wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 08:54 PM EDT

PDB ID	:	5TAZ
EMDB ID:	:	EMD-8390
Title	:	Structure of rabbit RyR1 (ryanodine dataset, class 3)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.30 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

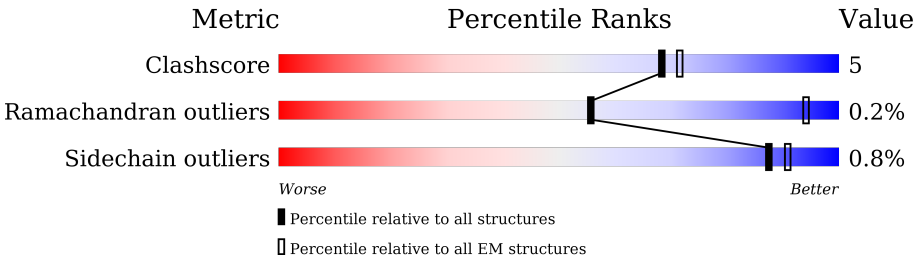
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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)	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	108	87% 12% •
1	F	108	89% 10% •
1	H	108	88% 11% •
1	J	108	89% 10% •
2	B	4416	84% 10% 5%
2	E	4416	84% 10% 5%
2	G	4416	84% 10% 5%
2	I	4416	85% 10% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

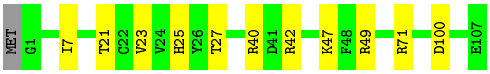
Mol	Chain	Residues	Atoms	AltConf
4	G	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0

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 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: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:

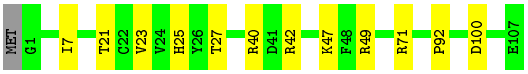


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:

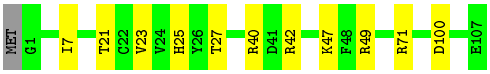
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



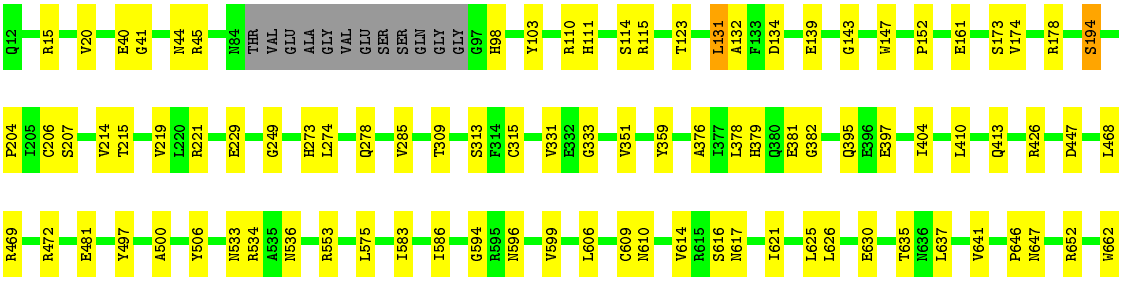
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

