

# Full wwPDB X-ray Structure Validation Report (i)

### Sep 6, 2023 – 09:04 AM EDT

PDB ID	:	4EKW
Title	:	Crystal structure of the NavAb voltage-gated sodium channel (wild-type, 3.2
		A)
Authors	:	Payandeh, J.; Gamal El-Din, T.M.; Scheuer, T.; Zheng, N.; Catterall, W.A.
Deposited on	:	2012-04-10
Resolution	:	3.21 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.21 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	285	11%	52%	23	% •	23%	
1	В	285	11%	41%	31%	•	23%	
1	С	285	8%	49%	24%	·	25%	
1	D	285	12%	43%	31%	·	24%	



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# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7218 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1 1	210	Total	С	Ν	0	Se	0	0	0
	A	219	1799	1228	268	292	11	0		0
1	В	210	Total	С	Ν	0	Se	0	0	Ο
	219	1799	1228	268	292	11	0	0	U	
1	1 0	C 912	Total	С	Ν	0	Se	0	0	0
	215	1756	1199	262	284	11	0	U	U	
1 D	217	Total	С	Ν	0	Se	0	0	0	
	217	1784	1219	266	288	11			U	

• Molecule 1 is a protein called Ion transport protein.

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	983	MSE	-	initiating methionine	UNP A8EVM5
А	984	ASP	-	expression tag	UNP A8EVM5
А	985	TYR	-	expression tag	UNP A8EVM5
А	986	LYS	-	expression tag	UNP A8EVM5
А	987	ASP	-	expression tag	UNP A8EVM5
А	988	ASP	-	expression tag	UNP A8EVM5
А	989	ASP	-	expression tag	UNP A8EVM5
А	990	ASP	-	expression tag	UNP A8EVM5
А	991	LYS	-	expression tag	UNP A8EVM5
А	992	GLY	-	expression tag	UNP A8EVM5
А	993	SER	-	expression tag	UNP A8EVM5
А	994	LEU	-	expression tag	UNP A8EVM5
А	995	VAL	-	expression tag	UNP A8EVM5
А	996	PRO	-	expression tag	UNP A8EVM5
А	997	ARG	-	expression tag	UNP A8EVM5
А	998	GLY	-	expression tag	UNP A8EVM5
А	999	SER	-	expression tag	UNP A8EVM5
А	1000	HIS	-	expression tag	UNP A8EVM5
В	983	MSE	-	initiating methionine	UNP A8EVM5
В	984	ASP	-	expression tag	UNP A8EVM5
В	985	TYR	-	expression tag	UNP A8EVM5



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Chain	Residue	Modelled	Actual	Comment	Reference
В	986	LYS	-	expression tag	UNP A8EVM5
В	987	ASP	-	expression tag	UNP A8EVM5
В	988	ASP	-	expression tag	UNP A8EVM5
В	989	ASP	-	expression tag	UNP A8EVM5
В	990	ASP	-	expression tag	UNP A8EVM5
В	991	LYS	-	expression tag	UNP A8EVM5
В	992	GLY	_	expression tag	UNP A8EVM5
В	993	SER	_	expression tag	UNP A8EVM5
В	994	LEU	_	expression tag	UNP A8EVM5
В	995	VAL	-	expression tag	UNP A8EVM5
В	996	PRO	-	expression tag	UNP A8EVM5
В	997	ARG	-	expression tag	UNP A8EVM5
В	998	GLY	-	expression tag	UNP A8EVM5
В	999	SER	-	expression tag	UNP A8EVM5
В	1000	HIS	-	expression tag	UNP A8EVM5
С	983	MSE	-	initiating methionine	UNP A8EVM5
С	984	ASP	-	expression tag	UNP A8EVM5
С	985	TYR	-	expression tag	UNP A8EVM5
С	986	LYS	-	expression tag	UNP A8EVM5
С	987	ASP	-	expression tag	UNP A8EVM5
С	988	ASP	-	expression tag	UNP A8EVM5
С	989	ASP	-	expression tag	UNP A8EVM5
С	990	ASP	-	expression tag	UNP A8EVM5
С	991	LYS	-	expression tag	UNP A8EVM5
С	992	GLY	-	expression tag	UNP A8EVM5
С	993	SER	-	expression tag	UNP A8EVM5
С	994	LEU	-	expression tag	UNP A8EVM5
С	995	VAL	-	expression tag	UNP A8EVM5
С	996	PRO	-	expression tag	UNP A8EVM5
С	997	ARG	-	expression tag	UNP A8EVM5
С	998	GLY	-	expression tag	UNP A8EVM5
C	999	SER	-	expression tag	UNP A8EVM5
С	1000	HIS	-	expression tag	UNP A8EVM5
D	983	MSE	-	initiating methionine	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 $A8EVM\overline{5}$
D	991	LYS	-	expression tag	UNP A8EVM5



