



Full wwPDB Geometry-Only Validation Report ⓘ

Mar 7, 2019 – 03:48 PM EST

PDB ID : 6N4U
Title : MicroED structure of Proteinase K at 2.75Å resolution from a single milled crystal.
Authors : Martynowycz, M.W.; Zhao, W.; Hattne, J.; Jensen, G.J.; Gonen, T.
Deposited on : 2018-11-20
Resolution : 2.75 Å(reported)

This is a Full wwPDB Geometry-Only 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

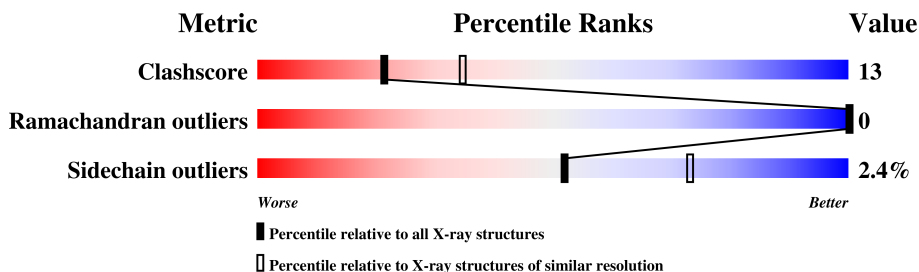
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	1029 (2.78-2.74)
Ramachandran outliers	120053	1013 (2.78-2.74)
Sidechain outliers	120020	1013 (2.78-2.74)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	279	 73% 25% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2057 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
			Total	C	N	O	S			
1	A	279	2027	1247	354	416	10	0	0	0

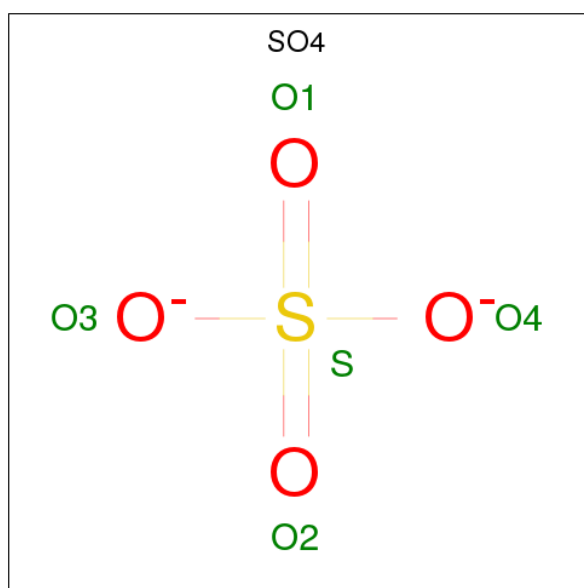
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	ASP	SER	conflict	UNP P06873

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



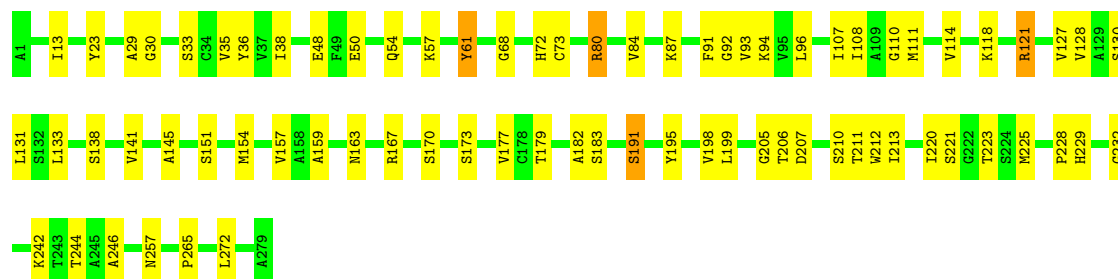
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		

Note EDS was not executed.

Chain A: 73% 25%



4 Model quality [i](#)

4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4

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	0.36	0/2066	0.52	1/2808 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	80	ARG	NE-CZ-NH2	-5.86	117.37	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2027	0	1927	51	0
2	A	2	0	0	0	0
3	A	5	0	0	0	0
4	A	23	0	0	1	0
All	All	2057	0	1927	51	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 13.

