wwPDB EM Validation Summary Report (i)

Feb 12, 2024 – 11:41 AM EST

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 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 (i) 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 (1)) were used in the production of this report:

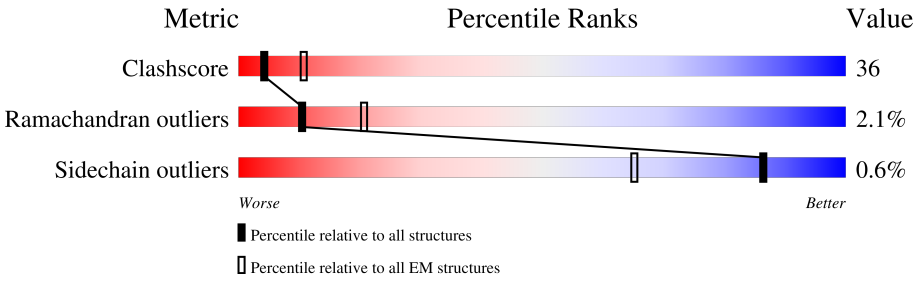
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	15% 30% 32% • 35%
1	B	747	10% 32% 31% • 36%
1	C	747	7% 31% 33% • 35%
1	D	747	7% 32% 31% • 36%
1	E	747	13% 28% 35% • 35%
1	F	747	36% 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 (i)

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.

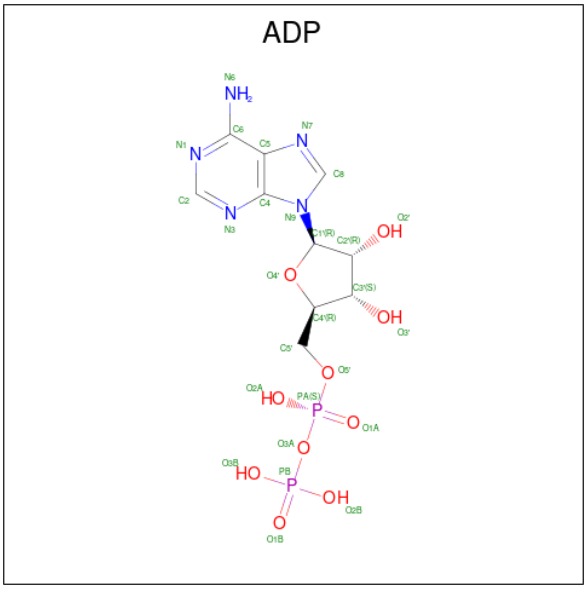
- Molecule 1 is a protein called Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	483	3513	2221	617	660	15	0	0
1	B	481	3517	2230	611	660	16	0	0
1	C	485	3535	2236	618	666	15	0	0
1	D	479	3467	2203	594	654	16	0	0
1	E	482	3516	2233	611	656	16	0	0
1	F	473	3467	2197	609	645	16	0	0

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: $C_{10}H_{15}N_5O_{10}P_2$).



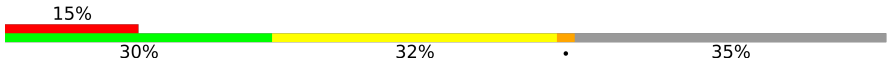
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

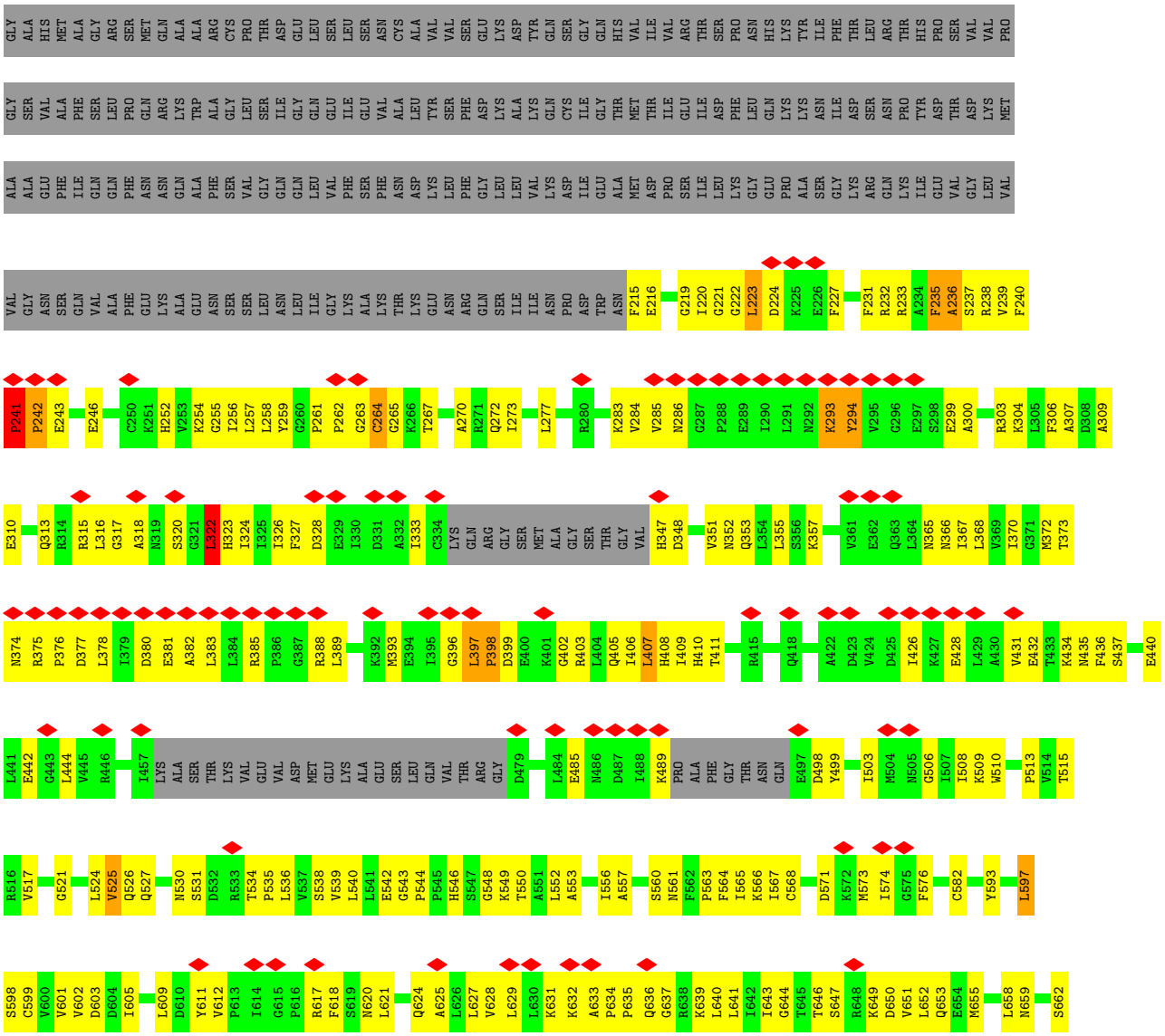
3 Residue-property plots (i)

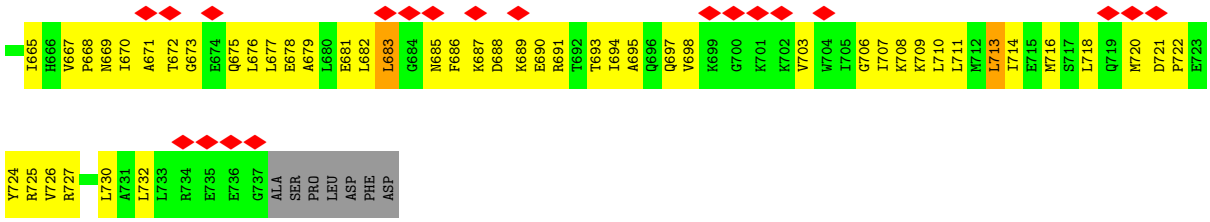
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

