



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:42 PM GMT

PDB ID : 3RW0
Title : Crystal structure of the NavAb voltage-gated sodium channel (Met221Cys, 2.95 Å)
Authors : Payandeh, J.; Scheuer, T.; Zheng, N.; Catterall, W.A.
Deposited on : 2011-05-06
Resolution : 2.95 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

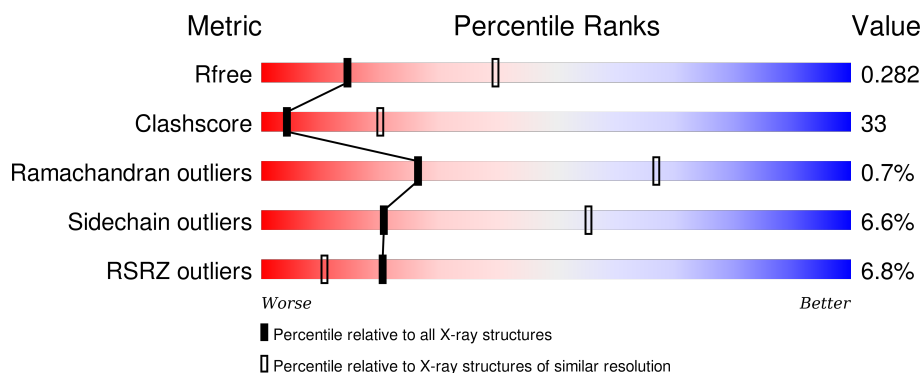
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	285	<div> <div>5%</div> <div>36%</div> <div>39%</div> <div>•</div> <div>22%</div> </div>
1	B	285	<div> <div>6%</div> <div>32%</div> <div>42%</div> <div>•</div> <div>22%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3781 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	223	Total	C	N	O	S	Se	0	0	0
			1826	1243	274	297	1	11			
1	B	223	Total	C	N	O	S	Se	0	0	0
			1826	1243	274	297	1	11			

There are 38 discrepancies between the modelled and reference sequences:

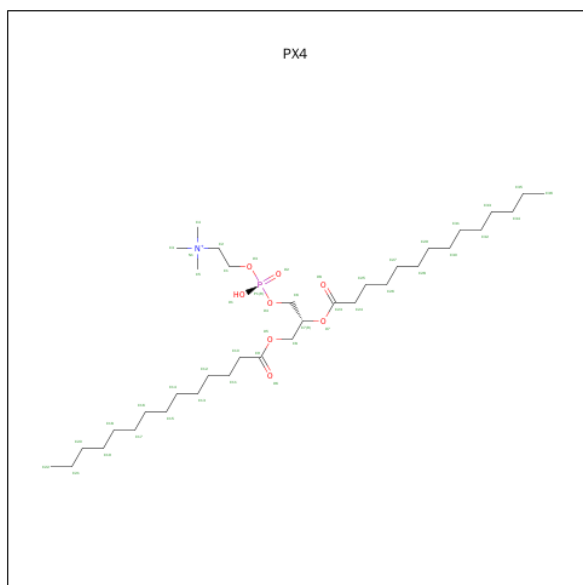
Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MSE	-	EXPRESSION TAG	UNP A8EVM5
A	984	ASP	-	EXPRESSION TAG	UNP A8EVM5
A	985	TYR	-	EXPRESSION TAG	UNP A8EVM5
A	986	LYS	-	EXPRESSION TAG	UNP A8EVM5
A	987	ASP	-	EXPRESSION TAG	UNP A8EVM5
A	988	ASP	-	EXPRESSION TAG	UNP A8EVM5
A	989	ASP	-	EXPRESSION TAG	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	1221	CYS	MET	ENGINEERED MUTATION	UNP A8EVM5
B	1983	MSE	-	EXPRESSION TAG	UNP A8EVM5
B	1984	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	1985	TYR	-	EXPRESSION TAG	UNP A8EVM5
B	1986	LYS	-	EXPRESSION TAG	UNP A8EVM5
B	1987	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	1988	ASP	-	EXPRESSION TAG	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1989	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	1990	ASP	-	EXPRESSION TAG	UNP A8EVM5
B	1991	LYS	-	EXPRESSION TAG	UNP A8EVM5
B	1992	GLY	-	EXPRESSION TAG	UNP A8EVM5
B	1993	SER	-	EXPRESSION TAG	UNP A8EVM5
B	1994	LEU	-	EXPRESSION TAG	UNP A8EVM5
B	1995	VAL	-	EXPRESSION TAG	UNP A8EVM5
B	1996	PRO	-	EXPRESSION TAG	UNP A8EVM5
B	1997	ARG	-	EXPRESSION TAG	UNP A8EVM5
B	1998	GLY	-	EXPRESSION TAG	UNP A8EVM5
B	1999	SER	-	EXPRESSION TAG	UNP A8EVM5
B	2000	HIS	-	EXPRESSION TAG	UNP A8EVM5
B	2221	CYS	MET	ENGINEERED MUTATION	UNP A8EVM5

- Molecule 2 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
2	A	1	Total C N O P 16 7 1 7 1	0	0
2	A	1	Total C O P 17 9 7 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total C 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 17 9 7 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total C O P 21 13 7 1	0	0
