wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 03:09 PM EDT

PDB ID	:	5T9S
EMDB ID:	:	EMD-8375
Title	:	Structure of rabbit RyR1 (Ca2+-only dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-09
Resolution	:	4.20 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

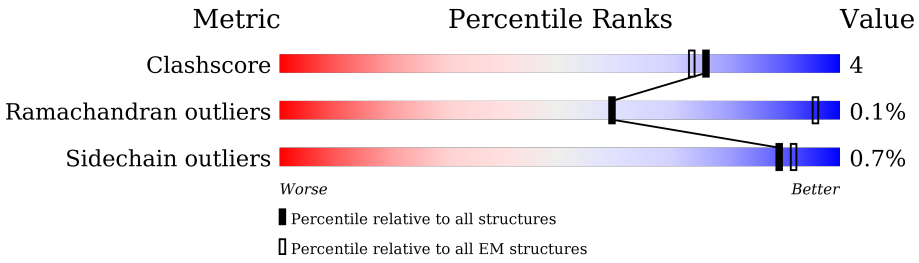
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.20 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	84% 15% .
1	F	108	83% 16% .
1	H	108	84% 15% .
1	J	108	84% 15% .
2	B	4676	80% 8% 11%
2	E	4676	80% 8% 11%
2	G	4676	81% 8% 11%
2	I	4676	81% 8% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	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).

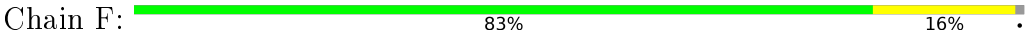
Mol	Chain	Residues	Atoms	AltConf
4	G	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0

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.

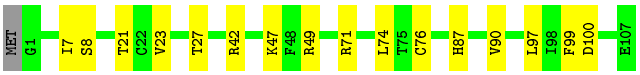
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



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

Chain A:



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

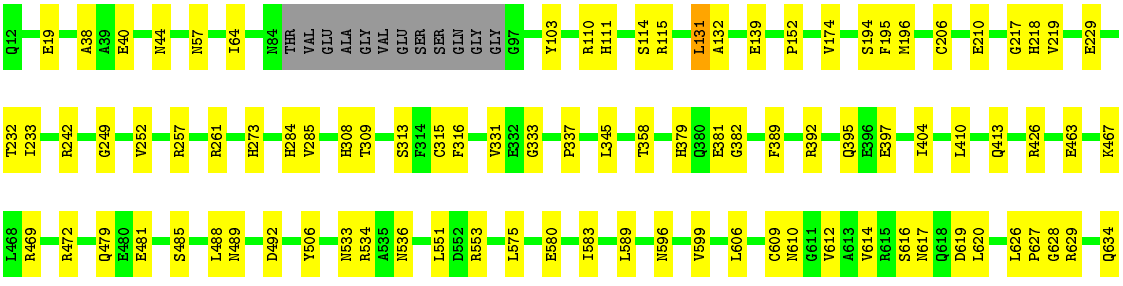
Chain H:

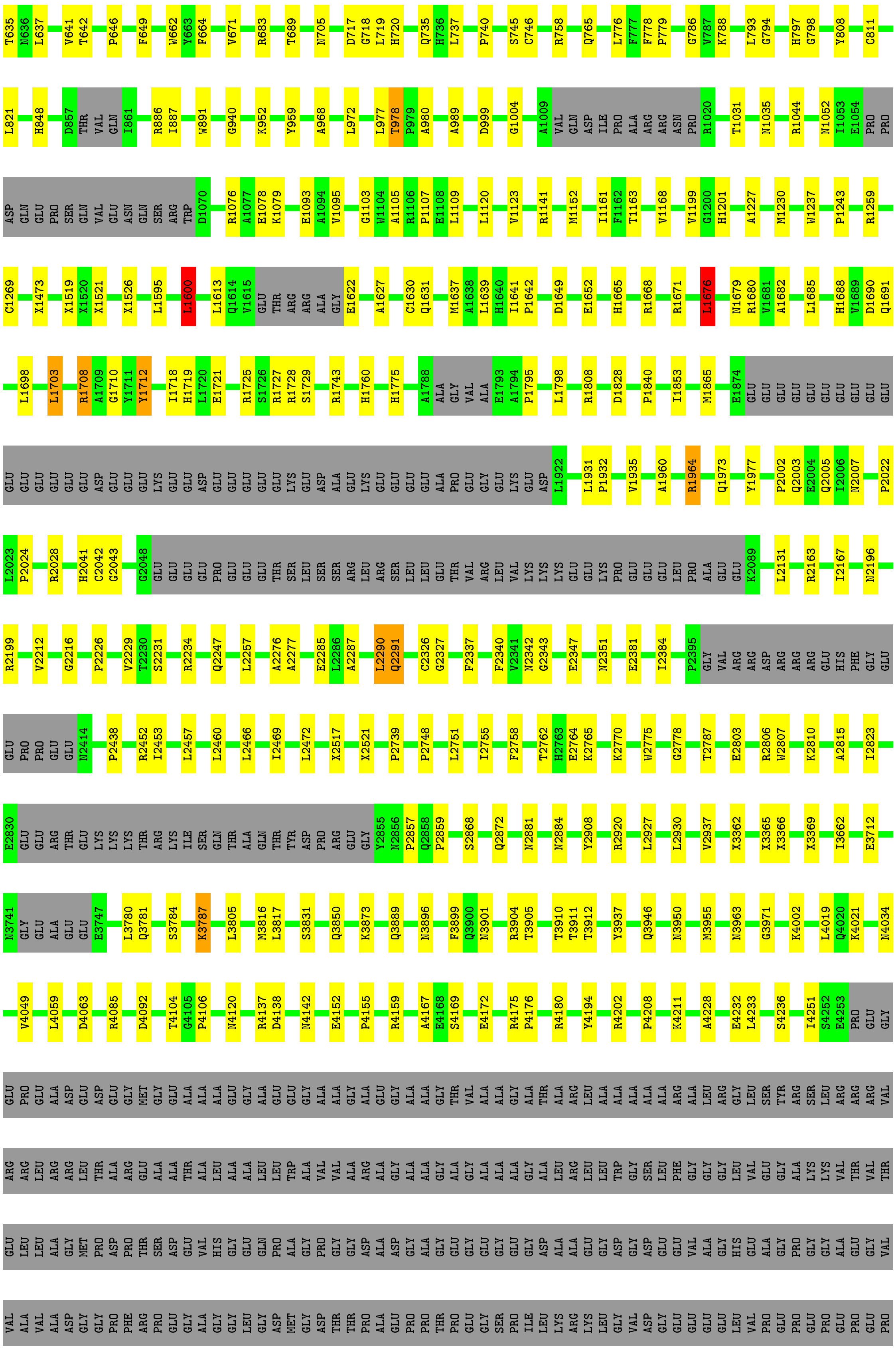
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

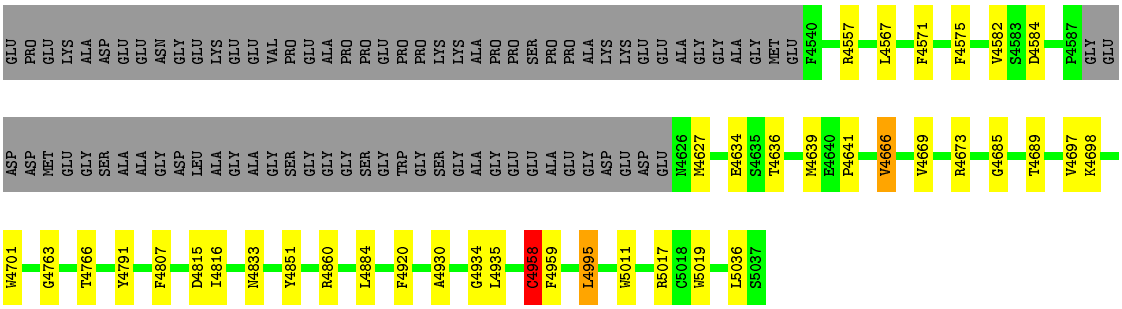
Chain J:

- Molecule 2: Ryanodine receptor 1

Chain B:

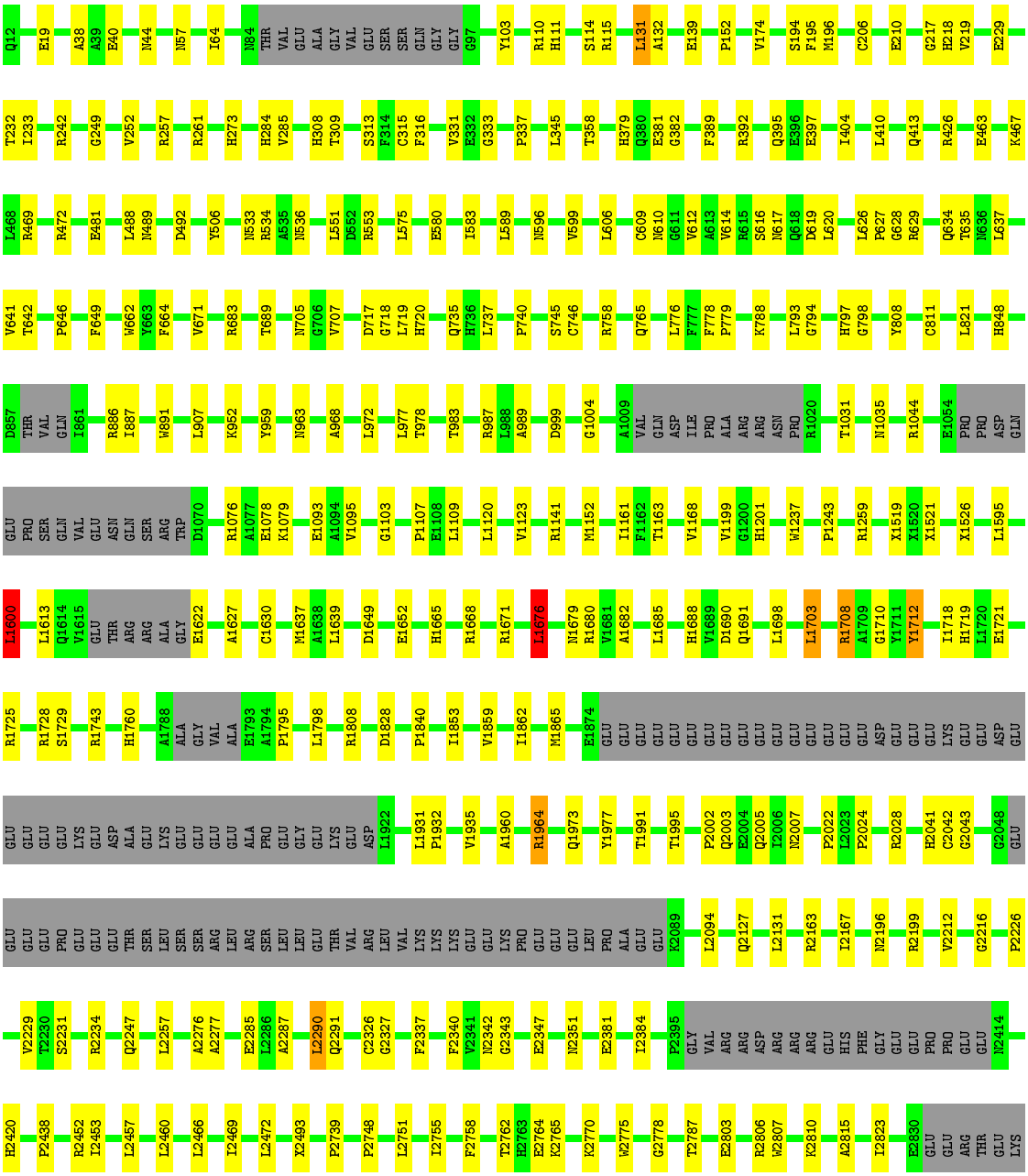


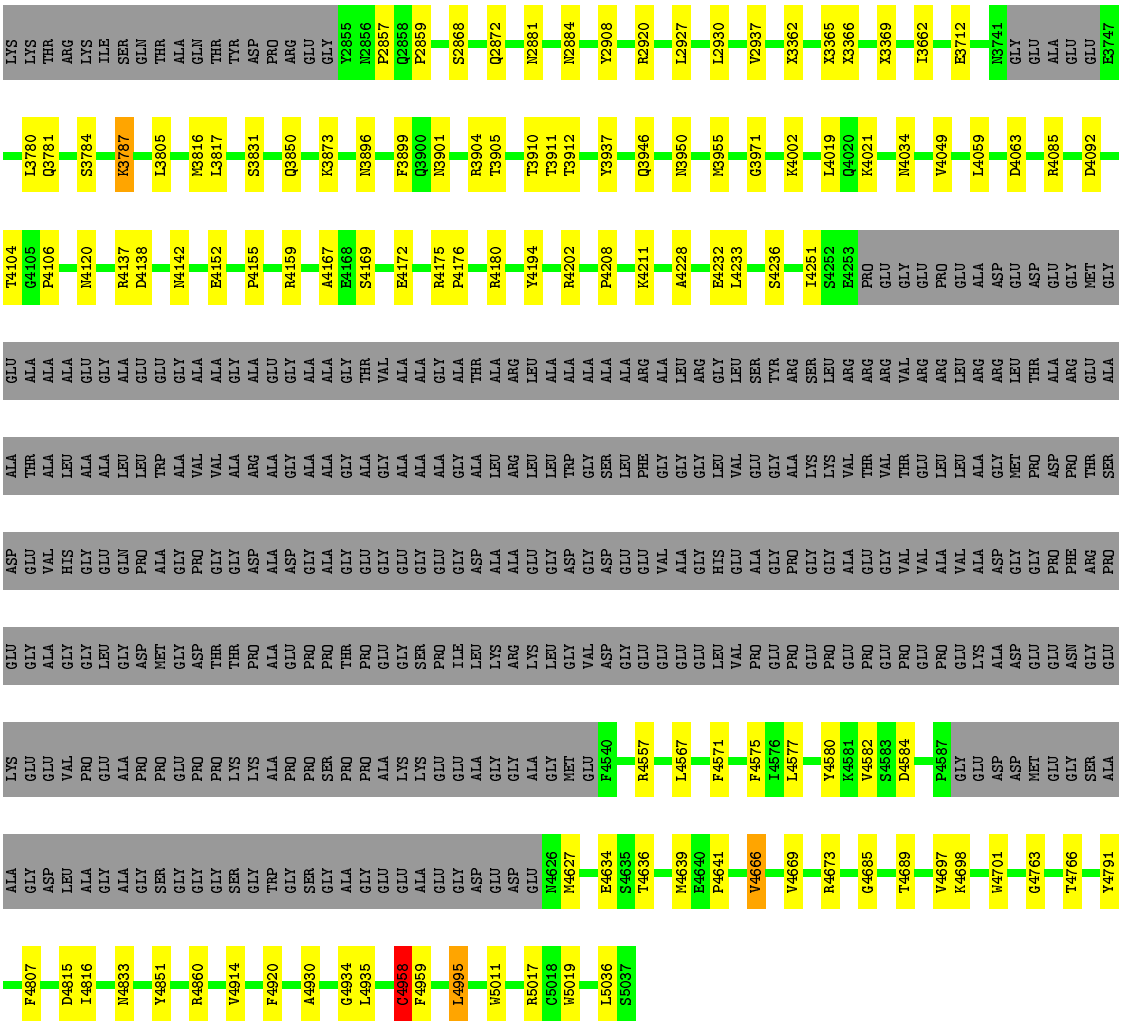

T635 N636 L637 V641 T642 P646 F649 W662 Y663 F664 V671 R683 T689 N705 D717 G718 L719 H720 Q735 H736 L737 P740 S745 C746 R758 Q765 L776 F777 F778 P779 G786 V787 K788 L793 G794 H797 G798 Y808 C811
L821 H848 D857 THR VAL GLN I861 R886 I887 W891 G940 K952 Y959 A968 L972 L977 T978 P979 A980 A989 D999 G1004 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 T1031 N1035 R1044 N1052 I1053 E1054 PRO PRO
ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1076 A1077 E1078 K1079 E1093 A1094 V1095 G1103 W1104 A1105 R1106 P1107 E1108 L1109 L1120 V1123 R1141 M1152 I1161 F1162 T1163 V1168 V1199 G1200 H1201 A1227 M1230 W1237 P1243 R1259
C1269 X1473 X1519 X1520 X1521 X1526 L1595 L1600 L1613 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 A1627 C1630 Q1631 M1637 A1638 L1639 H1640 I1641 P1642 D1649 E1652 H1665 R1668 R1671 L1676 N1679 R1680 V1681 A1682 L1685 H1688 V1689 D1690 Q1691
L1698 L1703 R1708 A1709 G1710 Y1711 Y1712 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728 S1729 R1743 H1760 H1775 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 R1808 D1828 P1840 I1853 M1865 E1874 GLU 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 ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1931 P1932 V1935 A1960 R1964 Q1973 Y1977 P2002 Q2003 E2004 Q2005 I2006 N2007 P2022