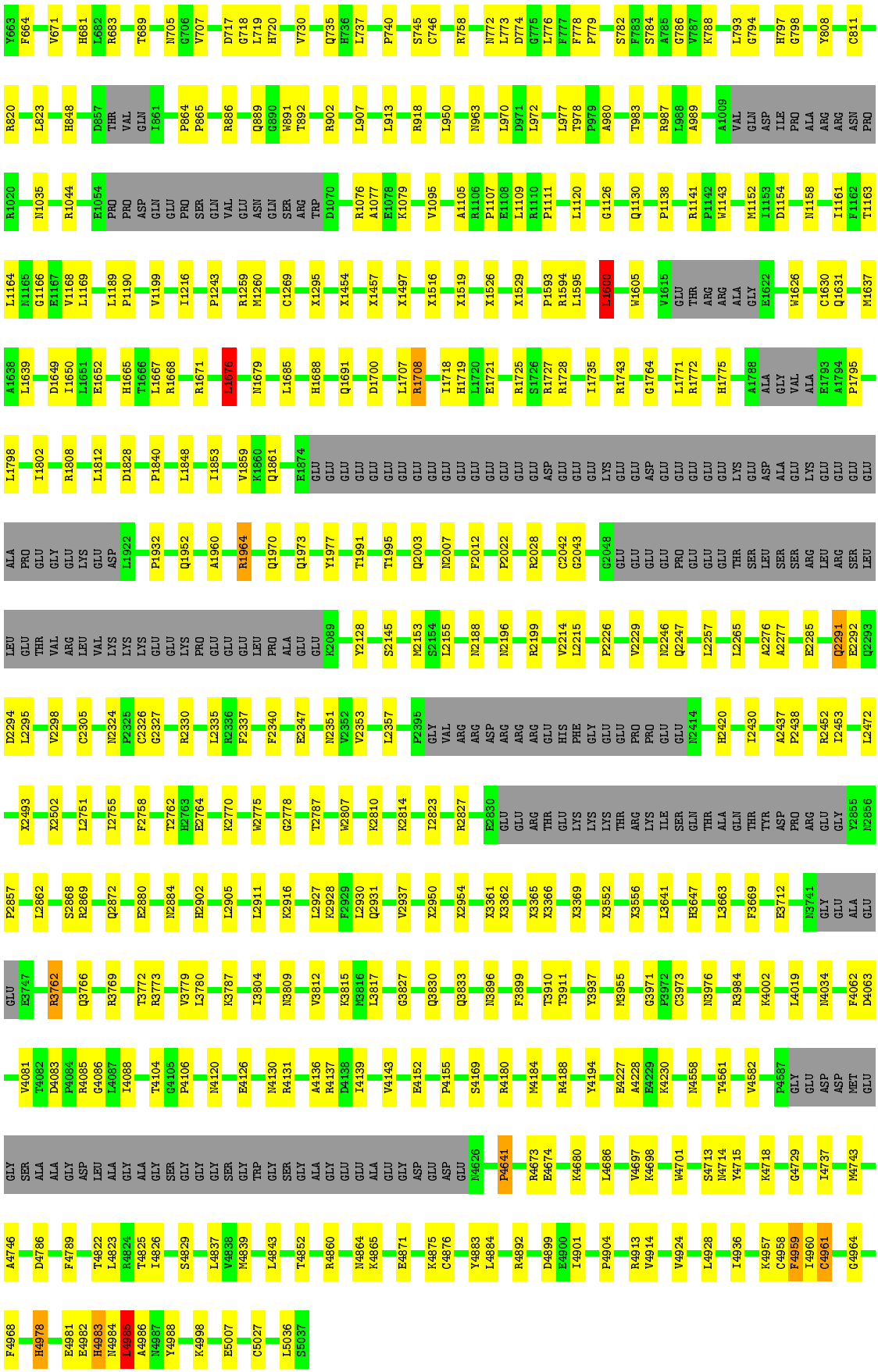
Chain J:



- Molecule 2: Ryanodine receptor 1

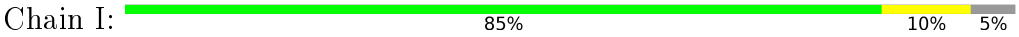
Chain B:

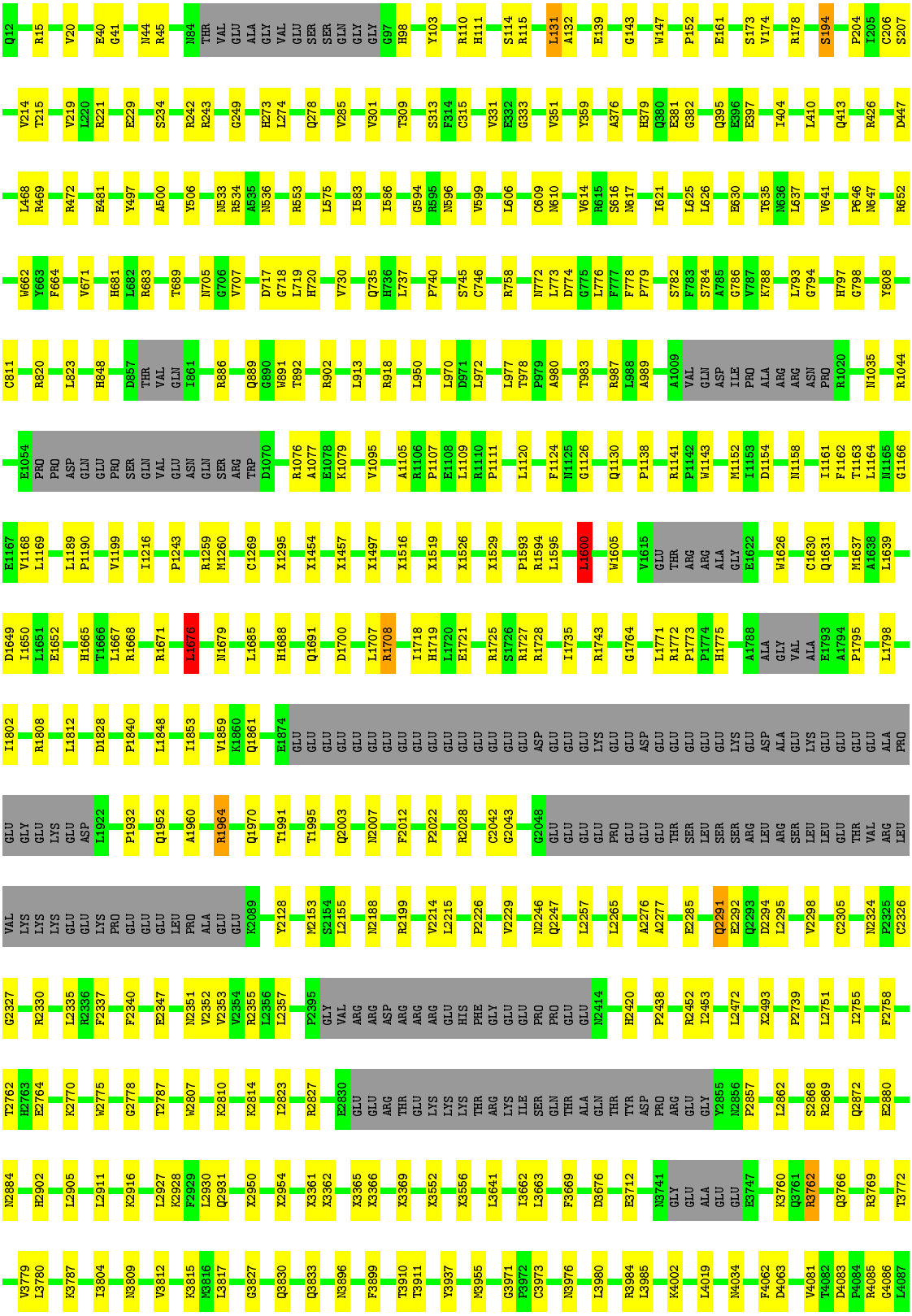


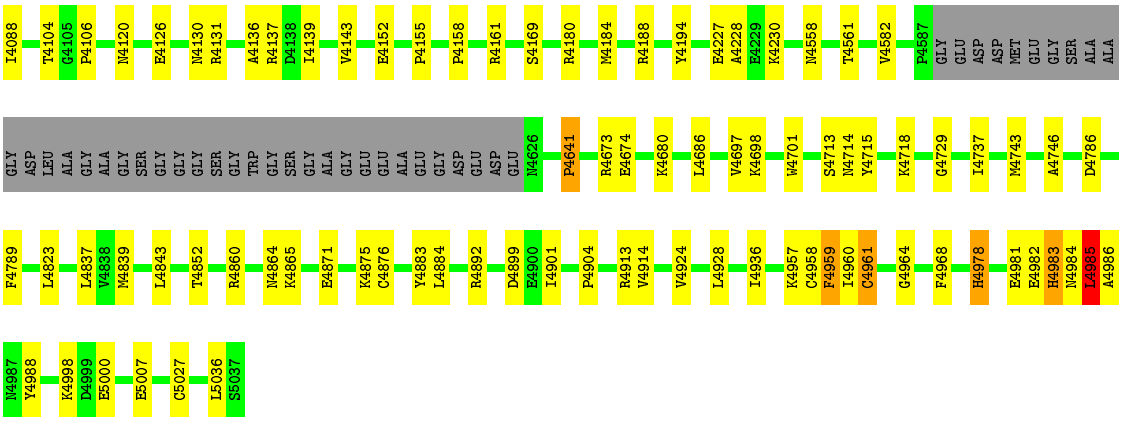


• Molecule 2: Ryanodine receptor 1

Chain I:

