



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:09 pm GMT

PDB ID : 5TB2
EMDB ID: : EMD-8393
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-11
Resolution : 4.60 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

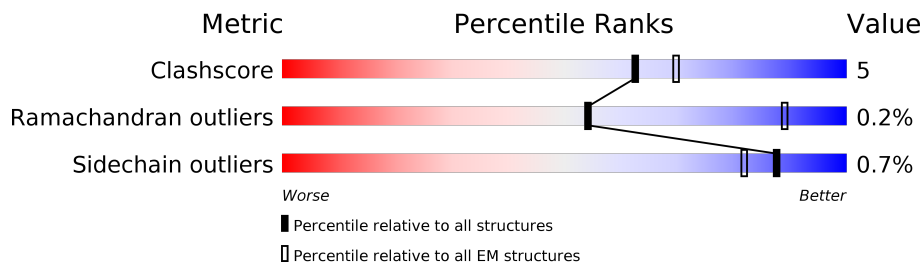
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	108	87% 12% .
1	F	108	87% 12% .
1	H	108	87% 12% .
1	J	108	90% 9% .
2	B	4416	84% 11% 5%
2	E	4416	84% 11% 5%
2	G	4416	84% 11% 5%
2	I	4416	84% 11% 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	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		
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


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: 




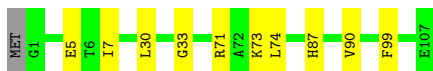
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




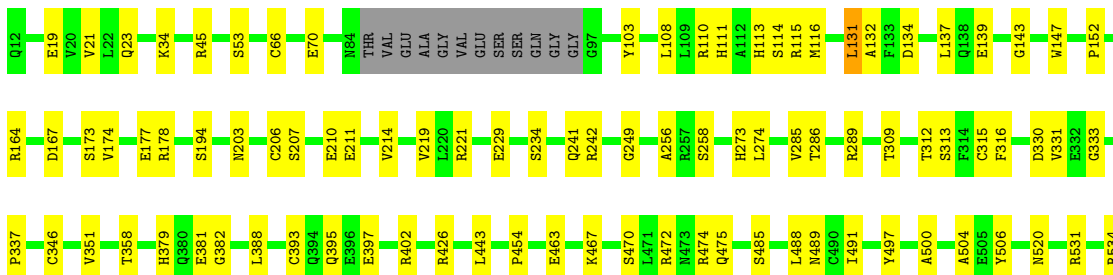
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



