	% 61% 29% • 8%
1	C	237	2% 59% 29% • 8%
1	D	237	2% 60% 30% • 8%

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
3	PX4	C	1304	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7386 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
			1799	1225	268	295	11			
1	B	219	Total	C	N	O	S	0	0	0
			1799	1225	268	295	11			
1	C	219	Total	C	N	O	S	0	0	0
			1799	1225	268	295	11			
1	D	219	Total	C	N	O	S	0	0	0
			1799	1225	268	295	11			

There are 84 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	1178	ASP	SER	CONFLICT	UNP A8EVM5
A	1181	ASP	MET	CONFLICT	UNP A8EVM5
A	1217	CYS	ILE	CONFLICT	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	1178	ASP	SER	CONFLICT	UNP A8EVM5
C	1181	ASP	MET	CONFLICT	UNP A8EVM5
C	1217	CYS	ILE	CONFLICT	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1178	ASP	SER	CONFLICT	UNP A8EVM5
D	1181	ASP	MET	CONFLICT	UNP A8EVM5
D	1217	CYS	ILE	CONFLICT	UNP A8EVM5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).

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

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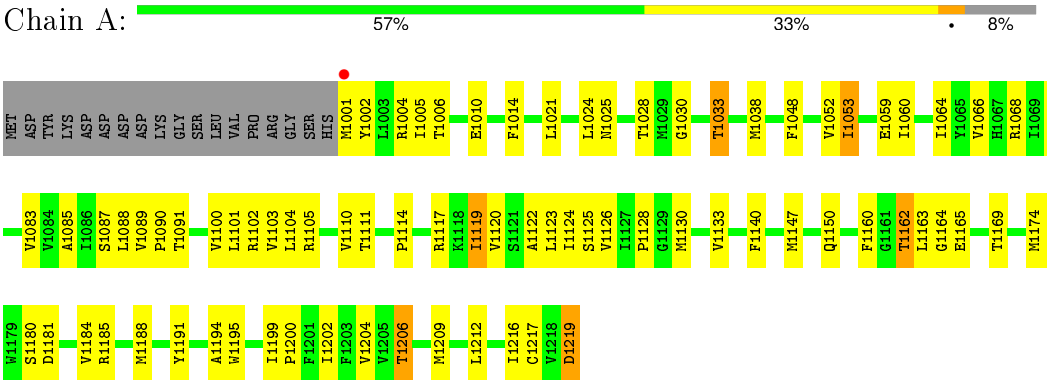
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C 6 6	0	0
3	D	1	Total C O P 10 3 6 1	0	0

3 Residue-property plots (i)

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

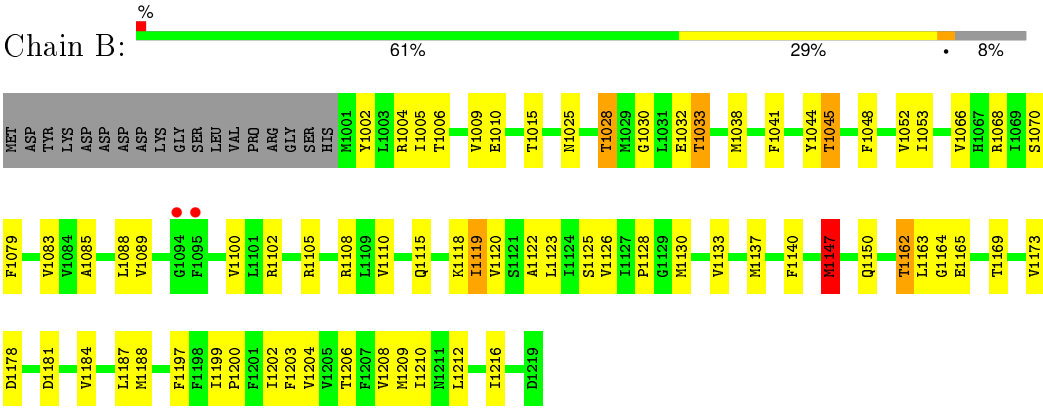
- Molecule 1: Ion transport protein

Chain A:



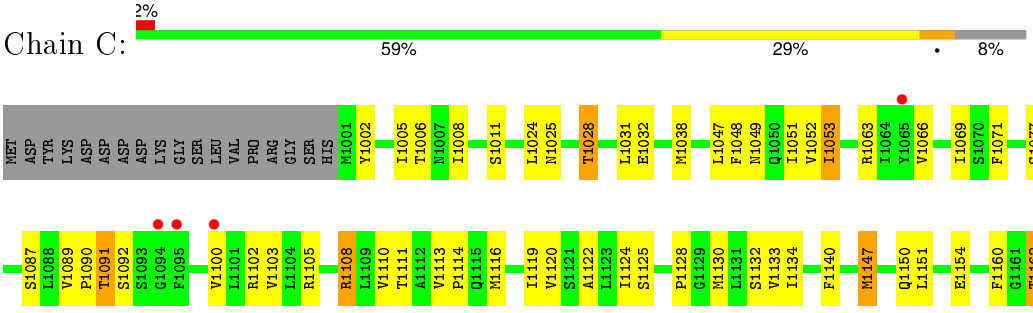
- Molecule 1: Ion transport protein

Chain B:



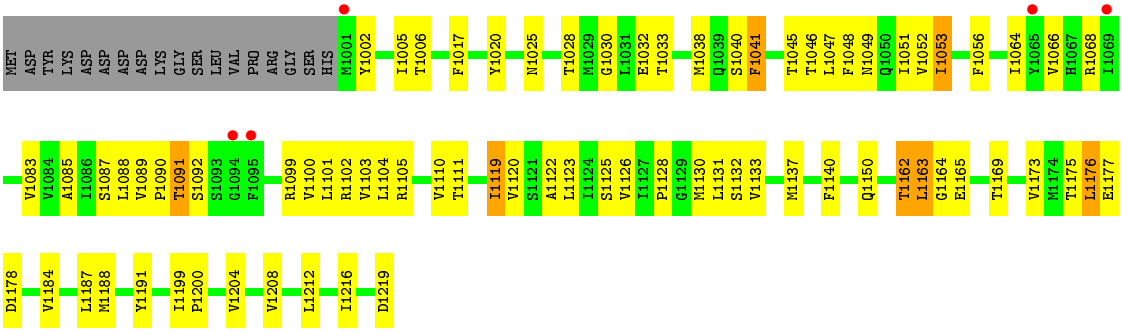
- Molecule 1: Ion transport protein

Chain C:



- Molecule 1: Ion transport protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	177.53Å 177.82Å 131.35Å 90.00° 132.57° 90.00°	Depositor
Resolution (Å)	29.90 – 3.30 29.88 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (29.90-3.30) 95.1 (29.88-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.242 , 0.280 0.240 , 0.271	Depositor DCC
R_{free} test set	2180 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	92.4	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 75.7	EDS
Estimated twinning fraction	0.438 for k,h,-1/2*h-1/2*k-l 0.428 for -k,-h,-1/2*h+1/2*k-l 0.428 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 43001 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7386	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 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, 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	0.74	0/1850	0.81	1/2518 (0.0%)
1	B	0.74	0/1850	0.82	1/2518 (0.0%)
1	C	0.70	0/1850	0.79	2/2518 (0.1%)
1	D	0.71	0/1850	0.79	1/2518 (0.0%)
All	All	0.72	0/7400	0.81	5/10072 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1147	MET	CG-SD-CE	5.39	108.82	100.20
1	D	1176	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	A	1174	MET	CG-SD-CE	-5.29	91.73	100.20
1	C	1151	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	C	1185	ARG	NE-CZ-NH2	-5.20	117.70	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1799	0	1863	56	0
1	B	1799	0	1863	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1799	0	1863	54	0
1	D	1799	0	1863	55	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	68	0	59	10	0
3	B	26	0	21	0	0
3	C	47	0	40	0	0
3	D	47	0	40	3	0
All	All	7386	0	7612	195	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 13.

