



# Full wwPDB X-ray Structure Validation Report

Nov 6, 2014 – 08:17 AM EST

PDB ID : 4MS2  
Title : Structural basis of Ca<sup>2+</sup> 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 : 2013-09-18  
Resolution : 2.75 Å(reported)

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

---

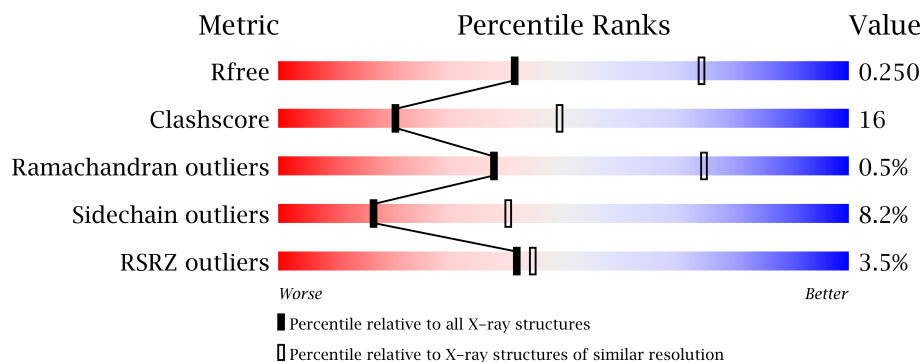
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.75 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	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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
2	PX4	A	1301	-	X
2	PX4	A	1305	-	X
2	PX4	A	1307	-	X
2	PX4	B	1301	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
2	PX4	B	1304	-	X
2	PX4	B	1305	-	X
2	PX4	B	1306	-	X
2	PX4	C	1301	-	X
2	PX4	C	1302	-	X
2	PX4	C	1304	-	X
2	PX4	C	1305	-	X
2	PX4	D	1301	-	X
2	PX4	D	1305	-	X
3	CA	A	1303	-	X
3	CA	A	1304	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7889 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	269	294	11			
1	B	219	Total	C	N	O	S	0	0	0
			1798	1224	269	294	11			
1	C	219	Total	C	N	O	S	0	0	0
			1798	1224	269	294	11			
1	D	219	Total	C	N	O	S	0	0	0
			1798	1224	269	294	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	ASN	MET	CONFLICT	UNP A8EVM5

*Continued on next page...*

*Continued from previous page...*

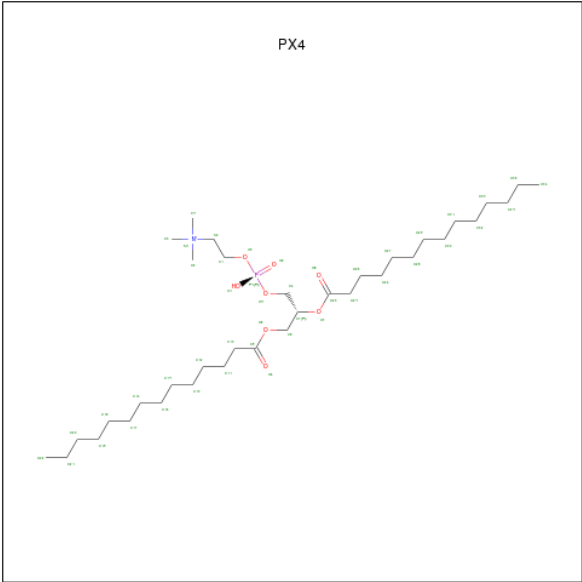
Chain	Residue	Modelled	Actual	Comment	Reference
A	1217	CYS	ILE	CONFLICT	UNP A8EVM5
B	983	MET	-	EXPRESSION TAG	UNP A8EVM5
B	984	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	985	TYR	-	EXPRESSION TAG	UNP A8EVM5
B	986	LYS	-	EXPRESSION TAG	UNP A8EVM5
B	987	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	988	ASP	-	EXPRESSION TAG	UNP 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	ASN	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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	1178	ASP	SER	CONFLICT	UNP A8EVM5
C	1181	ASN	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	ASN	MET	CONFLICT	UNP A8EVM5
D	1217	CYS	ILE	CONFLICT	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 21	C 13	O 7	P 1	0	0	
2	A	1	Total 41	C 32	O 8	P 1	0	0	
2	A	1	Total 41	C 31	N 1	O 8 P 1	0	0	
2	A	1	Total 46	C 36	N 1	O 8 P 1	0	0	
2	B	1	Total 21	C 13	O 7	P 1	0	0	
2	B	1	Total 41	C 32	O 8	P 1	0	0	
2	B	1	Total 40	C 30	N 1	O 8 P 1	0	0	
2	B	1	Total 46	C 36	N 1	O 8 P 1	0	0	
2	B	1	Total 14		C 14		0	0	
2	B	1	Total 14		C 14		0	0	
2	C	1	Total 21	C 13	O 7	P 1	0	0	
2	C	1	Total 41	C 32	O 8	P 1	0	0	
2	C	1	Total 43	C 33	N 1	O 8 P 1	0	0	
2	C	1	Total 42	C 32	N 1	O 8 P 1	0	0	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 46 36 1 8 1	0	0
2	C	1	Total C 14 14	0	0
2	D	1	Total C O P 21 13 7 1	0	0
2	D	1	Total C O P 41 32 8 1	0	0
2	D	1	Total C N O P 46 36 1 8 1	0	0
2	D	1	Total C 14 14	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0
3	D	2	Total Ca 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	B	8	Total O 8 8	0	0
4	C	9	Total O 9 9	0	0
4	D	11	Total O 11 11	0	0

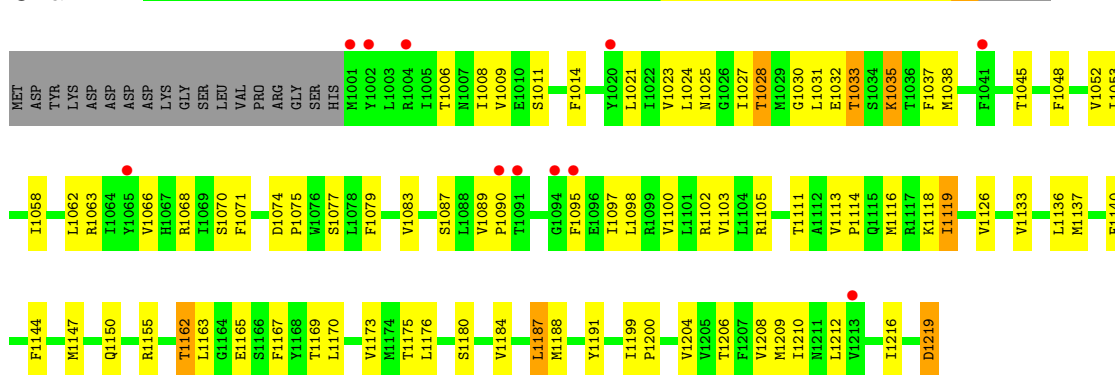


### 3 Residue-property plots

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.

