



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 06:46 PM UTC

PDB ID : 3J95 / pdb_00003j95
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 initial model : 1NSF

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:

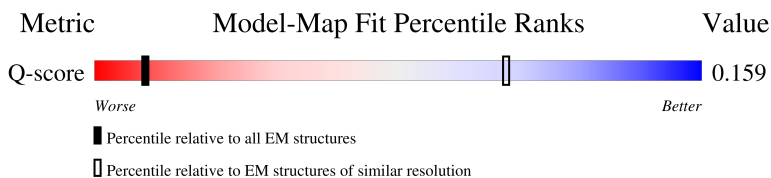
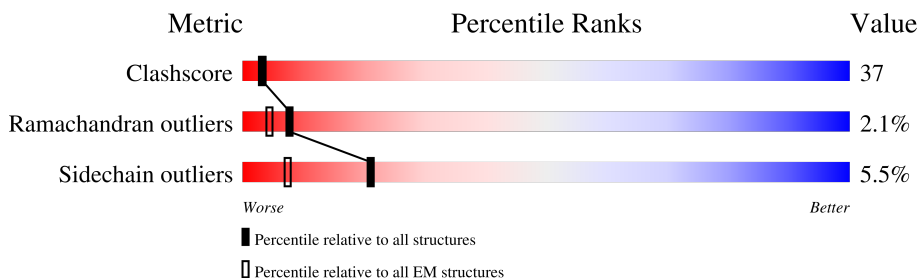
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	389 (7.10 - 8.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	747	
1	B	747	
1	C	747	
1	D	747	

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Mol	Chain	Length	Quality of chain
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	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.

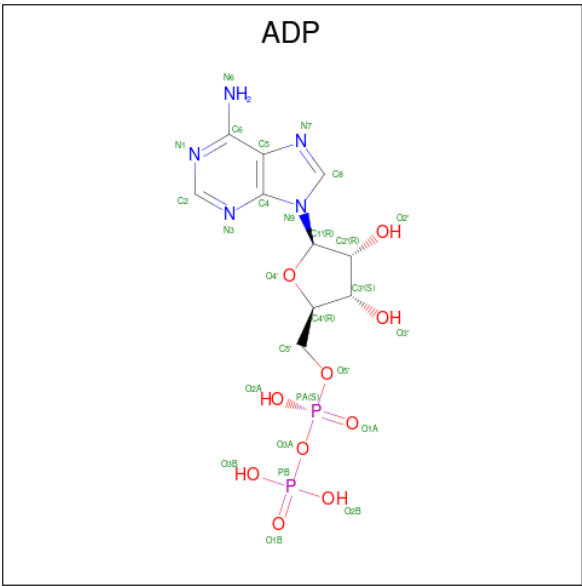
- Molecule 1 is a protein called Vesicle-fusing ATPase.

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		

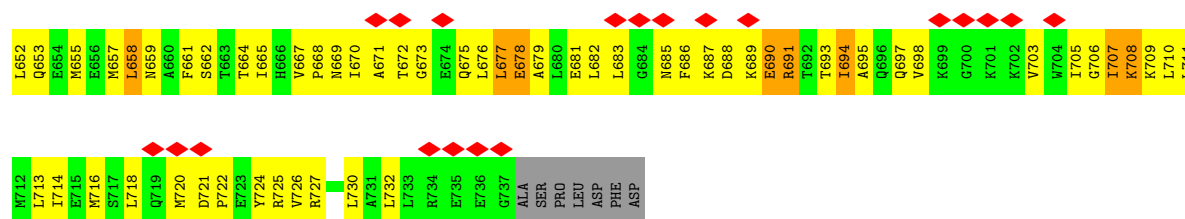
There are 18 discrepancies between the modelled and reference sequences:

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

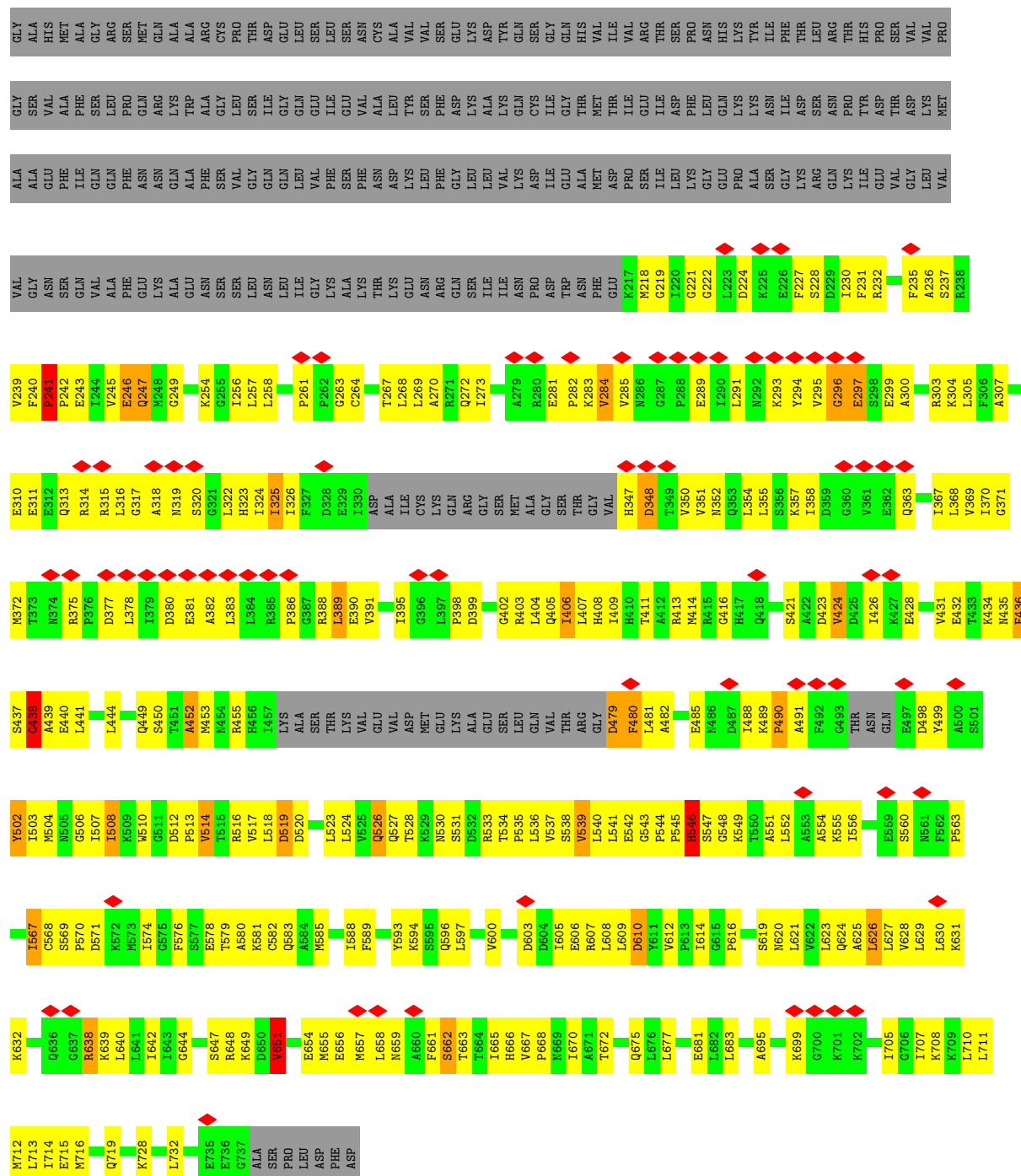
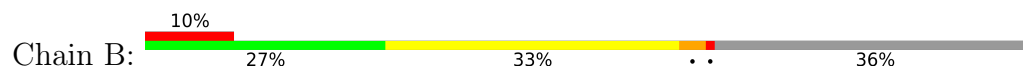
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



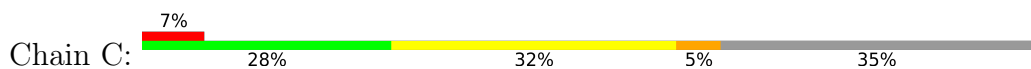
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	



