



## wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 07:39 PM EDT

PDB ID : 5TAV  
EMDB ID: : EMD-8386  
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA 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 : 4.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

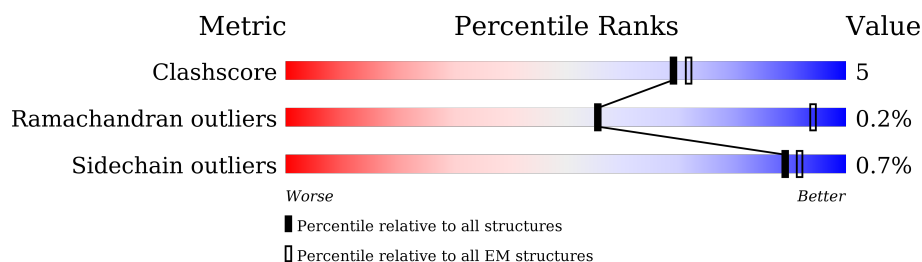
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 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  $\geq 3$ , 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	92% 7% .
1	F	108	91% 8% .
1	H	108	92% 7% .
1	J	108	93% 6% .
2	B	4416	84% 10% 5%
2	E	4416	84% 10% 5%
2	G	4416	85% 10% 5%
2	I	4416	84% 10% 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.

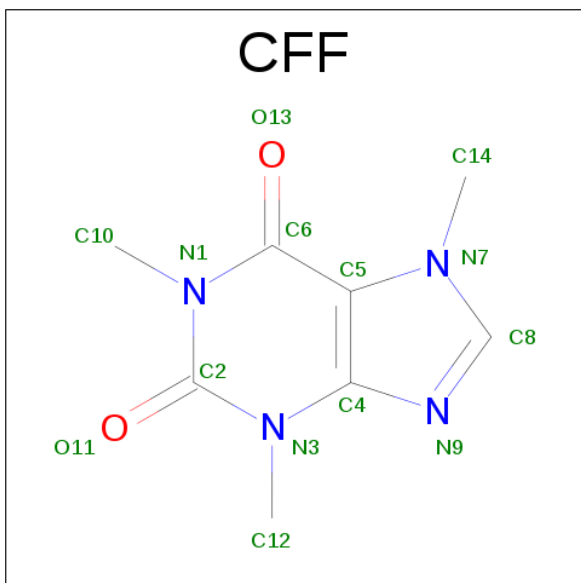
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (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	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 (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	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 (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 [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 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: 




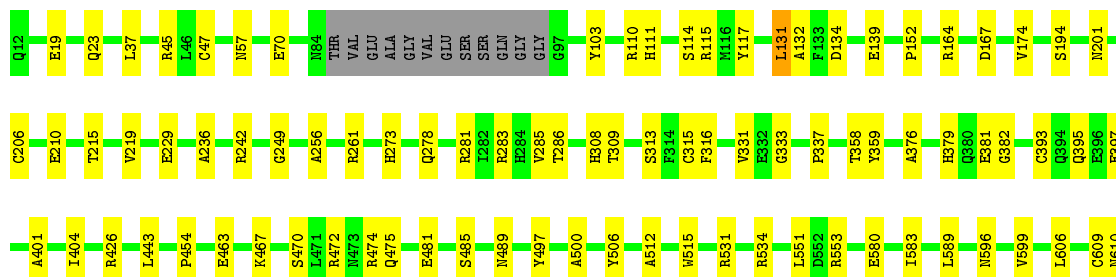
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 




