



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:12 pm GMT

PDB ID : 5TA3
EMDB ID: : EMD-8377
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ 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 : 4.40 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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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

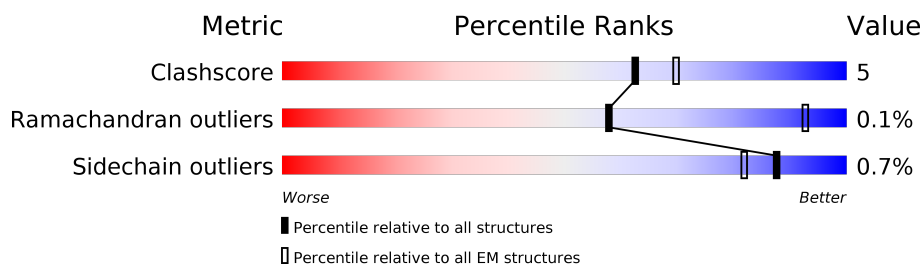
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	76% 23% .
1	F	108	72% 27% .
1	H	108	73% 26% .
1	J	108	71% 28% .
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 6 unique types of molecules in this entry. The entry contains 121456 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.

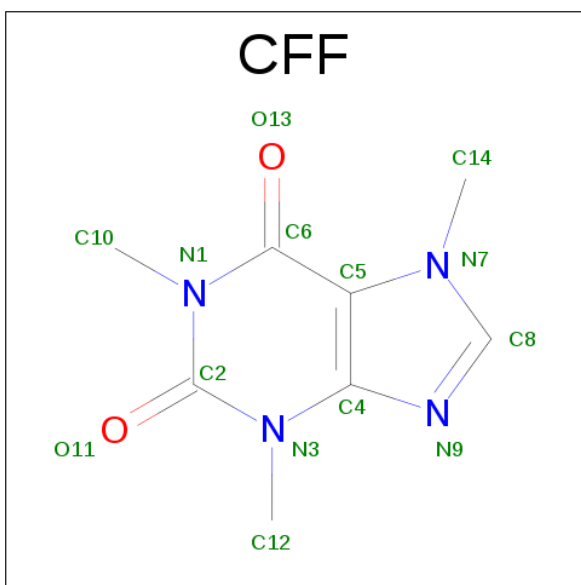
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

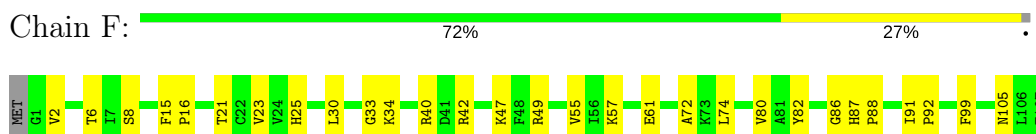
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

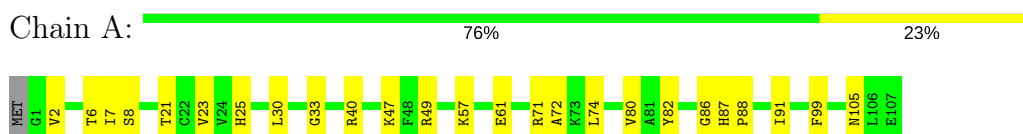
3 Residue-property plots [i](#)

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.

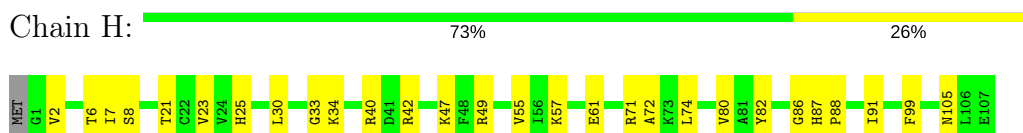
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



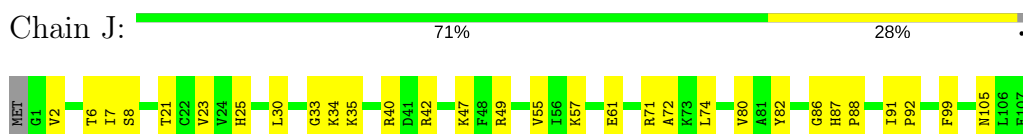
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