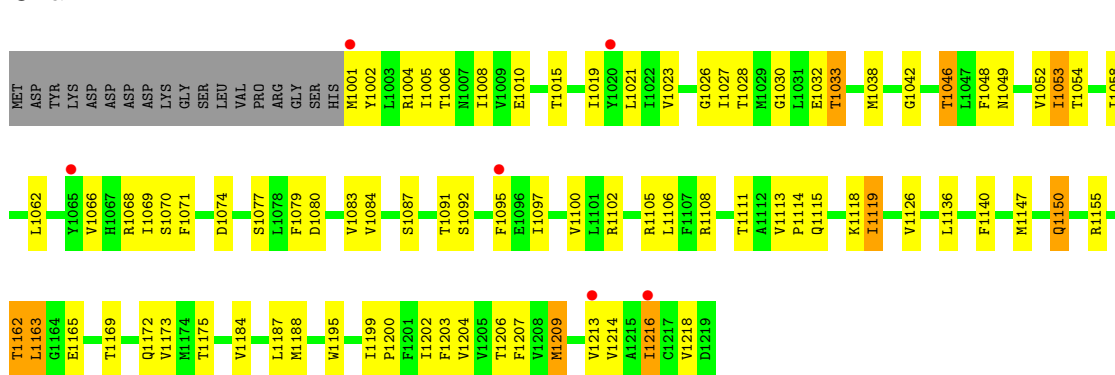
- Molecule 1: Ion transport protein

Chain A:



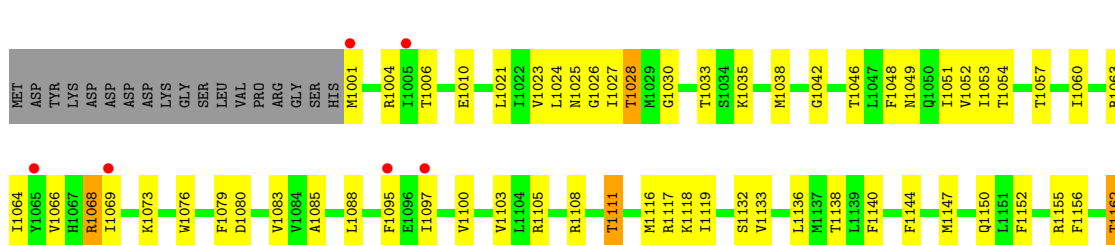
- Molecule 1: Ion transport protein

Chain B:



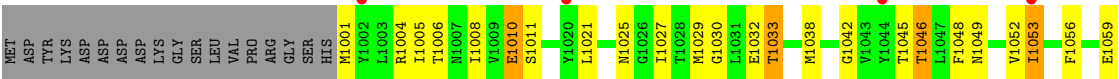
- Molecule 1: Ion transport protein

Chain C:





● Molecule 1: Ion transport protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.79Å 177.54Å 131.14Å 90.00° 132.69° 90.00°	Depositor
Resolution (Å)	40.37 – 2.75 40.37 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.0 (40.37-2.75) 93.8 (40.37-2.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.232 , 0.255 0.225 , 0.250	Depositor DCC
$R_{free}$ test set	3655 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.4	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.6	EDS
Estimated twinning fraction	0.447 for -k,-h,-1/2*h+1/2*k-l 0.457 for k,h,-1/2*h-1/2*k-l 0.457 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 72952 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: 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	0.60	0/1849	0.68	1/2517 (0.0%)
1	B	0.57	0/1849	0.65	0/2517
1	C	0.61	0/1849	0.67	0/2517
1	D	0.57	0/1849	0.63	0/2517
All	All	0.59	0/7396	0.66	1/10068 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1187	LEU	CB-CG-CD2	-5.77	101.19	111.00

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	1863	62	0
1	B	1798	0	1863	61	0
1	C	1798	0	1863	58	0
1	D	1798	0	1863	54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	149	0	206	24	0
2	B	176	0	258	21	0
2	C	207	0	298	25	0
2	D	122	0	177	22	0
3	A	3	0	0	0	0
3	D	2	0	0	0	0
4	A	10	0	0	0	0
4	B	8	0	0	0	0
4	C	9	0	0	0	0
4	D	11	0	0	0	0
All	All	7889	0	8391	255	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 16.

