



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 2WWV
EMDB ID: : EMD-1655
Title : Cryo-EM structure of the RbcL-RbcX complex
Authors : Liu, C.; Young, A.L.; Starling-Windhof, A.; Bracher, A.; Saschenbrecker, S.;
Rao, B.V.; Rao, K.V.; Berninghausen, O.; Mielke, T.; Hartl, F.U.; Beckmann,
R.; Hayer-Hartl, M.
Deposited on : 2009-10-20
Resolution : 9.00 Å(reported)
Based on PDB ID : 3HYB

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

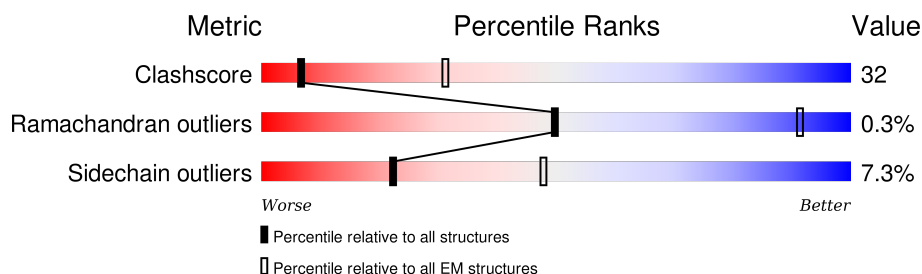
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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.







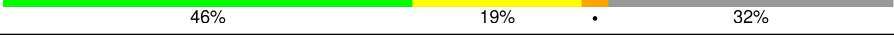



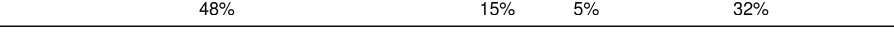
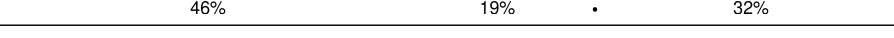

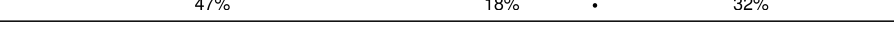
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	472	72% 22% . . .
1	B	472	71% 23% . . .
1	C	472	72% 22% . . .
1	D	472	71% 22% . . .
1	E	472	72% 22% . . .
1	F	472	71% 22% . . .
1	G	472	71% 22% . . .
1	H	472	71% 23% . . .
2	I	155	47% 18% . 32%

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Mol	Chain	Length	Quality of chain
2	J	155	
2	K	155	
2	L	155	
2	M	155	
2	N	155	
2	O	155	
2	P	155	
2	Q	155	
2	R	155	
2	S	155	
2	T	155	
2	U	155	
2	V	155	
2	W	155	
2	X	155	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 42856 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	B	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	C	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	D	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	E	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	F	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	G	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	H	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		

- Molecule 2 is a protein called RBCX PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	J	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	K	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	L	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	M	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	N	105	Total	C	N	O	S	4	0
			870	555	151	160	4		