Chain A:

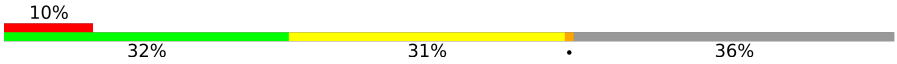


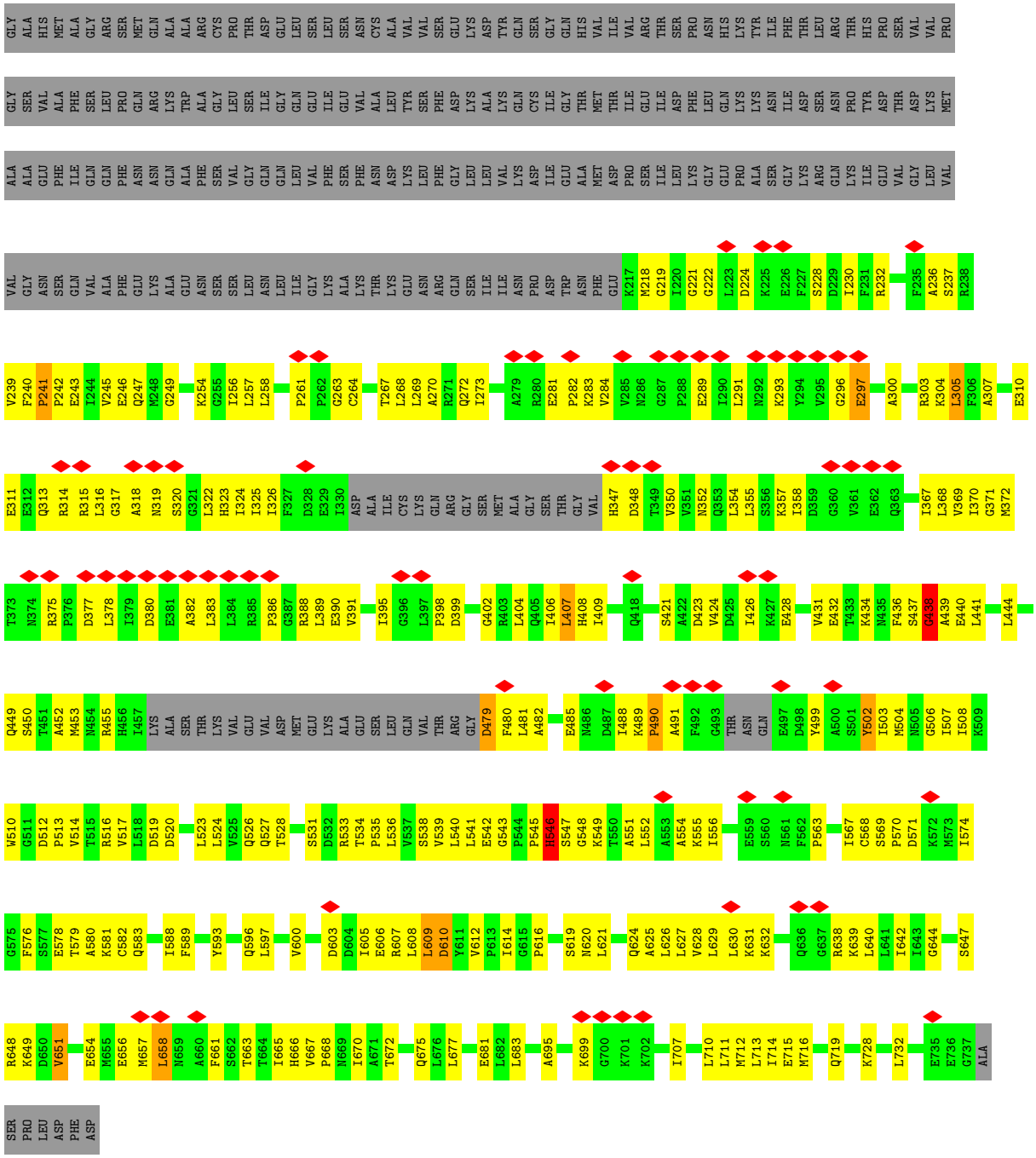




• Molecule 1: Vesicle-fusing ATPase

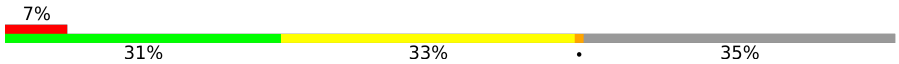
Chain B:

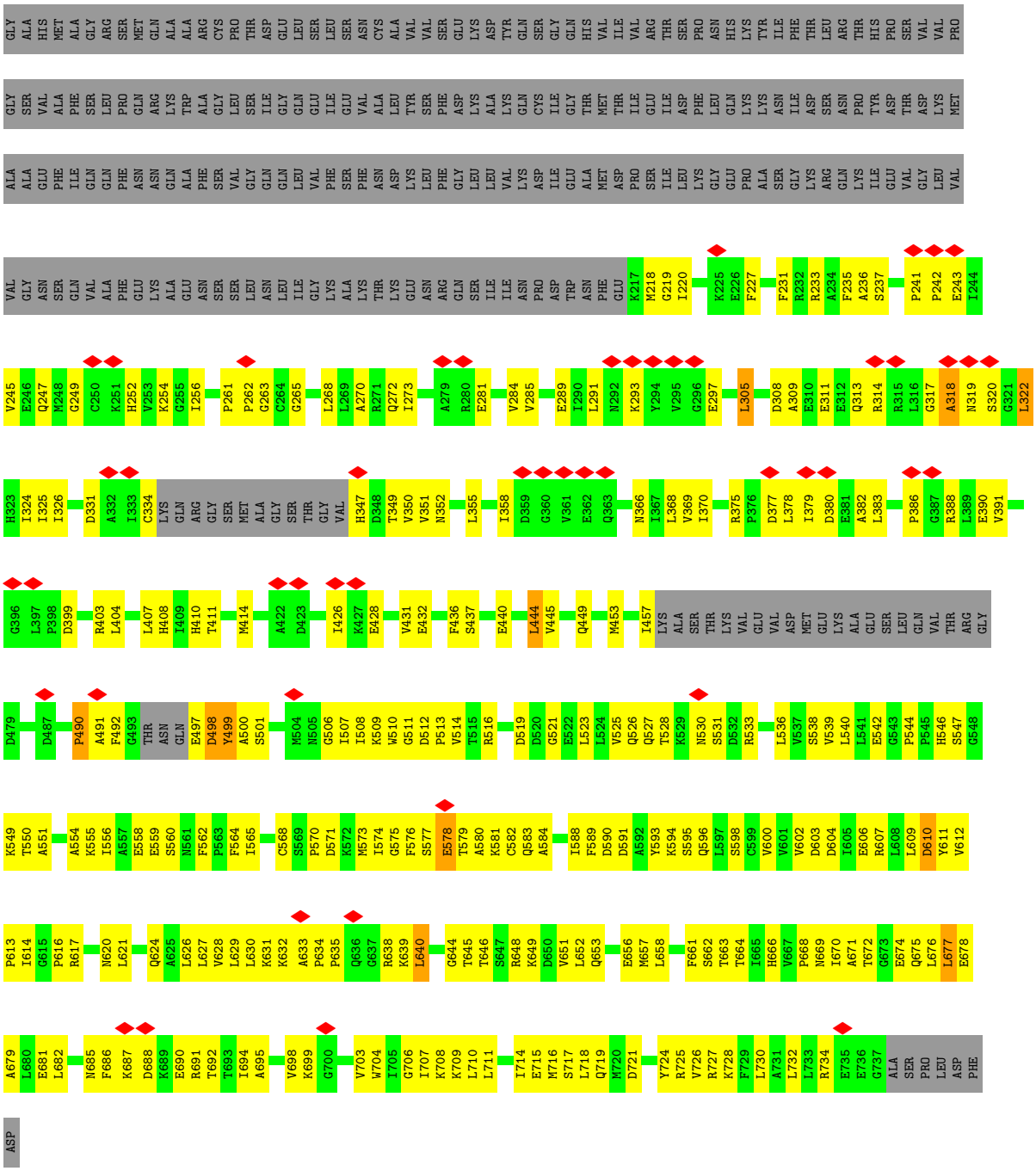




- Molecule 1: Vesicle-fusing ATPase

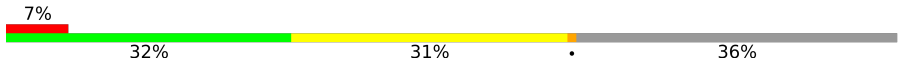
Chain C:

