



wwPDB EM Map/Model Validation Report ⓘ

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

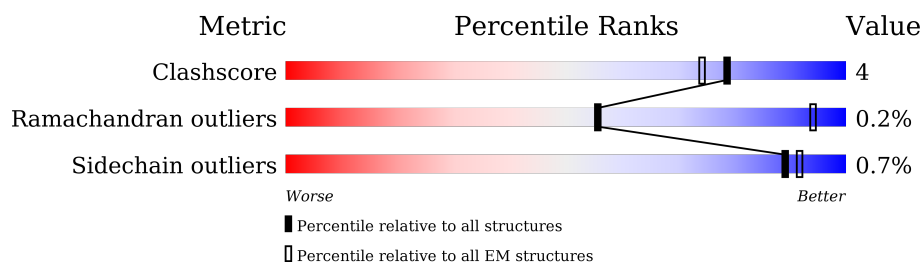
1 Overall quality at a glance

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 $\leq 5\%$.

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 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 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.

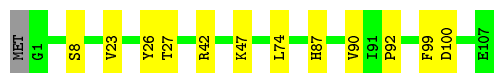
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 



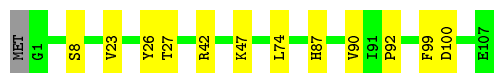
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




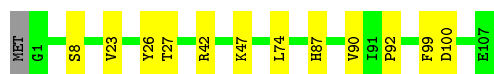
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




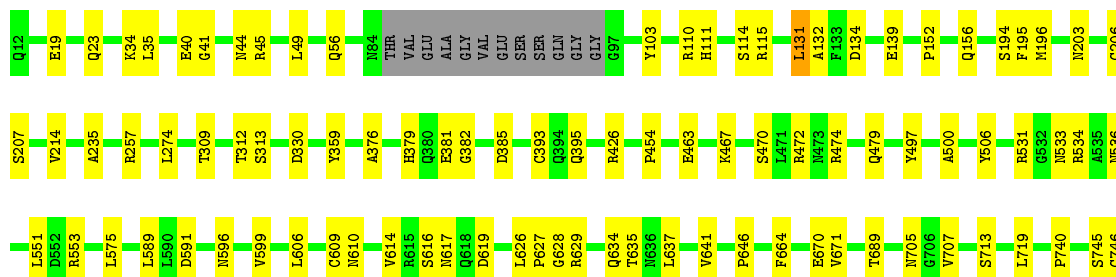
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 

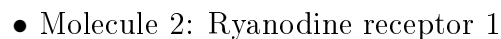


- Molecule 2: Ryanodine receptor 1

Chain B: 