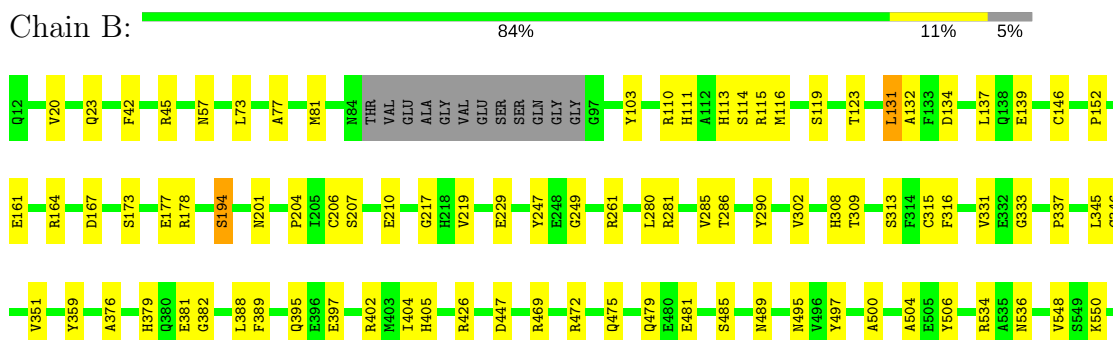
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



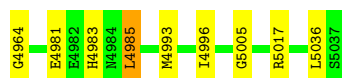
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B




