wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 07:38 PM EDT

PDB ID	:	5TAW
EMDB ID:	:	EMD-8387
Title	:	Structure of rabbit RyR1 (ryanodine dataset, all particles)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
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

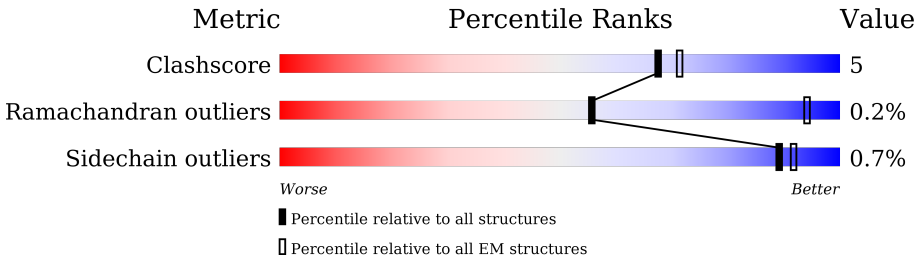
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	108	83% 16% .
1	F	108	81% 18% .
1	H	108	81% 18% .
1	J	108	81% 18% .
2	B	4416	84% 11% 5%
2	E	4416	84% 10% 5%
2	G	4416	84% 11% 5%
2	I	4416	84% 11% 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	G	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	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).

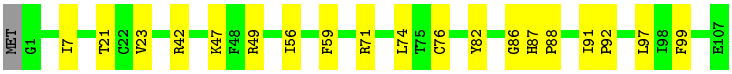
Mol	Chain	Residues	Atoms	AltConf
4	G	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0

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

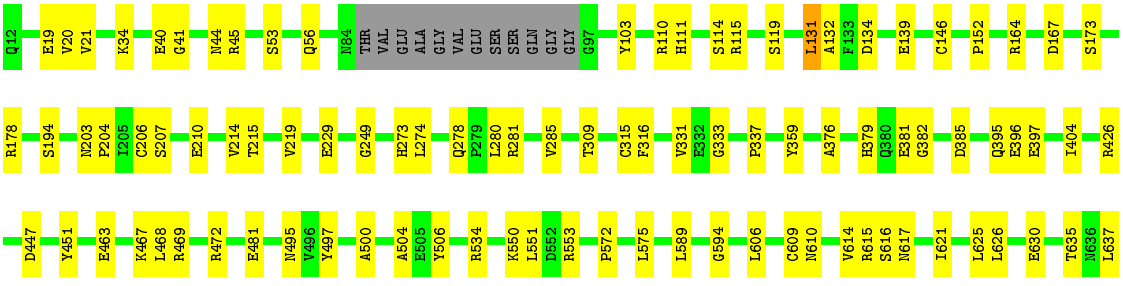
Chain H:

