wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 01:54 PM EDT

PDB ID	:	5T9N
EMDB ID:	:	EMD-8373
Title	:	Structure of rabbit RyR1 (Ca2+-only dataset, class 2)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-09
Resolution	:	3.80 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

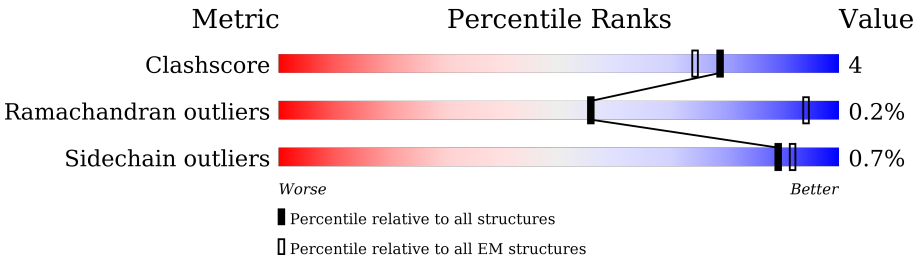
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.80 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	88% 11% .
1	F	108	88% 11% .
1	H	108	88% 11% .
1	J	108	88% 11% .
2	B	4676	81% 8% 11%
2	E	4676	81% 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)

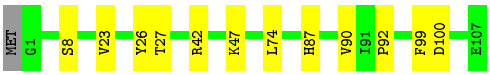
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

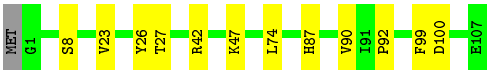
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



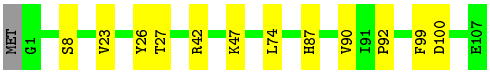
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



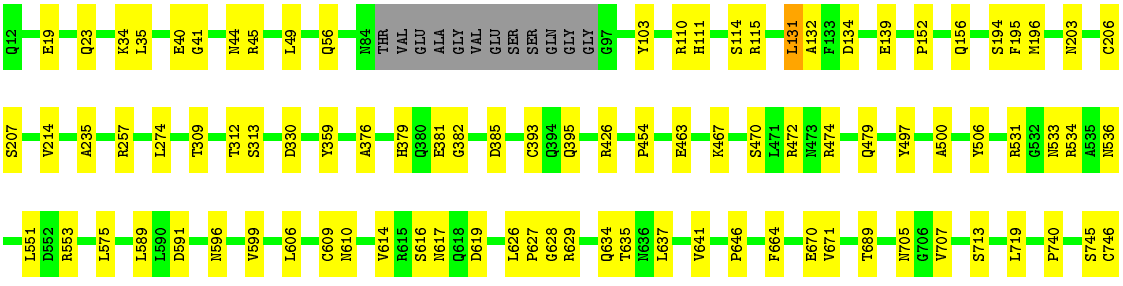
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

