



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:52 PM BST

PDB ID : 3J95  
EMDB ID: : EMD-6205  
Title : Structure of ADP-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 : 7.60 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

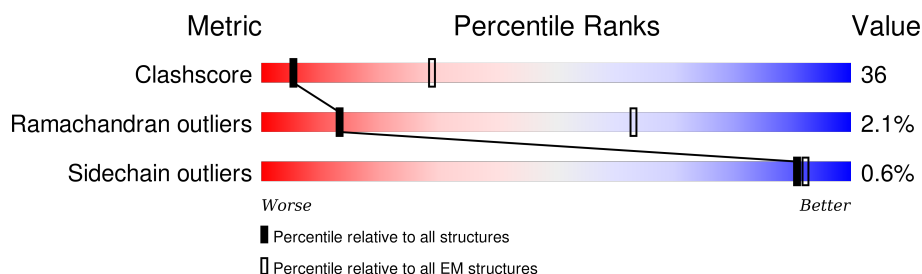
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.60 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	30% 32% . 35%
1	B	747	32% 31% . 36%
1	C	747	31% 33% . 35%
1	D	747	32% 31% . 36%
1	E	747	28% 35% . 35%
1	F	747	30% 32% .. 37%

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	ADP	B	801	-	-	X	-
2	ADP	D	801	-	-	X	-
2	ADP	E	801	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21123 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.

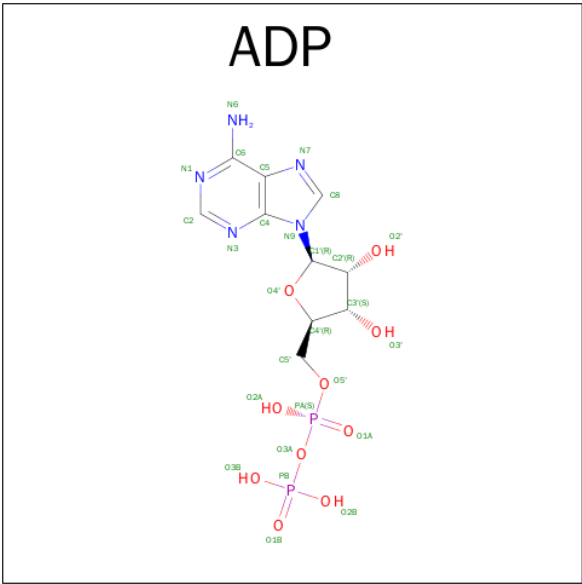
- Molecule 1 is a protein called Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	483	Total	C	N	O	S	0	0
			3513	2221	617	660	15		
1	B	481	Total	C	N	O	S	0	0
			3517	2230	611	660	16		
1	C	485	Total	C	N	O	S	0	0
			3535	2236	618	666	15		
1	D	479	Total	C	N	O	S	0	0
			3467	2203	594	654	16		
1	E	482	Total	C	N	O	S	0	0
			3516	2233	611	656	16		
1	F	473	Total	C	N	O	S	0	0
			3467	2197	609	645	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'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