Chain	Residue	Modelled	Actual	Comment	Reference
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

• 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	А	1	Total C O P 14 6 7 1	0	0
2	В	1	Total         C         O         P           9         3         5         1	0	0
2	В	1	Total         C         O         P           6         1         4         1	0	0
2	С	1	Total         C         O         P           20         12         7         1	0	0
2	D	1	Total         C         N         O         P           8         2         1         4         1	0	0

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total O 1 1	0	0
4	В	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0



# 3 Residue-property plots (i)

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



• Molecule 1: Ion transport protein







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42	Depositor
Cell constants	125.86Å 125.86Å 192.64Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	50.00 - 3.21	Depositor
Resolution (A)	48.60 - 3.21	EDS
% Data completeness	96.4 (50.00-3.21)	Depositor
(in resolution range)	96.6(48.60-3.21)	EDS
R <sub>merge</sub>	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.21 (at 3.19 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
D D	0.308 , $0.322$	Depositor
$\Lambda, \Lambda_{free}$	0.315 , $0.323$	DCC
$R_{free}$ test set	2401  reflections  (5.07%)	wwPDB-VP
Wilson B-factor $(Å^2)$	99.5	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, $62.9$	EDS
L-test for $twinning^2$	$< L >=0.44, < L^2>=0.26$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
Depented twinning fraction	0.496 for H, K, L	Deperitor
Reported twinning fraction	0.504 for K, H, -L	Depositor
Outliers	0 of 47387 reflections	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	7218	wwPDB-VP
Average B, all atoms $(Å^2)$	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 25.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1712e-03.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for a centric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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,  $\rm PO4$ 

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).

Mal	Chain	Bo	nd lengths	Bond	angles
1VIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.56	0/1840	0.63	0/2487
1	В	0.57	1/1840~(0.1%)	0.62	0/2487
1	С	0.54	0/1797	0.59	0/2427
1	D	0.55	1/1825~(0.1%)	0.60	0/2466
All	All	0.56	2/7302~(0.0%)	0.61	0/9867

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1195	TRP	CD2-CE2	5.07	1.47	1.41
1	В	1076	TRP	CD2-CE2	5.05	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1799	0	1875	47	1
1	В	1799	0	1875	68	1
1	С	1756	0	1826	47	0
1	D	1784	0	1862	69	0
2	А	14	0	5	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	15	0	4	0	0
2	С	20	0	17	0	0
2	D	8	0	4	0	0
3	А	5	0	0	0	0
3	В	5	0	0	0	0
3	С	5	0	0	0	0
3	D	5	0	0	0	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
4	D	1	0	0	0	0
All	All	7218	0	7468	210	1

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 14.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:1130:MSE:HE3	1:B:1212:LEU:HD11	1.36	1.07
1:A:1141:PHE:HZ	1:A:1174:MSE:SE	2.11	0.83
1:D:1131:LEU:HA	1:D:1134:ILE:HG22	1.62	0.82
1:C:1147:MSE:HE2	1:C:1147:MSE:HA	1.58	0.82
1:A:1174:MSE:HG3	1:A:1205:VAL:HG11	1.65	0.79
1:A:1107:PHE:CD1	1:B:1143:ILE:HD13	2.19	0.78
1:D:1174:MSE:HG3	1:D:1205:VAL:CG1	2.14	0.76
1:D:1174:MSE:HG3	1:D:1205:VAL:HG13	1.69	0.74
1:D:1183:ILE:O	1:D:1187:LEU:HB2	1.89	0.73
1:B:1018:ILE:HD11	1:B:1108:ARG:NH1	2.04	0.73
1:C:1103:VAL:HG21	1:D:1147:MSE:HG2	1.69	0.72
1:A:1058:ILE:O	1:A:1062:LEU:HG	1.90	0.72
1:A:1141:PHE:CZ	1:A:1174:MSE:SE	2.91	0.72
1:B:1018:ILE:HD11	1:B:1108:ARG:HH12	1.55	0.71
1:C:1209:MSE:HE2	1:C:1209:MSE:HA	1.71	0.71
1:D:1170:LEU:HB3	1:D:1201:PHE:CZ	2.26	0.70
1:D:1181:MSE:HA	1:D:1185:ARG:HG3	1.74	0.69
1:C:1200:PRO:HA	1:C:1203:PHE:HB2	1.74	0.69
1:D:1211:ASN:HA	1:D:1214:VAL:HG23	1.76	0.68
1:B:1130:MSE:CE	1:B:1212:LEU:HD11	2.22	0.67
1:A:1015:THR:O	1:A:1019:ILE:HG12	1.93	0.67
1:B:1060:ILE:O	1:B:1064:ILE:HG12	1.94	0.67
1:B:1076:TRP:HB3	1:B:1111:THR:HG23	1.75	0.67