2	B	1	Total C O P 21 13 7 1	0	0
2	B	1	Total C O P 13 5 7 1	0	0
2	B	1	Total C 6 6	0	0

- Molecule 3 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	125.50Å 125.81Å 191.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 42.23 – 2.96	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.95) 97.7 (42.23-2.96)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1 & 1.3	Depositor
R, R_{free}	0.259 , 0.272 0.268 , 0.282	Depositor DCC
R_{free} test set	1554 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	100.9	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 84.1	EDS
Estimated twinning fraction	0.477 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 31350 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3781	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.54	1/1867 (0.1%)	0.71	1/2522 (0.0%)
1	B	0.45	0/1867	0.61	0/2522
All	All	0.50	1/3734 (0.0%)	0.66	1/5044 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1041	PHE	CD2-CE2	6.63	1.52	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1042	GLY	N-CA-C	6.87	130.27	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1826	0	1897	137	0
1	B	1826	0	1897	145	0
2	A	66	0	46	2	0
2	B	61	0	54	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	1	0
3	B	1	0	0	0	0
All	All	3781	0	3894	253	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 33.

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:ALA:CB	1:B:2218:VAL:HG13	1.64	1.25
1:A:1217:ILE:HG22	1:B:2214:VAL:HG13	1.29	1.12
1:A:1032:GLU:HG3	1:A:1045:THR:HG21	1.26	1.07
1:A:1220:ALA:HB1	1:B:2218:VAL:HG13	1.07	1.06
1:A:1220:ALA:HB1	1:B:2218:VAL:CG1	1.87	1.04
1:B:2096:GLU:HG3	1:B:2099:ARG:HB3	1.39	1.04
1:A:1162:THR:HB	1:A:1165:GLU:HG3	1.39	1.02
1:B:2130:MSE:HE3	1:B:2216:ILE:HD11	1.42	1.00
1:A:1220:ALA:CB	1:B:2218:VAL:CG1	2.47	0.88
1:A:1074:ASP:HB3	1:A:1077:SER:OG	1.72	0.88
1:B:2001:MSE:HE2	1:B:2004:ARG:HD3	1.53	0.88
1:A:1185:ARG:HB2	1:A:1186:PRO:HD3	1.58	0.86
1:B:2002:TYR:HD1	1:B:2003:LEU:N	1.74	0.85
1:A:1217:ILE:CG2	1:B:2214:VAL:HG13	2.07	0.84
1:B:2074:ASP:HB3	1:B:2077:SER:OG	1.78	0.83
1:B:2076:TRP:HB3	1:B:2111:THR:HG23	1.62	0.82
1:A:1162:THR:HG22	1:A:1164:GLY:H	1.44	0.81
1:B:2100:VAL:O	1:B:2103:VAL:HG12	1.81	0.80
1:A:1005:ILE:HD13	1:A:1065:TYR:HD1	1.45	0.80
1:A:1022:ILE:HG21	1:A:1109:LEU:HB2	1.62	0.80
1:B:2002:TYR:CD1	1:B:2002:TYR:C	2.56	0.79
1:B:2028:THR:HG23	1:B:2045:THR:HG23	1.65	0.78
