



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 08:53 PM UTC

PDB ID : 5TAM / pdb_00005tam
EMDB ID : EMD-8379
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-10
Resolution : 4.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

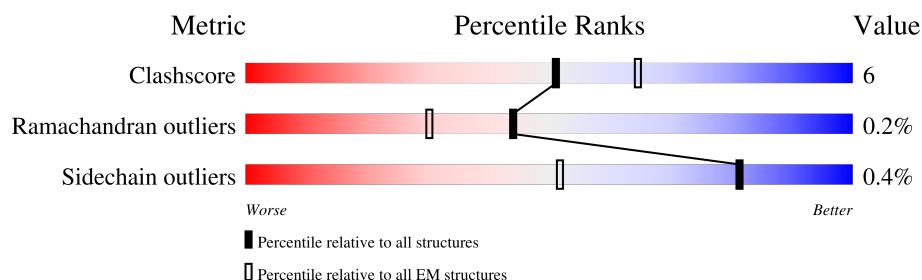
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	79% 20% .
1	F	108	79% 20% .
1	H	108	79% 20% .
1	J	108	79% 20% .
2	B	4416	83% 11% 5%
2	E	4416	83% 11% 5%
2	G	4416	83% 11% 5%
2	I	4416	83% 11% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	B	5102	-	X	-	-
4	CFF	E	5102	-	X	-	-
4	CFF	G	5102	-	X	-	-
4	CFF	I	5102	-	X	-	-

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.

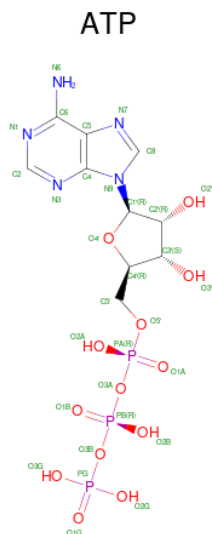
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

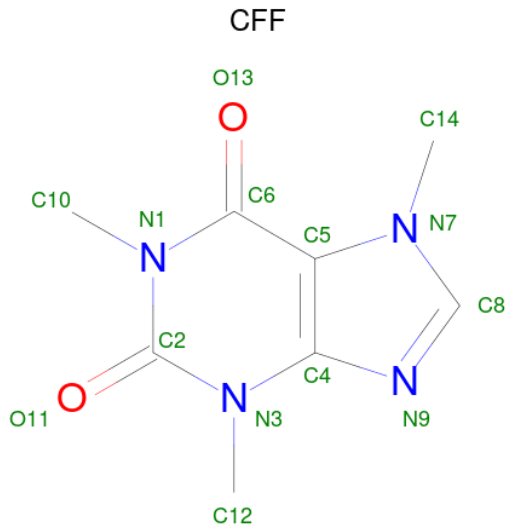
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
3	B	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	I	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 (CCD ID: 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	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 



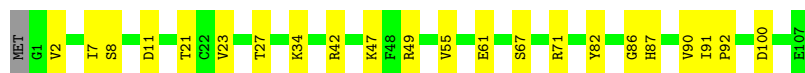
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 



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

Chain H: 



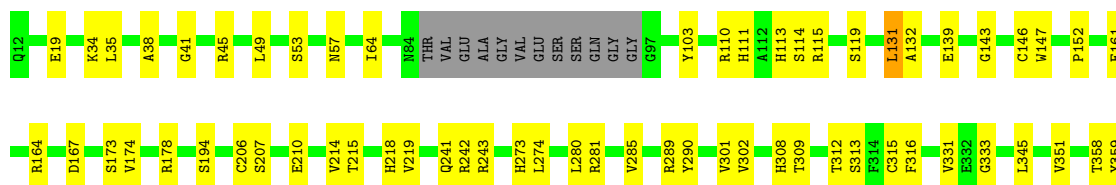
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 

