



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 08:06 PM EDT

PDB ID : 5TAS
EMDB ID: : EMD-8383
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA 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 : 6.20 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 : 1.7.1 (RC1), CSD as537be (2016)
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

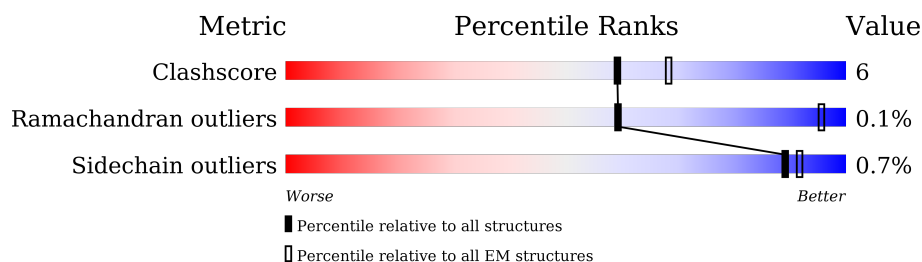
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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	69% 31% .
1	F	108	70% 29% .
1	H	108	71% 28% .
1	J	108	72% 27% .
2	B	4416	82% 12% 5%
2	E	4416	82% 12% 5%
2	G	4416	82% 12% 5%
2	I	4416	83% 12% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

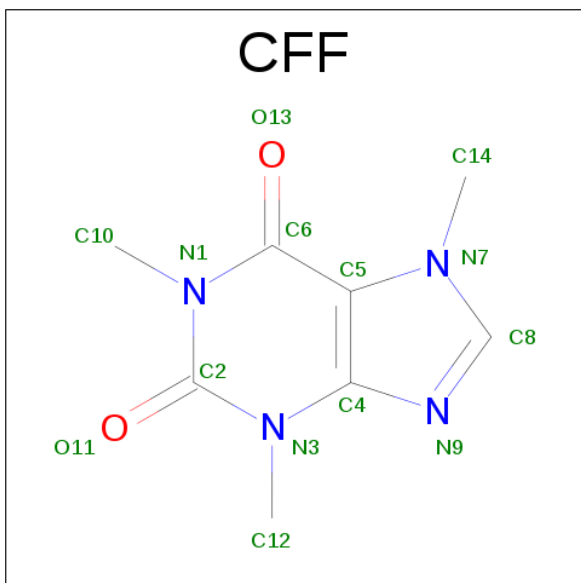
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is 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	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
3	G	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	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

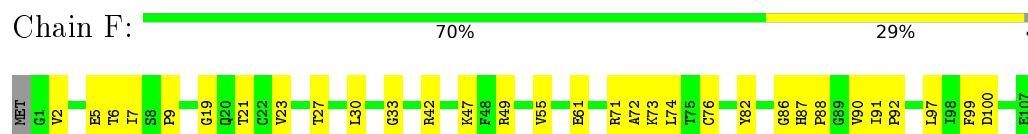
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	

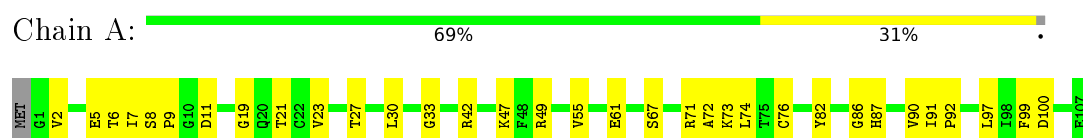
3 Residue-property plots

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.

