



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 09:31 AM EST

PDB ID : 4QAN
Title : Crystal structure of a cystatin-like protein (RUMGNA_02398) from *Ruminococcus gnavus* ATCC 29149 at 2.10 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2014-05-05
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

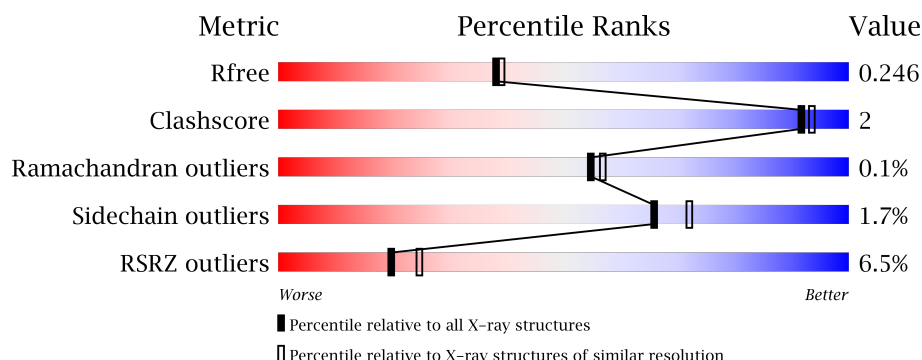
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	390	<div> <div>5%</div> <div>93%</div> <div>5%</div> </div>
1	B	390	<div> <div>7%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6302 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 hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	Se	0	7	0
			3089	1959	484	629	5	12			
1	B	372	Total	C	N	O	S	Se	0	1	0
			2954	1875	467	597	5	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP A7B4B4
B	0	GLY	-	leader sequence	UNP A7B4B4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

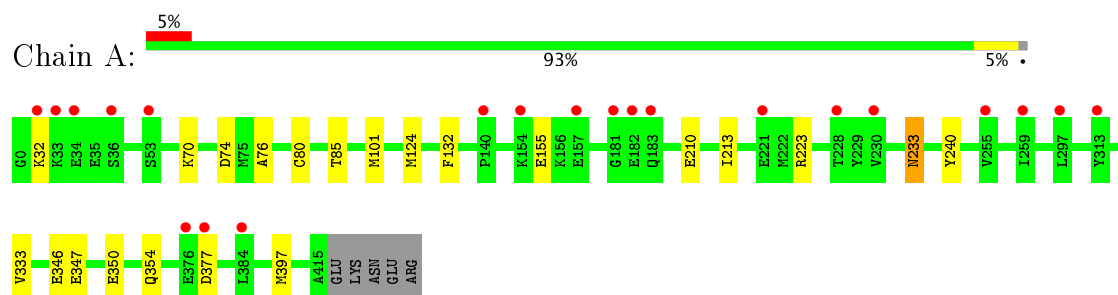
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	1
			119	119		
3	B	139	Total	O	0	0
			139	139		

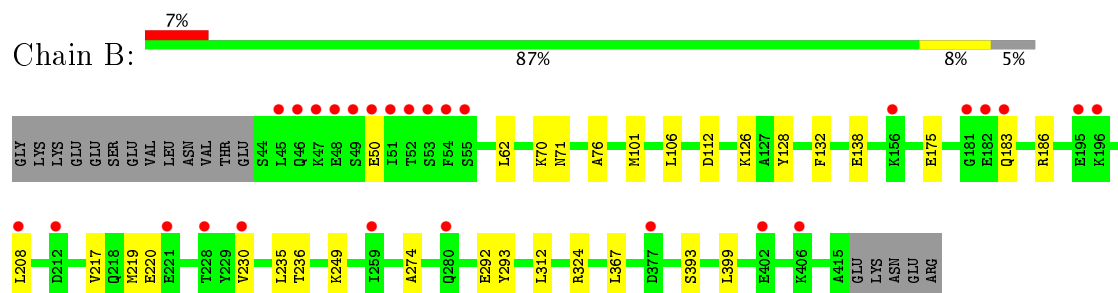
3 Residue-property plots

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: hypothetical protein



- Molecule 1: hypothetical protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.39Å 109.01Å 137.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.10 29.67 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.67-2.10) 98.1 (29.67-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.191 , 0.240 0.197 , 0.246	Depositor DCC
R_{free} test set	2271 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6302	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/3149	0.59	0/4235
1	B	0.44	0/2996	0.61	1/4030 (0.0%)
All	All	0.42	0/6145	0.60	1/8265 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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	B	101	MSE	CG-SE-CE	-5.50	86.81	98.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	ASN	Peptide