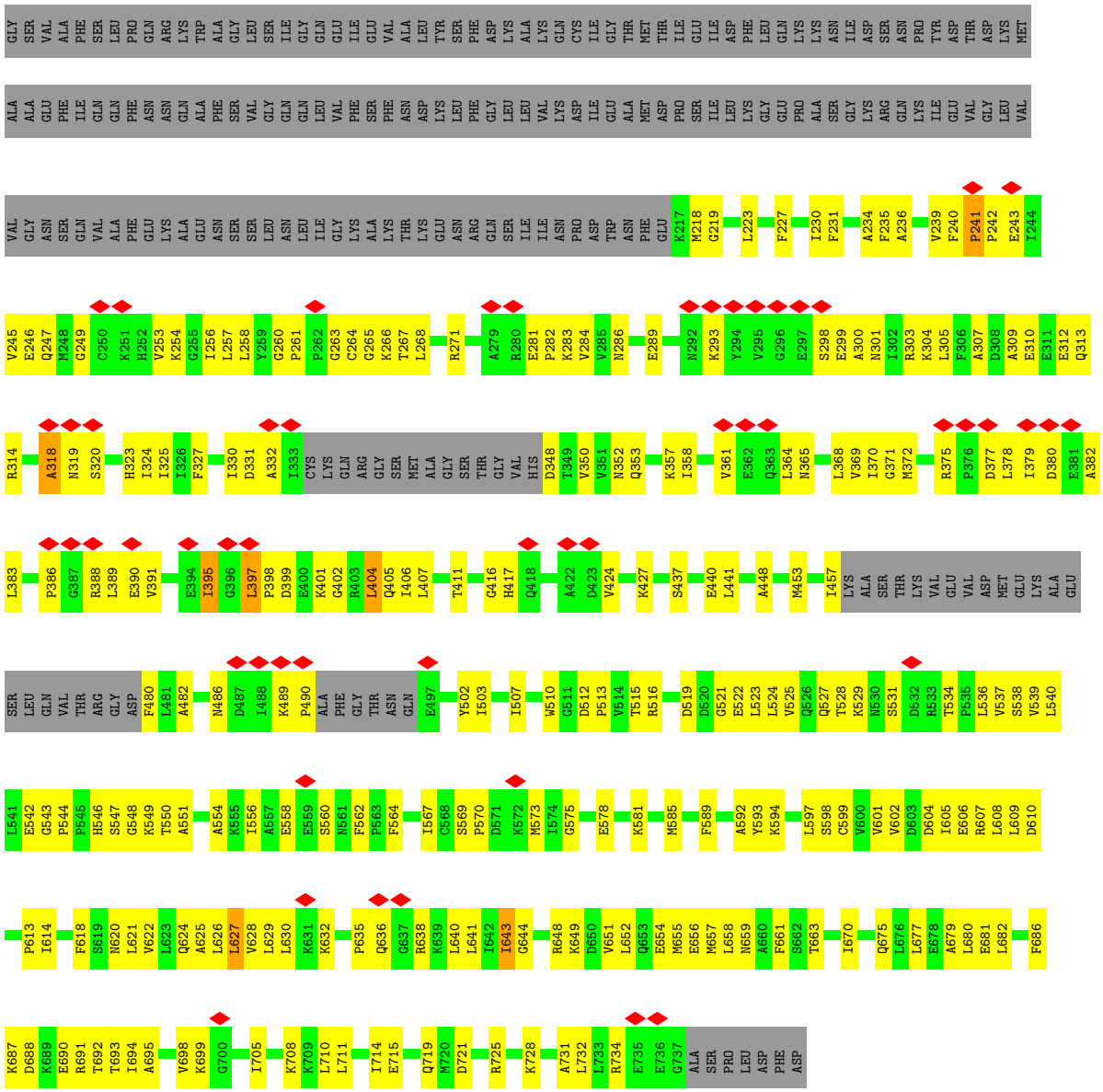




- Molecule 1: Vesicle-fusing ATPase

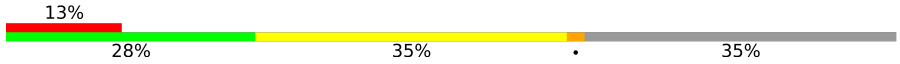
Chain D:

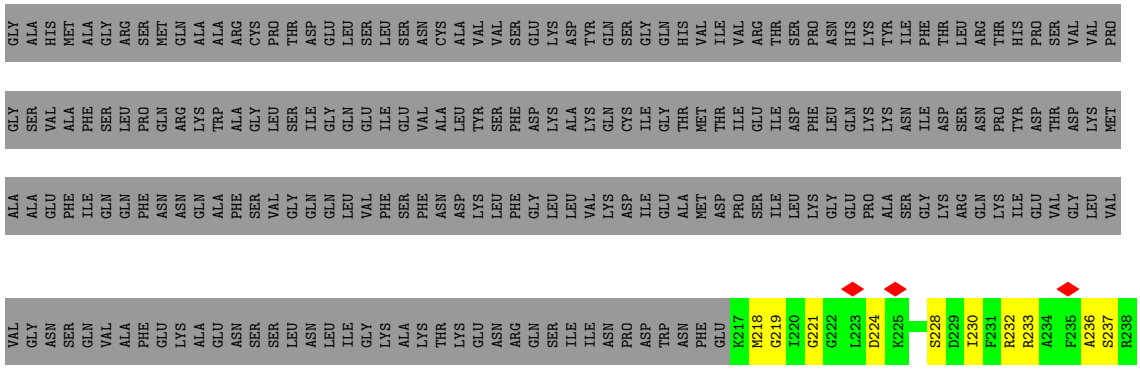


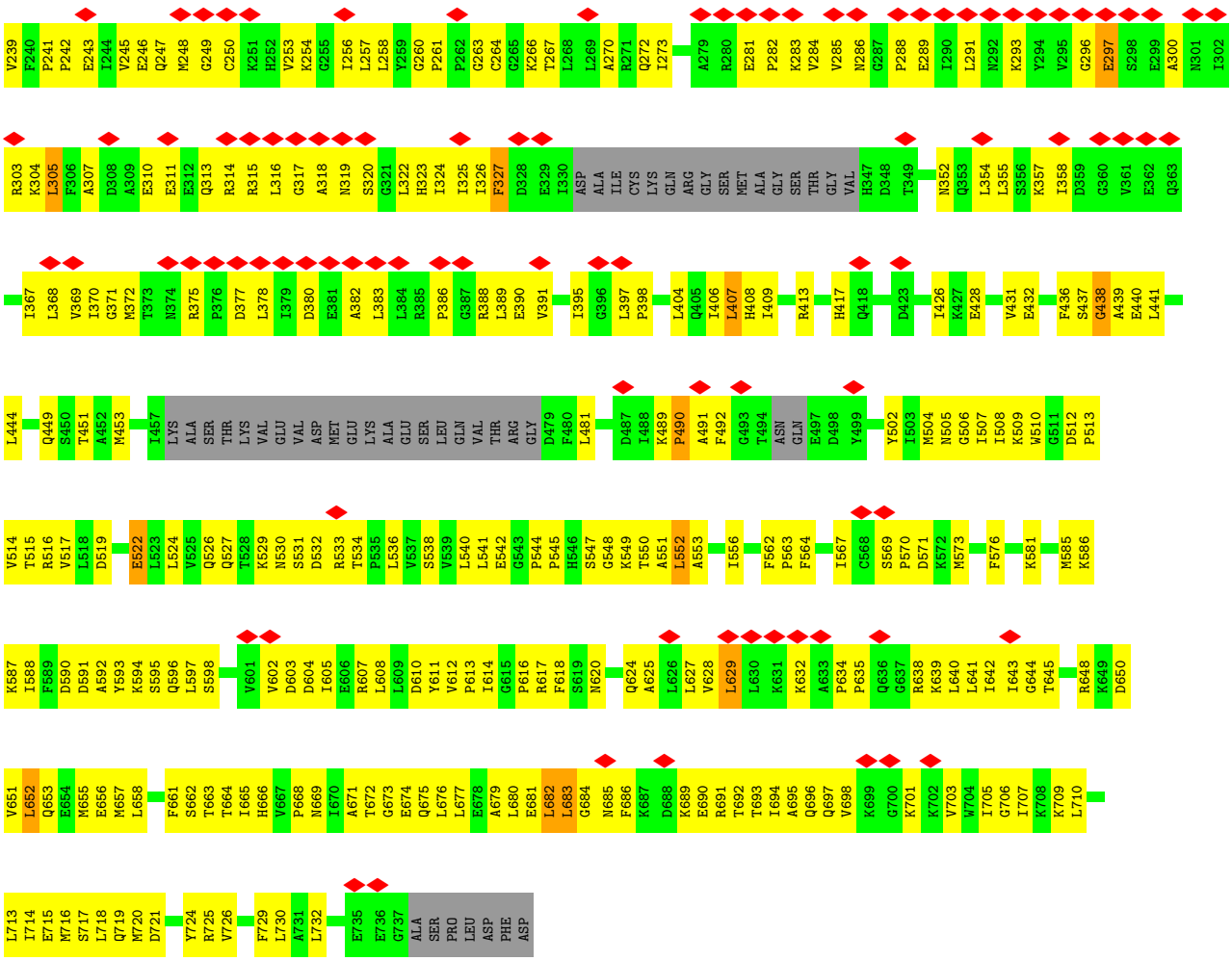


- Molecule 1: Vesicle-fusing ATPase

Chain E:

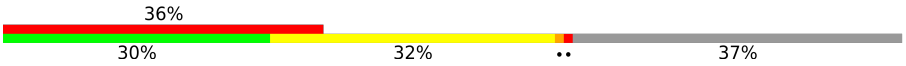


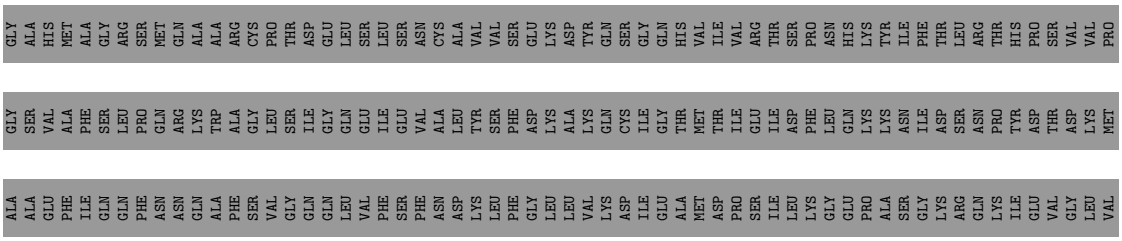


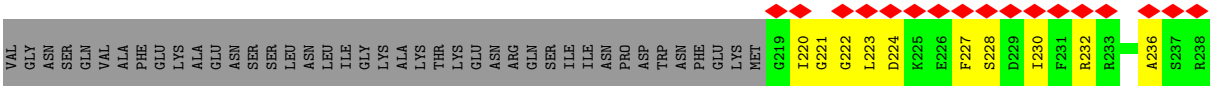


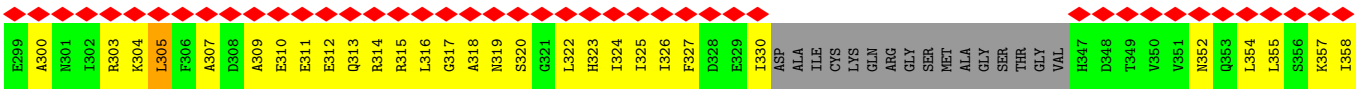
- Molecule 1: Vesicle-fusing ATPase

Chain F:









D359 G360 V361 E362 Q363 L364 N365 N366 I367 L368 V369 I370 G371 M372 T373 N374 R375 P376 D377 L378 I379 D380 E381 A382 L383 L384 R385 P386 G387 R388 L389 E390 V391 K392 M393 E394 I395 G396 L397 P398 D399 E400 K401 G402 R403 L404 Q405 I406 L407 H408 I409 H410 T411 M414 R415 G416 H417 Q418

A422 D423 I426 K427 E428 L429 A430 V431 E432 F436 S437 G438 A439 E440 L441 E442 G443 L444 V445 R446 Q449 S450 T451 A452 M453 N454 R455 H456 I457 LYS ALA SER THR LYS VAL GLU VAL ASP MET GLU LYS ALA GLU SER LEU GLN VAL THR ARG GLY D479 F480 L481 A482 S483 L484 E485

N486 D487 I488 K489 P490 ALA PHE GLY THR ASN GLN GLU ASP TYR A500 S501 Y502 I503 M504 N505 G506 I507 I508 K509 W510 G511 D512 P513 V514 T515 R516 V517 L518 G521 E522 V525 Q526 K529 N530 S531 D532 R533 T534 P535 L536 V537 S538 E542 G543 P544 P545 H546 S547 G548 K549 T550

A551 L552 A553 A554 K555 I556 A557 E558 E559 S560 N561 F562 P563 F564 I565 K566 I567 C568 S569 P570 D571 K572 M573 I574 G575 F576 S577 E578 T579 C582 Q583 K586 K587 I588 F589 D590 D591 A592 Y593 K594 S595 Q596 L597 S598 C599 V600 V601 V602 D603 D604 I605 E606 R607 L608 L609 D610 Y611 V612

P613 I614 R617 L621 V622 L623 Q624 A625 L626 L627 V628 L629 L630 K631 K632 A633 P634 P635 Q636 G637 R638 K639 L640 I643 G644 T645 T646 S647 R648 K649 D650 Q653 E654 M655 E656 M657 L658 N659 A660 F661 S662 T663 T664 I665 H666 V667 P668 N669 I670 A671 T672 Q675 L676 L677 E678

A679 L680 E681 L682 L683 G684 N685 F686 K687 D688 K689 E690 R691 T692 T693 I694 A695 Q696 Q697 V698 K699 G700 K701 K702 V703 W704 I705 G706 I707 K708 K709 L710 L711 M712 L713 I714 E715 M716 Q719 M720 D721 P722 E723 Y724 R725 V726 R727 K728 F729 L730 A731 L732 L733 R734 E735 E736 G737 ALA SER

PRO LEU ASP PHE ASP

4 Experimental information (i)

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 ($e^-/Å^2$)	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	6.0	Depositor
Map size (Å)	311.1936, 311.1936, 311.1936	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.4312, 2.4312, 2.4312	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	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
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(^{o})	Ideal(^{o})
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 (i)

