



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2024 – 11:24 AM EDT

PDB ID : 4DJ5
Title : Proteinase K by Langmuir-Blodgett Hanging Drop Method at 1.8Å resolution for Unique Water Distribution
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Deposited on : 2012-02-01
Resolution : 1.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

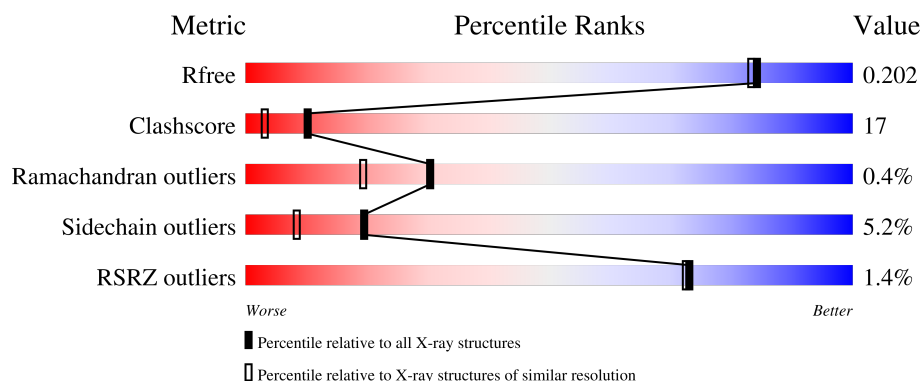
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 $\leq 5\%$. 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	X	279	<div> <div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="margin-left: 10px;"> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 83% 13% </div> </div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2485 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 Proteinase K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	279	Total	C	N	O	S	0	0	0
			2030	1247	357	416	10			

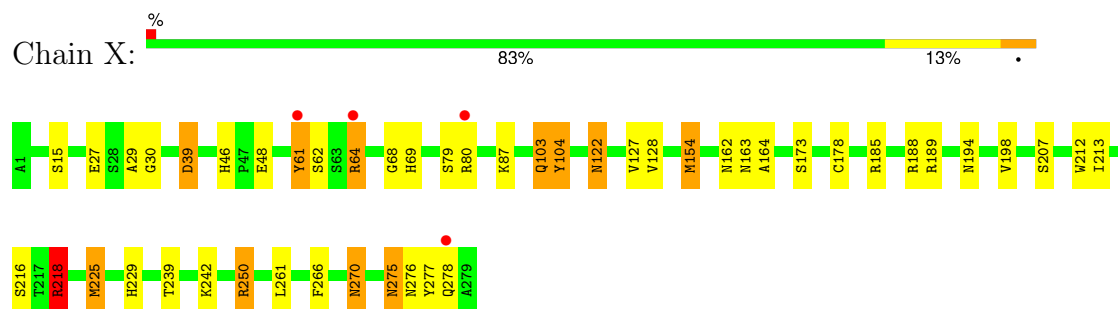
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	455	Total	O	0	0
			455	455		

3 Residue-property plots

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: Proteinase K



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	67.95Å 67.95Å 102.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 1.80 48.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.05-1.80) 99.3 (48.05-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.95 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.156 , 0.202 0.157 , 0.202	Depositor DCC
R_{free} test set	1166 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	5.5	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2485	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	X	1.24	7/2069 (0.3%)	1.05	7/2810 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	218	ARG	CD-NE	-8.44	1.32	1.46
1	X	266	PHE	CE2-CZ	8.34	1.53	1.37
1	X	218	ARG	CB-CG	-7.49	1.32	1.52
1	X	27	GLU	CG-CD	7.42	1.63	1.51
1	X	207	SER	CB-OG	7.14	1.51	1.42
1	X	104	TYR	CE1-CZ	5.58	1.45	1.38
1	X	27	GLU	CD-OE1	5.27	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	218	ARG	NE-CZ-NH2	-18.37	111.11	120.30
1	X	64	ARG	NE-CZ-NH2	9.72	125.16	120.30
1	X	64	ARG	NE-CZ-NH1	-9.45	115.58	120.30
1	X	218	ARG	CG-CD-NE	-8.57	93.79	111.80
1	X	188	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	X	188	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	X	218	ARG	NH1-CZ-NH2	6.09	126.10	119.40

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	X	2030	0	1935	67	2
2	X	455	0	0	39	2
All	All	2485	0	1935	67	3

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 17.