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	3089	0	3056	10	0
1	B	2954	0	2913	15	0
2	B	1	0	0	0	0
3	A	119	0	0	1	0
3	B	139	0	0	0	0
All	All	6302	0	5969	23	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 (23) 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:210:GLU:HB3	1:A:213:ILE:HD11	1.89	0.55
1:B:62:LEU:HD13	1:B:230:VAL:O	2.08	0.53
1:A:333:VAL:HG21	1:B:249:LYS:HG3	1.93	0.51
1:A:74:ASP:OD1	1:A:240:TYR:OH	2.17	0.50
1:B:126:LYS:HE3	1:B:292:GLU:HG3	1.93	0.50
1:A:347[B]:GLU:OE1	1:A:354:GLN:NE2	2.39	0.49
1:B:128:TYR:CE1	1:B:208:LEU:HD13	2.48	0.49
1:B:183:GLN:HE21	1:B:219:MSE:SE	2.46	0.48
1:B:175:GLU:HG3	1:B:186:ARG:HH11	1.80	0.47
1:A:76:ALA:HB1	1:A:132[B]:PHE:CZ	2.51	0.46
1:B:274:ALA:HB2	1:B:293:TYR:CZ	2.51	0.45
1:B:112:ASP:OD2	1:B:324:ARG:HD2	2.16	0.44
1:A:70:LYS:HE2	1:A:233:ASN:HB3	1.99	0.44
1:B:76:ALA:HB1	1:B:132[A]:PHE:CZ	2.53	0.42
1:B:367:LEU:HB2	1:B:399:LEU:HD11	2.02	0.42
1:A:85:THR:HB	1:A:124:MSE:HE1	2.02	0.42
1:B:70:LYS:O	1:B:71:ASN:C	2.58	0.42
1:B:183:GLN:HA	1:B:183:GLN:OE1	2.20	0.42
1:A:333:VAL:CG2	1:B:249:LYS:HG3	2.50	0.41
1:A:80:CYS:SG	1:A:132[B]:PHE:HZ	2.44	0.41
1:B:138:GLU:CB	1:B:217:VAL:HG11	2.51	0.41
1:B:106:LEU:CD1	1:B:312:LEU:HD11	2.51	0.41
1:A:397[B]:MSE:SE	3:A:597:HOH:O	2.89	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	390/390 (100%)	381 (98%)	8 (2%)	1 (0%)	44	44
1	B	371/390 (95%)	366 (99%)	5 (1%)	0	100	100
All	All	761/780 (98%)	747 (98%)	13 (2%)	1 (0%)	55	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	GLU

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	338/333 (102%)	331 (98%)	7 (2%)	59	64
1	B	320/333 (96%)	315 (98%)	5 (2%)	68	74
All	All	658/666 (99%)	646 (98%)	12 (2%)	66	70

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	101	MSE
1	A	155	GLU
1	A	223	ARG
1	A	350[A]	GLU

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Mol	Chain	Res	Type
1	A	350[B]	GLU
1	A	377	ASP
1	B	50	GLU
1	B	220	GLU
1	B	235	LEU
1	B	236	THR
1	B	393	SER

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

Mol	Chain	Res	Type
1	A	257	GLN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

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	375/390 (96%)	0.25	21 (5%) 25 31	26, 46, 86, 103	0
1	B	362/390 (92%)	0.29	27 (7%) 15 19	25, 43, 92, 165	0
All	All	737/780 (94%)	0.27	48 (6%) 20 25	25, 45, 89, 165	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	SER	8.0
1	B	51	ILE	7.4
1	B	52	THR	7.2
1	B	47	LYS	6.7
1	B	48	GLU	6.3
1	A	228	THR	6.0
1	B	46	GLN	5.9
1	B	50	GLU	5.8
1	B	45	LEU	5.3
1	B	53	SER	4.2
1	B	182	GLU	4.0
1	A	183	GLN	3.7
1	A	33	LYS	3.7
1	A	313	TYR	3.5
1	A	182	GLU	3.4
1	A	32	LYS	3.4
1	B	208	LEU	3.3
1	A	297	LEU	3.2
1	A	140	PRO	3.1
1	B	406	LYS	3.1
1	A	36	SER	3.0
1	B	280	GLN	3.0
1	A	221	GLU	2.9
1	A	181	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	157	GLU	2.8
1	B	402	GLU	2.8
1	B	55	SER	2.7
1	A	34	GLU	2.7
1	B	259	ILE	2.7
1	A	255	VAL	2.6
1	B	212	ASP	2.6
1	A	259	ILE	2.5
1	B	195	GLU	2.5
1	A	377	ASP	2.5
1	B	196	LYS	2.4
1	B	156	LYS	2.4
1	A	154	LYS	2.4
1	B	221	GLU	2.3
1	B	54	PHE	2.3
1	A	230	VAL	2.3
1	B	228	THR	2.2
1	B	183	GLN	2.1
1	B	230	VAL	2.1
1	A	384	LEU	2.1
1	A	53	SER	2.1
1	A	376	GLU	2.0
1	B	181	GLY	2.0
1	B	377	ASP	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	B	500	1/1	0.85	0.12	-	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.