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 (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	475/747 (64%)	443 (93%)	20 (4%)	12 (2%)	5 32
1	B	473/747 (63%)	429 (91%)	32 (7%)	12 (2%)	5 32
1	C	477/747 (64%)	450 (94%)	18 (4%)	9 (2%)	8 38
1	D	471/747 (63%)	439 (93%)	27 (6%)	5 (1%)	14 52
1	E	474/747 (64%)	441 (93%)	22 (5%)	11 (2%)	6 34
1	F	465/747 (62%)	428 (92%)	26 (6%)	11 (2%)	6 33
All	All	2835/4482 (63%)	2630 (93%)	145 (5%)	60 (2%)	10 36

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%)	343 (100%)	1 (0%)	92	95
1	B	349/638 (55%)	346 (99%)	3 (1%)	78	87
1	C	347/638 (54%)	346 (100%)	1 (0%)	92	95
1	D	340/638 (53%)	339 (100%)	1 (0%)	92	95
1	E	345/638 (54%)	342 (99%)	3 (1%)	78	87
1	F	345/638 (54%)	342 (99%)	3 (1%)	78	87
All	All	2070/3828 (54%)	2058 (99%)	12 (1%)	86	92

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

Mol	Chain	Res	Type
1	E	322	LEU
1	E	327	PHE
1	F	536	LEU
1	F	305	LEU
1	B	651	VAL

Sometimes 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	352	ASN
1	E	675	GLN
1	C	675	GLN
1	F	546	HIS
1	D	352	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides 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	D	801	-	24,29,29	1.08	1 (4%)	29,45,45	2.04	7 (24%)
2	ADP	E	801	-	24,29,29	1.27	3 (12%)	29,45,45	1.52	7 (24%)
2	ADP	C	801	-	24,29,29	1.22	4 (16%)	29,45,45	1.91	8 (27%)
2	ADP	B	801	-	24,29,29	1.06	2 (8%)	29,45,45	1.66	6 (20%)

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	D	801	-	-	3/12/32/32	0/3/3/3
2	ADP	E	801	-	-	2/12/32/32	0/3/3/3
2	ADP	C	801	-	-	1/12/32/32	0/3/3/3
2	ADP	B	801	-	-	5/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ADP	C5-C4	3.50	1.50	1.40

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	ADP	C5-C4	2.97	1.48	1.40
2	E	801	ADP	C2-N3	2.78	1.36	1.32
2	E	801	ADP	O4'-C1'	2.63	1.44	1.41
2	B	801	ADP	O4'-C1'	2.62	1.44	1.41

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	ADP	N3-C2-N1	-5.61	119.91	128.68
2	C	801	ADP	C3'-C2'-C1'	5.40	109.11	100.98
2	B	801	ADP	C4-C5-N7	-4.75	104.45	109.40
2	D	801	ADP	PA-O3A-PB	-4.69	116.74	132.83
2	D	801	ADP	C3'-C2'-C1'	4.12	107.17	100.98

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	ADP	C5'-O5'-PA-O1A
2	B	801	ADP	C3'-C4'-C5'-O5'
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.

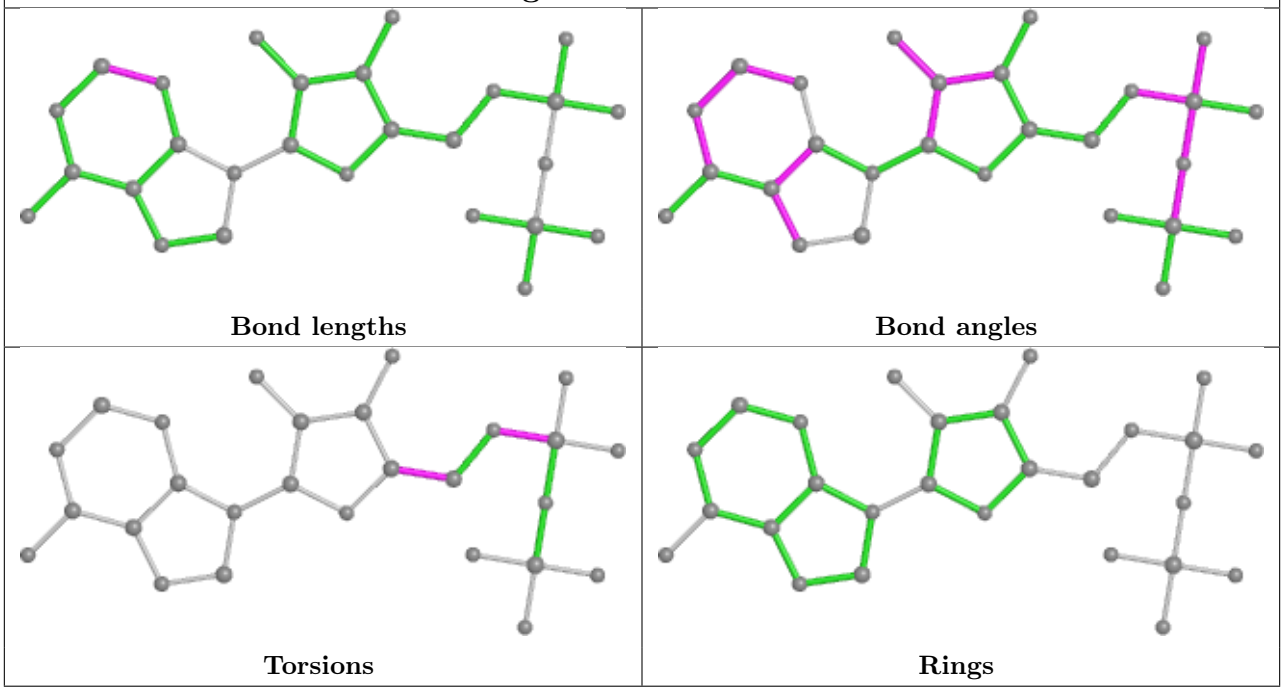
4 monomers are involved in 39 short contacts:

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

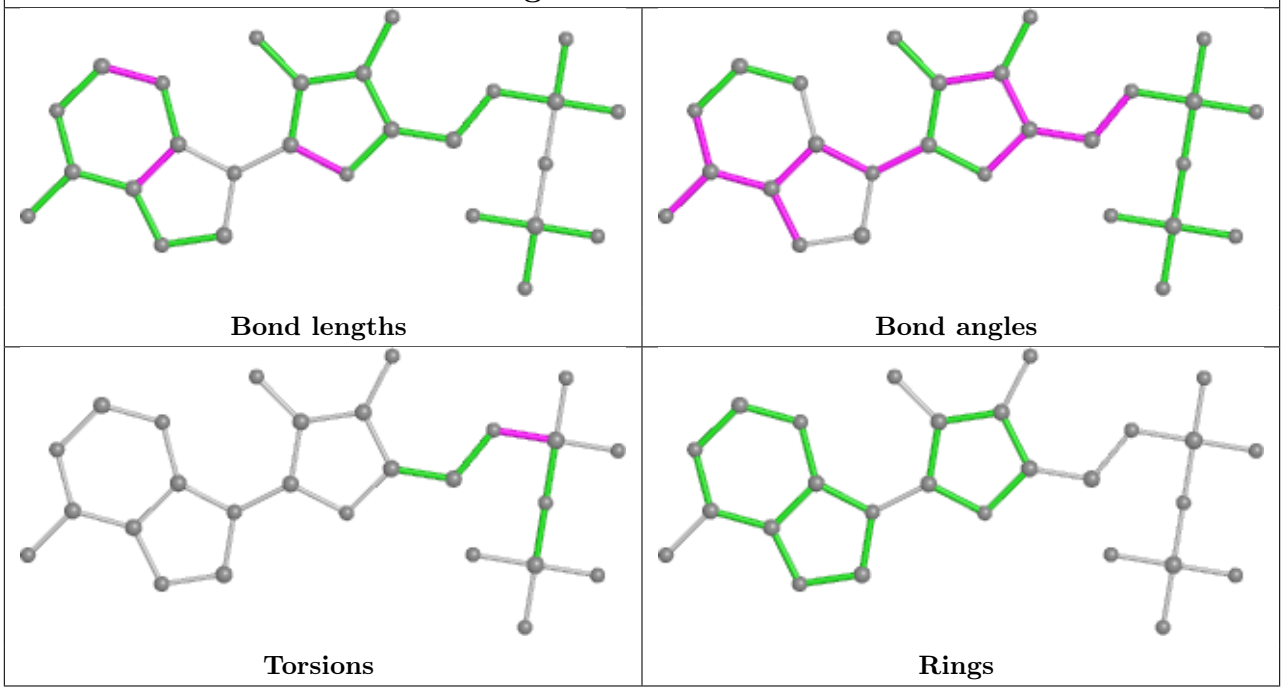
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