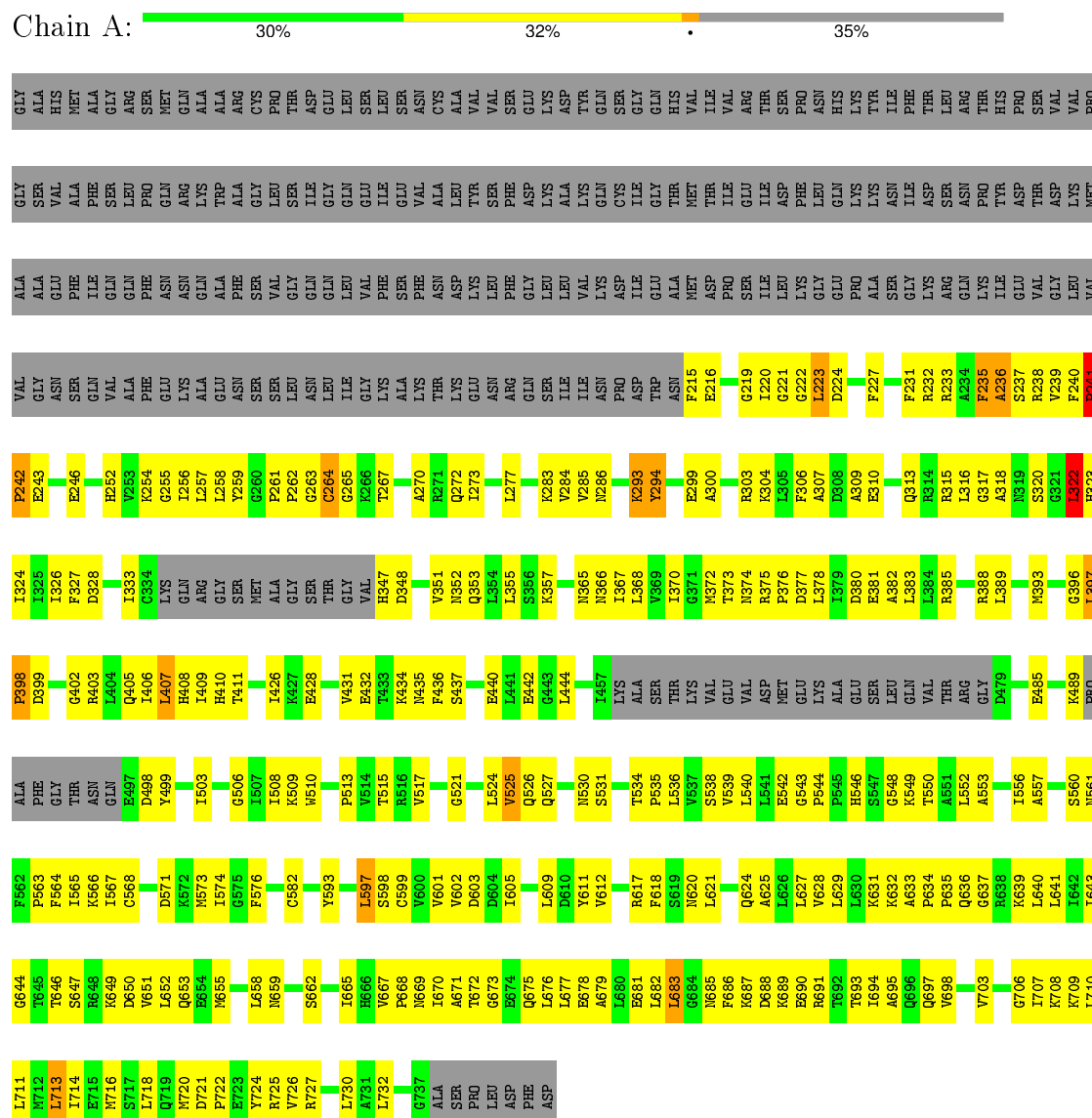


Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

### 3 Residue-property