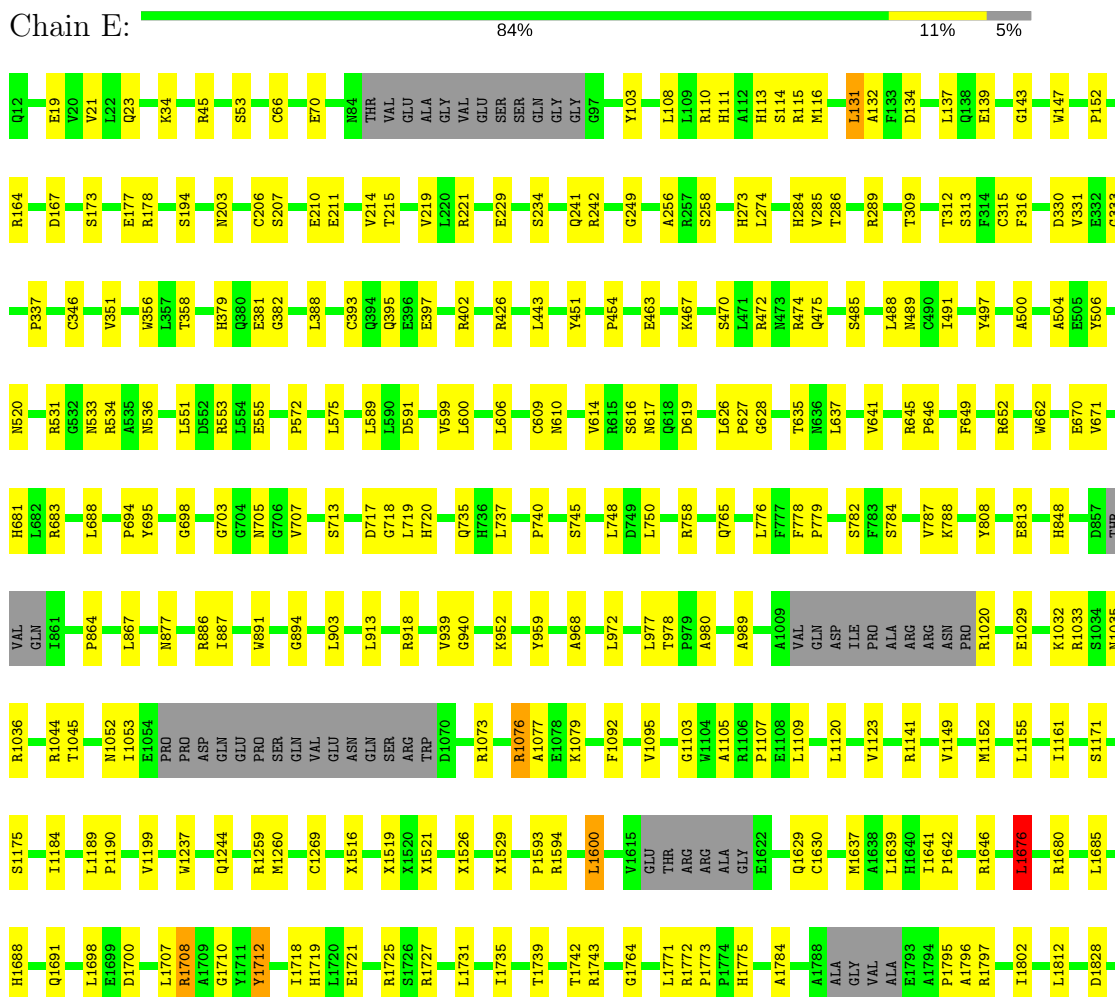
- Molecule 2: Ryanodine receptor 1

Chain B: 







Y4888	Gly	P4155	Q3833	L2930	K2770	G2343	Q2095	P2002	GLU	L1720	M1260	ASP	R886	G698
14897	ALA	R4180	L3842	X3362	W2775	V2346	R2104	Q2003	GLU	E1721	C1269	GLN	1887	G703
14901	GLU	14181	L3842	X3362	S2776	E2347	Q2107	E2004	GLU	R1725	PRD	SER	W891	G704
P4904	ALA	14190	Q3850	X3365	H2788	E2348	Q2121	Q2006	GLU	S1726	X1516	GLN	G894	N705
R4913	GLU	E4191	X3873	X3366	E2803	W2351	F2121	Q2007	GLU	R1727	X1519	VAL	7707	G706
A4930	ASP	R4192	Q3889	X3369	E2806	L2368	Q2127	P2024	GLU	L1731	X1520	GLU	L903	S713
A4930	ASP	Y4194	N3651	L2376	W2807	L2376	L2131	R2028	GLU	11735	X1521	ASN	L913	D717
Q4933	ASP	S4198	N3896	P2395	K2810	P2395	T2143	Q2029	GLU	T1739	X1526	ARG	R918	G718
G4934	GLU	N4201	F3899	GLY	E2823	VAL	T2167	D2033	GLU	T1742	X1529	TRP	V939	H720
R4944	GLU	E4227	T3907	ARG	E2830	ARG	K2189	C2042	GLU	R1743	P1593	R1073	G940	G734
D4945	GLU	A4228	L3662	ASP	GLU	ARG	Q2192	G2043	GLU	G1764	R1594	R1076	X952	H735
F4959	GLU	E4229	D3675	ARG	GLU	ASP	Q2196	G2048	GLU	L1771	L1600	A1077	Y959	L737
14960	GLU	K4230	E3712	ARG	GLU	ARG	R2199	GLU	GLU	R1772	Y1615	E1078	A969	P740
G4961	GLU	Y4231	Y3725	GLU	THR	ARG	HIS	GLU	GLU	P1774	THR	K1079	P758	H758
G4962	GLU	E4232	Y3725	GLU	GLU	GLU	PHE	GLU	GLU	H1775	ARG	F1092	L972	S745
14963	GLU	S4236	Q3946	GLU	LYS	GLU	GLY	GLU	GLU	A1764	ALA	V1095	L977	L748
F4968	GLU	E4239	N3950	GLU	THR	GLU	L2215	GLU	GLU	A1768	GLY	G1103	T978	D749
H4978	GLU	L4567	N3741	GLY	ARG	GLU	N2246	THR	GLU	ALA	E1622	W1104	P979	L750
E4981	GLU	F4571	GLU	GLU	LYS	PRO	L2265	GLU	GLU	VAL	Q1629	A1105	A980	R758
H4982	GLU	F4575	GLU	GLU	ILE	PRO	L2265	GLU	GLU	VAL	C1630	A1106	A989	Q765
H4983	GLU	F4575	GLU	GLU	THR	GLU	T2271	ARG	ASP	E1793	M1637	E1108	V1009	L776
L4985	GLU	V4582	E3747	GLU	ALA	GLU	P2272	LEU	ALA	A1794	A1638	L1109	VAL	F777
A4986	GLU	P4586	N3758	GLU	GLN	P2438	L2273	ARG	GLU	P1795	L1639	L1120	GLN	F778
Y4987	GLU	P4587	N3758	GLU	THR	R2452	D2274	ARG	LYS	A1796	R1646	V1123	ILE	P779
Y4988	GLU	GLY	K3762	GLU	ASP	R2453	V2275	LEU	GLU	R1797	L1676	VAL	PRO	Q765
T5004	ASP	L4031	Q3766	PRO	PRO	L2466	E2285	GLU	GLU	I1802	L1676	R1141	ALA	S782
G5005	ASP	N4034	Q3766	ARG	ARG	L2466	L2286	THR	GLU	L1812	R1680	V1149	ARG	V787
G5006	GLY	V4035	R3769	GLU	GLU	L2469	L2290	VAL	ALA	D1828	L1685	VAL	ASN	K788
E5007	GLY	L4068	R3769	GLU	GLU	L2472	Q2291	LEU	GLU	L1838	L1688	M1152	PRO	Y808
Y5014	SER	T4071	T3772	ASP	Y2855	L2472	D2294	VAL	GLY	F1838	H1688	L1155	R1020	Y808
R5017	ALA	14071	V3779	PRO	S2868	X2517	L2295	LYS	LYS	V1839	Q1691	I1161	E1029	E813
C5018	ALA	R4085	L3780	ARG	Q2872	X2521	C2326	LYS	GLU	V1841	Q1691	I1161	K1032	H848
Y5019	ASP	X3787	E2880	GLU	E2880	X2521	C2326	GLU	ASP	L1842	E1699	I1161	R1033	R848
D5026	LEU	Q4102	E2880	GLU	E2880	P2739	G2327	LYS	LYS	L1842	E1699	I1161	R1033	R848
C5027	ALA	N4120	H2883	GLU	H2883	P2748	R2330	PRO	P1932	V1859	D1700	L1184	R1035	D857
F5028	GLY	L3805	N2884	GLU	N2884	P2748	R2331	GLU	GLU	K1860	L1707	L1189	R1036	THR
Y5032	GLY	F4125	L2894	GLU	L2894	L2751	L2332	GLU	K1936	K1861	R1708	P1190	R1044	VAL
L5036	GLY	F4128	H2902	GLU	H2902	L2751	L2335	LEU	C1940	L1863	A1709	V1199	T1045	1861
S5037	GLY	F4132	V2906	GLU	V2906	L2751	L2335	ALA	A1960	L1864	G1710	V1199	R1044	P864
E4871	GLY	L3817	L2927	GLU	L2927	F2758	F2337	GLU	R1964	M1865	Y1712	V1237	M1052	L867
C4876	TRP	Q3830	L2927	GLU	L2927	T2762	F2340	GLU	R1964	V1870	I1718	Q1244	E1054	L867
							N2342	GLU	P2001	E1874	H1719	R1259	PRD	N877