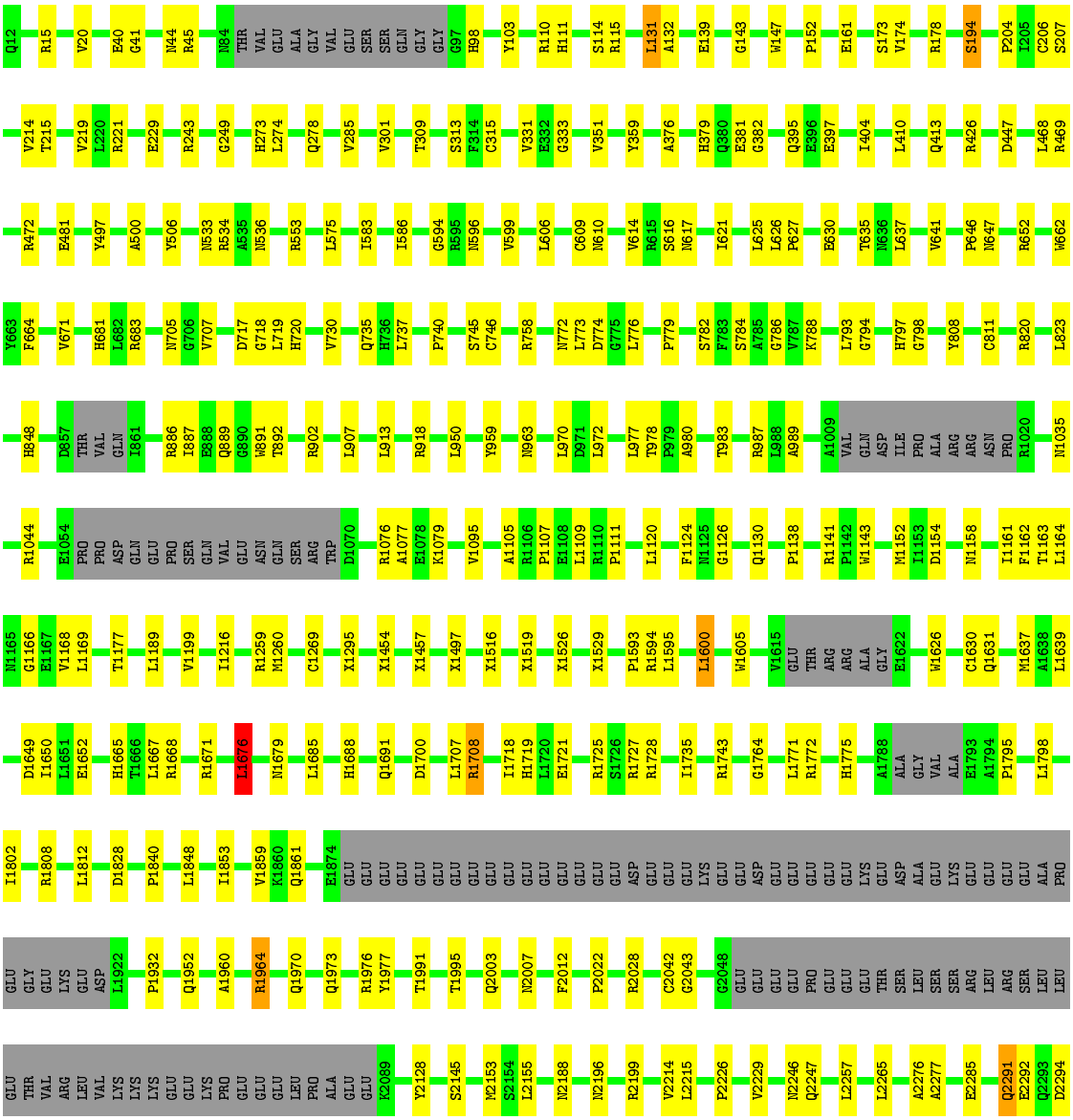


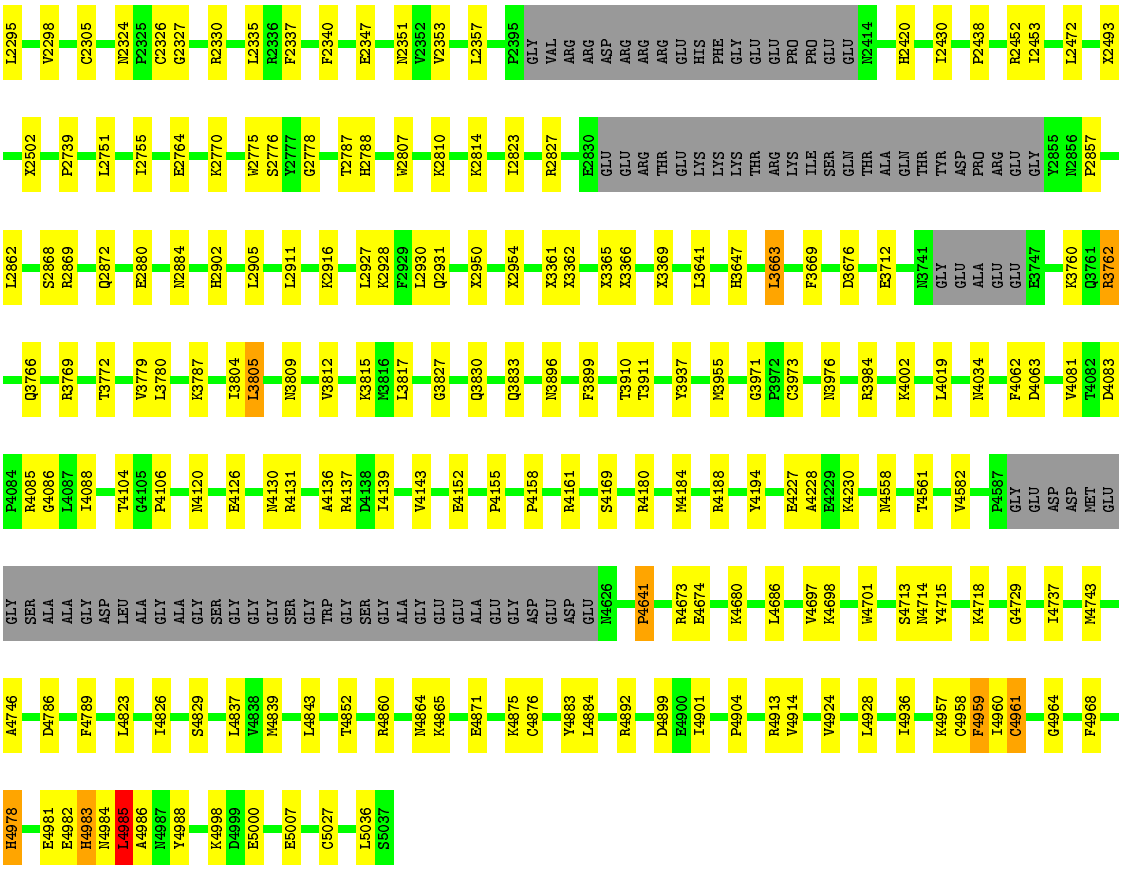




