wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 06:17 PM EDT

PDB ID	:	5TAM
EMDB ID:	:	EMD-8379
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/Ca2+ dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.30 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

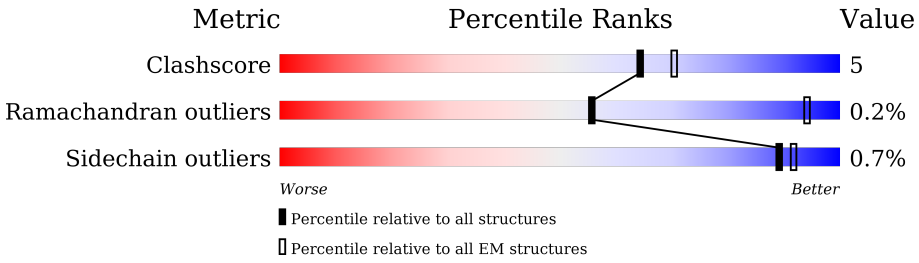
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.30 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	79% 20% .
1	F	108	81% 19% .
1	H	108	81% 19% .
1	J	108	81% 19% .
2	B	4416	83% 11% 5%
2	E	4416	84% 11% 5%
2	G	4416	83% 11% 5%
2	I	4416	84% 11% 5%

2 Entry composition

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.

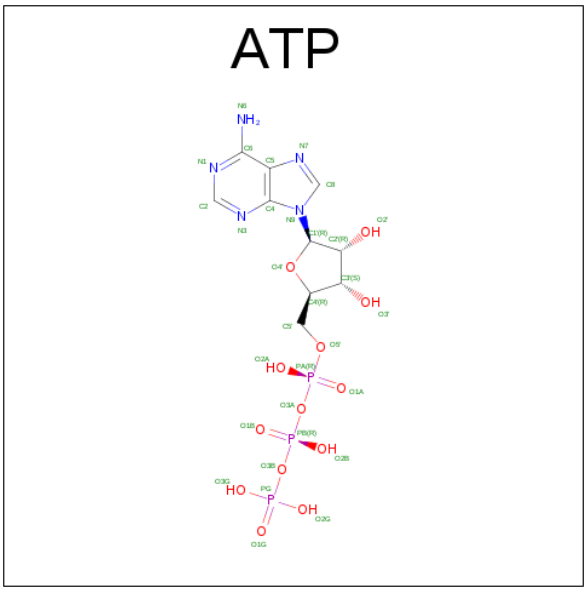
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

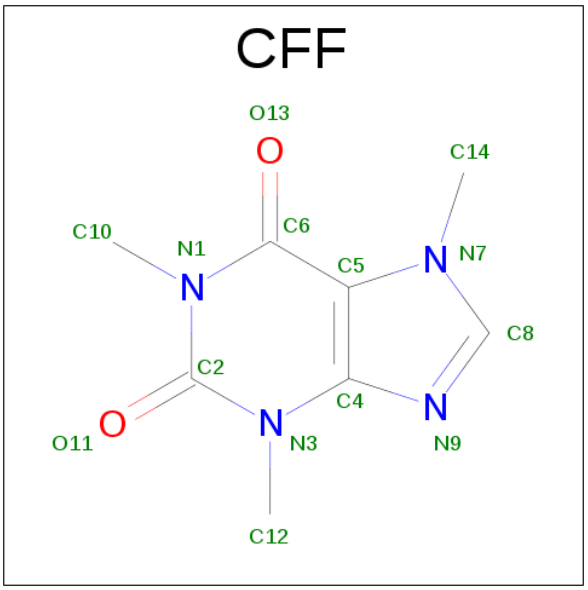
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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).

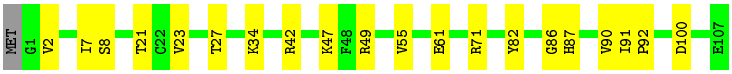
Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

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.