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.52	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	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	33/142628 (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	17
2	E	0	17
2	G	0	16
2	I	0	16
All	All	0	66

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.36	134.52	115.30
2	G	131	LEU	CA-CB-CG	8.35	134.51	115.30
2	B	131	LEU	CA-CB-CG	8.34	134.48	115.30
2	E	131	LEU	CA-CB-CG	8.33	134.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1676	LEU	CA-CB-CG	6.33	129.86	115.30

There are no chirality outliers.

5 of 66 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	312	THR	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide

5.2 Too-close contacts

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	8	0
1	F	818	0	824	8	0
1	H	818	0	824	8	0
1	J	818	0	824	5	0
2	B	29499	0	24751	284	0
2	E	29499	0	24751	290	0
2	G	29499	0	24751	288	0
2	I	29499	0	24751	286	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
All	All	121272	0	102300	1147	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 1147 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:E:4190:ILE:CD1	2:E:5026:ASP:OD2	1.77	1.33
2:I:4190:ILE:CD1	2:I:5026:ASP:OD2	1.76	1.33
2:G:4190:ILE:CD1	2:G:5026:ASP:OD2	1.77	1.32
2:B:4190:ILE:CD1	2:B:5026:ASP:OD2	1.76	1.31
2:B:4190:ILE:HD11	2:B:5026:ASP:OD2	1.31	1.26

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%)	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	3235/4416 (73%)	2892 (89%)	335 (10%)	8 (0%)	51	85
2	E	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	51	85
2	G	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	51	85
2	I	3235/4416 (73%)	2891 (89%)	336 (10%)	8 (0%)	51	85
All	All	13360/18096 (74%)	11941 (89%)	1387 (10%)	32 (0%)	54	85

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	I	5028	PHE
2	E	5028	PHE
2	G	5028	PHE
2	B	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%)	2474 (99%)	19 (1%)	85	92
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	85	92
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	85	92
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	85	92
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	87	93

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	4201	ASN
2	E	1141	ARG
2	G	4085	ARG
2	I	4959	PHE
2	E	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	3960	GLN
2	E	273	HIS
2	G	3781	GLN
2	I	4034	ASN
2	I	4553	ASN

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 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 [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	73.35
1	I	4345:UNK	C	4540:PHE	N	73.35
1	E	4345:UNK	C	4540:PHE	N	73.35
1	G	4345:UNK	C	4540:PHE	N	73.35

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	45.90