• Molecule 1: Vesicle-fusing ATPase

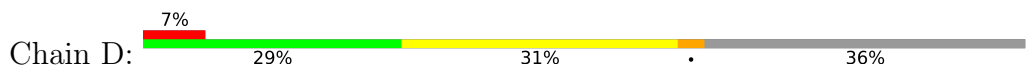


• Molecule 1: Vesicle-fusing ATPase

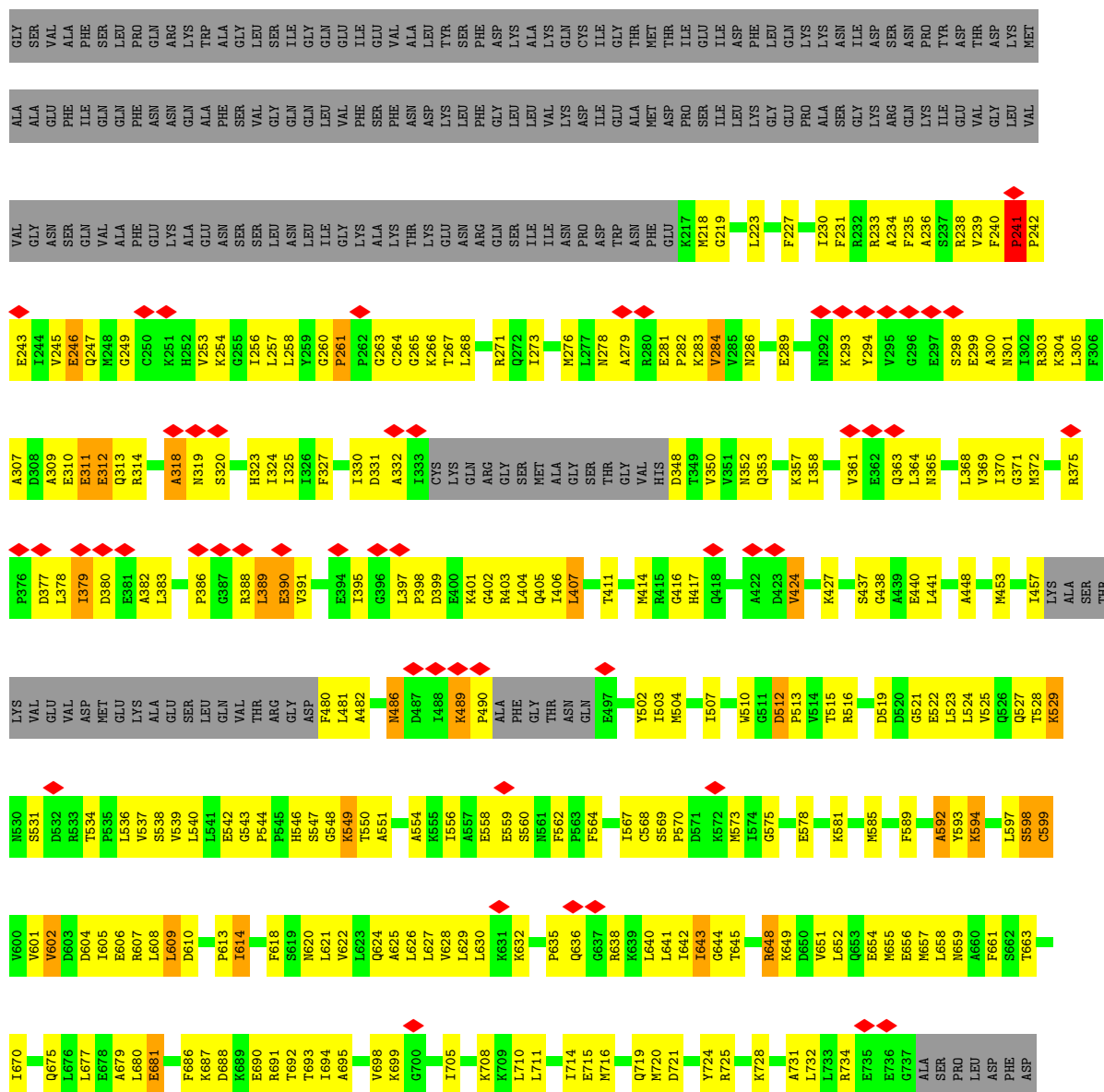


GLY	ALA	HIS	MET	ALA	PHE	GLN	GLY	ARG	PRO	GLN	ASN	GLN	ALA	LYS	TRP	ALA	ARG	CYS	PRO	THR	GLY	SER	LEU	SER	LEU	SER	ASN	VAL	CYS	ALA	ASP	LEU	VAL	VAL	SER	VAL	LEU	GLN	TYR	ASP	LYS	GLY	GLN	THR	HIS	VAL	THR	ILE	VAL	ARG	GLU	THR	ILE	ASP	SER	PRO	ASN	HIS	GLN	LEU	ASP	ILE	THR	ASP	GLY	ASN	ILE	PHE	THR	ASP	LEU	ARG	ASN	GLN	THR	PRO	THR	LYS	PRO	SER	VAL	VAL	LEU	ASP	MET	PRO																																																																																																																																																																																																																																																																																																																																																																																																						
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ALA	ALA	GLU	PHE	ILE	GLN	GLN	PHE	ASN	PHE	ASN	GLN	ALA	GLN	LYS	TRP	ALA	ARG	CYS	PRO	THR	GLY	ASP	GLU	LEU	SER	LEU	SER	ASN	VAL	CYS	ALA	ASP	LEU	VAL	VAL	SER	VAL	LEU	GLN	TYR	ASP	LYS	GLY	GLN	THR	HIS	VAL	THR	ILE	VAL	ARG	GLU	THR	ILE	ASP	SER	PRO	ASN	HIS	GLN	LEU	ASP	ILE	THR	ASP	GLY	ASN	ILE	PHE	THR	ASP	LEU	ARG	ASN	GLN	THR	PRO	THR	LYS	PRO	SER	VAL	VAL	LEU	ASP	MET	PRO																																																																																																																																																																																																																																																																																																																																																																																																					
VAL	GLY	ASN	SER	VAL	ILE	GLN	VAL	ALA	PHE	ASN	GLN	ALA	GLN	LYS	TRP	ALA	ARG	CYS	PRO	THR	GLY	ASP	GLU	LEU	SER	LEU	SER	ASN	VAL	CYS	ALA	ASP	LEU	VAL	VAL	SER	VAL	LEU	GLN	TYR	ASP	LYS	GLY	GLN	THR	HIS	VAL	THR	ILE	VAL	ARG	GLU	THR	ILE	ASP	SER	PRO	ASN	HIS	GLN	LEU	ASP	ILE	THR	ASP	GLY	ASN	ILE	PHE	THR	ASP	LEU	ARG	ASN	GLN	THR	PRO	THR	LYS	PRO	SER	VAL	VAL	LEU	ASP	MET	PRO																																																																																																																																																																																																																																																																																																																																																																																																					
P242	E243	E244	V245	V246	Q247	M248	G249	C250	G251	I332	I333	H252	V253	K254	G255	I256	P261	P262	G263	C264	G265	L268	L269	A270	R271	Q272	G273	A279	R280	E281	V284	V285	E289	L290	L291	N292	K293	Y294	V295	G296	E297	L305	D308	A309	E310	E311	Q312	Q313	R314	R315	L316	G317	A318	N319																																																																																																																																																																																																																																																																																																																																																																																																																																						
S320	G321	L322	H323	I324	I325	I326	D331	A332	I333	C334	L335	G336	H337	A338	G339	A340	A341	A342	A343	A344	A345	A346	A347	A348	A349	A350	A351	A352	A353	A354	A355	A356	A357	A358	A359	A360	A361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377	A378	A379	A380	A381	A382	A383	A384	A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800

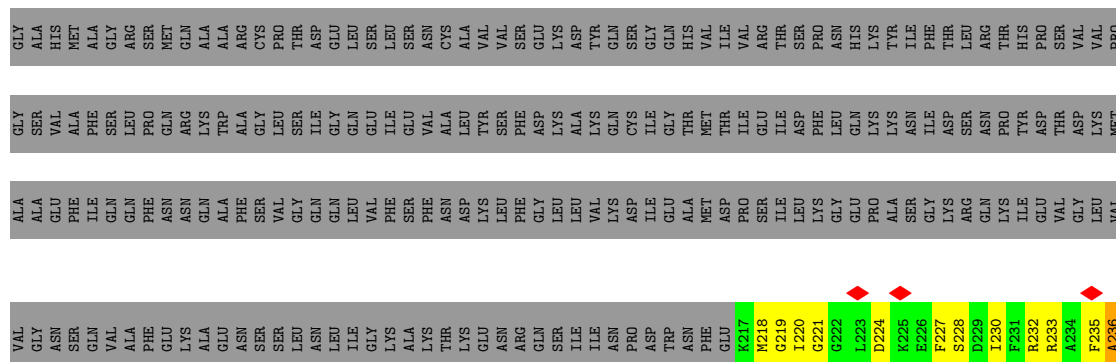
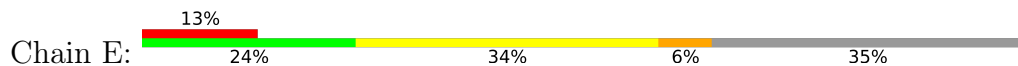
• Molecule 1: Vesicle-fusing ATPase