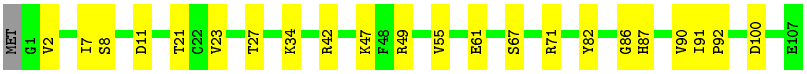
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



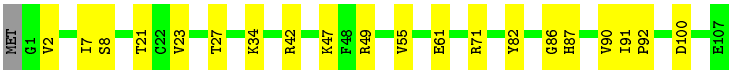
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



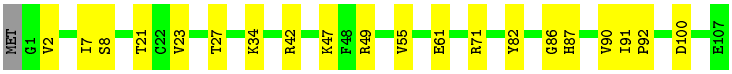
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



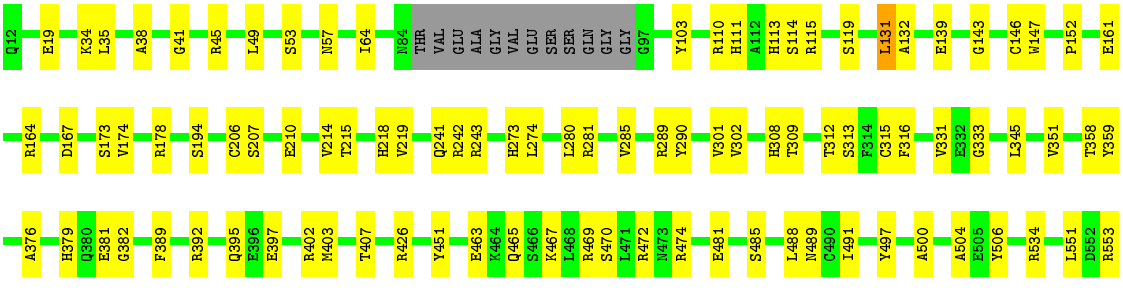
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

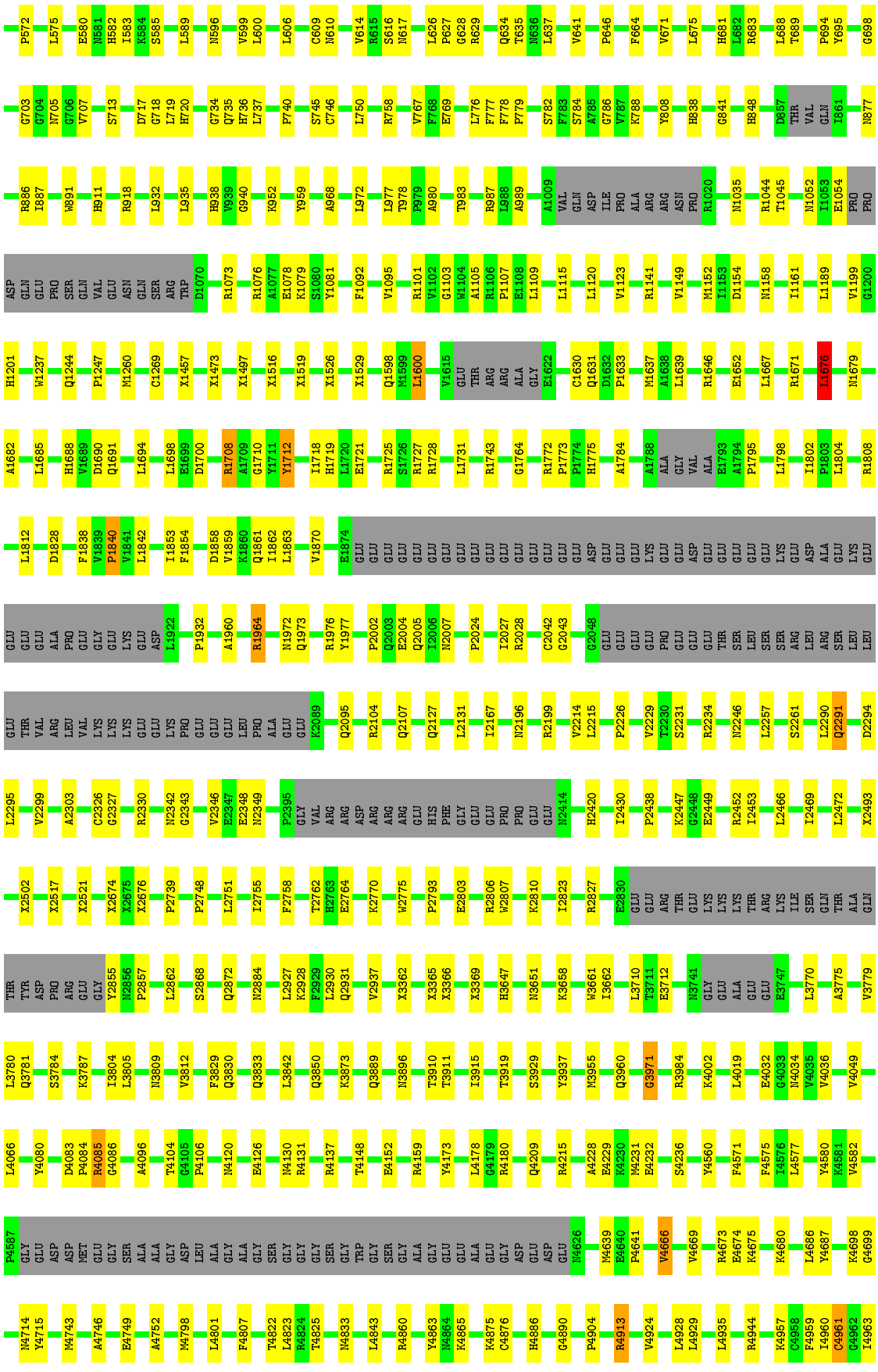
Chain J:



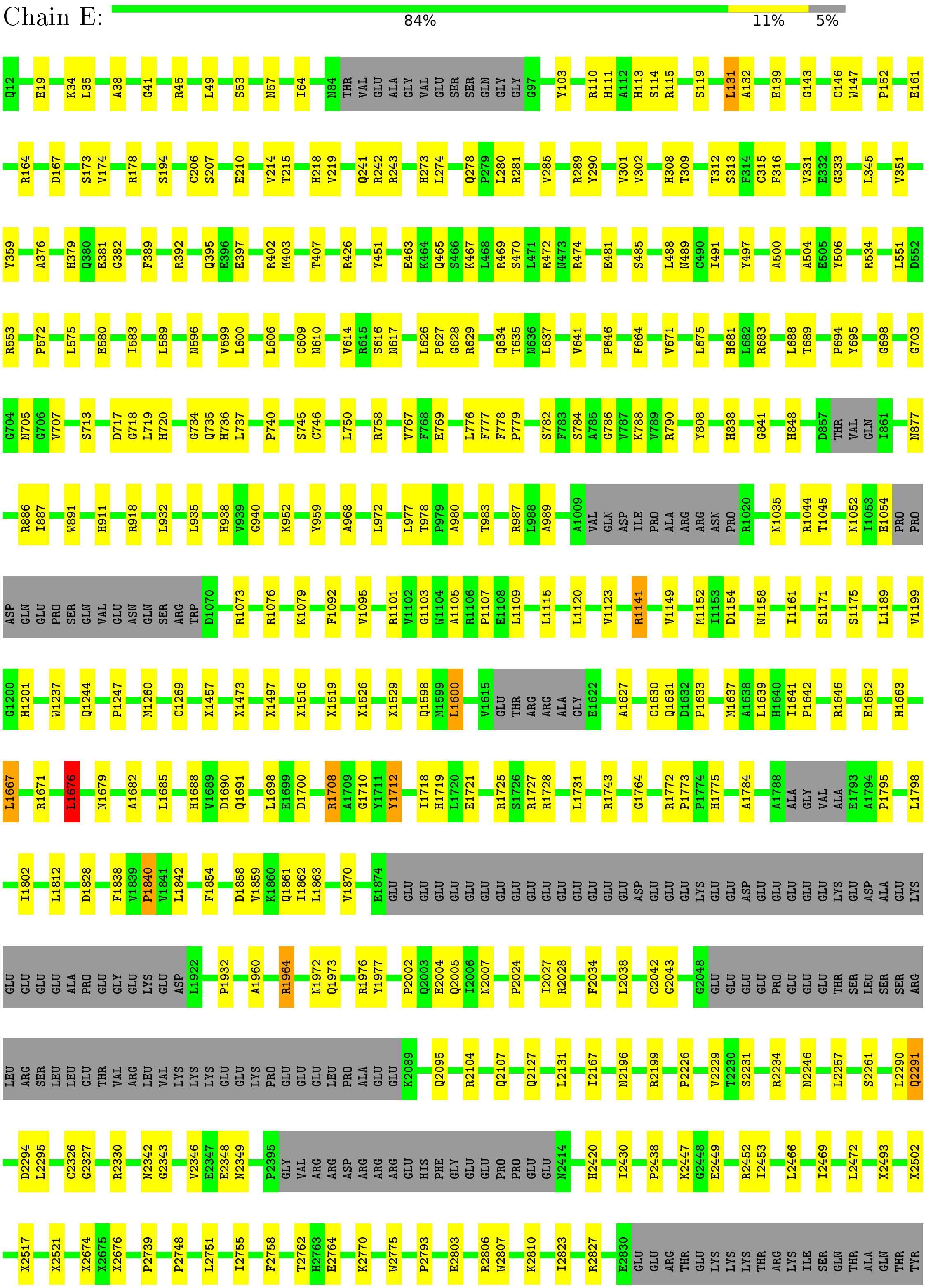
- Molecule 2: Ryanodine receptor 1

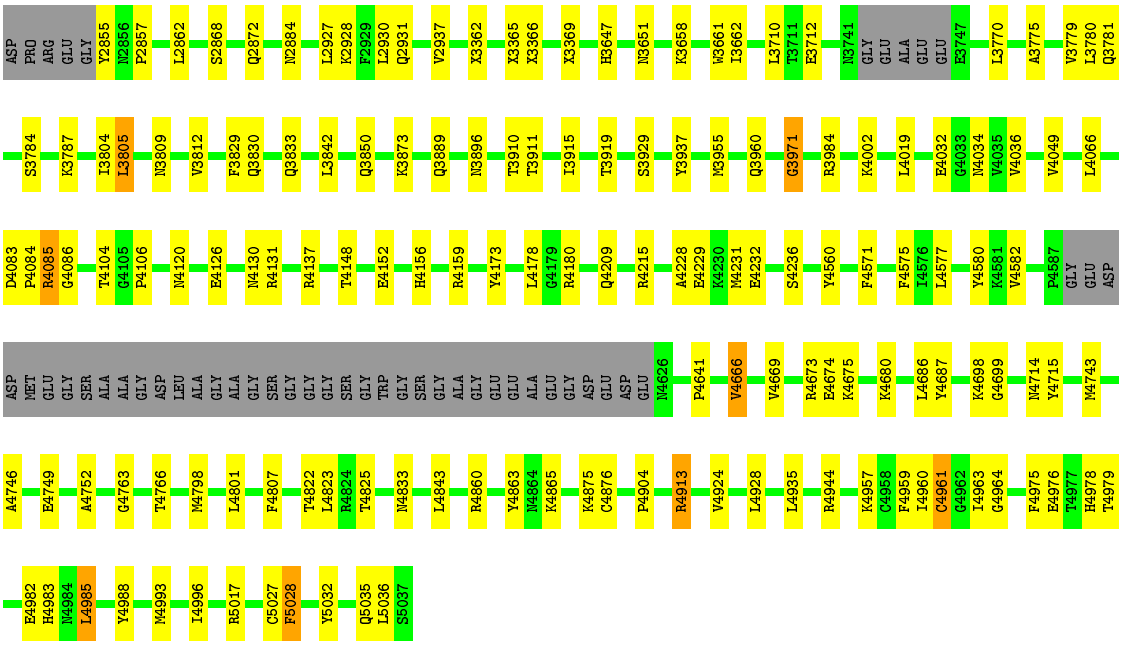
Chain B:




P572 L575 E580 N581 H582 I583 K584 S585 L589 N596 V599 L600 L606 C609 N610 V614 R615 S616 N617 L626 P627 G628 R629 Q634 T635 N636 L637 V641 P646 F664 V671 L675 H681 L682 R683 L688 T689 P694 Y695 G698
G703 G704 N705 G706 V707 S713 D717 G718 L719 H720 G734 Q735 H736 L737 P740 S745 C746 L750 R758 V767 F768 E769 L776 F777 F778 P779 S782 F783 S784 A785 G786 V787 K788 Y808 H838 G841 H848 D857 THR VAL GLN I861 N877
R886 I887 W891 H911 R918 L932 L935 H938 V939 G940 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 T1045 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 F1092 V1095 R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108 L1109 L1115 L1120 V1123 R1141 V1149 M1152 I1153 D1154 N1158 I1161 L1189 V1199 G1200
H1201 W1237 Q1244 P1247 M1260 C1269 X1457 X1473 X1497 X1516 X1519 X1526 X1529 Q1598 M1599 L1600 V1615 GLU THR ARG ARG ALA GLY E1622 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 R1646 E1652 L1667 R1671 L1676 N1679
A1682 L1685 H1688 V1689 D1690 Q1691 L1694 L1698 E1699 D1700 R1708 A1709 G1710 Y1711 V1712 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728 L1731 R1743 G1764 R1772 P1773 P1774 H1775 A1784 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 I1802 P1803 L1804 R1808
L1812 D1828 F1838 V1839 P1840 V1841 L1842 I1853 F1854 D1858 V1859 K1860 Q1861 I1862 L1863 V1870 E1874 GLU GLU GLU

