



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2019 – 07:33 PM EDT

PDB ID : 6I2M
Title : Crystal structure of vaccinia virus protein A55 BTB-Back domain in complex with human Cullin-3 N-terminus
Authors : Gao, G.; Graham, S.C.
Deposited on : 2018-11-01
Resolution : 2.30 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 : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

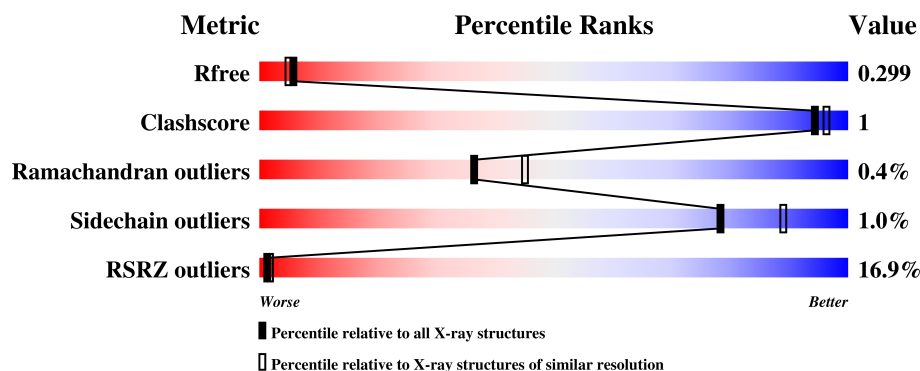
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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 $\leq 5\%$. 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	259	<div> <div>20%</div> <div>71%</div> <div>5%</div> <div>24%</div> </div>
2	B	388	<div> <div>10%</div> <div>84%</div> <div>•</div> <div>12%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4402 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 Kelch repeat and BTB domain-containing protein A55.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1587	1013	252	315	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	GLY	-	expression tag	UNP P24768
A	252	SER	-	expression tag	UNP P24768
A	253	LYS	-	expression tag	UNP P24768
A	254	HIS	-	expression tag	UNP P24768
A	255	HIS	-	expression tag	UNP P24768
A	256	HIS	-	expression tag	UNP P24768
A	257	HIS	-	expression tag	UNP P24768
A	258	HIS	-	expression tag	UNP P24768
A	259	HIS	-	expression tag	UNP P24768

- Molecule 2 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	343	Total	C	N	O	S	0	0	0
			2815	1771	491	529	24			

There are 24 discrepancies between the modelled and reference sequences:

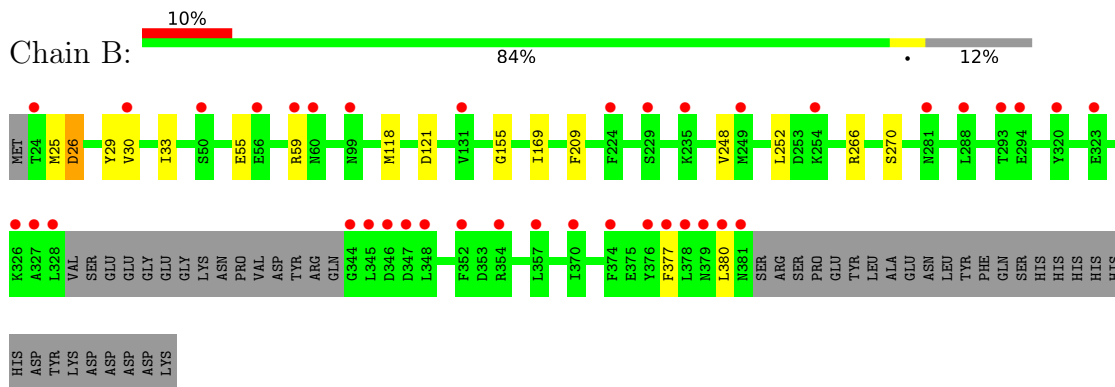
Chain	Residue	Modelled	Actual	Comment	Reference
B	342	ARG	ILE	engineered mutation	UNP Q13618
B	346	ASP	LEU	engineered mutation	UNP Q13618
B	389	ALA	-	expression tag	UNP Q13618
B	390	GLU	-	expression tag	UNP Q13618
B	391	ASN	-	expression tag	UNP Q13618
B	392	LEU	-	expression tag	UNP Q13618
B	393	TYR	-	expression tag	UNP Q13618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	394	PHE	-	expression tag	UNP Q13618
B	395	GLN	-	expression tag	UNP Q13618
B	396	SER	-	expression tag	UNP Q13618
B	397	HIS	-	expression tag	UNP Q13618
B	398	HIS	-	expression tag	UNP Q13618
B	399	HIS	-	expression tag	UNP Q13618
B	400	HIS	-	expression tag	UNP Q13618
B	401	HIS	-	expression tag	UNP Q13618
B	402	HIS	-	expression tag	UNP Q13618
B	403	ASP	-	expression tag	UNP Q13618
B	404	TYR	-	expression tag	UNP Q13618
B	405	LYS	-	expression tag	UNP Q13618
B	406	ASP	-	expression tag	UNP Q13618
B	407	ASP	-	expression tag	UNP Q13618
B	408	ASP	-	expression tag	UNP Q13618
B	409	ASP	-	expression tag	UNP Q13618
B	410	LYS	-	expression tag	UNP Q13618

- Molecule 1: Kelch repeat and BTB domain-containing protein A55



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.82Å 42.52Å 148.77Å 90.00° 128.41° 90.00°	Depositor
Resolution (Å)	58.29 – 2.30 58.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	53.0 (58.29-2.30) 53.0 (58.29-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.266 , 0.282 0.285 , 0.299	Depositor DCC
R_{free} test set	1170 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.5	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	0.88	EDS
Total number of atoms	4402	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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	0.41	0/1613	0.57	0/2183
2	B	0.40	0/2856	0.56	0/3833
All	All	0.41	0/4469	0.56	0/6016

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	1587	0	1562	4	0
2	B	2815	0	2805	8	0
All	All	4402	0	4367	12	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 1.

