



wwPDB EM Map/Model Validation Report

Sep 26, 2016 – 11:23 AM EDT

PDB ID : 5GO9
EMDB ID: : EMD-9528
Title : Cryo-EM structure of RyR2 in closed state
Authors : Peng, W.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-26
Resolution : 4.40 Å(reported)

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) : rb-20027939

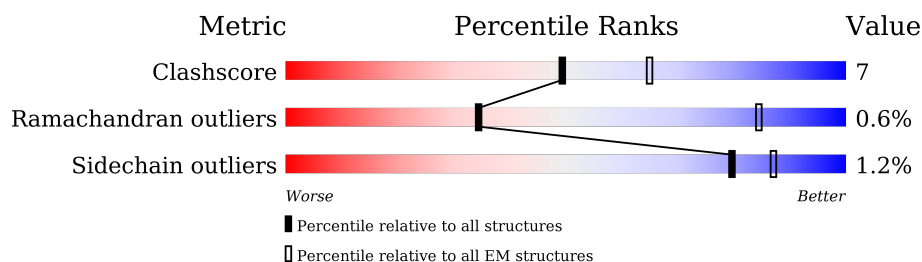
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	4968	54% 14% • 31%
1	B	4968	54% 14% • 31%
1	C	4968	54% 14% • 31%
1	D	4968	54% 14% • 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 105068 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3423	Total	C	N	O	S	0	0
			26266	16740	4498	4874	154		
1	B	3423	Total	C	N	O	S	0	0
			26266	16740	4498	4874	154		
1	C	3423	Total	C	N	O	S	0	0
			26266	16740	4498	4874	154		
1	D	3423	Total	C	N	O	S	0	0
			26266	16740	4498	4874	154		

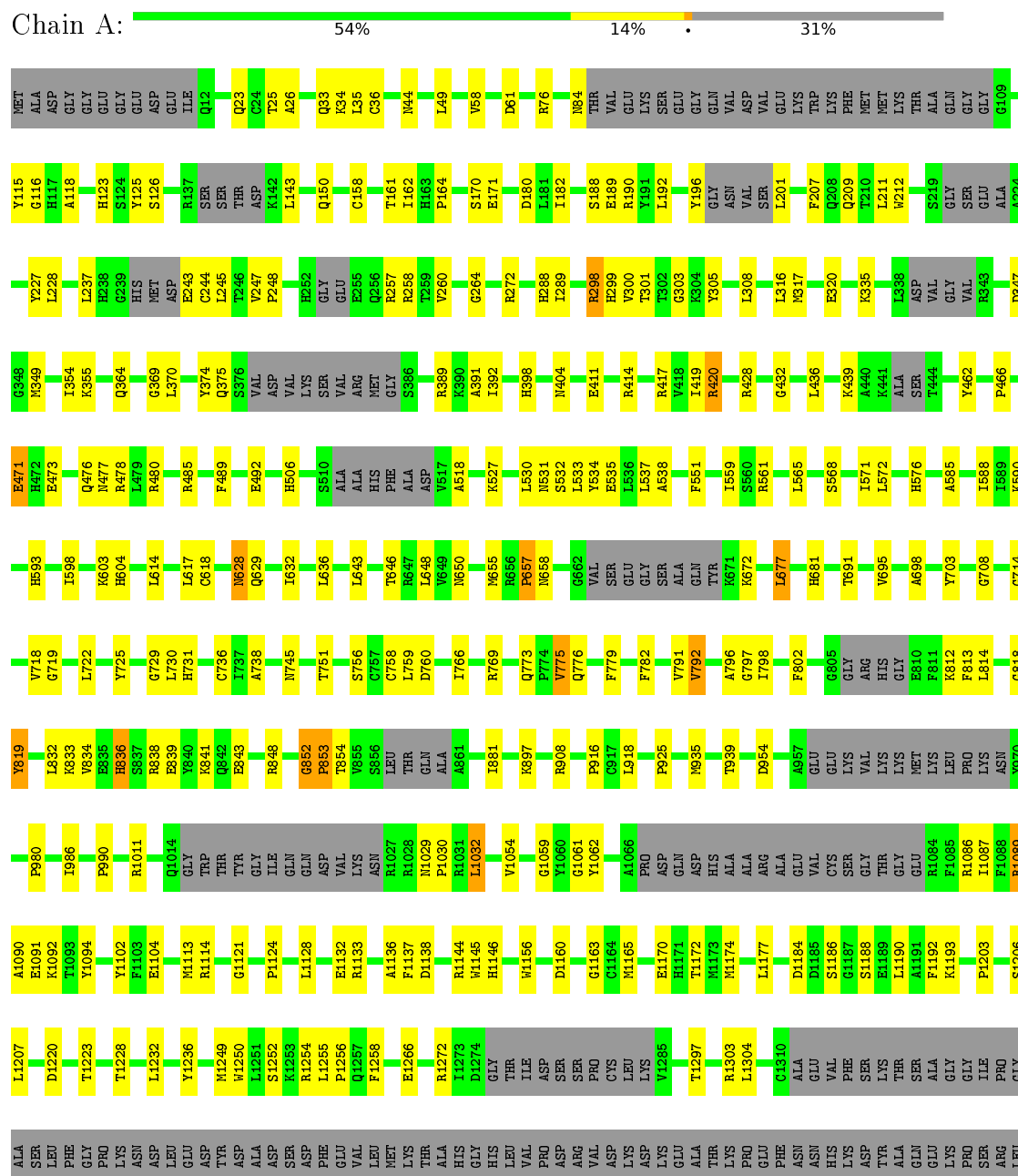
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	Zn	0
			1	1	
2	A	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	