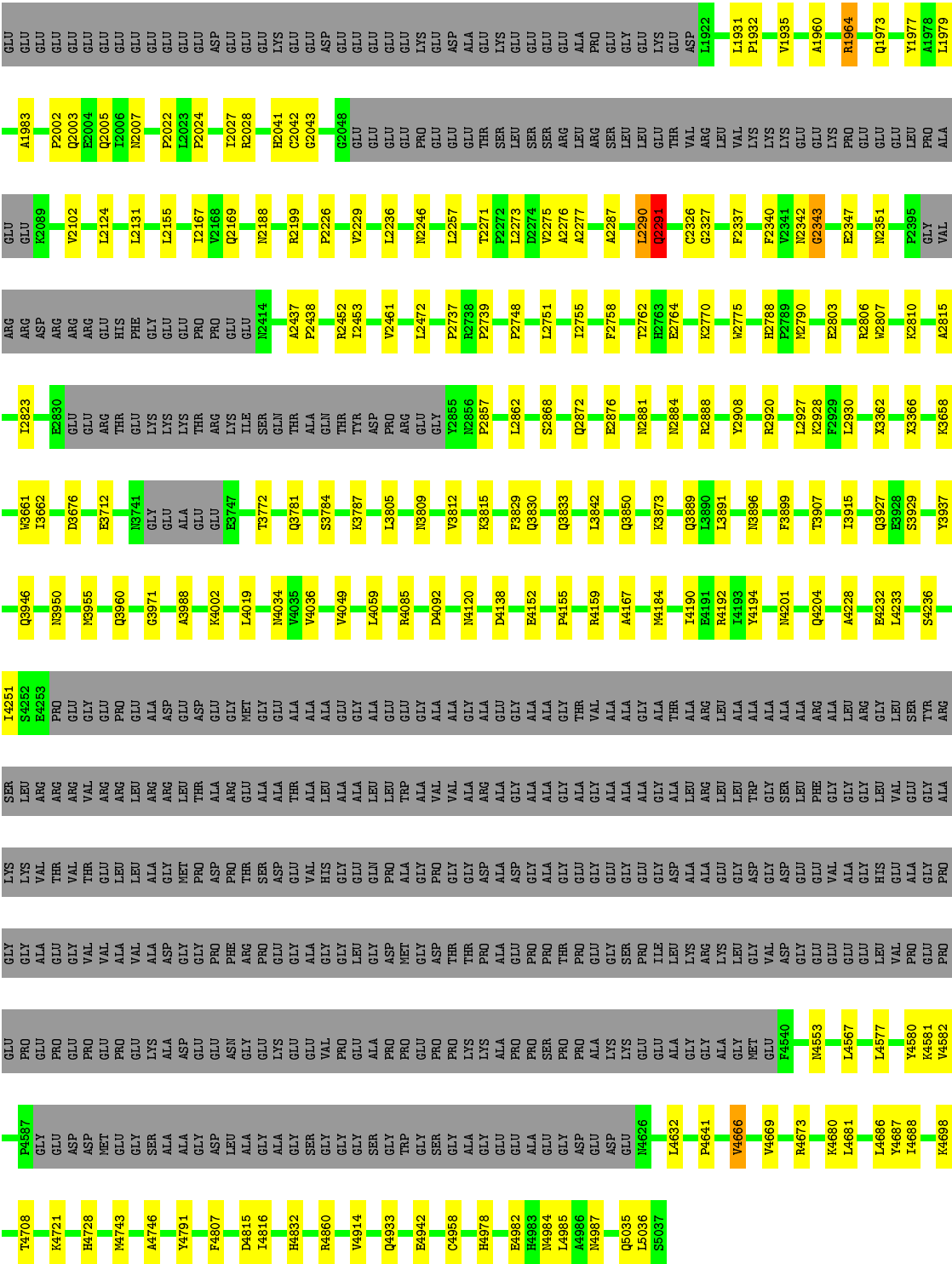


GLU	PRO	GLU	GLY	THR	VAL	ARG	ARG	E4253	Q3946	X3366	K2810	GLY	PRO	ALA	PRO	Q1691	A1178	M1035	R758
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PRO	GLU	VAL	ARG	GLU	VAL	ARG	ARG	GLU	M3955	V3661	I2823	ASP	ASP	ASP	ASP	L1707	R1212	M1052	P779
GLY	VAL	VAL	LEU	LEU	LEU	LEU	LEU	ALA	Q3960	I3662	E2830	ARG	ARG	ARG	ARG	R1708	W1237	I1053	K788
ALA	ASP	ALA	ARG	ALA	ASP	ARG	ALA	ALA	G3971	D3676	GLU	GLU	GLU	GLU	GLU	A1709	Q1244	E1084	I793
ASP	GLY	GLY	MET	GLY	GLY	LEU	THR	GLY	E3712	E3712	GLU	HIS	GLU	GLU	GLU	Y1712	F1245	PRO	L793
GLU	GLY	GLY	THR	THR	THR	THR	THR	ASP	K4002	E3712	GLU	PHE	ASP	ASP	ASP	D1713	X1516	ASP	H797
ASN	PHE	ARG	ARG	ARG	ARG	ARG	ARG	GLY	M3741	E3747	THR	GLY	GLY	GLY	GLY	GLN	GLU	GLN	Y808
GLY	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L4019	GLY	LYS	GLU	GLU	GLU	GLU	GLU	X1519	PRO	Y808
PRO	PRO	GLU	ALA	GLY	GLY	ALA	GLY	GLY	N4034	ALA	LYS	PRO	PRO	PRO	PRO	GLN	X1526	GLN	G841
LYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	V4035	GLU	THR	PRO	GLU	GLU	GLU	VAL	X1529	VAL	D857
GLU	GLU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	V4036	GLU	ALA	GLY	GLU	GLU	GLU	TRP	X1529	GLU	THR
VAL	VAL	GLY	LEU	ALA	ALA	LEU	ALA	ALA	V4049	E3747	LYS	LYS	LYS	LYS	LYS	ASN	VAL	VAL	GLN
PRO	PRO	GLY	ALA	ALA	ALA	ALA	ALA	ALA	GLY	T3772	ILE	ILE	GLU	GLU	GLU	GLN	R1594	GLN	I861
GLY	GLY	GLY	ALA	ALA	ALA	ALA	ALA	ALA	L4059	GLY	THR	THR	GLU	GLU	GLU	GLN	R1594	GLN	I861
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	R4085	Q3781	THR	THR	GLU	GLU	GLU	GLN	X1526	GLN	G841
PRO	PRO	GLY	ALA	ALA	ALA	ALA	ALA	ALA	D4082	S3784	ALA	ALA	GLY	GLY	GLY	GLN	X1526	GLN	G841
PRO	PRO	GLY	ALA	ALA	ALA	ALA	ALA	ALA	D4092	S3784	ALA	ALA	GLY	GLY	GLY	GLN	X1526	GLN	G841
PRO	PRO	GLY	ALA	ALA	ALA	ALA	ALA	ALA	N4120	K3787	THR	THR	GLU	GLU	GLU	GLN	X1526	GLN	G841
LYS	LYS	GLY	ALA	ALA	ALA	ALA	ALA	ALA	L4138	L3805	PRO	PRO	GLU	GLU	GLU	GLN	X1526	GLN	G841
PRO	PRO	GLY	ALA	ALA	ALA	ALA	ALA	ALA	D4138	L3805	PRO	PRO	GLU	GLU	GLU	GLN	X1526	GLN	G841
PRO	PRO	GLY	ALA	ALA	ALA	ALA	ALA	ALA	E4152	N3809	GLY	GLY	GLU	GLU	GLU	GLN	X1526	GLN	G841
SER	SER	GLY	ALA	ALA	ALA	ALA	ALA	ALA	V3812	V3812	GLY	GLY	GLU	GLU	GLU	GLN	X1526	GLN	G841
GLU	GLU	ILE	GLY	GLY	GLY	GLY	GLY	GLY	P4155	K3815	THR	THR	GLU	GLU	GLU	GLN	X1526	GLN	G841
ILE	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R4159	K3815	THR	THR	GLU	GLU	GLU	GLN	X1526	GLN	G841
LYS	LYS	GLY	ALA	ALA	ALA	ALA	ALA	ALA	A4167	F3829	L2862	GLY	GLU	GLU	GLU	GLN	X1526	GLN	G841
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GLU	GLU	ILE	GLY	GLY	GLY	GLY	GLY	GLY	M4184	Q3833	S2868	GLY	GLU	GLU	GLU	GLN	X1526	GLN	G841
ALA	ALA	LEU	GLY	GLY	GLY	GLY	GLY	GLY	I4190	L3842	Q2872	GLY	GLU	GLU	GLU	GLN	X1526	GLN	G841
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GLY	GLY	LEU	GLY	GLY	GLY														