- Molecule 2: Ryanodine receptor 1

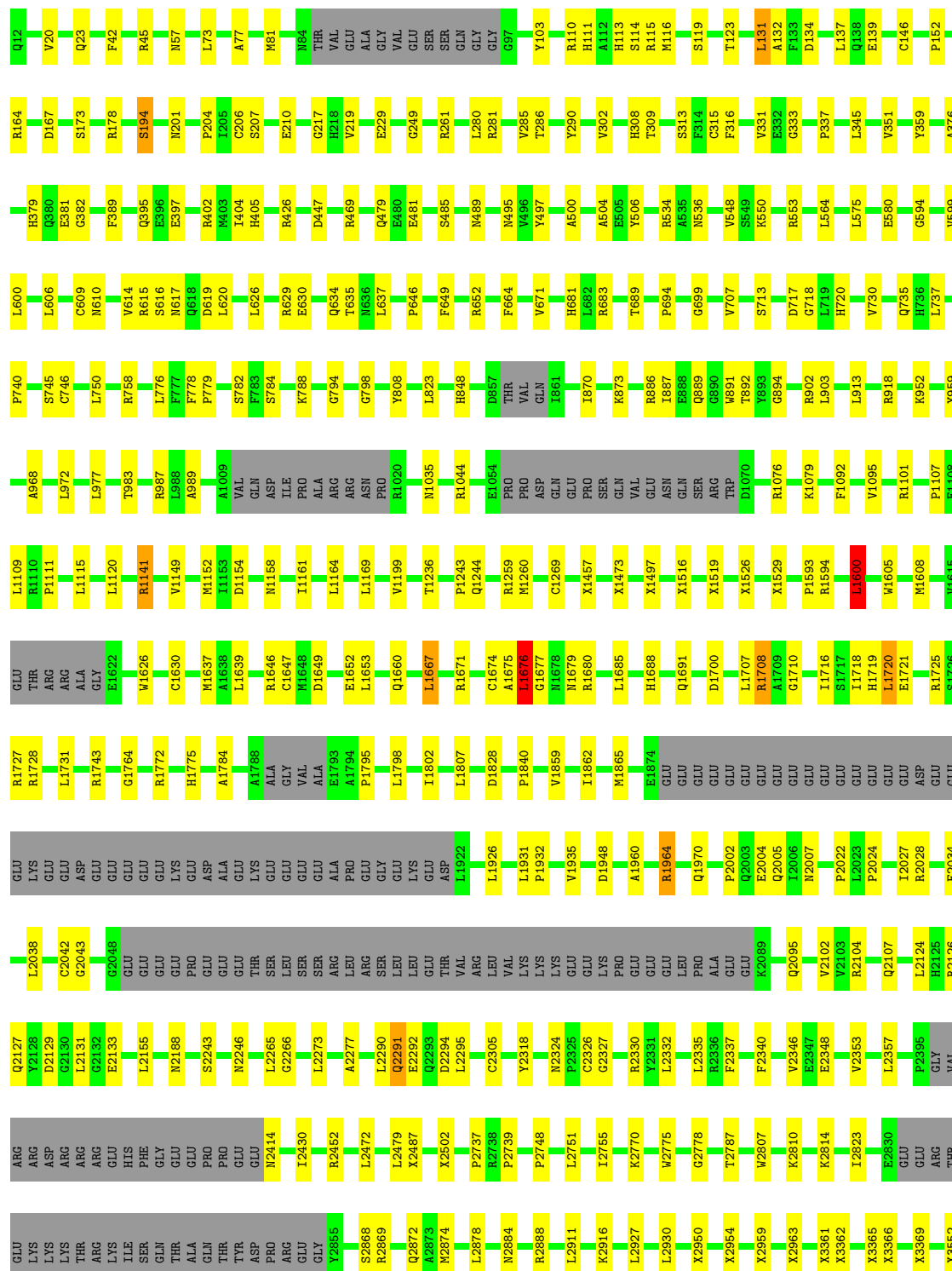


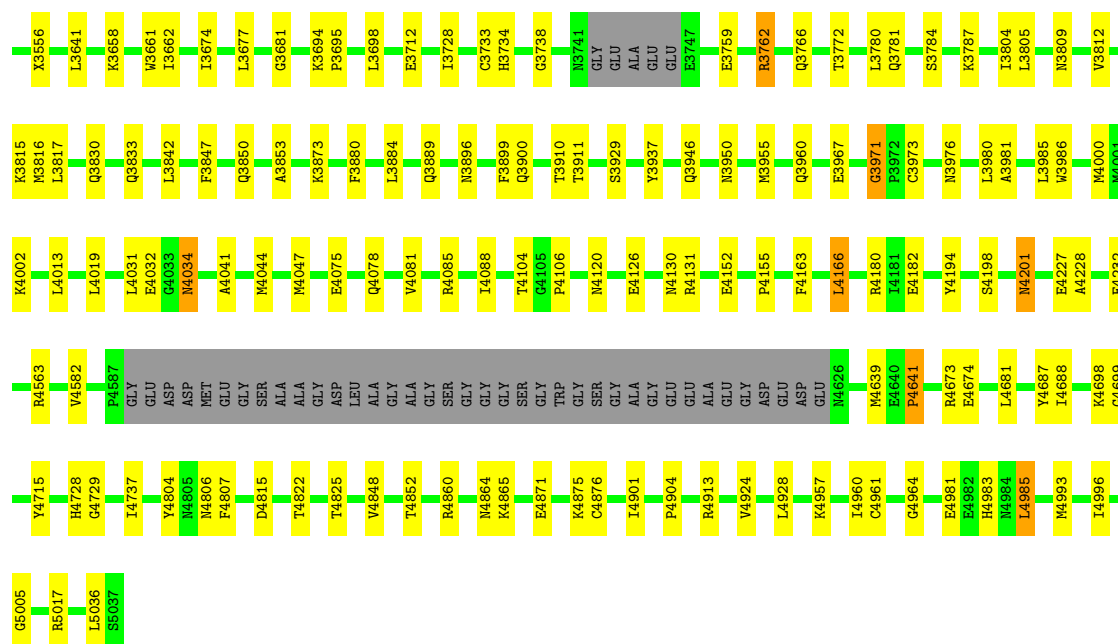


- Molecule 2: Ryanodine receptor 1

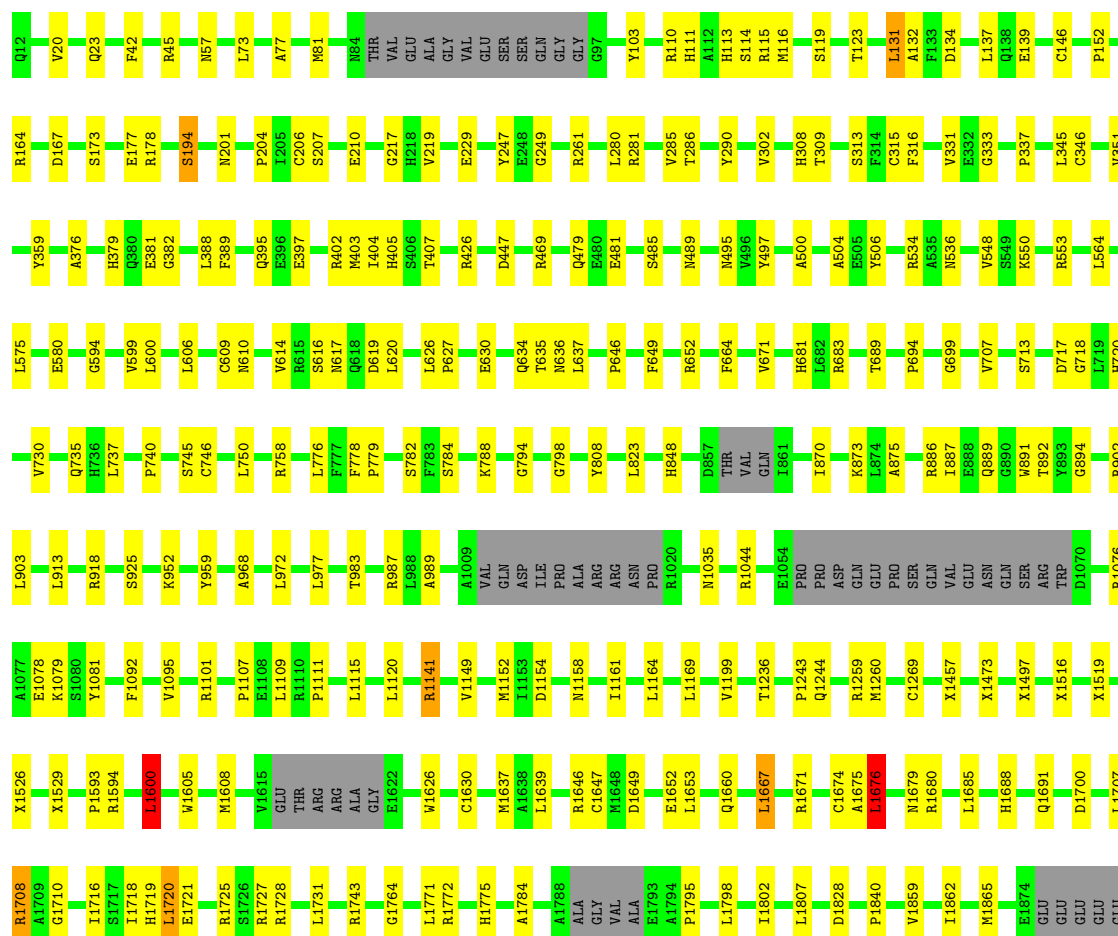
Chain G:  84% 11% 5%





• Molecule 2: Ryanodine receptor 1

Chain I: 84% 11% 5%



GLU	Q2003	GLU	L2335	W2775	L2930	H3771	N3950	E4152	GLU	D4899
GLU	E2004	GLU	L2336	W2776	L2931	T3772	E4900	GLY	E4900	
GLU	Q2005	GLU	F2337	G2778	X2950	R3773	I4901	ASP	I4901	
GLU	N2007	GLU	F2338	G2779	X2951	G3774	M3955	ASP	P4904	
GLU	P2022	GLU	F2339	T2787	X2952	L3780	Q3960	GLU	R4913	
GLU	L2023	GLU	V2340	W2807	X2953	Q3781	E3967	GLU	V4924	
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GLU	T2027	GLU	E2348	K2811	X2955	S3785	P3972	GLU	K4957	
ASP	R2028	GLU	V2353	K2812	X2956	K3787	C3973	GLU	I4960	
GLU	F2034	GLU	L2357	L2823	X2957	L3804	N3976	GLU	C4961	
GLU	L2038	GLU	P2395	E2830	X2958	L3805	L3980	GLU	G4964	
GLU	C2042	GLU	VAL	GLU	X2959	L3806	A3981	GLU	E4981	
ASP	G2043	GLU	ARG	ARG	X2960	N3809	A3982	GLU	E4982	
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V4924	E4640	E4181	P3972	S3784	X3361	W2807	L2357	L2124	T2027	E1721	V1615	P1107	P1107	Y959	V730
L4928	P4641	E4182	C3973	K3787	X3362	K2810	P2395	H2125	R2028	R1725	THR	E1108	E1108	Y959	H735
K4957	E4674	Y4194	N3976	L3804	X3365	K2814	VAL	R2126	F2034	S1726	GLU	R1109	R1109	A968	H736
L4681	L4681	S4198	L3980	L3805	X3366	K2823	ARG	Y2128	L2038	R1727	ARG	P1111	P1111	L972	L737
