wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 03:54 PM EDT

PDB ID	:	5TAQ
EMDB ID:	:	EMD-8382
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/Ca2+ dataset, class 3&4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.10 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

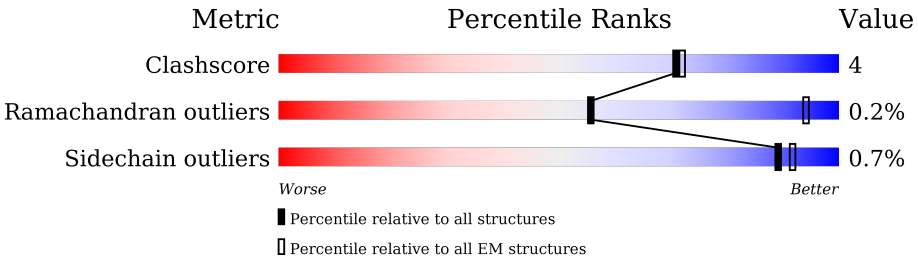
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.10 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	81% 17% ••
1	F	108	81% 17% ••
1	H	108	80% 19% ••
1	J	108	80% 19% ••
2	B	4416	85% 10% 5%
2	E	4416	85% 10% 5%
2	G	4416	85% 10% 5%
2	I	4416	85% 10% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

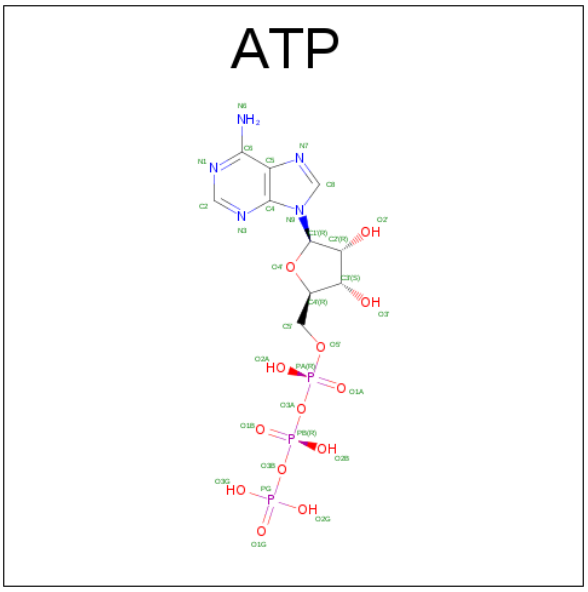
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

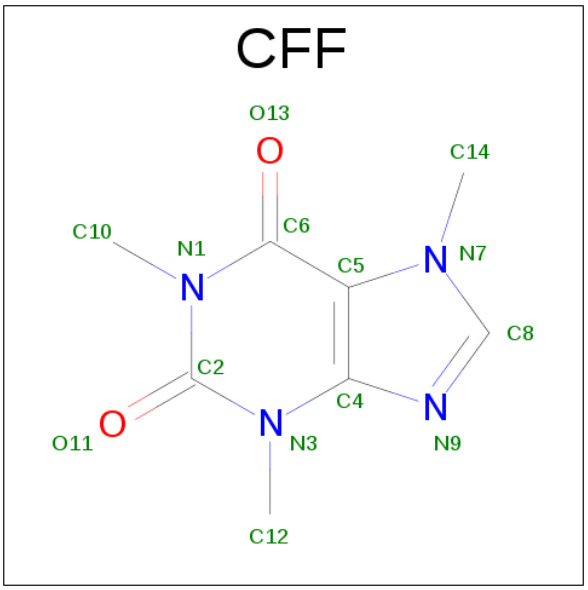
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

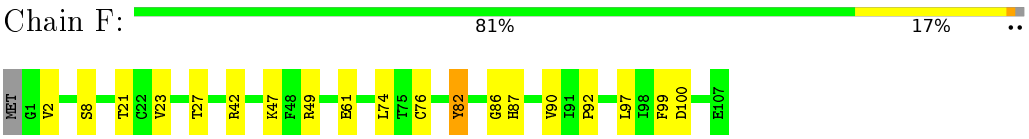
Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

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.

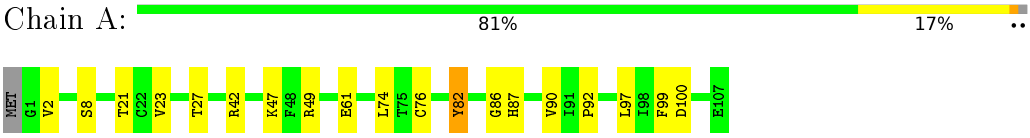
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



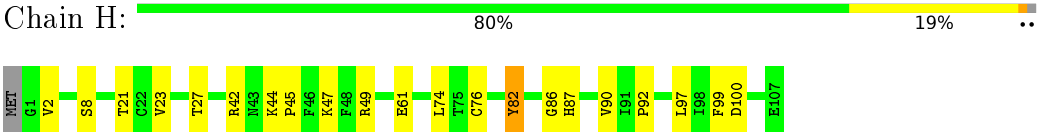
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