- Molecule 2: Ryanodine receptor 1

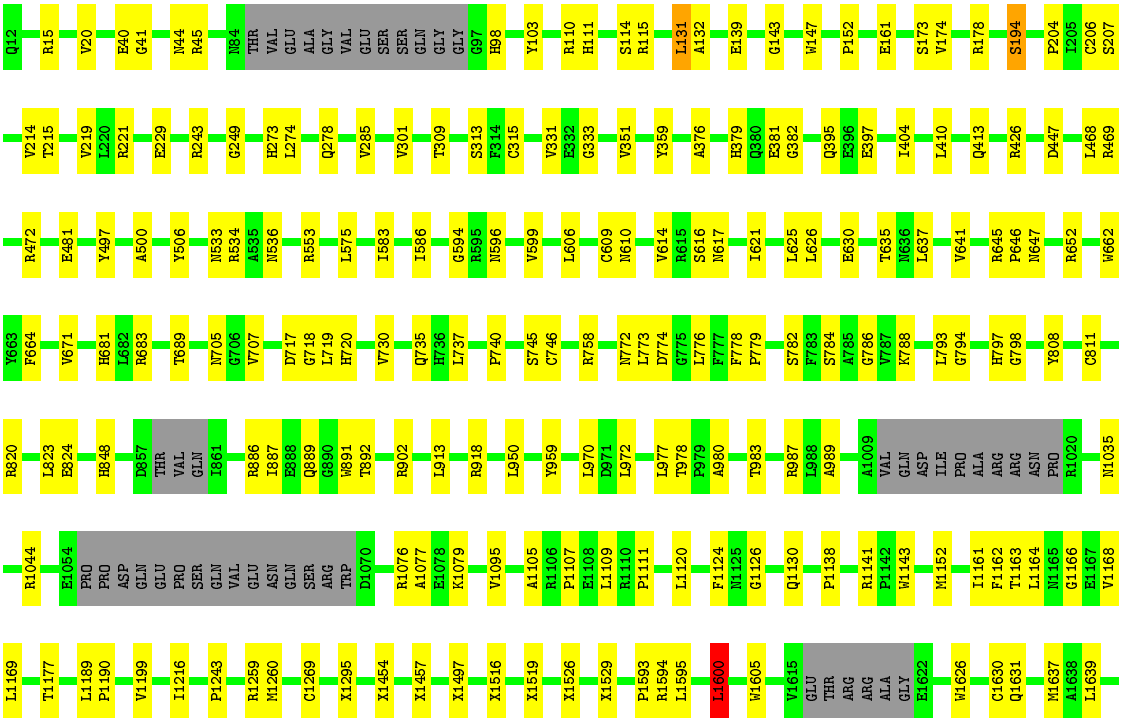
Chain G:

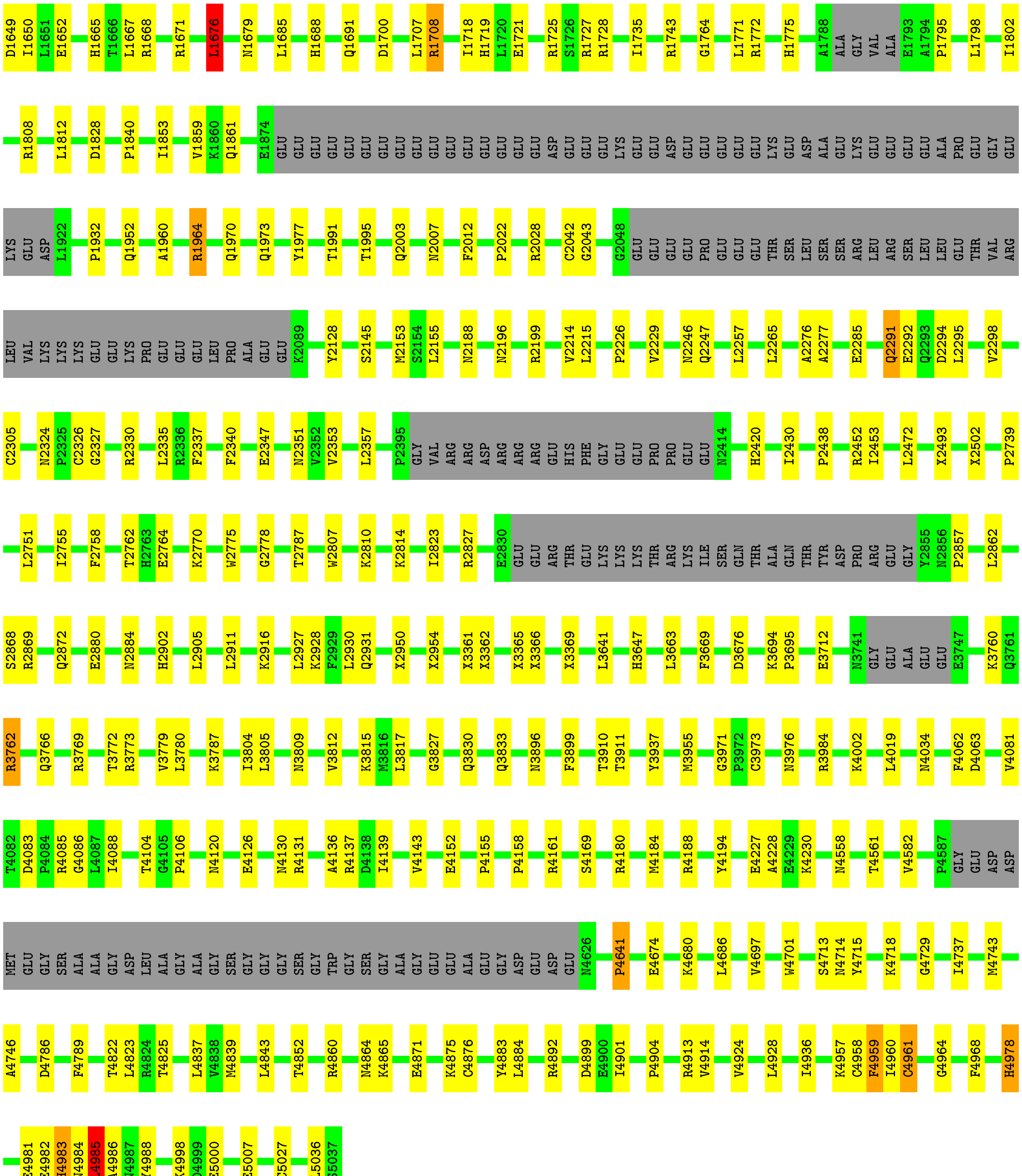




• Molecule 2: Ryanodine receptor 1

Chain E:




D1649 I1650 L1651 E1652 H1665 T1666 L1667 R1668 R1671 L1676 N1679 L1685 H1688 Q1691 D1700 L1707 R1708 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728 I1735 R1743 G1764 L1771 R1772 H1775 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 I1802
R1808 L1812 D1828 P1840 I1853 V1859 K1860 Q1861 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU GLU ALA PRO GLU GLY GLU
LYS GLU ASP L1922 P1932 Q1952 A1960 R1964 Q1970 Q1973 Y1977 T1991 T1995 Q2003 N2007 F2012 P2022 R2028 C2042 G2043 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG
LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 Y2128 S2145 M2153 S2154 L2155 N2188 N2196 R2199 V2214 L2215 P2226 V2229 N2246 Q2247 L2257 L2265 A2276 A2277 E2285 Q2291 E2292 Q2293 D2294 L2295 V2298
C2305 N2324 P2325 C2326 G2327 R2330 L2335 R2336 F2337 F2340 E2347 N2351 V2352 V2353 L2357 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 H2420 I2430 P2438 R2452 I2453 L2472 X2493 X2502 P2739
L2751 I2755 F2758 T2762 H2763 E2764 K2770 W2775 G2778 T2787 W2807 K2810 K2814 I2823 R2827 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 L2862