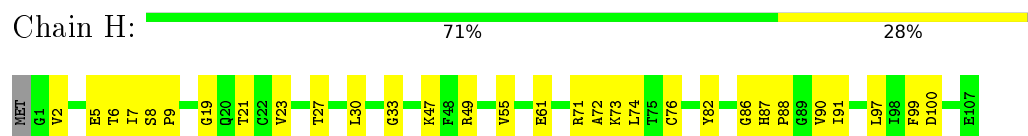
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



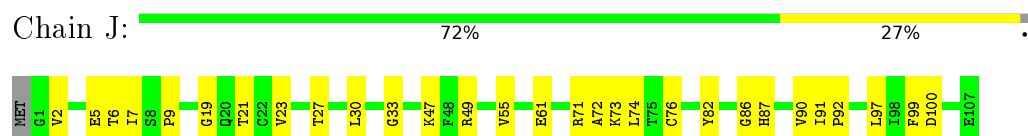
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



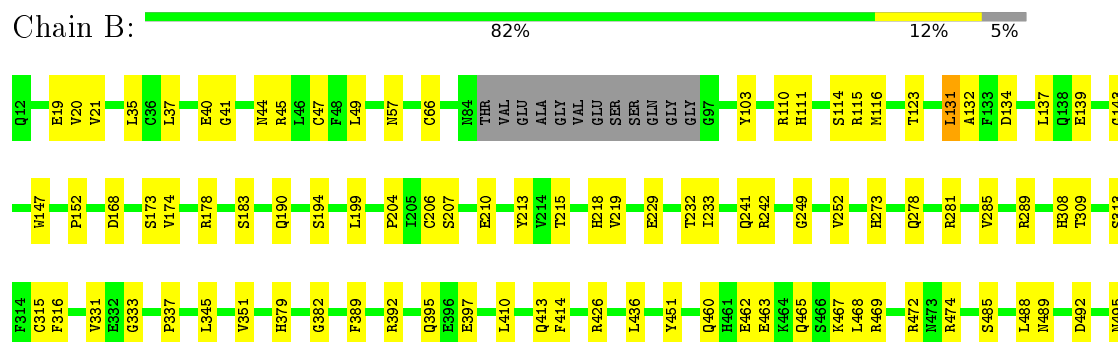
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



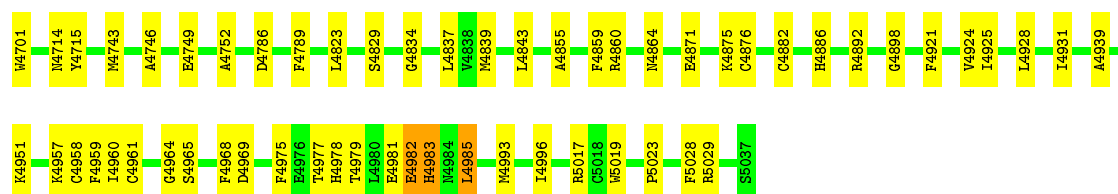
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1