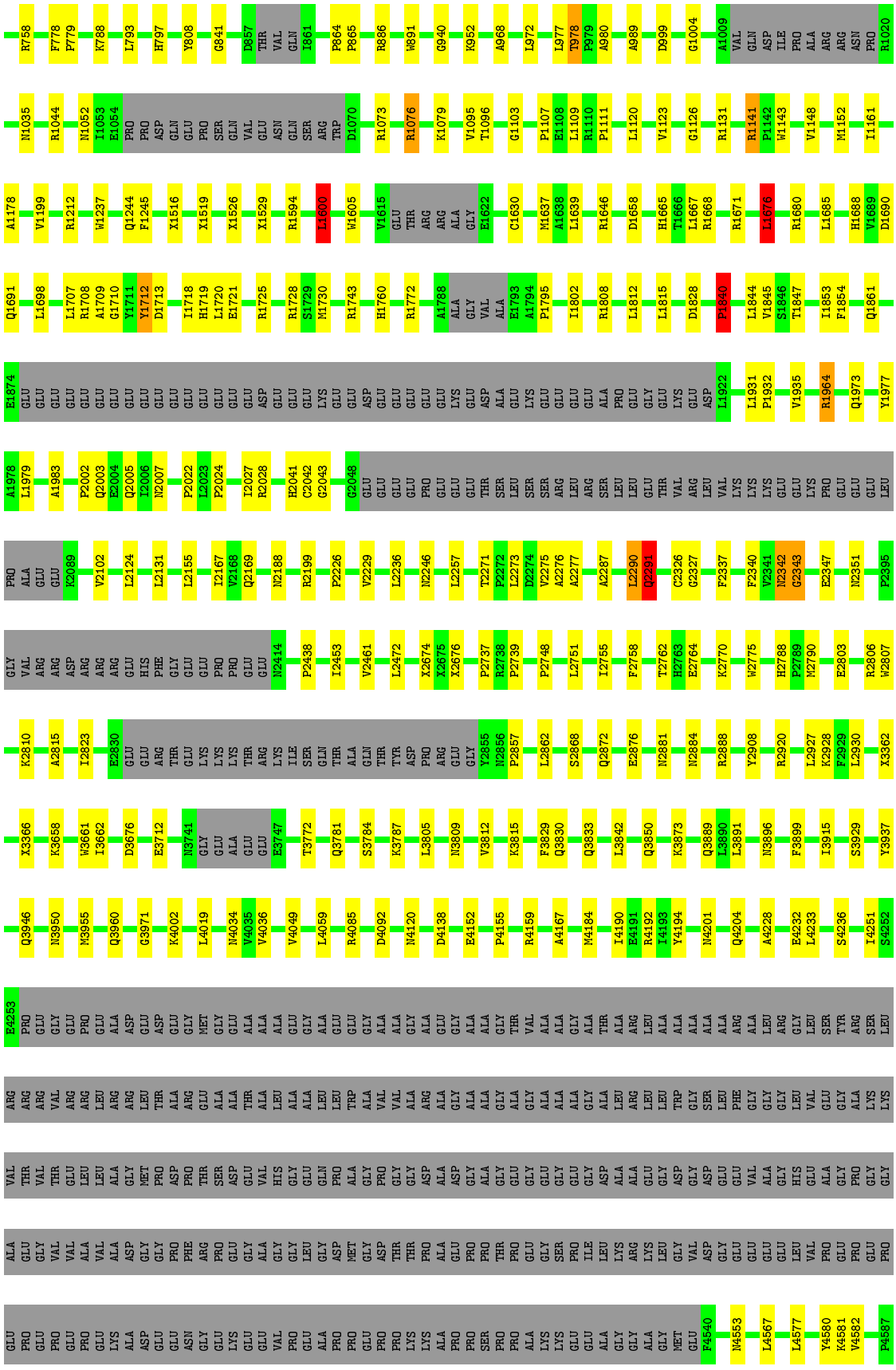
Chain J:

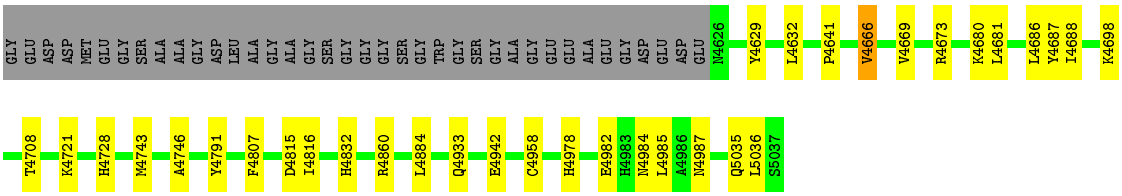


- Molecule 2: Ryanodine receptor 1

Chain B:

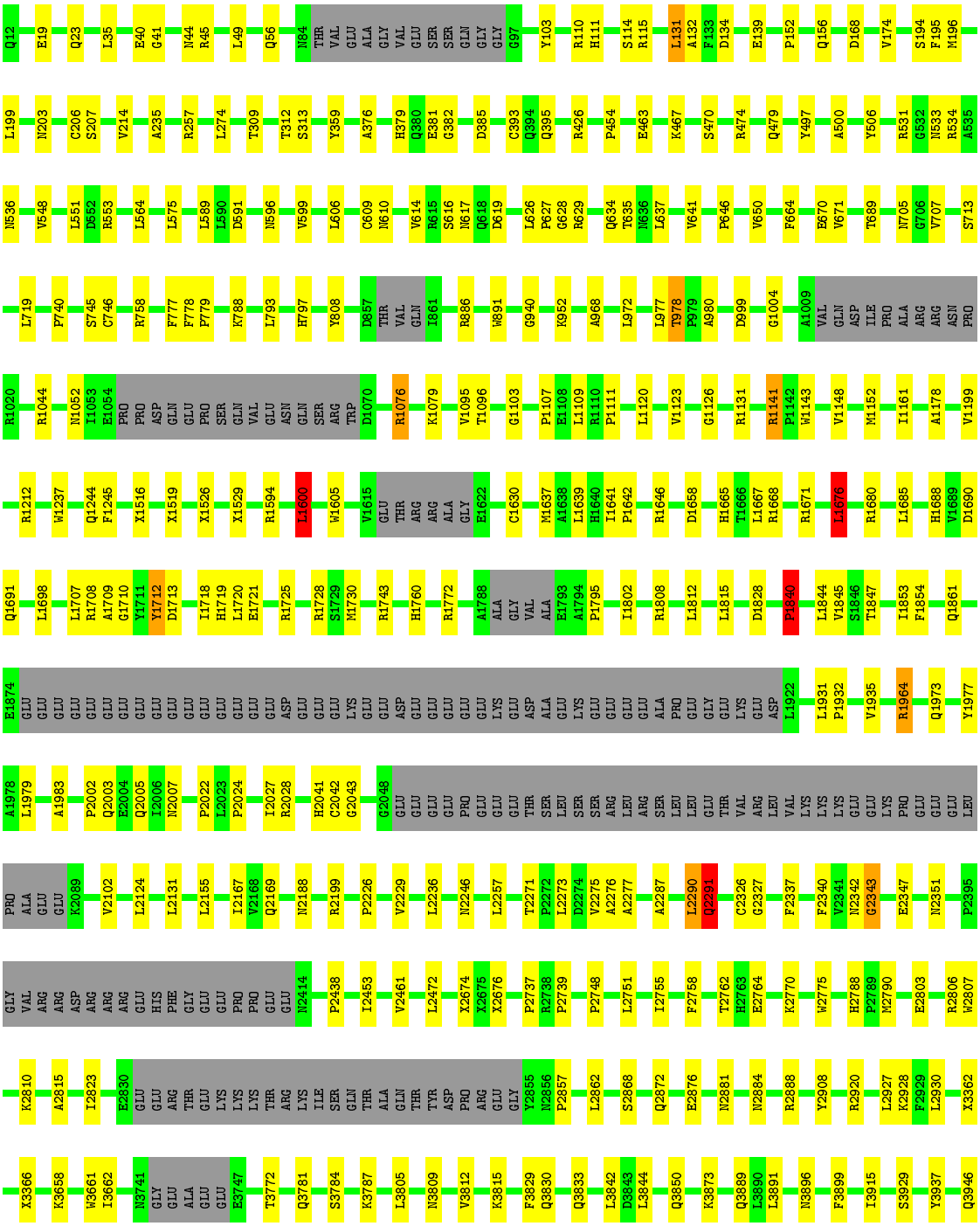


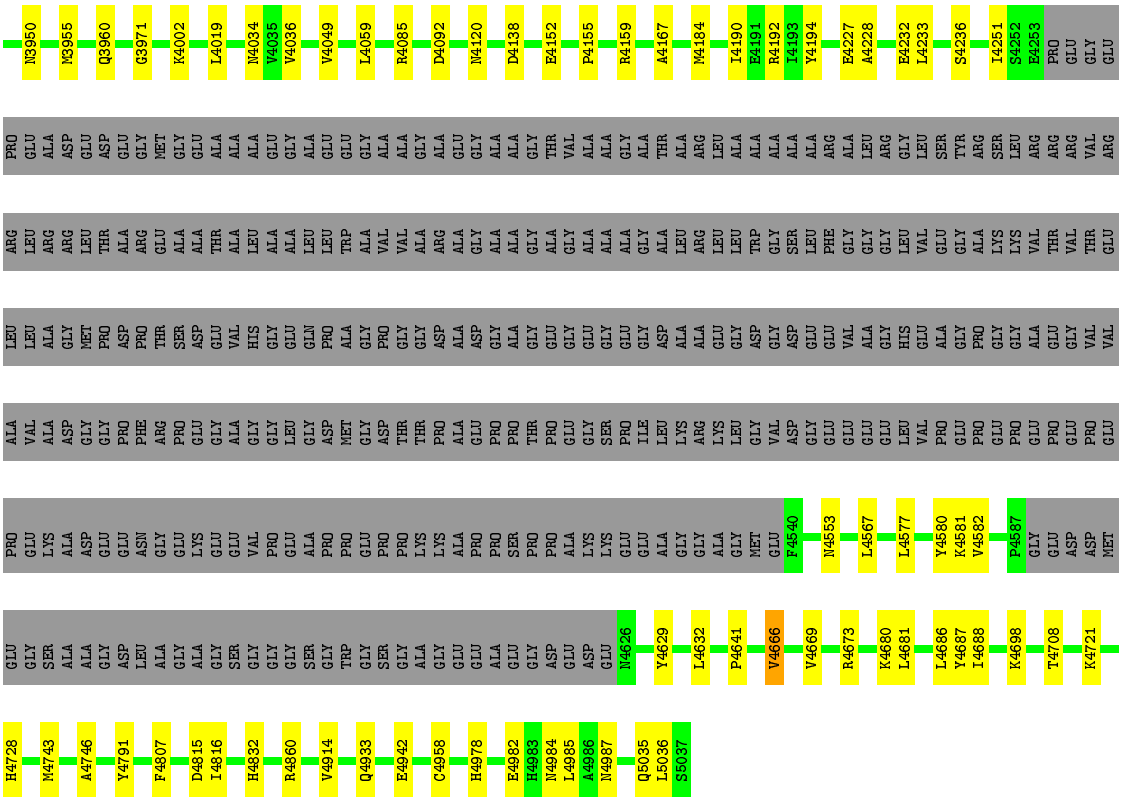