- Molecule 2: Ryanodine receptor 1

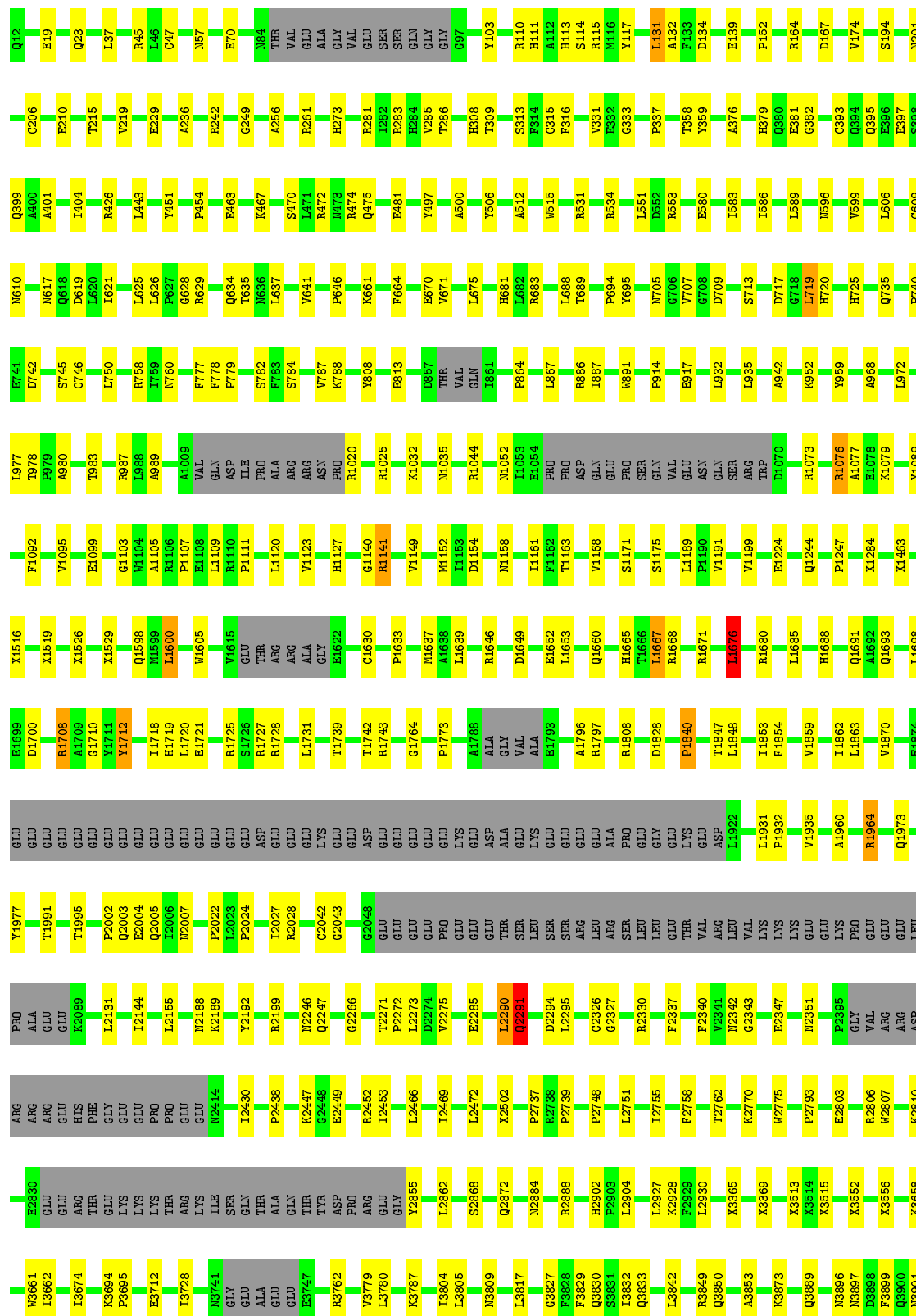
Chain B: 