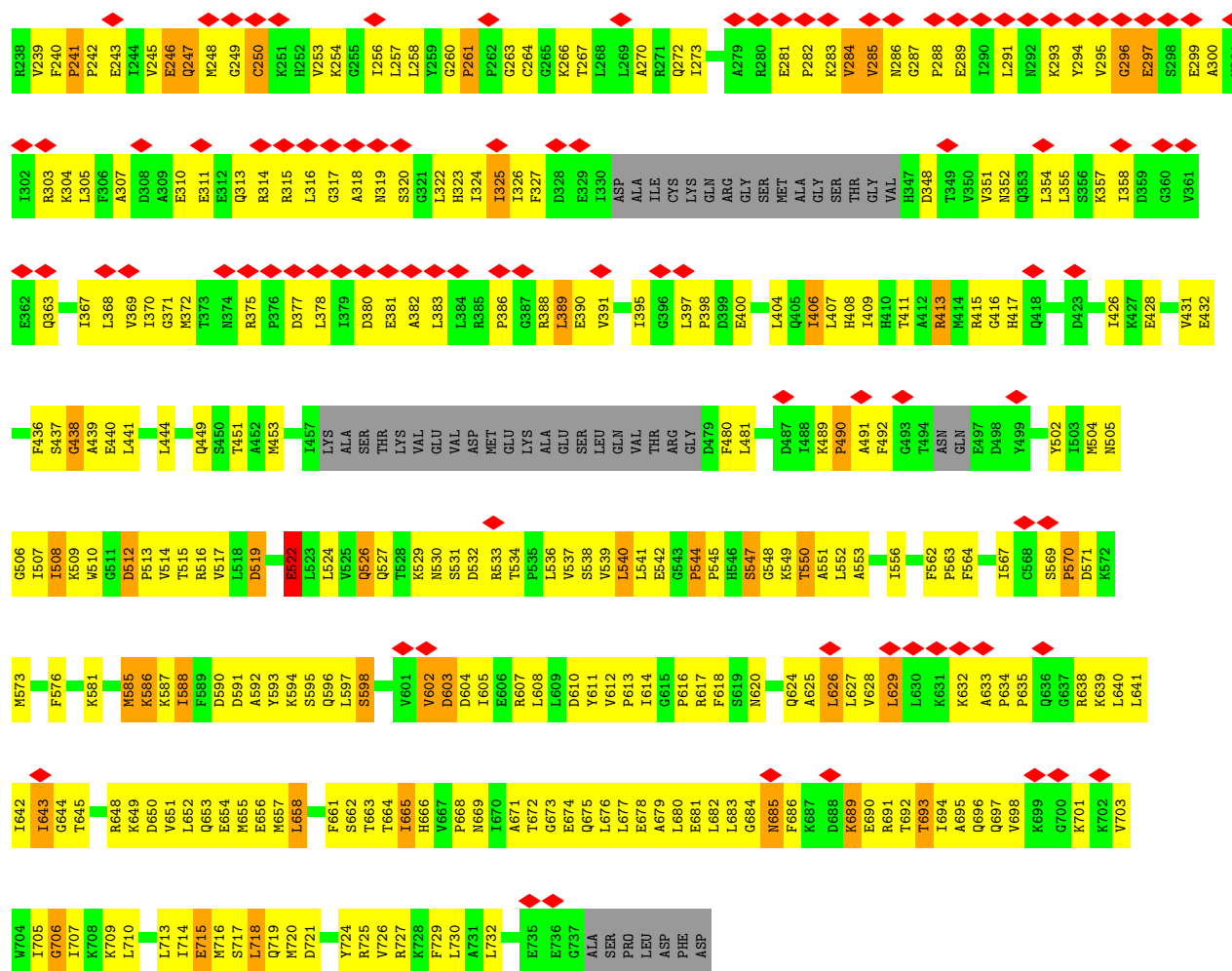


GLY	ALA	HIS	MET	ALA	PHE	GLN	GLY	ARG	PRO	GLN	ASN	GLN	ALA	LYS	TRP	ALA	ARG	CYS	PRO	THR	GLY	ASP	GLU	LEU	SER	LEU	SER	ASN	VAL	CYS	ALA	ASP	LEU	VAL	VAL	SER	VAL	LEU	GLN	TYR	ASP	LYS	GLY	GLN	THR	HIS	VAL	THR	ILE	VAL	ARG	GLU	THR	ILE	ASP	LEU	PRO	LYS	TYR	LYS	PRO	ASN	HIS	GLN	LEU	ASP	ILE	THR	ASP	GLY	ASN	ILE	PHE	THR	ASP	LEU	ARG	ASN	GLN	THR	PRO	THR	LYS	PRO	THR	ASP	PRO	SER	VAL	VAL	LEU	ASP	MET	PRO
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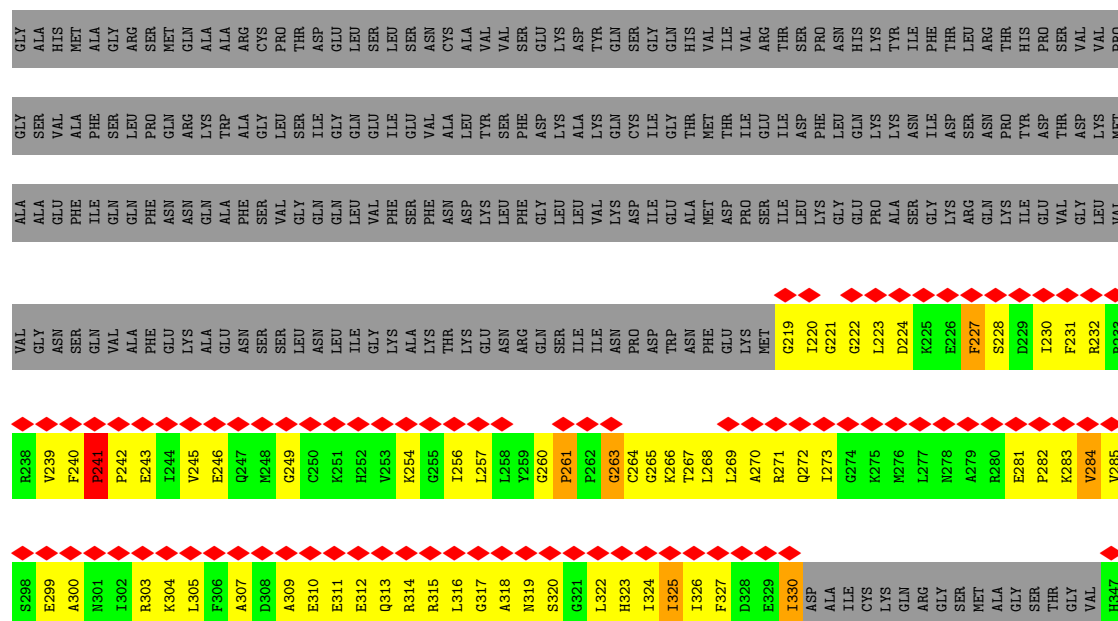
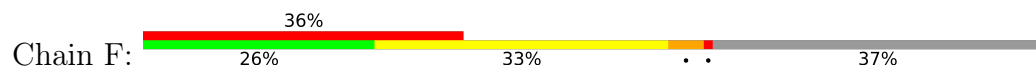