All (195) 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:C:1162:THR:HG22	1:C:1165:GLU:H	1.39	0.86
1:A:1162:THR:HG22	1:A:1165:GLU:H	1.46	0.80
1:B:1162:THR:HG22	1:B:1165:GLU:H	1.51	0.74
1:C:1175:THR:HB	1:D:1176:LEU:HD13	1.67	0.74
1:D:1162:THR:HG22	1:D:1165:GLU:H	1.53	0.73
1:B:1176:LEU:HD13	1:D:1175:THR:HB	1.73	0.69
1:C:1091:THR:O	1:C:1092:SER:OG	2.10	0.68
1:B:1130:MET:SD	1:B:1216:ILE:HD11	2.33	0.68
1:A:1164:GLY:CA	3:A:1304:PX4:H14	2.25	0.67
1:B:1126:VAL:HG11	1:B:1216:ILE:HG23	1.78	0.64
1:D:1091:THR:O	1:D:1099:ARG:NH2	2.30	0.64
1:A:1123:LEU:HD22	1:C:1211:ASN:HD22	1.62	0.64
1:A:1083:VAL:HG11	1:A:1105:ARG:HA	1.79	0.64
1:C:1083:VAL:HG11	1:C:1105:ARG:HA	1.81	0.62
1:A:1178:ASP:HA	1:B:1177:GLU:OE2	2.00	0.61
1:A:1176:LEU:HD13	1:B:1175:THR:HB	1.83	0.61
1:C:1006:THR:HG23	1:C:1066:VAL:HG13	1.82	0.61
1:D:1085:ALA:HA	1:D:1088:LEU:HD12	1.84	0.58
3:A:1303:PX4:O6	3:A:1303:PX4:H24	2.03	0.58
1:B:1006:THR:HG23	1:B:1066:VAL:HG13	1.86	0.58
1:B:1071:PHE:CE1	1:B:1077:SER:HB3	2.39	0.58
1:A:1133:VAL:HG11	1:A:1212:LEU:HD12	1.86	0.57
1:B:1125:SER:O	1:B:1128:PRO:HD2	2.04	0.57
1:C:1100:VAL:O	1:C:1103:VAL:HG12	2.04	0.57
3:A:1305:PX4:H63	1:C:1206:THR:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1089:VAL:HG13	1:D:1090:PRO:HD2	1.87	0.57
1:D:1083:VAL:HG11	1:D:1105:ARG:HA	1.87	0.57
1:A:1175:THR:HB	1:C:1176:LEU:HD13	1.87	0.56
1:A:1110:VAL:HG11	1:A:1120:VAL:HG21	1.87	0.56
1:A:1006:THR:HG23	1:A:1066:VAL:HG13	1.89	0.55
3:A:1303:PX4:H15	1:B:1164:GLY:CA	2.37	0.55
1:D:1128:PRO:HA	1:D:1131:LEU:HD12	1.88	0.55
1:A:1195:TRP:CH2	3:A:1303:PX4:H17	2.41	0.55
1:B:1133:VAL:HG11	1:B:1212:LEU:HD12	1.89	0.55
1:A:1085:ALA:HA	1:A:1088:LEU:HD12	1.89	0.55
1:C:1089:VAL:HG13	1:C:1090:PRO:HD2	1.88	0.55
1:A:1033:THR:HG21	1:C:1163:LEU:HB2	1.89	0.55
1:C:1188:MET:HA	1:C:1191:TYR:O	2.07	0.54
1:A:1217:CYS:SG	1:C:1214:VAL:HG22	2.46	0.54
1:C:1110:VAL:HG11	1:C:1120:VAL:HG21	1.90	0.54
1:B:1089:VAL:O	1:B:1102:ARG:NH2	2.41	0.54
1:D:1110:VAL:HG11	1:D:1120:VAL:HG21	1.90	0.54
1:C:1133:VAL:HG11	1:C:1212:LEU:HD12	1.91	0.53
1:A:1125:SER:O	1:A:1128:PRO:HD2	2.09	0.53
1:A:1130:MET:SD	1:A:1216:ILE:HD11	2.48	0.53
1:D:1091:THR:OG1	1:D:1099:ARG:NH2	2.40	0.53
1:B:1083:VAL:HG11	1:B:1105:ARG:HA	1.90	0.53
1:B:1169:THR:O	1:B:1173:VAL:HG23	2.09	0.53
1:B:1181:ASP:OD2	1:D:1178:ASP:OD2	2.28	0.52
1:D:1030:GLY:O	1:D:1033:THR:HB	2.10	0.52
1:C:1025:ASN:OD1	1:C:1105:ARG:HD2	2.10	0.52
1:A:1110:VAL:CG1	1:A:1120:VAL:HG21	2.40	0.52
1:D:1122:ALA:O	1:D:1125:SER:OG	2.28	0.51
1:A:1140:PHE:CZ	1:A:1204:VAL:HG11	2.45	0.51
1:A:1103:VAL:HG11	1:C:1147:MET:HG3	1.92	0.51
1:A:1195:TRP:CZ2	3:A:1303:PX4:H17	2.46	0.51
1:D:1188:MET:HA	1:D:1191:TYR:O	2.10	0.51
1:B:1123:LEU:O	1:B:1126:VAL:HG23	2.10	0.51
1:D:1164:GLY:CA	3:D:1302:PX4:H14	2.42	0.50
1:A:1119:ILE:HD11	1:C:1133:VAL:HG23	1.93	0.50
1:D:1041:PHE:CD1	1:D:1041:PHE:N	2.80	0.50
1:D:1164:GLY:HA3	3:D:1302:PX4:H14	1.93	0.50
1:A:1133:VAL:HG23	1:B:1119:ILE:HD11	1.94	0.50
1:A:1030:GLY:O	1:A:1033:THR:HB	2.10	0.50
1:B:1150:GLN:OE1	1:D:1100:VAL:HG22	2.11	0.50
1:A:1048:PHE:O	1:A:1052:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:SER:HB3	1:B:1177:GLU:OE1	2.11	0.50
1:A:1060:ILE:O	1:A:1064:ILE:HG13	2.11	0.50