S2868 R2869 Q2872 E2880 N2884 H2902 L2905 L2911 K2916 L2927 K2928 F2929 L2930 Q2931 X2950 X2954 X3361 X3362 X3365 X3366 X3369 L3641 H3647 L3663 F3669 D3676 K3694 P3695 E3712 N3741 GLY GLU ALA GLU GLU E3747 K3760 Q3761
R3762 Q3766 R3769 T3772 R3773 V3779 L3780 K3787 I3804 L3805 N3809 V3812 K3815 M3816 L3817 G3827 Q3830 Q3833 N3896 F3899 T3910 T3911 Y3937 M3955 G3971 P3972 C3973 N3976 R3984 K4002 L4019 N4034 F4062 D4063 V4081
T4082 D4083 P4084 R4085 G4086 L4087 I4088 T4104 G4105 P4106 N4120 E4126 N4130 R4131 A4136 R4137 D4138 I4139 V4143 E4152 P4155 P4158 R4161 S4169 R4180 M4184 R4188 Y4194 E4227 A4228 E4229 K4230 N4558 T4561 V4582 P4587 GLY GLU ASP ASP
MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 P4641 E4674 K4680 L4686 V4697 W4701 S4713 N4714 Y4715 K4718 G4729 I4737 M4743
A4746 D4786 F4789 T4822 L4823 R4824 T4825 L4837 V4838 M4839 L4843 T4852 R4860 N4864 K4865 E4871 K4875 C4876 Y4883 L4884 R4892 D4899 E4900 I4901 P4904 R4913 V4914 V4924 L4928 I4936 K4957 C4958 F4959 I4960 C4961 G4964 F4968 H4978
E4981 E4982 H4983 N4984 L4985 A4986 N4987 Y4988 K4998 D4999 E5000 E5007 C5027 L5036 S5037