C4961	L4681	N4201	A3981	N3809	X3369	L2823	ASP	D2129	C2042	R1728	ALA	L1115	L1115	L977	P740
G4964	Y4687	A4227	R3984	V3812	X3552	E2830	ARG	G2130	G2043	L1731	GLY	L1120	L1120	L987	S745
E4981	L4688	A4228	L3985	K3815	X3556	GLU	ARG	E2133	G2048	R1743	E1622	R1141	R1141	T983	C746
H4983	E4982	E4232	W3986	K3816	L3641	THR	ARG	L2155	GLU	G1764	W1626	V1149	V1149	L988	L750
H4984	E4983	E4563	N4001	L3817	L3641	GLU	HIS	L2188	GLU	R1772	C1630	V1149	V1149	A989	R758
L4985	Y4715	V4582	K4002	Q3830	X3658	GLU	PHE	N2188	GLU	H1775	M1637	M1152	M1152	A1009	L776
M4993	H4728	V4582	L4013	Q3833	X3661	LYS	GLU	S2243	PRO	H1775	A1638	L1153	L1153	VAL	F777
L4996	G4729	P4587	L4019	Q3833	L3662	LYS	GLU	G2246	GLU	A1764	L1639	D1154	D1154	GLN	F778
G5005	I4737	GLY	L4031	L3842	L3674	THR	PRO	N2246	THR	A1768	R1646	M1158	M1158	ASP	P779
R5017	M4743	ASP	E4032	F3847	D3675	LYS	GLU	L2265	SER	ALA	M1647	I1161	I1161	PRO	S782
L5036	A4746	ASP	G4033	Q3850	D3676	ILE	GLU	G2266	LEU	GLY	D1649	L1164	L1164	ALA	F783
S5037	Y4804	NET	N4034	Q3850	L3677	SER	N2414	L2273	SER	ALA	E1652	L1164	L1164	ARG	S784
	N4805	GLY	M4044	A3853	G3681	THR	L2430	L2277	ARG	E1793	L1653	L1169	L1169	ASN	K788
	N4806	SER	M4047	K3873	L3698	ALA	R2462	A2277	LEU	A1794	Q1660	V1199	V1199	PRO	G794
	F4807	ALA	M4047	K3873	L3698	THR	L2472	L2290	SER	PY795	Q1660	V1199	V1199	PRO	G794
	D4815	GLY	E4075	F3880	E3712	TYR	L2472	L2290	GLY	L1798	H1665	T1236	T1236	M1035	G798
	T4822	ASP	Q4078	L3884	I3728	PRO	L2479	E2292	LEU	L1798	T1666	P1243	P1243	R1044	Y808