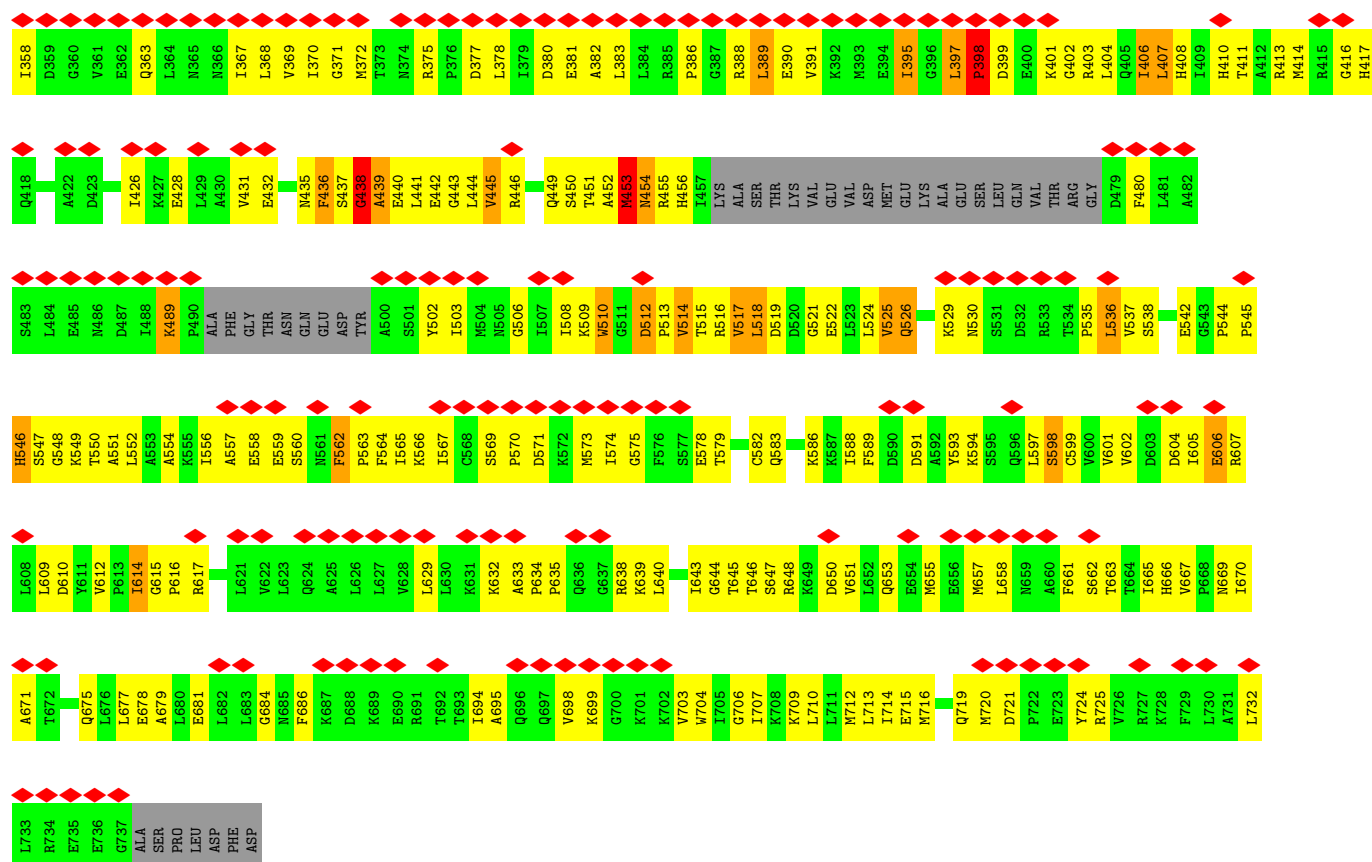
• Molecule 1: Vesicle-fusing ATPase





● Molecule 1: Vesicle-fusing ATPase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12830	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	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
Maximum map value	13.843	Depositor
Minimum map value	-5.160	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6	Depositor
Map size ($\text{\AA}$)	311.1936, 311.1936, 311.1936	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.4312, 2.4312, 2.4312	Depositor

5 Model quality

5.1 Standard geometry

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	4/3559 (0.1%)	1.46	51/4824 (1.1%)
1	B	0.66	2/3566 (0.1%)	1.35	40/4834 (0.8%)
1	C	0.65	1/3584 (0.0%)	1.35	44/4858 (0.9%)
1	D	0.61	0/3516	1.34	36/4775 (0.8%)
1	E	0.69	1/3566 (0.0%)	1.41	50/4833 (1.0%)
1	F	0.69	2/3514 (0.1%)	1.43	53/4759 (1.1%)
All	All	0.68	10/21305 (0.0%)	1.39	274/28883 (0.9%)

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	PHE	CA-C	-8.64	1.41	1.52
1	A	236	ALA	CA-CB	-8.41	1.40	1.53
1	C	507	ILE	CA-C	-7.14	1.47	1.53
1	F	456	HIS	CA-C	6.10	1.60	1.52
1	A	330	ILE	CA-CB	5.58	1.61	1.54

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	455	ARG	N-CA-C	12.80	125.31	111.36
1	A	239	VAL	N-CA-C	10.74	121.57	110.72
1	A	261	PRO	CA-C-N	10.72	133.42	120.23
1	A	261	PRO	C-N-CA	10.72	133.42	120.23
1	D	416	GLY	N-CA-C	-10.11	100.25	112.49

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	274	0
1	B	3517	0	3436	266	0
1	C	3535	0	3431	286	0
1	D	3467	0	3351	261	0
1	E	3516	0	3424	294	0
1	F	3467	0	3409	271	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	1543	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 37.

The worst 5 of 1543 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%)	4	26
1	B	473/747 (63%)	429 (91%)	32 (7%)	12 (2%)	4	26
1	C	477/747 (64%)	450 (94%)	18 (4%)	9 (2%)	6	32
1	D	471/747 (63%)	439 (93%)	27 (6%)	5 (1%)	11	46
1	E	474/747 (64%)	441 (93%)	22 (5%)	11 (2%)	5	28
1	F	465/747 (62%)	428 (92%)	26 (6%)	11 (2%)	4	27
All	All	2835/4482 (63%)	2630 (93%)	145 (5%)	60 (2%)	8	30

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 [i](#)

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%)	323 (94%)	21 (6%)	17	38
1	B	349/638 (55%)	334 (96%)	15 (4%)	26	47
1	C	347/638 (54%)	324 (93%)	23 (7%)	15	37
1	D	340/638 (53%)	327 (96%)	13 (4%)	29	50
1	E	345/638 (54%)	321 (93%)	24 (7%)	14	35
1	F	345/638 (54%)	328 (95%)	17 (5%)	22	43
All	All	2070/3828 (54%)	1957 (94%)	113 (6%)	21	41

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	691	ARG
1	F	606	GLU
1	D	716	MET
1	F	578	GLU
1	F	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	418	GLN
1	F	286	ASN
1	F	546	HIS
1	B	526	GLN
1	B	418	GLN

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](#)

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	E	801	-	28,29,29	1.89	5 (17%)	43,45,45	2.11	13 (30%)
2	ADP	C	801	-	28,29,29	1.81	6 (21%)	43,45,45	2.23	16 (37%)
2	ADP	D	801	-	28,29,29	1.44	5 (17%)	43,45,45	2.64	13 (30%)
2	ADP	B	801	-	28,29,29	1.57	5 (17%)	43,45,45	2.11	11 (25%)

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	E	801	-	-	4/16/32/32	0/3/3/3
2	ADP	C	801	-	-	2/16/32/32	0/3/3/3
2	ADP	D	801	-	-	4/16/32/32	0/3/3/3
2	ADP	B	801	-	-	7/16/32/32	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ADP	C5-C4	6.22	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	ADP	C5-C4	5.44	1.48	1.39
2	E	801	ADP	PA-O3A	5.37	1.65	1.59
2	B	801	ADP	C5-C4	4.62	1.47	1.39
2	D	801	ADP	C5-C4	4.00	1.46	1.39

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	801	ADP	C5-C4-N3	-6.69	117.50	126.72
2	D	801	ADP	C5-C4-N3	-6.49	117.78	126.72
2	B	801	ADP	C5-C4-N3	-6.49	117.78	126.72
2	D	801	ADP	N3-C2-N1	-5.73	119.91	128.58
2	D	801	ADP	C4-N9-C8	5.65	111.67	105.74

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	ADP	C5'-O5'-PA-O1A
2	B	801	ADP	C5'-O5'-PA-O3A
2	E	801	ADP	C5'-O5'-PA-O2A
2	E	801	ADP	C5'-O5'-PA-O3A
2	B	801	ADP	O4'-C4'-C5'-O5'

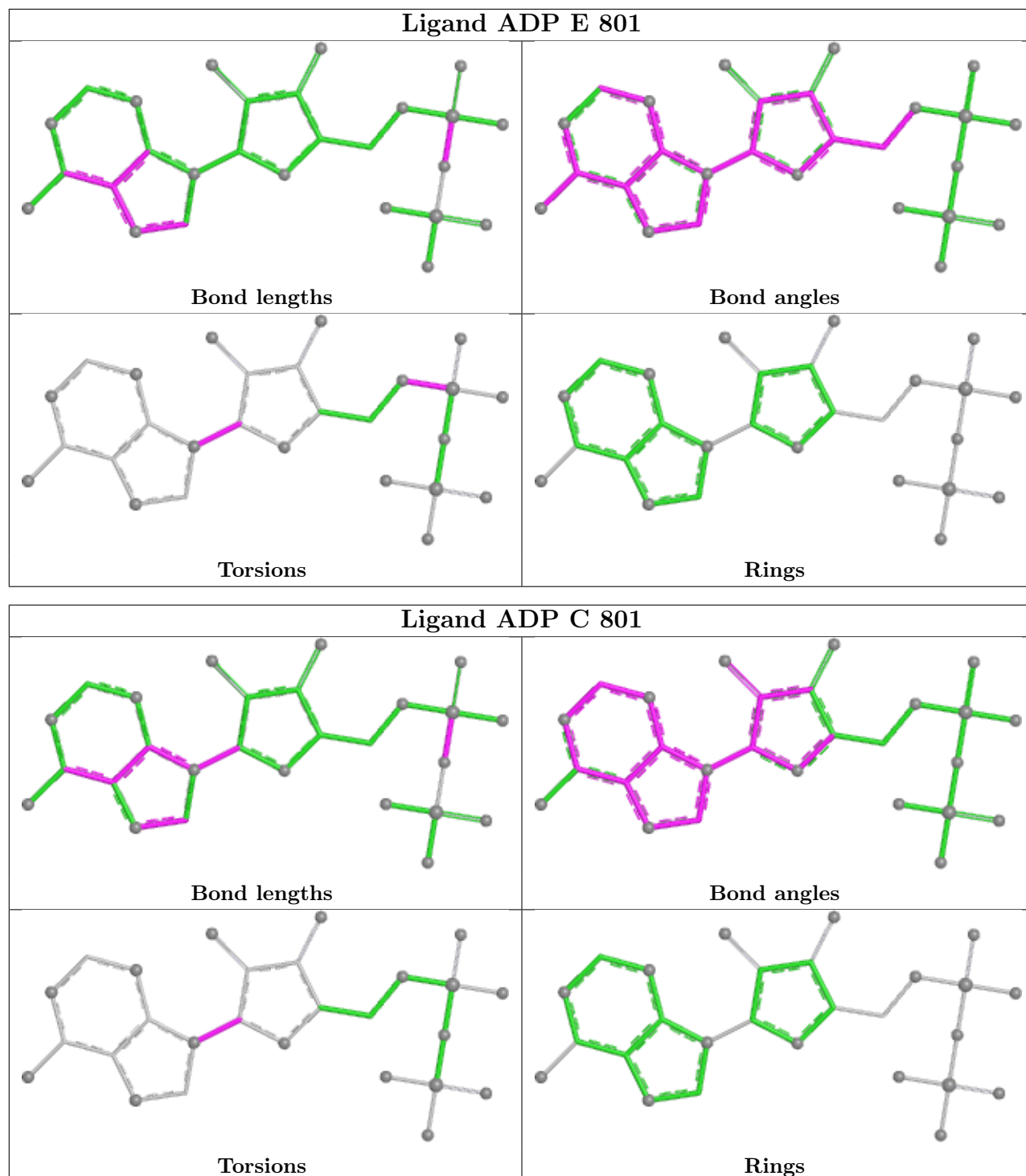
There are no ring outliers.