1:A:1133:VAL:CG1	1:A:1212:LEU:HD12	2.42	0.49
1:A:1188:MET:HA	1:A:1191:TYR:O	2.11	0.49
1:D:1110:VAL:CG1	1:D:1120:VAL:HG21	2.42	0.49
1:A:1025:ASN:OD1	1:A:1105:ARG:HD2	2.13	0.48
1:C:1089:VAL:O	1:C:1102:ARG:NH2	2.46	0.48
1:A:1100:VAL:HG22	1:C:1150:GLN:HG3	1.95	0.48
1:C:1206:THR:O	1:C:1210:ILE:HG13	2.13	0.48
1:B:1085:ALA:HA	1:B:1088:LEU:HD12	1.94	0.48
1:C:1063:ARG:HH12	1:C:1108:ARG:HH22	1.61	0.48
1:C:1110:VAL:CG1	1:C:1120:VAL:HG21	2.43	0.48
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.96	0.47
1:B:1110:VAL:CG1	1:B:1120:VAL:HG21	2.44	0.47
1:C:1125:SER:O	1:C:1128:PRO:HD2	2.14	0.47
1:C:1048:PHE:O	1:C:1052:VAL:HG23	2.13	0.47
1:D:1032:GLU:HG2	1:D:1045:THR:HG21	1.95	0.47
1:C:1202:ILE:O	1:C:1206:THR:OG1	2.27	0.47
1:D:1133:VAL:CG1	1:D:1212:LEU:HD12	2.43	0.47
1:A:1001:MET:HG3	1:A:1004:ARG:HD3	1.97	0.47
1:C:1053:ILE:HD11	1:C:1087:SER:HB2	1.95	0.47
1:C:1140:PHE:CZ	1:C:1204:VAL:HG11	2.49	0.47
1:D:1052:VAL:O	1:D:1056:PHE:HD1	1.97	0.47
1:B:1184:VAL:O	1:B:1188:MET:HG3	2.13	0.47
1:C:1162:THR:HB	1:C:1165:GLU:OE2	2.15	0.47
1:C:1185:ARG:HB2	1:C:1186:PRO:HD3	1.97	0.47
1:D:1101:LEU:HD22	1:D:1104:LEU:HD11	1.95	0.47
1:D:1128:PRO:HA	1:D:1131:LEU:CD1	2.44	0.47
1:A:1089:VAL:O	1:A:1102:ARG:NH2	2.48	0.47
1:B:1032:GLU:HG2	1:B:1045:THR:HG21	1.97	0.46
1:C:1071:PHE:CE1	1:C:1077:SER:HB3	2.50	0.46
1:C:1089:VAL:CG1	1:C:1090:PRO:HD2	2.45	0.46
1:C:1038:MET:HE2	1:C:1038:MET:HA	1.97	0.46
1:A:1181:ASP:OD2	1:B:1178:ASP:OD2	2.34	0.46
1:B:1048:PHE:O	1:B:1052:VAL:HG23	2.15	0.46
1:D:1199:ILE:HB	1:D:1200:PRO:HD3	1.96	0.46
1:D:1130:MET:SD	1:D:1216:ILE:HD11	2.56	0.46
1:B:1002:TYR:O	1:B:1005:ILE:HG12	2.15	0.46
1:A:1219:ASP:N	1:A:1219:ASP:OD1	2.49	0.46
1:C:1100:VAL:HG22	1:D:1150:GLN:HG3	1.97	0.46
1:B:1140:PHE:CZ	1:B:1204:VAL:HG11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:GLY:HA2	3:A:1304:PX4:H14	1.96	0.46
1:D:1133:VAL:HG11	1:D:1212:LEU:HD12	1.98	0.46
1:A:1038:MET:HE2	1:A:1038:MET:HA	1.97	0.46
1:C:1199:ILE:HB	1:C:1200:PRO:HD3	1.98	0.46
3:A:1303:PX4:H15	1:B:1164:GLY:HA3	1.97	0.45
1:A:1164:GLY:HA3	3:A:1304:PX4:H14	1.98	0.45
1:A:1114:PRO:HA	1:A:1117:ARG:HB2	1.98	0.45
1:B:1079:PHE:CZ	1:B:1083:VAL:HG21	2.52	0.45
1:C:1122:ALA:O	1:C:1125:SER:OG	2.31	0.45
1:A:1160:PHE:CZ	1:A:1169:THR:HG21	2.51	0.45
1:B:1216:ILE:HG22	1:B:1216:ILE:O	2.16	0.45
1:D:1032:GLU:HA	1:D:1038:MET:HE3	1.97	0.45
1:D:1006:THR:HG23	1:D:1066:VAL:HG13	1.97	0.45
1:B:1202:ILE:O	1:B:1206:THR:OG1	2.28	0.45
1:D:1002:TYR:O	1:D:1005:ILE:HG12	2.17	0.45
1:B:1041:PHE:O	1:B:1044:TYR:HB2	2.18	0.45
1:D:1089:VAL:O	1:D:1102:ARG:NH2	2.50	0.44
1:D:1017:PHE:O	1:D:1020:TYR:HB3	2.16	0.44
1:D:1090:PRO:C	1:D:1092:SER:H	2.21	0.44
1:A:1100:VAL:O	1:A:1103:VAL:HG12	2.18	0.44
1:B:1178:ASP:HA	1:D:1177:GLU:OE2	2.16	0.44
1:D:1053:ILE:HD11	1:D:1087:SER:HB2	2.00	0.44
1:A:1053:ILE:HD11	1:A:1087:SER:HB2	1.99	0.44
1:A:1202:ILE:O	1:A:1206:THR:OG1	2.24	0.43
1:D:1091:THR:HB	1:D:1102:ARG:HH12	1.83	0.43
1:D:1125:SER:O	1:D:1128:PRO:HD2	2.18	0.43
1:B:1206:THR:O	1:B:1210:ILE:HG13	2.18	0.43
1:D:1123:LEU:O	1:D:1126:VAL:HG23	2.17	0.43
1:C:1028:THR:O	1:C:1032:GLU:HG3	2.18	0.43
1:D:1184:VAL:HG12	1:D:1188:MET:HE2	2.00	0.43
1:B:1028:THR:O	1:B:1032:GLU:HG3	2.18	0.43
1:B:1133:VAL:HG23	1:D:1119:ILE:HD11	2.00	0.43