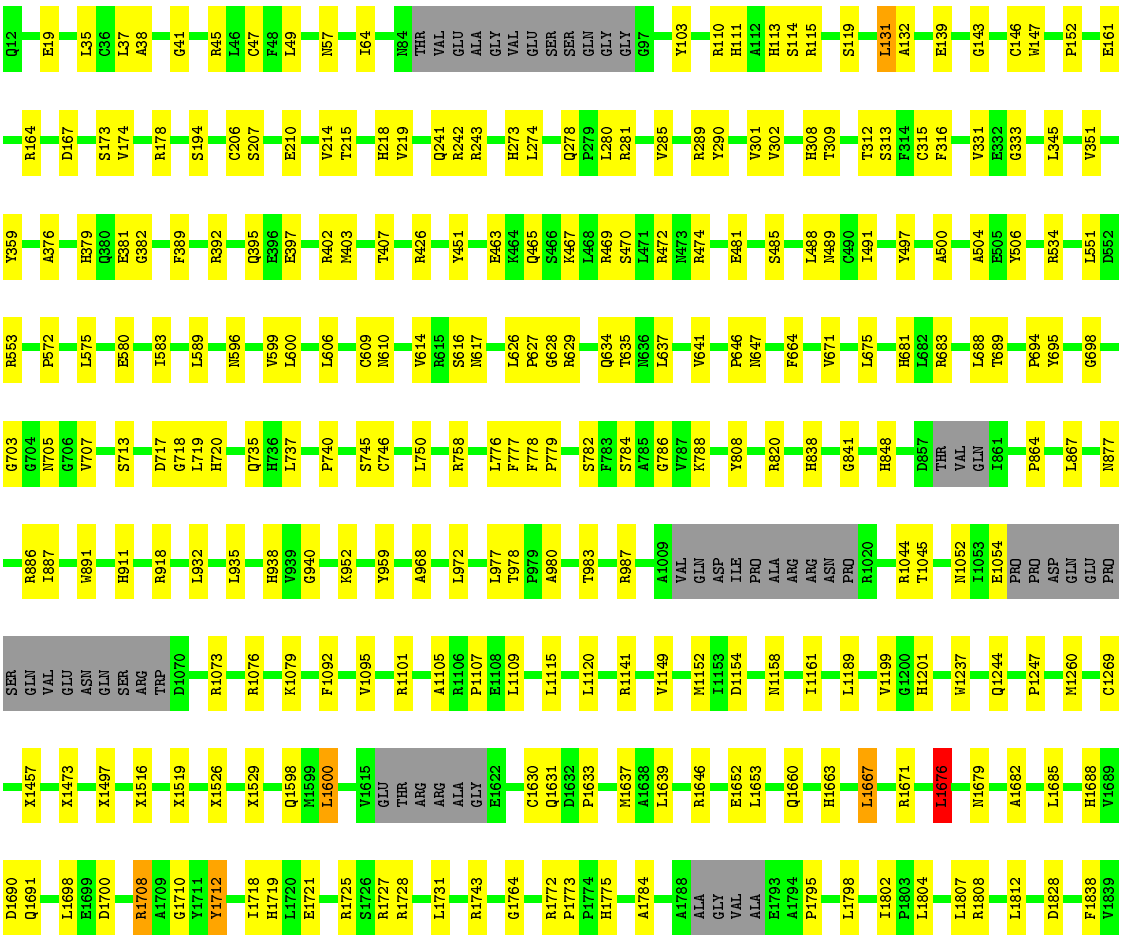
- Molecule 2: Ryanodine receptor 1

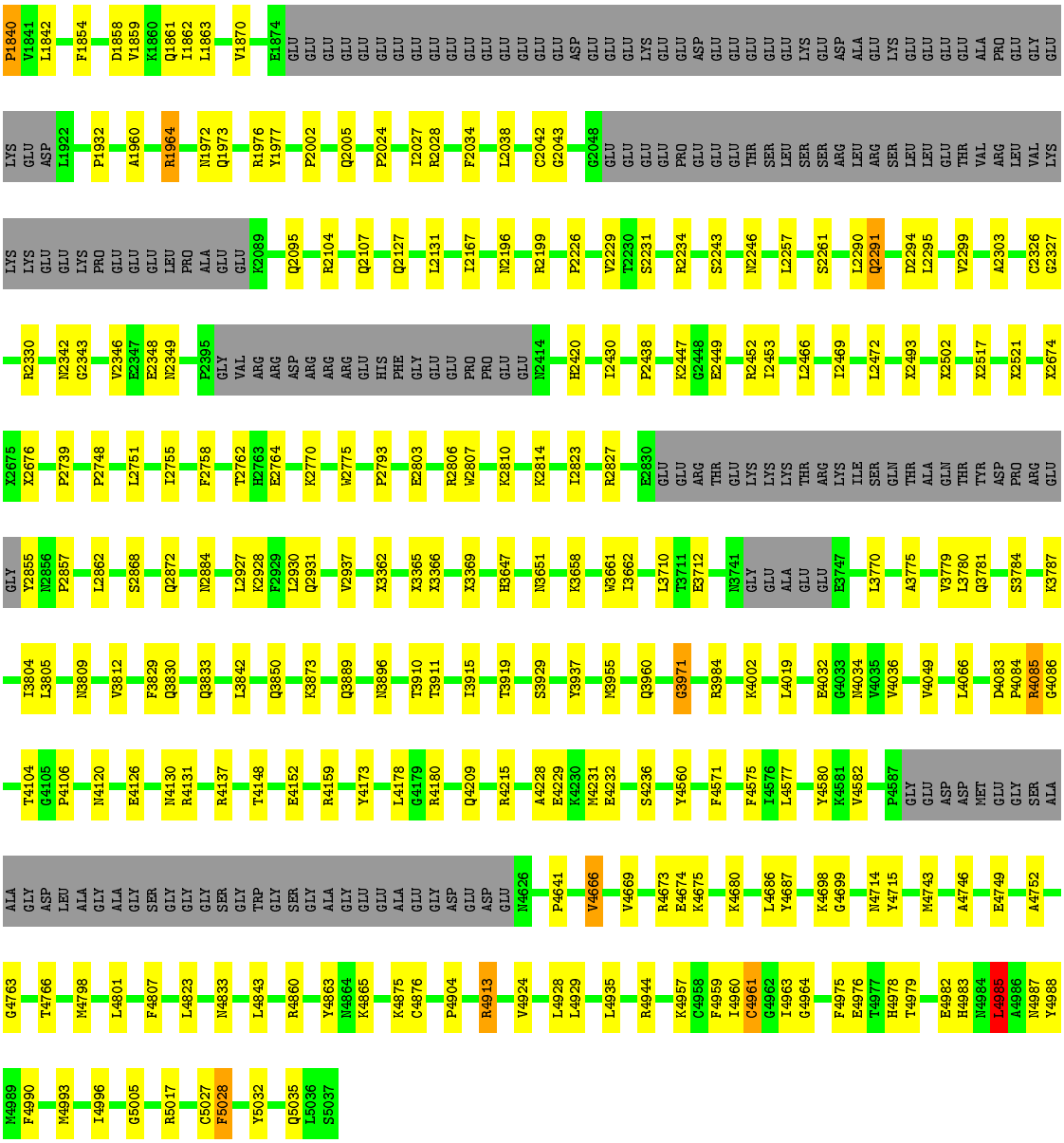