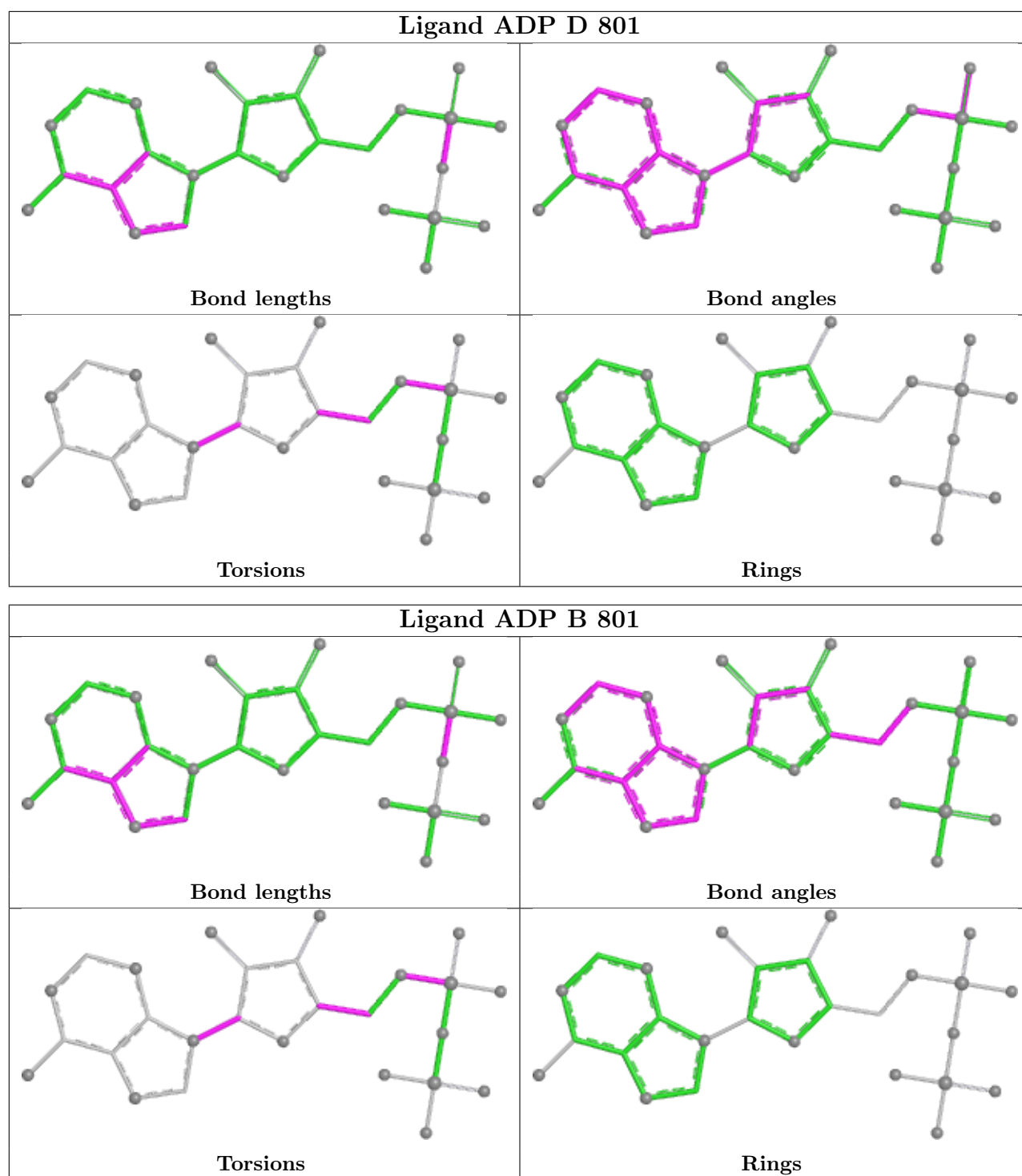
4 monomers are involved in 39 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

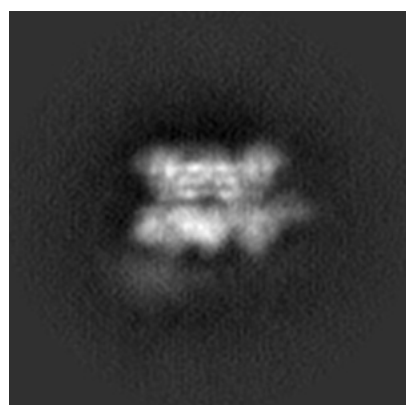
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6205. These allow visual inspection of the internal detail of the map and identification of artifacts.

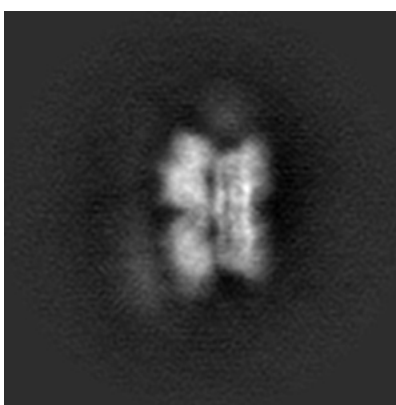
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

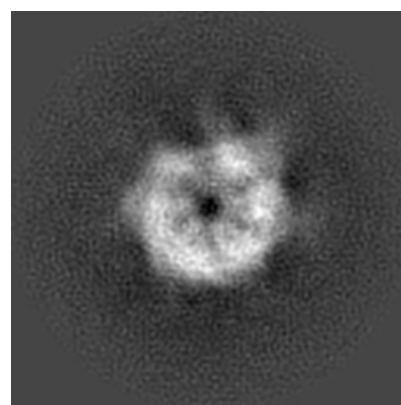
6.1.1 Primary map



X



Y

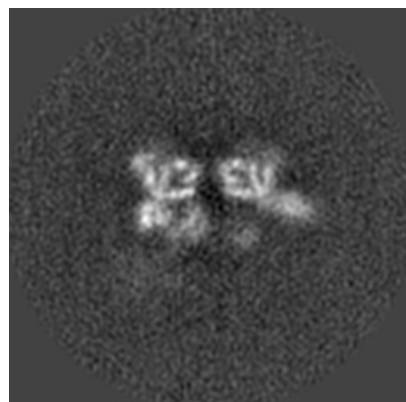


Z

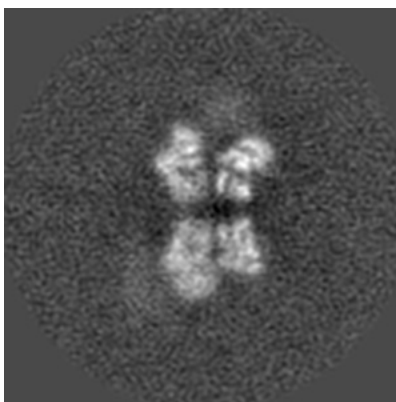
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