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1130:MSE:HE3	1:B:1212:LEU:CD1	2.21	0.66
1:D:1206:THR:O	1:D:1210:ILE:HG13	1.96	0.65
1:A:1177:GLU:OE1	1:B:1178:SER:HA	1.96	0.65
1:D:1028:THR:HA	1:D:1031:LEU:HD12	1.78	0.65
1:A:1119:ILE:HD13	1:B:1136:LEU:HB2	1.78	0.64
1:A:1185:ARG:HB2	1:A:1186:PRO:HD3	1.79	0.64
1:B:1130:MSE:HE2	1:B:1134:ILE:HD11	1.80	0.63
1:B:1005:ILE:HA	1:B:1008:ILE:HD12	1.79	0.63
1:C:1185:ARG:HB2	1:C:1186:PRO:HD3	1.80	0.63
1:B:1119:ILE:O	1:B:1123:LEU:HG	1.98	0.62
1:D:1144:PHE:CD2	1:D:1201:PHE:HD1	2.17	0.61
1:B:1052:VAL:O	1:B:1055:ILE:HG22	2.01	0.61
1:C:1147:MSE:HA	1:C:1147:MSE:CE	2.30	0.60
1:C:1144:PHE:CE2	1:C:1201:PHE:HB2	2.36	0.60
1:A:1152:PHE:HB3	1:A:1187:LEU:HD11	1.84	0.60
1:D:1137:MSE:HE2	1:D:1137:MSE:HA	1.84	0.59
1:B:1022:ILE:HG21	1:B:1109:LEU:HB2	1.85	0.59
1:B:1182:GLY:O	1:B:1183:ILE:HD13	2.03	0.59
1:D:1120:VAL:O	1:D:1124:ILE:HG13	2.03	0.58
1:D:1191:TYR:O	1:D:1193:TYR:N	2.37	0.58
1:B:1153:GLY:HA2	1:B:1156:PHE:O	2.04	0.58
1:C:1103:VAL:HG21	1:D:1147:MSE:CG	2.33	0.58
1:B:1101:LEU:HB3	1:B:1104:LEU:HD12	1.84	0.58
1:D:1185:ARG:HB2	1:D:1186:PRO:HD3	1.86	0.57
1:D:1008:ILE:HG22	1:D:1014:PHE:HD1	1.68	0.57
1:B:1176:LEU:HA	1:B:1179:TRP:HB3	1.86	0.57
1:A:1214:VAL:HA	1:A:1217:ILE:HD12	1.86	0.57
1:B:1183:ILE:HG22	1:B:1184:VAL:N	2.20	0.56
1:B:1053:ILE:HD11	1:B:1088:LEU:HD23	1.86	0.56
1:D:1177:GLU:OE2	1:D:1178:SER:OG	2.20	0.56
1:A:1184:VAL:O	1:A:1188:MSE:HG3	2.06	0.56
1:A:1107:PHE:CG	1:B:1143:ILE:HD13	2.41	0.56
1:B:1133:VAL:HG11	1:B:1212:LEU:HB2	1.88	0.55
1:C:1015:THR:HA	1:C:1018:ILE:HD12	1.89	0.55
1:A:1180:SER:OG	1:A:1181:MSE:N	2.38	0.55
1:C:1033:THR:HG23	1:D:1149:THR:HG21	1.89	0.55
1:C:1157:PRO:HA	1:C:1161:GLY:HA3	1.89	0.55
1:B:1127:ILE:HA	1:B:1130:MSE:HB2	1.88	0.55
1:D:1210:ILE:O	1:D:1213:VAL:HB	2.06	0.55
1:C:1188:MSE:HA	1:C:1191:TYR:O	2.06	0.54
1:C:1193:TYR:O	1:C:1195:TRP:N	2.39	0.54