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.

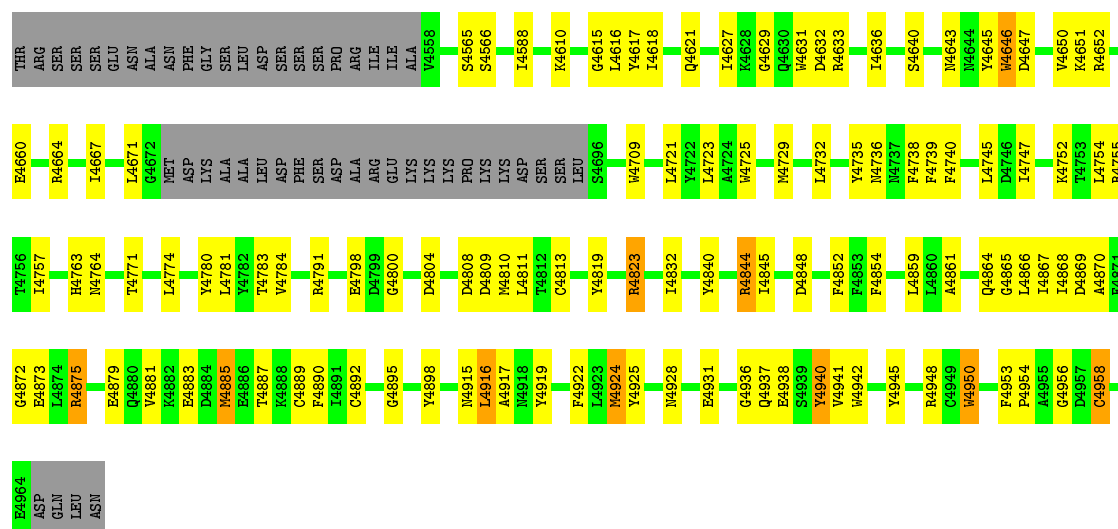
• Molecule 1: RyR2



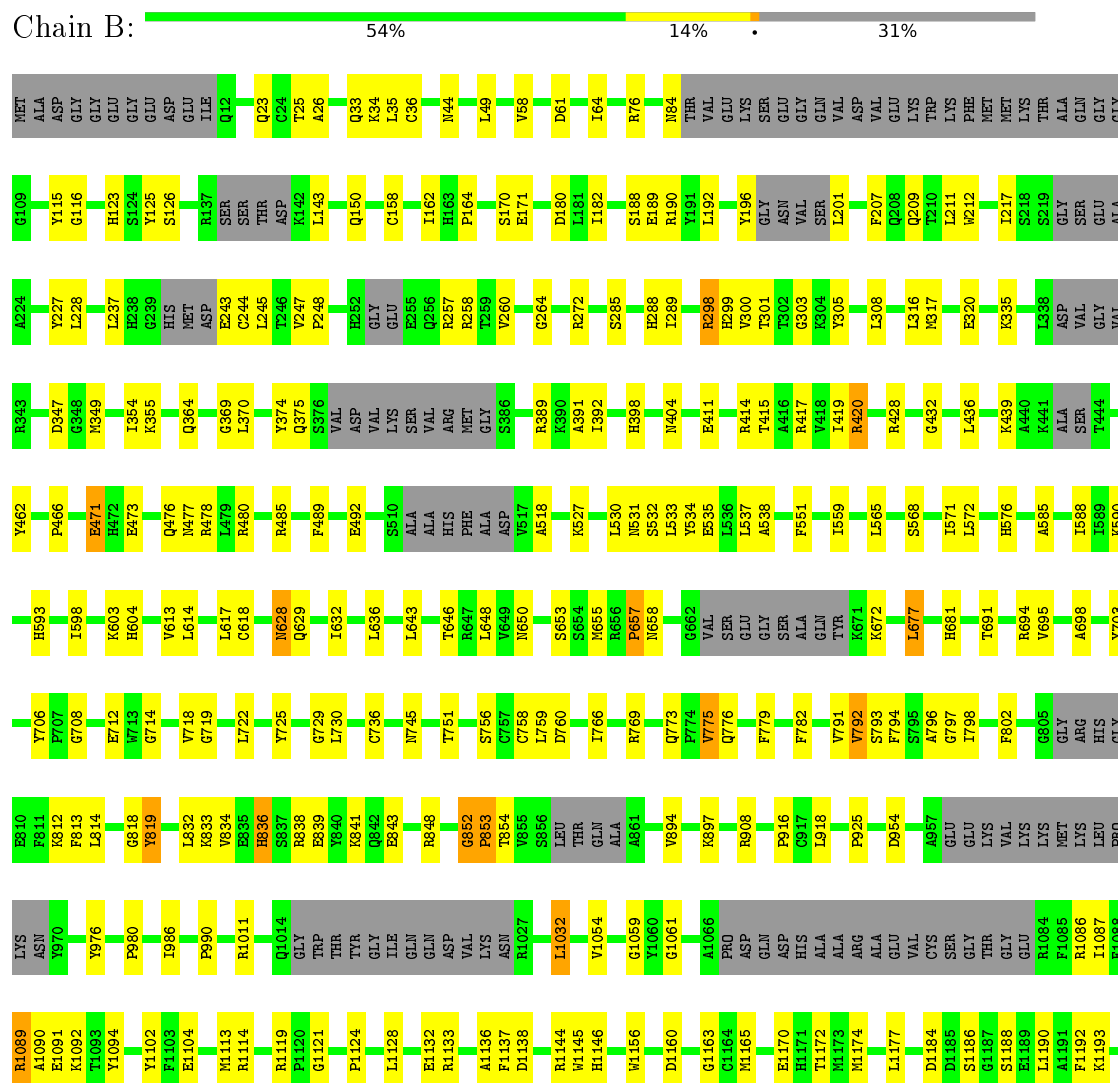








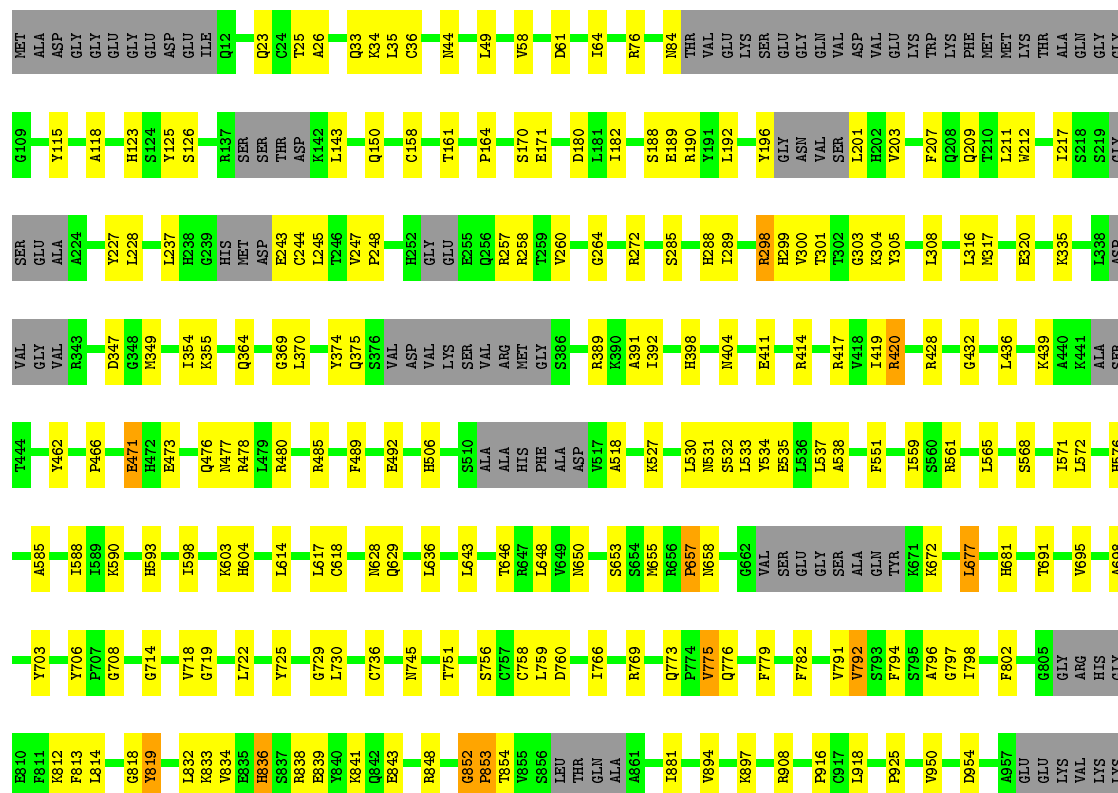
• Molecule 1: RyR2























G4956	D4869	R4755	E4660	PRO	ALA	LEU	ASN	LYS	GLU	E4108
D4957	A4870	T4756	E4660	THR	LYS	ILE	MET	MET	ARG	
C4958	F4871	I4757	R4664	ARG	GLU	PRO	PRO	THR	ALA	V4126
	G4872			SER	ASP	HIS	ASP	VAL	ASN	
K4961	E4873	H4763	I4667	SER	LYS	ASN	PRO	ARG	LYS	F4130
E4964	L4874	M4764		SER	GLY	PRO	THR	ASP	GLU	Q4131
ASP	R4875		L4671	GLU	LYS	ASN	GLN	MET	GLU	
GLN		T4771	G4672	ASN	GLN	ALA	ASP	VAL	GLU	L4134
LEU			MET	ALA	LYS	ALA	GLU	ALA	SER	G4135
ASN		L4774	ASP	ASN	ARG	LEU	VAL	ALA	GLU	R4136
			LYS	PHE	GLN	ASP	ARG	PHE	LYS	I4137
	K4882	Y4780	ALA	GLY	LEU	LEU	GLY	PHE	LYS	E4138
E4883	L4781		ALA	SER	HIS	MET	ASP	THR	LYS	I4139
D4884	Y4782		LEU	LEU	THR	SER	GLY	PRO	PRO	M4140
M4885	T4783		ASP	ASP	HIS	SER	TYR	GLU	GLU	G4141
E4886	V4784		SER	SER	ARG	PRO	GLY	TRP	GLU	S4142