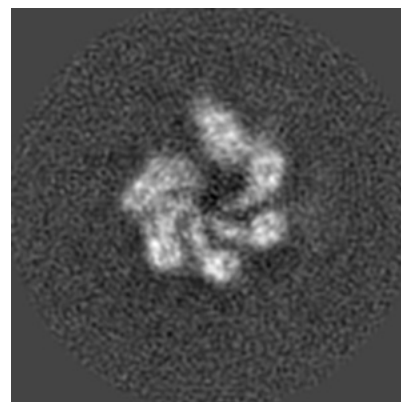
6.2.1 Primary map



X Index: 64



Y Index: 64

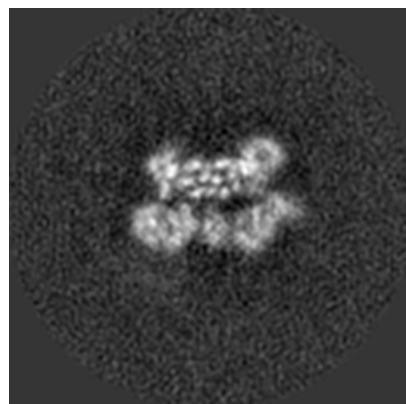


Z Index: 64

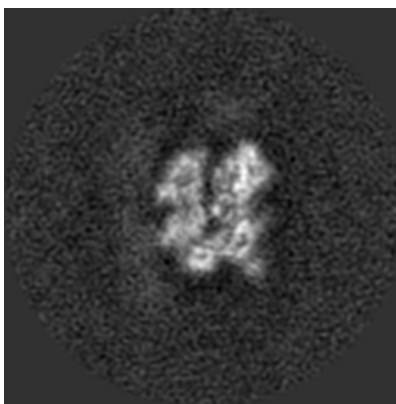
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

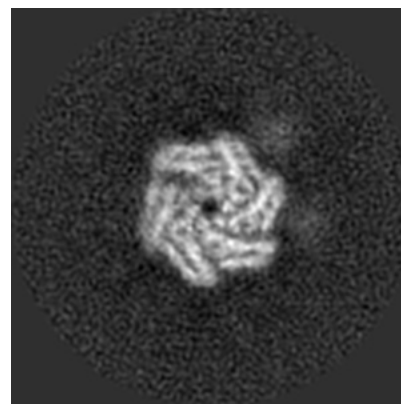
6.3.1 Primary map



X Index: 71



Y Index: 51

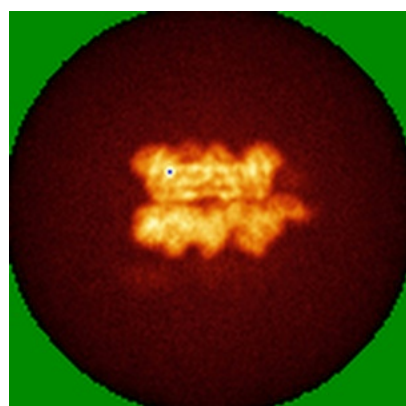


Z Index: 77

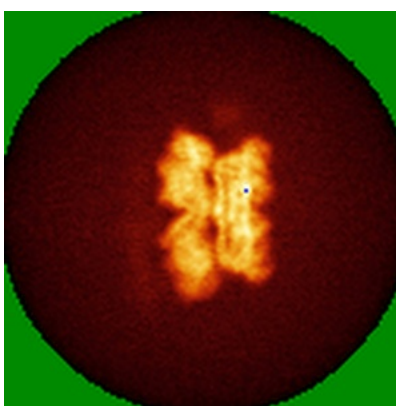
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

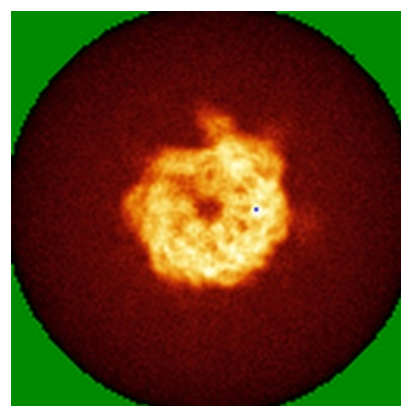
6.4.1 Primary map



X



Y

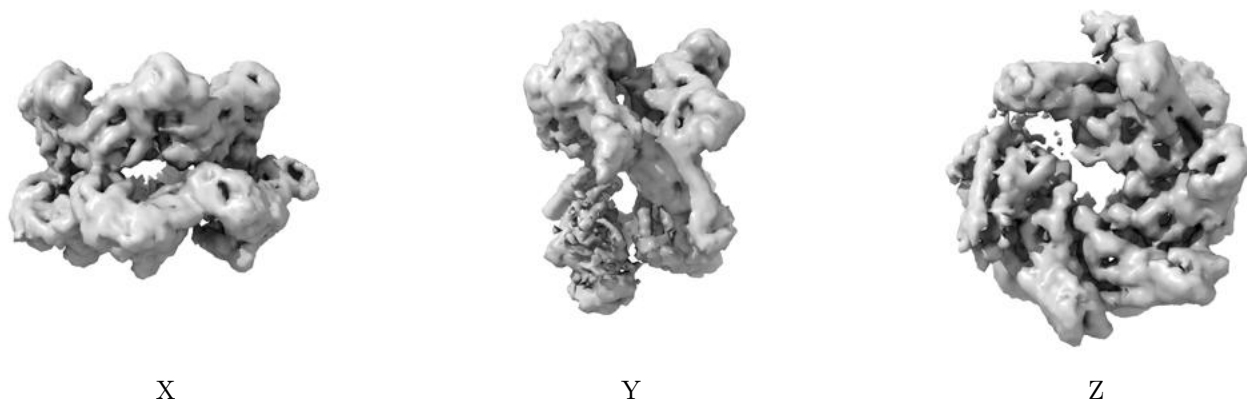


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

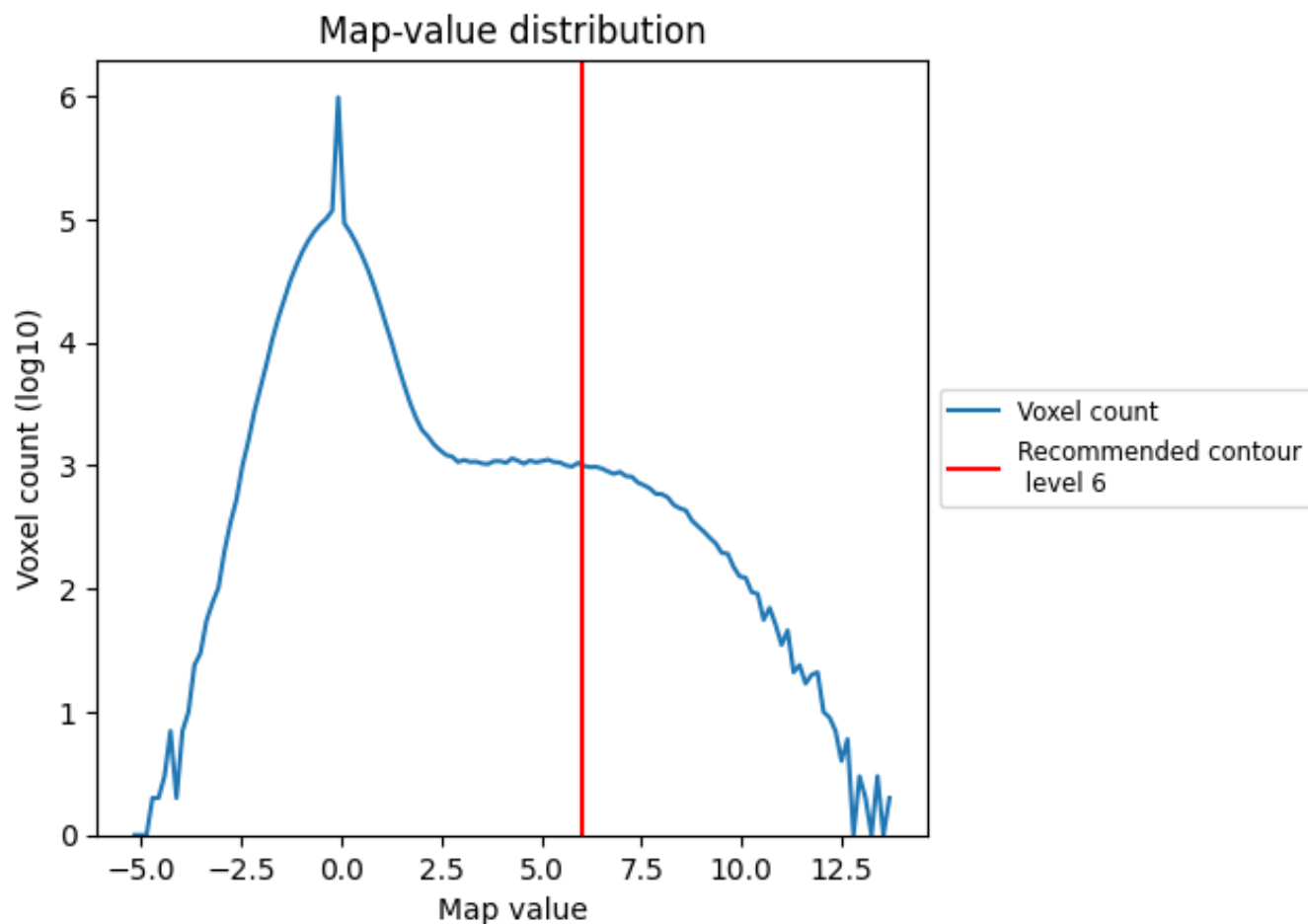
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

