



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:12 pm GMT

PDB ID : 5TAY
EMDB ID: : EMD-8389
Title : Structure of rabbit RyR1 (ryanodine dataset, class 2)
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/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

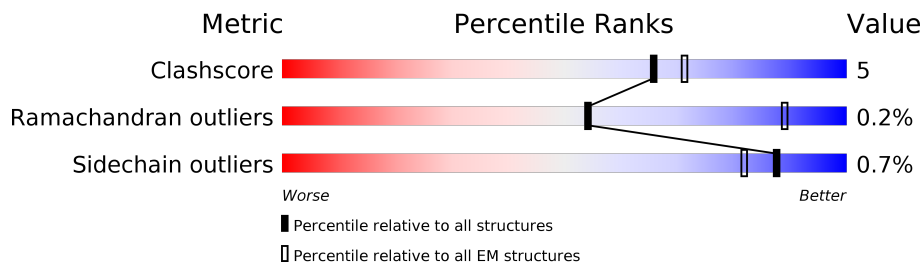
1 Overall quality at a glance

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	89% 10% .
1	F	108	86% 13% .
1	H	108	87% 12% .
1	J	108	86% 13% .
2	B	4416	84% 10% 5%
2	E	4416	84% 10% 5%
2	G	4416	84% 10% 5%
2	I	4416	85% 10% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 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	G	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		

- 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 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0

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: 




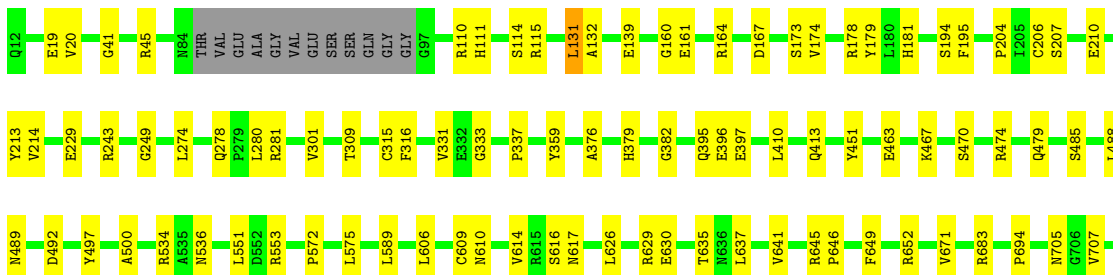
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



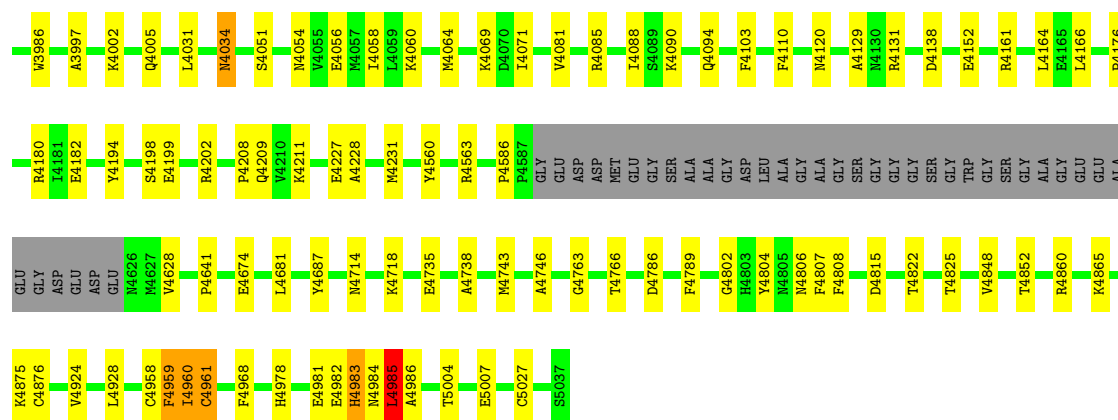
- Molecule 2: Ryanodine receptor 1

Chain B: 



