wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 02:09 PM EDT

PDB ID	:	5TB4
EMDB ID:	:	EMD-8395
Title	:	Structure of rabbit RyR1 (EGTA-only dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-11
Resolution	:	4.50 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

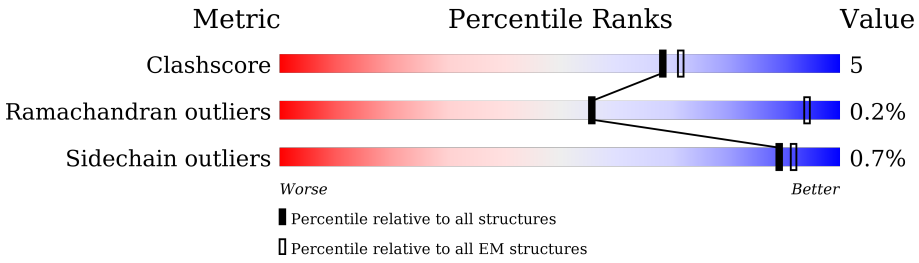
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.50 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	81% 19% .
1	H	108	85% 14% .
1	J	108	83% 16% .
2	B	4416	84% 10% 5%
2	E	4416	84% 10% 5%
2	G	4416	84% 10% 5%
2	I	4416	84% 10% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 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	E	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		

- 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	

3 Residue-property plots (i)

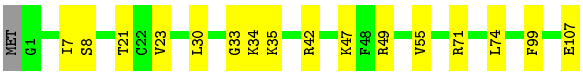
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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

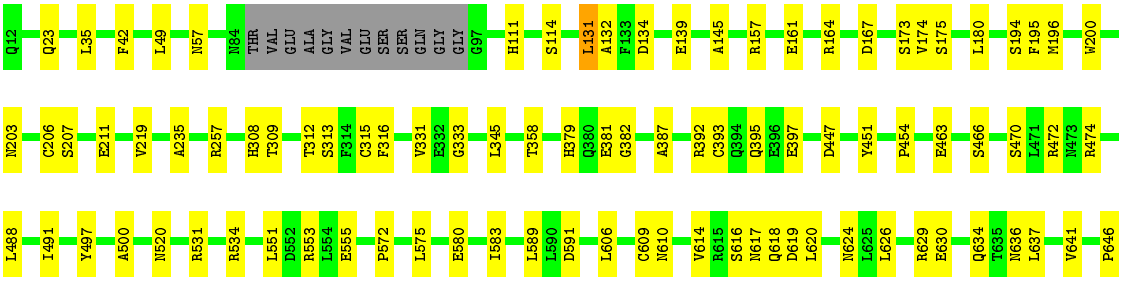
Chain H:

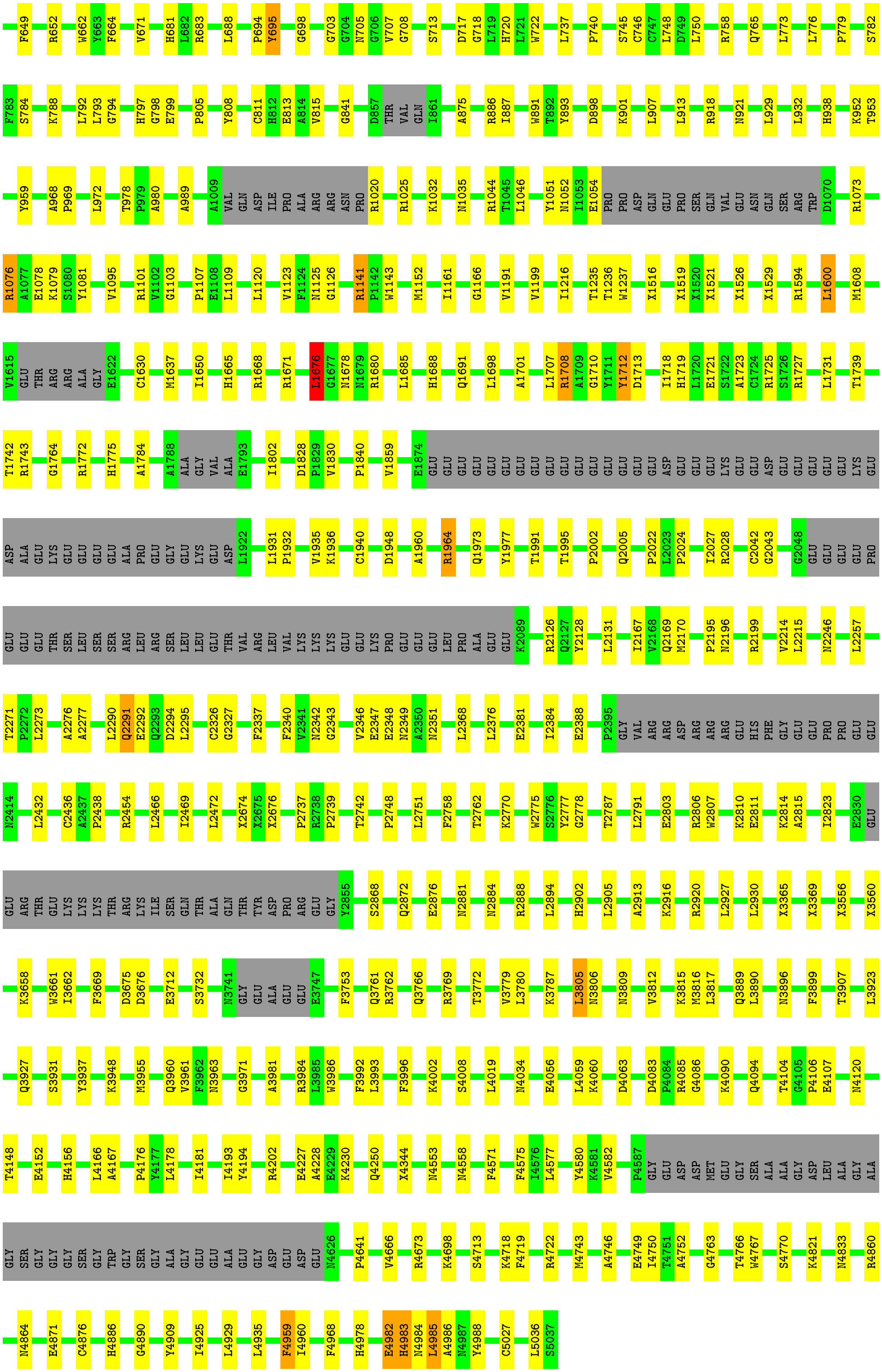
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J:

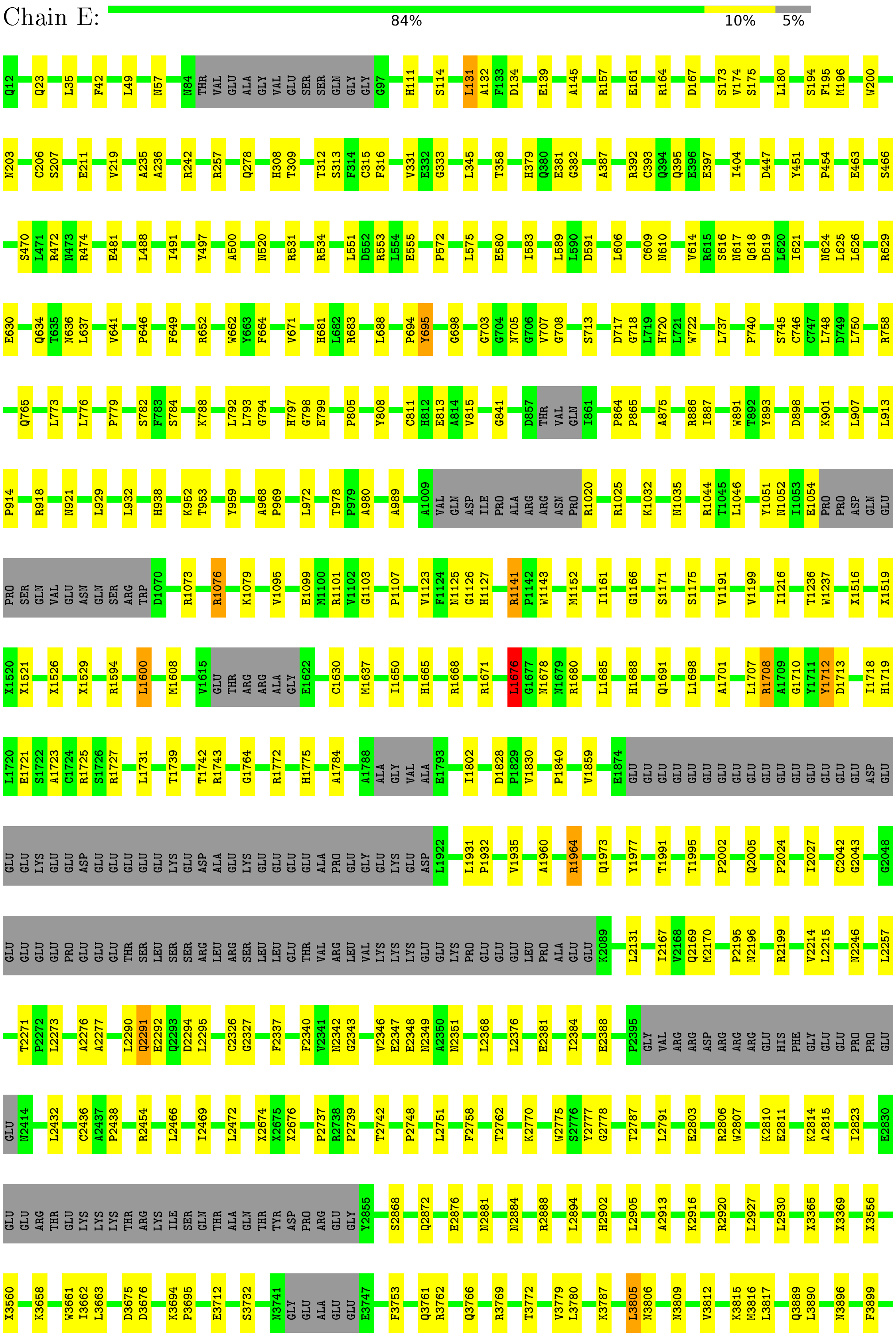
- Molecule 2: Ryanodine receptor 1

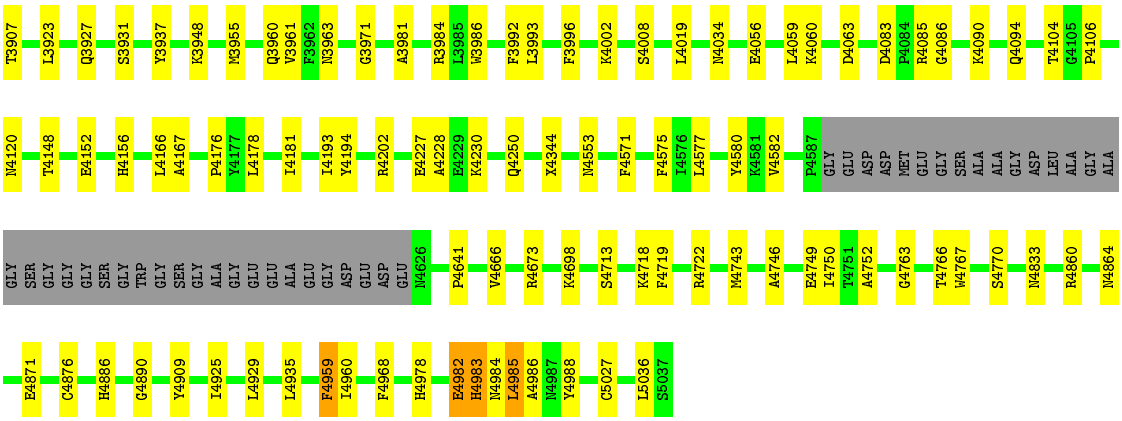
Chain B:




F649 R652 W662 Y663 F664 V671 H681 L682 R683 L688 P694 Y695 G698 G703 G704 N705 G706 V707 G708 S713 D717 G718 L719 H720 L721 W722 L737 P740 S745 C746 C747 L748 D749 L750 R758 Q765 L773 L776 P779 S782
F783 S784 K788 L792 L793 G794 H797 G798 E799 P805 Y808 C811 H812 E813 A814 V815 G841 D857 THR VAL GLN I861 A875 R886 I887 W891 T892 Y893 D898 K901 L907 L913 R918 N921 L929 L932 H938 K952 T953
Y959 A968 P969 L972 T978 P979 A980 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 R1025 K1032 N1035 R1044 T1045 L1046 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1073
R1076 A1077 E1078 K1079 S1080 Y1081 V1095 R1101 V1102 G1103 P1107 E1108 L1109 L1120 V1123 F1124 N1125 G1126 R1141 P1142 W1143 M1152 I1161 G1166 V1191 V1199 I1216 T1235 T1236 W1237 X1516 X1519 X1520 X1521 X1526 X1529 R1594 L1600 M1608
V1615 GLU THR ARG ARG ALA GLY E1622 C1630 M1637 I1650 H1665 R1668 R1671 L1676 G1677 N1678 N1679 R1680 L1685 H1688 Q1691 L1698 A1701 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721 S1722 A1723 C1724 R1725 S1726 R1727 L1731 T1739
T1742 R1743 G1764 R1772 H1775 A1784 A1788 ALA GLY VAL ALA E1793 I1802 D1828 P1829 V1830 P1840 V1859 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 K1936 C1940 D1948 A1960 R1964 Q1973 Y1977 T1991 T1995 P2002 Q2005 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 R2126 Q2127 Y2128 L2131 I2167 V2168 Q2169 M2170 P2195 N2196 R2199 V2214 L2215 N2246 L2257
T2271 P2272 L2273 A2276 A2277 L2290 Q2291 E2292 Q2293 D2294 L2295 C2326 G2327 F2337 F2340 V2341 N2342 G2343 V2346 E2347 E2348 N2349 A2350 N2351 L2368 L2376 E2381 I2384 E2388 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU
N2414 L2432 C2436 A2437 P2438 R2454 L2466 I2469 L2472 X2674 X2675 X2676 P2737 R2738 P2739 T2742 P2748 L2751 F2758 T2762 K2770 W2775 S2776 Y2777 G2778 T2787 L2791 E2803 R2806 W2807 K2810 E2811 K2814 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 S2868 Q2872 E2876 N2881 N2884 R2888 L2894 H2902 L2905 A2913 K2916 R2920 L2927 L2930 X3365 X3369 X3556 X3560
K3658 W3661 I3662 F3669 D3675 D3676 E3712 S3732 N3741 GLY GLU ALA GLU GLU E3747 F3753 Q3761 R3762 Q3766 R3769 T3772 V3779 L3780 K3787 L3805 N3806 N3809 V3812 K3815 M3816 L3817 Q3889 L3890 N3896 F3899 T3907 L3923
Q3927 S3931 Y3937 K3948 M3955 Q3960 V3961 F3962 N3963 G3971 A3981 R3984 L3985 W3986 F3992 L3993 F3996 K4002 S4008 L4019 N4034 E4056 L4059 K4060 D4063 D4083 P4084 R4085 G4086 K4090 Q4094 T4104 G4105 P4106 E4107 N4120
T4148 E4152 H4156 L4166 A4167 P4176 Y4177 L4178 I4181 I4193 Y4194 R4202 E4227 A4228 E4229 K4230 Q4250 X4344 N4553 N4558 F4571 F4575 I4576 L4577 Y4580 K4581 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 V4666 R4673 K4698 S4713 K4718 F4719 R4722 M4743 A4746 E4749 I4750 T4751 A4752 G4763 T4766 W4767 S4770 K4821 N4833 R4860
N4864 E4871 C4876 H4886 G4890 Y4909 I4925 L4929 L4935 F4959 I4960 F4968 H4978 E4982 H4983 N4984 L4985 A4986 N4987 Y4988 C5027 L5036 S5037