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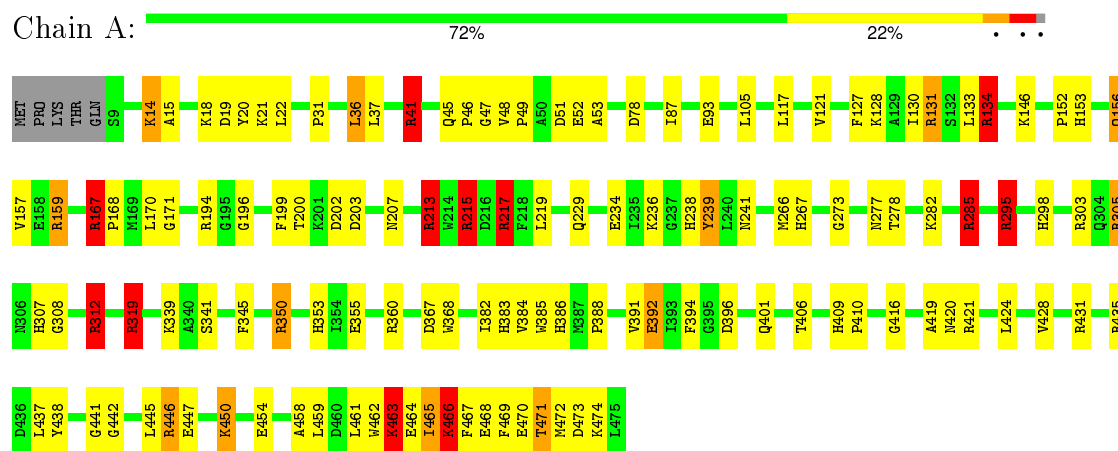
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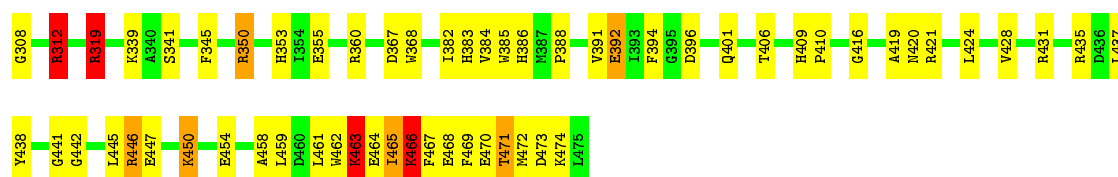
Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	P	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	Q	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	R	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	S	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	T	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	U	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	V	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	W	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	X	105	Total	C	N	O	S	4	0
			870	555	151	160	4		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

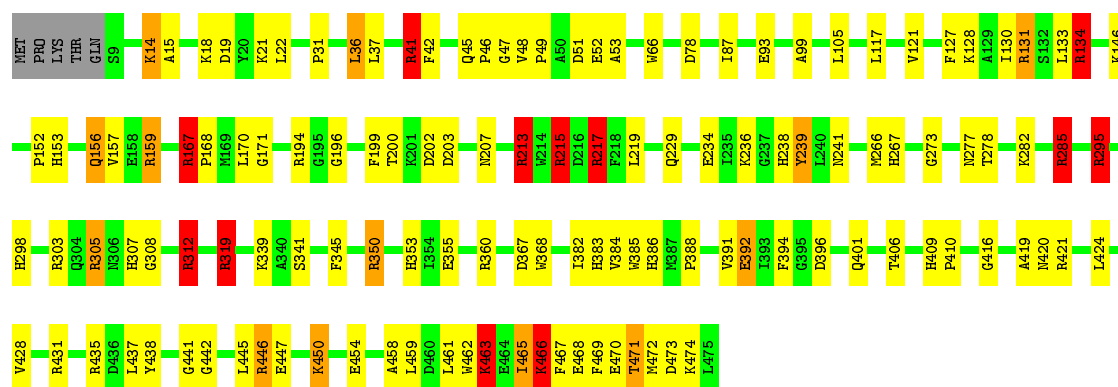
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN





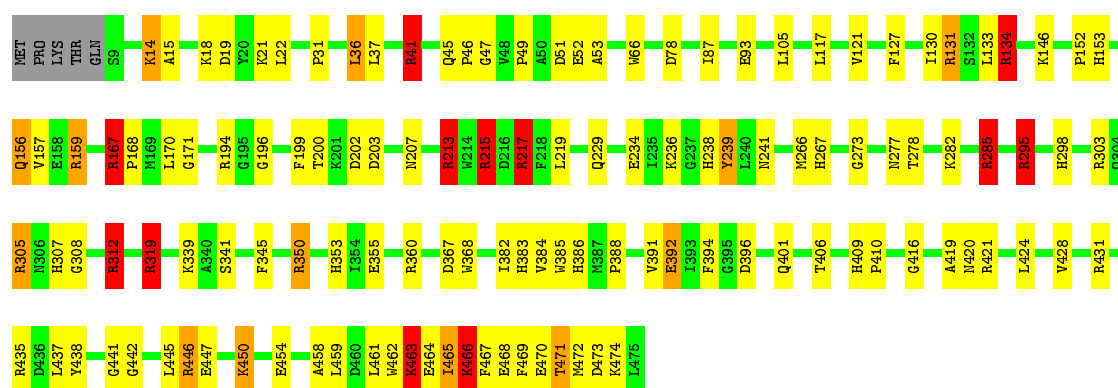
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain D: 71% 22%