L2023 P2024 R2028 H2041 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 K2089 L2131 R2163 I2167 N2196
R2199 V2212 G2216 P2226 V2229 T2230 S2231 R2234 Q2247 L2257 A2276 A2277 E2285 L2286 A2287 L2290 Q2291 C2326 G2327 F2337 F2340 V2341 N2342 G2343 E2347 N2351 E2381 I2384 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU
GLU PRO PRO GLU GLU N2414 P2438 R2452 I2453 L2457 L2460 L2466 I2469 L2472 X2517 X2521 P2739 P2748 L2751 I2755 F2758 T2762 H2763 E2764 K2765 K2770 W2775 G2778 T2787 E2803 R2806 W2807 K2810 A2815 I2823
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 Q2858 P2859 S2868 Q2872 N2881 N2884 Y2908 R2920 L2927 L2930 V2937 X3362 X3365 X3366 X3369 I3662 E3712
N3741 GLY GLU ALA GLU GLU E3747 L3780 Q3781 S3784 K3787 L3805 M3816 L3817 S3831 Q3850 K3873 Q3889 N3896 F3899 Q3900 N3901 R3904 T3905 T3910 T3911 T3912 Y3937 Q3946 N3950 M3955 N3963 G3971 K4002 L4019 Q4020 K4021 N4034
V4049 L4059 D4063 R4085 D4092 T4104 G4105 P4106 N4120 R4137 D4138 N4142 E4152 P4155 R4159 A4167 E4168 S4169 E4172 R4175 P4176 R4180 Y4194 R4202 P4208 K4211 A4228 E4232 L4233 S4236 I4251 S4252 E4253 PRO GLU GLY
GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG VAL
ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR
GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL
VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY LEU GLU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO



