



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:53 PM BST

PDB ID : 3J94  
EMDB ID: : EMD-6204  
Title : Structure of ATP-bound N-ethylmaleimide sensitive factor determined by single particle cryoelectron microscopy  
Authors : Zhao, M.; Wu, S.; Cheng, Y.; Brunger, A.T.  
Deposited on : 2014-12-05  
Resolution : 4.20 Å(reported)  
Based on PDB ID : 1NSF

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) : trunk27241

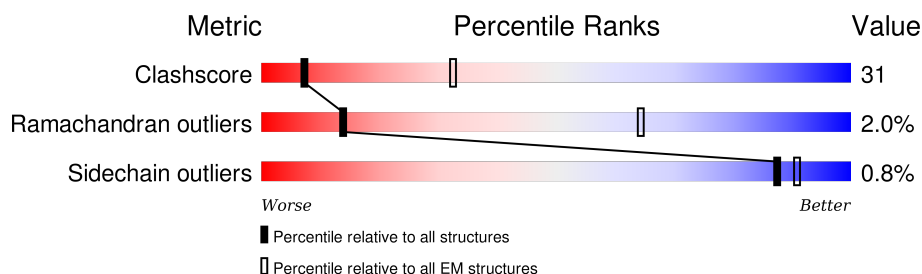
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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  $\geq 3$ , 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	747	
1	B	747	
1	C	747	
1	D	747	
1	E	747	
1	F	747	

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
2	ATP	D	801	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21509 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.

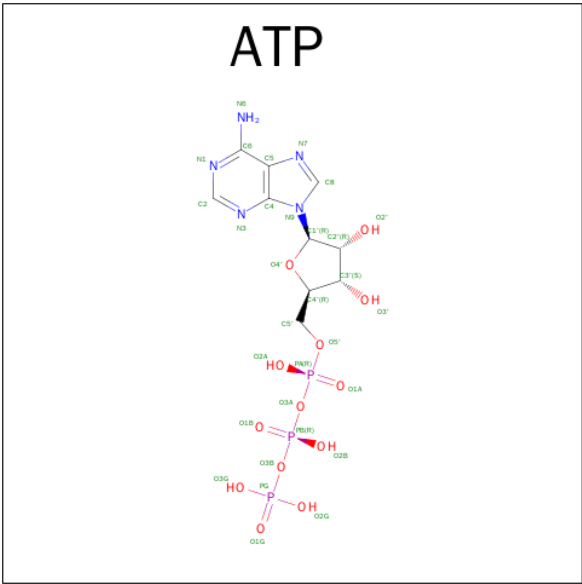
- Molecule 1 is a protein called Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	490	Total	C	N	O	S	0	0
			3559	2266	613	665	15		
1	B	484	Total	C	N	O	S	0	0
			3563	2264	618	665	16		
1	C	488	Total	C	N	O	S	0	0
			3573	2268	621	669	15		
1	D	485	Total	C	N	O	S	0	0
			3526	2244	603	663	16		
1	E	482	Total	C	N	O	S	0	0
			3529	2242	611	661	15		
1	F	466	Total	C	N	O	S	0	0
			3418	2164	598	640	16		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P18708
A	-1	ALA	-	EXPRESSION TAG	UNP P18708
A	0	HIS	-	EXPRESSION TAG	UNP P18708
B	-2	GLY	-	EXPRESSION TAG	UNP P18708
B	-1	ALA	-	EXPRESSION TAG	UNP P18708
B	0	HIS	-	EXPRESSION TAG	UNP P18708
C	-2	GLY	-	EXPRESSION TAG	UNP P18708
C	-1	ALA	-	EXPRESSION TAG	UNP P18708
C	0	HIS	-	EXPRESSION TAG	UNP P18708
D	-2	GLY	-	EXPRESSION TAG	UNP P18708
D	-1	ALA	-	EXPRESSION TAG	UNP P18708
D	0	HIS	-	EXPRESSION TAG	UNP P18708
E	-2	GLY	-	EXPRESSION TAG	UNP P18708
E	-1	ALA	-	EXPRESSION TAG	UNP P18708
E	0	HIS	-	EXPRESSION TAG	UNP P18708
F	-2	GLY	-	EXPRESSION TAG	UNP P18708
F	-1	ALA	-	EXPRESSION TAG	UNP P18708
F	0	HIS	-	EXPRESSION TAG	UNP P18708