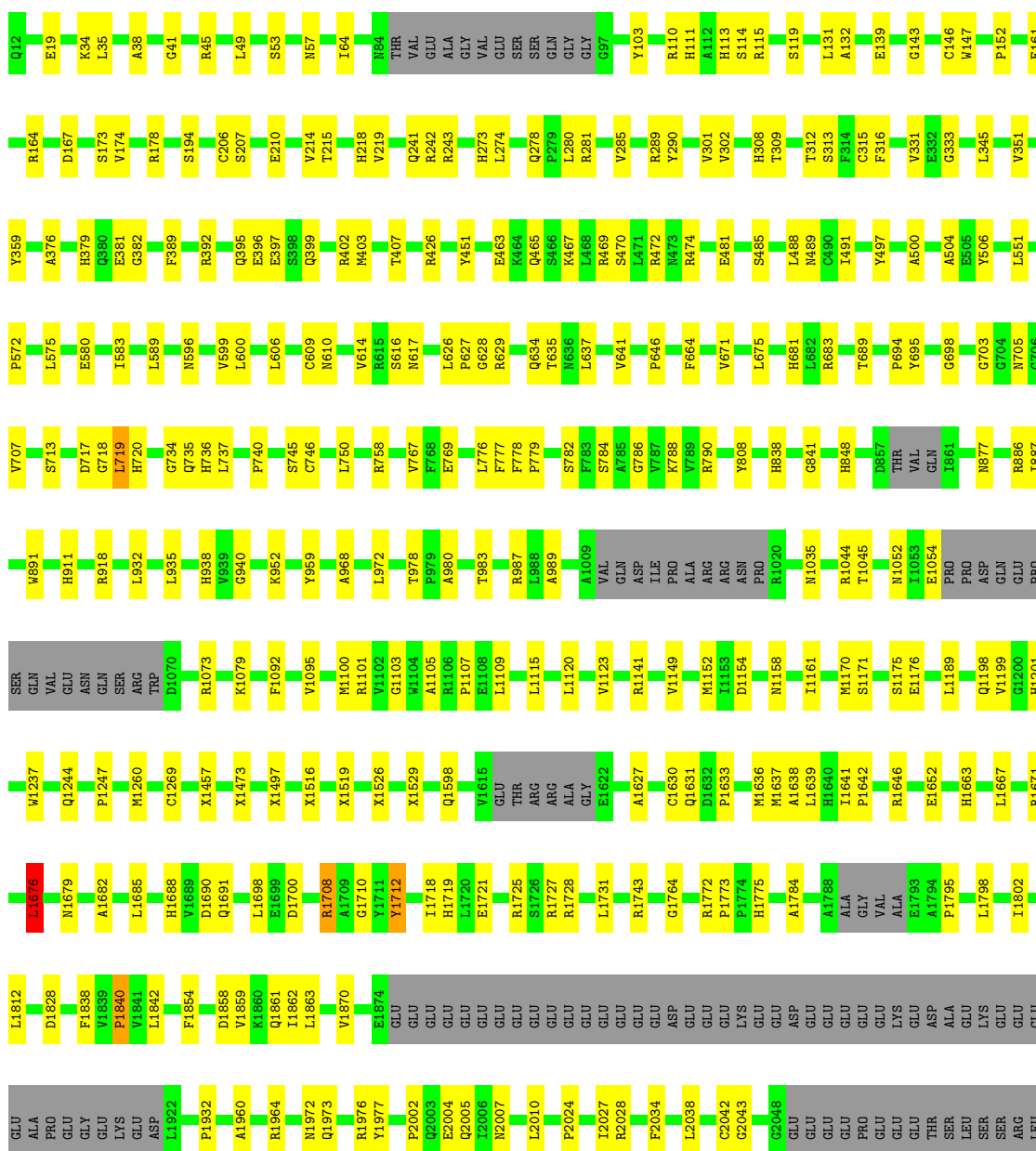


- Molecule 2: Ryanodine receptor 1

Chain B: 