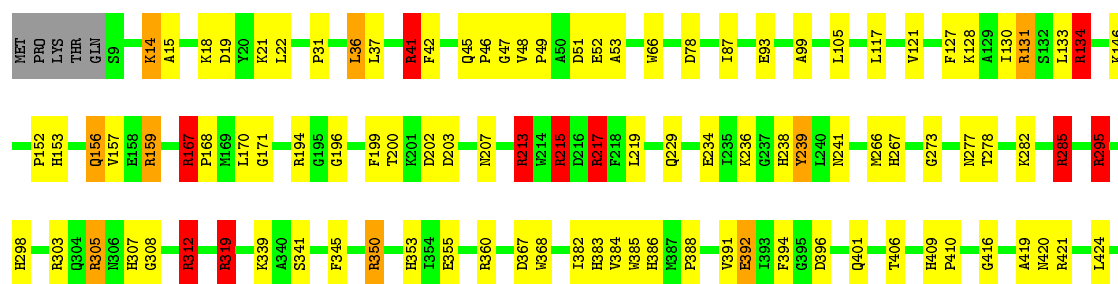
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain E: 72% 22%



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

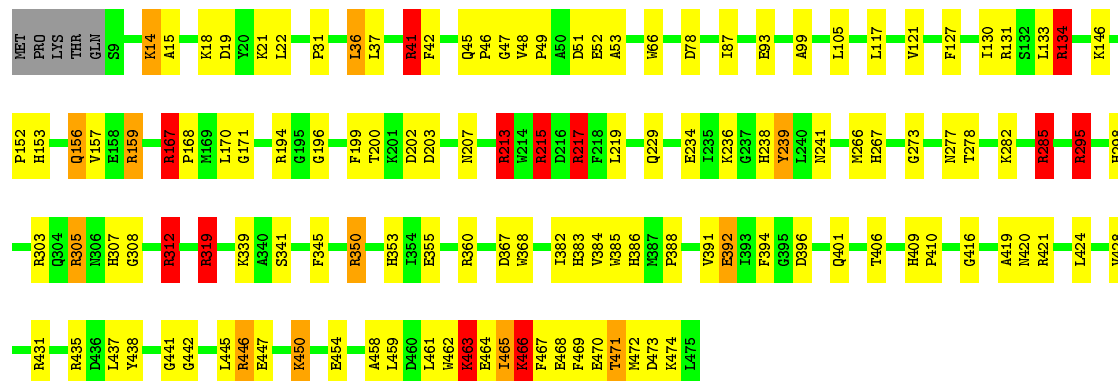
Chain F: 71% 22%





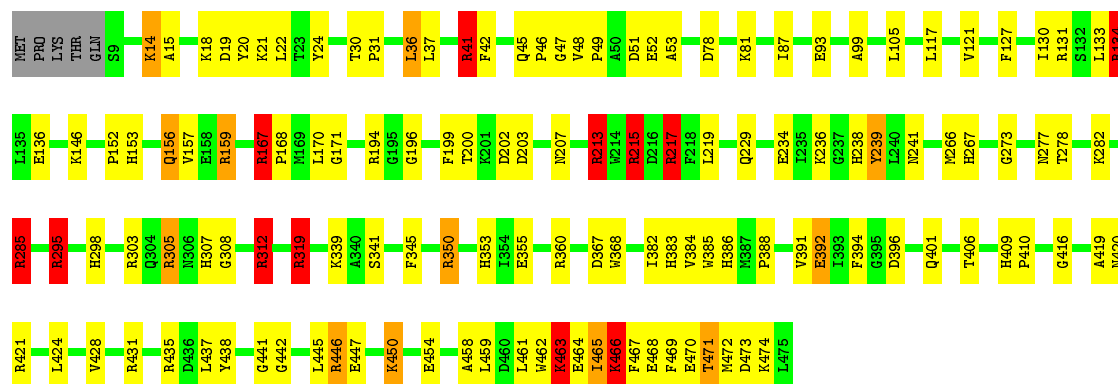
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain G: 71% 22%