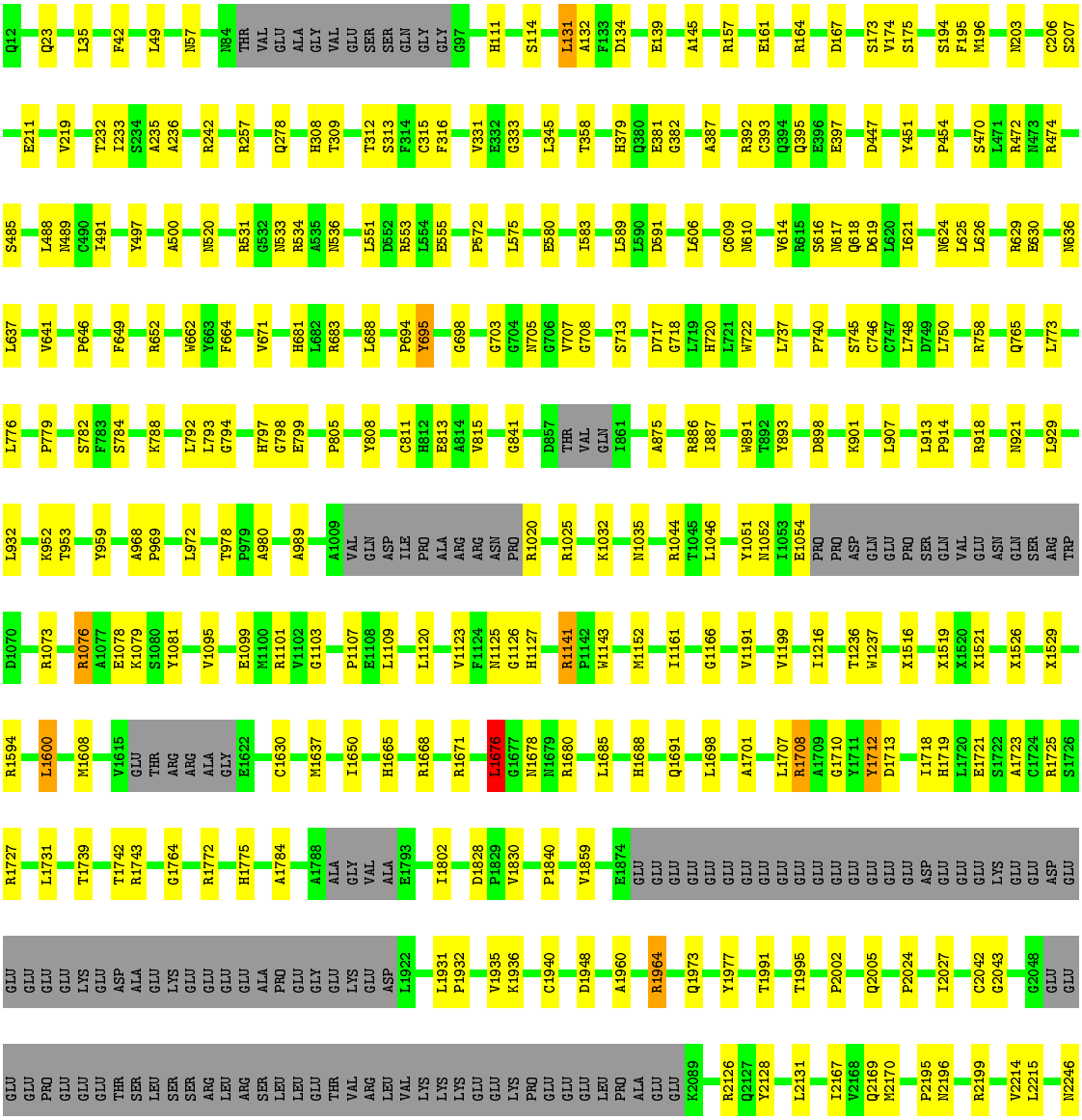
- Molecule 2: Ryanodine receptor 1

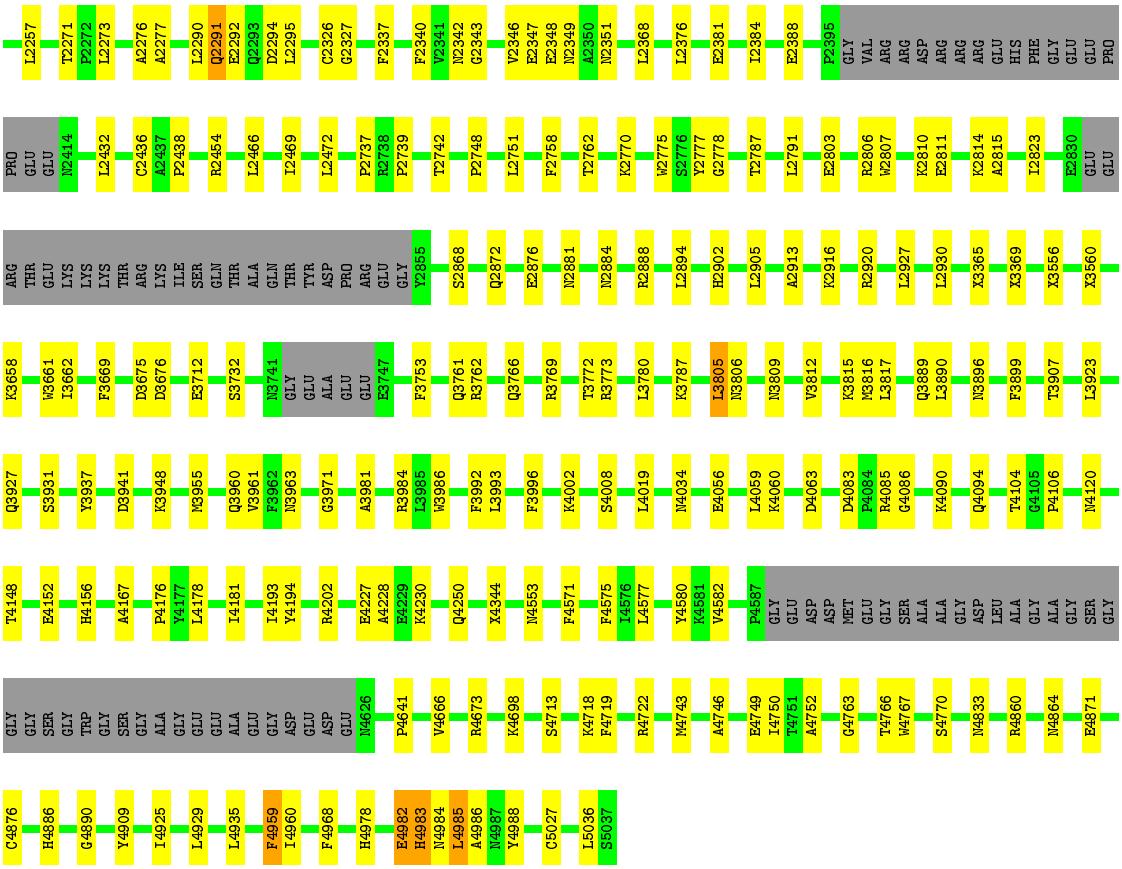