• Molecule 2: Ryanodine receptor 1

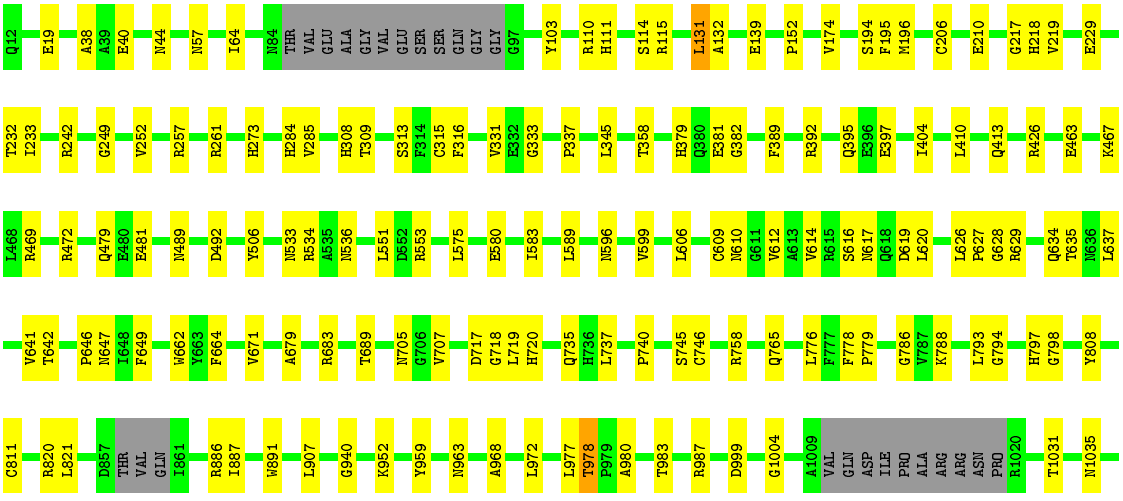
Chain E:

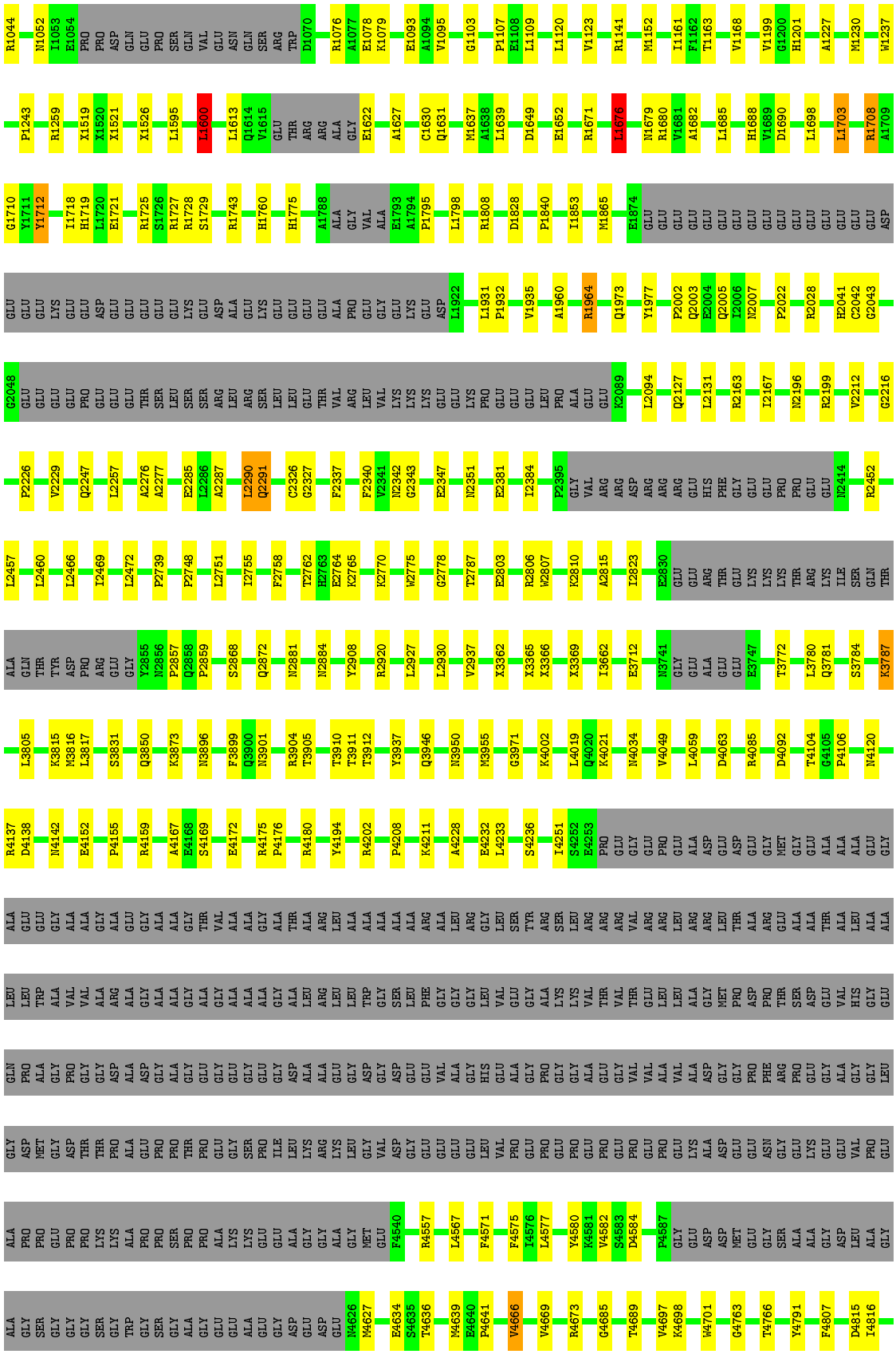




• Molecule 2: Ryanodine