1:A:1053:ILE:HD11	1:A:1088:LEU:HD23	1.65	0.78
1:B:2185:ARG:HB2	1:B:2186:PRO:HD3	1.67	0.77
1:A:1102:ARG:O	1:A:1105:ARG:HG2	1.85	0.77
1:A:1100:VAL:O	1:A:1103:VAL:HG12	1.85	0.76
1:A:1218:VAL:HG13	1:A:1219:ASP:N	2.00	0.76
1:A:1032:GLU:HG3	1:A:1045:THR:CG2	2.11	0.75
1:A:1005:ILE:HD13	1:A:1065:TYR:CD1	2.21	0.75
1:A:1127:ILE:HA	1:A:1130:MSE:HE2	1.68	0.75
1:B:2018:ILE:HD12	1:B:2059:GLU:OE1	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2022:ILE:HG21	1:B:2109:LEU:HB2	1.67	0.73
1:B:2056:PHE:CD2	1:B:2108:ARG:NH1	2.57	0.73
1:B:2214:VAL:O	1:B:2218:VAL:HG23	1.89	0.72
1:A:1030:GLY:O	1:A:1033:THR:HB	1.88	0.72
1:B:2001:MSE:CE	1:B:2004:ARG:HD3	2.19	0.71
1:B:2162:THR:HG22	1:B:2164:GLY:H	1.55	0.71
1:B:2048:PHE:O	1:B:2052:VAL:HG23	1.89	0.71
1:A:1025:ASN:OD1	1:A:1105:ARG:NH1	2.23	0.71
1:A:1162:THR:HG22	1:A:1164:GLY:N	2.05	0.71
1:A:1018:ILE:HD12	1:A:1059:GLU:OE1	1.91	0.71
1:B:2079:PHE:CE2	1:B:2083:VAL:HG21	2.27	0.70
1:B:2096:GLU:HG3	1:B:2099:ARG:CB	2.18	0.70
1:A:1033:THR:HG21	1:B:2163:LEU:HB2	1.74	0.69
1:B:2002:TYR:CD1	1:B:2003:LEU:N	2.60	0.69
1:A:1221:CYS:SG	1:B:2221:CYS:SG	2.66	0.69
1:A:1079:PHE:CE2	1:A:1083:VAL:HG21	2.28	0.68
1:B:2002:TYR:C	1:B:2002:TYR:HD1	1.94	0.68
1:A:1106:LEU:HB2	1:B:2143:ILE:CD1	2.23	0.68
1:A:1080:ASP:O	1:A:1084:VAL:HG23	1.93	0.68
1:A:1184:VAL:HG12	1:A:1188:MSE:HE2	1.76	0.67
1:B:2035:LYS:HG3	1:B:2036:THR:N	2.09	0.67
1:A:1028:THR:HG23	1:A:1045:THR:HG23	1.76	0.67
1:B:2079:PHE:CZ	1:B:2083:VAL:HG21	2.29	0.67
1:B:2018:ILE:CD1	1:B:2059:GLU:OE1	2.42	0.66
1:B:2155:ARG:HD2	1:B:2190:VAL:HG11	1.77	0.66
1:B:2214:VAL:O	1:B:2218:VAL:CG2	2.44	0.66
1:A:1103:VAL:HG11	1:B:2147:MSE:HG2	1.78	0.65
1:B:2162:THR:HG22	1:B:2164:GLY:N	2.10	0.65
1:A:1018:ILE:CD1	1:A:1059:GLU:OE1	2.44	0.65
1:A:1035:LYS:O	1:A:1039:GLN:HG3	1.97	0.65
1:A:1221:CYS:HG	1:B:2221:CYS:HG	0.76	0.64
1:B:2118:LYS:HE2	1:B:2118:LYS:HA	1.79	0.64
1:B:2056:PHE:HD2	1:B:2108:ARG:HH11	1.45	0.64
1:A:1079:PHE:CZ	1:A:1083:VAL:HG21	2.32	0.64
1:A:1031:LEU:HA	2:A:4013:PX4:O6	1.99	0.62
1:B:2050:GLN:O	1:B:2053:ILE:HG22	1.99	0.61
1:A:1023:VAL:O	1:A:1027:ILE:HG13	2.01	0.61
1:A:1218:VAL:CG1	1:A:1219:ASP:N	2.64	0.61
1:A:1083:VAL:HG11	1:A:1105:ARG:HA	1.81	0.60
1:A:1162:THR:CG2	1:A:1164:GLY:H	2.14	0.60
1:B:2028:THR:CG2	1:B:2045:THR:HG23	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2031:LEU:C	1:B:2033:THR:H	2.03	0.60
1:A:1137:MSE:HE1	1:A:1208:VAL:HB	1.83	0.60
1:A:1124:ILE:HA	1:A:1127:ILE:HG12	1.84	0.60
2:A:4013:PX4:H26	1:B:2142:TYR:OH	2.02	0.60