1:D:1025:ASN:OD1	1:D:1105:ARG:HD2	2.19	0.43
1:A:1184:VAL:O	1:A:1188:MET:HG3	2.18	0.43
1:D:1140:PHE:CZ	1:D:1204:VAL:HG11	2.53	0.43
1:A:1120:VAL:O	1:A:1124:ILE:HG13	2.19	0.43
1:D:1169:THR:O	1:D:1173:VAL:HG23	2.19	0.42
1:C:1080:ASP:OD1	1:C:1111:THR:HG21	2.20	0.42
1:C:1169:THR:O	1:C:1173:VAL:HG23	2.19	0.42
1:A:1101:LEU:HD22	1:A:1104:LEU:HD11	2.00	0.42
1:C:1133:VAL:CG1	1:C:1212:LEU:HD12	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1122:ALA:O	1:A:1125:SER:OG	2.37	0.42
1:D:1048:PHE:O	1:D:1052:VAL:HG23	2.19	0.42
1:A:1123:LEU:HD22	1:C:1211:ASN:ND2	2.33	0.42
1:A:1185:ARG:HA	1:A:1188:MET:HE3	2.01	0.42
1:C:1031:LEU:HD23	1:C:1031:LEU:HA	1.89	0.42
1:B:1212:LEU:O	1:B:1216:ILE:HG13	2.19	0.42
1:B:1122:ALA:O	1:B:1125:SER:OG	2.38	0.42
1:B:1199:ILE:HB	1:B:1200:PRO:HD3	2.01	0.42
1:D:1047:LEU:O	1:D:1051:ILE:HG13	2.20	0.42
1:C:1160:PHE:CZ	1:C:1169:THR:HG21	2.55	0.42
1:D:1137:MET:SD	1:D:1208:VAL:HG11	2.60	0.42
1:A:1014:PHE:CZ	1:A:1059:GLU:HG3	2.56	0.41
1:A:1071:PHE:CE1	1:A:1077:SER:HB3	2.55	0.41
1:D:1040:SER:C	1:D:1041:PHE:HD1	2.23	0.41
1:D:1038:MET:HE2	1:D:1038:MET:HA	2.03	0.41
1:C:1184:VAL:HG12	1:C:1188:MET:HE2	2.02	0.41
1:B:1150:GLN:HG3	1:D:1100:VAL:HG22	2.02	0.41
1:B:1137:MET:SD	1:B:1208:VAL:HG11	2.60	0.41
1:C:1130:MET:HE3	1:C:1134:ILE:HD11	2.02	0.41
1:C:1032:GLU:HA	1:C:1038:MET:HE3	2.03	0.41
1:A:1126:VAL:HG11	1:A:1216:ILE:HG23	2.03	0.41
1:B:1203:PHE:HZ	3:D:1302:PX4:H31	1.86	0.41
1:B:1147:MET:HB3	1:B:1197:PHE:HE2	1.85	0.41
1:D:1150:GLN:HE21	1:D:1150:GLN:HB3	1.58	0.41
1:B:1025:ASN:OD1	1:B:1105:ARG:HD2	2.21	0.41
1:B:1032:GLU:HA	1:B:1038:MET:HE3	2.02	0.41
1:C:1069:ILE:O	1:C:1069:ILE:HG12	2.21	0.41
1:C:1002:TYR:O	1:C:1005:ILE:HG12	2.20	0.41
1:A:1150:GLN:HG3	1:B:1100:VAL:HG22	2.02	0.41
1:B:1133:VAL:CG1	1:B:1212:LEU:HD12	2.51	0.41
1:D:1089:VAL:CG1	1:D:1090:PRO:HD2	2.50	0.41
1:B:1009:VAL:HG21	1:B:1066:VAL:HG21	2.02	0.41
1:C:1120:VAL:O	1:C:1124:ILE:HG13	2.20	0.41
1:B:1038:MET:HE2	1:B:1038:MET:HA	2.03	0.41
1:D:1163:LEU:HD23	1:D:1163:LEU:HA	1.92	0.41
1:B:1030:GLY:O	1:B:1033:THR:HB	2.20	0.41
1:D:1064:ILE:O	1:D:1068:ARG:N	2.44	0.41
1:A:1083:VAL:CG1	1:A:1105:ARG:HA	2.47	0.41
1:C:1219:ASP:OD1	1:C:1219:ASP:N	2.54	0.41
1:A:1021:LEU:HA	1:A:1021:LEU:HD23	1.88	0.40
1:D:1100:VAL:O	1:D:1103:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1113:VAL:HA	1:C:1114:PRO:HD3	1.87	0.40
1:C:1047:LEU:O	1:C:1051:ILE:HG13	2.22	0.40
3:A:1304:PX4:H17	3:A:1304:PX4:H20	1.77	0.40
1:C:1008:ILE:O	1:C:1011:SER:OG	2.20	0.40
1:C:1116:MET:O	1:C:1119:ILE:HG22	2.22	0.40
1:A:1002:TYR:O	1:A:1005:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	217/237 (92%)	200 (92%)	15 (7%)	2 (1%)	21 60
1	B	217/237 (92%)	201 (93%)	16 (7%)	0	100 100
1	C	217/237 (92%)	200 (92%)	17 (8%)	0	100 100
1	D	217/237 (92%)	199 (92%)	18 (8%)	0	100 100
All	All	868/948 (92%)	800 (92%)	66 (8%)	2 (0%)	52 85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1194	ALA
1	A	1090	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/218 (93%)	185 (92%)	17 (8%)	14	46
1	B	202/218 (93%)	184 (91%)	18 (9%)	12	43
1	C	202/218 (93%)	189 (94%)	13 (6%)	22	60
1	D	202/218 (93%)	189 (94%)	13 (6%)	22	60
All	All	808/872 (93%)	747 (92%)	61 (8%)	17	52