T4887			PHE	SER	TYR	ALA	GLY	VAL	GLN	A4143
K4888	R4791		SER	SER	GLY	PRO	ARG	PHE	GLY	K4144
C4889			ASP	PRO	GLY	ILE	LYS	MET	PRO	R4145
F4890	E4798		ALA	ARG	GLU	ILE	LYS	THR	ARG	I4146
I4891	D4799		ARG	ILE	PRO	GLU	VAL	THR	MET	
C4892	G4800		ILE	ALA	VAL	VAL	LEU	LEU	PHE	S4157
G4893			LYS	ALA	PRO	GLN	GLY	LEU	GLY	R4158
I4894	D4804		LYS	GLY	PRO	GLU	THR	PHE	SER	
G4895			LYS	SER	SER	LYS	LEU	ALA	LEU	I4161
			PRO	LYS	SER	LYS	PRO	ALA	VAL	E4162
Y4898	D4808		LYS	PRO	ALA	PHE	PRO	ALA	THR	R4163
	D4809		LYS	S4865	ALA	LYS	LYS	SER	VAL	R4164
N4915	M4810		LYS	S4866	PHE	GLN	SER	SER	VAL	
L4916	L4811		ASP	I4888	TRP	GLU	GLY	VAL	ARG	K4170
L4917	G4812		SER	K4610	LYS	GLN	ASP	SER	ARG	R4171
A4917	C4813		SER		LYS	LYS	LEU	ARG	ALA	
I4918			LEU		ILE	ALA	THR	GLY	ALA	I4174
Y4919	Y4819		S4896	G4615	LYS	LYS	ASP	PHE	LEU	
				L4616	GLU	GLU	LEU	SER	LEU	V4178
F4922	R4823		W4709	Y4617	GLU	LYS	ARG	ARG	ALA	
I4923				I4618	GLU	GLU	ILE	LEU	LEU	N4179
M4924	L4832		L4721		LYS	LYS	LEU	ILE	ARG	
Y4925			Y4722	Q4621	GLU	GLU	THR	GLY	TYR	M4187
	Y4840		L4723	I4627	GLU	LYS	GLU	GLY	ASN	E4188
