



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 01:41 PM EDT

PDB ID : 5T9M
EMDB ID: : EMD-8372
Title : Structure of rabbit RyR1 (Ca²⁺-only dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-09
Resolution : 4.00 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

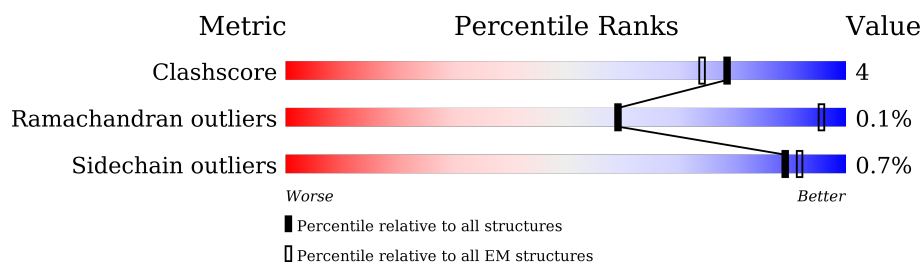
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY









The reported resolution of this entry is 4.00 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	
1	F	108	
1	H	108	
1	J	108	
2	B	4676	
2	E	4676	
2	G	4676	
2	I	4676	

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.

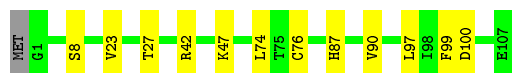
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 




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

Chain A: 




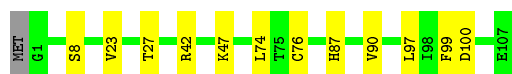
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




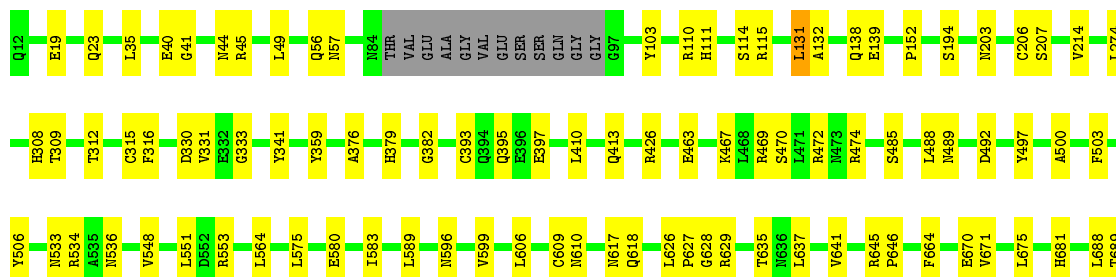
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 