• Molecule 2: Ryanodine receptor 1

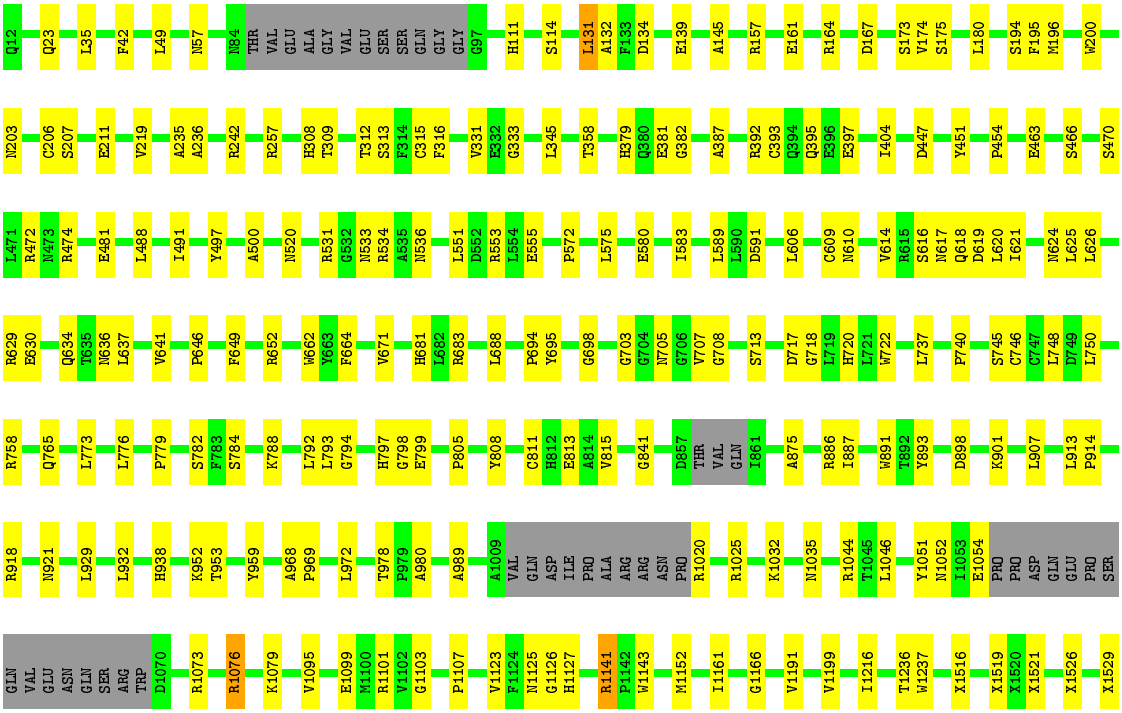
Chain I:

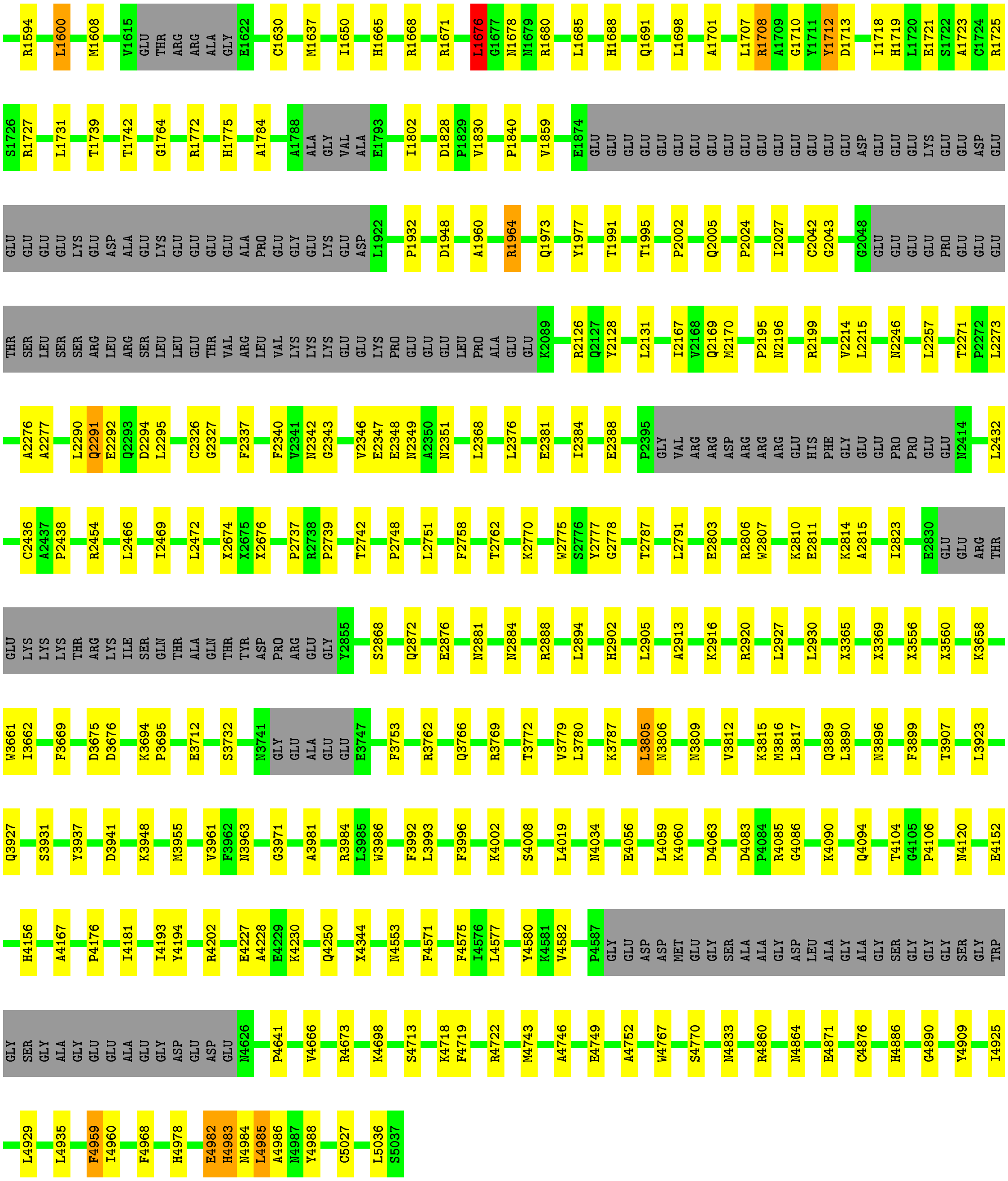




- Molecule 2: Ryanodine receptor 1

Chain G:




R1594 L1600 M1608 V1615 GLU THR ARG ARG ALA GLY E1622 C1630 M1637 I1650 H1665 R1668 R1671 L1676 G1677 N1678 N1679 R1680 L1685 H1688 Q1691 L1698 A1701 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721 S1722 A1723 C1724 R1725
S1726 R1727 L1731 T1739 T1742 G1764 R1772 H1775 A1784 A1788 ALA GLY VAL ALA E1793 I1802 D1828 P1829 V1830 P1840 V1859 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 P1932 D1948 A1960 R1964 Q1973 Y1977 T1991 T1995 P2002 Q2005 P2024 I2027 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 R2126 Q2127 Y2128 L2131 I2167 V2168 Q2169 M2170 P2195 N2196 R2199 V2214 L2215 N2246 L2257 T2271 P2272 L2273
A2276 A2277 L2290 Q2291 E2292 Q2293 D2294 L2295 C2326 G2327 F2337 F2340 V2341 N2342 G2343 V2346 E2347 E2348 N2349 A2350 N2351 L2368 L2376 E2381 I2384 E2388 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 L2432
C2436 A2437 P2438 R2454 L2466 I2469 L2472 X2674 X2675 X2676 P2737 R2738 P2739 T2742 P2748 L2751 F2758 T2762 K2770 W2775 S2776 Y2777 G2778 T2787 L2791 E2803 R2806 W2807 K2810 E2811 K2814 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 S2868 Q2872 E2876 N2881 N2884 R2888 L2894 H2902 L2905 A2913 K2916 R2920 L2927 L2930 X3365 X3369 X3556 X3560 K3658
W3661 I3662 F3669 D3675 D3676 K3694 P3695 E3712 S3732 N3741 GLY GLU ALA GLU GLU E3747 F3753 R3762 Q3766 R3769 T3772 V3779 L3780 K3787 L3805 N3806 N3809 V3812 K3815 M3816 L3817 Q3889 L3890 N3896 F3899 T3907 L3923
Q3927 S3931 Y3937 D3941 K3948 M3955 V3961 F3962 N3963 G3971 A3981 R3984 L3985 W3986 F3992 L3993 F3996 K4002 S4008 L4019 N4034 E4056 L4059 K4060 D4063 D4083 P4084 R4085 G4086 K4090 Q4094 T4104 G4105 P4106 N4120 E4152
H4156 A4167 P4176 I4181 I4193 Y4194 R4202 E4227 A4228 E4229 K4230 Q4250 X4344 N4553 F4571 F4575 I4576 L4577 Y4580 K4581 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 V4666 R4673 K4698 S4713 K4718 F4719 R4722 M4743 A4746 E4749 A4752 W4767 S4770 N4833 R4860 N4864 E4871 C4876 H4886 G4890 Y4909 I4925
L4929 L4935 F4959 I4960 F4968 H4978 E4982 H4983 N4984 L4985 A4986 N4987 Y4988 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

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	0.31	0/834	0.51	0/1123
1	J	0.31	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.55	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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	695	TYR	C-N	5.28	1.44	1.34
2	I	695	TYR	C-N	5.28	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	695	TYR	C-N	5.28	1.44	1.34
2	E	695	TYR	C-N	5.26	1.44	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	E	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	G	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	I	131	LEU	CA-CB-CG	8.21	134.18	115.30
2	I	1600	LEU	CA-CB-CG	6.73	130.78	115.30

There are no chirality outliers.

5 of 60 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	11	0
1	F	818	0	824	12	0
1	H	818	0	824	9	0
1	J	818	0	824	11	0
2	B	29499	0	24757	259	0
2	E	29499	0	24757	259	0
2	G	29499	0	24757	251	0
2	I	29499	0	24757	256	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1	0	0	0	0
All	All	121272	0	102324	1040	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 1040 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:G:2291:GLN:HB3	2:G:2294:ASP:H	1.51	0.76
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.51	0.76
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.51	0.75
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.51	0.74
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.57	0.70

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%)	97 (92%)	8 (8%)	0	100	100
1	F	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	J	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	52	86
2	E	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	52	86
2	G	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	52	86
2	I	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	52	86
All	All	13360/18096 (74%)	11956 (90%)	1376 (10%)	28 (0%)	56	86

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	I	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%)	2476 (99%)	17 (1%)	88	94
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%)	10256 (99%)	68 (1%)	89	94

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	4085	ARG
2	I	1141	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 105 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	3976	ASN
2	I	479	GLN
2	G	3960	GLN
2	E	4034	ASN
2	E	4987	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	14
2	B	14
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	74.04
1	E	4345:UNK	C	4540:PHE	N	74.04
1	I	4345:UNK	C	4540:PHE	N	74.04
1	G	4345:UNK	C	4540:PHE	N	74.04
1	B	3613:UNK	C	3639:THR	N	46.14