X3366	K2810	GLY VAL	A1978 L1979	Q1691	R1212	R1020	L719	M536	L199	Q12
	K3658	ARG GLU	A1983	L1698	M237	R1044	P740	V548	M203	E19
X3661	I2823	ARG ASP	P2002	L1707	Q1244	M1062	S745	L551	C206	Q23
	I3662	ARG ARG	P2003	A1708	F1245	I1053	C746	M552	S207	L35
X3741	E2830	GLU GLU	E2004	G1710	X1516	E1054	R758	L564	V214	E40
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GLU ARG		I2006	G1712	Y1712	GLN		F777	L575	R257	M44
GLU THR		M2007	D1713	D1713	X1549	GLU	P779	L589	L274	R45
GLU GLU		P2022	I1718	I1718	X1526	PRO				L49
GLY LYS		L2023	H1719	H1719	GLN	GLU	L590	D591	T309	
GLU LYS		P2024	L1720	L1720	X1529	GLN	K788			Q56
GLY THR		L2027	E1721	E1721	VAL	VAL	L793	M596	T312	M94
ARG ARG		R2028	R1725	R1725	R1594	ASN			S313	THR
GLY LYS			R1728	R1728	L1600	GLN	H797	V599	Y359	GLU
ILE		H2041	G1729	G1729	M1605	ARG	Y808	L606	A376	GLY
GLN SER		C2042	M1730	M1730	THR	THR	D557	M610	R379	VAL
GLN THR		G2043			V1635	R1076	R615	V614	Q380	GLU
ALA		G2048			ARG	GLN	R616	S616	G382	SER
GLN THR					ALA	K1079	R886	M617	GLN	GLY
ASP					GLY	V1095	Q618	D619	D385	GLY
PRO					GLY	T1096	M891		C393	G97
ARG ARG					ALA	G1103	G940	L626	Q394	Y103
GLU GLU					VAL	P1107	R952	G628	Q395	R110
GLY GLY					ALA	A1638	A968	Q634	P454	
THR					GLU	L1108	L972	T635	S114	S114
GLU					LYS	A1794	P1111	M636	E463	R115
GLU					GLU	P1795	L1120	L637	K467	L131
GLU					GLU	I1802	P1642	T978	F133	A132
GLU					ALA	R1808	R1646	A980	S470	D134
LEU					PRO	L1812	D1698	D699	R474	E139
LEU					GLY	L1815	H1665	V641	Q479	P152
THR					LYS	D1828	T1666	P646	Y497	Q156
GLU					GLU		L1667	V650	A500	D168
ARG					ASP		R1668	G1004	Y506	V174
LEU					ASP		R1141		R531	S194
VAL					L1922		P1152	F664	M532	M196
LYS					LYS		M1143			
LYS					LYS		VAL	D670	Q156	
LYS					P1932		GLN	V671	A500	
GLU					V1845		ASP	T689	D168	
GLU					V1846		ILE		Y506	
GLU					T1847		PRO			
LYS					V1935					
PRO					R1964		ALA	M705	R531	V174
GLU					F1854		ARG	G706	M532	S194
GLU					Q1973		ARG	V707	N533	F195
GLU							ASN	R534	M534	M196
GLU					Q1861		THR	S712	A552	
LEU					Y1077					











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	0.31	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($^{\circ}$)	Ideal($^{\circ}$)
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

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 ⓘ

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 [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 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 [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	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