Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 04:08 PM JST

PDB ID	:	9L78 / pdb_00009l78
Title	:	Crystal structure of nucleotide-free human kinesin-1 motor domain (G234A mutant)
Authors	:	Makino, T.; Miyazono, K.; Tanokura, M.; Tomishige, M.
Deposited on	:	2024-12-26
Resolution	:	2.82 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:

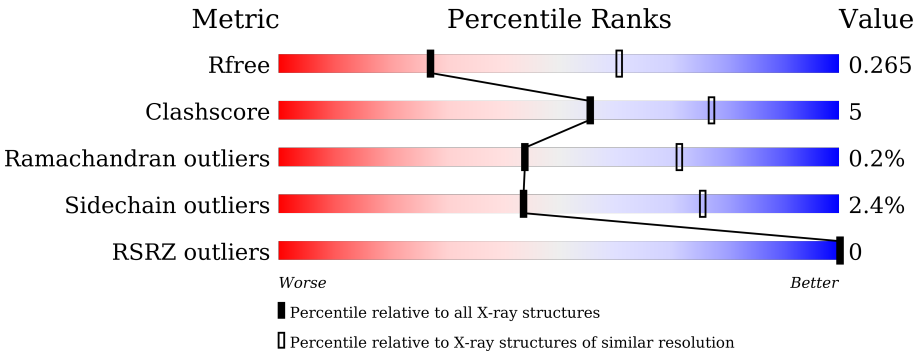
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4293 (2.84-2.80)
Clashscore	180529	4801 (2.84-2.80)
Ramachandran outliers	177936	4739 (2.84-2.80)
Sidechain outliers	177891	4741 (2.84-2.80)
RSRZ outliers	164620	4295 (2.84-2.80)

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 <=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	342	75% 15% 9%
1	B	342	75% 11% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4762 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 Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2439	1524	419	487	9			
1	B	295	Total	C	N	O	S	0	0	0
			2322	1457	396	460	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P33176
A	-4	HIS	-	expression tag	UNP P33176
A	-3	HIS	-	expression tag	UNP P33176
A	-2	HIS	-	expression tag	UNP P33176
A	-1	HIS	-	expression tag	UNP P33176
A	0	HIS	-	expression tag	UNP P33176
A	1	HIS	-	expression tag	UNP P33176
A	7	SER	CYS	conflict	UNP P33176
A	65	ALA	CYS	conflict	UNP P33176
A	168	ALA	CYS	conflict	UNP P33176
A	174	SER	CYS	conflict	UNP P33176
A	234	ALA	GLY	engineered mutation	UNP P33176
A	294	ALA	CYS	conflict	UNP P33176
A	330	SER	CYS	conflict	UNP P33176
B	-5	MET	-	initiating methionine	UNP P33176
B	-4	HIS	-	expression tag	UNP P33176
B	-3	HIS	-	expression tag	UNP P33176
B	-2	HIS	-	expression tag	UNP P33176
B	-1	HIS	-	expression tag	UNP P33176
B	0	HIS	-	expression tag	UNP P33176
B	1	HIS	-	expression tag	UNP P33176
B	7	SER	CYS	conflict	UNP P33176
B	65	ALA	CYS	conflict	UNP P33176
B	168	ALA	CYS	conflict	UNP P33176
B	174	SER	CYS	conflict	UNP P33176

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Chain	Residue	Modelled	Actual	Comment	Reference
B	234	ALA	GLY	engineered mutation	UNP P33176
B	294	ALA	CYS	conflict	UNP P33176
B	330	SER	CYS	conflict	UNP P33176

- Molecule 2 is water.