	the second se	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1130:MSE:HG3	1:B:1216:ILE:HD11	1.90	0.54
1:D:1067:HIS:ND1	1:D:1067:HIS:N	2.56	0.54
1:D:1191:TYR:O	1:D:1194:ALA:N	2.40	0.54
1:C:1119:ILE:HG13	1:D:1132:SER:HB3	1.90	0.53
1:D:1124:ILE:HG23	1:D:1127:ILE:HD12	1.90	0.53
1:D:1155:ARG:O	1:D:1157:PRO:HD3	2.07	0.53
1:A:1100:VAL:O	1:A:1103:VAL:HG22	2.09	0.53
1:D:1207:PHE:HA	1:D:1210:ILE:HD12	1.90	0.53
1:B:1083:VAL:HA	1:B:1086:ILE:HD12	1.90	0.53
1:D:1008:ILE:HG22	1:D:1014:PHE:CD1	2.44	0.53
1:D:1146:ILE:HG12	1:D:1163:LEU:HD21	1.90	0.53
1:D:1005:ILE:HG23	1:D:1006:THR:H	1.74	0.53
1:C:1064:ILE:HD11	1:C:1081:PHE:HE1	1.73	0.52
1:D:1005:ILE:HD11	1:D:1062:LEU:HA	1.91	0.52
1:B:1087:SER:HA	1:B:1102:ARG:HG2	1.91	0.52
1:C:1107:PHE:CE1	1:D:1143:ILE:HD13	2.45	0.52
1:C:1127:ILE:HB	1:C:1128:PRO:HD3	1.92	0.52
1:A:1172:GLN:HE22	1:B:1181:MSE:SE	2.43	0.51
1:D:1071:PHE:CE1	1:D:1077:SER:HB3	2.46	0.51
1:D:1025:ASN:HA	1:D:1028:THR:HG22	1.93	0.51
1:C:1179:TRP:O	1:C:1184:VAL:HG23	2.11	0.51
1:D:1160:PHE:CZ	1:D:1198:PHE:HZ	2.29	0.51
1:C:1121:SER:HA	1:C:1124:ILE:HD12	1.93	0.51
1:D:1025:ASN:O	1:D:1029:MSE:HB2	2.11	0.51
1:A:1176:LEU:O	1:A:1179:TRP:HD1	1.92	0.50
1:D:1065:TYR:HE2	1:D:1068:ARG:HH21	1.59	0.50
1:B:1193:TYR:O	1:B:1196:VAL:HG23	2.11	0.50
1:B:1004:ARG:O	1:B:1008:ILE:HG13	2.12	0.50
1:D:1069:ILE:O	1:D:1073:LYS:HG3	2.11	0.50
1:A:1097:ILE:O	1:A:1101:LEU:HD12	2.11	0.50
1:D:1201:PHE:O	1:D:1205:VAL:HB	2.12	0.50
1:D:1201:PHE:CE2	1:D:1205:VAL:HG21	2.47	0.50
1:A:1103:VAL:HG23	1:B:1147:MSE:HG2	1.94	0.50
1:D:1160:PHE:CZ	1:D:1198:PHE:CZ	2.99	0.50
1:B:1067:HIS:HB2	1:B:1070:SER:HB2	1.93	0.49
1:B:1207:PHE:O	1:B:1211:ASN:ND2	2.45	0.49
1:B:1045:THR:HA	1:B:1048:PHE:HB3	1.94	0.49
1:D:1160:PHE:CZ	1:D:1169:THR:HG21	2.47	0.49
1:C:1033:THR:OG1	1:D:1163:LEU:HD23	2.12	0.49
1:D:1048:PHE:HA	1:D:1051:ILE:HD12	1.93	0.49
1:A:1140:PHE:CZ	1:A:1201:PHE:HA	2.47	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1156:PHE:CZ	1:D:1158:GLU:OE2	2.65	0.49
1:D:1076:TRP:HB3	1:D:1111:THR:HG23	1.94	0.49
1:C:1130:MSE:O	1:C:1134:ILE:HG13	2.12	0.49
1:A:1109:LEU:HG	1:B:1139:LEU:HD21	1.95	0.48
1:A:1114:PRO:HA	1:A:1117:ARG:HB2	1.94	0.48
1:C:1209:MSE:HA	1:C:1209:MSE:CE	2.41	0.48
1:B:1207:PHE:HA	1:B:1210:ILE:HD12	1.94	0.48
1:B:1106:LEU:C	1:B:1108:ARG:H	2.17	0.48
1:A:1098:LEU:HA	1:A:1101:LEU:HD12	1.96	0.47
1:B:1206:THR:HG22	1:B:1210:ILE:HD11	1.96	0.47
1:D:1174:MSE:HE3	1:D:1209:MSE:HE3	1.95	0.47
1:B:1162:THR:HG22	1:B:1163:LEU:N	2.30	0.47
1:D:1174:MSE:HG3	1:D:1205:VAL:HG11	1.94	0.47
1:A:1179:TRP:O	1:A:1184:VAL:HG23	2.15	0.47
1:A:1057:THR:O	1:A:1060:ILE:HG22	2.14	0.47
1:B:1006:THR:HG23	1:B:1066:VAL:HG13	1.97	0.47
1:C:1071:PHE:CE2	1:C:1077:SER:HB3	2.50	0.47
1:B:1208:VAL:HG12	1:B:1208:VAL:O	2.14	0.47
1:A:1140:PHE:HZ	1:A:1201:PHE:HA	1.80	0.46
1:B:1029:MSE:C	1:B:1031:LEU:H	2.17	0.46
1:B:1199:ILE:HB	1:B:1200:PRO:HD3	1.96	0.46
1:B:1146:ILE:O	1:B:1149:THR:N	2.47	0.46
1:C:1162:THR:O	1:C:1165:GLU:N	2.47	0.46
1:D:1158:GLU:OE1	1:D:1158:GLU:HA	2.15	0.46
1:D:1179:TRP:O	1:D:1183:ILE:HB	2.15	0.46
1:B:1059:GLU:HA	1:B:1062:LEU:HD12	1.97	0.46
1:B:1138:THR:HA	1:B:1141:PHE:HB2	1.98	0.46
1:C:1207:PHE:O	1:C:1210:ILE:HB	2.15	0.46
1:C:1162:THR:O	1:C:1163:LEU:C	2.54	0.46
1:A:1110:VAL:HG22	1:B:1139:LEU:HD23	1.98	0.46
1:A:1005:ILE:HA	1:A:1008:ILE:HD12	1.98	0.46
1:D:1191:TYR:O	1:D:1192:PRO:C	2.54	0.46
1:D:1008:ILE:O	1:D:1014:PHE:HB2	2.16	0.46
1:B:1110:VAL:HG11	1:B:1120:VAL:HG21	1.97	0.45
1:C:1098:LEU:HA	1:C:1101:LEU:HD12	1.98	0.45
1:D:1130:MSE:HE3	1:D:1215:ALA:HB3	1.98	0.45
1:A:1103:VAL:CG2	1:B:1147:MSE:HG2	2.45	0.45
1:C:1104:LEU:HD23	1:C:1107:PHE:CD1	2.51	0.45
1:B:1029:MSE:HE1	1:B:1105:ARG:HH21	1.81	0.45
1:A:1071:PHE:CE1	1:A:1077:SER:HB3	2.52	0.45
1:A:1188:MSE:CE	1:A:1195:TRP:HD1	2.29	0.45