	T4825	ALA	V4081	Q3889	C3733	GLU	X2487	D2294	THR	I1802	L1667	Q1244	Q1244	R1044	Y808
	V4848	GLY	R4085	L3891	H3734	GLY	X2502	L2295	VAL	L1807	R1671	R1259	R1259	E1084	L823
	T4852	GLY	I4088	N3896	G3738	S2868	X2587	L2302	ARG	D1828	C1674	M1260	M1260	PRO	H848
	R4860	GLY	T4104	F3899	N3741	R2869	X2591	C2305	VAL	P1840	A1675	C1269	C1269	ASP	D857
	N4864	SER	G4105	Q3900	GLY	Q2872	X2674	N2318	LYS	V1859	L1676	X1457	X1457	GLN	THR
	K4865	GLY	P4106	T3910	ALA	N2884	X2676	N2324	LYS	I1862	R1680	X1473	X1473	PRO	VAL
	E4871	GLY	N4120	T3911	GLY	R2888	P2737	C2326	PRO	M1865	L1685	X1497	X1497	GLN	1870
	K4875	GLY	E4126	S3929	GLY	L2911	K2738	G2327	GLU	E1874	H1688	X1516	X1516	ASN	K873
	C4876	ALA	N4130	Y3937	E3759	K2916	P2739	R2330	GLU	GLU	Q1691	X1519	X1519	SER	K886
	Y4888	GLY	R4131	Y3937	R3762	K2916	P2748	L2332	PRO	GLU	Q1691	X1519	X1519	ARG	1887
	I4901	GLY	E4152	Q3946	Q3766	L2927	L2751	L2335	ALA	GLU	D1700	X1526	X1526	TRP	E888
	P4904	ASP	P4155	N3950	H3771	L2930	I2755	F2337	GLU	GLU	L1707	X1529	X1529	D1070	Q883
	R4913	ASP	H4156	K3955	T3772	K2950	K2770	F2340	GLU	GLU	R1708	P1593	P1593	R1076	G890
	D4917	ASP	F4163	Q3960	G3774	K2954	K2775	V2346	Q2095	GLU	A1709	G1710	G1710	K1079	W891
		GLY	L4166	E3967	L3780	K2959	G2778	E2347	Q2103	GLU	S1717	L1716	L1716	F1092	T892
			R4180	G3971	Q3781	K2963	T2787	E2348	R2104	GLU	H1718	W1605	W1605	V1095	G894
									Q2107	GLU	H1719	W1605	W1605	R1101	R902
										GLU	L1720	M1608	M1608	R1101	L903
										GLU					K952