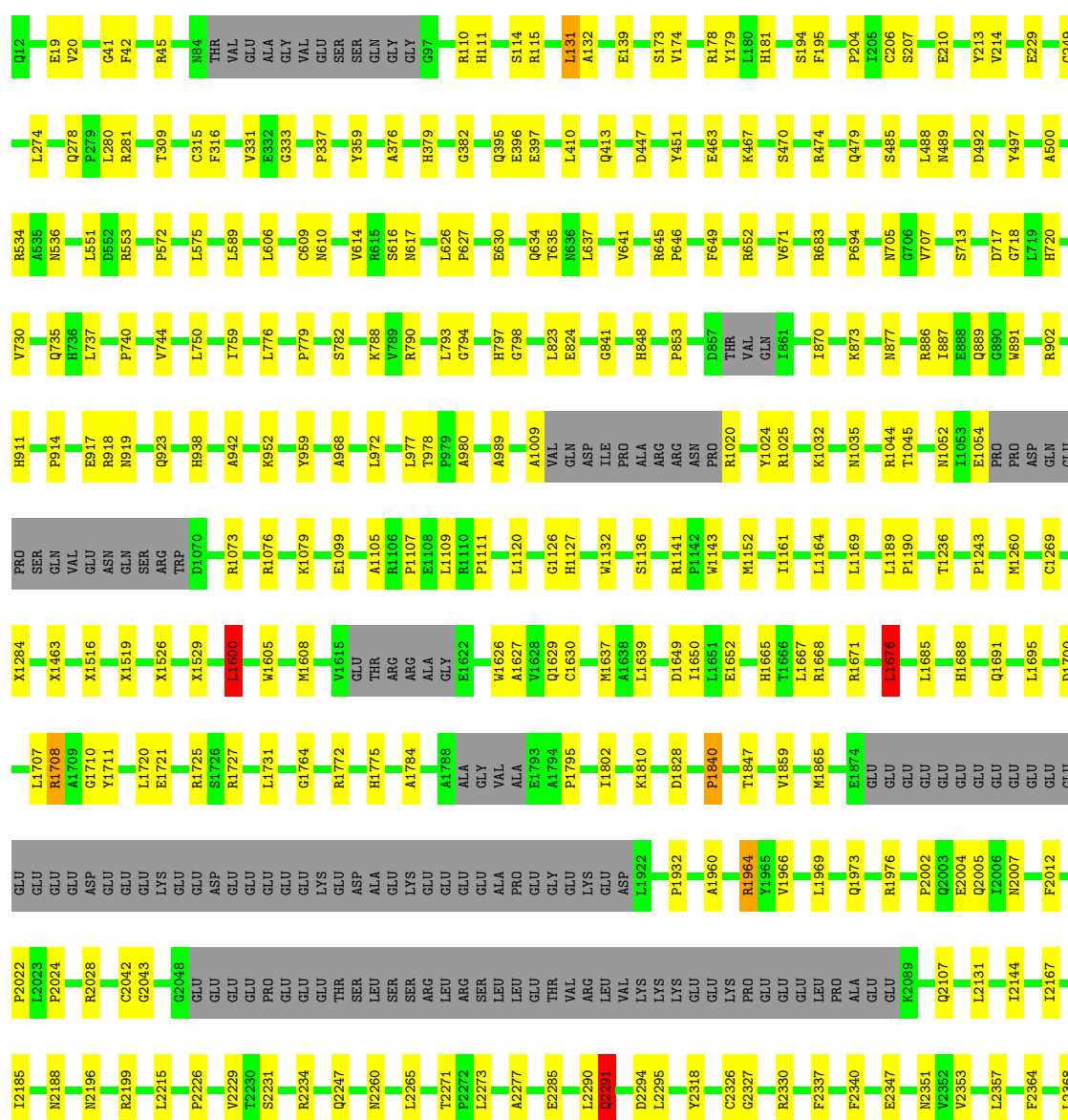

WORLDWIDE PDB
 PROTEIN DATA BANK