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1203:PHE:O	1:A:1204:VAL:C	2.55	0.45
1:D:1128:PRO:HA	1:D:1131:LEU:HD12	1.98	0.45
1:C:1097:ILE:H	1:C:1097:ILE:HG13	1.61	0.45
1:A:1200:PRO:O	1:A:1204:VAL:N	2.41	0.45
1:C:1118:LYS:O	1:C:1121:SER:HB2	2.17	0.45
1:C:1148:ALA:HB1	1:C:1160:PHE:HD2	1.81	0.45
1:D:1126:VAL:HG11	1:D:1216:ILE:HD13	1.97	0.45
1:C:1084:VAL:O	1:C:1087:SER:HB3	2.17	0.44
1:A:1074:ASP:HA	1:A:1075:PRO:HD3	1.88	0.44
1:B:1113:VAL:HA	1:B:1114:PRO:HD3	1.77	0.44
1:A:1174:MSE:CG	1:A:1205:VAL:HG11	2.43	0.44
1:B:1100:VAL:C	1:B:1102:ARG:H	2.19	0.44
1:B:1203:PHE:O	1:B:1207:PHE:HB2	2.17	0.44
1:B:1057:THR:O	1:B:1060:ILE:HG22	2.17	0.44
1:A:1159:TRP:O	1:A:1165:GLU:O	2.35	0.44
1:D:1181:MSE:O	1:D:1186:PRO:HD3	2.17	0.44
1:C:1162:THR:O	1:C:1164:GLY:N	2.50	0.44
1:B:1178:SER:O	1:B:1178:SER:OG	2.34	0.44
1:C:1113:VAL:HA	1:C:1114:PRO:HD3	1.80	0.44
1:C:1026:GLY:O	1:D:1142:TYR:OH	2.35	0.43
1:D:1139:LEU:O	1:D:1143:ILE:HD12	2.18	0.43
1:A:1157:PRO:HG2	1:D:1155:ARG:O	2.17	0.43
1:B:1095:PHE:HB2	1:B:1097:ILE:HG13	2.01	0.43
1:B:1108:ARG:HH11	1:B:1108:ARG:HB3	1.82	0.43
1:B:1139:LEU:O	1:B:1143:ILE:HD12	2.18	0.43
1:D:1211:ASN:HA	1:D:1214:VAL:CG2	2.47	0.43
1:B:1005:ILE:O	1:B:1009:VAL:HG23	2.18	0.43
1:C:1193:TYR:C	1:C:1195:TRP:H	2.22	0.43
1:D:1166:SER:C	1:D:1168:TYR:H	2.22	0.43
1:A:1113:VAL:HA	1:A:1114:PRO:HD3	1.92	0.43
1:D:1188:MSE:C	1:D:1190:VAL:H	2.22	0.42
1:D:1199:ILE:HB	1:D:1200:PRO:HD3	2.02	0.42
1:C:1198:PHE:O	1:C:1202:ILE:HG13	2.18	0.42
1:A:1203:PHE:O	1:A:1206:THR:N	2.51	0.42
1:D:1130:MSE:O	1:D:1134:ILE:N	2.42	0.42
1:A:1071:PHE:C	1:A:1073:LYS:H	2.22	0.42
1:C:1107:PHE:CE1	1:D:1143:ILE:HG21	2.54	0.42
1:B:1080:ASP:OD2	1:B:1111:THR:HG21	2.19	0.42
1:A:1207:PHE:O	1:A:1211:ASN:HB2	2.19	0.42
1:B:1034:SER:HB3	1:B:1037:PHE:HB2	2.02	0.42
1:B:1072:PHE:HD2	1:B:1078:LEU:HD21	1.85	0.42



