



## wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 02:36 PM EDT

PDB ID : 5TB1  
EMDB ID: : EMD-8392  
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 1)  
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.  
Deposited on : 2016-09-10  
Resolution : 4.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

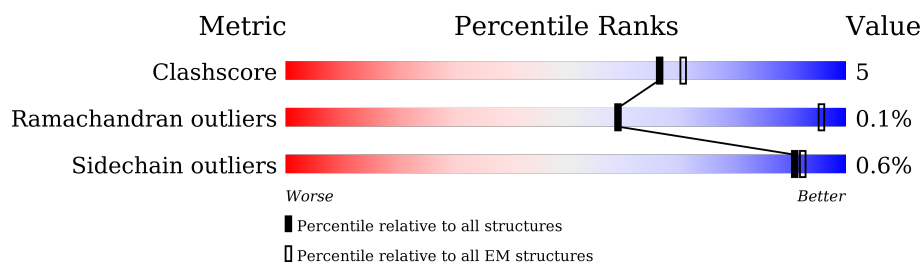
# 1 Overall quality at a glance

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	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  $\geq 3$ , 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	74% 25% .
1	F	108	73% 26% .
1	H	108	76% 23% .
1	J	108	77% 22% .
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		

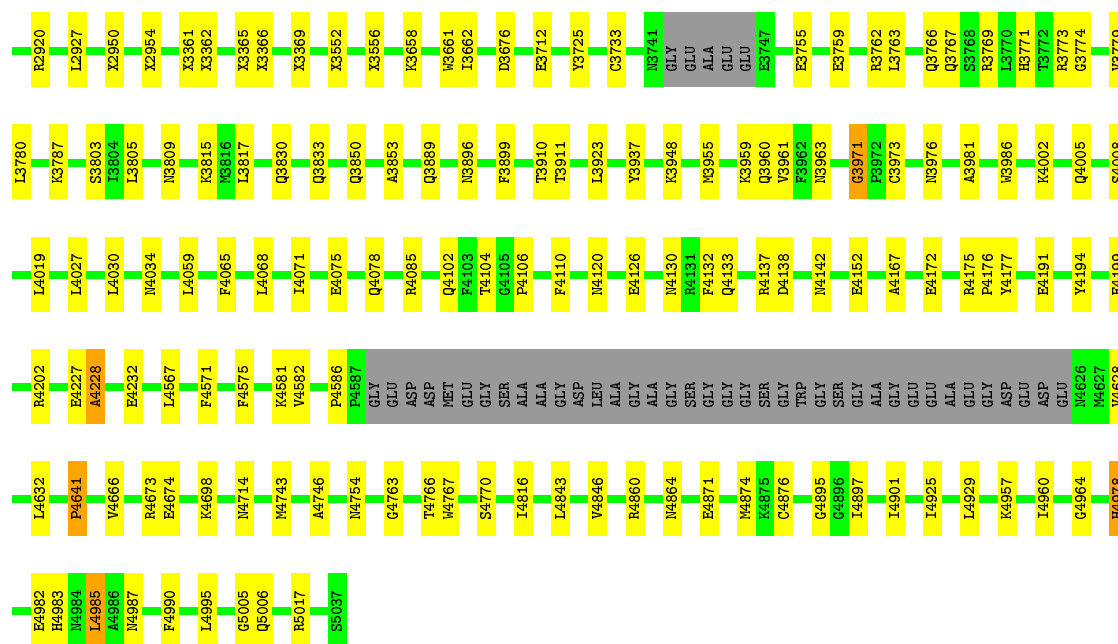
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	