E4032	N3741	S2261	L2466	LYS	VAL	PRO	F1838	D1690	P1247	GLU	H911	S713	L575	A376
V4036	GLY	M2267	L2469	LYS	ARG	GLY	V1839	Q1691	M1260	ASN	R918	D717	E580	H379
V4049	ALA	Q2268	I2469	GLY	LEU	GLY	P1840	L1695	P1840	GLN	R932	G718	E583	Q380
D4063	GLU	Q2291	L2472	LYS	LYS	LYS	V1841	L1698	C1269	ARG	L935	L719	L589	E381
L4066	ILE	D2294	X2493	ASP	LYS	ASP	L1842	E1699	X1487	TRP	H938	H720	L606	G382
Y4080	SER	L2295	X2502	L1922	GLY	L1922	F1854	D1700	X1473	D1070	G940	G734	L609	F389
D4083	GLN	V2299	X2517	P1932	LYS	P1932	D1858	A1708	X1497	R1073	V939	H735	N596	R392
P4084	ALA	A2303	X2521	A1960	PRO	A1960	V1859	G1710	X1516	E1078	G940	L737	V599	Q395
R4085	GLN	C2326	X2674	R1964	GLY	R1964	V1860	Y1711	X1519	K1079	K952	P740	L600	E396
G4086	THR	G2327	X2675	M1972	LEU	M1972	Q1861	Y1712	X1519	S1080	Y959	S745	L606	E397
A4096	ARG	R2330	X2676	Q1973	ALA	Q1973	I1863	H1718	X1526	F1092	A968	C746	C609	Q399
T4104	GLY	N2342	P2739	R1976	GLY	R1976	V1870	H1719	X1529	V1095	L972	L750	N610	R402
P4106	GLY	G2343	P2748	Y1977	GLY	Y1977	E1874	L1720	Q1598	M1100	L978	R758	V614	M403
E4126	GLY	V2346	L2751	P2002	GLY	P2002	GLY	R1725	Q1598	R1101	T978	E769	R615	T407
N4130	ARG	E2347	L2755	Q2003	GLY	Q2003	GLY	S1726	M1599	V1102	P979	F767	S616	N617
R4148	ARG	E2348	L2758	E2004	GLY	E2004	GLY	R1727	L1600	G1103	A980	F768	Q634	R426
E4152	ARG	N2349	L2762	Q2005	GLY	Q2005	GLY	R1728	Y1615	A1104	T983	E769	T635	Y451
R4159	ARG	P2395	L2763	I2006	GLY	I2006	GLY	L1731	GLY	R1106	R987	L776	L636	E463
S4169	ARG	GLY	H2763	N2007	GLY	N2007	GLY	R1743	THR	P1107	L988	F777	L637	K464
Y4173	ARG	VAL	E2764	L2010	GLY	L2010	GLY	G1764	ARG	L1109	A989	F779	L637	Q465
L4178	ARG	ARG	E2770	P2024	GLY	P2024	GLY	A1784	ALA	L1115	A1009	S782	L636	S466
R4180	ARG	ARG	K2770	I2027	GLY	I2027	GLY	A1788	GLY	L1120	VAL	F783	L637	K467
L4190	ARG	ARG	W2775	R2028	GLY	R2028	GLY	GLY	GLY	L1123	GLN	F783	L637	L468
Q4209	ARG	ARG	N2775	C2042	GLY	C2042	GLY	ALA	ALA	V1129	ASP	A785	L637	R469
R4215	ARG	ARG	N2780	G2043	GLY	G2043	GLY	ALA	ALA	V1149	PRO	G786	L637	S470
A4228	ARG	ARG	N2787	G2048	GLY	G2048	GLY	ALA	ALA	M1152	ALA	V787	L637	R472
E4232	ARG	ARG	T2787	GLY	GLY	GLY	GLY	ALA	ALA	M1153	ARG	K788	L637	M473
S4236	ARG	ARG	P2793	GLY	GLY	GLY	GLY	VAL	VAL	D1154	ASN	Y808	L637	R474
Y4560	ARG	ARG	E2803	PRO	GLY	PRO	GLY	ALA	ALA	M1158	PRO	H838	L637	S485
F4571	ARG	ARG	R2806	GLY	GLY	GLY	GLY	E1793	R1646	I1161	N1035	G841	L637	L488
	THR	THR	W2807	GLY	GLY	GLY	GLY	A1794	E1652	M1170	R1044	H848	L637	M489
	GLY	GLY	N2414	THR	THR	THR	THR	P1795	E1671	E1176	T1045	D857	L637	C490
	GLY	GLY	L2215	LEU	LEU	LEU	LEU	L1798	R1671	L1189	N1052	THR	L637	I491
	GLY	GLY	P2226	SER	SER	SER	SER	I1802	L1676	L1198	E1054	VAL	L637	Y497
	GLY	GLY	V2229	SER	SER	SER	SER	P1803	L1679	Q1198	PRO	GLN	L637	A500
	GLY	GLY	T2230	ARG	ARG	ARG	ARG	L1804	A1682	V1199	ASP	GLN	L637	A504
	GLY	GLY	S2231	LEU	LEU	LEU	LEU	R1808	A1682	H1200	GLN	GLN	L637	E505
	GLY	GLY	R2234	ARG	ARG	ARG	ARG	D1809	L1685	H1201	PRO	GLN	L637	Y506
	GLY	GLY	N2246	ARG	ARG	ARG	ARG	K1810	L1685	W1237	PRO	GLN	L637	G703
	GLY	GLY	K2447	LEU	LEU	LEU	LEU	A1811	H1688	Q1244	GLN	GLN	L637	G704
	GLY	GLY	E2449	LEU	LEU	LEU	LEU	L1812	H1688		VAL	GLN	L637	L551
	GLY	GLY	R2452	THR	THR	THR	THR	D1828	V1689			GLN	L637	P572
	GLY	GLY	I2453											