All (255) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1302:PX4:H51	2:C:1304:PX4:O8	1.49	1.12
2:A:1305:PX4:H51	2:C:1303:PX4:O8	1.51	1.10
1:C:1155:ARG:HH21	2:C:1305:PX4:H11	1.36	0.89
1:A:1027:ILE:HG12	2:A:1305:PX4:H33	1.53	0.89
1:D:1092:SER:HB3	1:D:1093:SER:HB2	1.54	0.89
2:B:1302:PX4:C26	2:C:1304:PX4:O8	2.26	0.83
1:A:1033:THR:HG21	1:C:1163:LEU:HB2	1.61	0.82
2:C:1305:PX4:O8	2:C:1305:PX4:O4	1.98	0.81
1:D:1109:LEU:HD22	2:D:1304:PX4:H43	1.64	0.79
1:B:1162:THR:HG22	1:B:1165:GLU:H	1.49	0.78
1:B:1026:GLY:HA3	2:B:1302:PX4:H41	1.66	0.78
1:D:1162:THR:HG22	1:D:1165:GLU:H	1.49	0.78
1:C:1162:THR:HG22	1:C:1165:GLU:H	1.50	0.76
1:D:1190:VAL:O	2:D:1305:PX4:H5	1.90	0.72
2:A:1306:PX4:C23	2:D:1304:PX4:H51	2.20	0.71
1:A:1162:THR:HG22	1:A:1165:GLU:H	1.56	0.70
1:A:1175:THR:HG22	2:C:1306:PX4:H52	1.73	0.69
1:D:1063:ARG:HH12	1:D:1108:ARG:HH22	1.42	0.68
1:A:1103:VAL:HG11	1:C:1147:MET:HG3	1.77	0.67
1:D:1027:ILE:HG12	2:D:1304:PX4:H31	1.76	0.67
1:A:1126:VAL:HG11	1:A:1216:ILE:HG23	1.76	0.67
1:A:1006:THR:HG23	1:A:1066:VAL:HG13	1.77	0.67
2:A:1306:PX4:O8	2:D:1304:PX4:C26	2.43	0.66
2:A:1306:PX4:O8	2:D:1304:PX4:H51	1.94	0.66
1:C:1103:VAL:HG11	1:D:1147:MET:HG2	1.76	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:1305:PX4:C26	2:C:1303:PX4:O8	2.39	0.65
2:B:1304:PX4:H72	2:B:1304:PX4:H38	1.78	0.65
1:A:1075:PRO:HB3	2:A:1301:PX4:O6	1.98	0.64
1:C:1026:GLY:HA3	2:C:1302:PX4:H41	1.80	0.64
1:B:1209:MET:HE1	2:B:1305:PX4:H62	1.82	0.62
2:A:1306:PX4:H6	1:B:1165:GLU:HG3	1.80	0.62
1:B:1147:MET:HG2	1:D:1103:VAL:HG11	1.83	0.60
1:A:1169:THR:O	1:A:1173:VAL:HG23	2.02	0.59
2:A:1307:PX4:H35	2:A:1307:PX4:H71	1.85	0.59
1:D:1127:ILE:HA	1:D:1130:MET:HE2	1.83	0.59
2:A:1306:PX4:H15	2:A:1306:PX4:O8	2.02	0.59
2:B:1303:PX4:O4	2:B:1303:PX4:O8	2.20	0.59
1:D:1059:GLU:OE2	1:D:1063:ARG:NH1	2.36	0.59
1:B:1095:PHE:HB3	1:B:1097:ILE:HG12	1.85	0.59
1:D:1190:VAL:O	2:D:1305:PX4:C3	2.51	0.59
1:D:1109:LEU:HD22	2:D:1304:PX4:C22	2.33	0.59
1:A:1167:PHE:HB3	2:C:1304:PX4:H20	1.85	0.58
1:C:1155:ARG:HH21	2:C:1305:PX4:C5	2.14	0.58
2:C:1304:PX4:H53	2:C:1304:PX4:H26	1.86	0.58
1:C:1095:PHE:HB3	1:C:1097:ILE:HG12	1.86	0.58
2:D:1305:PX4:H4	2:D:1305:PX4:O2	2.04	0.58
2:A:1305:PX4:O1	2:A:1305:PX4:H17	2.04	0.57
1:D:1169:THR:O	1:D:1173:VAL:HG23	2.04	0.57
1:A:1155:ARG:HH21	2:A:1307:PX4:H11	1.69	0.56
1:C:1100:VAL:HG12	1:D:1147:MET:HE3	1.87	0.56
1:C:1165:GLU:HG3	2:C:1303:PX4:H4	1.87	0.56
1:C:1042:GLY:O	1:C:1046:THR:OG1	2.21	0.56
2:A:1306:PX4:O3	2:A:1306:PX4:H9	2.05	0.56
1:C:1155:ARG:NH2	2:C:1305:PX4:H11	2.14	0.56
1:A:1212:LEU:O	1:A:1216:ILE:HG13	2.06	0.56
1:D:1144:PHE:HZ	2:D:1305:PX4:H38	1.71	0.55
1:A:1024:LEU:HD23	1:A:1048:PHE:CZ	2.41	0.55
1:C:1169:THR:O	1:C:1173:VAL:HG23	2.06	0.55
1:D:1113:VAL:HG12	1:D:1114:PRO:O	2.07	0.55
2:A:1305:PX4:H64	1:C:1138:THR:HG22	1.89	0.55
1:B:1150:GLN:HG3	1:D:1100:VAL:HG22	1.88	0.55
1:B:1199:ILE:HB	1:B:1200:PRO:HD3	1.89	0.55
1:B:1126:VAL:HG11	1:B:1216:ILE:HG23	1.87	0.55
2:B:1302:PX4:H51	2:C:1304:PX4:C23	2.35	0.55
1:D:1080:ASP:OD2	1:D:1108:ARG:NH2	2.40	0.55
1:A:1150:GLN:HG3	1:B:1100:VAL:HG22	1.89	0.55
1:A:1075:PRO:CB	2:A:1301:PX4:O6	2.54	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1064:ILE:O	1:C:1068:ARG:N	2.33	0.54
1:B:1203:PHE:CD1	2:B:1306:PX4:H60	2.42	0.54
1:D:1199:ILE:HB	1:D:1200:PRO:HD3	1.89	0.54
2:C:1303:PX4:O3	2:C:1303:PX4:H9	2.07	0.54
1:D:1184:VAL:HG12	1:D:1188:MET:HE2	1.88	0.54
1:B:1074:ASP:HB3	1:B:1077:SER:HB2	1.89	0.53
1:C:1100:VAL:O	1:C:1103:VAL:HG12	2.07	0.53
1:A:1188:MET:HA	1:A:1191:TYR:O	2.08	0.53
1:D:1083:VAL:HG11	1:D:1105:ARG:HA	1.91	0.53
1:C:1069:ILE:O	1:C:1073:LYS:HG3	2.09	0.53
1:A:1095:PHE:HB3	1:A:1097:ILE:HG12	1.91	0.53
1:B:1042:GLY:O	1:B:1046:THR:OG1	2.26	0.53
2:A:1306:PX4:O8	2:D:1304:PX4:H50	2.09	0.53
1:B:1163:LEU:HB2	1:D:1033:THR:HG21	1.90	0.53
1:A:1100:VAL:HG22	1:C:1150:GLN:HG3	1.90	0.52
1:C:1108:ARG:O	1:C:1111:THR:HG22	2.09	0.52
1:C:1001:MET:HG3	1:C:1004:ARG:HD3	1.91	0.52
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.92	0.52
1:B:1209:MET:HE1	2:B:1305:PX4:H58	1.92	0.52
1:B:1071:PHE:CE1	1:B:1077:SER:HB3	2.45	0.52
1:C:1083:VAL:HG11	1:C:1105:ARG:HA	1.92	0.52
1:D:1029:MET:SD	1:D:1106:LEU:HD21	2.51	0.51
1:C:1218:VAL:HG12	1:C:1219:ASP:OD1	2.11	0.51
2:C:1303:PX4:H8	1:D:1188:MET:SD	2.50	0.51
1:A:1083:VAL:HG11	1:A:1105:ARG:HA	1.93	0.50
1:D:1042:GLY:O	1:D:1046:THR:OG1	2.28	0.50
1:B:1030:GLY:O	1:B:1033:THR:HB	2.12	0.50
1:C:1206:THR:HG21	2:C:1306:PX4:H54	1.93	0.50
1:A:1008:ILE:O	1:A:1011:SER:OG	2.20	0.50
2:B:1304:PX4:H22	2:B:1304:PX4:H47	1.93	0.50
1:C:1054:THR:O	1:C:1057:THR:N	2.44	0.50
1:A:1140:PHE:CZ	1:A:1204:VAL:HG11	2.46	0.50
1:B:1079:PHE:CE2	1:B:1083:VAL:HG21	2.46	0.50
1:A:1071:PHE:CE1	1:A:1077:SER:HB3	2.47	0.50
1:A:1031:LEU:HD13	1:A:1037:PHE:CE1	2.47	0.49
1:A:1048:PHE:O	1:A:1052:VAL:HG23	2.12	0.49
1:B:1115:GLN:O	1:B:1118:LYS:HB3	2.13	0.49
1:C:1025:ASN:OD1	1:C:1105:ARG:HD2	2.11	0.49
1:C:1048:PHE:O	1:C:1052:VAL:HG23	2.13	0.49
1:A:1133:VAL:HG11	1:A:1212:LEU:HD12	1.94	0.49
1:A:1175:THR:HB	1:C:1176:LEU:HD13	1.93	0.49
1:C:1006:THR:HG23	1:C:1066:VAL:HG13	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1097:ILE:HD13	2:D:1305:PX4:H57	1.94	0.49
1:A:1176:LEU:HD13	1:B:1175:THR:HB	1.95	0.48
1:D:1219:ASP:N	1:D:1219:ASP:OD1	2.46	0.48
1:B:1113:VAL:HG12	1:B:1114:PRO:O	2.13	0.48
1:C:1203:PHE:CE1	2:C:1306:PX4:H59	2.48	0.48
1:C:1030:GLY:O	2:C:1302:PX4:O6	2.31	0.48
1:A:1137:MET:SD	1:A:1208:VAL:HG11	2.53	0.48
1:B:1203:PHE:CE1	2:B:1306:PX4:H60	2.49	0.48
1:B:1058:ILE:O	1:B:1062:LEU:HG	2.14	0.48
1:C:1165:GLU:HG3	2:C:1303:PX4:C2	2.43	0.48
1:B:1087:SER:CB	1:B:1105:ARG:HH21	2.27	0.48
1:D:1143:ILE:O	1:D:1147:MET:HG3	2.14	0.48
1:A:1030:GLY:O	1:A:1033:THR:HB	2.14	0.48
1:B:1079:PHE:O	1:B:1083:VAL:HG23	2.14	0.48
1:A:1219:ASP:N	1:A:1219:ASP:OD1	2.47	0.47
1:B:1053:ILE:HD11	1:B:1087:SER:HB2	1.95	0.47
2:B:1303:PX4:H2	2:B:1303:PX4:H13	1.32	0.47
1:C:1076:TRP:CD2	1:C:1117:ARG:HD3	2.49	0.47
1:A:1162:THR:HB	1:A:1165:GLU:OE2	2.14	0.47
1:B:1087:SER:HB3	1:B:1105:ARG:HH21	1.79	0.47
1:B:1087:SER:HA	1:B:1102:ARG:HG2	1.95	0.47
1:B:1202:ILE:O	1:B:1206:THR:OG1	2.24	0.47