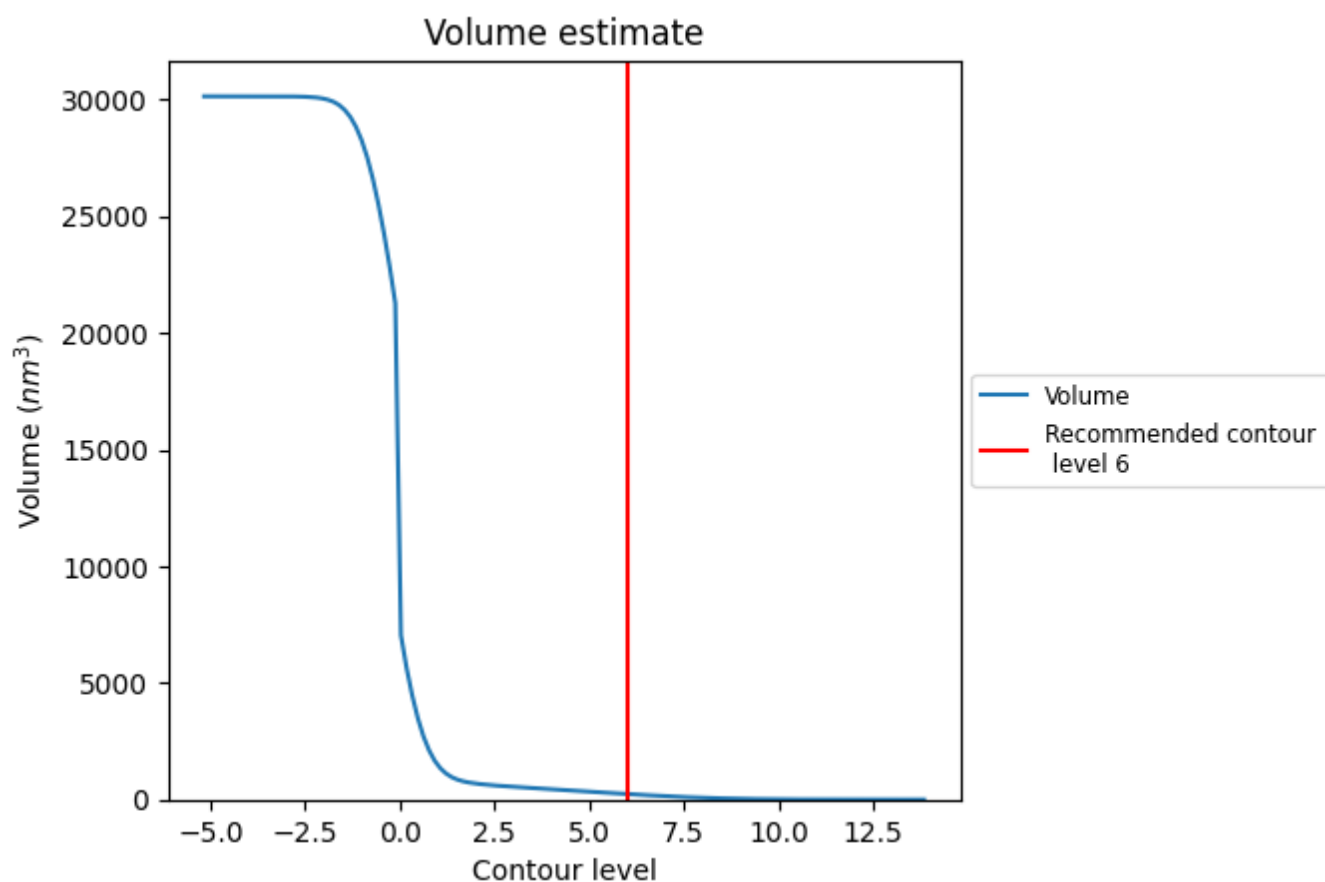
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

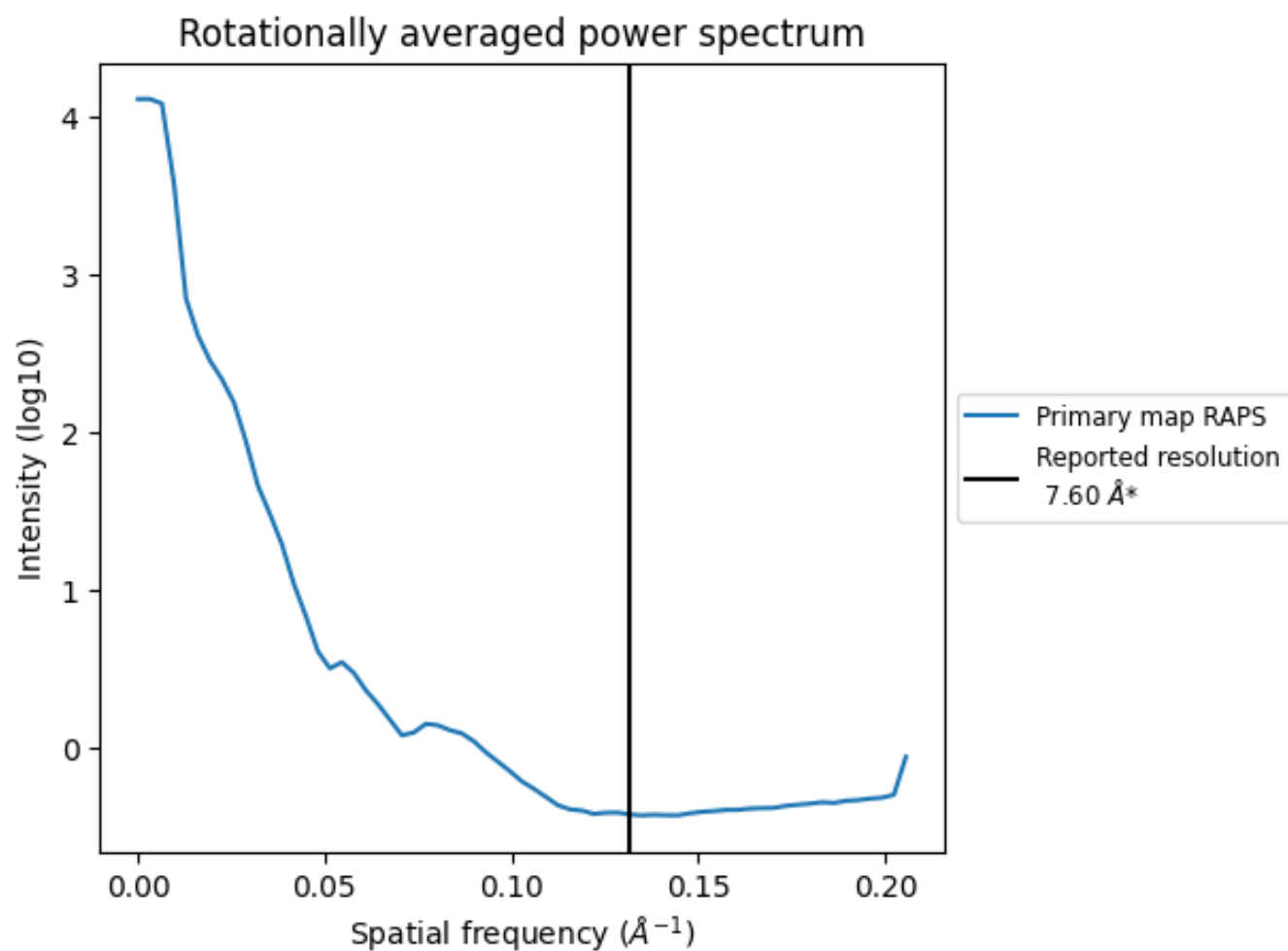
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 239 nm³; this corresponds to an approximate mass of 216 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.132 Å⁻¹