A 4 1	A t 9	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1083:VAL:HG12	1:B:1105:ARG:HA	2.01	0.42
1:C:1179:TRP:O	1:C:1183:ILE:HB	2.19	0.42
1:C:1207:PHE:HA	1:C:1210:ILE:HD12	2.02	0.42
1:B:1189:GLU:HB3	1:D:1189:GLU:OE1	2.20	0.41
1:C:1137:MSE:HA	1:C:1137:MSE:HE2	2.02	0.41
1:B:1014:PHE:HZ	1:B:1062:LEU:HD13	1.84	0.41
1:A:1108:ARG:HA	1:A:1111:THR:OG1	2.21	0.41
1:D:1162:THR:OG1	1:D:1165:GLU:OE2	2.38	0.41
1:A:1061:ILE:HA	1:A:1064:ILE:HD12	2.01	0.41
1:A:1216:ILE:HG22	1:B:1214:VAL:HG21	2.02	0.41
1:B:1116:MSE:H	1:B:1116:MSE:HG2	1.61	0.41
1:C:1054:THR:O	1:C:1058:ILE:HG12	2.20	0.41
1:C:1206:THR:HA	1:C:1209:MSE:HB2	2.02	0.41
1:D:1197:PHE:O	1:D:1200:PRO:HD2	2.21	0.41
1:A:1170:LEU:HD22	1:A:1201:PHE:CZ	2.56	0.41
1:B:1071:PHE:C	1:B:1073:LYS:H	2.24	0.41
1:C:1169:THR:O	1:C:1172:GLN:HB3	2.21	0.41
1:A:1029:MSE:SE	1:A:1103:VAL:HG12	2.71	0.41
1:C:1110:VAL:HG22	1:C:1116:MSE:HG2	2.02	0.40
1:C:1160:PHE:O	1:C:1162:THR:N	2.53	0.40
1:D:1195:TRP:O	1:D:1199:ILE:HG12	2.20	0.40
1:D:1018:ILE:HG13	1:D:1059:GLU:OE2	2.21	0.40
1:C:1006:THR:O	1:C:1010:GLU:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:SER:OG	1:B:1177:GLU:OE2[2_565]	2.09	0.11

## 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	Perce	entiles
1	А	217/285~(76%)	182 (84%)	30 (14%)	5(2%)	6	33
1	В	217/285~(76%)	180 (83%)	29~(13%)	8 (4%)	3	21
1	С	211/285~(74%)	185 (88%)	17 (8%)	9~(4%)	2	19
1	D	215/285~(75%)	185 (86%)	25~(12%)	5(2%)	6	33
All	All	860/1140~(75%)	732 (85%)	101 (12%)	27 (3%)	4	26

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1068	ARG
1	В	1153	GLY
1	С	1125	SER
1	С	1148	ALA
1	С	1161	GLY
1	С	1194	ALA
1	D	1153	GLY
1	D	1161	GLY
1	А	1093	SER
1	А	1180	SER
1	В	1157	PRO
1	С	1068	ARG
1	D	1141	PHE
1	В	1081	PHE
1	В	1107	PHE
1	С	1163	LEU
1	D	1192	PRO
1	В	1152	PHE
1	С	1167	PHE
1	А	1072	PHE
1	В	1065	TYR
1	С	1093	SER
1	D	1199	ILE
1	А	1200	PRO
1	В	1205	VAL
1	С	1157	PRO
1	В	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.

1

1

All

С

D

All

analysed, and the total number of residues.								
	Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles	
	1	А	202/251~(80%)	190~(94%)	12~(6%)	19	54	
	1	В	202/251~(80%)	189 (94%)	13 (6%)	17	51	

190 (96%)

187 (94%)

756 (94%)

The Analysed column shows the number of residues for which the sidechain conformation was

7 (4%)

13~(6%)

45 (6%)

35

17

21

68

50

56

All (45) residues with a non-rotameric sidechain are listed below:

197/251 (78%)

200/251 (80%)

801/1004 (80%)