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	E	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	E	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

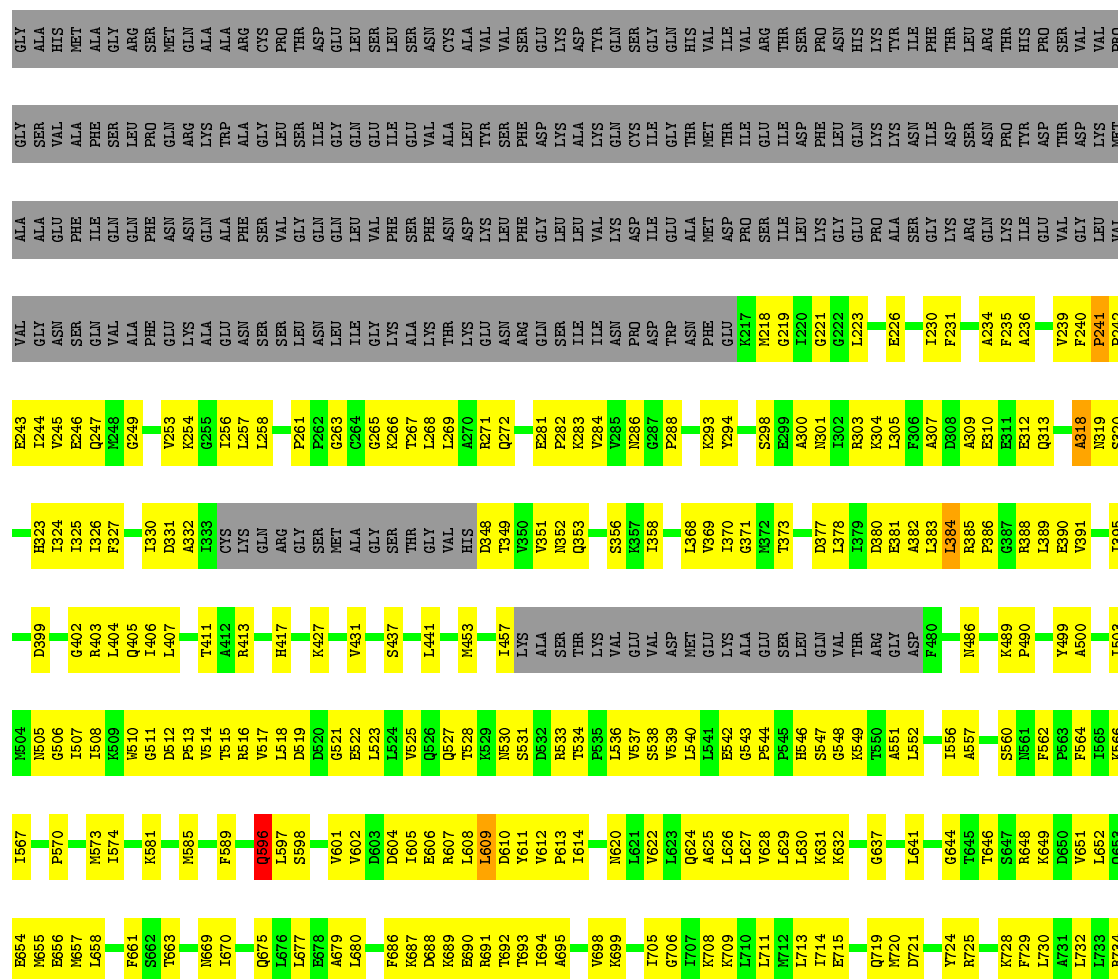


GLY	ALA	GLY	ALA	VAL	E246	1322	Q402	P490		R448	PHE
ALA	SER	SER	GLU	GLY	Q247	H323	R403	A491	I574	K649	ASP
HIS	VAL	ASN	PHE	ASN	G248	I324	L404		G575		
MET	ALA	SER	ILE	GLN	G249	I325	Q405	D498	S576	E656	
GLY	SER	GLN	ILE	VAL		I326	L406	Y499	S577	M657	
ARG	LEU	PRO	GLN	VAL	K254	F327	L407		S578	L658	
			PHE	ALA	G255		H408	Y502	T579		
SER	PRO	GLN	ASN	PHE	I256	I330		I503	A580	F661	
GLN	ARG	GLY	ASN	GLY	L257	ASP	R413	M504	K581	S662	
ALA	LYS	ASN	ALA	ALA	Y259	ILE	M414	G506	I588	T663	
ALA	TRP	GLY	GLY	CYS	G265	CYS	L426	I507	F589	V667	
ARG	ALA	GLY	ASN	LYS	K266	GLN	K427	I508	D590	P668	
CYS	GLY	SER	SER	SER	T267	ARG	E428	R516	Y593	M669	
PRO	LEU	VAL	LEU	GLY	L268	GLY	V431	V517	Q596	I670	
THR	ILE	GLY	LEU	ASN	L269	SER	E432	L518	L597	Q675	
ASP	GLY	GLN	LEU	LEU	A270	MET	F436	D519	S598	F686	
GLU	GLY	LEU	VAL	ILE	H271	ALA	S437	L523	C599	E690	
LEU	GLN	LEU	PHE	GLY	Q272	GLY	Q439	L524	V600	R691	
SER	LEU	LYS	PHE	ALA	I273	THR	A439	V525	V601	T692	
	GLU	ASN	LYS	GLY	E281	GLY	E440	Q526	V602	T693	
CYS	ALA	THR	ASN	THR	P282	VAL	L441	Q527	D603	I694	
ALA	LEU	LYS	ASP	GLY	K283	H347	L444	T528	E606	A695	
VAL	TYR	GLU	LYS	VAL	V284	D343	V445	T529	R607	Q696	
VAL	SER	LEU	LEU	ASP		T349		N530	L608	Q697	