- Molecule 2: Ryanodine receptor 1

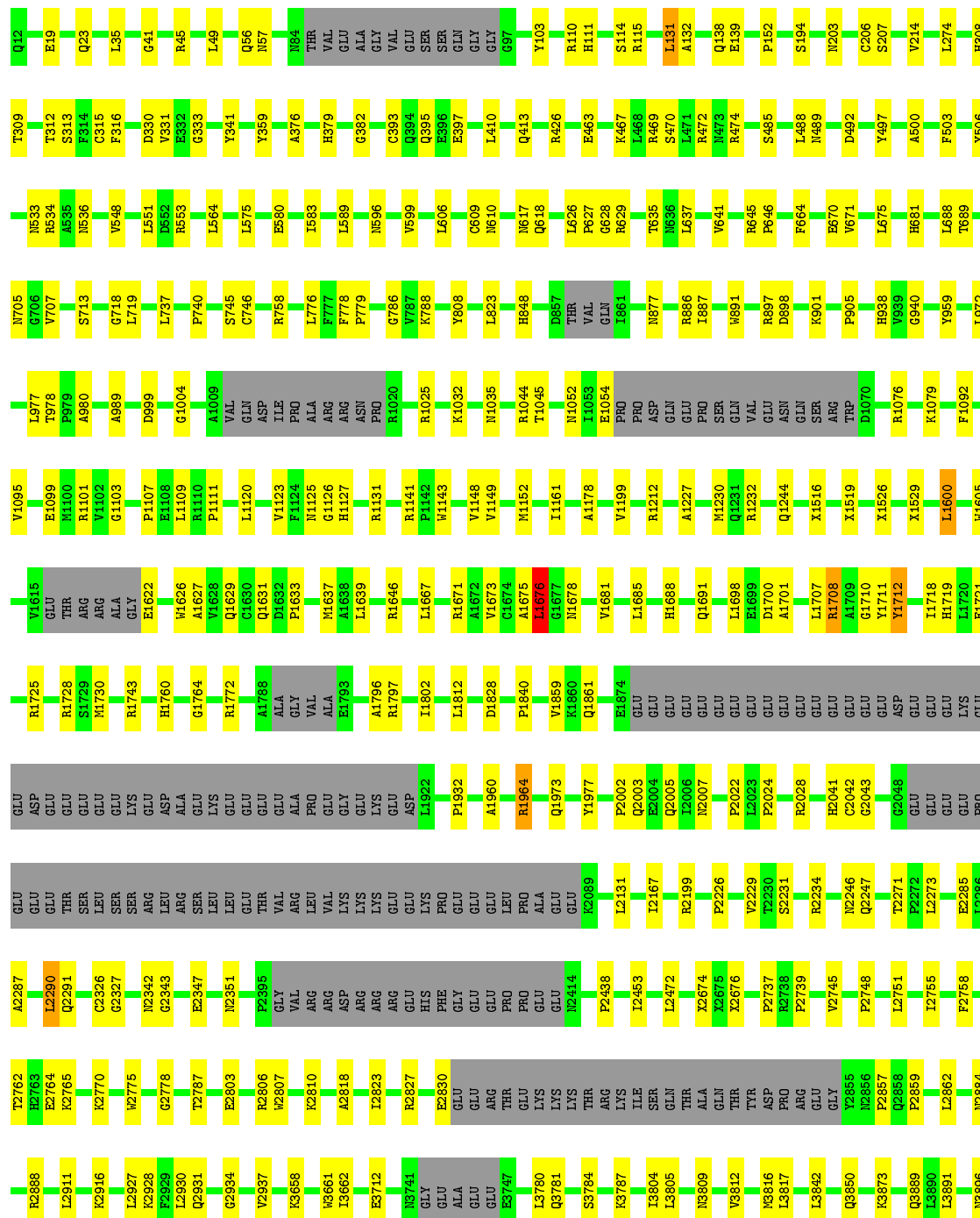
Chain B: 






- Molecule 2: Ryanodine receptor 1

Chain E:  81% 8% 11%





Q1244	GLN	R891	E870	Y487	L274	Q12
	VAL	R897	V671	A500	H308	E19
	GLU	D898	L675	F503	T309	Q23
	ASN	R901	H681	Y506	T312	L35
	GLN	P905	L688	S313	F314	G41
	SER	R938	T689	R531	C315	R45
	TRP	N939	N705	A532	F316	
	D1070	G940	G706	H533	D330	L49
	R1076	Y959	V707	H534	V331	Q56
	K1079	V1095	S713	A535	E332	N57
L1600	GLU	L972	G718	Y548	Y359	R64
	THR	E1099	L719	L551	A376	THR
	ARG	H1100	T978	D552	H379	VAL
	ARG	R1101	P979	R553	L564	GLU
	ALA	V1102	A980	P740	G382	ALA
	GLY	G1103		S745	G382	GLY
	E1622	P1107	A989	C746	L575	VAL
		E1108	D999	R758	E580	GLU
		R1109	G1004	L776	C933	SER
		P1110		F777	Q394	SER
W1626	ARG	R1110	L776	L583	Q395	GLN
	Q1629	P1111	R758	E580	E396	GLY
	Q1631	G1004	L776	L583	E397	GLY
	G1632	L1120	F777	L589	I404	Q97
	P1633	V1123	GLN	F778	L410	Y103
	M1637	F1124	ASP	P779	Q413	R110
	A1638	N1125	ILE	N596	R426	H111
	L1639	G1126	PRO	G786	C609	S114
		H1127	ALA	V787	N610	R115
	R1646	H1127	ARG	K788	P454	
L1667	R1131	ARG	Y808	L606		
	L1671	ASN	Y808	C609		
	R1672	PRO	L623	N610		
	A1673	R1020	L623	N610		
	V1673	R1025	H648	N617	E463	L131
	C1674	V1148	D857	Q618	A132	
	A1675	M1152	THR	L626	K467	Q138
	G1677	L1676	VAL	P627	L468	E139
	M1678	L1161	GLN	G628	R469	P152
			T661	R629	L471	
V1681	A1178	T1045	P864	T635	R472	S194
		N1052	P865	N636	M473	N203
	L1685	L1053	P865	L637	R474	
	H1688	R1212	E376	L637	E481	C206
		PRO	N977	V641		S207
	Q1691	A1227	E380	R645	S485	V214
	L1698	M1230	GLN	P646	L488	A235
	E1699	Q1231	GLU	R686	N489	
	D1700	R1232	PRO	I387	F664	
			PRO		P400	R357

