wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2024 – 02:59 am BST

PDB ID	:	5LB7
Title	:	Complex structure between p60N/p80C katanin and a peptide derived from ASPM
Authors	:	Rezabkova, L.; Capitani, G.; Kammerer, R.A.; Steinmetz, M.O.
Deposited on	:	2016-06-15
Resolution	:	1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

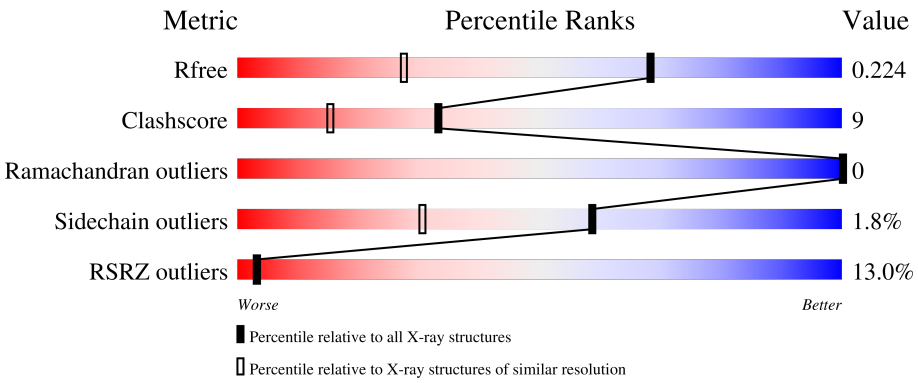
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (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 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	212	13%, 67%, 11%, 22%
2	B	80	2%, 85%, 11%, • •
3	C	9	22%, 22%, 11%, 67%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2413 atoms, of which 197 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 Katanin p80 WD40 repeat-containing subunit B1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	166	1448	832	137	230	242	7	5	3	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	MET	-	initiating methionine	UNP Q8BG40
A	448	GLY	-	expression tag	UNP Q8BG40
A	449	SER	-	expression tag	UNP Q8BG40
A	450	SER	-	expression tag	UNP Q8BG40
A	451	HIS	-	expression tag	UNP Q8BG40
A	452	HIS	-	expression tag	UNP Q8BG40
A	453	HIS	-	expression tag	UNP Q8BG40
A	454	HIS	-	expression tag	UNP Q8BG40
A	455	HIS	-	expression tag	UNP Q8BG40
A	456	HIS	-	expression tag	UNP Q8BG40
A	457	SER	-	expression tag	UNP Q8BG40
A	458	SER	-	expression tag	UNP Q8BG40
A	459	GLY	-	expression tag	UNP Q8BG40
A	460	LEU	-	expression tag	UNP Q8BG40
A	461	VAL	-	expression tag	UNP Q8BG40
A	462	PRO	-	expression tag	UNP Q8BG40
A	463	ARG	-	expression tag	UNP Q8BG40
A	464	GLY	-	expression tag	UNP Q8BG40
A	465	SER	-	expression tag	UNP Q8BG40
A	466	HIS	-	expression tag	UNP Q8BG40
A	467	MET	-	expression tag	UNP Q8BG40
A	468	ALA	-	expression tag	UNP Q8BG40
A	469	SER	-	expression tag	UNP Q8BG40
A	470	MET	-	expression tag	UNP Q8BG40
A	471	THR	-	expression tag	UNP Q8BG40
A	472	GLY	-	expression tag	UNP Q8BG40
A	473	GLY	-	expression tag	UNP Q8BG40

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Chain	Residue	Modelled	Actual	Comment	Reference
A	474	GLN	-	expression tag	UNP Q8BG40
A	475	GLN	-	expression tag	UNP Q8BG40
A	476	MET	-	expression tag	UNP Q8BG40
A	477	GLY	-	expression tag	UNP Q8BG40
A	478	ARG	-	expression tag	UNP Q8BG40
A	479	GLY	-	expression tag	UNP Q8BG40
A	480	SER	-	expression tag	UNP Q8BG40

- Molecule 2 is a protein called Katanin p60 ATPase-containing subunit A1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	78	721	426	60	110	120	5	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP Q9WV86
B	0	GLY	-	expression tag	UNP Q9WV86

- Molecule 3 is a protein called Abnormal spindle-like microcephaly-associated protein homolog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	25	18	3	4	0	0	0

- Molecule 4 is water.