• Molecule 2: Ryanodine receptor 1

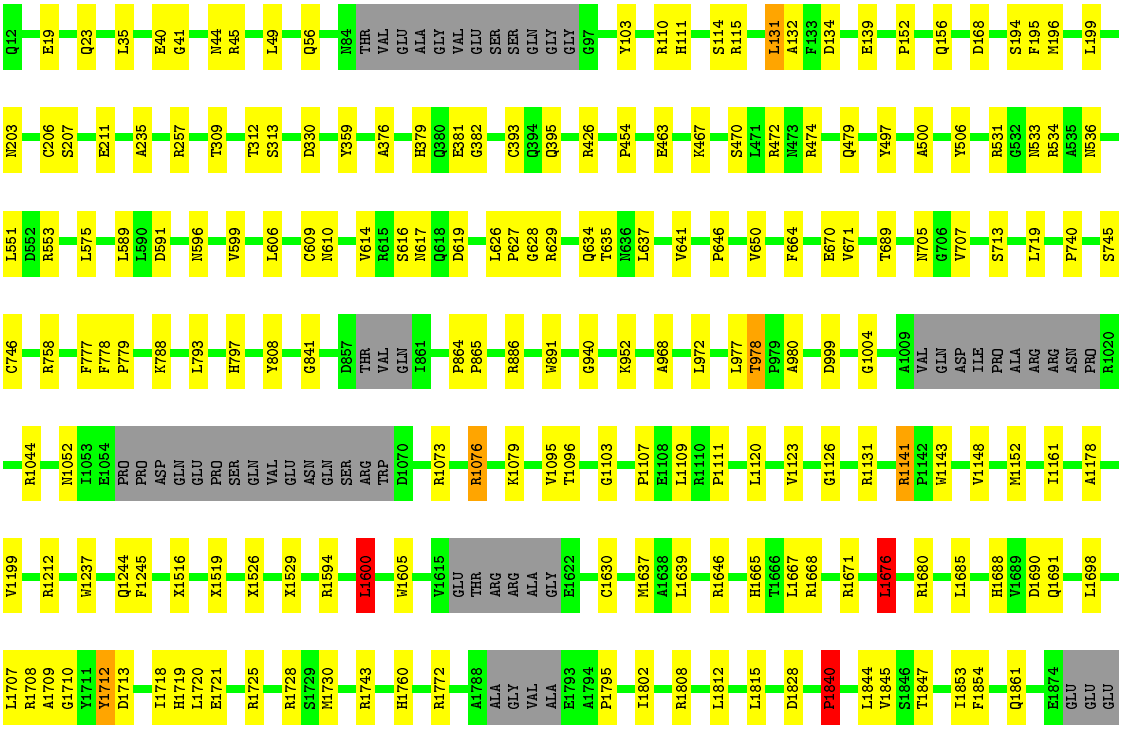
Chain E:

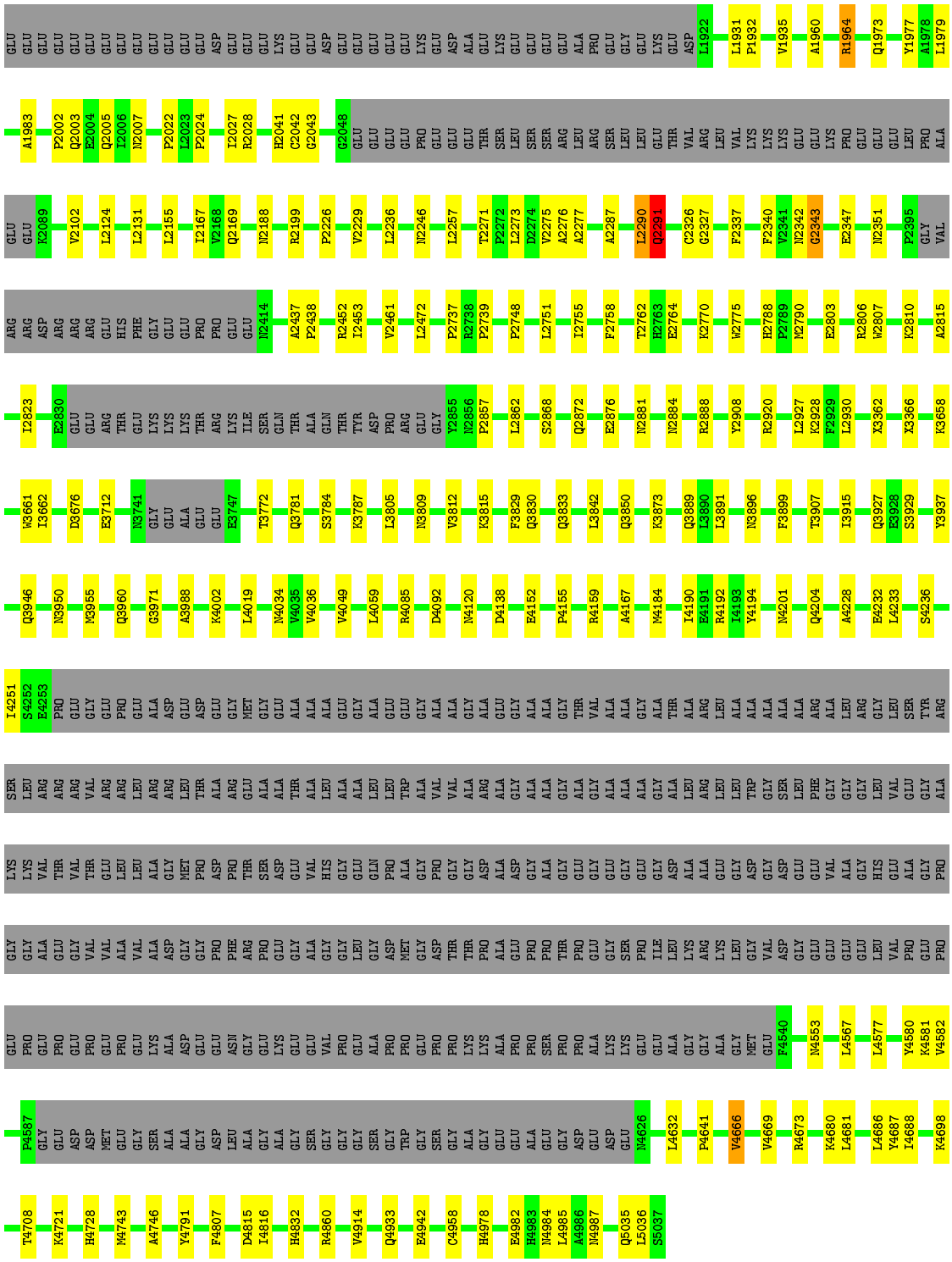




• Molecule 2: Ryanodine receptor 1

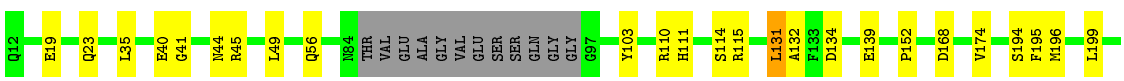
Chain I:

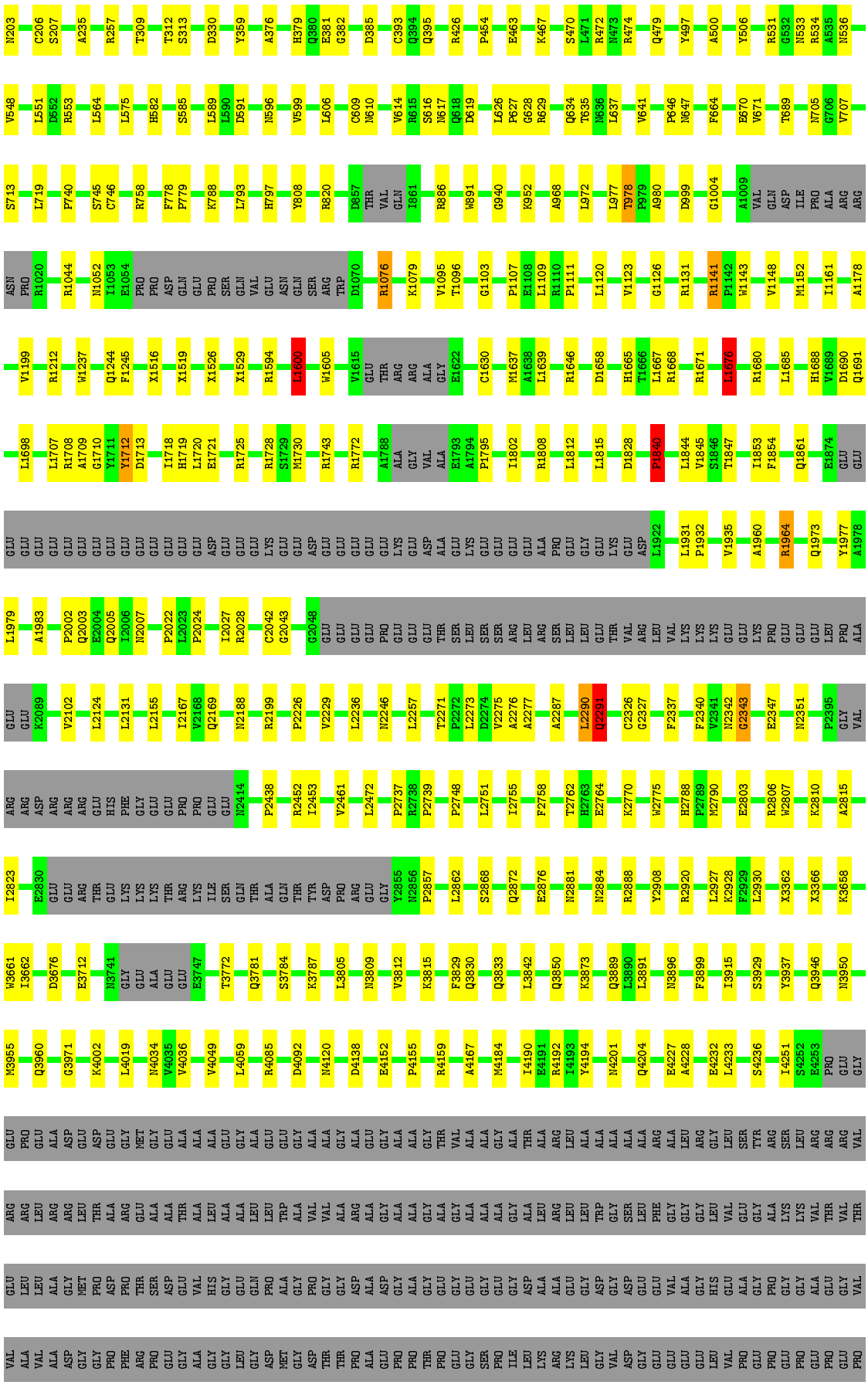


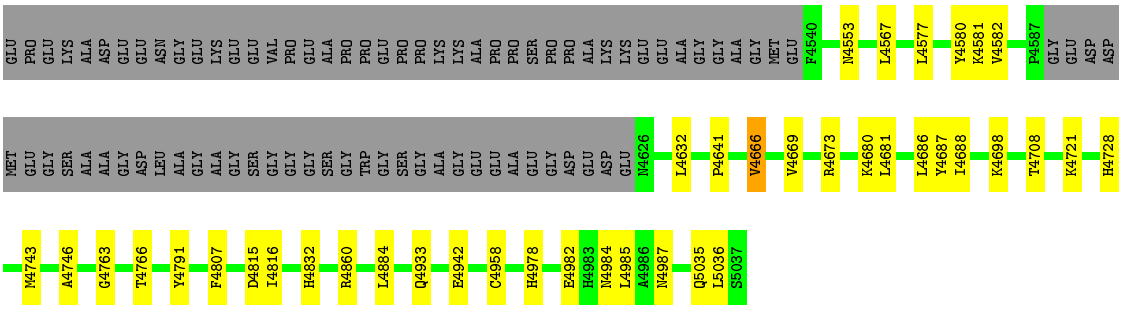


• Molecule 2: Ryanodine receptor 1

Chain G:






GLU PRO GLU LYS ALA ASP GLU GLU 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 M4553 L4567 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 L4632 P4641 V4666 V4669 R4673 K4680 L4681 L4686 Y4687 I4688 K4698 T4708 K4721 H4728
M4743 A4746 G4763 T4766 Y4791 F4807 D4815 I4816 H4832 R4860 L4884 Q4933 E4942 C4958 H4978 E4982 H4983 N4984 L4985 A4986 N4987 Q5035 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	0.52	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	8/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	32/142628 (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 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	131	LEU	CA-CB-CG	8.36	134.52	115.30
2	B	131	LEU	CA-CB-CG	8.34	134.49	115.30
2	I	131	LEU	CA-CB-CG	8.34	134.49	115.30
2	G	131	LEU	CA-CB-CG	8.34	134.49	115.30
2	I	1600	LEU	CA-CB-CG	6.97	131.32	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	6	0
1	F	818	0	824	7	0
1	H	818	0	824	6	0
1	J	818	0	824	6	0
2	B	29369	0	24723	198	0
2	E	29369	0	24722	194	0
2	G	29369	0	24722	196	0
2	I	29369	0	24722	198	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	102185	789	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 789 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:4958:CYS:SG	2:G:4978:HIS:CD2	2.67	0.87