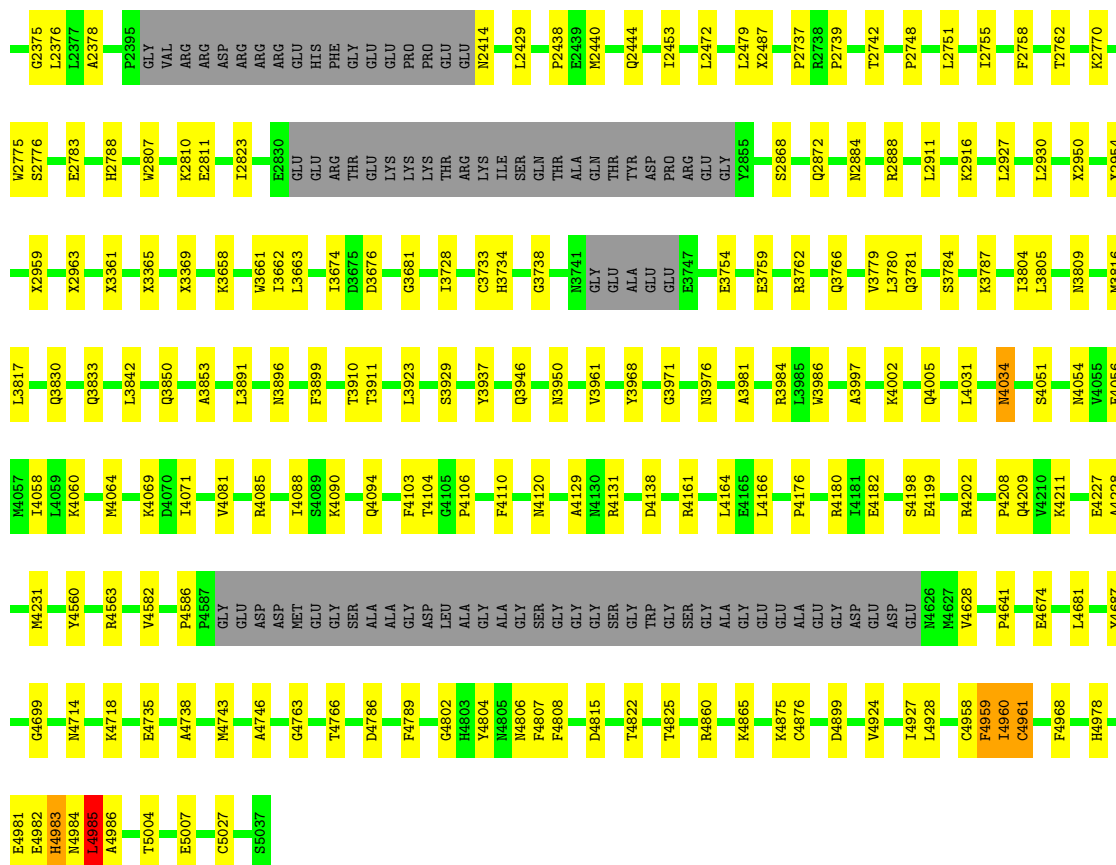
EMDataBank
 Unified Data Resource for 3DEM