plots

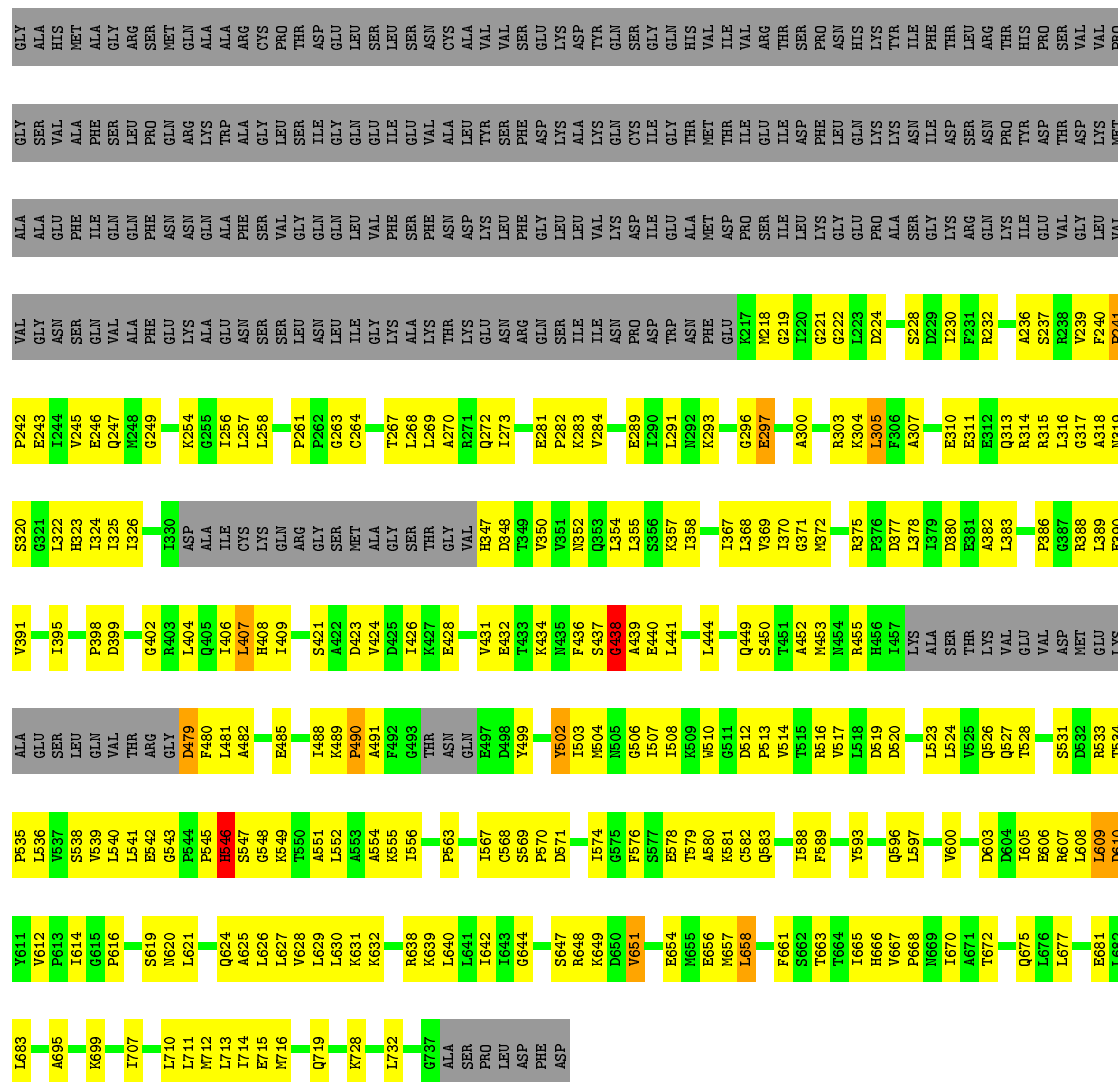
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: Vesicle-fusing ATPase