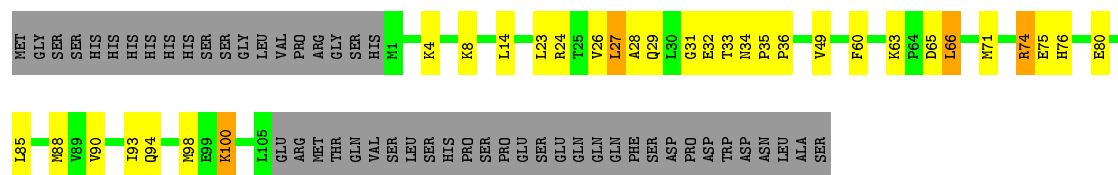
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain H: 71% 23%



• Molecule 2: RBCX PROTEIN

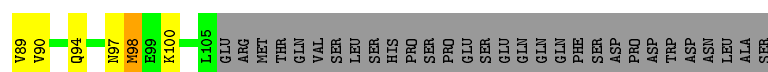
Chain I: 47% 18% 32%



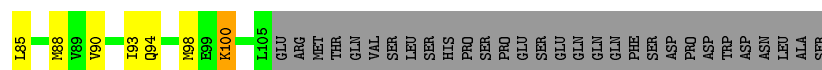
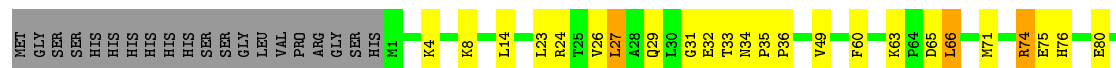
• Molecule 2: RBCX PROTEIN