• Molecule 2: Ryanodine receptor 1

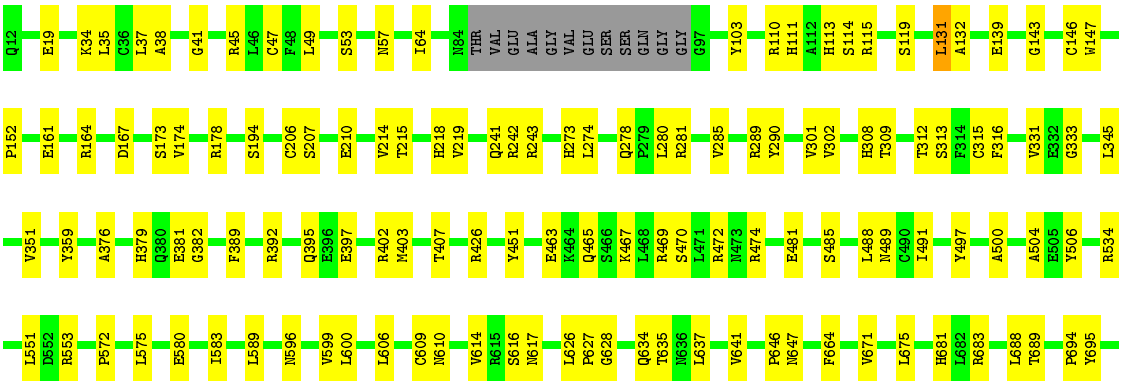