1:A:1220:ALA:HB3	1:B:2218:VAL:HG13	1.74	0.60
1:B:2113:VAL:HG12	1:B:2114:PRO:O	2.02	0.60
1:A:1035:LYS:HG3	1:A:1036:THR:N	2.17	0.60
1:B:2171:PHE:CD1	1:B:2174:MSE:HE2	2.37	0.60
1:B:2199:ILE:HB	1:B:2200:PRO:HD3	1.84	0.60
1:A:1005:ILE:CD1	1:A:1065:TYR:CD1	2.85	0.59
1:B:2080:ASP:OD2	1:B:2108:ARG:NE	2.36	0.59
1:A:1076:TRP:HB3	1:A:1111:THR:HG23	1.85	0.59
1:B:2127:ILE:N	1:B:2128:PRO:HD2	2.19	0.58
1:A:1001:MSE:SE	1:A:1004:ARG:HD3	2.53	0.58
1:B:2162:THR:CG2	1:B:2164:GLY:H	2.16	0.58
1:B:2079:PHE:O	1:B:2083:VAL:HG23	2.04	0.57
1:B:2184:VAL:HG12	1:B:2188:MSE:HE2	1.87	0.57
1:B:2096:GLU:OE2	1:B:2099:ARG:NE	2.38	0.57
1:B:2080:ASP:O	1:B:2084:VAL:HG23	2.04	0.57
1:B:2032:GLU:HB2	1:B:2045:THR:HG21	1.86	0.57
1:B:2030:GLY:O	1:B:2033:THR:HB	2.04	0.57
1:B:2195:TRP:O	1:B:2199:ILE:HG12	2.05	0.56
1:A:1057:THR:O	1:A:1060:ILE:HG22	2.04	0.56
1:B:2083:VAL:HG11	1:B:2105:ARG:HA	1.87	0.55
1:A:1114:PRO:O	1:A:1115:GLN:HB2	2.05	0.55
1:B:2002:TYR:CE1	1:B:2006:THR:OG1	2.59	0.55
1:B:2124:ILE:HA	1:B:2127:ILE:HG12	1.87	0.55
1:B:2130:MSE:HE3	1:B:2216:ILE:CD1	2.27	0.55
1:B:2032:GLU:HG3	1:B:2038:MSE:HE3	1.87	0.55
1:B:2080:ASP:OD1	1:B:2111:THR:HG21	2.06	0.55
1:B:2162:THR:HG22	1:B:2165:GLU:H	1.72	0.55
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.89	0.55
1:A:1068:ARG:HG3	1:A:1069:ILE:N	2.22	0.55
1:B:2137:MSE:HE3	1:B:2208:VAL:HG21	1.89	0.54
1:B:2007:ASN:O	1:B:2011:SER:HB3	2.07	0.54
1:A:1058:ILE:O	1:A:1062:LEU:HG	2.09	0.53
1:A:1171:PHE:CD1	1:A:1174:MSE:HE2	2.44	0.53
1:A:1217:ILE:HD12	1:B:2217:ILE:HG21	1.90	0.53
1:A:1063:ARG:NH2	1:A:1077:SER:HB3	2.24	0.53
1:A:1037:PHE:CE1	1:A:1041:PHE:HB2	2.43	0.53
1:B:2089:VAL:HG11	1:B:2098:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:MSE:O	1:A:1212:LEU:HB3	2.09	0.53
1:A:1182:GLY:HA3	1:B:2181:MSE:HE2	1.89	0.53
1:A:1137:MSE:HE3	1:A:1209:MSE:HE3	1.90	0.53
1:A:1209:MSE:HA	1:A:1209:MSE:HE2	1.91	0.53
1:B:2083:VAL:CG1	1:B:2105:ARG:HA	2.39	0.52
1:B:2068:ARG:HG3	1:B:2069:ILE:N	2.24	0.52
1:B:2137:MSE:HE2	1:B:2137:MSE:HA	1.92	0.52
1:A:1103:VAL:CG1	1:B:2147:MSE:HG2	2.40	0.52
1:B:2133:VAL:HG11	1:B:2212:LEU:HD12	1.92	0.52
1:A:1095:PHE:HB2	1:A:1097:ILE:HG12	1.91	0.51
1:A:1155:ARG:HD2	1:A:1190:VAL:HG11	1.93	0.51
1:A:1195:TRP:O	1:A:1199:ILE:HG12	2.10	0.51
1:A:1101:LEU:HD23	1:B:2147:MSE:HE1	1.93	0.51
1:A:1158:GLU:HB3	3:A:3001:HOH:O	2.10	0.51
1:A:1071:PHE:CE1	1:A:1077:SER:HB2	2.46	0.51
1:A:1177:GLU:CD	1:B:2178:SER:HA	2.31	0.51
1:A:1177:GLU:OE1	1:B:2178:SER:HA	2.11	0.51
1:A:1108:ARG:HB3	1:A:1108:ARG:HH11	1.74	0.51