Chain J: 48% 15% 5% 32%

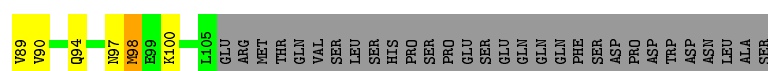




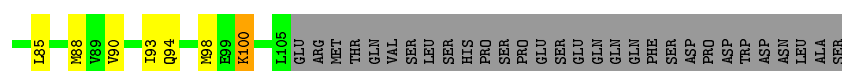
• Molecule 2: RBCX PROTEIN



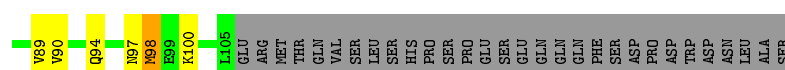
• Molecule 2: RBCX PROTEIN



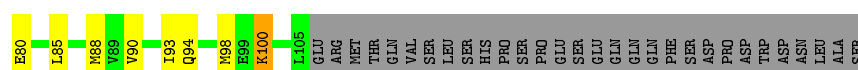
• Molecule 2: RBCX PROTEIN



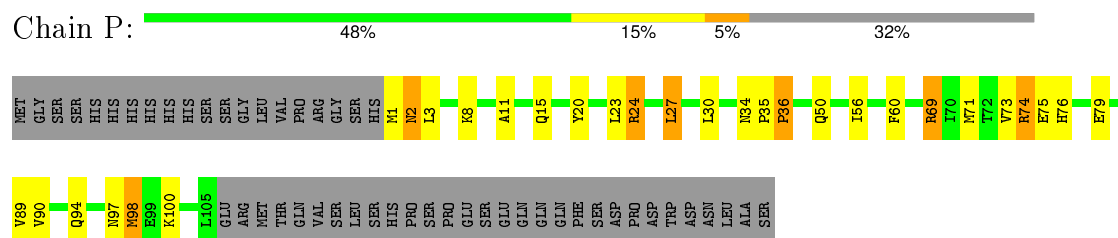
• Molecule 2: RBCX PROTEIN



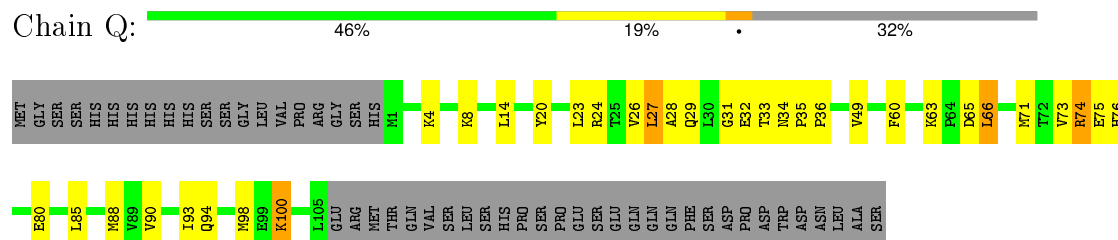
• Molecule 2: RBCX PROTEIN



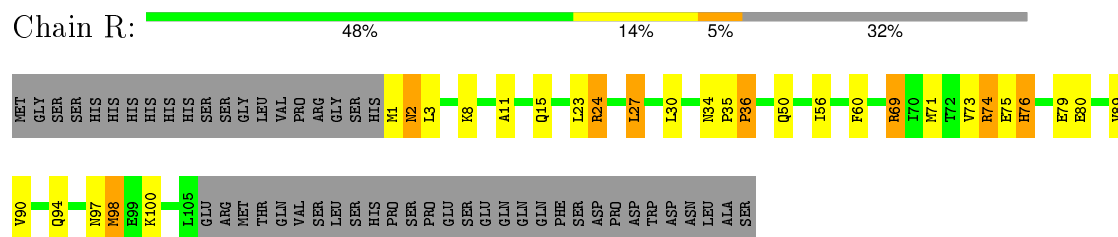
- Molecule 2: RBCX PROTEIN



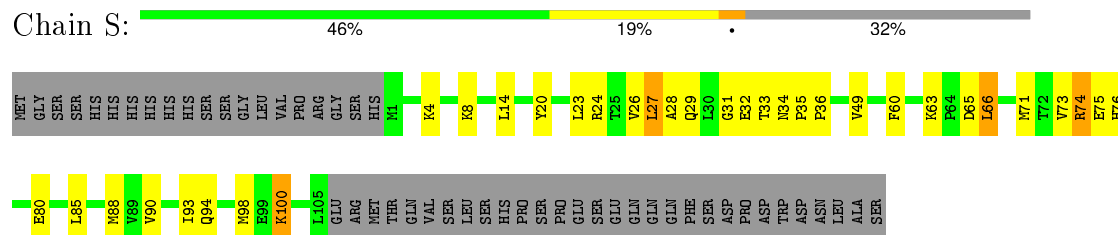
- Molecule 2: RBCX PROTEIN



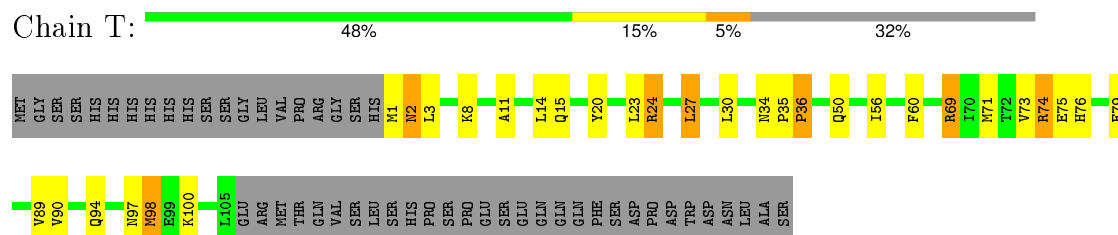
- Molecule 2: RBCX PROTEIN



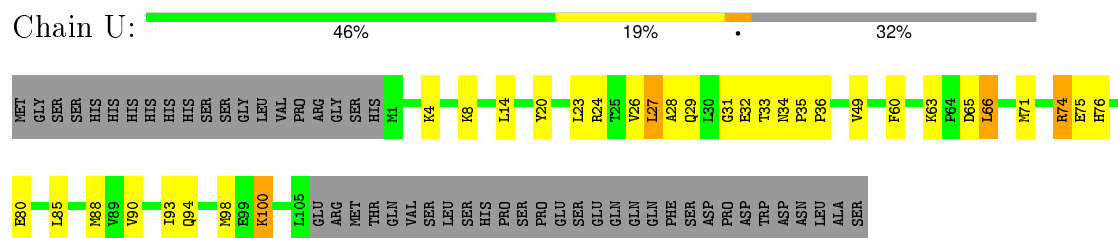
- Molecule 2: RBCX PROTEIN



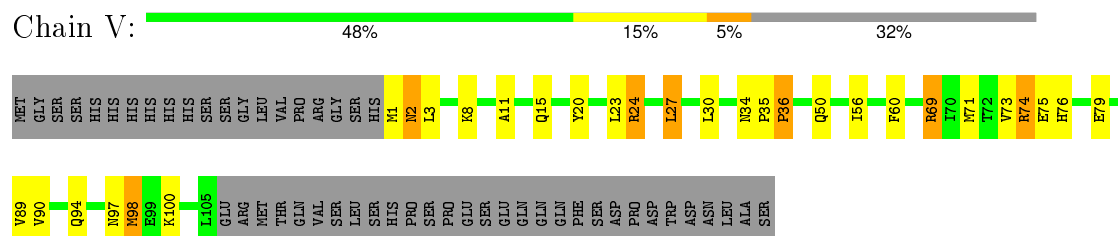
- Molecule 2: RBCX PROTEIN



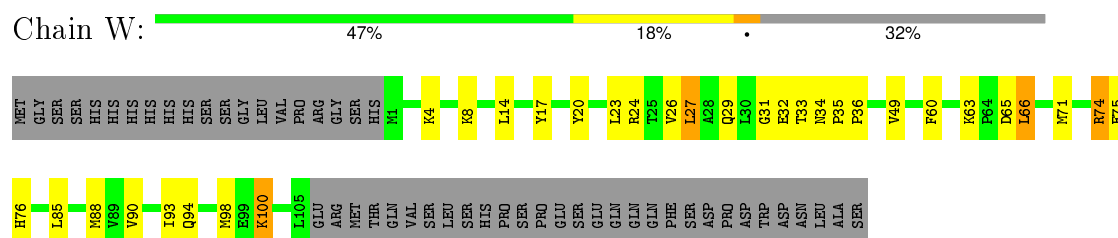
- Molecule 2: RBCX PROTEIN



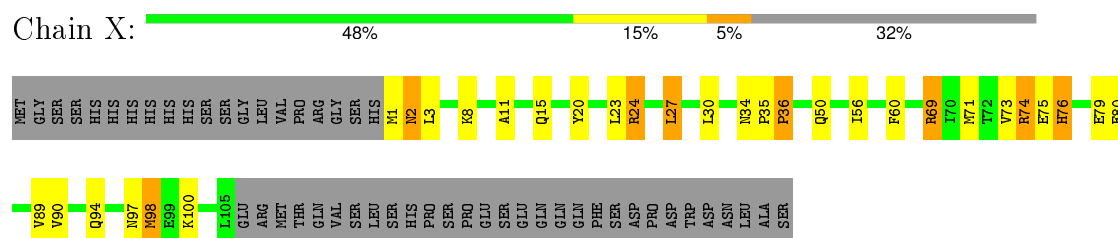
• Molecule 2: RBCX PROTEIN



• Molecule 2: RBCX PROTEIN



• Molecule 2: RBCX PROTEIN



4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO163	Depositor

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 >2	RMSZ	# Z >2