ALA	R44120	L3842	P2748	R2028	GLU	L1707	Q1244	ASN	D898	B670	A500	L274
LEU	R4159	Q3850	L2751	R2041	GLU	R1708	Q1244	GLN	X901	B671	A500	L274
GLY	A4228	Q3859	L2755	R2042	GLU	R1709	X1516	ARG	P905	H681	F503	Q278
VAL	E4232	L2862	P2758	R2043	GLU	Y1710	X1519	TRP	H938	L688	Y506	H308
THR	L4251	N2884	T2271	R2048	ASP	Y1712	X1526	D1070	H939	L689	R631	T309
ALA	E4252	N2888	L2272	GLU	GLU	I1718	X1529	R1076	G940	T689	G532	T312
ARG	E4253	R2763	L2273	GLU	GLU	H1719	X1529	K1079	Y959	N705	N533	S313
LEU	PRQ	E2764	E2285	GLU	LYS	L1720	L1600	R1101	Y959	G706	R534	F314
ARG	GLU	R2765	L2286	PRQ	GLU	E1721	L1600	E1093	L972	V707	A535	C315
ARG	GLU	L2287	A2287	GLU	GLU	R1725	V1605	A1094	L972	S713	N536	F316
VAL	GLU	L2290	L2290	GLU	ASP	R1728	V1615	V1095	L977	S713	V548	D330
ARG	GLU	Q2291	Q2291	THR	GLU	R1728	V1615	E1099	T978	G718	V548	D330
LEU	GLU	L2291	L2291	GLU	GLU	M1729	GLU	N1100	P979	L719	L551	V331
ALA	GLU	C2326	C2326	LEU	GLU	M1730	THR	R1101	A980	L719	L551	V331
GLY	GLU	C2327	C2327	GLU	GLU	R1743	ARG	V1102	A989	L737	R553	G333
THR	GLU	L2342	L2342	GLU	LYS	R1743	ARG	G1103	A989	P740	L564	Y359
ASP	GLU	E2343	E2343	ARG	ASP	H1760	ALA	P1107	D999	S745	L575	A376
GLY	GLU	E2347	E2347	ALA	ALA	G1764	E1622	E1108	G1004	C746	L575	A376
LEU	LEU	N2351	N2351	LEU	LYS	R1772	V1626	R1109	G1004	C746	E580	H379
GLU	GLU	L2395	L2395	GLU	GLU	R1772	A1627	R1110	A1009	R758	N581	G382
THR	THR	P2395	P2395	THR	GLU	A1788	V1628	L1120	VAL	L776	H582	C393
GLY	VAL	GLY	GLY	VAL	GLU	GLY	Q1629	ASP	ASP	F777	I583	C393
ARG	ARG	ARG	ARG	ARG	ALA	ALA	Q1631	ILE	ASP	F778	R585	Q394
LEU	LEU	ARG	ARG	LEU	PRQ	VAL	Q1631	F1124	PRQ	P779	S585	Q395
VAL	VAL	ASP	ASP	VAL	GLU	ALA	M1637	N1125	ALA	G786	L589	E397
LYS	LYS	ASP	ASP	LYS	GLY	E1793	A1639	G1126	ANG	G787	N596	L410
GLY	LYS	ARG	ARG	LYS	GLU	A1796	L1639	H1127	ASN	K788	V599	Q413
GLU	GLU	ARG	ARG	GLU	LYS	R1797	R1646	R1131	PRQ	Y808	L606	R426
GLU	GLU	GLU	GLU	GLU	ASP	L1922	R1671	R1141	R1020	L823	C609	P454
GLU	GLU	H1S	H1S	LYS	LYS	L1922	A1672	P1142	R1025	H848	N610	E463
THR	THR	PHE	PHE	PRQ	PRQ	L1812	V1673	W1143	R1044	D857	N617	K467
GLY	GLY	GLY	GLY	GLU	GLU	D1828	C1674	V1148	T1045	VAL	Q618	L466
LYS	GLU	GLU	GLU	GLU	GLU	A1960	A1675	V1148	T1045	GLN	I626	R469
PRQ	PRQ	PRQ	PRQ	LEU	PRQ	R1964	A1676	S1171	N1035	THR	P627	S470
THR	THR	PRQ	PRQ	PRQ	PRQ	P1840	G1677	S1171	N1035	GLN	G628	L471
ARG	ARG	GLU	GLU	ALA	ALA	Y1859	M1678	S1175	N1052	VAL	R629	R472
ILE	ILE	N2414	N2414	GLU	GLU	Q1861	V1681	A1178	T1053	R861	R629	R472
GLN	GLN	P2438	P2438	R2089	Y1977	Q1861	L1685	A1178	N1053	L870	T635	R473
THR	THR	P2438	P2438	R2089	Y1977	Q1861	L1685	V1199	E1054	L874	N636	R474
ALA	ALA	T2453	T2453	L2131	P2002	E1874	H1688	H1201	PRQ	L874	L637	S485
GLN	GLN	T2453	T2453	L2131	Q2003	GLU	H1688	H1201	PRQ	N877	V641	L488
THR	THR	L2472	L2472	L2167	Q2004	GLU	Q1691	R1212	ASP	R886	R645	I489
TVR	TVR	P2737	P2737	R2199	Q2005	GLU	Q1691	R1212	GLN	L887	P646	D492
ASP	ASP	P2737	P2737	R2199	Q2006	GLU	L1694	R1212	GLU	R887	F664	Y497
PRQ	PRQ	P2738	P2738	R2199	Q2007	GLU	L1694	R1212	GLU	R887	F664	Y497
ARG	ARG	P2739	P2739	P2226	Q2022	GLU	L1698	M1230	PRQ	R891	F664	Y497
GLY	GLY	P2739	P2739	P2226	Q2023	GLU	E1699	Q1231	VAL	R891	F664	Y497
GLY	GLY	V2745	V2745	P2229	Q2024	GLU	D1700	Q1231	VAL	R891	F664	Y497
GLY	GLY	V2745	V2745	P2229	Q2024	GLU	D1700	Q1231	VAL	R891	F664	Y497
GLY	GLY	V2855	V2855	S2231	P2024	GLU	A1701	R1232	GLU	R897	F664	Y497




