



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:27 PM GMT

PDB ID : 1P4O
Title : Structure of Apo unactivated IGF-1R KInase domain at 1.5A resolution.
Authors : Munshi, S.; Kornienko, M.; Hall, D.L.; Darke, P.L.; Waxman, L.; Kuo, L.C.
Deposited on : 2003-04-23
Resolution : 1.50 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

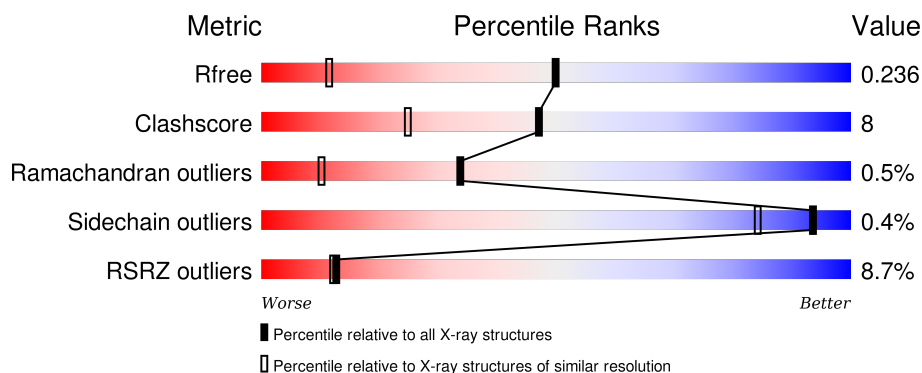
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	322	<div> <div>8%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
1	B	322	<div> <div>9%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5593 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 Insulin-like growth factor I receptor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2455	1562	408	462	23			
1	B	314	Total	C	N	O	S	0	0	0
			2503	1593	416	471	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	943	MET	-	INITIATING MET	UNP P08069
A	1067	ALA	GLU	ENGINEERED	UNP P08069
A	1069	ALA	GLU	ENGINEERED	UNP P08069
B	943	MET	-	INITIATING MET	UNP P08069
B	1067	ALA	GLU	ENGINEERED	UNP P08069
B	1069	ALA	GLU	ENGINEERED	UNP P08069

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	315	Total	O	0	0
			315	315		
2	B	320	Total	O	0	0
			320	320		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.95Å 85.56Å 78.88Å 90.00° 99.10° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 31.52 – 1.50	Depositor EDS
% Data completeness (in resolution range)	80.3 (20.00-1.50) 80.7 (31.52-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 1.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.236 0.209 , 0.236	Depositor DCC
R_{free} test set	10812 reflections (12.15%)	DCC
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	1 of 98622 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5593	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 50.68 % 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 6.2474e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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	0.29	0/2510	0.56	0/3390
1	B	0.29	0/2560	0.58	0/3460
All	All	0.29	0/5070	0.57	0/6850

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2455	0	2412	39	0
1	B	2503	0	2461	40	0
2	A	315	0	0	4	0
2	B	320	0	0	3	0
All	All	5593	0	4873	74	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 8.