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1010	GLU
1	A	1024	LEU
1	A	1028	THR
1	A	1033	THR
1	A	1053	ILE
1	A	1068	ARG
1	A	1070	SER
1	A	1091	THR
1	A	1111	THR
1	A	1119	ILE
1	A	1147	MET
1	A	1162	THR
1	A	1163	LEU
1	A	1177	GLU
1	A	1206	THR
1	A	1209	MET
1	A	1219	ASP
1	B	1004	ARG
1	B	1010	GLU
1	B	1015	THR
1	B	1028	THR
1	B	1033	THR
1	B	1045	THR
1	B	1053	ILE
1	B	1068	ARG
1	B	1070	SER
1	B	1108	ARG
1	B	1115	GLN
1	B	1118	LYS
1	B	1119	ILE

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Mol	Chain	Res	Type
1	B	1147	MET
1	B	1162	THR
1	B	1163	LEU
1	B	1187	LEU
1	B	1209	MET
1	C	1024	LEU
1	C	1028	THR
1	C	1049	ASN
1	C	1053	ILE
1	C	1091	THR
1	C	1108	ARG
1	C	1132	SER
1	C	1147	MET
1	C	1154	GLU
1	C	1162	THR
1	C	1163	LEU
1	C	1177	GLU
1	C	1214	VAL
1	D	1028	THR
1	D	1041	PHE
1	D	1046	THR
1	D	1049	ASN
1	D	1053	ILE
1	D	1091	THR
1	D	1111	THR
1	D	1119	ILE
1	D	1132	SER
1	D	1162	THR
1	D	1163	LEU
1	D	1187	LEU
1	D	1219	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1150	GLN
1	B	1115	GLN
1	C	1211	ASN
1	D	1211	ASN