1:B:1114:PRO:O	1:B:1115:GLN:HB2	2.13	0.47
1:A:1184:VAL:O	1:A:1188:MET:HG3	2.15	0.47
1:C:1152:PHE:O	1:C:1156:PHE:HB2	2.14	0.47
1:D:1198:PHE:O	1:D:1202:ILE:HG13	2.14	0.47
2:A:1306:PX4:H47	2:D:1304:PX4:H55	1.96	0.47
1:B:1048:PHE:O	1:B:1052:VAL:HG23	2.13	0.47
1:B:1080:ASP:O	1:B:1084:VAL:HG23	2.15	0.47
1:D:1008:ILE:O	1:D:1011:SER:OG	2.24	0.47
1:A:1009:VAL:HA	1:A:1014:PHE:CD2	2.50	0.47
1:C:1116:MET:O	1:C:1119:ILE:HG22	2.15	0.47
1:B:1105:ARG:HG3	1:B:1106:LEU:HD23	1.98	0.46
1:B:1002:TYR:O	1:B:1005:ILE:HG12	2.14	0.46
1:C:1051:ILE:O	1:C:1054:THR:OG1	2.25	0.46
1:C:1199:ILE:HB	1:C:1200:PRO:HD3	1.97	0.46
1:B:1209:MET:CE	2:B:1305:PX4:H58	2.45	0.46
1:C:1202:ILE:O	1:C:1206:THR:OG1	2.23	0.46
1:D:1206:THR:O	1:D:1210:ILE:HG13	2.16	0.46
1:C:1079:PHE:CE2	1:C:1083:VAL:HG21	2.51	0.46
1:A:1087:SER:HA	1:A:1102:ARG:HG2	1.97	0.46
1:A:1206:THR:O	1:A:1210:ILE:HG13	2.15	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1019:ILE:HD13	1:B:1113:VAL:HG22	1.98	0.45
1:D:1025:ASN:OD1	1:D:1105:ARG:HD2	2.15	0.45
1:B:1184:VAL:HG12	1:B:1188:MET:HE2	1.99	0.45
1:B:1184:VAL:O	1:B:1188:MET:HG3	2.17	0.45
2:A:1306:PX4:C23	2:D:1304:PX4:C26	2.92	0.45
1:C:1184:VAL:O	1:C:1188:MET:HG3	2.16	0.45
1:A:1113:VAL:HG12	1:A:1114:PRO:O	2.16	0.45
1:C:1063:ARG:HH12	1:C:1108:ARG:HH22	1.64	0.45
1:A:1035:LYS:H	1:A:1035:LYS:HG2	1.47	0.45
1:C:1079:PHE:CZ	1:C:1083:VAL:HG21	2.52	0.45
1:D:1032:GLU:HA	1:D:1038:MET:HE3	1.99	0.45
1:C:1133:VAL:HG11	1:C:1212:LEU:HD12	1.99	0.45
1:D:1030:GLY:O	1:D:1033:THR:HB	2.16	0.45
1:D:1056:PHE:HE2	1:D:1108:ARG:HH11	1.65	0.45
1:A:1023:VAL:O	1:A:1027:ILE:HG13	2.17	0.44
1:A:1038:MET:HE2	1:A:1038:MET:HA	1.99	0.44
2:B:1302:PX4:H49	2:B:1302:PX4:H19	1.98	0.44
1:A:1098:LEU:HD23	1:A:1098:LEU:HA	1.86	0.44
1:C:1144:PHE:HZ	2:C:1305:PX4:H40	1.83	0.44
1:B:1207:PHE:HB2	2:B:1306:PX4:H67	2.00	0.44
1:A:1119:ILE:HG23	1:C:1136:LEU:HD22	1.99	0.44
1:C:1147:MET:HE3	2:C:1305:PX4:H31	2.00	0.44
1:D:1053:ILE:HD11	1:D:1087:SER:HB2	2.00	0.44
1:B:1026:GLY:HA3	2:B:1302:PX4:C21	2.43	0.44
1:B:1080:ASP:OD2	1:B:1111:THR:HG21	2.18	0.44
2:B:1304:PX4:H53	1:D:1097:ILE:HD13	2.00	0.44
1:D:1063:ARG:HH12	1:D:1108:ARG:NH2	2.12	0.44
2:A:1307:PX4:H54	2:A:1307:PX4:H48	1.64	0.44
1:B:1140:PHE:CZ	1:B:1204:VAL:HG11	2.52	0.44
1:B:1169:THR:O	1:B:1173:VAL:HG23	2.17	0.44
1:C:1085:ALA:HA	1:C:1088:LEU:HD12	1.98	0.44
1:D:1144:PHE:CZ	2:D:1305:PX4:H38	2.52	0.44
1:D:1128:PRO:HA	1:D:1131:LEU:CD1	2.48	0.43
1:A:1188:MET:SD	2:A:1306:PX4:H11	2.58	0.43
1:D:1001:MET:O	1:D:1004:ARG:HB3	2.17	0.43
1:C:1076:TRP:CE2	1:C:1117:ARG:HD3	2.54	0.43
1:A:1032:GLU:HA	1:A:1038:MET:HE3	2.01	0.43
2:A:1306:PX4:H13	2:A:1306:PX4:H2	1.78	0.43
1:C:1162:THR:HB	1:C:1165:GLU:OE2	2.18	0.43
1:B:1032:GLU:HG2	1:B:1038:MET:HE3	2.01	0.43
1:D:1006:THR:O	1:D:1010:GLU:HB2	2.19	0.43
1:C:1038:MET:HE2	1:C:1038:MET:HA	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1021:LEU:HA	1:D:1021:LEU:HD23	1.83	0.43
1:A:1038:MET:HE1	1:A:1045:THR:HG21	2.01	0.43
1:C:1140:PHE:CZ	1:C:1204:VAL:HG11	2.53	0.42
1:A:1028:THR:O	1:A:1032:GLU:HG3	2.19	0.42
1:A:1116:MET:O	1:A:1119:ILE:HG22	2.19	0.42
1:A:1136:LEU:HD22	1:B:1119:ILE:HG23	2.00	0.42
1:D:1071:PHE:CE1	1:D:1077:SER:HB3	2.53	0.42
1:C:1025:ASN:O	1:C:1028:THR:HG22	2.20	0.42
1:D:1048:PHE:O	1:D:1052:VAL:HG23	2.18	0.42
2:D:1305:PX4:H61	2:D:1305:PX4:H67	1.75	0.42
1:A:1031:LEU:HD23	1:A:1031:LEU:HA	1.80	0.42
1:B:1006:THR:HG23	1:B:1066:VAL:HG13	2.01	0.42
2:D:1305:PX4:H1	2:D:1305:PX4:H7	1.79	0.42
2:C:1305:PX4:O8	2:C:1305:PX4:O6	2.38	0.42
1:D:1032:GLU:HG2	1:D:1045:THR:HG21	2.01	0.42
2:B:1302:PX4:H37	2:B:1302:PX4:H44	1.77	0.42
1:A:1074:ASP:HB3	1:A:1077:SER:HB2	2.01	0.42
1:A:1113:VAL:O	1:A:1116:MET:HB2	2.20	0.42
1:A:1144:PHE:HZ	2:A:1307:PX4:H38	1.84	0.42
1:C:1023:VAL:O	1:C:1027:ILE:HG13	2.20	0.42
1:B:1038:MET:HE1	1:B:1042:GLY:HA2	2.01	0.42
1:D:1203:PHE:HD1	2:D:1306:PX4:H65	1.85	0.42
1:A:1133:VAL:CG1	1:A:1212:LEU:HD12	2.50	0.41
1:B:1091:THR:O	1:B:1092:SER:OG	2.36	0.41
1:B:1027:ILE:HG12	2:B:1302:PX4:H31	2.01	0.41
1:C:1021:LEU:HD23	1:C:1021:LEU:HA	1.78	0.41
2:C:1305:PX4:H67	2:C:1305:PX4:H61	1.85	0.41
2:C:1303:PX4:C22	2:D:1306:PX4:H62	2.50	0.41
1:A:1025:ASN:OD1	1:A:1105:ARG:HD2	2.20	0.41
1:B:1136:LEU:HD22	1:D:1119:ILE:HG23	2.01	0.41
2:A:1307:PX4:O7	2:A:1307:PX4:O6	2.39	0.41
1:B:1155:ARG:NH2	2:B:1304:PX4:H11	2.36	0.41
2:B:1304:PX4:H1	2:B:1304:PX4:H10	1.88	0.41
1:D:1005:ILE:HG13	1:D:1066:VAL:HG22	2.01	0.41
1:B:1021:LEU:HD23	1:B:1021:LEU:HA	1.82	0.41
1:B:1023:VAL:O	1:B:1027:ILE:HG13	2.19	0.41
1:C:1057:THR:O	1:C:1060:ILE:HG22	2.20	0.41
2:D:1304:PX4:H49	2:D:1304:PX4:H19	2.02	0.41
1:C:1188:MET:HA	1:C:1191:TYR:O	2.20	0.41
1:A:1021:LEU:HA	1:A:1021:LEU:HD23	1.69	0.41
1:B:1195:TRP:O	1:B:1199:ILE:HG12	2.20	0.41
1:B:1209:MET:O	1:B:1213:VAL:HG23	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1058:ILE:O	1:A:1062:LEU:HG	2.21	0.41
1:D:1001:MET:HG3	1:D:1004:ARG:HD3	2.03	0.41
1:D:1066:VAL:HG12	1:D:1066:VAL:O	2.21	0.41
1:D:1082:PHE:O	1:D:1086:ILE:HG13	2.20	0.41
1:D:1111:THR:O	1:D:1117:ARG:NE	2.51	0.41
1:A:1089:VAL:HA	1:A:1090:PRO:HD3	1.91	0.41
1:B:1001:MET:O	1:B:1004:ARG:HB3	2.21	0.41
1:B:1079:PHE:CZ	1:B:1083:VAL:HG21	2.56	0.41
1:C:1103:VAL:CG1	1:D:1147:MET:HG2	2.48	0.41
1:A:1100:VAL:O	1:A:1103:VAL:HG12	2.21	0.41
1:A:1210:ILE:HG23	1:B:1213:VAL:HG13	2.03	0.41
2:A:1307:PX4:H1	2:A:1307:PX4:H7	1.80	0.41
1:A:1079:PHE:CE2	1:A:1083:VAL:HG21	2.55	0.40
1:A:1170:LEU:HA	1:A:1170:LEU:HD23	1.88	0.40
1:B:1216:ILE:HG22	1:B:1216:ILE:O	2.20	0.40
1:C:1080:ASP:OD1	1:C:1111:THR:HG21	2.21	0.40
1:B:1004:ARG:O	1:B:1008:ILE:HG13	2.22	0.40
2:D:1304:PX4:H37	2:D:1304:PX4:H44	1.77	0.40
1:D:1196:VAL:HB	2:D:1305:PX4:H24	2.02	0.40
1:A:1180:SER:CB	1:B:1172:GLN:HG3	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/237 (92%)	194 (89%)	22 (10%)	1 (0%)	38	74
1	B	217/237 (92%)	197 (91%)	19 (9%)	1 (0%)	38	74
1	C	217/237 (92%)	199 (92%)	17 (8%)	1 (0%)	38	74
1	D	217/237 (92%)	197 (91%)	19 (9%)	1 (0%)	38	74
All	All	868/948 (92%)	787 (91%)	77 (9%)	4 (0%)	38	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1218	VAL
1	A	1063	ARG
1	B	1216	ILE
1	D	1114	PRO