I4996	M4714	A4566	V3961	GLU	SER	N2414	R2199	C2042	GLU	L1731	ARG	R1106	T983	S745	M617
M4997	Y4715	L4567	F3962	GLU	GLN	I2430	N2246	G2043	ASP	L1739	ALA	P1107	T983	C746	M618
K4998	M4743	V4582	N3963	THR	ALA	I2438	Q2247	G2048	GLU	T1739	GLY	E1109	R987	I750	D619
E5007	A4746	P4587	G3971	GLN	THR	P2438	G2266	GLU	LYS	T1742	C1630	P1111	A989	R758	L620
R5017	K4757	GLY	L3980	TYR	T2447	K2447	G2266	GLU	GLU	R1743	P1633	L1120	A1009	I759	L621
M5019	ASP	GLU	I3985	ASP	G2446	E2449	T2271	GLU	ASP	G1764	M1637	V1123	VAL	M760	L625
P5023	M4767	MET	F3992	ARG	D2274	E2453	D2272	GLU	GLU	P1773	A1638	V1123	ASP	F777	L626
D5026	S4770	GLY	I3804	GLY	I2453	L2466	D2275	GLU	GLU	P1773	L1639	G1140	ILE	F778	P627
C5027	F4807	SER	L3805	Y2855	L2466	E2285	V2275	THR	GLU	A1788	R1646	R1141	PRO	P779	R629
F5028	M4816	ALA	N3809	L2862	I2469	L2290	E2285	THR	GLU	ALA	R1646	R1141	ALA	S782	Q634
Y5032	M4864	GLY	L3817	S2868	L2472	Q2291	L2290	SER	LYS	GLY	D1649	V1149	ARG	S784	T635
L5036	E4871	ASP	G3827	Q2872	X2502	D2294	D2294	SER	ASP	E1793	E1652	M1152	ASN	V787	L637
S5037	G4898	LEU	F3828	Q2872	P2737	L2295	L2295	ARG	GLU	A1796	L1653	D1154	PRO	K788	V641
	D4899	ALA	F3829	N2884	P2737	C2326	C2326	LEU	LYS	R1797	Q1660	N1158	ALA	E813	P646
	P4904	SER	Q3830	R2888	P2738	G2327	G2327	SER	GLU	I1802	H1665	I1161	ARG	D857	F664
	R4913	GLY	Q3833	R2902	P2748	R2330	R2330	THR	GLU	L1807	T1666	T1162	VAL	THR	E670
	I4925	GLY	L3842	F2903	L2751	F2337	F2337	VAL	GLY	R1808	R1668	T1163	I1053	GLN	V671
	L4928	TRP	Q3849	L2904	I2755	F2340	F2340	ARG	GLY	D1828	R1671	V1168	E1054	PRO	L675
	L4929	GLY	Q3850	L2927	V2341	V2341	V2341	LEU	LYS	I1853	L1676	L1189	ASP	P864	H681
	I4931	ALA	A3853	K2928	F2758	N2342	N2342	LYS	ASP	F1854	R1680	V1199	GLN	P865	L682
	R4944	GLY	K3873	F2938	T2762	G2343	G2343	LYS	ASP	T1847	R1680	E1224	GLU	H866	R683
	K4957	ALA	Q3889	L2930	K2770	E2347	E2347	LYS	GLU	L1846	L1685	Q1244	PRO	R886	L688
	F4958	ALA	N3896	X3365	K2770	E2347	E2347	GLU	GLU	I1853	L1685	Q1244	SER	R887	T689
	F4959	GLY	N3897	X3369	W2775	N2351	N2351	PRO	LYS	F1854	H1688	P1247	VAL	W891	P694
	I4960	ASP	D3898	X3513	P2793	A2378	A2378	GLU	GLU	V1859	Q1691	X1284	ASN	P914	V695
	C4961	GLU	F3899	X3515	E2803	E2382	E2382	LEU	ASP	I1862	A1692	X1284	GLN	N705	N705
	G4962	ASP	Q3900	X3552	E2806	P2395	P2395	PRO	PRO	L1863	Q1693	X1463	ARG	E917	G706
	I4963	GLU	N3901	X3556	W2807	GLY	GLY	ALA	VAL	V1870	E1698	X1516	TRP	V707	G708
	G4964	GLU	T3910	K3658	K2810	VAL	VAL	GLU	GLU	E1874	D1700	X1516	D1070	L932	D709
	Y4967		T3911	K3658	K2810	ARG	ARG	GLU	GLU	GLU	R1708	X1519	R1073	L935	S713
	F4975		L3923	W3661	E2830	ASP	ASP	K2089	Y1977	GLU	A1709	X1526	R1076	A942	S713
	E4976		S3929	I3662	GLU	ARG	ARG	V2103	P2002	GLU	G1710	X1529	A1077	P865	D717
	H4978		Y3937	I3674	ARG	ARG	ARG	Q2107	Q2003	GLU	Y1711	X1529	E1078	K952	G718
	T4979		Q3946	E3712	THR	GLU	GLU	L2131	E2004	GLU	Y1712	Q1598	K1079	K952	L719
	E4982		Q3946	E3712	THR	LYS	LYS	L2155	Q2005	GLU	I1718	M1599	Y1089	Y859	H720
	H4983		N3950	I3728	LYS	LYS	LYS	L2155	N2007	GLU	H1719	L1600	F1092	A968	H725
	N4984		M3955	N3741	THR	THR	THR	N2188	P2022	GLU	E1721	W1605	V1095	L972	Q735
	L4985		Q3960	GLY	ARG	ARG	ARG	K2189	P2024	GLU	R1725	V1615	G1103	L977	P740
	L4995			ALA	LYS	LYS	LYS	Y2192	I2027	GLU	S1726	GLU	W1104	T978	D742
					ILE	ILE	ILE		R2028	GLU	R1728	ARG	A1105	A980	