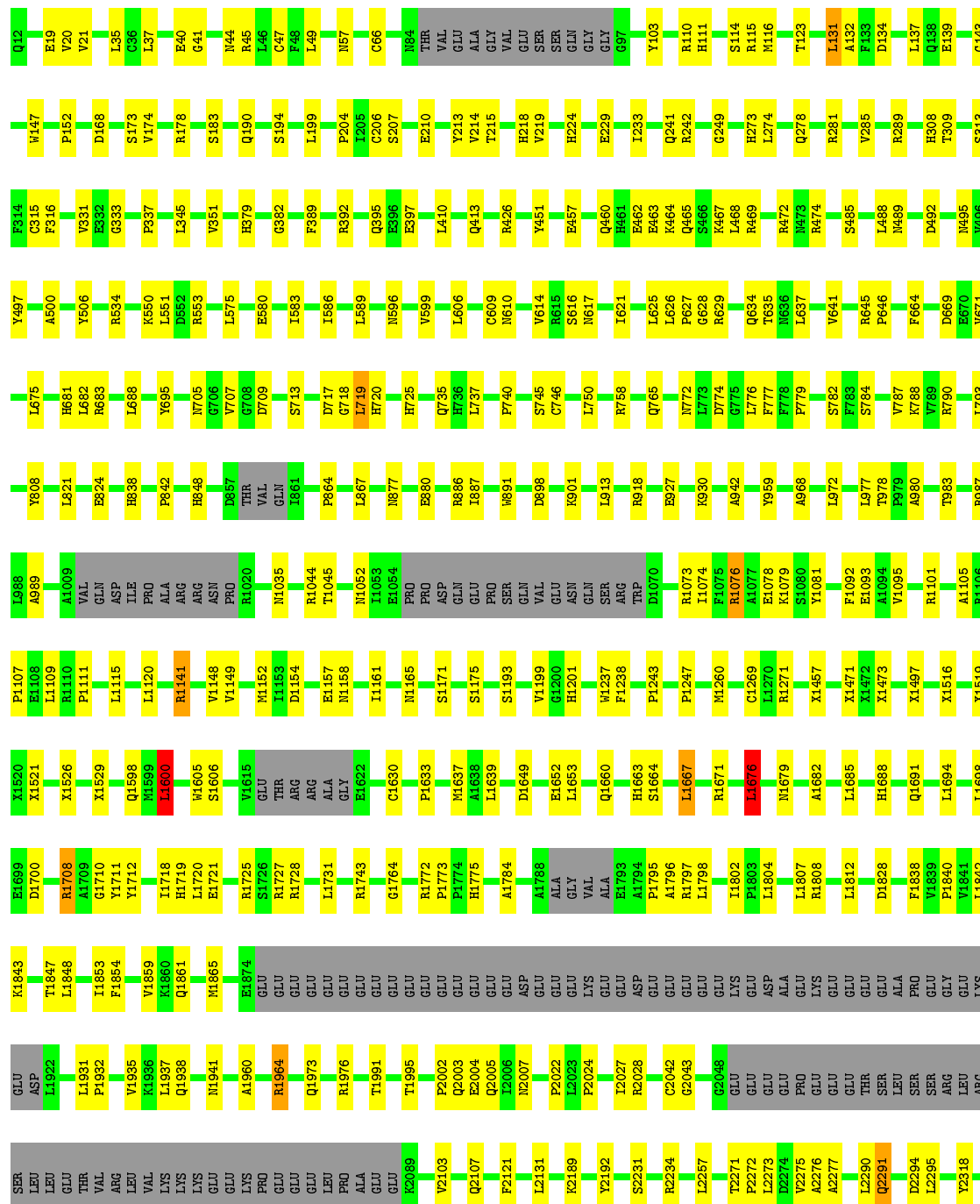


L4013	Q3850	T2762	C2326	LEU	GLU	V1839	Q1691	X1497	A1105	A989	L793	V671	Y496
L4019	A3853	K2770	G2327	ARG	GLY	P1840	Q1691	X1516	R1106	A989	L793	V671	Y497
L4031	K3873	K2775	R2330	LEU	LYS	V1841	L1694	X1516	E1108	A1009	L793	V671	Y497
Y4034	F3880	K2793	F2337	GLU	ASP	K1843	L1694	X1519	L1109	VAL	L821	H681	A500
E4056	L3884	E2803	E2342	VAL	ASP	T1847	L1698	X1520	R1110	GLN	E824	H682	A504
K4060	Q3889	R2806	G2343	VAL	ASP	L1848	E1699	X1521	P1111	ASP	E824	H683	E505
H4064	K3896	K2807	E2347	LYS	LYS	V1853	L1698	X1526	L1115	ILE	H838	L688	Y506
L4068	H3897	K2810	N2351	LYS	LYS	F1854	R1708	X1529	L1120	ALA	H842	Y695	H534
R4085	F3898	L2823	F2395	GLU	GLU	T1854	G1710	X1529	Q1130	ARG	H848	N705	K550
T4104	Q3900	E2830	G2395	GLU	GLU	V1859	Y1711	Q1598	Q1130	ASN	H848	N705	L551
G4105	Y3902	GLU	F2395	GLU	GLU	K1860	Y1712	H1599	P1138	PRO	H848	N705	L551
P4106	T3905	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
G1120	Q3906	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
E4126	T3910	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
N4130	T3911	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
R4131	T3912	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
E4152	Y3922	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
L3926	L3926	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
S3929	S3929	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
E4181	D3932	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
E4182	D3932	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
L4190	K3935	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
Y4194	Y3937	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
P4208	Q3946	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
K4211	K3947	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
R4215	K3949	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
K4230	K3955	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
E4232	Q3960	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
H4558	G3971	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
E4673	F3972	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
E4674	C3973	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
L4681	K3976	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
Y4687	K4002	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
Y4697	L4003	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
K4698	K4698	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
G4699	G4699	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551
Q4700	Q4700	GLU	G2395	GLU	GLU	Q1861	Y1712	H1599	P1138	PRO	H848	N705	L551