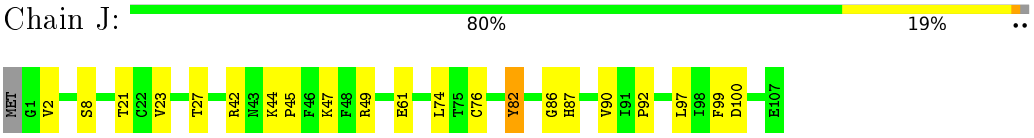
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



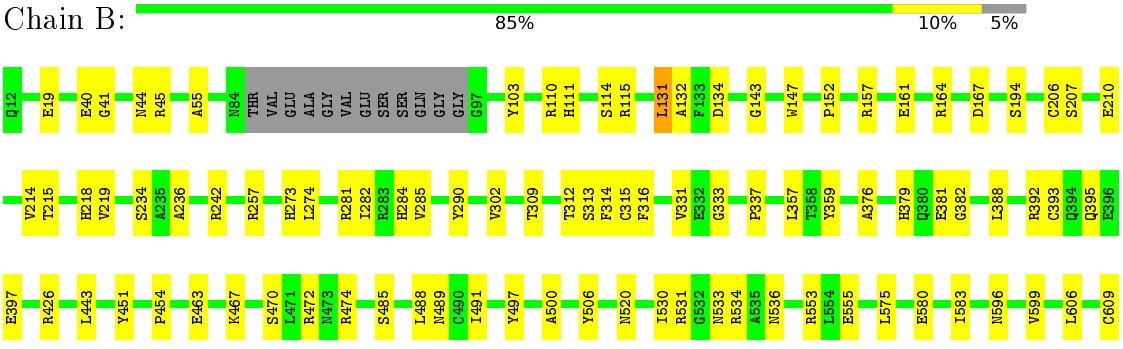
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

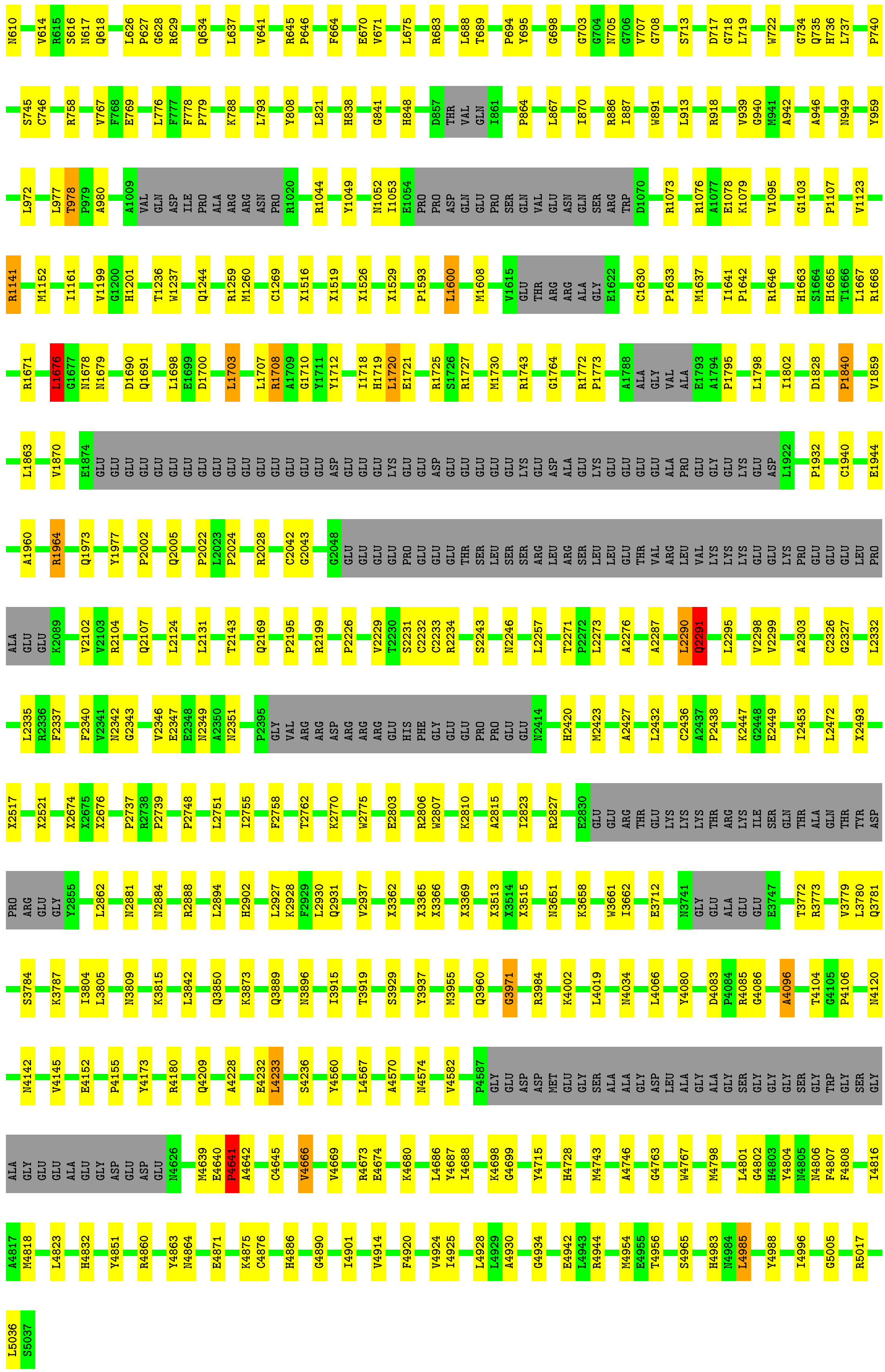
Chain J:



- Molecule 2: Ryanodine receptor 1

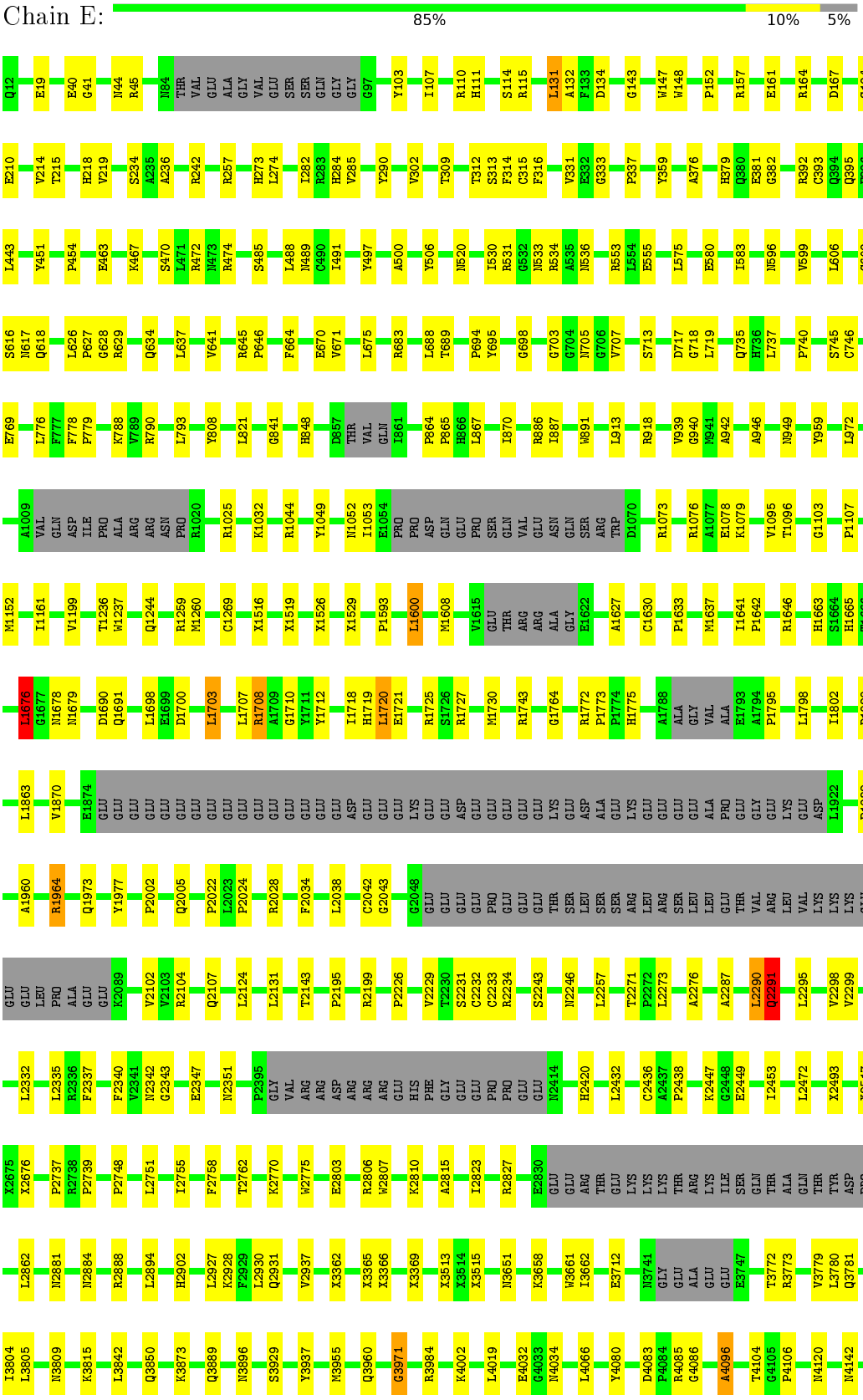
Chain B:

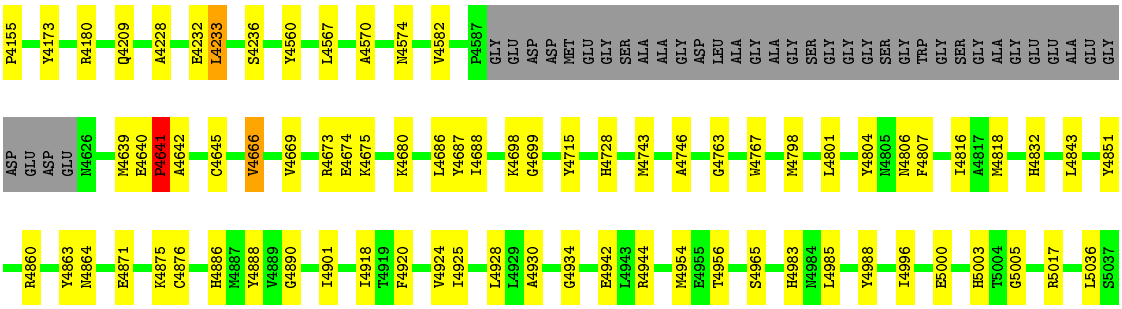



N610 V614 R615 S616 N617 Q618 L626 P627 G628 R629 Q634 L637 V641 R645 P646 F664 E670 V671 L675 R683 L688 T689 P694 Y695 G698 G703 G704 N705 G706 V707 G708 S713 D717 G718 L719 W722 G734 Q735 H736 L737 P740
S745 C746 R758 V767 F768 E769 L776 F777 F778 P779 K788 L793 Y808 L821 H838 G841 H848 D857 THR VAL GLN I861 P864 L867 I870 R886 I887 W891 L913 R918 V939 G940 M941 A942 A946 N949 Y959
L972 L977 T978 P979 A980 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 R1044 Y1049 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1073 R1076 A1077 E1078 K1079 V1095 G1103 P1107 V1123
R1141 M1152 I1161 V1199 G1200 H1201 T1236 W1237 Q1244 R1259 M1260 C1269 X1516 X1519 X1526 X1529 P1593 L1600 M1608 V1615 GLU THR ARG ARG ALA GLY E1622 C1630 P1633 M1637 I1641 P1642 R1646 H1663 S1664 H1665 T1666 L1667 R1668
R1671 L1676 G1677 N1678 N1679 D1690 Q1691 L1698 E1699 D1700 L1703 L1707 R1708 A1709 G1710 Y1711 Y1712 I1718 H1719 L1720 E1721 R1725 S1726 R1727 M1730 R1743 G1764 R1772 P1773 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 I1802 D1828 P1840 V1859
L1863 V1870 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 C1940 E1944
A1960 R1964 Q1973 Y1977 P2002 Q2005 P2022 L2023 P2024 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 V2102 V2103 R2104 Q2107 L2124 L2131 T2143 Q2169 P2195 R2199 P2226 V2229 T2230 S2231 C2232 C2233 R2234 S2243 N2246 L2257 T2271 P2272 L2273 A2276 A2287 L2290 Q2291 L2295 V2298 V2299 A2303 C2326 G2327 L2332
L2335 R2336 F2337 F2340 V2341 N2342 G2343 V2346 E2347 E2348 N2349 A2350 N2351 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 H2420 M2423 A2427 L2432 C2436 A2437 P2438 K2447 G2448 E2449 I2453 L2472 X2493
X2517 X2521 X2674 X2675 X2676 P2737 R2738 P2739 P2748 L2751 I2755 F2758 T2762 K2770 W2775 E2803 R2806 W2807 K2810 A2815 I2823 R2827 E2830 GLU GLU ARG THR THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP
PRO ARG GLU GLY Y2855 L2862 N2881 N2884 R2888 L2894 H2902 L2927 K2928 F2929 L2930 Q2931 V2937 X3362 X3365 X3366 X3369 X3513 X3514 X3515 N3651 K3658 W3661 I3662 E3712 N3741 GLY GLU ALA GLU GLU E3747 T3772 R3773 V3779 L3780 Q3781
S3784 K3787 I3804 L3805 N3809 K3815 L3842 Q3850 K3873 Q3889 N3896 I3915 T3919 S3929 Y3937 M3955 Q3960 G3971 R3984 K4002 L4019 N4034 L4066 Y4080 D4083 P4084 R4085 G4086 A4096 T4104 G4105 P4106 N4120
N4142 V4145 E4152 P4155 Y4173 R4180 Q4209 A4228 E4232 L4233 S4236 Y4560 L4567 A4570 N4574 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 M4639 E4640 P4641 A4642 C4645 V4666 V4669 R4673 E4674 K4680 L4686 Y4687 I4688 K4698 G4699 Y4715 H4728 M4743 A4746 G4763 W4767 M4798 L4801 G4802 H4803 Y4804 N4805 N4806 F4807 F4808 I4816
A4817 M4818 L4823 H4832 Y4851 R4860 Y4863 N4864 E4871 K4875 C4876 H4886 G4890 I4901 V4914 F4920 V4924 I4925 L4928 L4929 A4930 G4934 E4942 L4943 R4944 M4954 E4955 T4956 S4965 H4983 N4984 L4985 Y4988 I4996 G5005 R5017
L5036 S5037