receptor 1

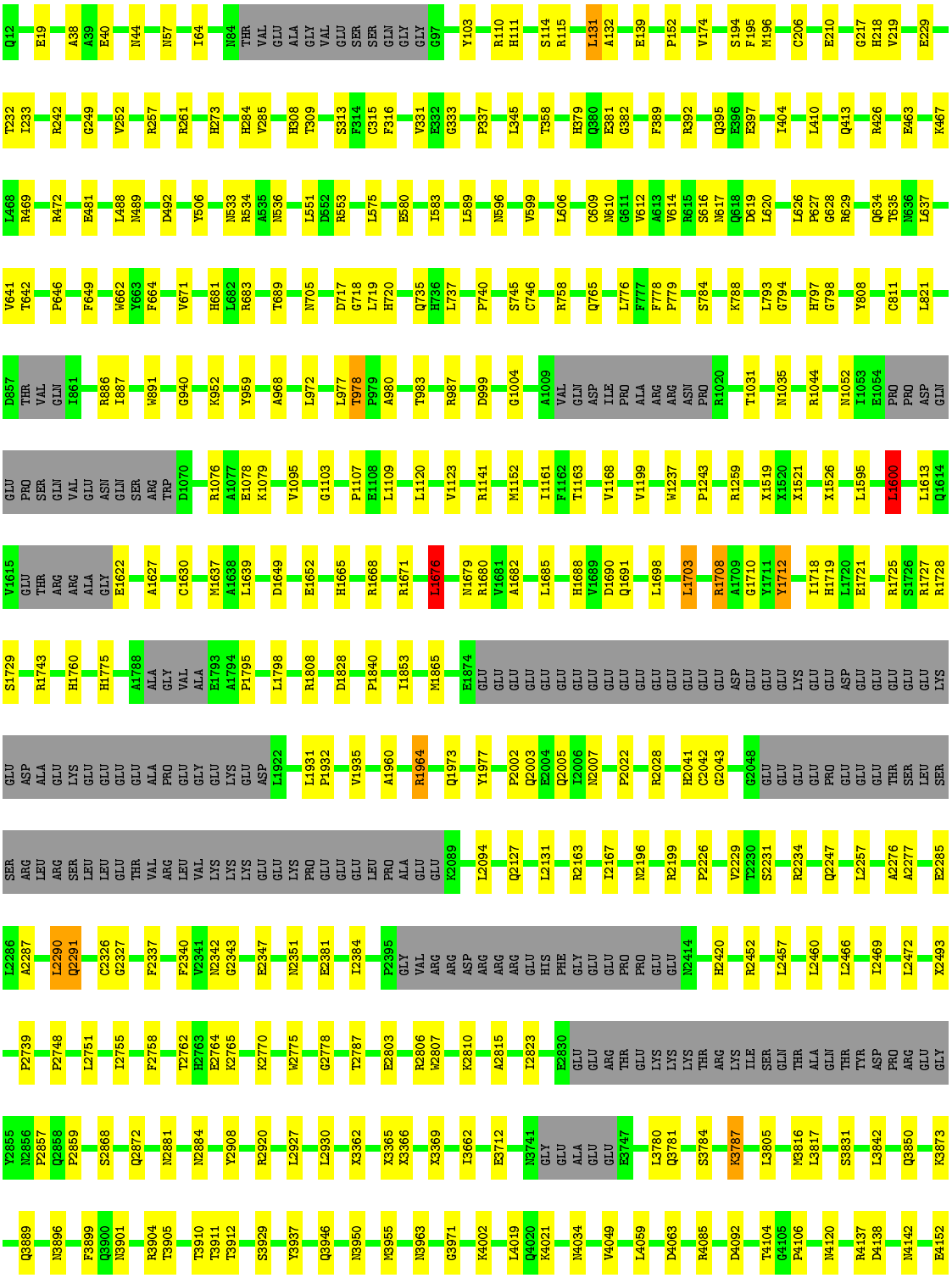
Chain I:

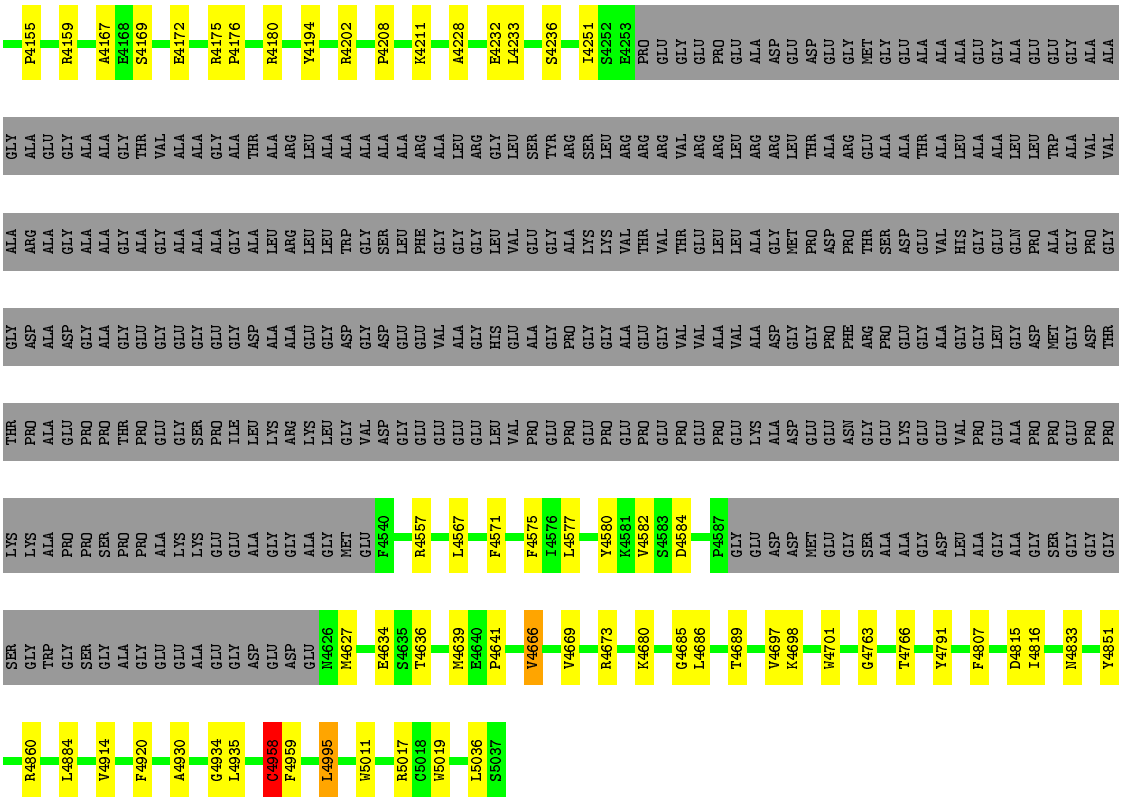




- Molecule 2: Ryanodine receptor 1

Chain G:




P4155 R4159 A4167 E4168 S4169 E4172 R4175 P4176 R4180 Y4194 R4202 P4208 K4211 A4228 E4232 L4233 S4236 I4251 S4252 E4253
GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL
ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY
GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR
THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLY PRO GLU PRO GLU GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU GLY ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO
LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 R4557 L4567 F4571 F4575 I4576 L4577 Y4580 K4581 V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA ALA GLY ALA SER GLY GLY GLY
SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 M4627 E4634 S4635 T4636 M4639 E4640 P4641 V4666 V4669 R4673 K4680 G4685 L4686 T4689 V4697 K4698 W4701 G4763 T4766 Y4791 F4807 D4815 I4816 N4833 Y4851
R4860 L4884 V4914 F4920 A4930 G4934 L4935 C4958 F4959 L4995 W5011 R5017 C5018 W5019 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	0.31	0/834	0.51	0/1123
1	F	0.31	0/834	0.51	0/1123
1	H	0.30	0/834	0.51	0/1123
1	J	0.31	0/834	0.51	0/1123
2	B	0.30	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.30	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	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
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	68

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	G	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	E	131	LEU	CA-CB-CG	8.11	133.96	115.30
2	I	131	LEU	CA-CB-CG	8.11	133.96	115.30
2	B	131	LEU	CA-CB-CG	8.10	133.94	115.30
2	E	1600	LEU	CA-CB-CG	7.05	131.51	115.30

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	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	8	0
1	F	818	0	824	9	0
1	H	818	0	824	8	0
1	J	818	0	824	9	0
2	B	29369	0	24721	212	0
2	E	29369	0	24721	206	0
2	G	29369	0	24719	205	0
2	I	29369	0	24721	208	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	120756	0	102178	849	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 4.

The worst 5 of 849 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:426:ARG:HB2	2:B:506:TYR:HA	1.78	0.66
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.78	0.66
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.78	0.66
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.78	0.65
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.77	0.64

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%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4676 (69%)	2894 (90%)	336 (10%)	5 (0%)	52	86
2	E	3235/4676 (69%)	2896 (90%)	334 (10%)	5 (0%)	52	86
2	G	3235/4676 (69%)	2894 (90%)	336 (10%)	5 (0%)	52	86
2	I	3235/4676 (69%)	2895 (90%)	335 (10%)	5 (0%)	52	86
All	All	13360/19136 (70%)	11959 (90%)	1381 (10%)	20 (0%)	59	90

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

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Continued from previous page...

Mol	Chain	Res	Type
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO

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	2493/3202 (78%)	2475 (99%)	18 (1%)	88 94
2	E	2493/3202 (78%)	2475 (99%)	18 (1%)	88 94
2	G	2493/3202 (78%)	2475 (99%)	18 (1%)	88 94
2	I	2493/3202 (78%)	2475 (99%)	18 (1%)	88 94
All	All	10324/13164 (78%)	10252 (99%)	72 (1%)	89 94

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	4085	ARG
2	I	1076	ARG
2	G	3896	ASN
2	E	4120	ASN
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	3960	GLN

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Mol	Chain	Res	Type
2	I	224	HIS
2	G	3896	ASN
2	E	3994	HIS
2	E	4553	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	12
2	B	12
2	I	12
2	E	12

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	44.23
1	G	3613:UNK	C	3639:THR	N	43.95
1	I	3613:UNK	C	3639:THR	N	43.88
1	E	3613:UNK	C	3639:THR	N	43.84
1	E	3163:UNK	C	3170:UNK	N	16.60