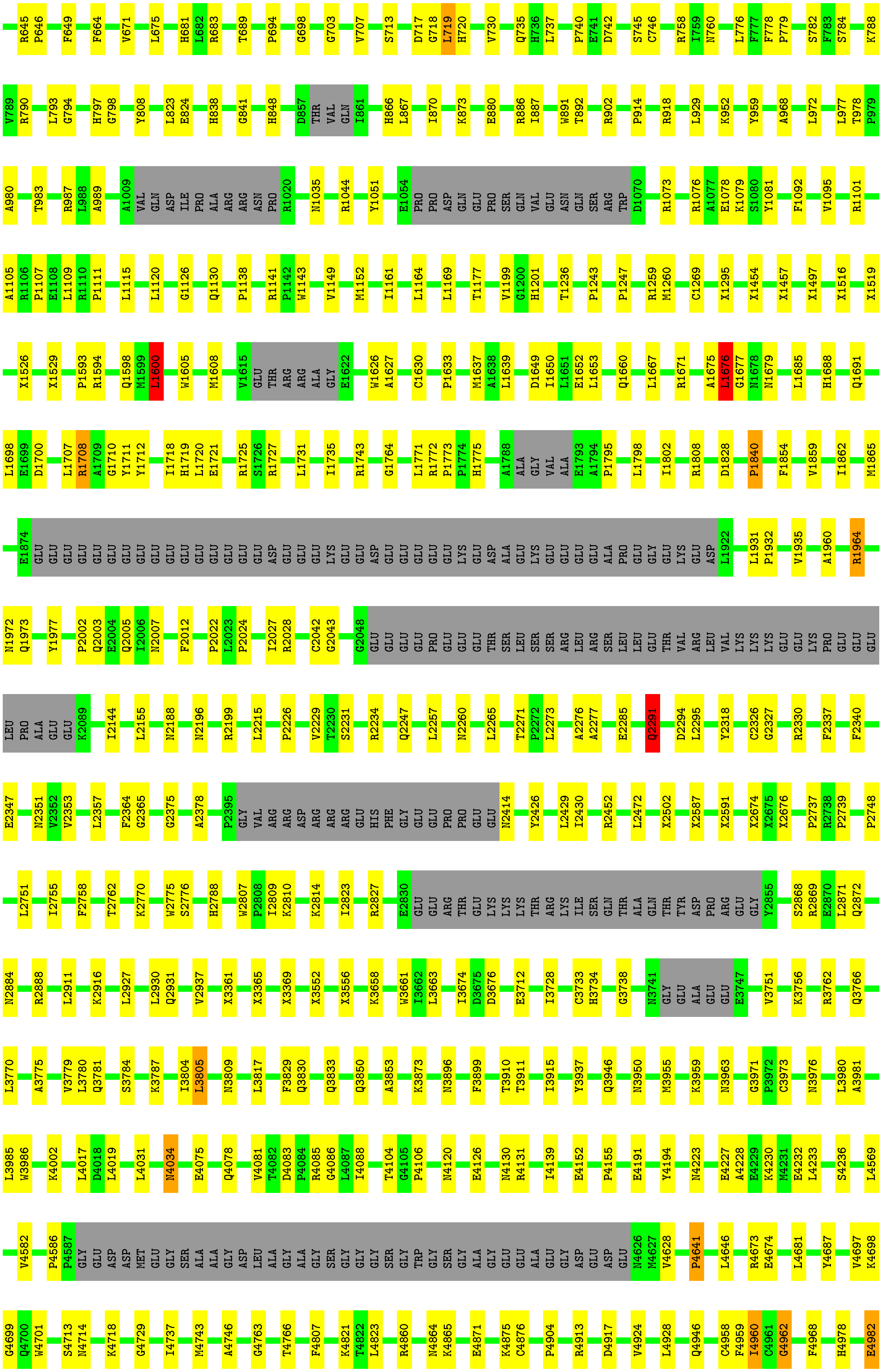
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J:

- Molecule 2: Ryanodine receptor 1

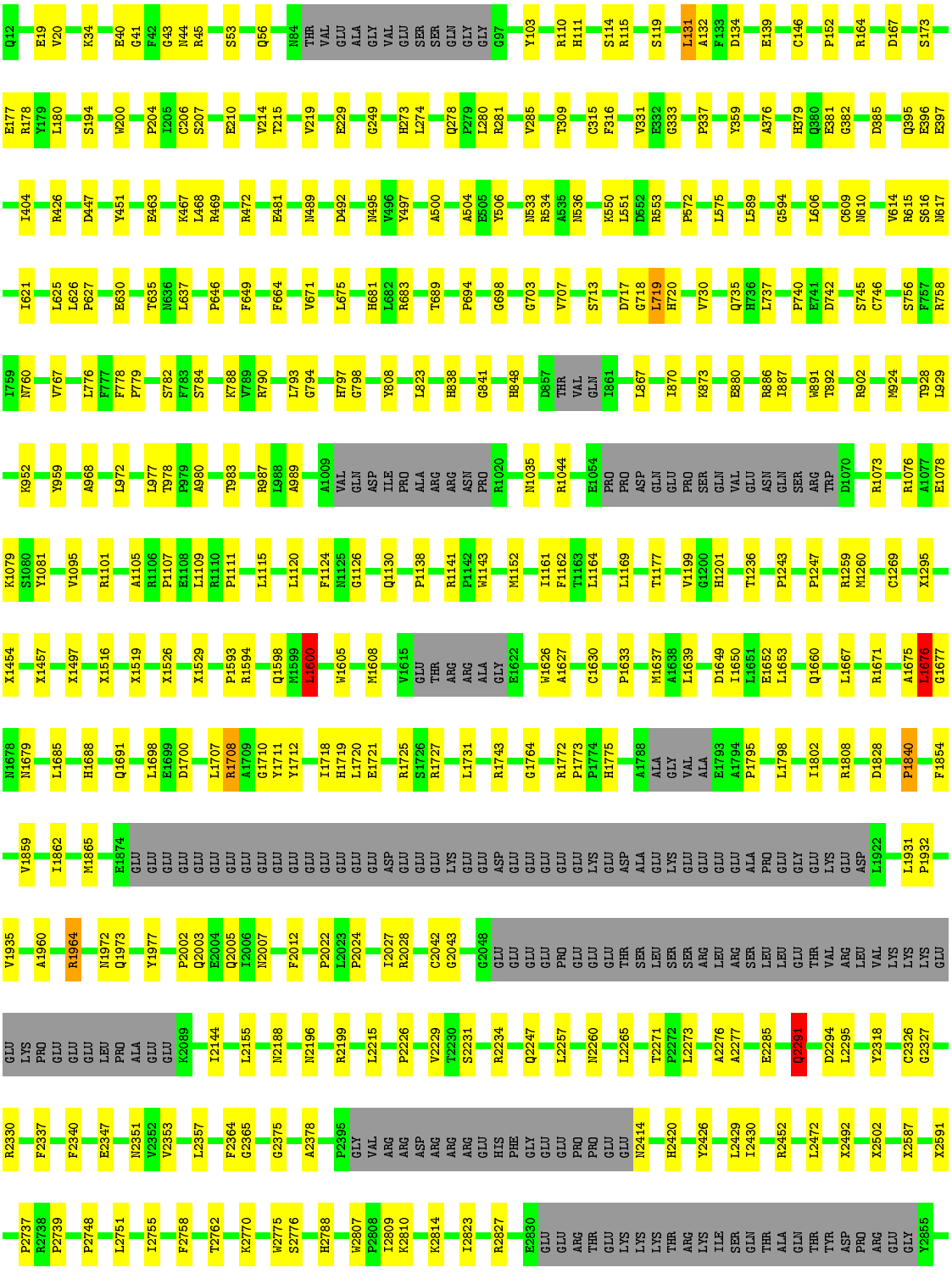
Chain B:

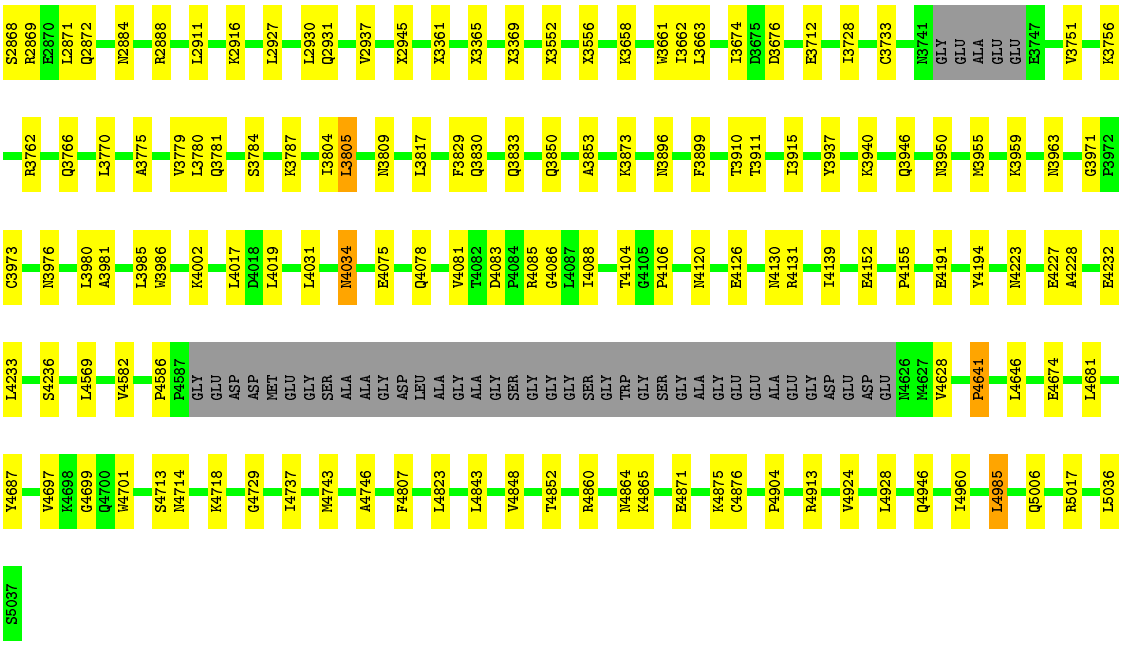



R645 P646 F649 F664 V671 L675 H681 L682 R683 T689 P694 G698 G703 V707 S713 D717 G718 L719 H720 V730 Q735 H736 L737 P740 E741 D742 S745 C746 R758 I759 N760 L776 F777 F778 P779 S782 F783 S784 K788
V789 R790 L793 G794 H797 G798 Y808 L823 E824 H838 G841 H848 D857 THR VAL GLN I861 H866 L867 I870 K873 E880 R886 I887 W891 T892 R902 P914 R918 L929 K952 Y959 A968 L972 L977 T978 P979
A980 T983 R987 L988 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 N1035 R1044 Y1051 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1073 R1076 A1077 E1078 K1079 S1080 Y1081 F1092 V1095 R1101
A1105 R1106 P1107 E1108 L1109 R1110 P1111 L1115 L1120 G1126 Q1130 P1138 R1141 P1142 W1143 V1149 M1152 I1161 L1164 L1169 T1177 V1199 G1200 H1201 T1236 P1243 P1247 R1259 M1260 C1269 X1295 X1454 X1457 X1497 X1516 X1519
X1526 X1529 P1593 R1594 Q1598 M1599 L1600 W1605 M1608 V1615 GLU THR ARG ARG ALA GLY E1622 W1626 A1627 C1630 P1633 M1637 A1638 L1639 D1649 I1650 L1651 E1652 L1653 Q1660 L1667 R1671 A1675 L1676 G1677 N1678 N1679 L1685 H1688 Q1691
L1698 E1699 D1700 L1707 R1708 A1709 G1710 Y1711 Y1712 I1718 H1719 L1720 E1721 R1725 S1726 R1727 L1731 I1735 R1743 G1764 L1771 R1772 P1773 P1774 H1775 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 I1802 R1808 D1828 P1840 F1854 V1859 I1862 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
N1972 Q1973 Y1977 P2002 Q2003 E2004 Q2005 I2006 N2007 F2012 P2022 L2023 P2024 I2027 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 I2144 L2155 N2188 N2196 R2199 L2215 P2226 V2229 T2230 S2231 R2234 Q2247 L2257 N2260 L2265 T2271 P2272 L2273 A2276 A2277 E2285 Q2291 D2294 L2295 Y2318 C2326 G2327 R2330 F2337 F2340
E2347 N2351 V2352 V2353 L2357 F2364 G2365 G2375 A2378 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 Y2426 L2429 I2430 R2452 L2472 X2502 X2587 X2591 X2674 X2675 X2676 P2737 R2738 P2739 P2748
L2751 I2755 F2758 T2762 K2770 W2775 S2776 H2788 W2807 P2808 I2809 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 S2868 R2869 E2870 L2871 Q2872
N2884 R2888 L2911 K2916 L2927 L2930 Q2931 V2937 X3361 X3365 X3369 X3552 X3556 K3658 W3661 I3662 L3663 I3674 D3675 D3676 E3712 I3728 C3733 H3734 G3738 N3741 GLY GLU ALA GLU GLU E3747 V3751 K3756 R3762 Q3766
L3770 A3775 V3779 L3780 Q3781 S3784 K3787 I3804 L3805 N3809 L3817 F3829 Q3830 Q3833 Q3850 A3853 K3873 N3896 F3899 T3910 T3911 I3915 Y3937 Q3946 N3950 M3955 K3959 N3963 G3971 P3972 C3973 N3976 L3980 A3981
L3985 W3986 K4002 L4017 D4018 L4019 L4031 N4034 E4075 Q4078 V4081 T4082 D4083 P4084 R4085 G4086 L4087 I4088 T4104 G4105 P4106 N4120 E4126 N4130 R4131 I4139 E4152 P4155 E4191 Y4194 N4223 E4227 A4228 E4229 K4230 M4231 E4232 L4233 S4236 L4569
V4582 P4586 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 M4627 V4628 P4641 L4646 R4673 E4674 L4681 Y4687 V4697 K4698
G4699 Q4700 W4701 S4713 N4714 K4718 G4729 I4737 M4743 A4746 G4763 T4766 F4807 K4821 T4822 L4823 R4860 N4864 K4865 E4871 K4875 C4876 P4904 R4913 D4917 V4924 L4928 Q4946 C4958 F4959 I4960 C4961 G4962 F4968 H4978 E4982