All (74) 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:B:1204:PRO:HG2	1:B:1207:CYS:HB2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:GLY:H	1:A:982:MET:HE3	1.47	0.80
1:A:976:GLY:H	1:A:982:MET:CE	1.97	0.77
1:A:1023:VAL:HG21	1:B:947:ASN:ND2	2.06	0.70
1:B:1209:ASP:O	1:B:1213:GLU:HG3	1.92	0.70
1:B:1188:ASN:O	1:B:1192:LEU:HD13	1.94	0.67
1:A:1245:ARG:HB2	1:A:1245:ARG:HH21	1.59	0.67
1:A:1245:ARG:HB2	1:A:1245:ARG:NH2	2.10	0.67
1:A:1020:GLU:CD	1:B:949:GLU:HB3	2.18	0.64
1:B:949:GLU:HG2	1:B:950:TYR:N	2.12	0.64
1:B:1065:ARG:HB3	1:B:1066:PRO:HD3	1.80	0.63
1:B:947:ASN:ND2	1:B:951:PHE:O	2.30	0.62
1:B:1097:ASN:ND2	1:B:1161:THR:OG1	2.32	0.62
1:B:1204:PRO:HG2	1:B:1207:CYS:CB	2.29	0.59
1:A:1138:LYS:HB3	1:A:1144:LEU:HD12	1.85	0.58
1:B:1187:SER:H	1:B:1190:GLN:HE21	1.52	0.57
1:A:1097:ASN:OD1	1:A:1161:THR:OG1	2.21	0.57
1:B:1005:VAL:HG11	1:B:1014:ARG:HG2	1.87	0.56
1:A:1172:LEU:CD1	1:A:1214:LEU:HD22	2.37	0.55
1:A:1020:GLU:OE1	1:B:949:GLU:HB3	2.07	0.55
1:A:976:GLY:N	1:A:982:MET:CE	2.69	0.55
1:B:1017:PHE:CE2	1:B:1047:VAL:HG23	2.42	0.54
1:A:1017:PHE:CE2	1:A:1047:VAL:HG23	2.43	0.53
1:B:949:GLU:HG2	1:B:950:TYR:H	1.73	0.52
1:A:1172:LEU:HD11	1:A:1214:LEU:HD22	1.93	0.51
1:A:1209:ASP:O	1:A:1213:GLU:HG3	2.10	0.51
1:B:1253:GLU:HA	1:B:1256:LYS:HG3	1.92	0.51
1:A:1103:HIS:O	1:A:1104:ARG:HB2	2.10	0.51
1:B:1097:ASN:ND2	1:B:1229:PHE:HD2	2.09	0.51
1:B:1257:LEU:CD1	1:B:1260:PRO:HG3	2.41	0.50
1:B:1103:HIS:O	1:B:1104:ARG:HB2	2.12	0.50
1:A:1245:ARG:CB	1:A:1245:ARG:HH21	2.24	0.49
1:A:1071:ASN:HB2	2:A:233:HOH:O	2.11	0.49
1:B:1187:SER:H	1:B:1190:GLN:NE2	2.11	0.49
1:A:1214:LEU:HD23	1:A:1214:LEU:O	2.13	0.49
1:A:996:PRO:HG2	2:A:359:HOH:O	2.13	0.49
1:A:1030:HIS:HE1	2:A:92:HOH:O	1.96	0.48
1:A:976:GLY:N	1:A:982:MET:HE1	2.27	0.48
1:A:974:GLU:HB3	1:A:982:MET:CE	2.44	0.48
1:A:1011:MET:HB2	1:B:1156:ASP:HB3	1.95	0.47
1:B:949:GLU:CG	1:B:950:TYR:H	2.25	0.47
1:B:1181:GLN:O	1:B:1184:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1177:THR:HG22	1:A:1204:PRO:HB3	1.96	0.47
1:A:1188:ASN:O	1:A:1192:LEU:HG	2.15	0.47
1:B:1007:GLU:HG3	2:B:241:HOH:O	2.14	0.47
1:B:1116:ASP:O	1:B:1117:PHE:HB2	2.15	0.47
1:B:960:ASP:HB2	1:B:961:GLU:OE1	2.16	0.46
1:B:1193:ARG:HG2	2:B:556:HOH:O	2.15	0.46
1:A:1116:ASP:O	1:A:1117:PHE:HB2	2.15	0.46
1:B:1258:PRO:O	1:B:1259:GLU:HB3	2.17	0.45
1:A:1041:GLN:HA	1:A:1041:GLN:NE2	2.31	0.45
1:A:1193:ARG:HG2	1:A:1197:GLU:OE2	2.16	0.45
1:B:1097:ASN:ND2	1:B:1229:PHE:CD2	2.84	0.45
1:B:1257:LEU:HD12	1:B:1260:PRO:HG3	1.98	0.45
1:B:1177:THR:HG22	1:B:1204:PRO:HB3	1.98	0.45
1:B:977:GLN:HE22	1:B:981:GLY:HA2	1.82	0.44
1:B:1079:LEU:O	1:B:1083:ILE:HG13	2.19	0.43
1:B:947:ASN:ND2	2:B:273:HOH:O	2.51	0.43
1:A:1065:ARG:N	1:A:1066:PRO:HD2	2.33	0.43
1:A:1023:VAL:HG21	1:B:947:ASN:HD22	1.82	0.43
1:A:982:MET:CE	1:A:983:VAL:O	2.67	0.42
1:B:947:ASN:HA	1:B:948:PRO:HD3	1.76	0.42
1:A:1075:ALA:HB1	1:A:1076:PRO:HD2	2.02	0.42
1:A:1041:GLN:HA	1:A:1041:GLN:HE21	1.85	0.41
1:B:1259:GLU:HG3	1:B:1259:GLU:O	2.21	0.41
1:A:1004:THR:HG22	1:A:1046:LEU:HD22	2.03	0.41
1:B:1004:THR:HG22	1:B:1046:LEU:CD2	2.51	0.41
1:A:1014:ARG:NH2	1:A:1043:GLN:NE2	2.69	0.41
1:B:1091:ASP:HA	1:B:1233:ILE:HD11	2.03	0.41
1:B:1177:THR:CG2	1:B:1204:PRO:HB3	2.51	0.41
1:A:1004:THR:HG22	1:A:1046:LEU:CD2	2.51	0.41
1:A:1161:THR:HG23	2:A:163:HOH:O	2.21	0.40
1:A:1044:PRO:HG2	1:A:1046:LEU:HD21	2.01	0.40
1:A:960:ASP:HB2	1:A:961:GLU:OE1	2.21	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	306/322 (95%)	298 (97%)	8 (3%)	0	100	100
1	B	312/322 (97%)	302 (97%)	7 (2%)	3 (1%)	19	3
All	All	618/644 (96%)	600 (97%)	15 (2%)	3 (0%)	34	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	949	GLU
1	B	1259	GLU
1	B	948	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	267/280 (95%)	265 (99%)	2 (1%)	88	73
1	B	273/280 (98%)	273 (100%)	0	100	100
All	All	540/560 (96%)	538 (100%)	2 (0%)	93	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1184	GLN
1	A	1253	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	977	GLN
1	A	1019	ASN