VAL	PHE	GLY	PHE	GLY	P288		Q449	T534	L609	K699	
SER	ASP	ASN	GLN	ASN	E289	Q353		P535	D610	G706	
GLU	LYS	ILE	ILE	ILE	I290	L354	A452	S538	V611	I707	
LYS	ALA	ILE	ASP	ASP	I291	K357	M453	V539	V612	L710	
ASP	ALA	THR	LEU	THR	E292	I358	R454	L540	G615	L711	
TYR	GLN	MET	VAL	GLY	G296	N366	L456	L541	P616	M712	
GLN	THR	ASP	VAL	ILE	S298	I367	L457	E542	R617	L713	
SER	MET	PHE	ILE	ASN	E299	L368	ALA	R543	S619	I714	
VAL	THR	ASP	THR	PHE	A300	V369	SER	S547	M620	E715	
ILE	ILE	PRO	ILE	GLY	N301	I370	THR	G548	L621	M716	
ARG	GLU	SER	GLU	ILE	I302	G371	LYS	K349	L622	S717	
THR	ILE	THR	ILE	THR	R303		VAL	T550	V623	L718	
SER	ASP	SER	LEU	SER	K304	P376	GLY	A551	L624	Q719	
PRO	PHE	PRO	LYS	PRO	I220	D377	VAL	L552	A625	M720	
ASN	LEU	ASN	GLY	ASN	G221	L378	ASP	K555	L626	D721	
HIS	LEU	GLN	LYS	GLY	D224	I379	MET	I556	L627		
LYS	ASN	PRO	LYS	THR		D380	GLY	L566	V628	Y724	
TYR	ASN	LYS	ALA	SER	S228	E381	LYS	E559	L629	R725	
ILE	ASN	ILE	SER	ILE	R233	L383	GLY	S560	L630	K728	
PHE	ILE	LYS	GLY	THR	E312	R384	SER	M561	K631		
THR	ASP	ARG	LYS	ASP	Q313	R385	LEU	P562	R632	L732	
LEU	SER	GLN	ARG	SER	A236	G387	GLN	P563	R638		
ARG	ASN	LYS	LYS	ASN	V239	R388	VAL	K566	K639	G737	
THR	PRO	ILE	ILE	THR	P240	L316	THR	I567		ALA	
HIS	ASP	GLY	GLY	ASP	P241	L389	ARG	K567		SER	
PRO	THR	VAL	VAL	THR	P242	E390	GLY	C568	I643	PRO	
SER	ASP	GLY	GLY	ASP	E243	N319	D479	S569	G644	LEU	
VAL	LYS	LEU	LYS	VAL	I244	S320		P570		SER	
PRO	MET	VAL	VAL	VAL	V245	G321	K489	D571	S647	ASP	