All (67) 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:X:128:VAL:HA	2:X:681:HOH:O	1.22	1.31
1:X:61:TYR:CZ	2:X:611:HOH:O	1.87	1.24
1:X:239:THR:HB	2:X:653:HOH:O	1.06	1.21
1:X:276:ASN:HB3	2:X:482:HOH:O	1.48	1.10
1:X:278:GLN:OE1	2:X:473:HOH:O	1.69	1.09
1:X:61:TYR:CE2	2:X:611:HOH:O	2.07	1.02
1:X:61:TYR:CE1	2:X:611:HOH:O	2.09	0.97
1:X:62:SER:OG	1:X:64:ARG:HG2	1.65	0.96
1:X:80:ARG:CD	2:X:676:HOH:O	2.14	0.93
1:X:80:ARG:HD2	2:X:676:HOH:O	1.70	0.92
1:X:122:ASN:CG	2:X:511:HOH:O	2.08	0.92
1:X:154:MET:HB3	2:X:681:HOH:O	1.70	0.91
1:X:261:LEU:H	1:X:270:ASN:HD21	1.25	0.84
1:X:276:ASN:OD1	2:X:707:HOH:O	1.95	0.82
1:X:218:ARG:HD2	2:X:318:HOH:O	1.80	0.80
1:X:46:HIS:HD2	1:X:48:GLU:H	1.29	0.79
1:X:122:ASN:CB	2:X:511:HOH:O	2.31	0.79
1:X:122:ASN:HB2	2:X:511:HOH:O	1.82	0.78
1:X:250:ARG:HD3	2:X:594:HOH:O	1.83	0.78
1:X:276:ASN:CB	2:X:482:HOH:O	2.14	0.77
1:X:278:GLN:CD	2:X:473:HOH:O	2.19	0.76
1:X:185:ARG:NH1	2:X:658:HOH:O	2.05	0.72
1:X:80:ARG:CZ	2:X:676:HOH:O	2.38	0.71
1:X:218:ARG:CD	2:X:318:HOH:O	2.36	0.71
1:X:103:GLN:H	1:X:103:GLN:CD	1.92	0.70
1:X:127:VAL:O	2:X:681:HOH:O	2.08	0.69
1:X:80:ARG:NE	2:X:676:HOH:O	2.24	0.67
1:X:30:GLY:C	1:X:239:THR:HG21	2.16	0.65
1:X:250:ARG:CD	2:X:594:HOH:O	2.42	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:173:SER:HA	1:X:198:VAL:HG21	1.80	0.63
1:X:61:TYR:CD1	2:X:611:HOH:O	2.47	0.62
1:X:39:ASP:OD1	1:X:69:HIS:HD2	1.82	0.61
1:X:163:ASN:ND2	1:X:189:ARG:HH12	1.99	0.60
1:X:154:MET:CB	2:X:681:HOH:O	2.40	0.60
1:X:80:ARG:NH1	2:X:676:HOH:O	2.33	0.60
1:X:87:LYS:HG3	2:X:688:HOH:O	2.01	0.60
1:X:62:SER:OG	1:X:64:ARG:CG	2.47	0.56
1:X:29:ALA:HB3	1:X:87:LYS:HD3	1.87	0.56
1:X:46:HIS:HE1	1:X:216:SER:O	1.89	0.55
1:X:103:GLN:H	1:X:103:GLN:NE2	2.04	0.55
1:X:64:ARG:HG3	2:X:398:HOH:O	2.07	0.55
1:X:278:GLN:OE1	1:X:278:GLN:N	2.40	0.54
1:X:162:ASN:HB2	1:X:194:ASN:HD21	1.73	0.53
1:X:154:MET:N	2:X:681:HOH:O	2.40	0.53
1:X:61:TYR:CD2	2:X:611:HOH:O	2.46	0.53
1:X:225:MET:O	1:X:229:HIS:HD2	1.93	0.51
1:X:128:VAL:CA	2:X:681:HOH:O	2.08	0.50
1:X:30:GLY:HA2	1:X:239:THR:HG21	1.94	0.49
1:X:30:GLY:CA	1:X:239:THR:HG21	2.43	0.49
1:X:275:ASN:ND2	1:X:277:TYR:H	2.12	0.47
1:X:212:TRP:CG	1:X:218:ARG:HD3	2.50	0.47
1:X:163:ASN:HD22	1:X:189:ARG:HH12	1.62	0.47
1:X:218:ARG:HD3	2:X:318:HOH:O	2.10	0.47
1:X:164:ALA:H	1:X:194:ASN:HD22	1.62	0.45
1:X:164:ALA:H	1:X:194:ASN:ND2	2.14	0.45
1:X:46:HIS:CD2	1:X:48:GLU:H	2.20	0.45
1:X:48:GLU:HB3	1:X:79:SER:HB2	1.97	0.45
1:X:162:ASN:H	1:X:194:ASN:ND2	2.15	0.44
1:X:68:GLY:HA2	1:X:213:ILE:HG23	1.99	0.44
1:X:46:HIS:CD2	1:X:48:GLU:HB2	2.54	0.43
1:X:128:VAL:HG22	2:X:681:HOH:O	2.19	0.42
1:X:87:LYS:CG	2:X:688:HOH:O	2.65	0.41
1:X:154:MET:CA	2:X:681:HOH:O	2.68	0.41
1:X:239:THR:CB	2:X:653:HOH:O	1.95	0.41
1:X:242:LYS:HD2	2:X:492:HOH:O	2.20	0.40
1:X:261:LEU:N	1:X:270:ASN:HD21	2.05	0.40
1:X:64:ARG:NH1	2:X:304:HOH:O	2.38	0.40

All (3) 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:X:15:SER:OG	1:X:122:ASN:ND2[5_454]	1.59	0.61
1:X:250:ARG:NH1	2:X:598:HOH:O[3_554]	2.03	0.17
2:X:619:HOH:O	2:X:745:HOH:O[3_554]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	X	277/279 (99%)	271 (98%)	5 (2%)	1 (0%)	30 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	39	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	X	213/213 (100%)	202 (95%)	11 (5%)	19 8

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	61	TYR
1	X	103	GLN
1	X	104	TYR

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Mol	Chain	Res	Type
1	X	122	ASN
1	X	154	MET
1	X	178	CYS
1	X	218	ARG
1	X	225	MET
1	X	250	ARG
1	X	270	ASN
1	X	275	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	31	GLN
1	X	46	HIS
1	X	54	GLN
1	X	69	HIS
1	X	119	ASN
1	X	162	ASN
1	X	163	ASN
1	X	194	ASN
1	X	229	HIS
1	X	257	ASN
1	X	270	ASN
1	X	275	ASN
1	X	276	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 [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, 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	X	279/279 (100%)	-0.75	4 (1%) 73 72	2, 3, 11, 26	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	61	TYR	7.3
1	X	278	GLN	3.3
1	X	64	ARG	2.7
1	X	80	ARG	2.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.