5.3.3 RNA

There are no RNA molecules 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 18 ligands modelled in this entry, 2 are 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	0.61	0	10,12,53	1.19	1 (10%)
3	PX4	A	1303	-	20,20,45	1.57	3 (15%)	21,24,53	1.43	2 (9%)
3	PX4	A	1304	-	20,20,45	1.45	3 (15%)	21,24,53	1.81	2 (9%)
3	PX4	A	1305	-	5,5,45	0.36	0	4,4,53	0.21	0
3	PX4	A	1306	-	9,9,45	0.56	0	10,12,53	1.22	2 (20%)
3	PX4	B	1301	-	9,9,45	0.50	0	10,12,53	1.10	0
3	PX4	B	1302	-	5,5,45	0.40	0	4,4,53	0.23	0
3	PX4	B	1303	-	9,9,45	0.59	0	10,12,53	0.98	0
3	PX4	C	1302	-	9,9,45	0.58	0	10,12,53	0.94	0
3	PX4	C	1303	-	20,20,45	1.49	1 (5%)	21,24,53	1.78	2 (9%)
3	PX4	C	1304	-	5,5,45	0.32	0	4,4,53	0.23	0
3	PX4	C	1305	-	9,9,45	0.55	0	10,12,53	1.23	1 (10%)
3	PX4	D	1301	-	9,9,45	0.49	0	10,12,53	0.81	0
3	PX4	D	1302	-	20,20,45	1.49	2 (10%)	21,24,53	1.74	2 (9%)
3	PX4	D	1303	-	5,5,45	0.35	0	4,4,53	0.23	0
3	PX4	D	1304	-	9,9,45	0.58	0	10,12,53	1.08	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
3	PX4	A	1302	-	-	0/8/8/49	0/0/0/0
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	1302	-	-	0/8/8/49	0/0/0/0
3	PX4	C	1303	-	-	0/22/22/49	0/0/0/0
3	PX4	C	1304	-	-	0/3/3/49	0/0/0/0
3	PX4	C	1305	-	-	0/8/8/49	0/0/0/0
3	PX4	D	1301	-	-	0/8/8/49	0/0/0/0
3	PX4	D	1302	-	-	0/22/22/49	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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1304	PX4	O5-C8	-2.61	1.39	1.45
3	A	1303	PX4	O5-C8	-2.30	1.40	1.45
3	A	1304	PX4	O5-C9	2.10	1.39	1.33
3	A	1303	PX4	O5-C9	2.18	1.39	1.33
3	D	1302	PX4	O5-C9	2.45	1.40	1.33
3	A	1304	PX4	O6-C9	5.14	1.38	1.22
3	D	1302	PX4	O6-C9	5.61	1.39	1.22
3	C	1303	PX4	O6-C9	5.78	1.39	1.22
3	A	1303	PX4	O6-C9	5.86	1.40	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1303	PX4	O5-C9-O6	-6.87	105.76	123.49
3	A	1304	PX4	O5-C9-O6	-6.67	106.28	123.49
3	D	1302	PX4	O5-C9-O6	-6.23	107.41	123.49
3	A	1303	PX4	O5-C9-O6	-4.90	110.85	123.49
3	A	1304	PX4	O6-C9-C10	-4.38	106.20	123.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1302	PX4	O6-C9-C10	-4.24	106.77	123.72
3	A	1303	PX4	O6-C9-C10	-3.88	108.20	123.72
3	C	1303	PX4	O6-C9-C10	-3.49	109.75	123.72
3	A	1306	PX4	O4-P1-O2	2.03	112.31	107.14
3	A	1302	PX4	O4-P1-O2	2.34	113.11	107.14
3	A	1306	PX4	O3-P1-O4	2.71	114.38	106.56
3	C	1305	PX4	O1-P1-O4	2.92	114.96	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1303	PX4	5	0
3	A	1304	PX4	4	0
3	A	1305	PX4	1	0
3	D	1302	PX4	3	0