### 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%)	187 (93%)	15 (7%)	20	45
1	B	202/218 (93%)	182 (90%)	20 (10%)	11	29
1	C	202/218 (93%)	186 (92%)	16 (8%)	18	42
1	D	202/218 (93%)	187 (93%)	15 (7%)	20	45
All	All	808/872 (93%)	742 (92%)	66 (8%)	17	40

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1028	THR
1	A	1033	THR
1	A	1035	LYS
1	A	1053	ILE
1	A	1068	ARG
1	A	1070	SER
1	A	1111	THR
1	A	1118	LYS
1	A	1119	ILE
1	A	1147	MET
1	A	1162	THR
1	A	1163	LEU
1	A	1187	LEU
1	A	1209	MET
1	A	1219	ASP
1	B	1010	GLU
1	B	1015	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1028	THR
1	B	1033	THR
1	B	1046	THR
1	B	1049	ASN
1	B	1053	ILE
1	B	1054	THR
1	B	1068	ARG
1	B	1069	ILE
1	B	1070	SER
1	B	1108	ARG
1	B	1119	ILE
1	B	1150	GLN
1	B	1162	THR
1	B	1163	LEU
1	B	1187	LEU
1	B	1209	MET
1	B	1214	VAL
1	B	1218	VAL
1	C	1010	GLU
1	C	1024	LEU
1	C	1028	THR
1	C	1033	THR
1	C	1035	LYS
1	C	1049	ASN
1	C	1053	ILE
1	C	1068	ARG
1	C	1111	THR
1	C	1118	LYS
1	C	1132	SER
1	C	1162	THR
1	C	1167	PHE
1	C	1192	PRO
1	C	1214	VAL
1	C	1219	ASP
1	D	1010	GLU
1	D	1033	THR
1	D	1046	THR
1	D	1049	ASN
1	D	1053	ILE
1	D	1068	ARG
1	D	1069	ILE
1	D	1111	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	1119	ILE
1	D	1132	SER
1	D	1162	THR
1	D	1163	LEU
1	D	1187	LEU
1	D	1209	MET
1	D	1219	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1211	ASN
1	D	1150	GLN