1:A:1091:THR:HA	1:A:1102:ARG:HH22	1.76	0.51
1:B:2114:PRO:O	1:B:2115:GLN:HB2	2.11	0.51
1:B:1999:SER:HA	1:B:2002:TYR:HB3	1.93	0.50
1:B:2104:LEU:O	1:B:2107:PHE:HB2	2.10	0.50
1:A:1079:PHE:O	1:A:1083:VAL:HG23	2.11	0.50
1:A:1028:THR:CG2	1:A:1045:THR:HG23	2.40	0.50
1:A:1083:VAL:CG1	1:A:1105:ARG:HA	2.42	0.50
1:B:2139:LEU:O	1:B:2143:ILE:HG12	2.11	0.50
1:B:2023:VAL:O	1:B:2027:ILE:HG13	2.11	0.50
1:B:2041:PHE:CD1	1:B:2041:PHE:N	2.80	0.50
1:A:1107:PHE:CE2	1:B:2143:ILE:HG13	2.47	0.49
1:B:2060:ILE:O	1:B:2064:ILE:HG12	2.12	0.49
1:A:1101:LEU:O	1:A:1104:LEU:HB2	2.12	0.49
1:B:2057:THR:O	1:B:2060:ILE:HG22	2.12	0.49
1:B:2085:ALA:O	1:B:2088:LEU:HB2	2.12	0.49
1:B:2035:LYS:HG3	1:B:2036:THR:H	1.78	0.49
1:A:1127:ILE:N	1:A:1128:PRO:HD2	2.28	0.49
1:A:1018:ILE:HG13	1:A:1059:GLU:OE1	2.13	0.48
1:A:1217:ILE:HG22	1:B:2214:VAL:CG1	2.20	0.48
1:A:1052:VAL:O	1:A:1056:PHE:HD1	1.96	0.48
1:B:2103:VAL:HG22	1:B:2103:VAL:O	2.12	0.48
1:A:1177:GLU:HG3	1:B:2179:TRP:CD1	2.49	0.48
1:B:2115:GLN:O	1:B:2119:ILE:HG12	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:LEU:HA	1:B:2147:MSE:HE3	1.94	0.48
1:A:1177:GLU:OE2	1:B:2180:SER:HB3	2.12	0.48
1:A:1019:ILE:HD11	1:A:1112:ALA:O	2.14	0.48
1:B:2000:HIS:O	1:B:2004:ARG:HB2	2.14	0.48
1:A:1103:VAL:HG11	1:B:2147:MSE:CG	2.44	0.48
1:A:1113:VAL:HG12	1:A:1114:PRO:O	2.13	0.48
1:A:1068:ARG:HG3	1:A:1069:ILE:H	1.79	0.48
1:A:1110:VAL:HG11	1:A:1120:VAL:HG21	1.94	0.47
1:B:2031:LEU:C	1:B:2033:THR:N	2.67	0.47
1:A:1182:GLY:CA	1:B:2181:MSE:HE2	2.45	0.47
1:B:2096:GLU:CG	1:B:2099:ARG:HD2	2.44	0.47
1:A:1100:VAL:O	1:B:2147:MSE:HE3	2.15	0.47
1:A:1018:ILE:CG1	1:A:1059:GLU:OE1	2.62	0.47
1:A:1216:ILE:HG22	1:B:2214:VAL:HG11	1.97	0.47
1:A:1218:VAL:CG1	1:A:1219:ASP:H	2.28	0.47
1:A:1218:VAL:HG13	1:A:1219:ASP:H	1.79	0.47
1:A:1109:LEU:O	1:A:1109:LEU:HG	2.15	0.47
1:A:1014:PHE:CZ	1:A:1059:GLU:HG3	2.50	0.47
1:B:2142:TYR:O	1:B:2146:ILE:HG13	2.14	0.47
1:A:1078:LEU:O	1:A:1081:PHE:HB3	2.14	0.47
1:A:1171:PHE:CE1	1:A:1174:MSE:HE2	2.49	0.47
1:A:999:SER:HA	1:A:1002:TYR:HB3	1.97	0.47
1:B:2014:PHE:CZ	1:B:2059:GLU:HG3	2.49	0.47
1:A:1027:ILE:O	1:A:1031:LEU:CD1	2.63	0.47
1:B:2156:PHE:CD1	1:B:2187:LEU:HD12	2.50	0.47
1:B:2068:ARG:HG3	1:B:2069:ILE:H	1.81	0.46
1:B:2032:GLU:CG	1:B:2038:MSE:HE3	2.46	0.46
1:A:1106:LEU:HB2	1:B:2143:ILE:HD12	1.96	0.46
1:A:1087:SER:HA	1:A:1102:ARG:HG2	1.98	0.46
1:A:1035:LYS:O	1:A:1038:MSE:HB2	2.16	0.46
1:A:1137:MSE:CE	1:A:1209:MSE:HE3	2.46	0.46
1:A:1048:PHE:O	1:A:1052:VAL:HG23	2.15	0.46
1:A:1101:LEU:HA	1:B:2147:MSE:CE	2.45	0.46