1	A	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	B	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	C	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	D	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	E	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	F	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	G	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	H	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
2	I	0.59	0/847	0.66	0/1148
2	J	0.76	5/884 (0.6%)	0.69	0/1194
2	K	0.59	0/847	0.66	0/1148
2	L	0.76	5/884 (0.6%)	0.69	0/1194
2	M	0.59	0/847	0.66	0/1148
2	N	0.76	5/884 (0.6%)	0.69	0/1194
2	O	0.59	0/847	0.66	0/1148
2	P	0.76	5/884 (0.6%)	0.69	0/1194
2	Q	0.59	0/847	0.66	0/1148
2	R	0.76	5/884 (0.6%)	0.69	0/1194
2	S	0.59	0/847	0.66	0/1148
2	T	0.76	5/884 (0.6%)	0.69	0/1194
2	U	0.59	0/847	0.66	0/1148
2	V	0.76	5/884 (0.6%)	0.69	0/1194
2	W	0.59	0/847	0.66	0/1148
2	X	0.76	5/884 (0.6%)	0.69	0/1194
All	All	0.60	64/43752 (0.1%)	0.91	144/59128 (0.2%)

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	20

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	20
1	C	0	20
1	D	0	20
1	E	0	20
1	F	0	20
1	G	0	20
1	H	0	20
2	J	0	1
2	L	0	1
2	N	0	1
2	P	0	1
2	R	0	1
2	T	0	1
2	V	0	1
2	X	0	1
All	All	0	168

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	471	THR	C-N	20.46	1.81	1.34