• Molecule 2: Ryanodine receptor 1

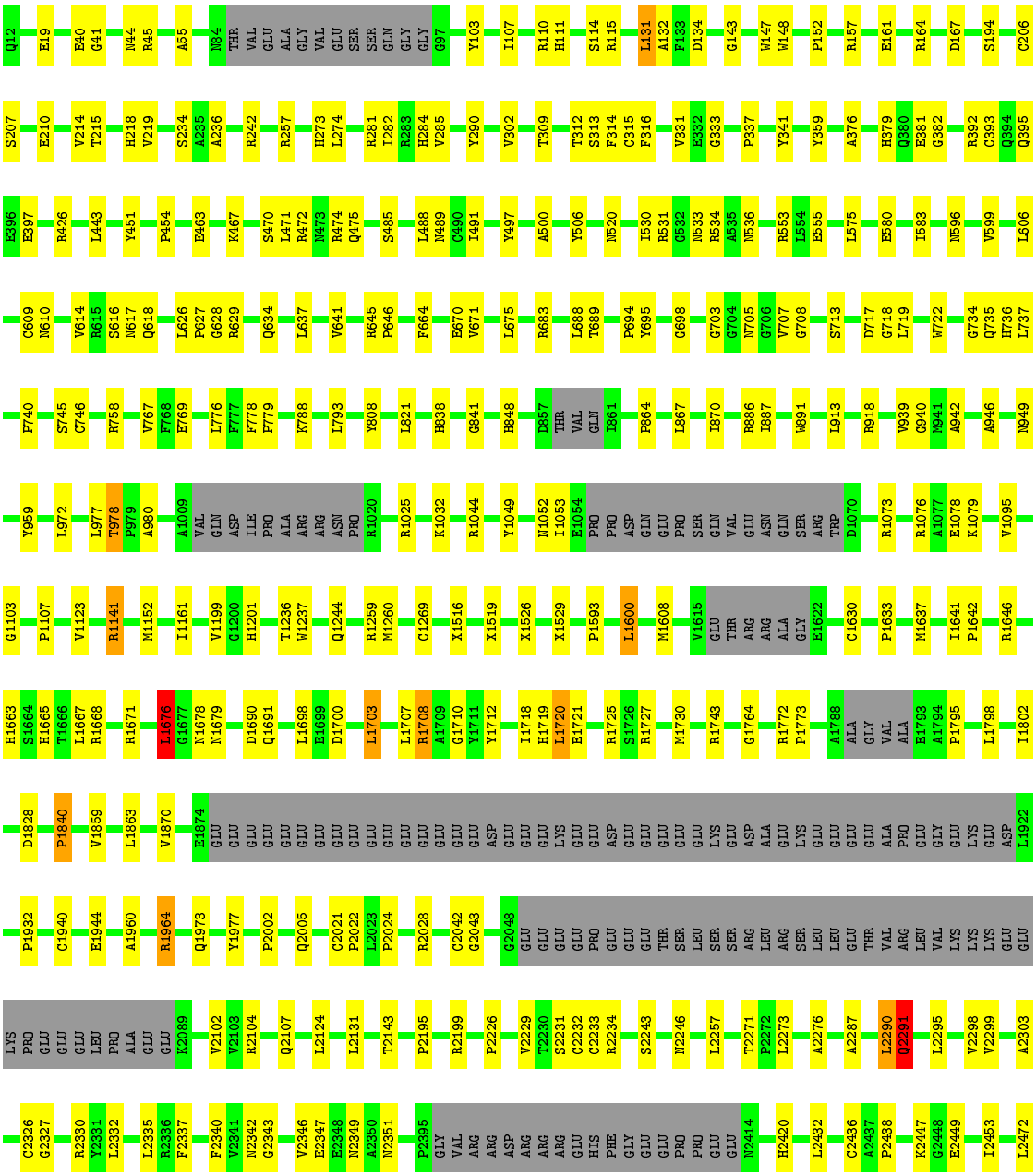
Chain E:

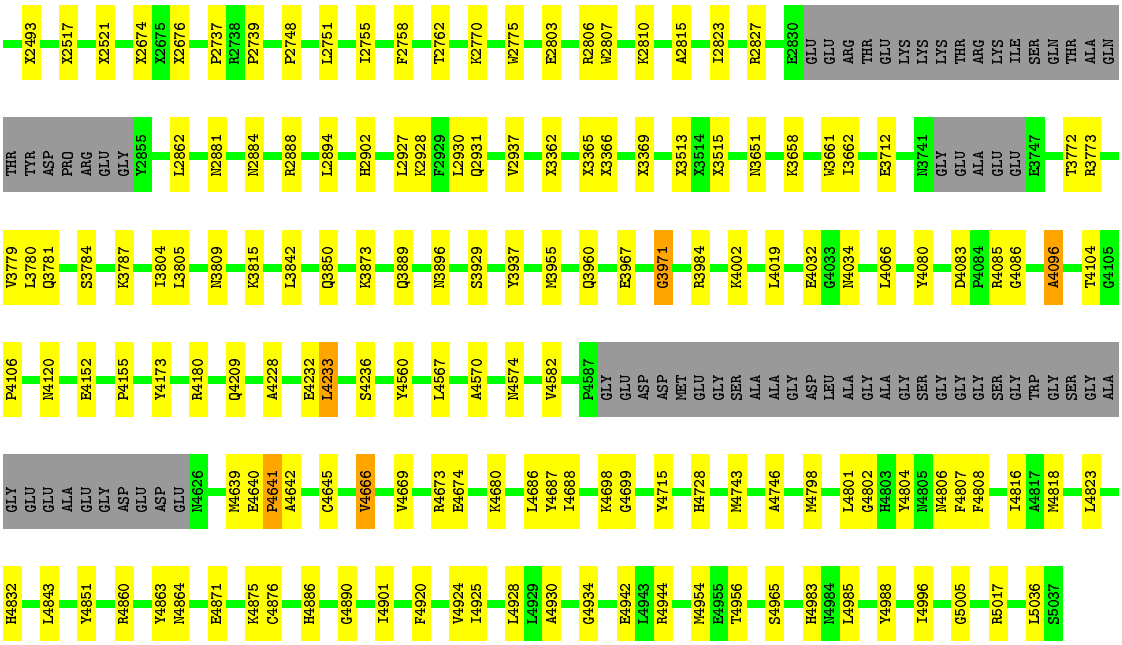




• Molecule 2: Ryanodine receptor 1

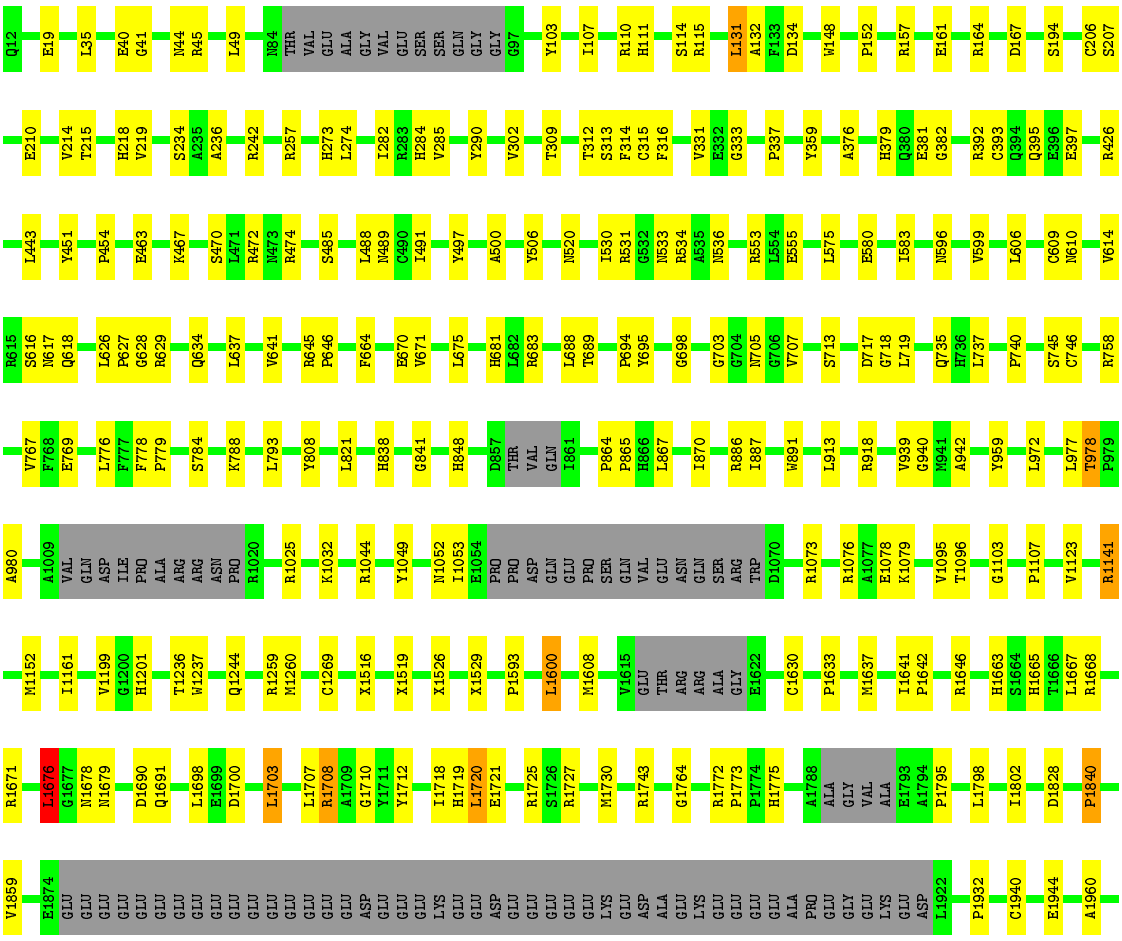
Chain I:

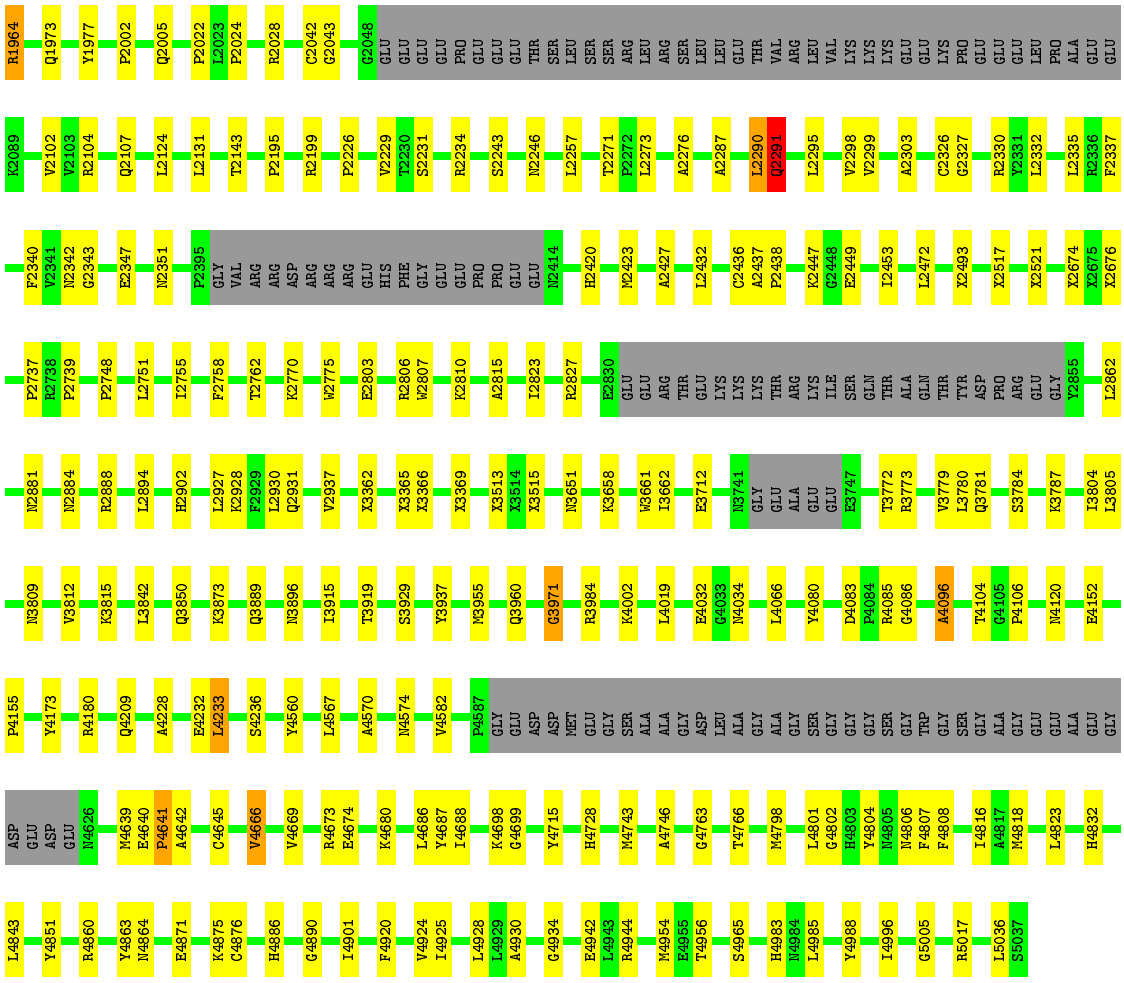




• Molecule 2: Ryanodine receptor 1

Chain G:




R1964 Q1973 Y1977 P2002 Q2005 P2022 L2023 P2024 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 V2102 V2103 R2104 Q2107 L2124 L2131 T2143 P2195 R2199 P2226 V2229 T2230 S2231 R2234 S2243 M2246 L2257 T2271 P2272 L2273 A2276 A2287 L2290 Q2291 L2295 V2298 V2299 A2303 C2326 G2327 R2330 Y2331 L2332 L2335 R2336 F2337
F2340 V2341 N2342 G2343 E2347 N2351 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 H2420 M2423 A2427 L2432 C2436 A2437 P2438 K2447 G2448 E2449 I2453 L2472 X2493 X2517 X2521 X2674 X2675 X2676
P2737 R2738 P2739 P2748 L2751 I2755 F2758 T2762 K2770 W2775 E2803 R2806 W2807 K2810 A2815 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 GLU GLY Y2855 L2862
N2881 N2884 R2888 L2894 H2902 L2927 K2928 F2929 L2930 Q2931 V2937 X3362 X3365 X3366 X3369 X3513 X3514 X3515 N3651 K3658 W3661 I3662 E3712 N3741 GLY GLU ALA GLU GLU E3747 T3772 R3773 V3779 L3780 Q3781 S3784 K3787 I3804 L3805
N3809 V3812 K3815 L3842 Q3850 K3873 Q3889 N3896 I3915 T3919 S3929 Y3937 M3955 Q3960 G3971 R3984 K4002 L4019 E4032 G4033 N4034 L4066 Y4080 D4083 P4084 R4085 G4086 A4096 T4104 G4105 P4106 N4120 E4152
P4155 Y4173 R4180 Q4209 A4228 E4232 L4233 S4236 Y4560 L4567 A4570 N4574 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 M4639 E4640 P4641 A4642 C4645 V4666 V4669 R4673 E4674 K4680 L4686 Y4687 I4688 K4698 G4699 Y4715 H4728 M4743 A4746 G4763 T4766 M4798 L4801 G4802 H4803 Y4804 N4805 N4806 F4807 F4808 I4816 A4817 M4818 L4823 H4832
L4843 Y4851 R4860 Y4863 N4864 E4871 K4875 C4876 H4886 G4890 I4901 F4920 V4924 I4925 L4928 L4929 A4930 G4934 E4942 L4943 R4944 M4954 E4955 T4956 S4965 H4983 N4984 L4985 Y4988 I4996 G5005 R5017 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: CFF, ZN, CA, ATP