All (12) 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)
2:B:266:ARG:HA	2:B:270:SER:HB2	1.93	0.49
2:B:26:ASP:HA	2:B:29:TYR:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:PHE:HA	2:B:380:LEU:HD12	1.97	0.47
2:B:55:GLU:O	2:B:59:ARG:HG2	2.15	0.47
1:A:23:ILE:HD11	1:A:62:VAL:HG23	1.98	0.46
1:A:67:LEU:HD22	1:A:97:THR:HG23	1.99	0.45
2:B:169:ILE:HG21	2:B:209:PHE:HE1	1.84	0.43
2:B:30:VAL:HA	2:B:33:ILE:HG12	2.00	0.43
1:A:84:LEU:HD21	1:A:94:ILE:HG21	2.03	0.41
2:B:248:VAL:HG22	2:B:252:LEU:HD12	2.02	0.41
2:B:118:MET:HA	2:B:121:ASP:HB2	2.03	0.40
1:A:76:ILE:HA	1:A:79:ILE:HD12	2.04	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	194/259 (75%)	182 (94%)	11 (6%)	1 (0%)	31	38
2	B	339/388 (87%)	330 (97%)	8 (2%)	1 (0%)	43	53
All	All	533/647 (82%)	512 (96%)	19 (4%)	2 (0%)	36	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	155	GLY
1	A	28	ASN

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	183/244 (75%)	180 (98%)	3 (2%)	65	81
2	B	313/355 (88%)	311 (99%)	2 (1%)	87	94
All	All	496/599 (83%)	491 (99%)	5 (1%)	78	89

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

Mol	Chain	Res	Type
1	A	86	LEU
1	A	139	GLU
1	A	176	LEU
2	B	25	MET
2	B	26	ASP

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

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 [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 ⓘ

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	196/259 (75%)	1.40	53 (27%) 0 0	68, 85, 109, 143	0
2	B	343/388 (88%)	0.99	38 (11%) 5 7	33, 60, 104, 140	0
All	All	539/647 (83%)	1.14	91 (16%) 1 2	33, 75, 106, 143	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	345	LEU	12.5
2	B	374	PHE	7.3
2	B	328	LEU	7.1
1	A	184	ALA	6.7
1	A	60	TYR	6.4
2	B	24	THR	6.3
2	B	378	LEU	6.3
1	A	172	SER	5.5
2	B	348	LEU	5.3
1	A	183	PHE	4.7
1	A	191	TRP	4.6
1	A	147	LEU	4.5
2	B	379	ASN	4.5
1	A	188	LEU	4.3
1	A	153	LEU	4.2
2	B	323	GLU	4.1
2	B	235	LYS	4.0
1	A	1	MET	3.9
1	A	144	ASN	3.7
2	B	376	TYR	3.7
1	A	175	MET	3.7
2	B	380	LEU	3.6
1	A	187	ILE	3.6
1	A	196	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	86	LEU	3.6
1	A	82	ILE	3.5
2	B	288	LEU	3.4
1	A	95	LEU	3.4
2	B	327	ALA	3.3
1	A	178	ILE	3.2
1	A	171	LEU	3.1
1	A	151	LEU	3.1
1	A	186	LEU	3.0
2	B	229	SER	3.0
2	B	60	ASN	3.0
1	A	11	ILE	3.0
2	B	352	PHE	3.0
2	B	347	ASP	2.9
1	A	84	LEU	2.9
2	B	30	VAL	2.9
1	A	70	GLN	2.9
1	A	8	ILE	2.9
1	A	123	CYS	2.9
1	A	169	LYS	2.8
2	B	326	LYS	2.8
1	A	146	ILE	2.8
1	A	91	VAL	2.7
2	B	357	LEU	2.7
1	A	189	ILE	2.7
2	B	320	TYR	2.7
2	B	346	ASP	2.7
1	A	179	LYS	2.7
1	A	165	GLU	2.7
2	B	344	GLY	2.7
1	A	170	ILE	2.6
2	B	254	LYS	2.6
2	B	381	ASN	2.6
1	A	41	GLY	2.6
1	A	78	TYR	2.6
1	A	113	TYR	2.6
2	B	50	SER	2.6
1	A	39	LEU	2.6
2	B	281	ASN	2.6
1	A	162	LEU	2.5
1	A	81	GLY	2.5
1	A	58	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	128	ILE	2.5
1	A	129	TYR	2.5
2	B	294	GLU	2.4
2	B	249	MET	2.4
1	A	103	ILE	2.4
1	A	152	ARG	2.4
1	A	148	GLN	2.4
2	B	131	VAL	2.4
1	A	154	ILE	2.3
1	A	108	THR	2.3
2	B	377	PHE	2.3
2	B	370	ILE	2.3
1	A	37	LEU	2.2
2	B	354	ARG	2.2
1	A	107	ILE	2.2
2	B	293	THR	2.2
2	B	59	ARG	2.2
1	A	176	LEU	2.2
2	B	56	GLU	2.2
1	A	122	ASN	2.1
1	A	185	PRO	2.1
1	A	9	ALA	2.0
2	B	224	PHE	2.0
2	B	99	ASN	2.0
1	A	124	ILE	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.