V4924	K4680	L4577	E4032	GLY	THR	L2472	Q2291	LYS	GLU	V1841	Q1691	X1473	ASN	H891
L4928	L4686	Y4580	V4036	ALA	ARG	X2493	D2294	LYS	ASP	L1842	L1698	X1497	GLN	H911
L4935	Y4687	V4582	GLU	ILE	GLU	L2295	L2295	GLU	L1922	F1854	E1699	H911	SER	H911
K4698	K4699	P4587	M4047	GLN	GLN	X2502	V2299	LYS	P1932	D1858	D1700	X1516	TRP	R918
C4968	Y4714	ASP	L4048	THR	ALA	X2517	A2303	PRO	A1960	V1859	R1708	X1519	R1073	L932
F4969	Y4715	ASP	D4063	GLN	GLN	X2521	C2326	GLU	R1964	Q1861	G1710	X1526	K1079	L935
C4961	A4738	MET	L4066	THR	THR	X2674	C2327	LEU	N1972	L1862	Y1712	X1529	F1092	H938
I4963	M4743	GLY	D4083	PRO	ASP	X2675	R2330	PRO	Q1973	L1863	I1718	Q1598	V1095	G940
G4964	A4746	ALA	P4084	ARG	ARG	X2676	N2342	ALA	R1976	V1870	H1719	L1600	M1100	K952
E4975	E4976	GLY	G4086	GLY	GLY	P2739	G2343	GLU	Y1977	E1874	E1721	L1599	R1101	K952
T4977	E4749	GLY	Y2855	GLU	GLU	P2748	Y2856	GLU	P2002	GLU	R1725	V1615	Y959	Y959
H4978	A4752	LEU	P2857	GLU	GLU	L2751	F2347	Q2095	Q2005	GLU	S1726	GLU	A1105	A968
T4979	A4763	GLY	L2862	GLY	GLY	I2755	E2348	R2104	L2010	GLU	R1727	THR	R1106	A968
E4982	G4763	ALA	S2868	GLY	GLY	F2758	N2349	Q2107	L2038	GLU	R1728	ARG	P1107	L972
H4983	T4766	GLY	Q2872	GLY	GLY	T2762	P2395	Q2127	C2042	ASP	L1731	GLY	L1109	L972
L4985	M4796	GLY	N2884	GLY	GLY	H2763	VAL	L2131	G2043	GLU	R1743	E1622	L1115	P978
A4986	V4797	GLY	L2927	GLY	GLY	E2764	ARG	L2167	G2048	GLU	G1764	C1630	L1120	A980
Y4988	M4798	SER	K2928	GLY	GLY	K2770	ASP	I2167	F2034	GLU	P1772	P1633	V1149	T983
F4990	L4801	TRP	F2929	GLY	GLY	W2775	ARG	M2178	L2038	GLU	P1773	P1633	L1152	R987
M4993	F4807	SER	L2930	GLY	GLY	N2780	GLU	N2196	C2042	ASP	H1775	M1636	L1153	A1009
I4996	T4822	GLY	Q2931	GLY	GLY	T2787	HIS	R2199	G2043	GLU	A1784	M1637	D1154	VAL
G5005	L4824	GLY	V2937	GLY	GLY	T2787	PHE	R2199	G2048	GLU	A1788	A1638	N1158	GLN
R5017	T4825	GLU	X3362	GLY	GLY	P2783	GLU	E2208	GLU	LYS	ALA	L1646	I1161	ILE
D5026	M4833	ALA	X3365	GLY	GLY	E2803	PRO	E2209	GLU	ASP	VAL	E1652	M170	ARG
C5027	L4843	GLY	X3366	GLY	GLY	R2806	PRO	V2210	PRO	GLU	ALA	L1653	ARG	ALA
F5028	V4848	ASP	X3369	GLY	GLY	W2807	GLU	P2226	GLU	GLU	E1793	Q1660	ASN	ARG
Y5032	T4852	GLU	H3647	GLY	GLY	K2810	N2414	V2229	GLU	GLU	A1794	Q1660	PRO	ASN
Q5035	R4860	GLY	N3651	GLY	GLY	K2814	H2420	T2230	THR	GLU	P1795	H1663	R1020	R1020
S5037	Y4863	GLY	N3658	GLY	GLY	L2823	T2430	S2231	SER	LYS	L1798	L1667	Q1198	R1044
	M4864	GLY	X3661	GLY	GLY	R2827	P2438	N2246	LEU	ASP	I1802	L1671	V1199	T1045
	K4865	GLY	I3662	GLY	GLY	E2830	S2448	H2283	SER	ASP	P1803	R1671	G1200	N1052
	K4875	GLY	L3710	GLY	GLY	GLU	K2447	H2283	SER	ALA	L1804	L1676	H1201	N1053
	C4876	GLY	T3711	GLY	GLY	ARG	G2448	H2283	LEU	GLY	L1812	N1679	W1237	E1054
	P4904	GLY	E3712	GLY	GLY	THR	E2449	L2257	LEU	ALA	P1247	A1682	Q1244	PRO
	R4913	GLY	Y3722	GLY	GLY	GLU	L2466	S2261	THR	PRO	M1260	L1685	M1260	PRO
		GLY	K3741	GLY	GLY	LYS	L2469	M2287	VAL	GLY	C1269	H1688	C1269	SER
		GLY	N3741	GLY	GLY	LYS	T2469	Q2268	ARG	GLY	V1689	Y1689	GLN	GLN
		GLY		GLY	GLY	LYS			VAL	LYS	P1840	D1690	VAL	VAL
		GLY		GLY	GLY	LYS			VAL	LYS			GLU	GLU

Chain G: 83% 11% 5%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, CA, CFF, ZN