● Molecule 1: Vesicle-fusing ATPase



GLY	ALA	VAL	VAL	VAL	V245	GLY	ALA	GLY	ALA	GLY	GLY
ALA	SER	GLY	ALA	ALA	E246	ALA	HIS	SER	GLU	SER	GLY
HIS	VAL	ASN	PHE	PHE	Q247	GLU	MET	VAL	ILE	THR	ILE
MET	ALA	SER	ILE	ILE	M248	GLN	ALA	GLY	GLN	GLY	GLY
GLY	SER	GLN	GLN	GLN	G249	VAL	ARG	LEU	TRP	ALA	ALA
ARG	LEU	ALA	GLN	GLN	K254	ALA	SER	PRO	ALA	ALA	ALA
		PHE	ASN	ASN	G255	PHE	MET	ASN	ALA	ALA	ALA
SER	PRO	GLN	ASN	LYS	I256	GLY	GLN	LEU	LYS	TRP	TRP
GLN	ARG	LYS	GLY	ALA	L257	ASN	GLY	GLY	ASN	ALA	ALA
ALA	LYS	ALA	ALA	GLY	G263	ILE	ASN	ILE	SER	ALA	ALA
ALA	TRP	GLY	PHE	ASN		GLY	SER	GLY	GLY	ALA	ALA
ARG	ALA	SER	VAL	THR	T267	THR	VAL	LEU	VAL	ALA	ALA
CYS	GLY	GLY	GLY	GLY	A270	ASN	GLY	ILE	VAL	ALA	ALA
PRO	LEU	SER	GLY	GLY	Q271	LEU	GLN	GLY	PHE	ALA	ALA
THR	ILE	THR	ILE	ILE	Q272	LEU	GLN	GLY	SER	ALA	ALA
ASP	GLY	THR	GLY	GLY	I273	ILE	LEU	GLN	ASP	ALA	ALA
GLU	GLN	GLY	VAL	VAL	V284	GLY	VAL	LEU	VAL	ALA	ALA
LEU	GLY	ALA	PHE	PHE	V285	ILE	ILE	LEU	VAL	ALA	ALA
SER	ILE	ALA	SER	SER	E289	LYS	THR	LEU	LYS	ALA	ALA
	GLU	LYS	LEU	TYR	I290	ASN	LYS	LEU	LEU	ALA	ALA
CYS	ALA	LYS	ASP	ASP	L291	GLY	LYS	LEU	LYS	ALA	ALA
ALA	LEU	GLY	LYS	VAL	E292	THR	ASN	ASP	ILE	ALA	ALA
VAL	TYR	GLU	ILE	VAL	K293	ASN	ARG	GLY	ILE	ALA	ALA
VAL	SER	ASN	PHE	PHE	Y294	GLN	GLY	GLY	ILE	ALA	ALA
VAL	PHE	LYS	GLY	GLY	V295	SER	GLY	LEU	THR	ALA	ALA
VAL	ASP	LYS	LEU	LEU	G296	ILE	LYS	LEU	ASP	ALA	ALA
VAL	LYS	ILE	VAL	VAL	E297	ILE	ILE	VAL	VAL	ALA	ALA
VAL	LYS	ASN	GLN	GLN	S298	ASN	ILE	VAL	VAL	ALA	ALA
VAL	CYS	PRO	ASP	ASP	E299	PRO	ASP	PRO	PRO	ALA	ALA
GLY	ILE	THR	ILE	ILE	A300	ASP	ILE	ILE	ILE	ALA	ALA
GLY	GLY	TRP	GLY	GLY	N301	TRP	GLY	GLY	GLY	ALA	ALA
GLY	GLY	ASN	ALA	ALA	L305	ASN	ALA	MET	MET	ALA	ALA
GLN	THR	PHE	MET	VAL		THR	HIS	THR	THR	ALA	ALA
GLN	ILE	GLY	MET	VAL	D308	GLY	VAL	THR	THR	ALA	ALA
ILE	THR	THR	THR	THR	A309	PRO	ILE	ILE	ILE	ALA	ALA
ILE	VAL	ILE	ILE	VAL	M218	ILE	VAL	ILE	ILE	ALA	ALA
ARG	VAL	GLY	GLY	VAL	G219	THR	ARG	GLY	GLY	ALA	ALA
THR	THR	THR	THR	THR	E310	ILE	THR	ILE	ILE	ALA	ALA
SER	SER	SER	ASP	SER	E311	THR	THR	ASP	ASP	ALA	ALA
PRO	PRO	PRO	PHE	PRO	G221	ASN	PRO	LEU	LEU	ALA	ALA
ASN	ASN	ASN	LEU	ASN		PHE	ASN	LEU	LEU	ALA	ALA
HIS	HIS	HIS	GLN	HIS	F227	GLY	HIS	GLN	GLY	ALA	ALA
LYS	LYS	LYS	LYS	LYS	I230	THR	LYS	GLN	GLY	ALA	ALA
TYR	TYR	TYR	ILE	TYR	F231	ASN	ASN	ASN	GLY	ALA	ALA
ILE	ILE	ILE	ASP	ILE	R232	THR	ILE	ILE	ILE	ALA	ALA
PHE	PHE	PHE	THR	THR	R233	ASP	LYS	ASP	THR	ALA	ALA
THR	THR	THR	THR	THR	A234	SER	ARG	SER	ASP	ALA	ALA
LEU	LEU	LEU	ARG	ARG	F235	GLN	GLY	GLY	LEU	ALA	ALA
LEU	GLN	GLN	ASN	ASN	G321	LYS	LYS	ASN	ASN	ALA	ALA
THR	THR	THR	PRO	PRO	L322	THR	LYS	PRO	PRO	ALA	ALA
HIS	THR	THR	ILE	THR	A236	ASN	ILE	THR	THR	ALA	ALA
PRO	ASP	ASP	GLY	GLY		GLY	GLY	ASP	ASP	ALA	ALA
SER	THR	THR	VAL	VAL	F240	THR	VAL	THR	THR	ALA	ALA
VAL	ASP	ASP	GLY	GLY	P241	THR	VAL	ASP	THR	ALA	ALA
LYS	LYS	LYS	LEU	LEU	E242	ASP	GLY	ASP	ASP	ALA	ALA
VAL	MET	VAL	VAL	VAL	E243	LYS	LYS	VAL	VAL	ALA	ALA
PRO		VAL	VAL	VAL	F327	THR	THR	THR	THR	ALA	ALA