2:I:4958:CYS:SG	2:I:4978:HIS:CD2	2.67	0.87
2:E:4958:CYS:SG	2:E:4978:HIS:CD2	2.67	0.87
2:B:4958:CYS:SG	2:B:4978:HIS:CD2	2.67	0.87
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.75	0.68

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%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	52	86
2	E	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	52	86
2	G	3235/4676 (69%)	2898 (90%)	331 (10%)	6 (0%)	52	86
2	I	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	52	86
All	All	13360/19136 (70%)	11967 (90%)	1369 (10%)	24 (0%)	56	86

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

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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%)	2476 (99%)	17 (1%)	88	95
2	E	2493/3202 (78%)	2476 (99%)	17 (1%)	88	95
2	G	2493/3202 (78%)	2476 (99%)	17 (1%)	88	95
2	I	2493/3202 (78%)	2476 (99%)	17 (1%)	88	95
All	All	10324/13164 (78%)	10256 (99%)	68 (1%)	89	95

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

Mol	Chain	Res	Type
2	E	3896	ASN
2	I	978	THR
2	G	3787	LYS
2	E	4034	ASN
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	2127	GLN

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Mol	Chain	Res	Type
2	I	156	GLN
2	G	2127	GLN
2	E	3896	ASN
2	E	4120	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	I	3613:UNK	C	3639:THR	N	43.02
1	B	3613:UNK	C	3639:THR	N	43.01
1	E	3613:UNK	C	3639:THR	N	43.01
1	G	3613:UNK	C	3639:THR	N	42.96
1	B	3163:UNK	C	3170:UNK	N	16.39