



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:24 am BST

PDB ID : 6CPY
Title : Structure of apo GRMZM2G135359 pseudokinase
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Deposited on : 2018-03-14
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

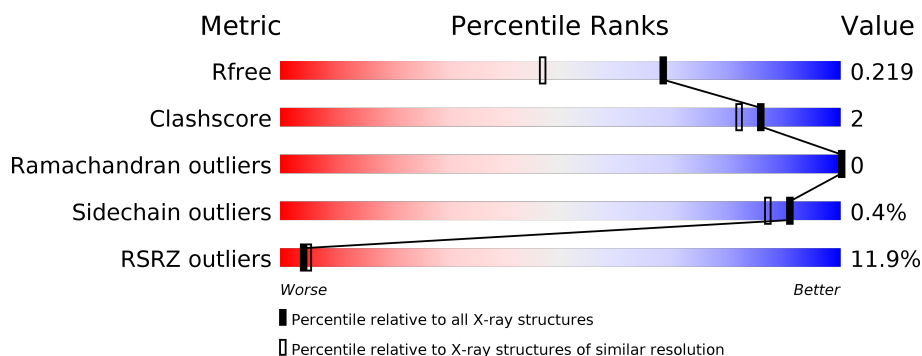
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	A	308	<div> <div>12%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>
1	B	308	<div> <div>9%</div> <div>82%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4432 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 GRMZM2G135359 pseudokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	2	0
			2162	1365	370	406	21			
1	B	262	Total	C	N	O	S	0	3	0
			2074	1313	351	391	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	SER	-	expression tag	UNP B4F901
A	186	MET	-	expression tag	UNP B4F901
B	185	SER	-	expression tag	UNP B4F901
B	186	MET	-	expression tag	UNP B4F901

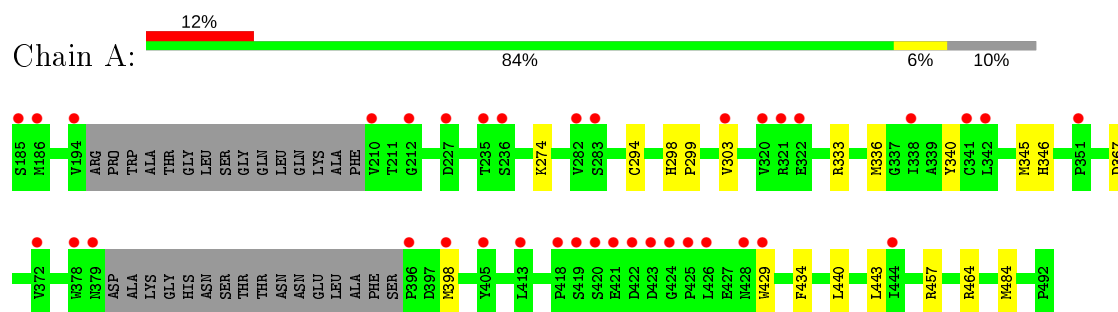
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	88	Total	O	0	0
			88	88		
2	B	108	Total	O	0	0
			108	108		

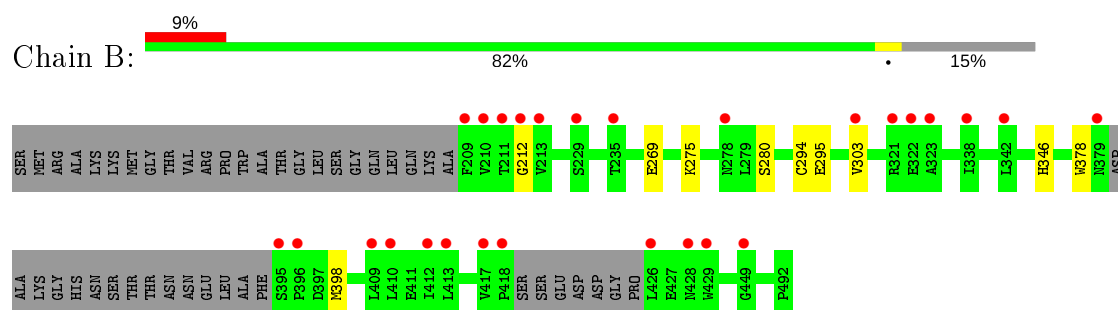
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: GRMZM2G135359 pseudokinase



- Molecule 1: GRMZM2G135359 pseudokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.49 Å 61.50 Å 144.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.82 – 1.70 19.82 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.82-1.70) 99.9 (19.82-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.199 , 0.215 0.208 , 0.219	Depositor DCC
R_{free} test set	2974 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4432	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% 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

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	0.39	0/2209	0.60	0/2982
1	B	0.37	0/2116	0.56	0/2861
All	All	0.38	0/4325	0.58	0/5843

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	2162	0	2116	13	0
1	B	2074	0	2008	5	0
2	A	88	0	0	0	0
2	B	108	0	0	0	0
All	All	4432	0	4124	18	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 2.