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	219/237 (92%)	0.21	1 (0%)	91	90	36, 93, 141, 179	0
1	B	219/237 (92%)	0.21	2 (0%)	85	82	34, 92, 147, 178	0
1	C	219/237 (92%)	0.30	4 (1%)	71	65	39, 95, 148, 197	0
1	D	219/237 (92%)	0.22	5 (2%)	64	57	39, 93, 142, 190	0
All	All	876/948 (92%)	0.23	12 (1%)	78	73	34, 94, 147, 197	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1065	TYR	4.3
1	C	1095	PHE	4.0
1	D	1065	TYR	3.1
1	D	1094	GLY	2.9
1	D	1095	PHE	2.7
1	B	1095	PHE	2.6
1	B	1094	GLY	2.5
1	D	1069	ILE	2.5
1	C	1100	VAL	2.4
1	D	1001	MET	2.1
1	A	1001	MET	2.1
1	C	1094	GLY	2.1

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PX4	C	1304	6/46	0.79	0.34	2.89	57,63,64,65	0
3	PX4	A	1305	6/46	0.78	0.33	2.00	61,64,68,69	0
3	PX4	D	1303	6/46	0.87	0.30	0.74	59,65,69,71	0
3	PX4	C	1303	21/46	0.80	0.27	0.56	94,120,140,147	0
3	PX4	B	1302	6/46	0.89	0.29	0.36	58,62,66,71	0
3	PX4	D	1301	10/46	0.74	0.31	0.28	89,115,141,145	0
3	PX4	A	1304	21/46	0.86	0.26	-0.12	88,100,124,130	0
3	PX4	C	1302	10/46	0.61	0.28	-0.18	86,112,147,148	0
3	PX4	C	1305	10/46	0.75	0.20	-0.48	93,125,132,134	0
3	PX4	A	1303	21/46	0.80	0.24	-0.55	86,105,126,130	0
3	PX4	D	1304	10/46	0.79	0.18	-0.60	95,119,136,141	0
3	PX4	D	1302	21/46	0.84	0.23	-0.61	98,115,126,130	0
3	PX4	B	1301	10/46	0.69	0.23	-0.93	81,107,155,162	0
2	CA	C	1301	1/1	0.81	0.19	-1.10	184,184,184,184	0
3	PX4	B	1303	10/46	0.80	0.17	-1.12	83,116,134,138	0
3	PX4	A	1306	10/46	0.82	0.17	-1.14	83,119,129,145	0
3	PX4	A	1302	10/46	0.72	0.19	-1.64	71,100,129,137	0
2	CA	A	1301	1/1	0.95	0.45	-	134,134,134,134	0

6.5 Other polymers (i)

There are no such residues in this entry.