1:B:2096:GLU:OE2	1:B:2099:ARG:CD	2.64	0.46
1:A:1066:VAL:HG12	1:A:1066:VAL:O	2.14	0.46
1:A:1097:ILE:HG13	1:A:1098:LEU:N	2.32	0.45
1:B:2118:LYS:CA	1:B:2118:LYS:HE2	2.46	0.45
1:B:2064:ILE:HD12	1:B:2072:PHE:CE1	2.52	0.45
1:A:1110:VAL:CG1	1:A:1120:VAL:HG21	2.47	0.45
1:B:2209:MSE:HE2	1:B:2209:MSE:HA	1.98	0.45
1:B:2071:PHE:C	1:B:2073:LYS:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2126:VAL:C	1:B:2128:PRO:HD2	2.36	0.44
1:B:2115:GLN:H	1:B:2118:LYS:HG2	1.82	0.44
1:B:2002:TYR:HD1	1:B:2003:LEU:CA	2.30	0.44
1:A:1036:THR:HG22	1:A:1037:PHE:N	2.33	0.44
1:B:2156:PHE:CE1	1:B:2187:LEU:HD12	2.51	0.44
1:A:1085:ALA:O	1:A:1088:LEU:HB2	2.18	0.44
1:B:2087:SER:OG	1:B:2105:ARG:NH2	2.51	0.44
1:A:1174:MSE:HG3	1:A:1205:VAL:HG11	1.98	0.44
1:A:1103:VAL:HG22	1:A:1103:VAL:O	2.18	0.44
1:A:1217:ILE:HG13	1:A:1218:VAL:N	2.33	0.43
1:A:1027:ILE:O	1:A:1031:LEU:HD12	2.18	0.43
1:B:2003:LEU:O	1:B:2007:ASN:OD1	2.36	0.43
1:B:2071:PHE:CE1	1:B:2077:SER:HB2	2.53	0.43
1:B:2085:ALA:HA	1:B:2088:LEU:HD12	1.99	0.43
1:A:1047:LEU:HD23	1:A:1047:LEU:HA	1.80	0.43
1:A:1184:VAL:O	1:A:1188:MSE:HG3	2.19	0.43
1:B:2056:PHE:CE2	1:B:2108:ARG:NH1	2.87	0.43
1:B:2184:VAL:O	1:B:2188:MSE:HG3	2.19	0.43
1:B:2084:VAL:O	1:B:2088:LEU:HG	2.18	0.43
1:B:2169:THR:O	1:B:2173:VAL:HG23	2.18	0.43
1:B:2043:VAL:HA	1:B:2046:THR:OG1	2.18	0.43
1:A:1085:ALA:HA	1:A:1088:LEU:HD12	2.01	0.43
1:A:1104:LEU:O	1:A:1107:PHE:HB2	2.19	0.43
1:B:2025:ASN:OD1	1:B:2105:ARG:HD2	2.19	0.43
1:B:2114:PRO:O	1:B:2115:GLN:CB	2.67	0.43
1:B:2123:LEU:O	1:B:2126:VAL:HG23	2.19	0.42
1:A:1204:VAL:O	1:A:1208:VAL:HG23	2.19	0.42
1:A:1116:MSE:HE2	1:A:1116:MSE:HA	2.01	0.42
1:B:2005:ILE:O	1:B:2008:ILE:N	2.52	0.42
1:B:2185:ARG:HB2	1:B:2186:PRO:CD	2.45	0.42
1:B:2109:LEU:O	1:B:2109:LEU:HG	2.19	0.42
1:B:2029:MSE:SE	1:B:2106:LEU:HD21	2.69	0.42
1:A:1092:SER:O	1:A:1093:SER:HB2	2.19	0.42
1:B:2206:THR:O	1:B:2210:ILE:HG13	2.20	0.42
1:A:1114:PRO:O	1:A:1115:GLN:CB	2.66	0.42
1:B:2116:MSE:HA	1:B:2116:MSE:HE2	2.01	0.42
1:B:2103:VAL:CG2	1:B:2103:VAL:O	2.67	0.42
1:B:2092:SER:O	1:B:2093:SER:HB2	2.19	0.42
1:A:1096:GLU:HG3	1:A:1099:ARG:HB3	2.00	0.42
1:B:2012:SER:O	1:B:2013:PHE:C	2.58	0.42
1:A:1199:ILE:O	1:A:1203:PHE:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:VAL:O	1:A:1023:VAL:HG12	2.21	0.41
1:A:1068:ARG:HA	1:A:1068:ARG:HD2	1.93	0.41
1:A:1198:PHE:O	1:A:1202:ILE:HG13	2.20	0.41
1:A:1069:ILE:O	1:A:1069:ILE:HG12	2.21	0.41
1:B:2110:VAL:HG11	1:B:2120:VAL:HG21	2.01	0.41
1:B:2066:VAL:HG12	1:B:2066:VAL:O	2.21	0.41