- Molecule 2: Ryanodine receptor 1

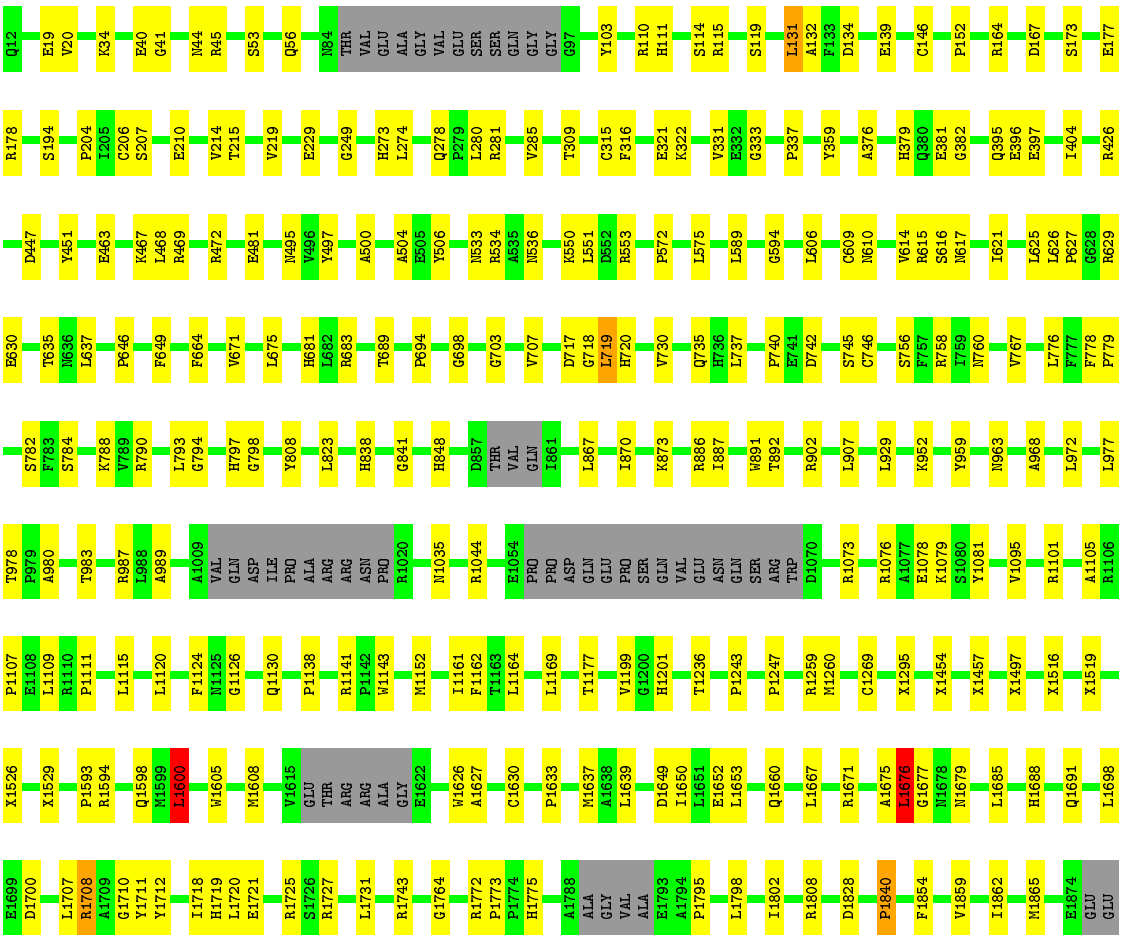
Chain G:

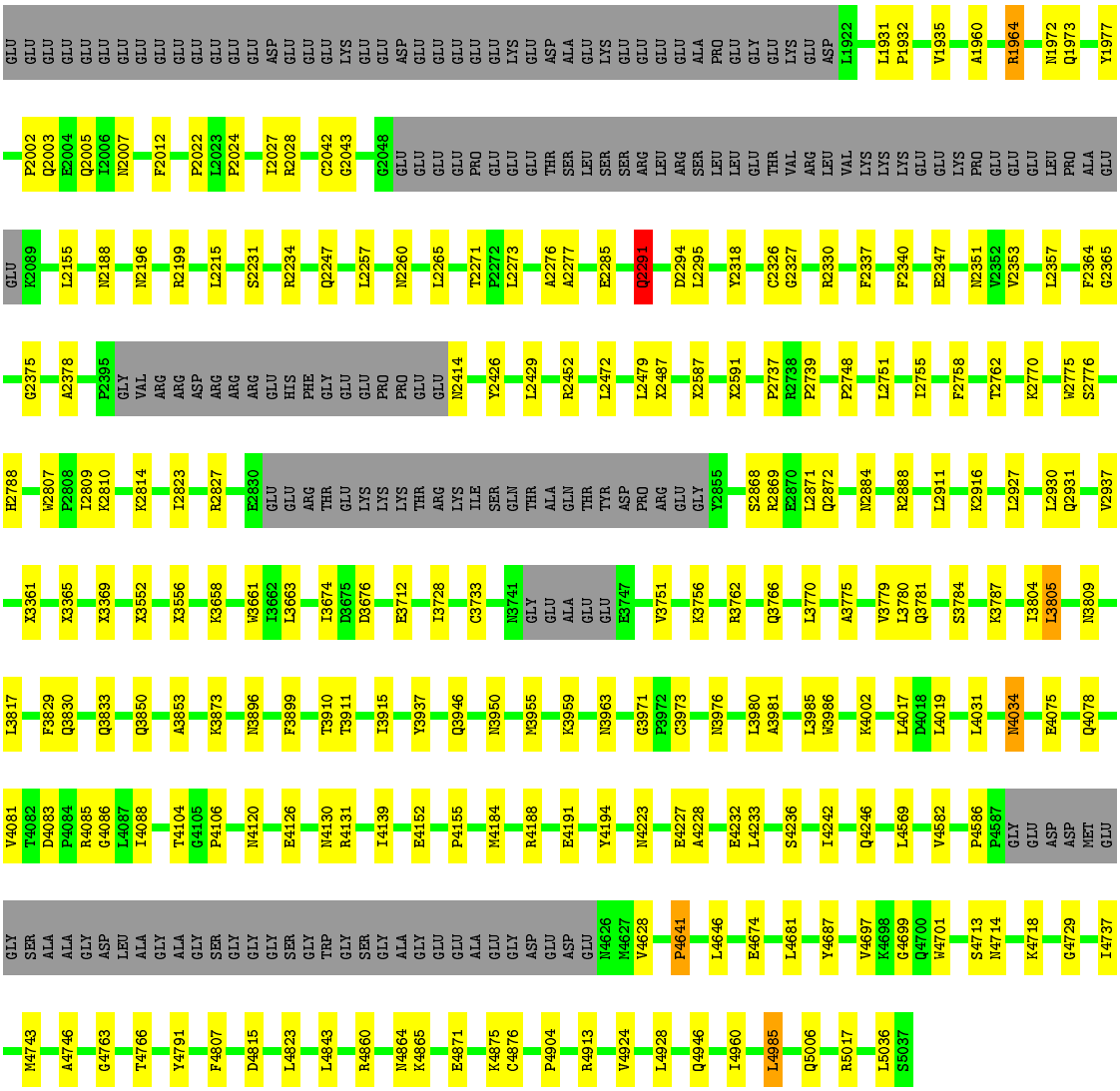




- Molecule 2: Ryanodine receptor 1

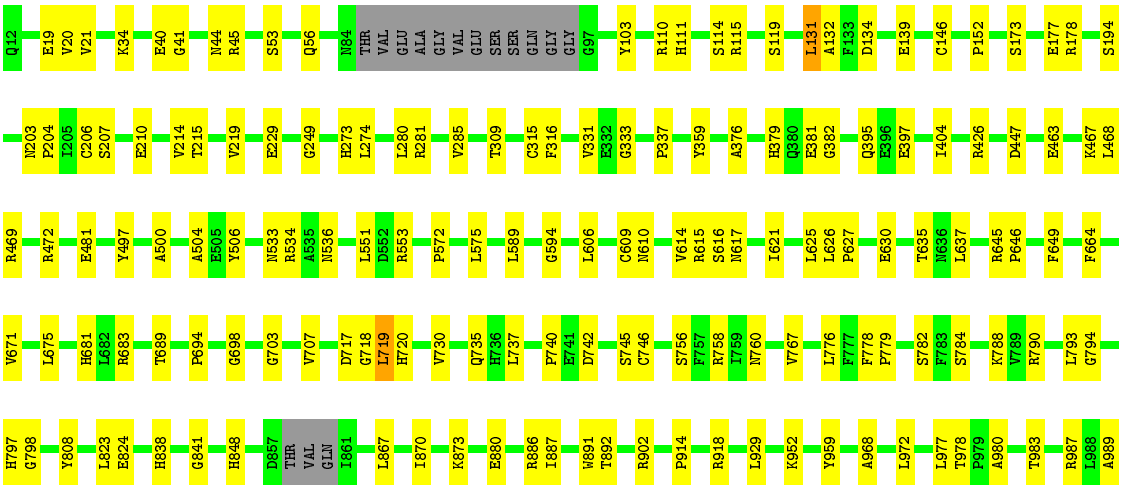
Chain I:

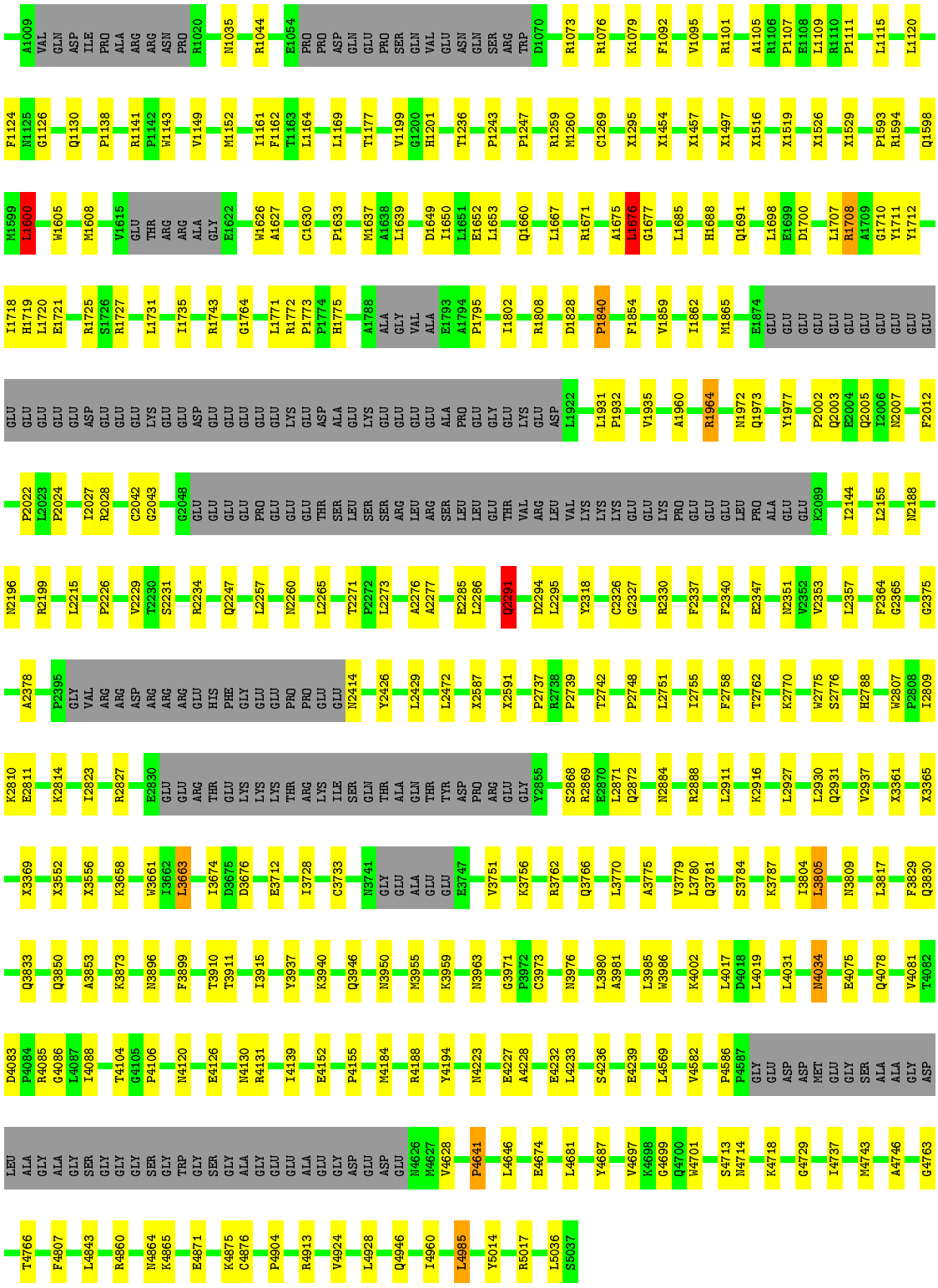




• Molecule 2: Ryanodine receptor 1

Chain E:





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	0.54	0/1123
1	F	0.31	0/834	0.54	0/1123
1	H	0.31	0/834	0.54	0/1123
1	J	0.31	0/834	0.54	0/1123
2	B	0.30	0/25428	0.54	5/34534 (0.0%)
2	E	0.30	0/25428	0.54	5/34534 (0.0%)
2	G	0.30	0/25428	0.54	5/34534 (0.0%)
2	I	0.30	0/25428	0.54	5/34534 (0.0%)
All	All	0.30	0/105048	0.54	20/142628 (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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	131	LEU	CA-CB-CG	7.62	132.81	115.30
2	I	131	LEU	CA-CB-CG	7.61	132.79	115.30
2	B	131	LEU	CA-CB-CG	7.59	132.75	115.30
2	G	131	LEU	CA-CB-CG	7.59	132.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1600	LEU	CA-CB-CG	6.68	130.67	115.30

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1720	LEU	Peptide
2	B	694	PRO	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	10	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	12	0
2	B	29499	0	24749	281	0
2	E	29499	0	24749	253	0
2	G	29499	0	24750	262	0
2	I	29499	0	24749	257	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	102293	1081	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 1081 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:4968:PHE:CE2	2:B:4978:HIS:CE1	2.28	1.20
2:B:4230:LYS:HD2	2:B:4959:PHE:HE2	0.99	1.10
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	1.92	1.04