M712	M713	L714	L715	M716	S717	L718	L719	M720	D721	Y724	R725	K728	L732	L733	R734	G737	ALA	SER	PRO	LEU	ASP	PHE	ASP																																
K639	L640	L641	L642	L643	G644	T645	T646	S647	K648	K649	D650	Q653	E654	M655	E656	M657	L658	F661	S662	T663	T664	L665	H666	V667	M669	L670	G673	E674	Q675	L676	L677	E678	E681	L682	L683	G684	M685	P686	E689	I694	A695	V698	K699	W704	I707	K708	K709	L710	L711						
K566	I567	C568	S569	P570	D571	K572	M573	I574	S577	E578	T579	A580	K581	Q582	Q583	K586	F589	Y593	L597	S598	C599	V600	V601	V602	D603	D604	I605	E606	R607	L608	L609	D610	Y611	V612	P613	I614	G615	P616	R617	F618	S619	N620	Q624	V628	L629	K632	A633	P634	P635	R638					
Y499	Y502	I503	Y504	M505	G506	L507	L508	K509	M510	G511	D512	F513	V514	T515	R516	V517	L518	G521	E522	L523	L524	V525	Q526	Q527	T528	K529	N530	P535	L536	V537	S538	V539	L540	L541	E542	G543	P544	P545	H546	S547	G548	K549	T550	A551	L552	A553	A554	K555	L556	A557	E558	E559	S560	F564	L565
V431	E432	S437	G438	A439	E440	L441	E442	V445	R446	A452	M453	R454	H456	I457	LYS	ALA	SER	THR	LYS	VAL	GLU	VAL	ASP	MET	T373	N374	R375	P376	D377	L378	L379	D380	R385	P386	G387	R388	L389	E390	V391	S392	M393	L397	P398	L404	Q405	L406	H407	I408	THR	ASN	GLN	E497	D498		
ARG	GLY	SER	MET	ALA	GLY	THR	GLY	VAL	H347	V350	V351	L354	T358	D359	R365	R366	T367	L368	V369	L370	G371	H372	T373	N374	R375	P376	D377	L378	L379	D380	R385	P386	G387	R388	L389	E390	V391	S392	M393	L397	P398	L404	Q405	L406	H407	I409	ALA	ILE	CYS	LYS	F240	GN			
VAL	P242	E243	I244	V245	G249	I256	L257	L258	Y259	G260	P261	A270	I273	E281	P282	K283	V284	K293	G296	E297	K304	L305	F306	A307	D308	A309	E310	E311	TRP	ASN	PHE	GLU	R314	R315	L316	G317	A318	N319	S320	G321	L322	H323	I324	I325	F327	I330	ASP	ALA	ILE	CYS	V239	F240	P241		