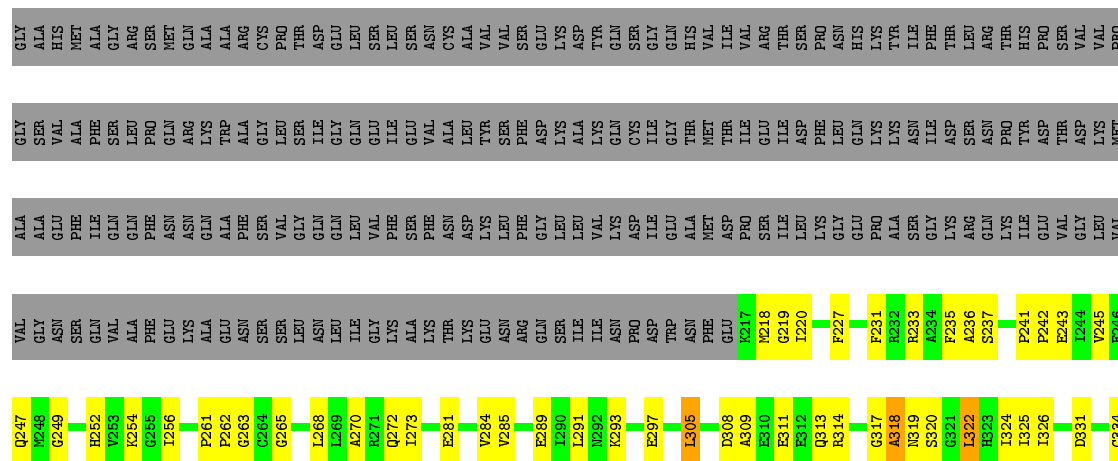
- Molecule 1: Vesicle-fusing ATPase





### • Molecule 1: Vesicle-fusing ATPase

Chain C: 31% 33% 35%

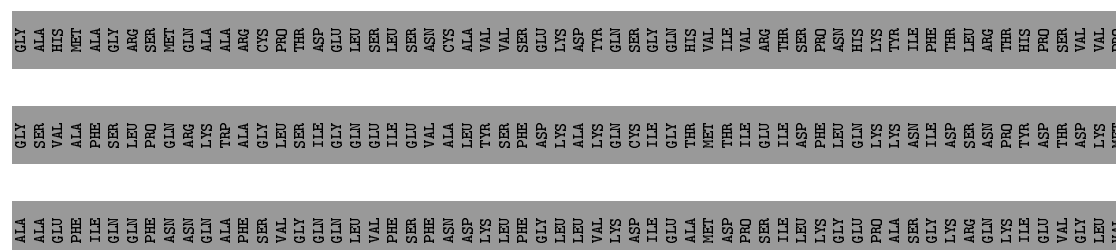


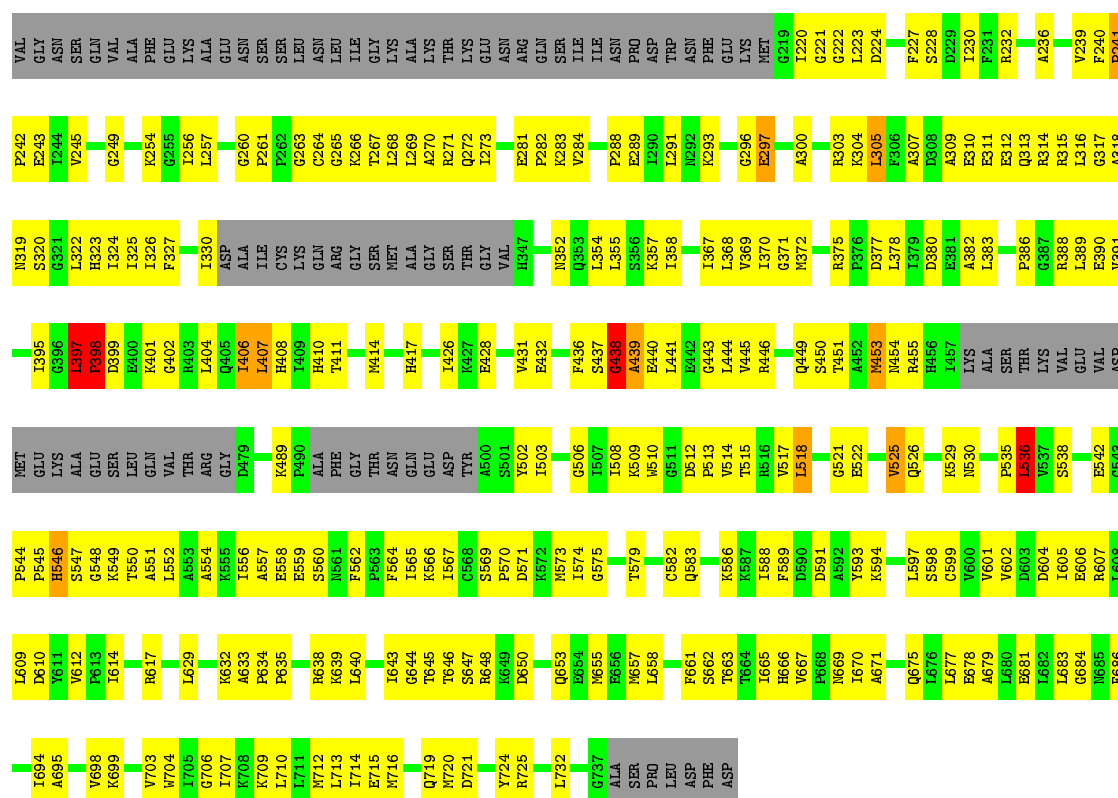
K708	K709	L710	L711	L714	E715	M716	S717	L718	Q719	M720	D721	Y724	V725	T726	R727	K728	F729	A731	L732	L733	R734	G737	ALA	SER	PRO	LEU	ASP	PHE	ASP	LYS GLN ARG GLY SER MET ALA GLY SER THR GLY VAL H347 D348 T349 V350 V351 N352 L355 L358 N366 L367 L368 V369 I370 R375 P376 D377 L378 L379 LEU D380 E381 A382 L383 P386 G387 R388 E389 V391 D399 R403 L404 L407 H408 L409 H410 T411 M414 L426	G511	D512	P513	V514	T515	R516	D519	D520	G521	E522	L523	F524	V525	Q526	T527	T528	K529	N530	S531	D532	R533	L536	V537	S538	V539	L540	E541	E542	G543	P544	P545	A554	K555	L556	A557	E558	E559	S560	N561	L562	L563	F564	L565	C568	S569	P570	D571	I572	L574
G575	F576	S577	E578	T579	A580	K581	C582	Q583	A584	I588	F589	D590	D591	A592	Y593	K594	S595	Q596	L597	S598	C599	V600	V601	V602	D603	D604	L605	E606	R607		L608	L609	D610	V611	V612	P613	I614	G615	P616	R617	N620	L621	Q624	A625	L626	L627	V628	L629	L630	K631	K632	A633	P634	P635	R638	K639																							
L640	G644	T645	T646	S647	R648	K649	D650	V651	L652	Q653	E656	L657	L658	F661	S662	T663	T664	L665	H666	V667	P668	H669	L670	A671	T672	G673	E674	Q675	L676		L677	A679	L680	E681	L682	N685	F686	D688	R689	B690	H691	T692	T693	L694	A695	V698	K699	V703	W704	I705	G706	L707																											
K708	K709	L710	L711	L714	E715	M716	S717	L718	Q719	M720	D721	Y724	V725	T726	R727	K728	F729	A731	L732	L733	R734	G737	ALA	SER	PRO	LEU	ASP	PHE	ASP		N685	F686	D688	R689	B690	H691	T692	T693	L694	A695	V698	K699	V703	W704	I705	G706	L707																																