1:B:2126:VAL:HG11	1:B:2216:ILE:HD13	2.03	0.41
1:B:2068:ARG:HD2	1:B:2068:ARG:HA	1.94	0.41
1:A:1065:TYR:HA	1:A:1065:TYR:HD2	1.75	0.41
1:A:1034:SER:O	1:A:1038:MSE:HG2	2.21	0.41
1:A:1137:MSE:HG2	2:B:4001:PX4:C17	2.51	0.41
1:A:1076:TRP:CH2	1:A:1117:ARG:HA	2.56	0.40
1:A:1157:PRO:O	1:A:1165:GLU:OE2	2.39	0.40
1:B:2101:LEU:O	1:B:2104:LEU:HB2	2.21	0.40
1:B:2068:ARG:O	1:B:2071:PHE:HB3	2.21	0.40
1:A:1031:LEU:C	1:A:1033:THR:N	2.75	0.40
1:A:1014:PHE:CZ	1:A:1059:GLU:CG	3.04	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	221/285 (78%)	203 (92%)	18 (8%)	0	100	100
1	B	221/285 (78%)	187 (85%)	31 (14%)	3 (1%)	14	49
All	All	442/570 (78%)	390 (88%)	49 (11%)	3 (1%)	26	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2220	ALA

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Mol	Chain	Res	Type
1	B	2072	PHE
1	B	2178	SER

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	205/252 (81%)	192 (94%)	13 (6%)	22	58
1	B	205/252 (81%)	191 (93%)	14 (7%)	20	54
All	All	410/504 (81%)	383 (93%)	27 (7%)	21	55

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1012	SER
1	A	1028	THR
1	A	1032	GLU
1	A	1033	THR
1	A	1036	THR
1	A	1065	TYR
1	A	1070	SER
1	A	1080	ASP
1	A	1095	PHE
1	A	1107	PHE
1	A	1108	ARG
1	A	1167	PHE
1	A	1177	GLU
1	B	2001	MSE
1	B	2002	TYR
1	B	2028	THR
1	B	2033	THR
1	B	2041	PHE
1	B	2046	THR
1	B	2070	SER
1	B	2080	ASP

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Mol	Chain	Res	Type
1	B	2095	PHE
1	B	2107	PHE
1	B	2126	VAL
1	B	2163	LEU
1	B	2167	PHE
1	B	2177	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1000	HIS
1	A	1150	GLN
1	B	2007	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PX4	A	4002	-	15,15,45	0.90	1 (6%)	15,19,53	1.01	0
2	PX4	A	4003	-	16,16,45	1.04	1 (6%)	18,20,53	1.23	2 (11%)
2	PX4	A	4004	-	4,4,45	1.98	2 (50%)	6,6,53	1.22	1 (16%)
2	PX4	A	4007	-	5,5,45	0.39	0	4,4,53	0.21	0
2	PX4	A	4013	-	16,16,45	1.02	1 (6%)	18,20,53	1.23	2 (11%)
2	PX4	A	4014	-	4,4,45	1.93	2 (50%)	6,6,53	1.24	1 (16%)
2	PX4	B	4001	-	20,20,45	0.79	1 (5%)	21,24,53	0.84	0
2	PX4	B	4011	-	20,20,45	0.77	1 (5%)	21,24,53	0.88	1 (4%)
2	PX4	B	4012	-	12,12,45	1.28	2 (16%)	14,16,53	1.18	1 (7%)
2	PX4	B	4017	-	5,5,45	0.40	0	4,4,53	0.21	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	4002	-	-	0/17/17/49	0/0/0/0
2	PX4	A	4003	-	-	0/16/16/49	0/0/0/0
2	PX4	A	4004	-	-	0/0/0/49	0/0/0/0
2	PX4	A	4007	-	-	0/3/3/49	0/0/0/0
2	PX4	A	4013	-	-	0/16/16/49	0/0/0/0
2	PX4	A	4014	-	-	0/0/0/49	0/0/0/0
2	PX4	B	4001	-	-	0/22/22/49	0/0/0/0