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/834	0.47	0/1123
1	F	0.20	0/834	0.47	0/1123
1	H	0.20	0/834	0.47	0/1123
1	J	0.20	0/834	0.47	0/1123
2	B	0.23	0/25428	0.53	3/34534 (0.0%)
2	E	0.23	0/25428	0.53	3/34534 (0.0%)
2	G	0.23	0/25428	0.53	3/34534 (0.0%)
2	I	0.23	0/25428	0.53	3/34534 (0.0%)
All	All	0.23	0/105048	0.53	12/142628 (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 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4639	MET	CA-C-N	5.09	134.21	121.80
2	G	4639	MET	C-N-CA	5.09	134.21	121.80
2	B	4639	MET	CA-C-N	5.08	134.21	121.80
2	B	4639	MET	C-N-CA	5.08	134.21	121.80
2	I	4639	MET	CA-C-N	5.08	134.20	121.80

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	15	0
1	F	818	0	824	14	0
1	H	818	0	824	13	0
1	J	818	0	824	15	0
2	B	29499	0	24747	302	0
2	E	29499	0	24747	303	0
2	G	29499	0	24747	304	0
2	I	29499	0	24748	304	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	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	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	102373	1235	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 1235 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:4975:PHE:O	2:B:4979:THR:HG23	1.85	0.77
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.85	0.76
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.86	0.76
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.86	0.76
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.78	0.71

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%)	98 (93%)	7 (7%)	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%)	98 (93%)	7 (7%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2892 (89%)	338 (10%)	5 (0%)	43	77
2	G	3235/4416 (73%)	2890 (89%)	340 (10%)	5 (0%)	43	77
2	I	3235/4416 (73%)	2889 (89%)	340 (10%)	6 (0%)	43	77
All	All	13360/18096 (74%)	11954 (90%)	1384 (10%)	22 (0%)	44	77

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
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	2033/3022 (67%)	2026 (100%)	7 (0%)	86	84
2	E	1878/3022 (62%)	1871 (100%)	7 (0%)	84	82
2	G	2470/3022 (82%)	2461 (100%)	9 (0%)	84	82
2	I	2016/3022 (67%)	2007 (100%)	9 (0%)	84	82
All	All	8749/12444 (70%)	8717 (100%)	32 (0%)	81	82

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	3663	LEU

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Mol	Chain	Res	Type
2	G	3805	LEU
2	E	4960	ILE
2	E	3805	LEU
2	G	4960	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 208 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	1678	ASN
2	I	4246	GLN
2	G	4246	GLN
2	I	1693	GLN
2	I	3809	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 oligosaccharides 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	E	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.66	9 (18%)
4	CFF	I	5102	-	15,15,15	1.99	7 (46%)	23,23,23	2.74	11 (47%)
4	CFF	B	5102	-	15,15,15	1.99	7 (46%)	23,23,23	2.74	11 (47%)
4	CFF	G	5102	-	15,15,15	1.99	7 (46%)	23,23,23	2.75	11 (47%)
3	ATP	G	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.67	9 (18%)
3	ATP	B	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.67	9 (18%)
3	ATP	I	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.67	9 (18%)
4	CFF	E	5102	-	15,15,15	1.99	7 (46%)	23,23,23	2.74	11 (47%)

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	E	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	6/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	6/22/38/38	0/3/3/3
3	ATP	I	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	ATP	C5-C4	4.46	1.47	1.39
3	I	5101	ATP	C5-C4	4.46	1.47	1.39
3	G	5101	ATP	C5-C4	4.43	1.47	1.39
3	E	5101	ATP	C5-C4	4.41	1.46	1.39
4	G	5102	CFF	C6-N1	-3.85	1.32	1.40

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	5102	CFF	C14-N7-C8	-7.78	111.73	126.28
4	B	5102	CFF	C14-N7-C8	-7.76	111.76	126.28
4	E	5102	CFF	C14-N7-C8	-7.76	111.76	126.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-7.75	111.77	126.28
3	I	5101	ATP	C5-C4-N3	-5.48	119.17	126.72