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	0.30	0/25428	0.55	8/34534 (0.0%)
2	E	0.30	0/25428	0.55	8/34534 (0.0%)
2	G	0.30	0/25428	0.55	8/34534 (0.0%)
2	I	0.30	0/25428	0.55	8/34534 (0.0%)
All	All	0.30	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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

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	G	131	LEU	CA-CB-CG	8.47	134.78	115.30
2	B	131	LEU	CA-CB-CG	8.46	134.76	115.30
2	E	131	LEU	CA-CB-CG	8.46	134.76	115.30
2	I	131	LEU	CA-CB-CG	8.46	134.75	115.30
2	B	1600	LEU	CA-CB-CG	7.43	132.39	115.30

There are no chirality outliers.

5 of 60 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	7	0
1	J	818	0	824	6	0
2	B	29369	0	24721	194	0
2	E	29369	0	24721	194	0
2	G	29369	0	24721	197	0
2	I	29369	0	24721	192	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	102180	783	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 783 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:4958:CYS:SG	2:E:4978:HIS:CD2	2.72	0.83
2:G:4958:CYS:SG	2:G:4978:HIS:CD2	2.72	0.83
2:I:4958:CYS:SG	2:I:4978:HIS:CD2	2.72	0.82
2:B:4958:CYS:SG	2:B:4978:HIS:CD2	2.72	0.82
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.72	0.70

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%)	97 (92%)	8 (8%)	0	100	100
1	F	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	H	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	J	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	B	3235/4676 (69%)	2881 (89%)	349 (11%)	5 (0%)	52	86
2	E	3235/4676 (69%)	2883 (89%)	347 (11%)	5 (0%)	52	86
2	G	3235/4676 (69%)	2879 (89%)	351 (11%)	5 (0%)	52	86
2	I	3235/4676 (69%)	2880 (89%)	350 (11%)	5 (0%)	52	86
All	All	13360/19136 (70%)	11913 (89%)	1427 (11%)	20 (0%)	59	90

5 of 20 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	94
2	E	2493/3202 (78%)	2476 (99%)	17 (1%)	88	94
2	G	2493/3202 (78%)	2476 (99%)	17 (1%)	88	94
2	I	2493/3202 (78%)	2476 (99%)	17 (1%)	88	94
All	All	10324/13164 (78%)	10256 (99%)	68 (1%)	89	94

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

Mol	Chain	Res	Type
2	E	4085	ARG
2	I	1076	ARG
2	G	3896	ASN
2	E	4120	ASN
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	3950	ASN

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Mol	Chain	Res	Type
2	I	379	HIS
2	G	3809	ASN
2	E	4034	ASN
2	E	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	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	42.97
1	B	3613:UNK	C	3639:THR	N	42.95
1	G	3613:UNK	C	3639:THR	N	42.95
1	E	3613:UNK	C	3639:THR	N	42.94
1	B	3163:UNK	C	3170:UNK	N	16.52