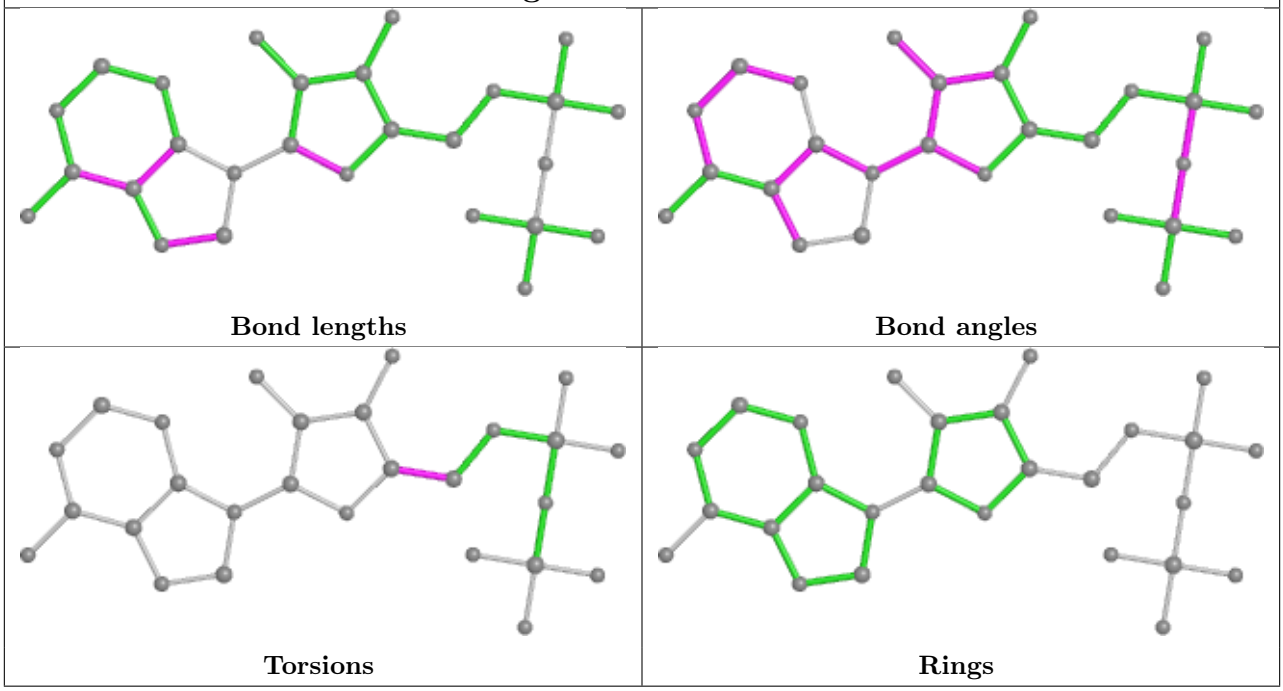
Ligand ADP D 801



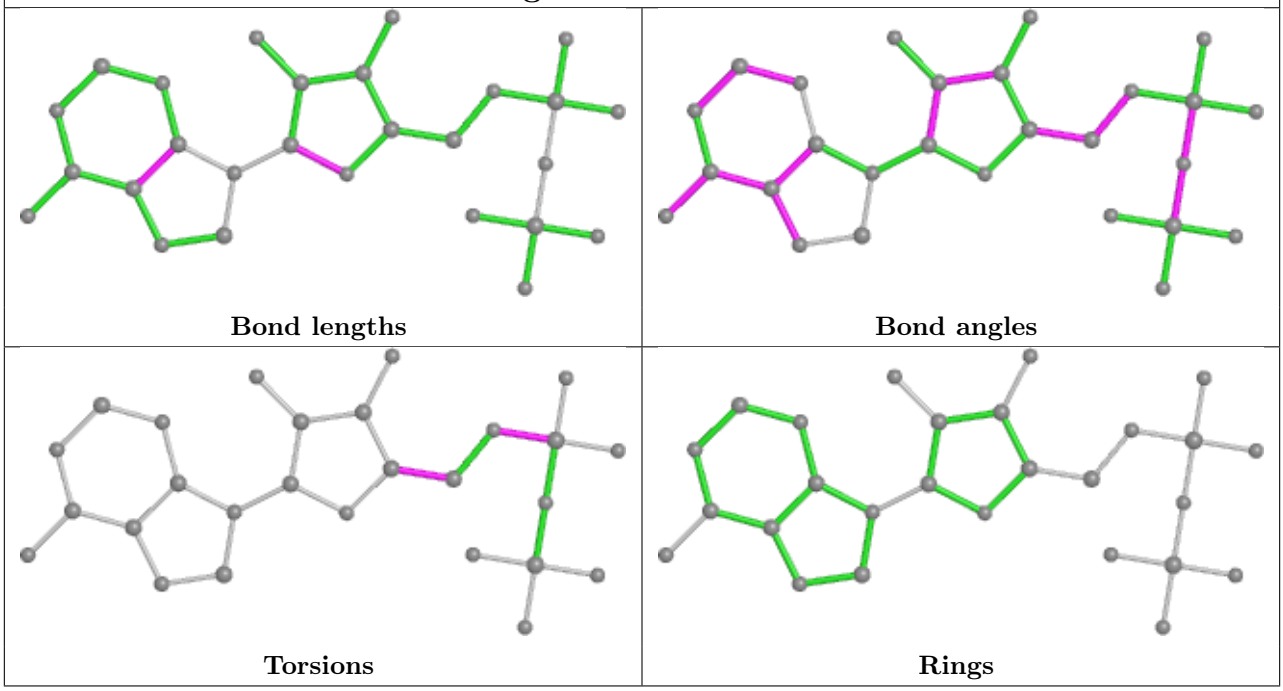
Ligand ADP E 801



Ligand ADP C 801



Ligand ADP B 801



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.

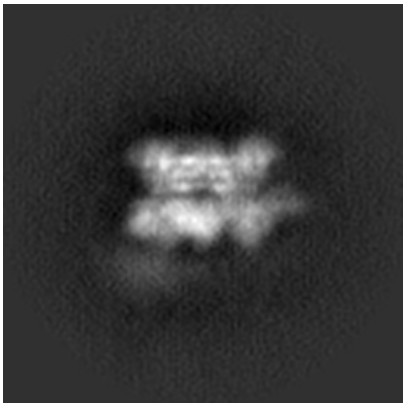
6 Map visualisation (i)

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.