• Molecule 1: Vesicle-fusing ATPase

Chain D: 

L630	A557	K489	I395	I325	V245	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY	ALA	GLY
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	12830	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 ( $e^-/\text{\AA}^2$ )	44	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.52	3/3559 (0.1%)	0.95	11/4824 (0.2%)
1	B	0.47	0/3566	0.89	6/4834 (0.1%)
1	C	0.46	0/3584	0.87	5/4858 (0.1%)
1	D	0.43	0/3516	0.84	8/4775 (0.2%)
1	E	0.48	0/3566	0.93	8/4833 (0.2%)
1	F	0.49	0/3514	0.92	13/4759 (0.3%)
All	All	0.48	3/21305 (0.0%)	0.90	51/28883 (0.2%)

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	B	0	2
1	E	0	1
1	F	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	PHE	CD1-CE1	-7.83	1.23	1.39
1	A	236	ALA	CA-CB	-5.78	1.40	1.52
1	A	235	PHE	CB-CG	-5.41	1.42	1.51

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	235	PHE	CB-CG-CD1	-10.55	113.42	120.80
1	C	677	LEU	CB-CG-CD2	-9.07	95.58	111.00
1	A	235	PHE	CB-CG-CD2	8.18	126.52	120.80
1	E	629	LEU	CB-CG-CD1	-8.14	97.16	111.00
1	C	322	LEU	CA-CB-CG	8.13	134.00	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	PRO	Peptide
1	B	438	GLY	Peptide
1	B	546	HIS	Mainchain
1	E	438	GLY	Peptide
1	F	438	GLY	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	3513	0	3416	260	0
1	B	3517	0	3436	261	0
1	C	3535	0	3431	278	0
1	D	3467	0	3351	250	0
1	E	3516	0	3424	286	0
1	F	3467	0	3409	263	0
2	B	27	0	10	11	0
2	C	27	0	12	8	0
2	D	27	0	9	11	0
2	E	27	0	10	9	0
All	All	21123	0	20508	1497	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 36.