• Molecule 2: Ryanodine receptor 1

Chain I: 83% 12% 5%

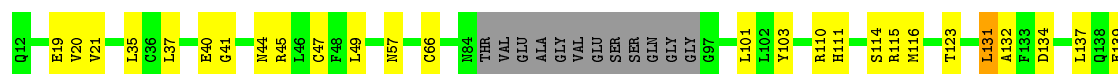


C2326	K2770	L2930	Q3850	S4008	Y4580	V4697	I4931	Q12
G2327	K2775	X3362	Q3853	L4013	K4581	K4698	A4939	E19
R2330	W2775	X3365	A3853	L4019	V4582	G4699	A4957	V20
F2337	P2793	X3366	K3873	L4031	D4584	W4700	K4957	V21
N2342	E2803	X3369	F3880	L4031	P4587	N4714	C4958	L35
G2343	R2806	X3552	L3884	N4034	GLY	Y4715	F4959	C36
E2347	W2807	X3556	L3884	E4056	ASP	I4960	C4961	L37
N2351	K2810	I3662	Q3889	E4056	MET	M4743	G4964	E40
P2395	K2814	I3663	N3896	K4060	GLY	A4746	S4965	G41
GLY	I2823	L3710	N3897	M4064	SER	E4749	F4968	N44
ARG	E2830	T3711	F3899	L4068	ALA	A4752	D4969	R45
ASP	GLU	E3712	Q3900	R4085	GLY	D4786	F4975	C47
ARG	GLU	Y3725	N3901	T4104	ASP	F4789	E4976	F48
ASP	THR	N3741	Y3902	G4105	LEU	T4977	T4977	L49
ARG	GLU	GLY	T3905	P4106	ALA	H4978	L4980	N84
ARG	LYS	ALA	T3910	N4120	GLY	T4979	E4981	THR
GLU	LYS	GLU	T3911	E4126	SER	L4982	E4982	VAL
PHE	LYS	E3747	T3912	N4130	GLY	H4983	L4985	GLU
GLY	THR	Q3767	Y3922	R4131	GLY	M4993	I4996	VAL
GLU	LYS	L3770	L3926	E4152	TRP	I4996	R5017	GLU
PRO	ILE	T3772	S9929	P4155	GLY	R5017	C5018	SER
PRO	SER	L3780	D3932	R4180	GLY	W5019	W5019	GLN
GLU	THR	Q3781	Y3935	E4182	GLU	P5023	P5023	GLY
N2414	TYR	ASP	Y3937	E4182	ALA	F4859	F5028	G97
E2420	ASP	GLY	Q3946	I4190	GLY	N4864	L5036	Y103
L2466	PRO	GLY	K3947	Y4194	ASP	E4871	L5036	R110
I2469	GLY	L3805	K3948	P4208	ASP	K4875	S5037	H111
L2472	Y2855	N3809	K3949	K4211	GLU	C4876		S114
X2493	I2862	K3815	N3950	R4215	M4627	C4882		R115
P2737	S2868	N3816	M3955	R4215	P4641	H4886		M116
E2738	Q2872	L3817	Q3960	K4230	V4666	R4892		T123
P2739	E2880	G3827	G3971	M4231	V4669	G4898		L131
P2748	N2884	Q3830	P3972	E4232	F4673	F4921		A132
L2751	R2888	Q3833	C3973	M4558	E4674	R308		F133
I2756	L2927	S3840	N3976	T4561	L4681	T309		D134
F2758	F2929	L3842	R3984	L4577	Y4687	S313		V301