### 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 25 ligands modelled in this entry, 5 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PX4	A	1301	-	19,20,45	2.68	3 (15%)	23,24,53	8.33	5 (21%)
2	PX4	A	1305	-	39,40,45	1.52	4 (10%)	44,45,53	1.51	6 (13%)
2	PX4	A	1306	-	40,40,45	1.68	7 (17%)	48,48,53	1.74	7 (14%)
2	PX4	A	1307	-	45,45,45	1.63	5 (11%)	53,53,53	1.47	5 (9%)
2	PX4	B	1301	-	19,20,45	2.06	3 (15%)	23,24,53	7.69	5 (21%)
2	PX4	B	1302	-	39,40,45	1.45	4 (10%)	44,45,53	1.86	7 (15%)
2	PX4	B	1303	-	39,39,45	1.98	7 (17%)	47,47,53	1.68	7 (14%)
2	PX4	B	1304	-	45,45,45	1.57	5 (11%)	53,53,53	1.56	7 (13%)
2	PX4	B	1305	-	12,13,45	0.79	0	11,12,53	0.54	0
2	PX4	B	1306	-	12,13,45	0.79	0	11,12,53	0.50	0
2	PX4	C	1301	-	19,20,45	2.55	3 (15%)	23,24,53	8.11	5 (21%)
2	PX4	C	1302	-	39,40,45	1.62	4 (10%)	44,45,53	1.51	5 (11%)
2	PX4	C	1303	-	42,42,45	1.83	6 (14%)	50,50,53	1.75	8 (16%)
2	PX4	C	1304	-	41,41,45	1.85	7 (17%)	49,49,53	1.53	5 (10%)
2	PX4	C	1305	-	45,45,45	1.50	6 (13%)	53,53,53	1.65	5 (9%)
2	PX4	C	1306	-	12,13,45	0.74	0	11,12,53	0.47	0
2	PX4	D	1301	-	19,20,45	2.39	3 (15%)	23,24,53	7.30	6 (26%)
2	PX4	D	1304	-	39,40,45	1.48	4 (10%)	44,45,53	1.60	5 (11%)
2	PX4	D	1305	-	45,45,45	1.63	5 (11%)	53,53,53	1.47	5 (9%)
2	PX4	D	1306	-	12,13,45	0.79	0	11,12,53	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PX4	A	1301	-	-	0/22/22/49	0/0/0/0
2	PX4	A	1305	-	-	0/44/44/49	0/0/0/0
2	PX4	A	1306	-	-	0/44/44/49	0/0/0/0
2	PX4	A	1307	-	-	0/49/49/49	0/0/0/0
2	PX4	B	1301	-	-	0/22/22/49	0/0/0/0
2	PX4	B	1302	-	-	0/44/44/49	0/0/0/0
2	PX4	B	1303	-	-	0/43/43/49	0/0/0/0
2	PX4	B	1304	-	-	0/49/49/49	0/0/0/0
2	PX4	B	1305	-	-	0/11/11/49	0/0/0/0
2	PX4	B	1306	-	-	0/11/11/49	0/0/0/0
2	PX4	C	1301	-	-	0/22/22/49	0/0/0/0
2	PX4	C	1302	-	-	0/44/44/49	0/0/0/0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PX4	C	1303	-	-	1/46/46/49	0/0/0/0
2	PX4	C	1304	-	-	1/45/45/49	0/0/0/0
2	PX4	C	1305	-	-	0/49/49/49	0/0/0/0
2	PX4	C	1306	-	-	0/11/11/49	0/0/0/0
2	PX4	D	1301	-	-	0/22/22/49	0/0/0/0
2	PX4	D	1304	-	-	0/44/44/49	0/0/0/0
2	PX4	D	1305	-	-	0/49/49/49	0/0/0/0
2	PX4	D	1306	-	-	0/11/11/49	0/0/0/0

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	PX4	C17-C16	-9.20	1.51	1.55
2	C	1301	PX4	C17-C16	-8.53	1.51	1.55
2	D	1301	PX4	C17-C16	-7.34	1.52	1.55
2	D	1301	PX4	O6-C9	6.46	1.41	1.22
2	B	1303	PX4	O8-C23	6.45	1.41	1.22
2	C	1303	PX4	O6-C9	6.23	1.41	1.22
2	B	1301	PX4	O6-C9	6.19	1.41	1.22
2	C	1301	PX4	O6-C9	6.19	1.41	1.22
2	C	1303	PX4	O8-C23	6.13	1.40	1.22
2	B	1303	PX4	O6-C9	6.10	1.40	1.22
2	C	1304	PX4	O6-C9	5.97	1.40	1.22
2	A	1307	PX4	O6-C9	5.96	1.40	1.22
2	D	1305	PX4	O6-C9	5.96	1.40	1.22
2	C	1302	PX4	O6-C9	5.96	1.40	1.22
2	A	1307	PX4	O8-C23	5.88	1.40	1.22
2	D	1305	PX4	O8-C23	5.88	1.40	1.22
2	C	1304	PX4	O8-C23	5.86	1.40	1.22
2	C	1302	PX4	O8-C23	5.86	1.40	1.22
2	B	1304	PX4	O8-C23	5.84	1.40	1.22
2	A	1301	PX4	O6-C9	5.83	1.40	1.22
2	A	1305	PX4	O6-C9	5.64	1.39	1.22
2	B	1304	PX4	O6-C9	5.59	1.39	1.22
2	C	1305	PX4	O8-C23	5.57	1.39	1.22
2	B	1301	PX4	C17-C16	-5.45	1.53	1.55
2	D	1304	PX4	O6-C9	5.45	1.38	1.22
2	A	1305	PX4	O8-C23	5.32	1.38	1.22
2	D	1304	PX4	O8-C23	5.31	1.38	1.22
2	B	1302	PX4	O6-C9	5.29	1.38	1.22
2	A	1306	PX4	O8-C23	5.20	1.38	1.22
2	C	1305	PX4	O6-C9	5.11	1.37	1.22