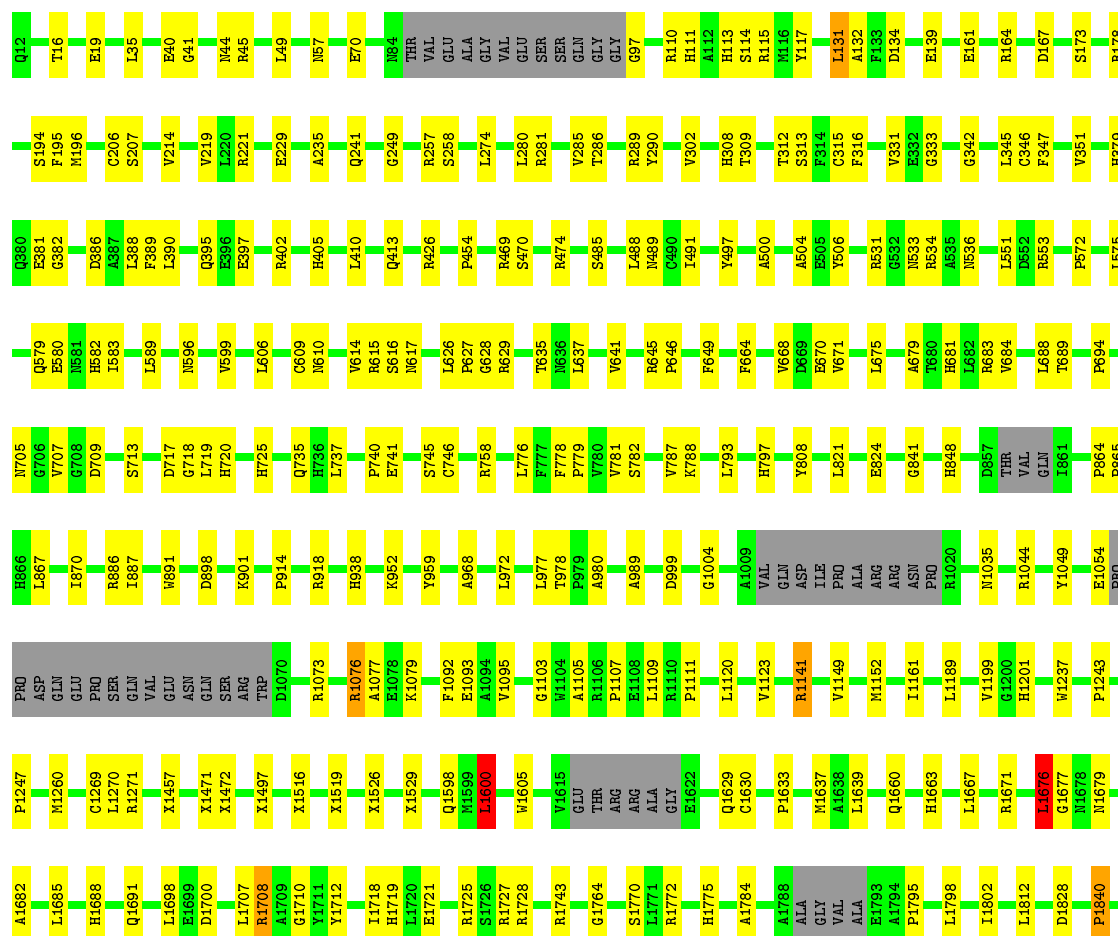




• Molecule 2: Ryanodine receptor 1

Chain E: 84% 11% 5%







I4987	R4673	F4551	I4059	Q3830	X3365	K2810	R2104	Q2003	GLU	L1707	X1457	TRP	H891	D709
F4990	E4674	L4567	F4065	Q3833	X3366	K2814	Q2107	E2004	GLU	R1708	X1471	D1070	H891	S713
L4995	K4698	F4571	F4068	Q3850	X3369	A2815	F2121	I2006	GLU	G1710	X1472	R1073	D898	D717
G5005	I4714	F4575	I4071	Q3853	X3552	I2823	Q2127	I2007	GLU	Y1711	X1497	R1076	K901	G718
Q5006	K4743	K4581	E4075	Q3889	X3556	E2830	Q2131	P2022	GLU	A1077	X1516	A1077	H938	L719
R5017	A4746	V4582	E4078	Q3896	K3658	GLU	L2155	P2024	ASP	K1079	X1519	K1079	K952	H720
S5037	I4754	P4586	Q4078	Q3899	K3661	THR	L2155	R2028	GLU	F1092	X1526	E1093	K959	H725
	G4763	P4587	R4085	F3910	I3662	GLU	K2188	C2042	LYS	E1093	X1526	A1094	Y959	O735
	E4763	GLY	Q4102	T3911	I3676	THR	K2189	G2043	GLU	V1095	X1529	V1095	A968	L737
	K4767	ASP	F4103	T3911	E3712	LYS	Y2192	G2048	GLU	G1103	Q1598	G1103	L972	P740
	S4770	NET	T4104	L3923	E3712	THR	K2208	GLU	GLU	A1104	R1599	A1104	L972	E741
	G4770	GLY	G4105	Y3937	X3725	LYS	P2226	GLU	GLU	A1105	R1600	R1106	L977	S745
	I4816	GLY	P4106	Y3937	I3741	LYS	Y2229	GLU	GLU	P1107	W1605	P1107	P979	C746
	L4843	ALA	F4110	K3948	GLY	ILE	H2253	GLU	LYS	L1109	V1615	L1109	A980	R758
	R4860	GLY	I4120	Y3955	ALA	THR	H2253	GLU	ASP	R1110	THR	R1110	A989	L776
	M4864	LEU	E4126	K3959	GLU	GLN	L2257	THR	ALA	P1111	ARG	P1111	D999	F777
	E4871	ALA	I4130	Q3960	GLY	THR	S2261	SER	LYS	L1120	ARG	L1120	G1004	F778
	K4871	ALA	R4131	Y3961	GLY	TYR	E2261	SER	GLY	V1123	GLY	V1123	P779	W780
	G4875	GLY	F4132	Y3962	ASP	ASP	P2272	LEU	GLU	R1141	E1622	R1141	W781	W781
	C4876	GLY	D4138	Y3963	ARG	GLY	Y2275	ARG	GLU	Q1629	C1630	Q1629	S782	
	R4892	TRP	E4152	Y3976	GLY	GLY	Y2290	LEU	ALA	C1630	C1630	C1630	VAL	
	L4897	GLY	A4167	Y3981	I3767	GLY	Q2291	THR	VAL	L1798	M1637	M1637	GLN	
	I4901	GLY	E4172	Y3984	S3768	I2881	D2294	VAL	ASP	S1175	Q1660	S1175	PRO	Y809
	L4925	ALA	R4175	Y3985	I3770	I2884	L2295	VAL	PRO	L1189	R1671	L1189	ASP	L821
	L4928	GLY	P4176	Y3986	T3772	K2888	C2326	LYS	GLY	P1190	R1671	P1190	ILE	
	L4929	GLY	Y4177	K4002	K3773	L2884	G2327	LYS	GLY	R1671	R1671	R1671	ALA	L793
	K4957	ALA	E4191	Q4005	G3774	L2894	N2342	LYS	LYS	L1637	L1637	L1637	ARG	H797
	L4960	GLY	Y4194	Q4008	V3779	H2902	G2343	GLU	ASP	L1802	Q1660	S1175	ASN	
	G4964	ASP	E4199	Y4019	I3780	Y2908	E2347	GLU	GLU	L1812	Q1660	S1175	PRO	Y809
	H4973	GLY	R4202	L4027	S3803	R2920	N2351	LYS	LYS	D1828	R1671	L1189	M1035	L821
	K4978	V4627	E4227	L4030	I3804	L2927	G2343	GLU	GLU	P1932	R1671	P1190	R1044	E824
	L4982	V4628	A4228	Y4034	L3805	X2950	E2347	PRO	PRO	Y1935	L1677	H1201	E1054	
	H4983	L4632	E4232	I4034	I3809	X2954	N2351	GLU	GLU	V1935	L1677	H1201	PRO	H848
	I4984	P4641	E4232	Y4053	K3815	X3361	E2381	LEU	LEU	Q1973	L1685	P1243	ASP	D857
	L4985	V4666	Q4547	E4056	I3816	X3361	L2376	ALA	ALA	Q1973	L1685	P1247	GLN	THR
	J4986				L3817	X3362	L2376	GLU	GLU	Y1977	H1688	P1247	PRO	VAL
							E2381	GLU	GLU	GLU	Q1691	M1260	GLN	L861
							E2803	GLU	GLU	GLU	Q1691	M1260	VAL	P864
							R2806	GLU	GLU	GLU	L1698	C1269	ASN	L867
							R2807	GLU	GLU	GLU	E1699	L1270	ASN	
								Q2095	GLU	GLU	D1700	L1271	SER	R886
									P2002	GLU			ARG	L887