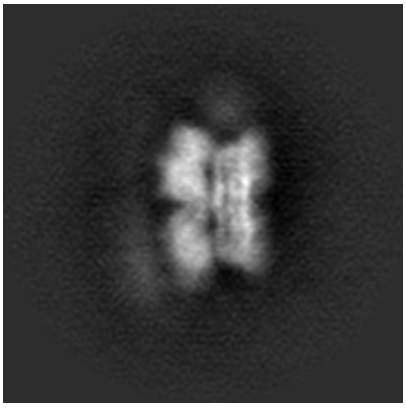
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

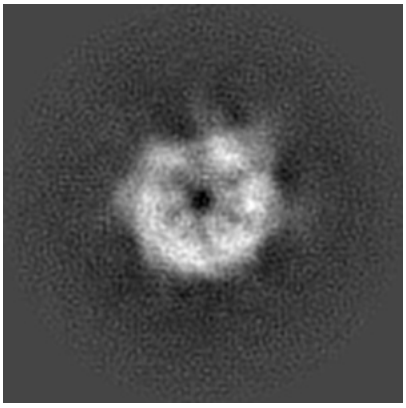
6.1.1 Primary map



X



Y

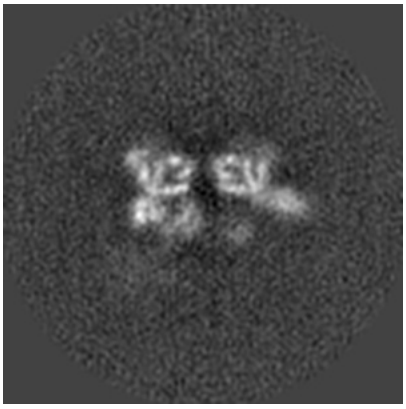


Z

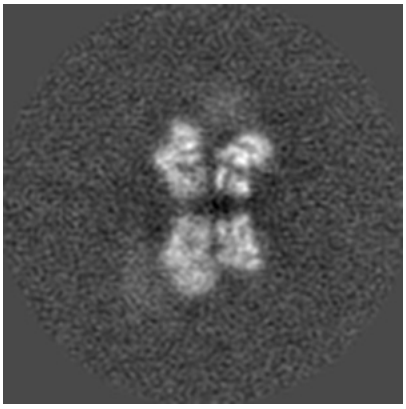
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

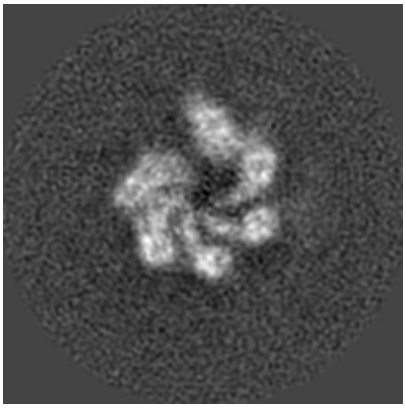
6.2.1 Primary map



X Index: 64



Y Index: 64

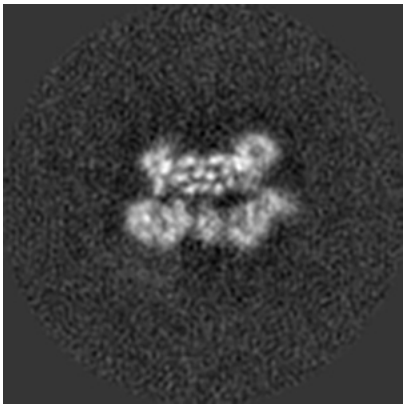


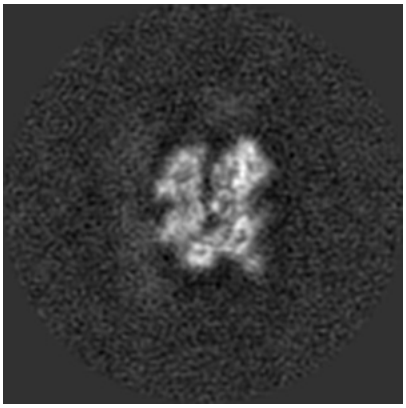
Z Index: 64

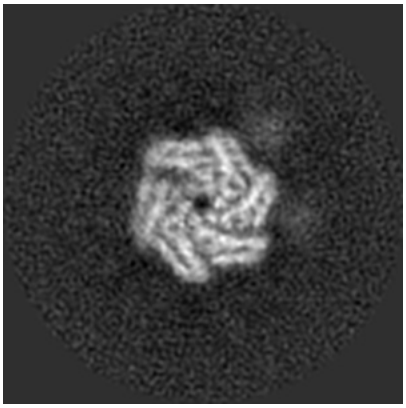
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 71

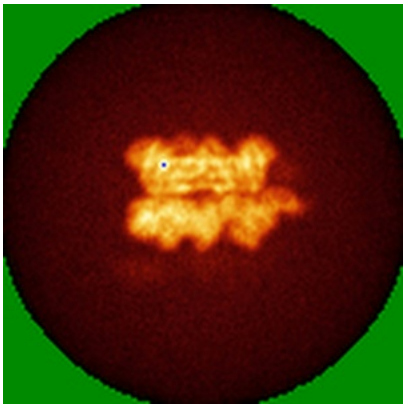

Y Index: 51

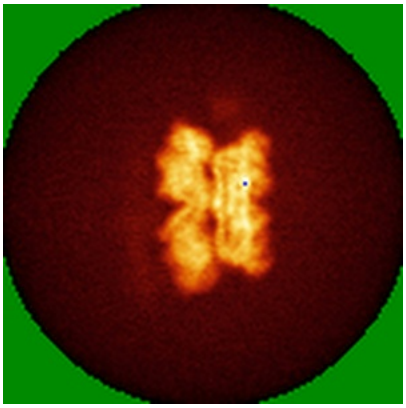

Z Index: 77

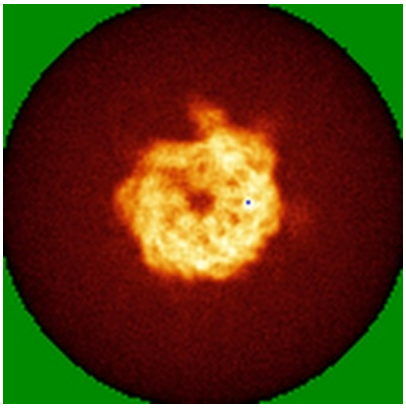
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

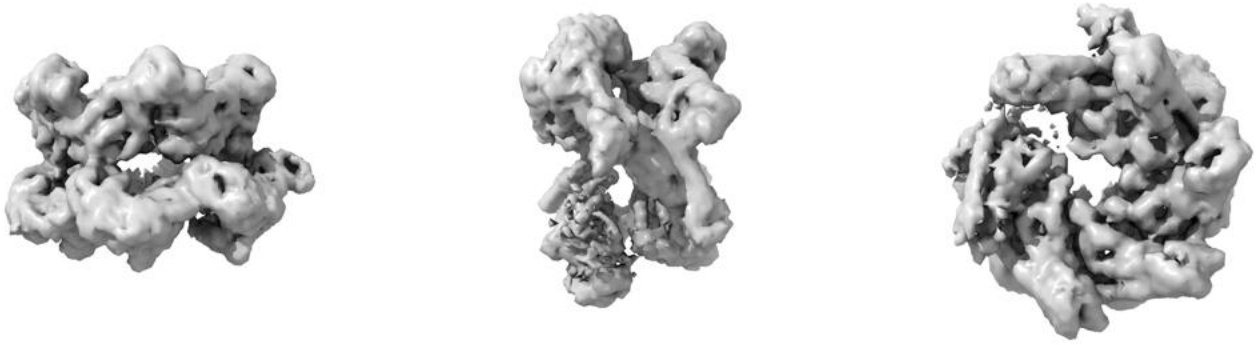

Y


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



X Y Z

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.