• Molecule 2: Ryanodine receptor 1

Chain E:  82% 12% 5%

Q12	W147	F314	Y496	V671	L793	R987
E19	P152	C315	Y497	L675	Y808	L988
V20	D168	F316	A500	H681	L821	A989
V21	S173	V331	A504	R682	E824	A1009
L35	V174	E332	E505	R683	P842	VAL
C36	R178	G333	Y506	L688	H848	GLN
L37	E40	P337	R534	Y695	P857	ASP
E40	G41	L345	K550	N705	THR	ILE
G41	N44	V351	L551	G706	VAL	ALA
N44	R45	H379	R553	V707	GLN	ARG
R45	L46	G382	L575	G708	I861	ASN
C47	F48	F389	E580	D709	P864	PRO
L49	L49	R392	I583	S713	L867	N1035
N84	N87	Q395	L589	D717	N877	R1044
THR	C66	E396	N596	G718	E880	T1045
VAL	Y213	E397	W599	H720	R886	N1052
GLU	V214	L410	L606	H725	I887	I1053
ALA	T215	Q413	S616	Q735	W891	E1054
GLY	E229	F414	N617	H736	D898	PRO
VAL	T232	R426	I621	L737	R901	PRO
GLU	T233	R426	L625	P740	L913	ASP
SER	Q241	Y451	L626	Q746	R918	GLN
GLN	R242	Q460	P627	L750	E927	GLU
GLY	R243	H461	L628	R758	R930	ASN
G97	Y103	E462	P628	Q765	G940	SER
	R110	K464	Q628	N772	P941	D1070
	H111	Q465	R629	L773	A942	R1073
	S114	K467	Q634	D774	Y959	I1074
	R115	L468	T635	G775	K1078	F1075
	M116	R469	N636	F777	K1079	A1076
	T123	R472	L637	F778	S1080	A1077
	L131	R474	V641	P779	Y1081	E1078
	A132	S485	R645	S782	F1092	K1079
	F133	R289	P646	S784	E1093	S1080
	D134	V301	N488	T787	T978	Y1094
	L137	R308	N489	K788	P979	Y1095
	Q138	T309	D492	R790	R101	R101
	E139	S313	N495		A1105	A1105






V4924	Q3960	E4232	V4666
I4925	G3971	E4239	V4669
L4928	P3972	N4558	R4673
I4931	C3973	T4561	E4674
A4939	N3976	L4577	L4681
K4957	K4002	Y4580	Y4687
C4958	L4003	K4581	V4697
F4959	S4008	V4582	K4698
I4960	L4013	S4583	G4699
C4961	L4019	D4584	Q4700
G4964	L4019	P4587	M4701
S4965	L4031	GLY	M4714
F4968	L4031	GLU	Y4715
D4969	M4034	ASP	Y4715
F4975	E4056	ASP	M4743
T4977	K4060	MET	A4746
H4978	M4064	GLU	E4749
T4979	L4068	GLY	E4749
L4980	R4085	SER	A4752
E4981	T4104	ALA	K4821
E4982	G4105	ALA	T4822
H4983	P4106	ASP	L4823
M4984	N4120	LEU	L4823
L4985	E4126	ALA	S4829
M4993	M4130	GLY	G4834
I4996	R4131	SER	G4834
Y5014	E4152	GLY	L4837
R5017	R4180	GLY	M4838
C5018	I4181	SER	M4839
W5019	E4182	TRP	A4855
P5023	E4182	GLY	F4859
F5028	R4180	SER	R4860
S5037	I4181	GLY	M4864
	E4182	ALA	E4871
	I4190	GLU	K4875
	Y4194	ALA	C4876
	P4208	GLU	C4882
	K4211	ASP	R4892
	R4215	GLU	G4898
	K4230	M4626	F4921
	M4231	M4627	
		P4641	