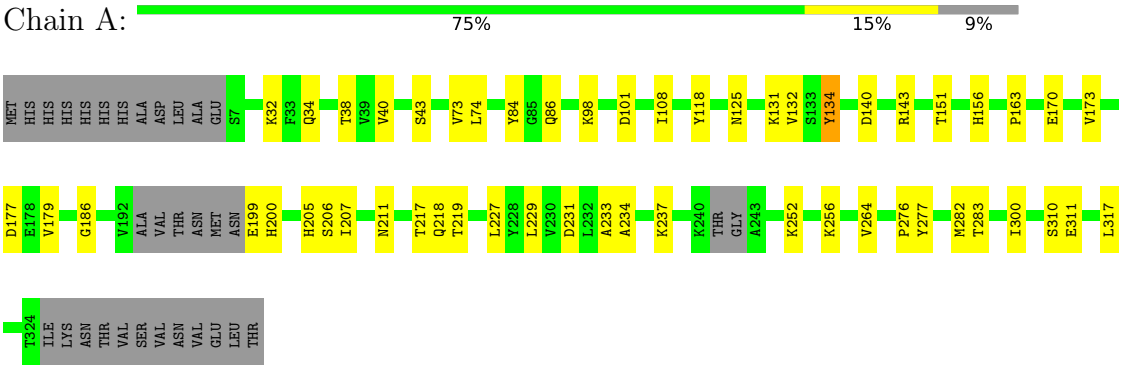
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0

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.

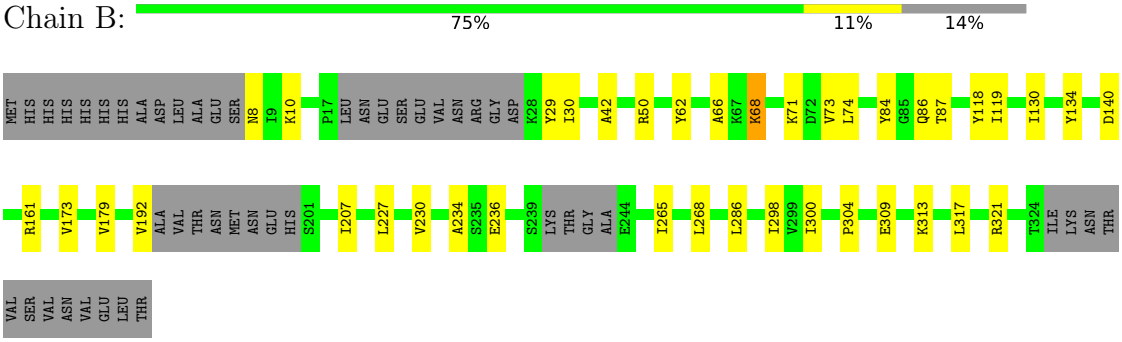
• Molecule 1: Kinesin-1 heavy chain

Chain A:



• Molecule 1: Kinesin-1 heavy chain

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.22Å 156.90Å 52.96Å 90.00° 114.56° 90.00°	Depositor
Resolution (Å)	19.58 – 2.82 19.58 – 2.83	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.58-2.82) 96.0 (19.58-2.83)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.05 (at 2.83Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.207 , 0.265 0.207 , 0.265	Depositor DCC
R_{free} test set	757 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 9.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.267 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4762	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.30	0/2476	0.51	0/3334
1	B	0.28	0/2357	0.49	0/3173
All	All	0.29	0/4833	0.50	0/6507

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	2439	0	2415	28	0
1	B	2322	0	2309	16	0
2	A	1	0	0	0	0
All	All	4762	0	4724	44	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 5.