Mol	Chain	Res	Type
1	А	1024	LEU
1	А	1025	ASN
1	А	1029	MSE
1	А	1036	THR
1	А	1095	PHE
1	А	1098	LEU
1	А	1107	PHE
1	А	1111	THR
1	А	1133	VAL
1	А	1142	TYR
1	А	1192	PRO
1	А	1203	PHE
1	В	1010	GLU
1	В	1015	THR
1	В	1045	THR
1	В	1060	ILE
1	В	1067	HIS
1	В	1095	PHE
1	В	1108	ARG
1	В	1116	MSE
1	В	1141	PHE
1	В	1163	LEU
1	В	1187	LEU
1	В	1196	VAL
1	В	1211	ASN
1	С	1029	MSE
1	С	1060	ILE
1	С	1095	PHE



Mol	Chain	Res	Type
1	С	1134	ILE
1	С	1154	GLU
1	С	1171	PHE
1	С	1203	PHE
1	D	1002	TYR
1	D	1036	THR
1	D	1040	SER
1	D	1047	LEU
1	D	1067	HIS
1	D	1083	VAL
1	D	1101	LEU
1	D	1121	SER
1	D	1127	ILE
1	D	1141	PHE
1	D	1163	LEU
1	D	1167	PHE
1	D	1212	LEU

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

Mol	Chain	Res	Type
1	А	1172	GLN
1	А	1211	ASN
1	В	1025	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 monosaccharides in this entry.



## 5.6 Ligand geometry (i)

9 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).

Mal	Turne	Chain	Dec	Link	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
INIOI	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PX4	В	1302	-	$5,\!5,\!45$	0.76	0	7,7,53	1.04	0
2	PX4	D	1301	-	7,7,45	0.72	0	9,9,53	0.81	0
3	PO4	А	1302	-	4,4,4	0.77	0	$6,\!6,\!6$	0.59	0
2	PX4	С	1301	-	19,19,45	1.13	1 (5%)	21,23,53	0.89	1 (4%)
3	PO4	В	1303	-	4,4,4	0.75	0	6,6,6	0.64	0
2	PX4	В	1301	-	8,8,45	0.51	0	$10,\!10,\!53$	1.03	0
2	PX4	А	1301	-	13,13,45	1.22	1 (7%)	13,16,53	0.88	1 (7%)
3	PO4	С	1302	-	4,4,4	0.95	0	6,6,6	0.62	0
3	PO4	D	1302	-	4,4,4	0.73	0	6,6,6	0.55	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	В	1302	-	-	0/1/3/49	-
2	PX4	D	1301	-	-	0/5/5/49	-
2	PX4	С	1301	-	-	9/21/21/49	-
2	PX4	В	1301	-	-	2/6/6/49	-
2	PX4	А	1301	-	-	5/15/15/49	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	С	1301	PX4	O5-C9	4.29	1.45	1.33
2	А	1301	PX4	O5-C9	3.60	1.47	1.33

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	1301	PX4	O5-C9-C10	2.19	118.78	111.91
2	А	1301	PX4	O5-C8-C7	2.01	114.28	108.43

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
2	А	1301	PX4	O6-C9-O5-C8
2	В	1301	PX4	O4-C6-C7-C8
2	В	1301	PX4	C6-C7-C8-O5
2	С	1301	PX4	O4-C6-C7-O7
2	С	1301	PX4	O4-C6-C7-C8
2	А	1301	PX4	C6-C7-C8-O5
2	С	1301	PX4	C10-C9-O5-C8
2	С	1301	PX4	C1-O3-P1-O2
2	С	1301	PX4	C12-C13-C14-C15
2	С	1301	PX4	O6-C9-O5-C8
2	А	1301	PX4	O7-C7-C8-O5
2	С	1301	PX4	C11-C12-C13-C14
2	А	1301	PX4	C6-C7-O7-C23
2	А	1301	PX4	C8-C7-O7-C23
2	С	1301	PX4	C11-C10-C9-O5
2	С	1301	PX4	O7-C7-C8-O5

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and similar rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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	А	208/285~(72%)	1.00	32 (15%) 2 1	67, 101, 119, 131	0
1	В	208/285~(72%)	0.96	30 (14%) 2 1	71, 106, 126, 145	0
1	С	202/285~(70%)	0.92	24 (11%) 4 3	67, 117, 132, 147	0
1	D	206/285~(72%)	1.11	33 (16%) 1 1	65, 105, 126, 135	0
All	All	824/1140~(72%)	1.00	119 (14%) 2 1	65, 106, 128, 147	0

All (119) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ	
1	D	1007	ASN	6.8	
1	В	1006	THR	6.4	
1	А	1009	VAL	6.1	
1	D	1033	THR	6.1	
1	D	1009	VAL	6.0	
1	В	1073	LYS	5.8	
1	D	1094	GLY	5.6	
1	D	1183	ILE	5.2	
1	А	1014	PHE	5.2	
1	D	1162	THR	5.0	
1	А	1005	ILE	4.8	
1	D	1006	THR	4.8	
1	С	1115	GLN	4.7	
1	D	1150	GLN	4.6	
1	С	1040	SER	4.5	
1	А	1036	THR	4.4	
1	В	1093	SER	4.2	
1	А	1002	TYR	4.2	
1	С	1092	SER	4.0	
1	В	1160	PHE	4.0	
1	С	1114	PRO	4.0	