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

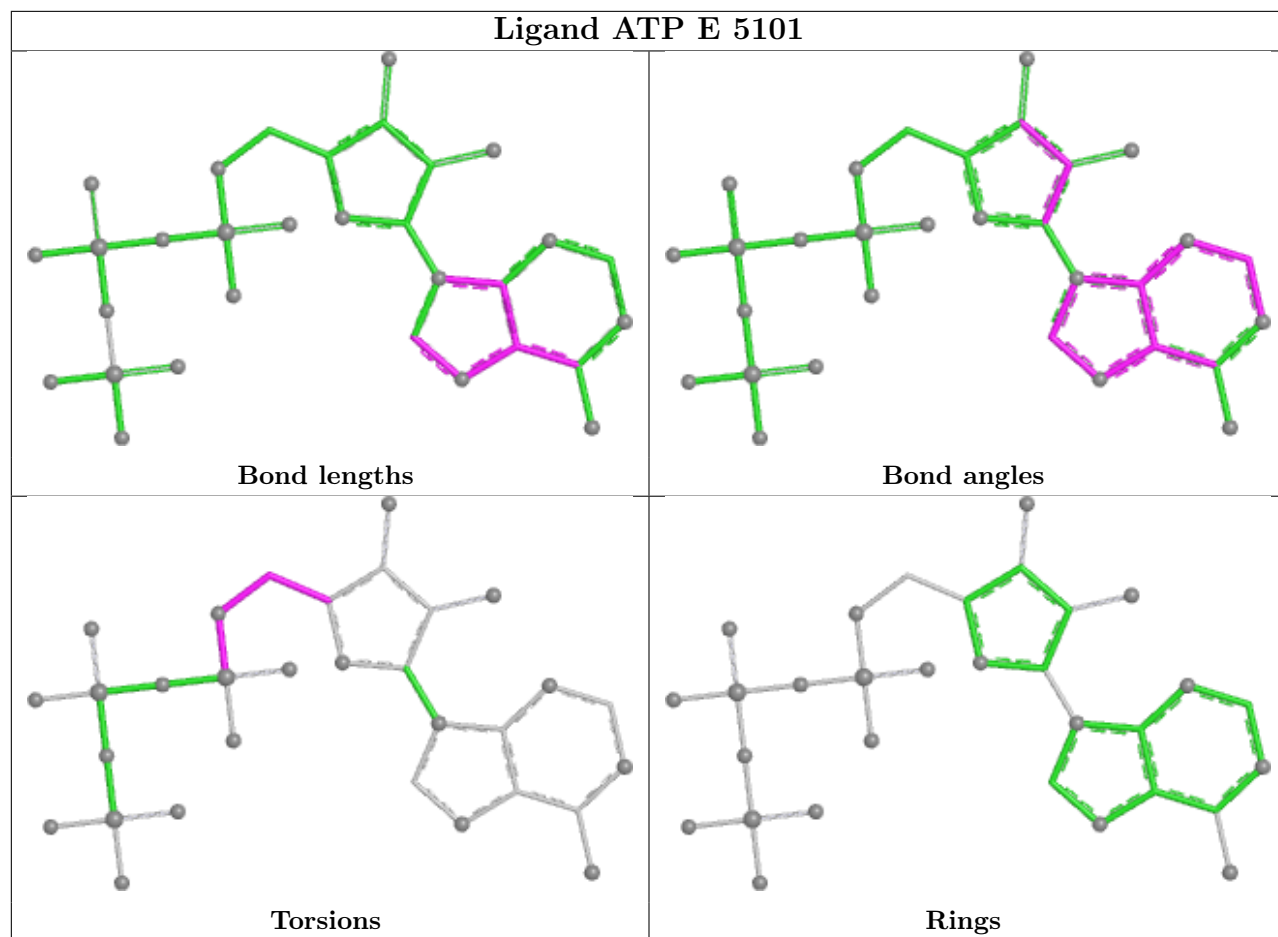
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O2A

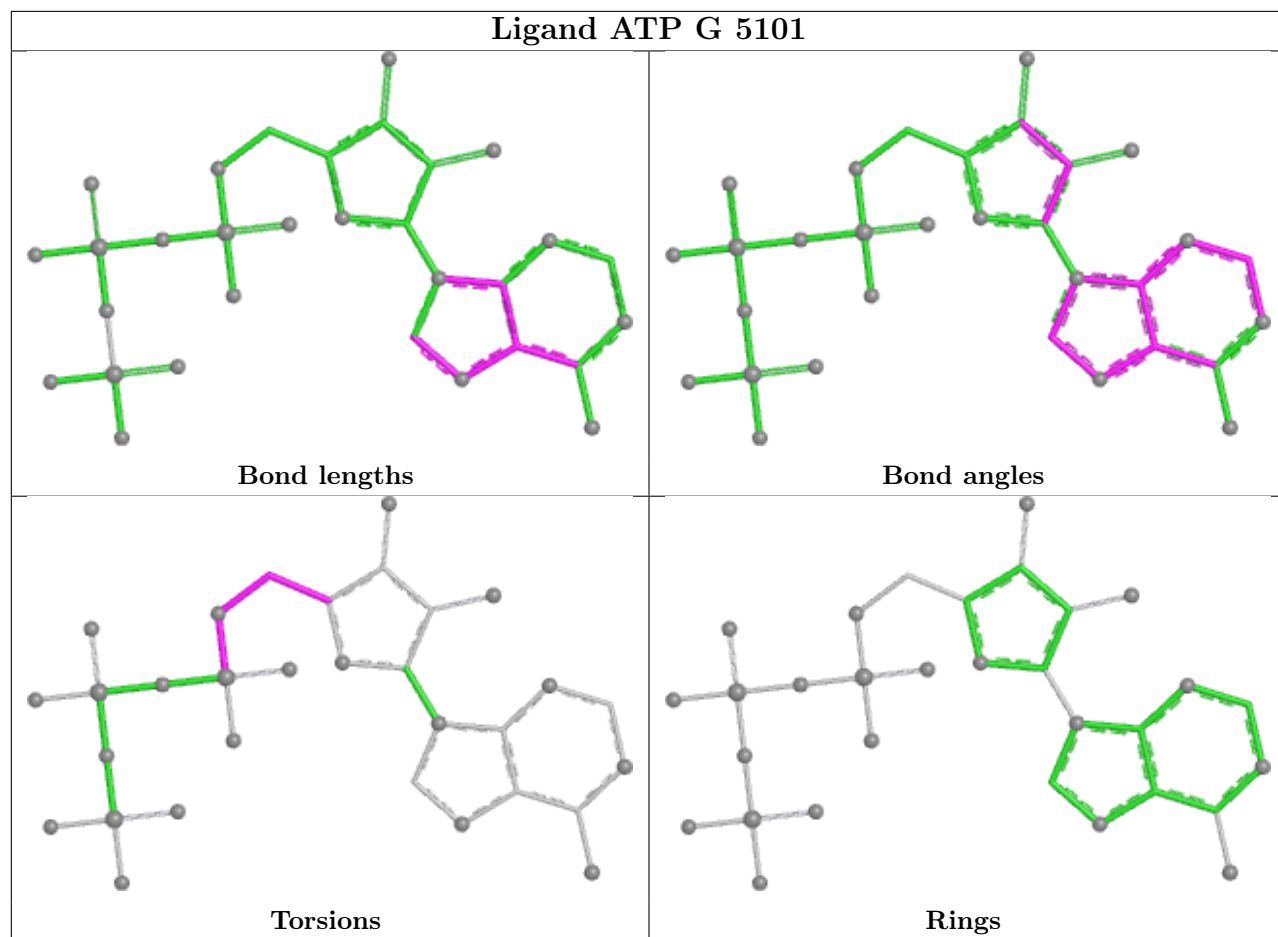
There are no ring outliers.