Chain I:

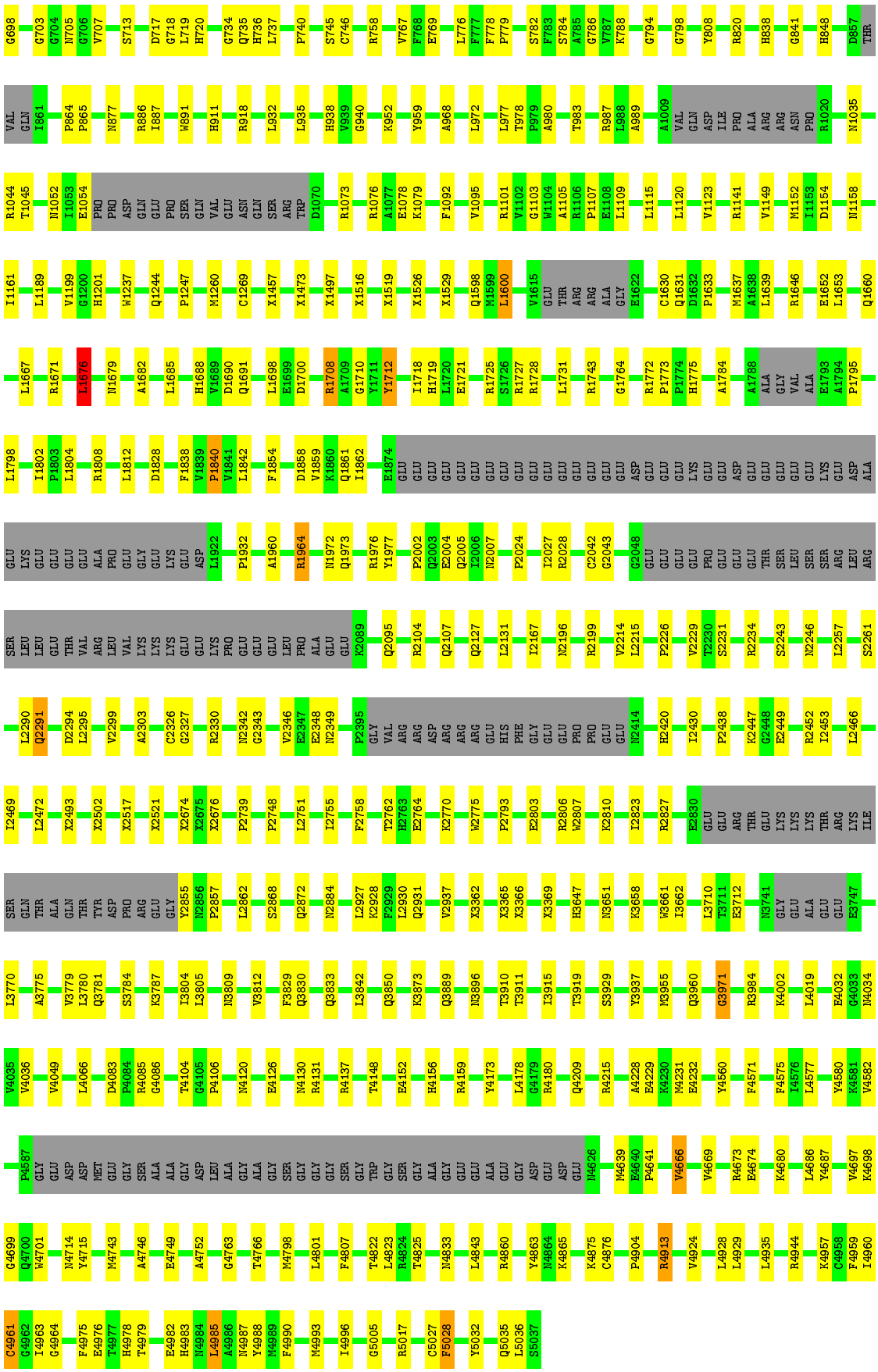




• Molecule 2: Ryanodine receptor 1

Chain G:





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	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.31	0/25428	0.55	9/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	9/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	34/142628 (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	17
2	E	0	17
2	G	0	17
2	I	0	17
All	All	0	72

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	131	LEU	CA-CB-CG	8.16	134.07	115.30
2	G	131	LEU	CA-CB-CG	8.16	134.07	115.30
2	B	131	LEU	CA-CB-CG	8.15	134.04	115.30
2	I	131	LEU	CA-CB-CG	8.13	133.99	115.30
2	E	4985	LEU	CA-CB-CG	7.48	132.50	115.30

There are no chirality outliers.

5 of 72 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	15	0
1	F	818	0	824	13	0
1	H	818	0	824	12	0
1	J	818	0	824	14	0
2	B	29499	0	24747	289	0
2	E	29499	0	24747	286	0
2	G	29499	0	24747	288	0
2	I	29499	0	24748	285	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	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

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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	102373	1167	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 1167 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:4975:PHE:O	2:B:4979:THR:HG23	1.85	0.77
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.85	0.76
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.86	0.76
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.86	0.76
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.78	0.71

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%)	98 (93%)	7 (7%)	0	100	100
1	F	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	H	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	J	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	52	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2892 (89%)	338 (10%)	5 (0%)	52	86
2	G	3235/4416 (73%)	2890 (89%)	340 (10%)	5 (0%)	52	86
2	I	3235/4416 (73%)	2889 (89%)	340 (10%)	6 (0%)	52	86
All	All	13360/18096 (74%)	11954 (90%)	1384 (10%)	22 (0%)	56	86

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
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	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
All	All	10324/12444 (83%)	10251 (99%)	73 (1%)	89	94

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	4137	ARG

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Mol	Chain	Res	Type
2	I	1076	ARG
2	G	4120	ASN
2	I	131	LEU
2	I	1600	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	3950	ASN
2	I	395	GLN
2	G	3896	ASN
2	E	3976	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	0.91	1 (3%)	26,52,52	1.59	2 (7%)
4	CFF	B	5102	-	8,15,15	2.55	3 (37%)	8,23,23	1.16	1 (12%)
3	ATP	E	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.58	2 (7%)
4	CFF	E	5102	-	8,15,15	2.55	3 (37%)	8,23,23	1.16	1 (12%)
3	ATP	G	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.59	2 (7%)
4	CFF	G	5102	-	8,15,15	2.54	3 (37%)	8,23,23	1.17	1 (12%)
3	ATP	I	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.59	2 (7%)
4	CFF	I	5102	-	8,15,15	2.55	3 (37%)	8,23,23	1.16	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	B	5102	CFF	C4-N3	-5.03	1.33	1.39
4	I	5102	CFF	C4-N3	-5.03	1.33	1.39
4	E	5102	CFF	C4-N3	-5.03	1.33	1.39
4	G	5102	CFF	C4-N3	-5.00	1.33	1.39
4	G	5102	CFF	C6-N1	-3.95	1.32	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5101	ATP	N3-C2-N1	-6.35	123.88	128.87
3	B	5101	ATP	N3-C2-N1	-6.33	123.90	128.87
3	I	5101	ATP	N3-C2-N1	-6.30	123.92	128.87
3	E	5101	ATP	N3-C2-N1	-6.29	123.93	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	5102	CFF	C14-N7-C8	-2.60	111.73	125.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
4	B	5102	CFF	1	0
3	E	5101	ATP	2	0
4	E	5102	CFF	1	0
3	G	5101	ATP	2	0
4	G	5102	CFF	1	0
3	I	5101	ATP	2	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	B	4345:UNK	C	4540:PHE	N	72.88
1	E	4345:UNK	C	4540:PHE	N	72.88
1	I	4345:UNK	C	4540:PHE	N	72.88
1	G	4345:UNK	C	4540:PHE	N	72.88
1	B	3613:UNK	C	3639:THR	N	43.44