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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, CA

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	0.30	0/834	0.54	0/1123
1	F	0.30	0/834	0.54	0/1123
1	H	0.30	0/834	0.54	0/1123
1	J	0.30	0/834	0.54	0/1123
2	B	0.29	0/25428	0.53	6/34534 (0.0%)
2	E	0.29	0/25428	0.53	6/34534 (0.0%)
2	G	0.29	0/25428	0.53	6/34534 (0.0%)
2	I	0.29	0/25428	0.53	6/34534 (0.0%)
All	All	0.29	0/105048	0.53	24/142628 (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
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	131	LEU	CA-CB-CG	7.91	133.50	115.30
2	G	131	LEU	CA-CB-CG	7.91	133.49	115.30
2	B	131	LEU	CA-CB-CG	7.90	133.47	115.30
2	E	131	LEU	CA-CB-CG	7.89	133.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1600	LEU	CA-CB-CG	6.81	130.95	115.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	194	SER	Peptide
2	B	808	TYR	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	818	0	824	7	0
1	F	818	0	824	6	0
1	H	818	0	824	7	0
1	J	818	0	824	6	0
2	B	29499	0	24749	265	0
2	E	29499	0	24749	262	0
2	G	29499	0	24749	265	0
2	I	29499	0	24748	262	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102291	1047	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 5.

The worst 5 of 1047 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:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.18	1.32
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.18	1.32
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.18	1.30
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.18	1.30
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	1.67	1.02

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	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2899 (90%)	330 (10%)	6 (0%)	52	86
2	E	3235/4416 (73%)	2900 (90%)	329 (10%)	6 (0%)	52	86
2	G	3235/4416 (73%)	2900 (90%)	329 (10%)	6 (0%)	52	86
2	I	3235/4416 (73%)	2899 (90%)	330 (10%)	6 (0%)	52	86
All	All	13360/18096 (74%)	11973 (90%)	1363 (10%)	24 (0%)	56	86

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4985	LEU
2	I	4985	LEU
2	G	4985	LEU
2	E	4985	LEU

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Mol	Chain	Res	Type
2	B	1708	ARG

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2472 (99%)	21 (1%)	86	93
2	E	2493/3022 (82%)	2471 (99%)	22 (1%)	84	92
2	G	2493/3022 (82%)	2471 (99%)	22 (1%)	84	92
2	I	2493/3022 (82%)	2472 (99%)	21 (1%)	86	93
All	All	10324/12444 (83%)	10238 (99%)	86 (1%)	87	93

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	4959	PHE
2	G	1676	LEU
2	E	4120	ASN
2	I	4978	HIS
2	G	534	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	3781	GLN
2	G	273	HIS
2	E	3809	ASN
2	I	3830	GLN

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Mol	Chain	Res	Type
2	I	4120	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 8 ligands modelled in this entry, 8 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	14
2	B	14

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Mol	Chain	Number of breaks
2	I	14
2	E	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.83
1	I	4345:UNK	C	4540:PHE	N	73.83
1	G	4345:UNK	C	4540:PHE	N	73.83
1	E	4345:UNK	C	4540:PHE	N	73.83
1	B	3613:UNK	C	3639:THR	N	45.16