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	50781	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	26.4	Depositor
Minimum defocus (nm)	-1800	Depositor
Maximum defocus (nm)	-2800	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 (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

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	0.37	0/3612	0.81	4/4904 (0.1%)
1	B	0.37	0/3615	0.77	1/4898 (0.0%)
1	C	0.38	0/3625	0.77	3/4915 (0.1%)
1	D	0.36	0/3577	0.77	3/4856 (0.1%)
1	E	0.35	0/3580	0.79	2/4854 (0.0%)
1	F	0.39	0/3467	0.82	3/4697 (0.1%)
All	All	0.37	0/21476	0.79	16/29124 (0.1%)

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	2
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	8

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	223	LEU	CA-CB-CG	6.62	130.52	115.30
1	F	536	LEU	CA-CB-CG	6.52	130.31	115.30
1	F	518	LEU	CA-CB-CG	6.32	129.84	115.30
1	C	385	ARG	NE-CZ-NH2	6.20	123.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	609	LEU	CA-CB-CG	6.07	129.27	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	PRO	Peptide
1	A	261	PRO	Peptide
1	B	438	GLY	Peptide
1	B	546	HIS	Sidechain
1	C	530	ASN	Sidechain

## 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	3559	0	3451	224	0
1	B	3563	0	3497	215	0
1	C	3573	0	3487	212	0
1	D	3526	0	3429	251	0
1	E	3529	0	3439	263	0
1	F	3418	0	3332	228	0
2	A	62	0	23	11	0
2	B	62	0	21	11	0
2	C	62	0	22	9	0
2	D	62	0	20	18	0
2	E	62	0	17	9	0
2	F	31	0	9	5	0
All	All	21509	0	20747	1292	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 31.

The worst 5 of 1292 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)
1:A:505:ASN:HB2	2:A:801:ATP:H1'	1.39	1.01
1:C:257:LEU:HB2	1:C:389:LEU:HD13	1.56	0.87
1:B:526:GLN:HE21	1:C:719:GLN:HB3	1.39	0.85
1:B:386:PRO:HA	1:B:390:GLU:HA	1.58	0.84
1:A:705:ILE:HD13	1:A:710:LEU:HD12	1.59	0.84

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	484/747 (65%)	452 (93%)	20 (4%)	12 (2%)	7	48
1	B	478/747 (64%)	436 (91%)	31 (6%)	11 (2%)	8	50
1	C	482/747 (64%)	454 (94%)	19 (4%)	9 (2%)	10	54
1	D	479/747 (64%)	448 (94%)	25 (5%)	6 (1%)	15	60
1	E	474/747 (64%)	443 (94%)	21 (4%)	10 (2%)	9	52
1	F	460/747 (62%)	425 (92%)	26 (6%)	9 (2%)	9	53
All	All	2857/4482 (64%)	2658 (93%)	142 (5%)	57 (2%)	14	53