• Molecule 2: Ryanodine receptor 1

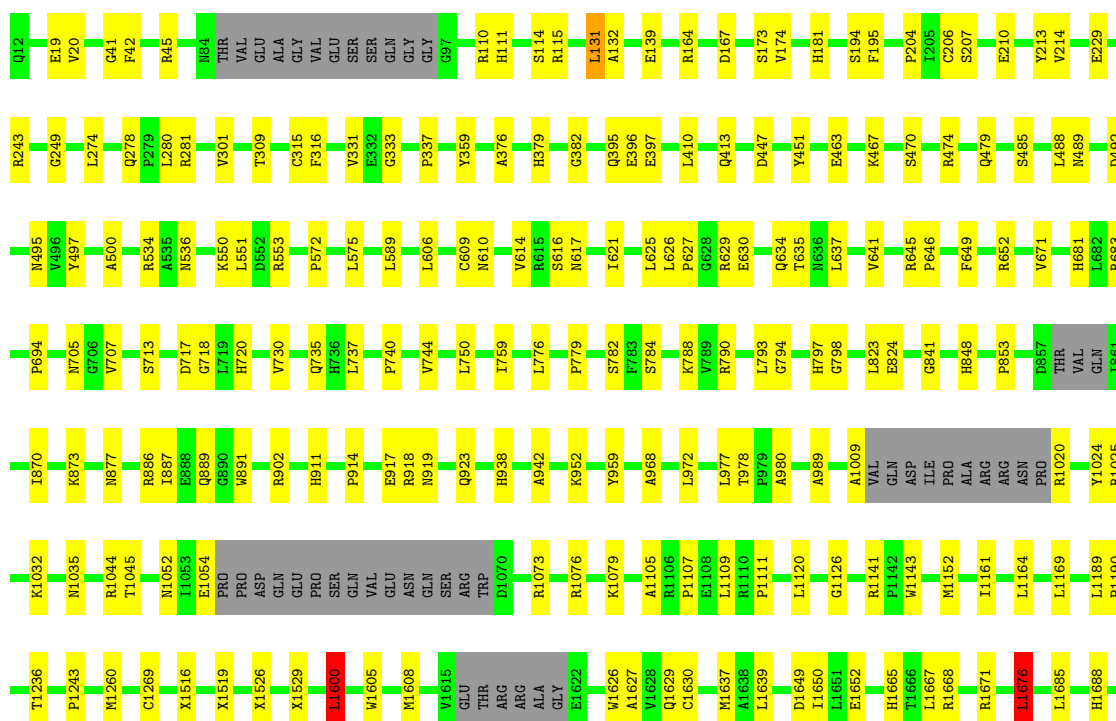
Chain I:





• Molecule 2: Ryanodine receptor 1

Chain E: 84% 10% 5%



R4860	L4166	L3763	Q2872	E2758	F2340	Q2107	Q2005	GLU	Q1691
K4865	P4176	Q3766	N2884	P2739	F2347	Q2127	L2006	GLU	L1695
K4875	R4180	V3779	R2888	T2742	E2347	Y2128	N2007	GLU	D1700
C4876	A3997	L3780	L2911	P2748	N2351	D2129	F2012	GLU	L1707
Y4888	E4182	Q3781	L2916	L2751	V2352	G2130	P2022	GLU	R1708
V4924	S4198	S3784	K2916	L2755	V2353	L2131	L2023	GLU	A1709
L4928	E4199	K3787	L2927	F2758	L2357	E2133	P2024	GLU	Y1711
C4958	R4202	L3804	L2930	T2762	R2359	I2144	R2028	ASP	L1720
F4959	P4208	L3805	X2950	K2770	F2364	I2167	C2042	GLU	E1721
I4960	Q4209	N3809	X2954	S2776	L2368	I2185	G2043	LYS	R1725
C4961	K4211	M3816	X2959	S2776	G2375	N2188	G2048	GLU	S1726
F4968	E4227	L3817	X2963	E2783	L2376	N2196	GLU	ASP	R1727
H4978	A4228	Q3830	X2963	H2788	L2377	R2199	GLU	GLU	R1728
E4981	M4231	Q3833	X3361	H2788	A2378	L2215	GLU	GLU	G1764
E4982	Y4560	L3842	X3365	W2807	P2395	P2226	GLU	LYS	R1772
H4983	R4563	F3847	X3369	K2810	GLY	V2229	THR	ASP	H1775
N4984	V4582	Q3850	K3658	E2811	ARG	T2230	LEU	ALA	A1784
A4986	P4586	A3853	K3658	I2823	ASP	S2231	SER	LYS	A1784
T5004	P4587	A3853	W3661	E2830	ARG	R2234	ARG	GLU	A1788
E5007	GLY	L3891	L3662	GLU	GLU	Q2247	ARG	GLU	ALA
C5027	ASP	N3896	I3674	GLU	HIS	N2260	SER	GLU	GLY
S5037	ASP	F3899	D3675	THR	PHE	L2265	LEU	ALA	ALA
	MET	T3910	D3676	LYS	GLY	L2265	THR	GLU	E1793
	GLY	T3911	G3681	LYS	GLU	T2271	VAL	GLY	A1794
	SER	L3923	I3728	LYS	PRO	P2272	ARG	GLU	P1795
	ALA	S3929	G3738	THR	PRO	L2273	LEU	LYS	I1802
	ALA	Y3937	N3741	THR	GLU	A2277	VAL	ASP	K1810
	GLY	Q3946	GLY	GLN	N2414	E2285	LYS	LYS	D1828
	GLY	N3950	GLU	THR	L2429	L2290	GLU	GLU	P1840
	SER	A4129	ALA	TTR	A2437	Q2291	LYS	PRO	T1847
	GLY	N4130	GLU	ASP	P2438	D2294	GLU	GLU	V1859
	SER	R4131	GLU	PRO	M2440	L2295	GLU	GLU	M1865
	GLY	D4138	GLU	ARG	Q2444	Y2318	LEU	PRO	E1874
	TRP	R4161	E3747	GLY	I2453	C2326	ALA	ALA	Q1973
	SER	L4164	E3754	GLY	L2472	G2327	GLU	GLU	R1976
	GLY	E4165	E3759	S2868	L2479	R2330	E2089	GLU	GLU
	ALA		R3762		X2487	F2337	Q2095	GLU	GLU
	GLY						Q2003	GLU	GLU
							E2004	GLU	GLU