1	G	471	THR	C-N	20.45	1.81	1.34
1	F	471	THR	C-N	20.45	1.81	1.34
1	A	471	THR	C-N	20.43	1.81	1.34
1	E	471	THR	C-N	20.43	1.81	1.34

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	463	LYS	O-C-N	-34.97	66.75	122.70
1	F	463	LYS	O-C-N	-34.96	66.77	122.70
1	H	463	LYS	O-C-N	-34.96	66.77	122.70
1	B	463	LYS	O-C-N	-34.95	66.79	122.70
1	E	463	LYS	O-C-N	-34.95	66.79	122.70

There are no chirality outliers.

5 of 168 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	A	134	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	159	ARG	Sidechain
1	A	167	ARG	Sidechain
1	A	41	ARG	Sidechain

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	3653	0	3547	317	0
1	B	3653	0	3546	322	0
1	C	3653	0	3547	286	0
1	D	3653	0	3548	332	0
1	E	3653	0	3548	334	0
1	F	3653	0	3547	313	0
1	G	3653	0	3547	312	0
1	H	3653	0	3547	296	0
2	I	834	0	820	110	0
2	J	870	0	880	43	0
2	K	834	0	821	140	0
2	L	870	0	880	40	0
2	M	834	0	822	95	0
2	N	870	0	880	41	0
2	O	834	0	820	139	0
2	P	870	0	880	46	0
2	Q	834	0	821	120	0
2	R	870	0	880	50	0
2	S	834	0	820	120	0
2	T	870	0	880	54	0
2	U	834	0	820	118	0
2	V	870	0	880	49	0
2	W	834	0	822	101	0
2	X	870	0	880	38	0
All	All	42856	0	41983	2709	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 32.