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Mol	Chain	Res	Type
1	A	1030	HIS
1	A	1041	GLN
1	A	1043	GLN
1	A	1206	ASN
1	B	947	ASN
1	B	977	GLN
1	B	1019	ASN
1	B	1070	ASN
1	B	1097	ASN
1	B	1190	GLN

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](#)

There are no ligands in this entry.

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	308/322 (95%)	0.49	26 (8%) 14 13	8, 17, 33, 45	0
1	B	314/322 (97%)	0.52	28 (8%) 12 11	8, 16, 33, 53	0
All	All	622/644 (96%)	0.50	54 (8%) 13 12	8, 17, 33, 53	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	948	PRO	19.4
1	B	947	ASN	11.7
1	B	1260	PRO	11.6
1	A	1139	GLY	9.8
1	A	948	PRO	7.7
1	A	1141	LYS	7.2
1	B	1259	GLU	5.6
1	B	1257	LEU	4.8
1	A	1138	LYS	4.7
1	B	1256	LYS	4.6
1	A	1140	GLY	4.6
1	B	949	GLU	4.1
1	B	1139	GLY	4.1
1	A	1185	GLY	3.9
1	A	1184	GLN	3.9
1	B	1258	PRO	3.8
1	B	1184	GLN	3.7
1	A	1065	ARG	3.7
1	B	1069	ALA	3.6
1	A	1070	ASN	3.6
1	A	949	GLU	3.5
1	A	994	ASP	3.4
1	B	1065	ARG	3.2
1	B	994	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1253	GLU	3.2
1	B	1072	PRO	3.2
1	A	1136	TYR	3.1
1	B	1070	ASN	3.1
1	B	1007	GLU	3.1
1	B	1205	ASP	3.0
1	B	1008	ALA	2.8
1	A	1162	TYR	2.8
1	A	1239	GLU	2.8
1	B	1026	GLU	2.6
1	B	1141	LYS	2.6
1	A	1026	GLU	2.6
1	A	1193	ARG	2.6
1	B	1043	GLN	2.6
1	B	1246	GLU	2.5
1	A	1242	PRO	2.5
1	A	1137	ARG	2.5
1	A	1066	PRO	2.5
1	B	1106	LEU	2.4
1	A	1069	ALA	2.3
1	A	1238	GLU	2.3
1	A	1206	ASN	2.3
1	A	1106	LEU	2.3
1	A	1205	ASP	2.3
1	A	1043	GLN	2.3
1	B	1242	PRO	2.2
1	B	1140	GLY	2.1
1	B	1193	ARG	2.0
1	A	1007	GLU	2.0
1	B	1206	ASN	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.