2	PX4	B	4011	-	-	0/22/22/49	0/0/0/0
2	PX4	B	4012	-	-	0/12/12/49	0/0/0/0
2	PX4	B	4017	-	-	0/3/3/49	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4002	PX4	O7-C23	2.09	1.40	1.35
2	B	4001	PX4	P1-O3	2.14	1.67	1.59
2	B	4011	PX4	P1-O3	2.18	1.67	1.59
2	B	4012	PX4	O7-C23	2.46	1.40	1.35
2	A	4014	PX4	P1-O3	2.63	1.64	1.54
2	A	4014	PX4	P1-O4	2.67	1.64	1.54
2	A	4004	PX4	P1-O4	2.70	1.64	1.54
2	A	4003	PX4	P1-O3	2.71	1.64	1.54
2	A	4013	PX4	P1-O3	2.72	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4004	PX4	P1-O3	2.74	1.64	1.54
2	B	4012	PX4	P1-O3	2.77	1.64	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4013	PX4	O5-C9-C10	-2.47	104.38	111.90
2	A	4003	PX4	O5-C9-C10	-2.41	104.55	111.90
2	B	4011	PX4	O5-C9-C10	-2.01	105.78	111.90
2	A	4004	PX4	O1-P1-O2	2.06	119.88	111.05
2	A	4014	PX4	O1-P1-O2	2.16	120.31	111.05
2	A	4013	PX4	O1-P1-O2	2.79	119.57	110.58
2	A	4003	PX4	O1-P1-O2	2.84	119.71	110.58
2	B	4012	PX4	O1-P1-O2	2.94	120.03	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4013	PX4	2	0
2	B	4001	PX4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	212/285 (74%)	0.45	13 (6%)	25 13	56, 106, 177, 249	0
1	B	212/285 (74%)	0.45	16 (7%)	17 9	56, 106, 171, 266	0
All	All	424/570 (74%)	0.45	29 (6%)	20 11	56, 106, 174, 266	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2098	LEU	8.0
1	A	1095	PHE	5.0
1	B	2090	PRO	4.8
1	B	2093	SER	4.7
1	B	2088	LEU	4.4
1	A	1098	LEU	3.8
1	B	2094	GLY	3.5
1	A	1217	ILE	3.4
1	A	1221	CYS	3.2
1	A	1094	GLY	3.1
1	B	2053	ILE	2.8
1	A	1060	ILE	2.7
1	A	1047	LEU	2.6
1	A	1064	ILE	2.6
1	A	1065	TYR	2.6
1	B	2092	SER	2.5
1	B	2097	ILE	2.5
1	A	1005	ILE	2.5
1	B	2013	PHE	2.4
1	B	2061	ILE	2.4
1	B	2054	THR	2.3
1	B	2035	LYS	2.3
1	B	2072	PHE	2.3
1	B	2214	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1045	THR	2.2
1	A	1051	ILE	2.2
1	A	1218	VAL	2.1
1	B	2218	VAL	2.1
1	B	2065	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PX4	A	4003	17/46	0.68	0.36	1.43	63,136,136,136	0
2	PX4	B	4011	21/46	0.76	0.24	0.96	63,115,115,115	0
2	PX4	A	4013	17/46	0.71	0.21	0.27	63,140,140,140	0
2	PX4	B	4001	21/46	0.80	0.21	0.10	63,117,117,117	0
2	PX4	B	4017	6/46	0.78	0.22	-0.16	86,86,86,86	0
2	PX4	B	4012	13/46	0.72	0.24	-0.33	135,135,135,135	0
2	PX4	A	4002	16/46	0.73	0.19	-0.72	138,138,138,138	0
2	PX4	A	4007	6/46	0.73	0.20	-0.80	88,88,88,88	0
2	PX4	A	4004	5/46	0.56	0.28	-	165,165,165,165	0
2	PX4	A	4014	5/46	0.84	0.16	-	161,161,161,161	0

6.5 Other polymers [i](#)

There are no such residues in this entry.