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1302	PX4	O8-C23	5.02	1.37	1.22
2	A	1306	PX4	O6-C9	4.98	1.37	1.22
2	C	1303	PX4	C33-C32	4.53	1.57	1.55
2	B	1303	PX4	C33-C32	4.35	1.56	1.55
2	C	1304	PX4	C33-C32	4.12	1.56	1.55
2	A	1306	PX4	C4-N1	-3.68	1.38	1.50
2	C	1305	PX4	C4-N1	-3.46	1.39	1.50
2	C	1303	PX4	O7-C23	3.38	1.44	1.34
2	A	1306	PX4	C33-C32	3.38	1.56	1.55
2	B	1303	PX4	O7-C23	3.28	1.44	1.34
2	C	1304	PX4	C4-N1	-3.23	1.40	1.50
2	D	1305	PX4	C4-N1	-3.21	1.40	1.50
2	B	1303	PX4	C4-N1	-3.21	1.40	1.50
2	A	1307	PX4	C4-N1	-3.18	1.40	1.50
2	B	1301	PX4	O5-C9	3.10	1.42	1.33
2	D	1301	PX4	O5-C9	2.95	1.42	1.33
2	B	1304	PX4	C4-N1	-2.92	1.41	1.50
2	B	1304	PX4	O7-C23	2.92	1.43	1.34
2	B	1303	PX4	O5-C9	2.91	1.42	1.33
2	C	1302	PX4	O7-C23	2.83	1.42	1.34
2	A	1307	PX4	O7-C23	2.82	1.42	1.34
2	D	1305	PX4	O7-C23	2.82	1.42	1.34
2	C	1304	PX4	O7-C23	2.81	1.42	1.34
2	B	1304	PX4	O5-C9	2.65	1.41	1.33
2	A	1307	PX4	O5-C9	2.63	1.41	1.33
2	C	1303	PX4	C4-N1	-2.63	1.42	1.50
2	D	1305	PX4	O5-C9	2.63	1.41	1.33
2	C	1304	PX4	O5-C9	2.62	1.41	1.33
2	C	1302	PX4	O5-C9	2.62	1.41	1.33
2	C	1305	PX4	O7-C23	2.62	1.42	1.34
2	A	1305	PX4	O5-C9	2.60	1.41	1.33
2	C	1303	PX4	O5-C9	2.59	1.41	1.33
2	C	1301	PX4	O5-C9	2.51	1.41	1.33
2	A	1306	PX4	O7-C23	2.49	1.41	1.34
2	A	1305	PX4	O7-C23	2.43	1.41	1.34
2	B	1303	PX4	C19-C18	-2.43	1.54	1.55
2	A	1301	PX4	O5-C9	2.38	1.40	1.33
2	D	1304	PX4	O7-C23	2.34	1.41	1.34
2	A	1306	PX4	C3-N1	-2.34	1.42	1.50
2	D	1304	PX4	O5-C9	2.31	1.40	1.33
2	B	1302	PX4	O7-C23	2.29	1.41	1.34
2	C	1304	PX4	C21-C20	-2.28	1.54	1.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1305	PX4	C3-N1	-2.14	1.43	1.50
2	B	1302	PX4	O5-C9	2.12	1.39	1.33
2	A	1306	PX4	O7-C7	-2.02	1.41	1.46
2	C	1305	PX4	O7-C7	-2.02	1.41	1.46

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1301	PX4	O7-C7-C6	-28.79	108.79	119.54
2	A	1301	PX4	O7-C7-C8	-28.02	109.08	119.54
2	B	1301	PX4	O7-C7-C6	-27.51	109.26	119.54
2	A	1301	PX4	O7-C7-C6	-27.37	109.32	119.54
2	C	1301	PX4	O7-C7-C8	-27.09	109.42	119.54
2	C	1301	PX4	O7-C7-C6	-26.94	109.48	119.54
2	B	1301	PX4	O7-C7-C8	-23.42	110.79	119.54
2	D	1301	PX4	O7-C7-C8	-18.58	112.60	119.54
2	C	1305	PX4	O5-C9-O6	-6.85	105.57	123.48
2	C	1303	PX4	O5-C9-O6	-6.80	105.71	123.48
2	B	1302	PX4	O5-C9-O6	-6.61	106.21	123.48
2	A	1306	PX4	O5-C9-O6	-6.10	107.53	123.48
2	A	1301	PX4	O5-C9-O6	-6.04	107.71	123.48
2	B	1302	PX4	O7-C23-O8	-5.97	107.73	123.66
2	B	1303	PX4	O5-C9-O6	-5.60	108.85	123.48
2	C	1305	PX4	O7-C23-O8	-5.49	109.01	123.66
2	A	1305	PX4	O7-C23-O8	-5.41	109.23	123.66
2	D	1305	PX4	O5-C9-O6	-5.36	109.47	123.48
2	A	1307	PX4	O5-C9-O6	-5.36	109.47	123.48
2	C	1302	PX4	O5-C9-O6	-5.36	109.47	123.48
2	C	1301	PX4	O5-C9-O6	-5.35	109.50	123.48
2	D	1304	PX4	O7-C23-O8	-5.35	109.40	123.66
2	C	1304	PX4	O5-C9-O6	-5.34	109.51	123.48
2	D	1304	PX4	O5-C9-O6	-5.33	109.54	123.48
2	A	1307	PX4	O7-C23-O8	-5.33	109.44	123.66
2	C	1304	PX4	O7-C23-O8	-5.32	109.47	123.66
2	D	1305	PX4	O7-C23-O8	-5.31	109.50	123.66
2	C	1302	PX4	O7-C23-O8	-5.30	109.52	123.66
2	D	1301	PX4	O5-C9-O6	-5.21	109.87	123.48
2	B	1301	PX4	O5-C9-O6	-5.17	109.96	123.48
2	B	1303	PX4	O7-C23-O8	-4.98	110.38	123.66
2	A	1306	PX4	O7-C23-O8	-4.97	110.39	123.66
2	B	1304	PX4	O7-C23-O8	-4.74	111.02	123.66
2	C	1303	PX4	O7-C23-O8	-4.67	111.19	123.66