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	293	LYS
1	A	294	TYR
1	A	318	ALA
1	A	320	SER

### 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	348/638 (54%)	344 (99%)	4 (1%)	80	91
1	B	356/638 (56%)	353 (99%)	3 (1%)	86	93
1	C	353/638 (55%)	351 (99%)	2 (1%)	90	95
1	D	348/638 (54%)	347 (100%)	1 (0%)	94	97
1	E	350/638 (55%)	349 (100%)	1 (0%)	94	97
1	F	339/638 (53%)	334 (98%)	5 (2%)	72	89
All	All	2094/3828 (55%)	2078 (99%)	16 (1%)	87	93

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	305	LEU
1	C	676	LEU
1	F	322	LEU
1	B	456	HIS
1	F	365	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	272	GLN
1	D	319	ASN
1	E	505	ASN
1	C	319	ASN
1	E	527	GLN

### 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 ⓘ

11 ligands are modelled in this entry.

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$
2	ATP	A	801	-	26,33,33	1.12	2 (7%)	26,52,52	1.80	4 (15%)
2	ATP	A	802	-	26,33,33	0.94	1 (3%)	26,52,52	1.67	1 (3%)
2	ATP	B	801	-	26,33,33	1.00	1 (3%)	26,52,52	1.91	2 (7%)
2	ATP	B	802	-	26,33,33	0.99	1 (3%)	26,52,52	1.40	2 (7%)
2	ATP	C	801	-	26,33,33	0.93	1 (3%)	26,52,52	1.85	4 (15%)
2	ATP	C	802	-	26,33,33	1.06	1 (3%)	26,52,52	1.71	2 (7%)
2	ATP	D	801	-	26,33,33	0.94	1 (3%)	26,52,52	1.41	2 (7%)
2	ATP	D	802	-	26,33,33	1.02	1 (3%)	26,52,52	2.34	5 (19%)
2	ATP	E	801	-	26,33,33	1.02	2 (7%)	26,52,52	2.67	4 (15%)
2	ATP	E	802	-	26,33,33	1.00	1 (3%)	26,52,52	1.69	1 (3%)
2	ATP	F	801	-	26,33,33	1.01	1 (3%)	26,52,52	1.71	4 (15%)

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
2	ATP	A	801	-	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	802	-	-	0/18/38/38	0/3/3/3
2	ATP	B	801	-	-	0/18/38/38	0/3/3/3
2	ATP	B	802	-	-	0/18/38/38	0/3/3/3
2	ATP	C	801	-	-	0/18/38/38	0/3/3/3
2	ATP	C	802	-	-	0/18/38/38	0/3/3/3
2	ATP	D	801	-	-	0/18/38/38	0/3/3/3
2	ATP	D	802	-	-	0/18/38/38	0/3/3/3
2	ATP	E	801	-	-	0/18/38/38	0/3/3/3
2	ATP	E	802	-	-	0/18/38/38	0/3/3/3
2	ATP	F	801	-	-	0/18/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ATP	O2'-C2'	2.31	1.48	1.43
2	E	801	ATP	O4'-C1'	2.33	1.44	1.41
2	C	801	ATP	C5-C4	2.79	1.46	1.40
2	D	801	ATP	C5-C4	2.97	1.47	1.40
2	A	802	ATP	C5-C4	2.99	1.47	1.40

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	801	ATP	N3-C2-N1	-10.51	120.62	128.87
2	D	802	ATP	N3-C2-N1	-9.44	121.46	128.87
2	B	801	ATP	N3-C2-N1	-7.30	123.14	128.87
2	C	801	ATP	N3-C2-N1	-6.95	123.41	128.87
2	A	802	ATP	N3-C2-N1	-6.71	123.60	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ATP	8	0
2	A	802	ATP	3	0
2	B	801	ATP	7	0
2	B	802	ATP	4	0
2	C	801	ATP	1	0
2	C	802	ATP	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	ATP	13	0
2	D	802	ATP	5	0
2	E	801	ATP	5	0
2	E	802	ATP	4	0
2	F	801	ATP	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.