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, 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	0.30	0/834	0.53	0/1123
1	F	0.30	0/834	0.53	0/1123
1	H	0.30	0/834	0.53	0/1123
1	J	0.30	0/834	0.53	0/1123
2	B	0.30	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.30	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	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

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	E	131	LEU	CA-CB-CG	7.94	133.56	115.30
2	I	131	LEU	CA-CB-CG	7.93	133.53	115.30
2	B	131	LEU	CA-CB-CG	7.92	133.53	115.30
2	G	131	LEU	CA-CB-CG	7.91	133.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1676	LEU	CA-CB-CG	6.62	130.52	115.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	694	PRO	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	6	0
1	F	818	0	824	10	0
1	H	818	0	824	9	0
1	J	818	0	824	9	0
2	B	29499	0	24750	264	0
2	E	29499	0	24750	264	0
2	G	29499	0	24750	256	0
2	I	29499	0	24750	256	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	121276	0	102296	1050	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 1050 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:4968:PHE:HE2	2:B:4978:HIS:CE1	1.29	1.49
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	1.29	1.48
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	1.29	1.48
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	1.29	1.48
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.09	1.41

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	3235/4416 (73%)	2892 (89%)	337 (10%)	6 (0%)	51	85
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	51	85
2	G	3235/4416 (73%)	2895 (90%)	334 (10%)	6 (0%)	51	85
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	51	85
All	All	13360/18096 (74%)	11944 (89%)	1392 (10%)	24 (0%)	54	85

5 of 24 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
2	E	4985	LEU

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%)	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	G	4959	PHE
2	I	1141	ARG
2	E	4120	ASN
2	G	4960	ILE
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	3960	GLN
2	I	383	HIS
2	E	3946	GLN
2	G	3994	HIS

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Mol	Chain	Res	Type
2	G	4806	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	14
2	B	14

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Mol	Chain	Number of breaks
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	73.85
1	G	4345:UNK	C	4540:PHE	N	73.85
1	I	4345:UNK	C	4540:PHE	N	73.85
1	E	4345:UNK	C	4540:PHE	N	73.85
1	B	3613:UNK	C	3639:THR	N	45.57