The worst 5 of 2709 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:D:167:ARG:CG	1:D:428:VAL:HG22	1.22	1.65
1:H:167:ARG:CG	1:H:428:VAL:HG22	1.21	1.64
1:G:167:ARG:CG	1:G:428:VAL:HG22	1.22	1.64
1:E:22:LEU:CD2	2:K:33:THR:CA	1.77	1.63
1:C:47:GLY:HA3	2:N:1:MET:SD	1.34	1.63

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 PDB entries followed by that with respect to all EM entries.

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	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	52	86
1	B	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	52	86
1	C	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	52	86
1	D	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	52	86
1	E	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	52	86
1	F	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	52	86
1	G	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	52	86
1	H	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	52	86
2	I	106/155 (68%)	104 (98%)	2 (2%)	0	100	100
2	J	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	21	67
2	K	106/155 (68%)	104 (98%)	2 (2%)	0	100	100
2	L	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	21	67
2	M	106/155 (68%)	104 (98%)	2 (2%)	0	100	100
2	N	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	21	67
2	O	106/155 (68%)	104 (98%)	2 (2%)	0	100	100
2	P	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	21	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	106/155 (68%)	104 (98%)	2 (2%)	0	100	100
2	R	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	21	67
2	S	106/155 (68%)	104 (98%)	2 (2%)	0	100	100
2	T	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	21	67
2	U	106/155 (68%)	104 (98%)	2 (2%)	0	100	100
2	V	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	21	67
2	W	106/155 (68%)	104 (98%)	2 (2%)	0	100	100
2	X	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	21	67
All	All	5336/6256 (85%)	5192 (97%)	128 (2%)	16 (0%)	50	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	LYS
1	B	463	LYS
1	C	463	LYS
1	D	463	LYS
1	E	463	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	377/383 (98%)	355 (94%)	22 (6%)	25	61
1	B	377/383 (98%)	355 (94%)	22 (6%)	25	61
1	C	377/383 (98%)	355 (94%)	22 (6%)	25	61
1	D	377/383 (98%)	355 (94%)	22 (6%)	25	61
1	E	377/383 (98%)	355 (94%)	22 (6%)	25	61
1	F	377/383 (98%)	355 (94%)	22 (6%)	25	61
1	G	377/383 (98%)	355 (94%)	22 (6%)	25	61
1	H	377/383 (98%)	355 (94%)	22 (6%)	25	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	85/137 (62%)	76 (89%)	9 (11%)	8	36
2	J	91/137 (66%)	82 (90%)	9 (10%)	10	39
2	K	85/137 (62%)	76 (89%)	9 (11%)	8	36
2	L	91/137 (66%)	82 (90%)	9 (10%)	10	39
2	M	85/137 (62%)	76 (89%)	9 (11%)	8	36
2	N	91/137 (66%)	82 (90%)	9 (10%)	10	39
2	O	85/137 (62%)	76 (89%)	9 (11%)	8	36
2	P	91/137 (66%)	82 (90%)	9 (10%)	10	39
2	Q	85/137 (62%)	76 (89%)	9 (11%)	8	36
2	R	91/137 (66%)	82 (90%)	9 (10%)	10	39
2	S	85/137 (62%)	76 (89%)	9 (11%)	8	36
2	T	91/137 (66%)	82 (90%)	9 (10%)	10	39
2	U	85/137 (62%)	76 (89%)	9 (11%)	8	36
2	V	91/137 (66%)	82 (90%)	9 (10%)	10	39
2	W	85/137 (62%)	76 (89%)	9 (11%)	8	36
2	X	91/137 (66%)	82 (90%)	9 (10%)	10	39
All	All	4424/5256 (84%)	4104 (93%)	320 (7%)	22	55

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	219	LEU
2	I	60	PHE
2	V	24	ARG
1	G	319	ARG
1	H	203	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	212	GLN
1	F	212	GLN
2	P	2	ASN
1	E	238	HIS
1	E	353	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 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 [i](#)

There are no chain breaks in this entry.