All (18) 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:346:HIS:CD2	1:B:398:MET:HG3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HD11	1:A:457:ARG:HG3	1.88	0.54
1:A:336[A]:MET:CE	1:A:484:MET:HB3	2.40	0.52
1:A:336[B]:MET:HG3	1:A:340:TYR:CE2	2.46	0.51
1:A:346:HIS:ND1	1:A:398:MET:HG3	2.27	0.50
1:A:336[A]:MET:HG3	1:A:340:TYR:CE2	2.46	0.49
1:B:294:CYS:HB3	1:B:303:VAL:HG22	1.96	0.48
1:A:336[A]:MET:HE1	1:A:484:MET:HB3	1.98	0.46
1:B:269:GLU:OE2	1:B:295:GLU:OE1	2.33	0.45
1:A:336[A]:MET:HB2	1:A:336[A]:MET:HE3	1.67	0.45
1:A:434:PHE:CE1	1:A:464:ARG:HB2	2.52	0.45
1:A:333:ARG:NH2	1:A:367:ASP:O	2.50	0.45
1:A:294:CYS:HB3	1:A:303:VAL:HG22	1.99	0.43
1:A:298:HIS:HA	1:A:299:PRO:HA	1.92	0.42
1:A:336[A]:MET:HA	1:A:336[A]:MET:HE2	2.01	0.42
1:B:212:GLY:HA3	1:B:280:SER:HB2	2.02	0.41
1:A:429:TRP:CH2	1:A:443:LEU:HD12	2.56	0.40
1:B:275:LYS:HD2	1:B:378:TRP:CD1	2.56	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	273/308 (89%)	268 (98%)	5 (2%)	0	100	100
1	B	259/308 (84%)	258 (100%)	1 (0%)	0	100	100
All	All	532/616 (86%)	526 (99%)	6 (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	233/268 (87%)	231 (99%)	2 (1%)	78	70
1	B	224/268 (84%)	224 (100%)	0	100	100
All	All	457/536 (85%)	455 (100%)	2 (0%)	91	87

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

Mol	Chain	Res	Type
1	A	274	LYS
1	A	345	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	ASN
1	B	356	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 carbohydrates 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 ⓘ

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	277/308 (89%)	0.88	37 (13%) 3 3	22, 34, 56, 76	0
1	B	262/308 (85%)	0.63	27 (10%) 6 7	21, 33, 51, 67	0
All	All	539/616 (87%)	0.76	64 (11%) 4 5	21, 34, 55, 76	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	422	ASP	7.7
1	B	211	THR	6.4
1	B	426	LEU	6.3
1	A	424	GLY	6.3
1	A	194	VAL	6.0
1	A	420	SER	5.9
1	A	429	TRP	5.7
1	B	395	SER	5.5
1	A	419	SER	5.2
1	A	425	PRO	5.0
1	A	378	TRP	5.0
1	B	409	LEU	4.6
1	B	428	ASN	4.6
1	A	426	LEU	4.5
1	B	209	PHE	4.2
1	A	423	ASP	4.1
1	A	342	LEU	4.0
1	A	185	SER	3.9
1	A	396	PRO	3.8
1	A	421	GLU	3.7
1	A	418	PRO	3.6
1	B	418	PRO	3.6
1	A	379	ASN	3.5
1	B	413	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	429	TRP	3.5
1	B	396	PRO	3.4
1	A	210	VAL	3.4
1	B	342	LEU	3.3
1	B	321	ARG	3.3
1	A	351	PRO	3.3
1	B	210	VAL	3.2
1	A	413	LEU	3.1
1	A	212	GLY	3.1
1	A	321	ARG	3.0
1	A	236	SER	3.0
1	A	322	GLU	3.0
1	B	212	GLY	3.0
1	B	303	VAL	2.8
1	B	410	LEU	2.8
1	A	282	VAL	2.8
1	B	235	THR	2.8
1	A	338	ILE	2.7
1	A	235	THR	2.7
1	A	303	VAL	2.7
1	A	283	SER	2.7
1	B	323	ALA	2.6
1	B	379	ASN	2.5
1	A	320	VAL	2.5
1	B	338	ILE	2.5
1	B	213	VAL	2.5
1	A	444	ILE	2.5
1	A	398	MET	2.4
1	A	341	CYS	2.4
1	B	229	SER	2.3
1	B	412	ILE	2.3
1	B	449	GLY	2.3
1	A	227	ASP	2.3
1	A	186	MET	2.3
1	A	428	ASN	2.3
1	B	322	GLU	2.1
1	A	405	TYR	2.1
1	B	278	ASN	2.1
1	A	372	VAL	2.1
1	B	417	VAL	2.0

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 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.