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	0.32	0/834	0.54	0/1123
1	F	0.32	0/834	0.54	0/1123
1	H	0.32	0/834	0.54	0/1123
1	J	0.32	0/834	0.54	0/1123
2	B	0.32	0/25428	0.57	13/34534 (0.0%)
2	E	0.32	0/25428	0.57	13/34534 (0.0%)
2	G	0.32	0/25428	0.57	13/34534 (0.0%)
2	I	0.32	0/25428	0.57	13/34534 (0.0%)
All	All	0.32	0/105048	0.57	52/142628 (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	2
1	F	0	2
1	H	0	2
1	J	0	2
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	80

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	131	LEU	CA-CB-CG	8.14	134.03	115.30
2	B	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	E	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	I	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	E	4639	MET	C-N-CA	6.84	138.79	121.70

There are no chirality outliers.

5 of 80 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
1	A	82	TYR	Peptide
1	F	8	SER	Peptide
1	F	82	TYR	Peptide
1	H	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	10	0
1	F	818	0	824	10	0
1	H	818	0	824	11	0
1	J	818	0	824	11	0
2	B	29499	0	24752	242	0
2	E	29499	0	24752	242	0
2	G	29499	0	24752	241	0
2	I	29499	0	24752	243	0
3	B	31	0	12	1	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102392	986	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 986 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:646:PRO:HD2	2:G:779:PRO:HB2	1.73	0.70
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.69
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.69
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.75	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.73	0.69

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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2877 (89%)	352 (11%)	6 (0%)	52	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2878 (89%)	351 (11%)	6 (0%)	52	86
2	G	3235/4416 (73%)	2877 (89%)	352 (11%)	6 (0%)	52	86
2	I	3235/4416 (73%)	2878 (89%)	351 (11%)	6 (0%)	52	86
All	All	13360/18096 (74%)	11884 (89%)	1452 (11%)	24 (0%)	56	86

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1840	PRO
2	B	1932	PRO
2	B	4641	PRO
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%)	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

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Mol	Chain	Res	Type
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 156 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	3946	GLN
2	I	405	HIS
2	G	3781	GLN
2	E	4034	ASN
2	E	5003	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ATP	B	5101	-	26,33,33	0.90	1 (3%)	26,52,52	1.73	3 (11%)
4	CFF	B	5102	-	8,15,15	2.59	3 (37%)	8,23,23	1.13	1 (12%)
3	ATP	E	5101	-	26,33,33	0.90	1 (3%)	26,52,52	1.68	2 (7%)
4	CFF	E	5102	-	8,15,15	2.60	3 (37%)	8,23,23	1.14	1 (12%)
3	ATP	G	5101	-	26,33,33	0.90	1 (3%)	26,52,52	1.69	3 (11%)
4	CFF	G	5102	-	8,15,15	2.57	3 (37%)	8,23,23	1.13	1 (12%)
3	ATP	I	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.68	2 (7%)
4	CFF	I	5102	-	8,15,15	2.58	3 (37%)	8,23,23	1.13	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	E	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	G	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	I	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	0/0/0/0	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C4-N3	-5.02	1.33	1.39
4	B	5102	CFF	C4-N3	-5.01	1.33	1.39
4	I	5102	CFF	C4-N3	-4.92	1.33	1.39
4	G	5102	CFF	C4-N3	-4.89	1.33	1.39
4	E	5102	CFF	C6-N1	-4.34	1.31	1.38

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5101	ATP	N3-C2-N1	-6.67	123.64	128.87
3	G	5101	ATP	N3-C2-N1	-6.49	123.77	128.87
3	E	5101	ATP	N3-C2-N1	-6.46	123.80	128.87
3	I	5101	ATP	N3-C2-N1	-6.42	123.83	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	5102	CFF	C14-N7-C8	-2.57	111.89	125.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
4	B	5102	CFF	1	0
4	E	5102	CFF	1	0
4	G	5102	CFF	1	0
4	I	5102	CFF	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	E	4345:UNK	C	4540:PHE	N	72.62
1	B	4345:UNK	C	4540:PHE	N	72.61
1	I	4345:UNK	C	4540:PHE	N	72.60
1	G	4345:UNK	C	4540:PHE	N	72.60
1	E	3613:UNK	C	3639:THR	N	43.07