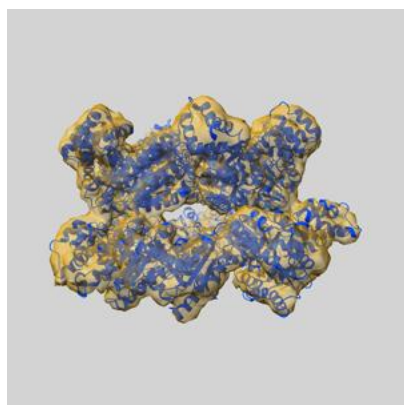
8 Fourier-Shell correlation

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

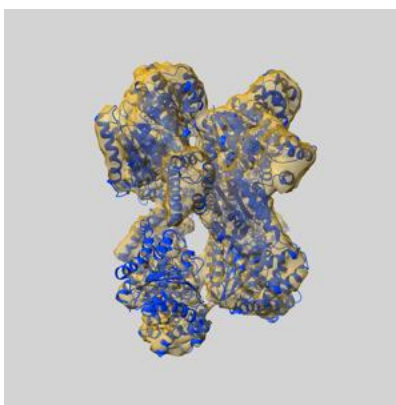
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6205 and PDB model 3J95. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

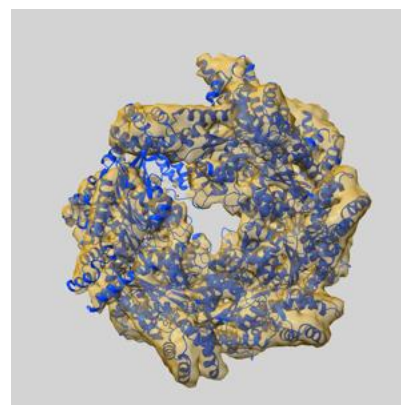
9.1 Map-model overlay [i](#)



X



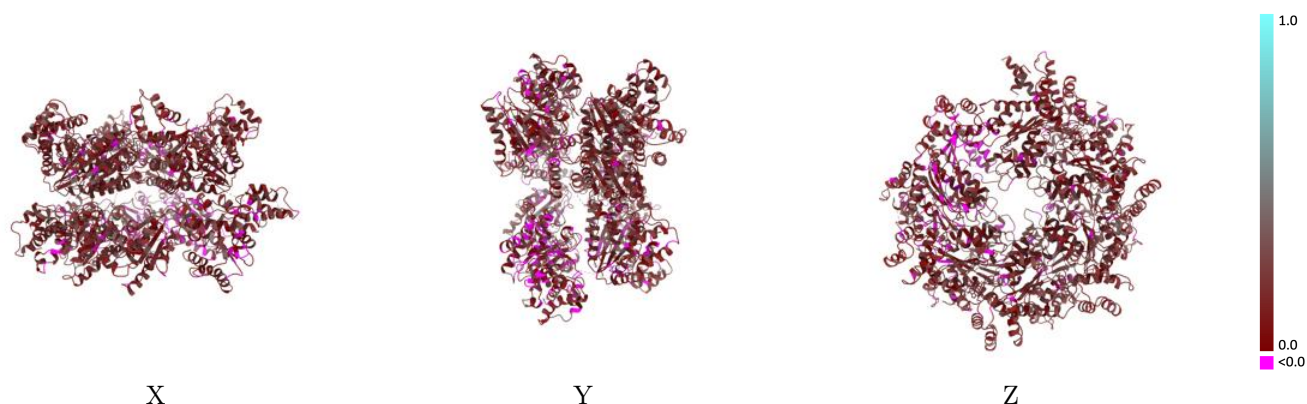
Y



Z

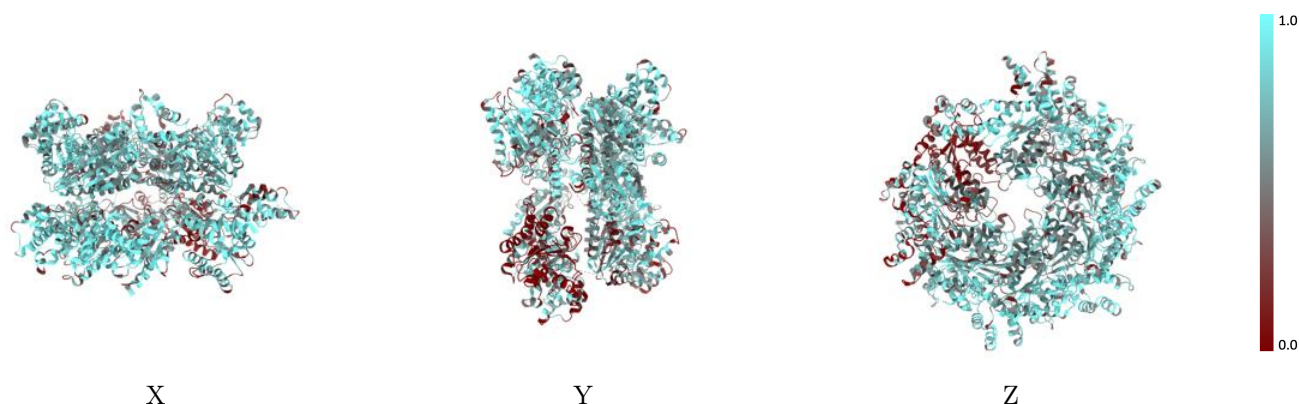
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



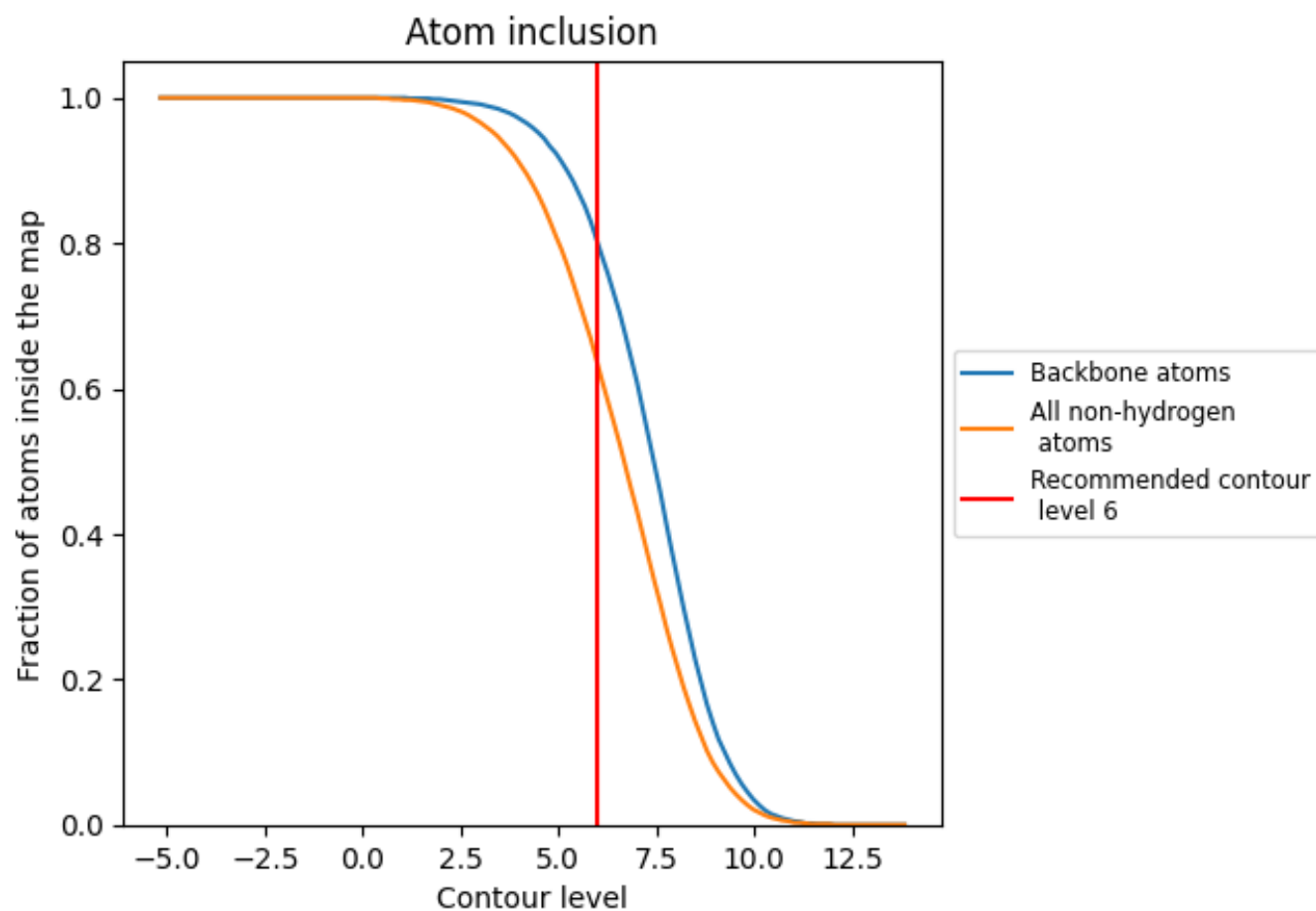
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6340	0.1590
A	0.6410	0.1540
B	0.6920	0.1590
C	0.7250	0.1840
D	0.7220	0.1800
E	0.6600	0.1560
F	0.3590	0.1170

1.0
0.0
-0.0