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1303	PX4	C5-N1-C4	4.61	121.23	108.99
2	B	1304	PX4	O5-C9-O6	-4.42	111.92	123.48
2	A	1306	PX4	C5-N1-C4	4.38	120.62	108.99
2	B	1303	PX4	O6-C9-C10	-4.31	106.30	123.78
2	B	1304	PX4	O6-C9-C10	-4.22	106.66	123.78
2	A	1306	PX4	O6-C9-C10	-4.16	106.91	123.78
2	B	1301	PX4	O6-C9-C10	-4.16	106.93	123.78
2	B	1303	PX4	C5-N1-C4	4.10	119.87	108.99
2	C	1305	PX4	O8-C23-C24	-4.07	107.28	123.78
2	B	1302	PX4	O8-C23-C24	-4.04	107.42	123.78
2	B	1302	PX4	O3-P1-O4	4.03	113.36	102.86
2	B	1304	PX4	O8-C23-C24	-3.99	107.59	123.78
2	A	1305	PX4	O8-C23-C24	-3.99	107.60	123.78
2	D	1304	PX4	O8-C23-C24	-3.88	108.03	123.78
2	A	1301	PX4	O6-C9-C10	-3.87	108.09	123.78
2	B	1304	PX4	C5-N1-C4	3.84	119.18	108.99
2	A	1306	PX4	O8-C23-C24	-3.83	108.26	123.78
2	C	1304	PX4	C5-N1-C4	3.82	119.14	108.99
2	A	1305	PX4	O3-P1-O4	3.81	112.78	102.86
2	D	1305	PX4	C5-N1-C4	3.75	118.94	108.99
2	A	1307	PX4	C5-N1-C4	3.72	118.86	108.99
2	B	1302	PX4	O6-C9-C10	-3.70	108.79	123.78
2	C	1303	PX4	C8-O5-C9	-3.65	106.58	116.99
2	A	1305	PX4	O5-C9-O6	-3.57	114.14	123.48
2	D	1304	PX4	O3-P1-O4	3.56	112.13	102.86
2	D	1304	PX4	O6-C9-C10	-3.53	109.47	123.78
2	C	1302	PX4	O6-C9-C10	-3.53	109.48	123.78
2	C	1302	PX4	O8-C23-C24	-3.52	109.50	123.78
2	C	1301	PX4	O6-C9-C10	-3.52	109.50	123.78
2	D	1305	PX4	O8-C23-C24	-3.52	109.49	123.78
2	A	1307	PX4	O8-C23-C24	-3.52	109.50	123.78
2	C	1304	PX4	O8-C23-C24	-3.52	109.52	123.78
2	A	1307	PX4	O6-C9-C10	-3.51	109.53	123.78
2	C	1304	PX4	O6-C9-C10	-3.51	109.53	123.78
2	D	1305	PX4	O6-C9-C10	-3.51	109.54	123.78
2	C	1305	PX4	C5-N1-C4	3.45	118.16	108.99
2	C	1305	PX4	O6-C9-C10	-3.44	109.84	123.78
2	D	1301	PX4	O6-C9-C10	-3.40	110.00	123.78
2	B	1303	PX4	O8-C23-C24	-3.36	110.18	123.78
2	C	1303	PX4	O8-C23-C24	-2.93	111.88	123.78
2	B	1302	PX4	O7-C7-C8	2.93	119.33	108.50
2	A	1305	PX4	O6-C9-C10	-2.90	112.02	123.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1303	PX4	C1-C2-N1	-2.81	106.08	115.85
2	B	1301	PX4	O3-P1-O4	2.70	109.90	102.86
2	C	1303	PX4	O6-C9-C10	-2.56	113.40	123.78
2	C	1301	PX4	O3-P1-O4	2.53	109.45	102.86
2	B	1304	PX4	C8-C7-C6	-2.53	106.05	111.86
2	C	1302	PX4	O3-P1-O4	2.53	109.44	102.86
2	B	1302	PX4	O5-C8-C7	2.47	115.29	108.80
2	C	1303	PX4	C8-C7-C6	-2.44	106.25	111.86
2	A	1305	PX4	O1-P1-O3	2.42	112.91	104.85
2	B	1304	PX4	O5-C8-C7	-2.23	102.94	108.80
2	D	1301	PX4	O3-P1-O4	2.23	108.66	102.86
2	D	1301	PX4	O1-P1-O3	2.22	112.25	104.85
2	A	1301	PX4	O3-P1-O4	2.10	108.32	102.86
2	C	1303	PX4	P1-O3-C1	-2.08	109.96	121.66
2	A	1306	PX4	C8-C7-C6	2.07	116.60	111.86
2	B	1303	PX4	C4-N1-C3	-2.02	103.63	108.99
2	A	1306	PX4	O5-C9-C10	-2.00	105.76	111.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1304	PX4	C7-O7-C23-O8
2	C	1303	PX4	C7-O7-C23-O8

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%)	0.51	11 (5%) 28 29	29, 77, 112, 139	0
1	B	219/237 (92%)	0.48	6 (2%) 52 55	30, 76, 115, 135	0
1	C	219/237 (92%)	0.46	6 (2%) 52 55	28, 76, 112, 143	0
1	D	219/237 (92%)	0.47	8 (3%) 39 42	30, 78, 116, 137	0
All	All	876/948 (92%)	0.48	31 (3%) 42 44	28, 77, 115, 143	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1095	PHE	5.9
1	D	1069	ILE	4.6
1	C	1065	TYR	4.5
1	A	1020	TYR	3.4
1	D	1065	TYR	3.4
1	C	1095	PHE	3.4
1	B	1001	MET	3.2
1	A	1065	TYR	3.1
1	D	1044	TYR	3.0
1	C	1069	ILE	2.8
1	B	1065	TYR	2.6
1	A	1094	GLY	2.6
1	A	1090	PRO	2.6
1	B	1020	TYR	2.5
1	D	1131	LEU	2.4
1	A	1004	ARG	2.4
1	D	1002	TYR	2.4
1	B	1213	VAL	2.4
1	C	1001	MET	2.4
1	D	1020	TYR	2.4
1	A	1001	MET	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	1095	PHE	2.3
1	A	1002	TYR	2.3
1	C	1005	ILE	2.3
1	A	1091	THR	2.2
1	A	1041	PHE	2.1
1	A	1213	VAL	2.1
1	B	1216	ILE	2.1
1	C	1097	ILE	2.1
1	D	1053	ILE	2.1
1	D	1097	ILE	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(Å <sup>2</sup> )	Q<0.9
3	CA	A	1304	1/1	1.12	73.09	99,99,99,99	0
3	CA	A	1303	1/1	0.36	7.73	81,81,81,81	0
2	PX4	D	1301	21/46	0.40	4.42	79,99,116,123	0
2	PX4	B	1301	21/46	0.42	3.83	74,95,112,122	0
2	PX4	A	1307	46/46	0.37	3.80	55,73,86,94	0
2	PX4	C	1301	21/46	0.37	3.57	74,94,111,124	0
2	PX4	A	1301	21/46	0.36	3.44	68,96,111,120	0
2	PX4	B	1306	14/46	0.30	3.42	51,62,82,83	0
2	PX4	B	1304	46/46	0.34	3.37	53,72,82,91	0
2	PX4	C	1305	46/46	0.33	3.11	57,73,85,96	0
2	PX4	D	1305	46/46	0.40	2.93	56,75,91,109	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PX4	B	1305	14/46	0.33	2.77	47,65,74,79	0
2	PX4	C	1302	41/46	0.32	2.38	60,74,93,109	0
2	PX4	A	1305	41/46	0.31	2.12	62,76,92,101	0
2	PX4	C	1304	42/46	0.26	2.06	49,68,79,83	0
2	PX4	B	1302	41/46	0.29	2.00	64,75,94,105	0
2	PX4	D	1304	41/46	0.26	1.32	62,74,90,100	0
2	PX4	D	1306	14/46	0.26	1.16	47,70,75,79	0
2	PX4	B	1303	40/46	0.23	0.99	44,68,76,78	0
2	PX4	C	1306	14/46	0.21	0.32	47,63,75,77	0
2	PX4	C	1303	43/46	0.22	0.29	48,71,76,84	0
2	PX4	A	1306	41/46	0.21	0.00	44,69,78,81	0
3	CA	A	1302	1/1	0.10	-2.78	63,63,63,63	0
3	CA	D	1302	1/1	0.09	-7.58	59,59,59,59	0
3	CA	D	1303	1/1	0.50	-	113,113,113,113	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.