			W4725	K4628	GLU	GLU	SER	LEU	VAL	L4189
	R4844			G4629	GLU	GLU	ASP	LEU	LEU	F4190
	I4845			W4630	ASN	ASN	LEU	GLY	THR	V4191
E4931			M4729	W4631	LYS	LYS	LEU	GLY	LEU	
	D4848			D4632	LYS	LYS	LEU	SER	MET	C4194
G4936			L4732	R4633	GLU	GLU	SER	ARG	ARG	
Q4937				I4636	SER	PRO	ASP	LEU	MET	T4197
E4938	F4852		Y4735		GLU	GLU	ILE	VAL	LEU	
S4939	F4853		M4736		GLU	GLU	PHE	GLU	SER	M4201
Y4940	F4854		N4737	I4636	GLU	GLU	GLY	GLY	LEU	Q4202
V4941			F4738	S4640	ALA	ALA	LEU	LYS	SER	I4203
W4942	V4857		F4739		GLU	GLY	ASP	LYS	LEU	A4204
	I4858		F4740	N4643	THR	GLY	LEU	LYS	LEU	A4205
Y4945	L4859			M4644	SER	ASP	LYS	ILE	LYS	Q4206
	L4860		L4745	Y4645	VAL	ASP	ARG	LYS	LYS	I4207
R4948	A4861		D4746	W4646	VAL	GLY	GLY	VAL	GLU	SER
C4949			I4747	D4647	GLY	GLY	GLY	ALA	MET	GLU
W4950	Q4864				LYS	LYS	GLY	GLY	LYS	SER
	G4865				GLU	GLU	GLY	GLY	LYS	GLU
F4953	L4866		K4752	V4650	LYS	GLU	GLY	GLY	LYS	SER
P4954	I4867		T4753	K4651	GLU	GLU	TYR	LEU	VAL	ASP
A4955	I4868		L4754	R4652	LEU	LYS	LYS	LEU	VAL	LEU
									ASN	ASN