All (44) 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:265:ILE:HD13	1:B:298:ILE:HD11	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:HG21	1:B:227:LEU:HB2	1.69	0.74
1:A:32:LYS:NZ	1:A:43:SER:H	1.93	0.67
1:A:86:GLN:HG3	1:A:311:GLU:HB3	1.77	0.65
1:A:277:TYR:O	1:A:283:THR:HG23	1.98	0.63
1:A:143:ARG:HG2	1:A:151:THR:HG23	1.81	0.61
1:A:252:LYS:HE3	1:A:256:LYS:HD2	1.81	0.61
1:A:173:VAL:HG21	1:A:179:VAL:HG22	1.86	0.57
1:A:98:LYS:HD3	1:A:101:ASP:HB2	1.86	0.57
1:A:32:LYS:HZ2	1:A:43:SER:H	1.53	0.56
1:A:73:VAL:HG21	1:A:227:LEU:HB2	1.88	0.56
1:B:173:VAL:HG21	1:B:179:VAL:HG22	1.89	0.54
1:A:207:ILE:HD11	1:A:282:MET:HG3	1.91	0.53
1:A:32:LYS:HD2	1:A:40:VAL:HB	1.91	0.53
1:A:84:TYR:HB3	1:A:300:ILE:HG22	1.90	0.53
1:B:119:ILE:HD11	1:B:130:ILE:HD11	1.90	0.53
1:A:237:LYS:HE3	1:A:310:SER:HB3	1.91	0.53
1:A:264:VAL:HG22	1:A:276:PRO:HD2	1.90	0.53
1:A:34:GLN:HB2	1:A:38:THR:HB	1.91	0.52
1:B:29:TYR:CE2	1:B:304:PRO:HB2	2.44	0.52
1:A:156:HIS:O	1:A:163:PRO:HA	2.11	0.51
1:A:134:TYR:CD2	1:A:186:GLY:HA3	2.46	0.50
1:B:207:ILE:HG12	1:B:230:VAL:HG22	1.95	0.49
1:A:74:LEU:HD13	1:A:118:TYR:CG	2.51	0.46
1:B:317:LEU:O	1:B:321:ARG:HB2	2.15	0.46
1:B:309:GLU:HG2	1:B:313:LYS:HE3	1.97	0.46
1:A:200:HIS:CD2	1:A:200:HIS:H	2.33	0.46
1:B:62:TYR:CD1	1:B:66:ALA:HB3	2.51	0.46
1:A:108:ILE:HG12	1:A:229:LEU:HD13	1.99	0.45
1:B:86:GLN:HB3	1:B:87:THR:H	1.61	0.44
1:A:132:VAL:O	1:A:170:GLU:HA	2.18	0.44
1:A:205:HIS:CE1	1:A:233:ALA:H	2.35	0.44
1:A:218:GLN:HG3	1:A:219:THR:N	2.32	0.44
1:B:8:ASN:N	1:B:10:LYS:HZ1	2.16	0.43
1:B:234:ALA:O	1:B:236:GLU:HG3	2.18	0.43
1:B:74:LEU:HD13	1:B:118:TYR:CG	2.53	0.43
1:A:131:LYS:HE3	1:A:170:GLU:OE1	2.19	0.43
1:B:84:TYR:HB3	1:B:300:ILE:HG22	2.01	0.42
1:B:68:LYS:NZ	1:B:71:LYS:HD2	2.34	0.42
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.91	0.41
1:B:230:VAL:HG21	1:B:286:LEU:HD11	2.01	0.41
1:A:84:TYR:CE2	1:A:234:ALA:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:O	1:A:217:THR:HG23	2.21	0.40
1:A:206:SER:OG	1:A:231:ASP:HB3	2.22	0.40

There are no symmetry-related clashes.

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	A	304/342 (89%)	288 (95%)	16 (5%)	0	100 100
1	B	287/342 (84%)	273 (95%)	13 (4%)	1 (0%)	37 65
All	All	591/684 (86%)	561 (95%)	29 (5%)	1 (0%)	44 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	ALA

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	A	275/303 (91%)	270 (98%)	5 (2%)	54 82
1	B	262/303 (86%)	254 (97%)	8 (3%)	35 68
All	All	537/606 (89%)	524 (98%)	13 (2%)	44 76

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	TYR
1	A	140	ASP
1	A	177	ASP
1	A	199	GLU
1	A	211	ASN
1	B	30	ILE
1	B	50	ARG
1	B	68	LYS
1	B	134	TYR
1	B	140	ASP
1	B	161	ARG
1	B	192	VAL
1	B	268	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	125	ASN
1	A	200	HIS
1	A	221	GLN
1	B	53	GLN
1	B	152	ASN
1	B	218	GLN
1	B	253	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 oligosaccharides 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, 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	A	310/342 (90%)	-1.94	0	100	100	8, 20, 46, 64	0
1	B	295/342 (86%)	-1.93	0	100	100	9, 21, 49, 80	0
All	All	605/684 (88%)	-1.94	0	100	100	8, 20, 48, 80	0

There are no RSRZ outliers to report.

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.