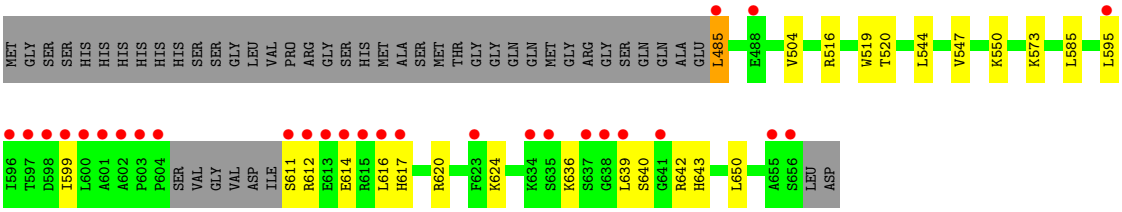
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	146	146	146	0	0
4	B	66	66	66	0	0
4	C	7	7	7	0	0

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.

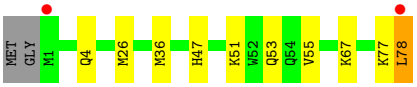
• Molecule 1: Katanin p80 WD40 repeat-containing subunit B1

Chain A:



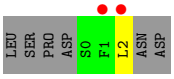
• Molecule 2: Katanin p60 ATPase-containing subunit A1

Chain B:



• Molecule 3: Abnormal spindle-like microcephaly-associated protein homolog

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	104.09Å 145.12Å 37.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.87 – 1.50 43.87 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (43.87-1.50) 97.7 (43.87-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 1.50Å)	Xtriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, R_{free}	0.183 , 0.223 0.183 , 0.224	Depositor DCC
R_{free} test set	903 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2413	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.58% 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 (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	A	0.27	0/1334	0.43	0/1800
2	B	0.27	0/676	0.40	0/909
3	C	0.36	0/25	0.36	0/32
All	All	0.27	0/2035	0.42	0/2741

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 (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	1311	137	1383	30	0
2	B	661	60	672	11	0
3	C	25	0	27	1	0
4	A	146	0	0	6	0
4	B	66	0	0	1	0
4	C	7	0	0	0	0
All	All	2216	197	2082	35	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 9.

The worst 5 of 35 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:516:ARG:HH12	1:A:520:THR:HB	1.38	0.87
1:A:636:LYS:NZ	4:A:703:HOH:O	2.16	0.78
1:A:516:ARG:NH1	1:A:520:THR:HB	1.98	0.78
1:A:640:SER:OG	4:A:701:HOH:O	2.05	0.74
1:A:636:LYS:O	4:A:702:HOH:O	2.07	0.73

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	165/212 (78%)	163 (99%)	2 (1%)	0	100	100
2	B	77/80 (96%)	77 (100%)	0	0	100	100
3	C	1/9 (11%)	1 (100%)	0	0	100	100
All	All	243/301 (81%)	241 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	153/186 (82%)	151 (99%)	2 (1%)	69	44
2	B	73/73 (100%)	71 (97%)	2 (3%)	44	15
3	C	3/9 (33%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	229/268 (85%)	225 (98%)	4 (2%)	59 33

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	485	LEU
1	A	639	LEU
2	B	53	GLN
2	B	78	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	643	HIS

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)

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 (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	A	166/212 (78%)	0.82	28 (16%)	1	1	19, 32, 61, 79	0
2	B	78/80 (97%)	0.23	2 (2%)	56	61	19, 25, 40, 57	0
3	C	3/9 (33%)	2.51	2 (66%)	0	0	42, 42, 45, 47	0
All	All	247/301 (82%)	0.65	32 (12%)	3	3	19, 29, 57, 79	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	639	LEU	8.0
1	A	638	GLY	7.9
1	A	637	SER	6.3
1	A	612	ARG	5.8
2	B	78	LEU	5.8

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.