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: CFF, ZN, CA, ATP

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	0.52	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.30	0/25428	0.54	9/34534 (0.0%)
2	E	0.30	0/25428	0.54	9/34534 (0.0%)
2	G	0.30	0/25428	0.54	9/34534 (0.0%)
2	I	0.30	0/25428	0.54	9/34534 (0.0%)
All	All	0.30	0/105048	0.54	36/142628 (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 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	LEU	CA-CB-CG	7.43	132.38	115.30
2	G	131	LEU	CA-CB-CG	7.42	132.36	115.30
2	I	131	LEU	CA-CB-CG	7.42	132.36	115.30
2	E	131	LEU	CA-CB-CG	7.41	132.34	115.30
2	G	4985	LEU	CA-CB-CG	6.93	131.25	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	13	0
1	F	818	0	824	18	0
1	H	818	0	824	17	0
1	J	818	0	824	19	0
2	B	29499	0	24746	271	0
2	E	29499	0	24745	276	0
2	G	29499	0	24745	266	0
2	I	29499	0	24745	278	0
3	B	31	0	12	2	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102365	1132	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 1132 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:4985:LEU:HB2	3:I:5101:ATP:HN61	1.52	0.74
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.51	0.74
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.51	0.73
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.71	0.73
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.52	0.73

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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	51	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	51	85
2	G	3235/4416 (73%)	2881 (89%)	349 (11%)	5 (0%)	51	85
2	I	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	51	85
All	All	13360/18096 (74%)	11903 (89%)	1437 (11%)	20 (0%)	58	89

5 of 20 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
2	B	4641	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%)	2476 (99%)	17 (1%)	87	93
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	87	93

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

Mol	Chain	Res	Type
2	G	4120	ASN

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Mol	Chain	Res	Type
2	I	1141	ARG
2	E	4034	ASN
2	G	4131	ARG
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	3946	GLN
2	I	479	GLN
2	E	3889	GLN
2	G	3960	GLN
2	G	4806	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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	5101	-	27,33,33	0.89	1 (3%)	25,52,52	1.72	3 (12%)
4	CFF	B	5102	-	7,15,15	1.94	2 (28%)	8,23,23	1.24	1 (12%)
3	ATP	E	5101	-	27,33,33	0.89	1 (3%)	25,52,52	1.70	3 (12%)
4	CFF	E	5102	-	7,15,15	1.95	2 (28%)	8,23,23	1.24	1 (12%)
3	ATP	G	5101	-	27,33,33	0.89	1 (3%)	25,52,52	1.71	3 (12%)
4	CFF	G	5102	-	7,15,15	1.94	2 (28%)	8,23,23	1.23	1 (12%)
3	ATP	I	5101	-	27,33,33	0.89	1 (3%)	25,52,52	1.71	3 (12%)
4	CFF	I	5102	-	7,15,15	1.95	2 (28%)	8,23,23	1.24	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	E	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	G	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	I	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	0/0/0/0	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C6-N1	-4.05	1.32	1.38
4	E	5102	CFF	C6-N1	-4.03	1.32	1.38
4	B	5102	CFF	C6-N1	-4.00	1.32	1.38
4	G	5102	CFF	C6-N1	-3.98	1.32	1.38
4	B	5102	CFF	O13-C6	-2.33	1.18	1.24

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	ATP	N3-C2-N1	-6.29	123.38	128.86
3	G	5101	ATP	N3-C2-N1	-6.27	123.40	128.86
3	I	5101	ATP	N3-C2-N1	-6.25	123.42	128.86
3	E	5101	ATP	N3-C2-N1	-6.20	123.46	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-2.92	111.56	125.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
4	B	5102	CFF	1	0
3	E	5101	ATP	1	0
4	E	5102	CFF	1	0
3	G	5101	ATP	1	0
4	G	5102	CFF	1	0
3	I	5101	ATP	1	0
4	I	5102	CFF	1	0

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	E	4345:UNK	C	4540:PHE	N	73.04
1	B	4345:UNK	C	4540:PHE	N	73.02
1	I	4345:UNK	C	4540:PHE	N	73.01
1	G	4345:UNK	C	4540:PHE	N	73.00
1	E	3613:UNK	C	3639:THR	N	45.97