● Molecule 2: Ryanodine receptor 1


Chain E:  84% 10% 5%





I4963	GLU	I4193	T3910																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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• Molecule 2: Ryanodine receptor 1

Chain I:  84% 10% 5%

P2024	I2027	R2028	C2042	G2043	G2048	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
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R2199	P2438	GLN	G3971	Y4560	Y4687	T4977	T4978	Y4687	Y4560	GLN	E3747	V3779	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199
N2246	K2447	THR	L3980	T4561	K4698	H4978	T4979	K4698	T4561	THR	E3747	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
Q2247	E2449	ASP	L3985	F4564	G4699	E4982	H4983	G4699	F4564	ASP	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
G2266	L2453	PRO	F3992	A4566	S4713	E4982	H4983	S4713	A4566	PRO	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
T2271	L2466	ARG	F3996	L4567	K4714	E4982	H4983	K4714	L4567	ARG	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
P2272	L2469	GLU	K4002	V4582	Y4715	E4982	H4983	Y4715	V4582	GLU	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
D2273	L2472	GLY	L4019	P4587	M4743	E4982	H4983	M4743	P4587	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
V2275	L2502	GLY	L4019	P4587	A4746	E4982	H4983	A4746	P4587	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
E2285	X2502	ASP	L4019	P4587	K4757	E4982	H4983	K4757	P4587	ASP	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
L2290	P2737	ASP	M4034	GLY	G4763	E4982	H4983	G4763	GLY	ASP	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
Q2291	P2737	GLY	M4034	GLY	G4763	E4982	H4983	G4763	GLY	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
D2294	P2739	GLY	V4049	SER	T4766	E4982	H4983	T4766	SER	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
L2295	P2748	ALA	R4085	ALA	S4770	E4982	H4983	S4770	ALA	ALA	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
C2326	P2751	GLY	K4090	GLY	Y4775	E4982	H4983	Y4775	GLY	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
G2327	L2751	LEU	Q4094	ASP	F4807	E4982	H4983	F4807	ASP	LEU	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
R2330	L2755	ALA	T4104	ALA	Y4807	E4982	H4983	Y4807	ALA	ALA	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
F2337	F2758	GLY	G4105	GLY	I4846	E4982	H4983	I4846	GLY	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
F2340	T2762	GLY	P4106	SER	R4860	E4982	H4983	R4860	SER	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
V2341	K2770	GLY	M4120	GLY	M4864	E4982	H4983	M4864	GLY	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
N2342	W2775	GLY	E4126	GLY	E4871	E4982	H4983	E4871	GLY	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
G2343	P2793	GLY	M4130	TRP	P4904	E4982	H4983	P4904	TRP	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
E2347	E2803	GLY	E4152	SER	R4913	E4982	H4983	R4913	SER	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
N2351	R2806	GLY	H4156	GLY	I4925	E4982	H4983	I4925	GLY	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
P2395	W2807	GLY	R4159	ALA	L4928	E4982	H4983	L4928	ALA	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
GLY	K2810	VAL	R4192	GLY	L4929	E4982	H4983	L4929	GLY	VAL	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	E2830	ARG	I4193	GLY	A4930	E4982	H4983	A4930	GLY	ARG	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	GLU	ARG	Y4194	ASP	I4931	E4982	H4983	I4931	ASP	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	GLU	ARG	I4197	ASP	R4944	E4982	H4983	R4944	ASP	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	GLU	ARG	K4957	ASP	C4958	E4982	H4983	C4958	ASP	GLY	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	THR	ARG	F4959	ASP	I4960	E4982	H4983	I4960	ASP	THR	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	C4961	ASP	G4962	E4982	H4983	G4962	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	I4963	ASP	G4964	E4982	H4983	I4963	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453	E2449	G2448	K2447	R2199	
ARG	LYS	ARG	E4232	ASP	Y4967	E4982	H4983	Y4967	ASP	LYS	R3762	L3780	L3805	L3804	Y2855	L2453					