2:B:4983:HIS:CE1	2:B:5027:CYS:SG	2.57	0.98
2:B:4230:LYS:CD	2:B:4959:PHE:HE2	1.87	0.87

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	94 (90%)	11 (10%)	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%)	2894 (90%)	333 (10%)	8 (0%)	52	86
2	E	3235/4416 (73%)	2898 (90%)	332 (10%)	5 (0%)	52	86
2	G	3235/4416 (73%)	2896 (90%)	334 (10%)	5 (0%)	52	86
2	I	3235/4416 (73%)	2898 (90%)	332 (10%)	5 (0%)	52	86
All	All	13360/18096 (74%)	11962 (90%)	1375 (10%)	23 (0%)	56	86

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4962	GLY
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG

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Mol	Chain	Res	Type
2	E	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%)	2473 (99%)	20 (1%)	86	93
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
All	All	10324/12444 (83%)	10253 (99%)	71 (1%)	89	94

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	3896	ASN
2	I	553	ARG
2	E	3805	LEU
2	G	4034	ASN
2	G	4131	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	3950	ASN
2	I	395	GLN
2	E	3896	ASN
2	G	3963	ASN

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Mol	Chain	Res	Type
2	G	4983	HIS

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	G	4345:UNK	C	4540:PHE	N	73.65
1	B	4345:UNK	C	4540:PHE	N	73.61
1	I	4345:UNK	C	4540:PHE	N	73.61
1	E	4345:UNK	C	4540:PHE	N	73.59
1	G	3613:UNK	C	3639:THR	N	45.21