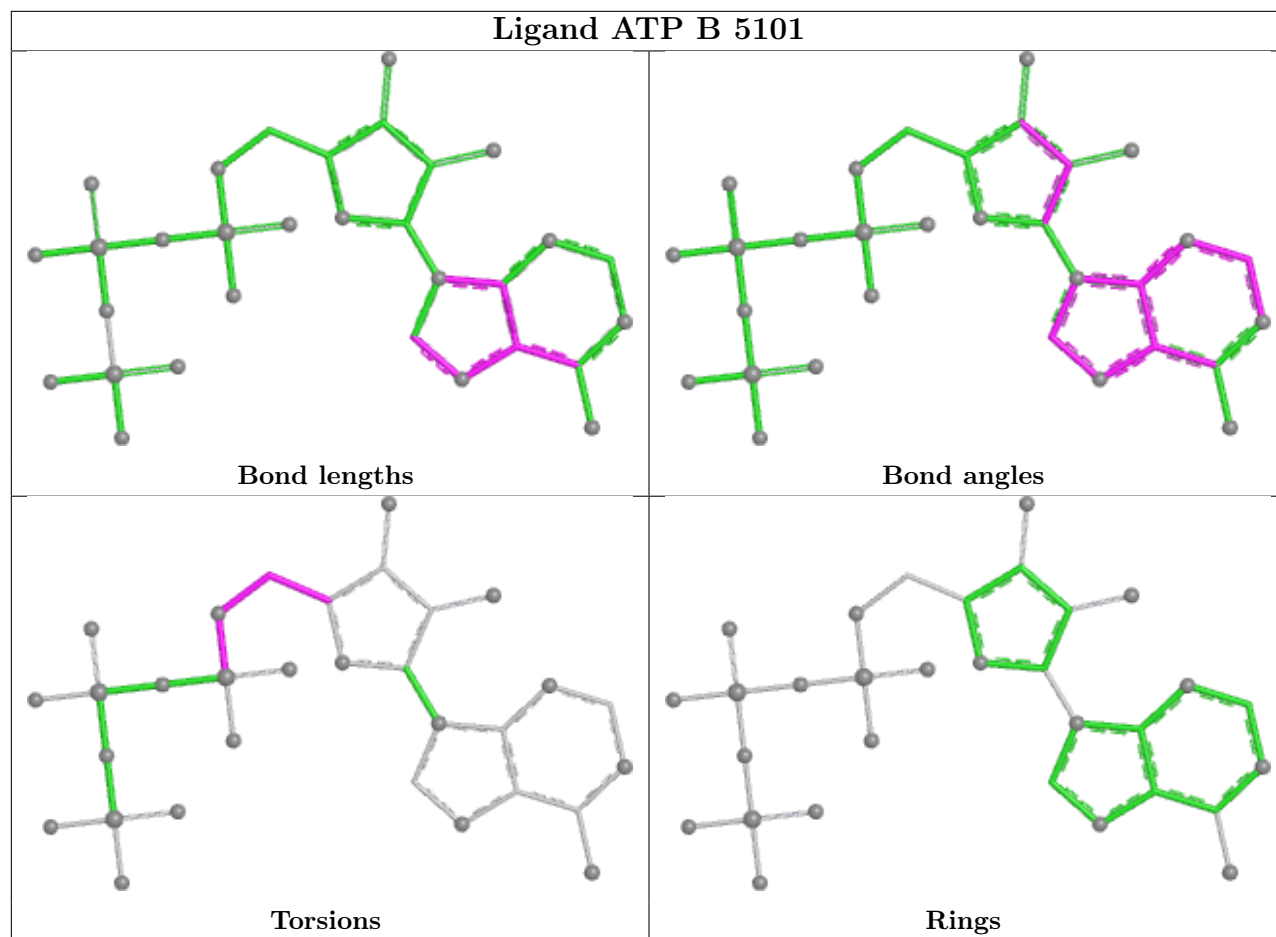
4 monomers are involved in 8 short contacts:

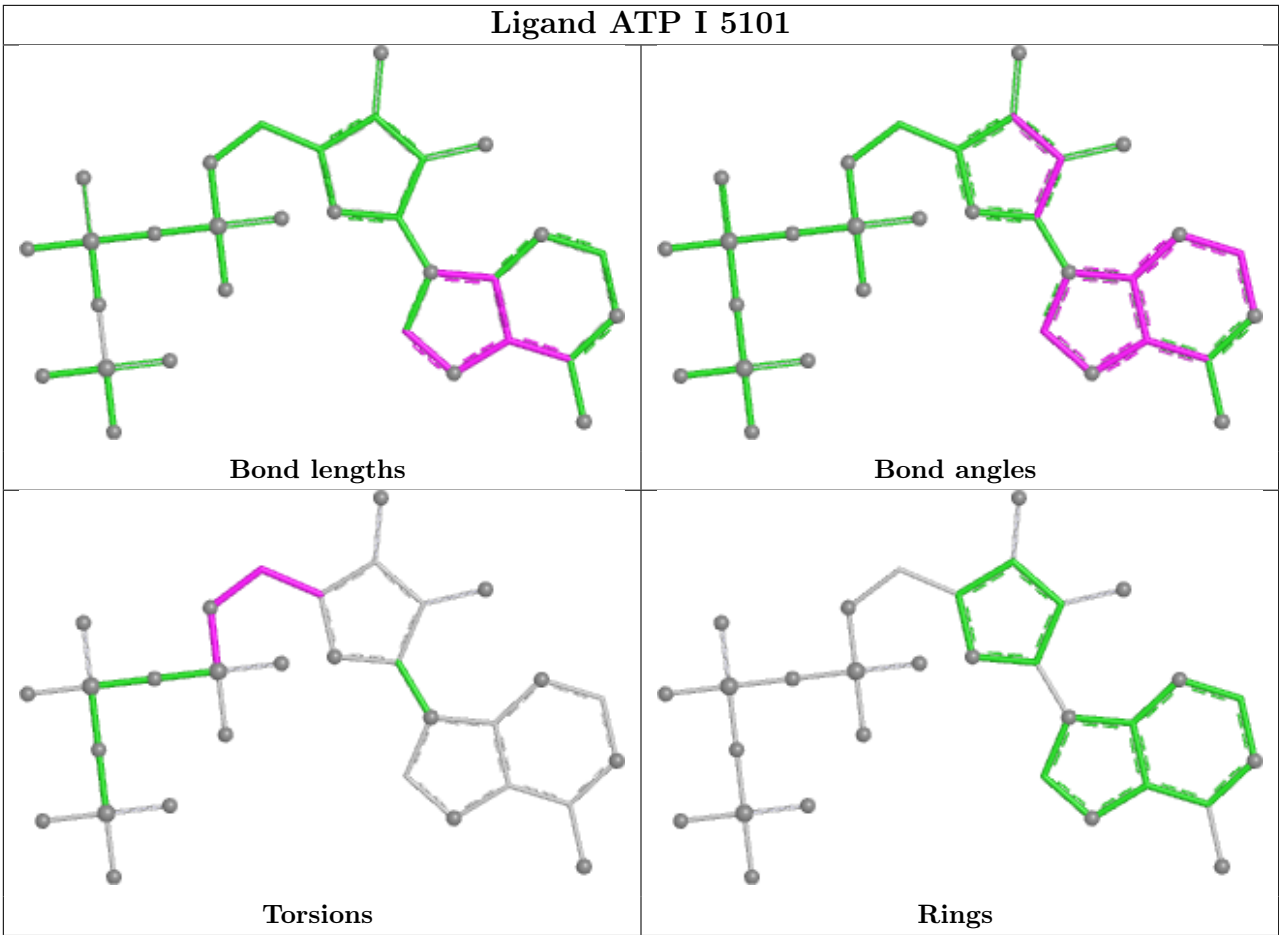
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	2	0
3	G	5101	ATP	2	0
3	B	5101	ATP	2	0
3	I	5101	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	B	14
2	E	14
2	I	14
2	G	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	72.88
1	E	4345:UNK	C	4540:PHE	N	72.88

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.88
1	G	4345:UNK	C	4540:PHE	N	72.88
1	B	3613:UNK	C	3639:THR	N	43.44

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8379. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.