All (51) 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:173:SER:HA	1:A:198:VAL:HG11	1.67	0.77
1:A:138:SER:HB2	1:A:141:VAL:HG22	1.70	0.73
1:A:72:HIS:ND1	1:A:225:MET:SD	2.62	0.70
1:A:207:ASP:H	1:A:221:SER:HB3	1.57	0.69
1:A:141:VAL:CG2	1:A:170:SER:HB3	2.29	0.63
1:A:94:LYS:NZ	1:A:96:LEU:O	2.33	0.61
1:A:50:GLU:CD	1:A:80:ARG:HD2	2.22	0.60
1:A:38:ILE:HA	1:A:93:VAL:HG23	1.84	0.59
1:A:91:PHE:CZ	1:A:121:ARG:HG2	2.36	0.59
1:A:50:GLU:OE1	1:A:80:ARG:HD2	2.03	0.59
1:A:242:LYS:NZ	4:A:401:HOH:O	2.36	0.57
1:A:108:ILE:HG13	1:A:141:VAL:HG12	1.87	0.57
1:A:30:GLY:O	1:A:33:SER:OG	2.23	0.57
1:A:57:LYS:HB3	1:A:93:VAL:HG12	1.88	0.56
1:A:244:THR:HG22	1:A:246:ALA:H	1.70	0.56
1:A:68:GLY:HA2	1:A:213:ILE:HG23	1.88	0.55
1:A:118:LYS:NZ	1:A:151:SER:O	2.40	0.54
1:A:38:ILE:HD13	1:A:131:LEU:HG	1.91	0.53
1:A:131:LEU:HB2	1:A:157:VAL:HG12	1.91	0.53
1:A:179:THR:HB	1:A:199:LEU:HA	1.91	0.52
1:A:29:ALA:HB3	1:A:87:LYS:HE2	1.91	0.52
1:A:84:VAL:HG13	1:A:232:GLY:HA3	1.91	0.51
1:A:13:ILE:HD11	1:A:229:HIS:HB3	1.93	0.51
1:A:107:ILE:HD13	1:A:133:LEU:HD13	1.94	0.49
1:A:107:ILE:HG22	1:A:111:MET:HE2	1.94	0.49
1:A:145:ALA:HB1	1:A:177:VAL:HG11	1.96	0.48
1:A:141:VAL:HG23	1:A:170:SER:HB3	1.96	0.48
1:A:182:ALA:HB1	1:A:205:GLY:HA3	1.96	0.48
1:A:23:TYR:OH	1:A:84:VAL:HG23	2.15	0.46
1:A:167:ARG:HA	1:A:173:SER:HB3	1.97	0.46
1:A:210:SER:OG	1:A:211:THR:N	2.48	0.46
1:A:212:TRP:HZ3	1:A:220:ILE:HD13	1.82	0.45
1:A:48:GLU:HG3	1:A:80:ARG:H	1.80	0.45
1:A:159:ALA:HB1	1:A:199:LEU:HD11	1.98	0.45
1:A:72:HIS:CD2	1:A:210:SER:HB3	2.52	0.45
1:A:110:GLY:O	1:A:114:VAL:HG23	2.17	0.45
1:A:118:LYS:HG3	1:A:127:VAL:HG11	1.98	0.45
1:A:206:THR:HA	1:A:221:SER:HB3	2.00	0.43
1:A:195:TYR:CG	1:A:265:PRO:HG2	2.53	0.43
1:A:35:VAL:HG13	1:A:128:VAL:HB	2.00	0.43
1:A:163:ASN:ND2	1:A:191:SER:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASN:HB2	1:A:272:LEU:HB3	2.00	0.43
1:A:54:GLN:O	1:A:92:GLY:N	2.45	0.43
1:A:182:ALA:HB2	1:A:223:THR:HA	2.01	0.42
1:A:61:TYR:C	1:A:61:TYR:CD1	2.93	0.42
1:A:128:VAL:HG13	1:A:154:MET:HG3	2.01	0.42
1:A:138:SER:N	1:A:170:SER:OG	2.46	0.42
1:A:36:TYR:CD1	1:A:114:VAL:HG22	2.55	0.42
1:A:73:CYS:HB2	1:A:228:PRO:CG	2.50	0.42
1:A:72:HIS:NE2	1:A:210:SER:HB3	2.36	0.41
1:A:72:HIS:CE1	1:A:210:SER:HB3	2.56	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	A	277/279 (99%)	265 (96%)	12 (4%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	A	212/213 (100%)	207 (98%)	5 (2%)	52	73

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	TYR
1	A	121	ARG
1	A	130	SER
1	A	183	SER
1	A	191	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	303	-	4,4,4	0.17	0	6,6,6	0.12	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
3	SO4	A	303	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.