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	48454	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	B	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	C	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	D	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
All	All	0.98	116/107004 (0.1%)	0.94	312/144596 (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	30
1	B	0	30
1	C	0	30
1	D	0	30
All	All	0	120

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	B	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	C	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	D	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	A	4950	TRP	CE3-CZ3	-9.89	1.21	1.38

The worst 5 of 312 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	B	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	C	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	D	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	A	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	471	GLU	Peptide
1	A	657	PRO	Peptide
1	A	729	GLY	Peptide
1	A	775	VAL	Peptide
1	A	791	VAL	Peptide

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	26266	0	24898	409	0
1	B	26266	0	24898	421	0
1	C	26266	0	24898	414	0
1	D	26266	0	24898	401	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	105068	0	99592	1515	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 7.

The worst 5 of 1515 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:4873:GLU:HA	1:B:4875:ARG:NH1	1.62	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4875:ARG:NH1	1:D:4873:GLU:HA	1.62	1.14
1:B:4873:GLU:HA	1:C:4875:ARG:NH1	1.62	1.13
1:C:4873:GLU:OE1	1:D:4875:ARG:HD3	1.49	1.12
1:C:4873:GLU:HA	1:D:4875:ARG:NH1	1.62	1.12

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	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	B	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	C	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	D	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
All	All	13156/19872 (66%)	11932 (91%)	1140 (9%)	84 (1%)	34	74

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4071	ALA
1	B	4071	ALA
1	C	4071	ALA
1	D	4071	ALA
1	A	730	LEU

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 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	2659/4355 (61%)	2628 (99%)	31 (1%)	78	90
1	B	2658/4355 (61%)	2627 (99%)	31 (1%)	78	90
1	C	2659/4355 (61%)	2627 (99%)	32 (1%)	78	90
1	D	2660/4355 (61%)	2628 (99%)	32 (1%)	78	90
All	All	10636/17420 (61%)	10510 (99%)	126 (1%)	79	90

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4499	ASN
1	C	658	ASN
1	D	4136	ARG
1	B	4652	ARG
1	C	84	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3976	GLN
1	C	593	HIS
1	D	3916	GLN
1	B	4179	ASN
1	C	44	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are 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.