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, 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	0.31	0/834	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.29	0/25428	0.53	9/34534 (0.0%)
2	E	0.29	0/25428	0.53	9/34534 (0.0%)
2	G	0.29	0/25428	0.53	9/34534 (0.0%)
2	I	0.29	0/25428	0.53	9/34534 (0.0%)
All	All	0.29	0/105048	0.53	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
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 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.04	133.78	115.30
2	B	131	LEU	CA-CB-CG	8.02	133.75	115.30
2	I	131	LEU	CA-CB-CG	8.01	133.73	115.30
2	E	131	LEU	CA-CB-CG	8.00	133.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1600	LEU	CA-CB-CG	7.20	131.87	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	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	21	0
1	F	818	0	824	20	0
1	H	818	0	824	18	0
1	J	818	0	824	18	0
2	B	29499	0	24746	316	0
2	E	29499	0	24746	322	0
2	G	29499	0	24746	319	0
2	I	29499	0	24746	317	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	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
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102368	1324	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 6.

The worst 5 of 1324 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:4230:LYS:HD2	2:G:4959:PHE:CE2	1.25	1.69
2:E:4230:LYS:HD2	2:E:4959:PHE:CE2	1.25	1.64
2:I:4230:LYS:HD2	2:I:4959:PHE:CE2	1.25	1.60
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	1.25	1.58
2:B:4230:LYS:HD2	2:B:4959:PHE:CZ	1.55	1.42

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%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2929 (90%)	302 (9%)	4 (0%)	56	90
2	E	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	56	90
2	G	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	56	90
2	I	3235/4416 (73%)	2928 (90%)	303 (9%)	4 (0%)	56	90
All	All	13360/18096 (74%)	12101 (91%)	1243 (9%)	16 (0%)	59	90

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

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Mol	Chain	Res	Type
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	1840	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%)	2475 (99%)	18 (1%)	88	94
2	E	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
All	All	10324/12444 (83%)	10252 (99%)	72 (1%)	89	94

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	4131	ARG
2	E	1141	ARG
2	G	4085	ARG
2	I	4839	MET
2	E	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	3946	GLN

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Mol	Chain	Res	Type
2	E	379	HIS
2	G	3946	GLN
2	I	3960	GLN
2	I	4142	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 12 ligands modelled in this entry, 4 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	-	26,33,33	0.94	1 (3%)	26,52,52	1.66	2 (7%)
4	CFF	B	5102	-	8,15,15	2.21	3 (37%)	8,23,23	1.25	1 (12%)
3	ATP	E	5101	-	26,33,33	0.94	1 (3%)	26,52,52	1.65	2 (7%)
4	CFF	E	5102	-	8,15,15	2.20	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	G	5101	-	26,33,33	0.95	1 (3%)	26,52,52	1.66	2 (7%)
4	CFF	G	5102	-	8,15,15	2.21	3 (37%)	8,23,23	1.25	1 (12%)
3	ATP	I	5101	-	26,33,33	0.95	1 (3%)	26,52,52	1.67	2 (7%)
4	CFF	I	5102	-	8,15,15	2.20	3 (37%)	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 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C4-N3	-4.04	1.34	1.39
4	G	5102	CFF	C4-N3	-4.03	1.34	1.39
4	B	5102	CFF	C4-N3	-4.00	1.34	1.39
4	E	5102	CFF	C4-N3	-4.00	1.34	1.39
4	B	5102	CFF	C6-N1	-3.79	1.32	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	N3-C2-N1	-6.79	123.54	128.87
3	G	5101	ATP	N3-C2-N1	-6.73	123.58	128.87
3	B	5101	ATP	N3-C2-N1	-6.73	123.58	128.87
3	E	5101	ATP	N3-C2-N1	-6.69	123.61	128.87
4	B	5102	CFF	C14-N7-C8	-2.58	111.86	125.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 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	2	0
4	E	5102	CFF	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	5101	ATP	2	0
4	G	5102	CFF	1	0
3	I	5101	ATP	2	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	B	4345:UNK	C	4540:PHE	N	73.19
1	I	4345:UNK	C	4540:PHE	N	73.19
1	E	4345:UNK	C	4540:PHE	N	73.19
1	G	4345:UNK	C	4540:PHE	N	73.19
1	B	3613:UNK	C	3639:THR	N	44.63