## 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	0.29	0/834	0.52	0/1123
1	F	0.29	0/834	0.52	0/1123
1	H	0.29	0/834	0.52	0/1123
1	J	0.29	0/834	0.52	0/1123
2	B	0.29	0/25428	0.54	10/34534 (0.0%)
2	E	0.29	0/25428	0.54	10/34534 (0.0%)
2	G	0.29	0/25428	0.54	10/34534 (0.0%)
2	I	0.29	0/25428	0.54	10/34534 (0.0%)
All	All	0.29	0/105048	0.54	40/142628 (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	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	52

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.42	134.66	115.30
2	B	131	LEU	CA-CB-CG	8.41	134.65	115.30
2	E	131	LEU	CA-CB-CG	8.41	134.63	115.30
2	I	131	LEU	CA-CB-CG	8.39	134.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1600	LEU	CA-CB-CG	6.97	131.33	115.30

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	694	PRO	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	5	0
1	F	818	0	824	5	0
1	H	818	0	824	4	0
1	J	818	0	824	4	0
2	B	29499	0	24746	252	0
2	E	29499	0	24746	258	0
2	G	29499	0	24746	248	0
2	I	29499	0	24746	255	0
3	B	31	0	12	0	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	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	1020	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 1020 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:5028:PHE:HE1	2:G:5032:TYR:CD2	1.87	0.93
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.87	0.93
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.87	0.92
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.87	0.92
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.58	0.92

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%)	2916 (90%)	311 (10%)	8 (0%)	52	86
2	E	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	52	86
2	G	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	52	86
2	I	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	52	86
All	All	13360/18096 (74%)	12037 (90%)	1291 (10%)	32 (0%)	56	86

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE

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Mol	Chain	Res	Type
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG

### 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%)	88	94
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	89	94

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

Mol	Chain	Res	Type
2	E	4944	ARG
2	I	1141	ARG
2	G	4085	ARG
2	E	4983	HIS
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	3946	GLN

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Mol	Chain	Res	Type
2	I	395	GLN
2	G	3889	GLN
2	E	3960	GLN
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 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	0.92	1 (3%)	26,52,52	1.75	1 (3%)
4	CFF	B	5102	-	8,15,15	2.40	3 (37%)	8,23,23	1.18	1 (12%)
3	ATP	E	5101	-	26,33,33	0.92	1 (3%)	26,52,52	1.77	1 (3%)
4	CFF	E	5102	-	8,15,15	2.40	3 (37%)	8,23,23	1.18	1 (12%)
3	ATP	G	5101	-	26,33,33	0.92	1 (3%)	26,52,52	1.75	1 (3%)
4	CFF	G	5102	-	8,15,15	2.40	3 (37%)	8,23,23	1.18	1 (12%)
3	ATP	I	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.75	1 (3%)
4	CFF	I	5102	-	8,15,15	2.40	3 (37%)	8,23,23	1.18	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	G	5102	CFF	C4-N3	-4.53	1.33	1.39
4	I	5102	CFF	C4-N3	-4.53	1.33	1.39
4	B	5102	CFF	C4-N3	-4.53	1.33	1.39
4	E	5102	CFF	C4-N3	-4.51	1.33	1.39
4	I	5102	CFF	C6-N1	-4.00	1.32	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	N3-C2-N1	-7.26	123.17	128.87
3	I	5101	ATP	N3-C2-N1	-7.20	123.22	128.87
3	B	5101	ATP	N3-C2-N1	-7.19	123.22	128.87
3	G	5101	ATP	N3-C2-N1	-7.19	123.22	128.87
4	G	5102	CFF	C14-N7-C8	-2.55	112.02	125.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5102	CFF	1	0
4	E	5102	CFF	1	0
4	G	5102	CFF	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	B	4345:UNK	C	4540:PHE	N	72.89
1	E	4345:UNK	C	4540:PHE	N	72.89
1	I	4345:UNK	C	4540:PHE	N	72.89
1	G	4345:UNK	C	4540:PHE	N	72.89
1	B	3613:UNK	C	3639:THR	N	44.63