## 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	0.30	0/834	0.52	0/1123
1	F	0.30	0/834	0.52	0/1123
1	H	0.30	0/834	0.53	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.29	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.29	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	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
2	B	0	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	64

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.01	133.72	115.30
2	B	131	LEU	CA-CB-CG	8.00	133.69	115.30
2	E	131	LEU	CA-CB-CG	7.99	133.68	115.30
2	I	131	LEU	CA-CB-CG	7.99	133.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4985	LEU	CA-CB-CG	7.25	131.97	115.30

There are no chirality outliers.

5 of 64 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	16	0
1	F	818	0	824	18	0
1	H	818	0	824	15	0
1	J	818	0	824	14	0
2	B	29499	0	24746	268	0
2	E	29499	0	24746	273	0
2	G	29499	0	24746	261	0
2	I	29499	0	24746	262	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	102280	1100	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 1100 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:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.68
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.67
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.67
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.66
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.61	0.65

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%)	92 (88%)	13 (12%)	0	100	100
1	F	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	H	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	J	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	B	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	56	90
2	E	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	56	90
2	G	3235/4416 (73%)	2887 (89%)	344 (11%)	4 (0%)	56	90
2	I	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	56	90
All	All	13360/18096 (74%)	11919 (89%)	1425 (11%)	16 (0%)	59	90

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	1932	PRO

### 5.3.2 Protein sidechains ⓘ

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%)	2477 (99%)	16 (1%)	90	95
2	E	2493/3022 (82%)	2477 (99%)	16 (1%)	90	95
2	G	2493/3022 (82%)	2477 (99%)	16 (1%)	90	95
2	I	2493/3022 (82%)	2477 (99%)	16 (1%)	90	95
All	All	10324/12444 (83%)	10260 (99%)	64 (1%)	91	95

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	4120	ASN
2	E	1076	ARG
2	G	4085	ARG
2	I	4978	HIS
2	E	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	3950	ASN
2	E	413	GLN
2	G	3946	GLN
2	I	3963	ASN
2	I	4142	ASN

### 5.3.3 RNA ⓘ

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	73.36
1	I	4345:UNK	C	4540:PHE	N	73.36
1	E	4345:UNK	C	4540:PHE	N	73.36
1	G	4345:UNK	C	4540:PHE	N	73.36

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	46.46