Mol	Chain	Res	Type	RSRZ
1	С	1009	VAL	3.9
1	С	1071	PHE	3.9
1	В	1098	LEU	3.8
1	А	1065	TYR	3.8
1	С	1086	ILE	3.8
1	С	1005	ILE	3.7
1	D	1160	PHE	3.6
1	А	1183	ILE	3.5
1	D	1093	SER	3.5
1	В	1019	ILE	3.4
1	В	1150	GLN	3.4
1	В	1062	LEU	3.4
1	В	1094	GLY	3.3
1	D	1161	GLY	3.3
1	А	1076	TRP	3.3
1	В	1095	PHE	3.2
1	D	1045	THR	3.2
1	В	1002	TYR	3.2
1	В	1066	VAL	3.2
1	А	1149	THR	3.2
1	В	1037	PHE	3.1
1	D	1216	ILE	3.1
1	D	1037	PHE	3.1
1	С	1036	THR	3.1
1	А	1128	PRO	3.1
1	В	1126	VAL	3.0
1	В	1069	ILE	3.0
1	С	1064	ILE	2.9
1	В	1183	ILE	2.9
1	D	1098	LEU	2.9
1	С	1002	TYR	2.8
1	С	1008	ILE	2.8
1	С	1168	TYR	2.8
1	A	1068	ARG	2.8
1	А	1047	LEU	2.8
1	A	1071	PHE	2.8
1	В	1117	ARG	2.8
1	С	1149	THR	2.8
1	D	1069	ILE	2.8
1	A	1217	ILE	2.7
1	А	1112	ALA	2.7
1	В	1005	ILE	2.7



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Mol	Chain	Res	Type	RSRZ
1	В	1151	LEU	2.7
1	В	1121	SER	2.7
1	С	1091	THR	2.6
1	А	1070	SER	2.6
1	С	1150	GLN	2.6
1	А	1069	ILE	2.6
1	А	1120	VAL	2.6
1	D	1072	PHE	2.6
1	С	1112	ALA	2.6
1	D	1113	VAL	2.6
1	В	1016	LYS	2.5
1	С	1033	THR	2.5
1	D	1173	VAL	2.5
1	В	1216	ILE	2.5
1	В	1114	PRO	2.5
1	D	1114	PRO	2.4
1	А	1008	ILE	2.4
1	А	1113	VAL	2.4
1	В	1097	ILE	2.4
1	D	1034	SER	2.4
1	D	1119	ILE	2.4
1	D	1047	LEU	2.4
1	D	1070	SER	2.4
1	В	1063	ARG	2.4
1	D	1074	ASP	2.3
1	В	1033	THR	2.3
1	С	1127	ILE	2.3
1	D	1187	LEU	2.3
1	В	1051	ILE	2.3
1	С	1184	VAL	2.3
1	В	1003	LEU	2.3
1	С	1006	THR	2.2
1	С	1075	PRO	2.2
1	D	1149	THR	2.2
1	D	1071	PHE	2.2
1	A	1160	PHE	2.2
1	C	1082	PHE	2.2
1	A	1019	ILE	2.2
1	В	1065	TYR	2.2
1	A	1161	GLY	2.1
1	A	1072	PHE	2.1
1	D	1112	ALA	2.1



Mol	Chain	Res	Type	RSRZ
1	А	1086	ILE	2.1
1	А	1146	ILE	2.1
1	А	1077	SER	2.1
1	А	1150	GLN	2.1
1	С	1152	PHE	2.1
1	А	1095	PHE	2.1
1	А	1162	THR	2.1
1	А	1109	LEU	2.0
1	D	1041	PHE	2.0
1	D	1022	ILE	2.0
1	В	1009	VAL	2.0
1	D	1003	LEU	2.0
1	D	1124	ILE	2.0
1	А	1041	PHE	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 monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	PX4	В	1301	9/46	0.83	0.29	91,99,111,115	0
2	PX4	D	1301	8/46	0.83	0.27	82,101,119,125	0
3	PO4	D	1302	5/5	0.84	0.23	95,99,105,113	0
2	PX4	С	1301	20/46	0.87	0.30	73,86,97,107	0
3	PO4	В	1303	5/5	0.88	0.20	107,107,118,123	0
3	PO4	С	1302	5/5	0.90	0.27	106,107,118,120	0
2	PX4	В	1302	6/46	0.90	0.23	102,104,111,114	0
2	PX4	А	1301	14/46	0.92	0.21	65,75,94,96	0
3	PO4	А	1302	5/5	0.94	0.24	87,95,98,102	0



The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









## 6.5 Other polymers (i)

There are no such residues in this entry.