The worst 5 of 1497 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:F:222:GLY:H	1:F:402:GLY:HA3	1.24	1.02
1:A:222:GLY:HA3	1:A:402:GLY:HA2	1.51	0.93
1:E:263:GLY:O	1:E:437:SER:HB2	1.71	0.89
1:D:448:ALA:HA	1:D:482:ALA:HB3	1.53	0.89
1:C:490:PRO:HA	1:C:491:ALA:HB3	1.53	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	475/747 (64%)	443 (93%)	20 (4%)	12 (2%)	7	46
1	B	473/747 (63%)	429 (91%)	32 (7%)	12 (2%)	7	46
1	C	477/747 (64%)	450 (94%)	18 (4%)	9 (2%)	10	52
1	D	471/747 (63%)	439 (93%)	27 (6%)	5 (1%)	17	63
1	E	474/747 (64%)	441 (93%)	22 (5%)	11 (2%)	8	48
1	F	465/747 (62%)	428 (92%)	26 (6%)	11 (2%)	7	47
All	All	2835/4482 (63%)	2630 (93%)	145 (5%)	60 (2%)	13	50

5 of 60 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	344/638 (54%)	343 (100%)	1 (0%)	94	96
1	B	349/638 (55%)	346 (99%)	3 (1%)	84	93
1	C	347/638 (54%)	346 (100%)	1 (0%)	94	96
1	D	340/638 (53%)	339 (100%)	1 (0%)	94	96
1	E	345/638 (54%)	342 (99%)	3 (1%)	84	93
1	F	345/638 (54%)	342 (99%)	3 (1%)	84	93
All	All	2070/3828 (54%)	2058 (99%)	12 (1%)	91	95

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	305	LEU
1	E	305	LEU
1	F	305	LEU
1	C	305	LEU
1	E	327	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	319	ASN
1	C	352	ASN
1	D	527	GLN
1	B	620	ASN
1	D	352	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 ⓘ

4 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	ADP	B	801	-	24,29,29	1.07	2 (8%)	23,45,45	1.45	4 (17%)
2	ADP	C	801	-	24,29,29	1.27	2 (8%)	23,45,45	2.37	5 (21%)
2	ADP	D	801	-	24,29,29	1.06	2 (8%)	23,45,45	2.79	6 (26%)
2	ADP	E	801	-	24,29,29	1.28	3 (12%)	23,45,45	1.86	8 (34%)

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	ADP	B	801	-	-	0/12/32/32	0/3/3/3
2	ADP	C	801	-	-	0/12/32/32	0/3/3/3
2	ADP	D	801	-	-	0/12/32/32	0/3/3/3
2	ADP	E	801	-	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	ADP	C2-N3	2.11	1.35	1.32
2	C	801	ADP	O4'-C1'	2.36	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ADP	O4'-C1'	2.44	1.44	1.41
2	E	801	ADP	O4'-C1'	2.46	1.44	1.41
2	E	801	ADP	C2-N3	2.50	1.36	1.32

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	ADP	N3-C2-N1	-11.41	119.91	128.87
2	C	801	ADP	N3-C2-N1	-7.18	123.23	128.87
2	C	801	ADP	C1'-N9-C4	-5.35	120.83	126.81
2	B	801	ADP	N3-C2-N1	-4.33	125.47	128.87
2	D	801	ADP	C1'-N9-C4	-2.80	123.68	126.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	ADP	11	0
2	C	801	ADP	8	0
2	D	801	ADP	11	0
2	E	801	ADP	9	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.