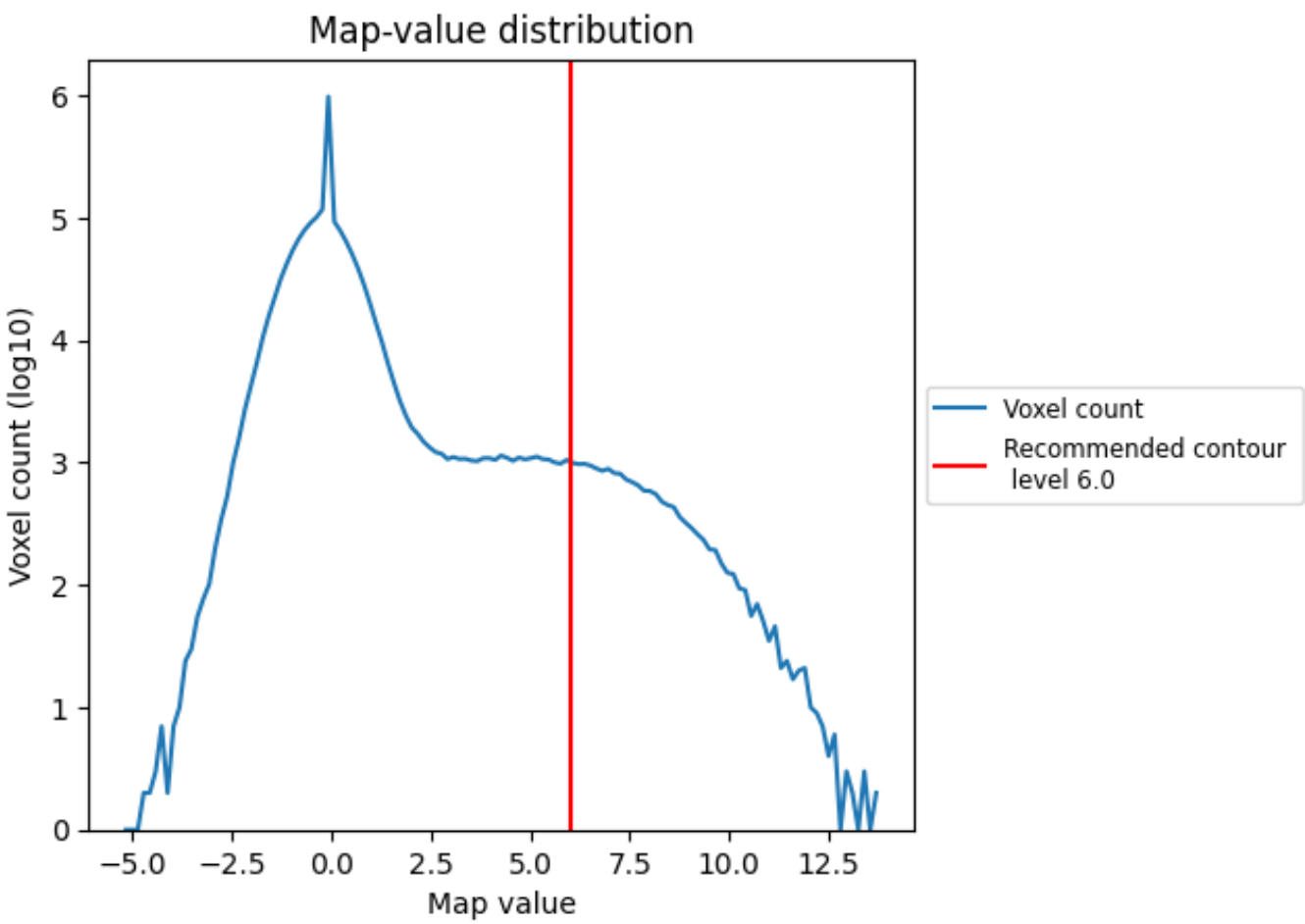
6.6 Mask visualisation (i)

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

7 Map analysis (i)

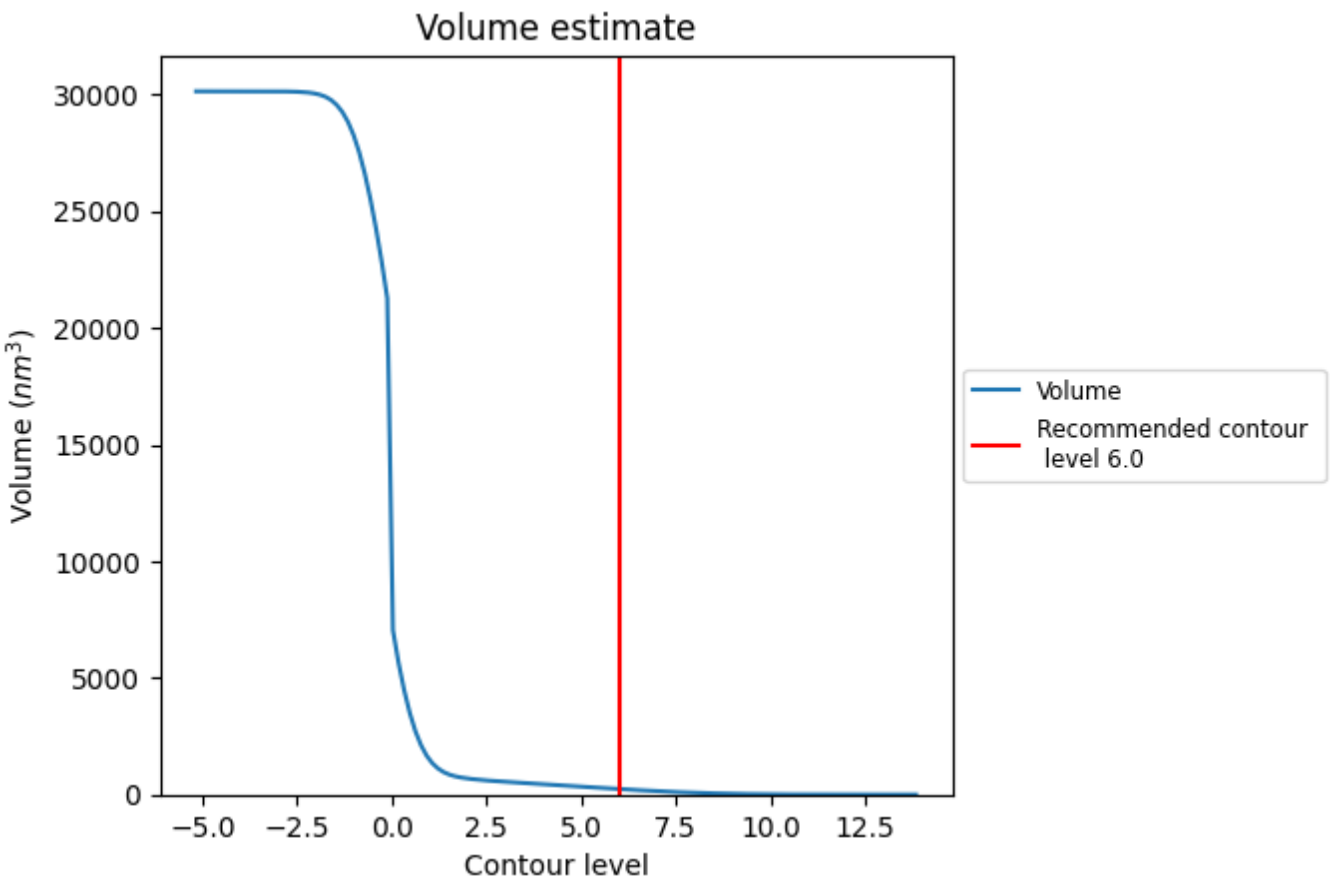
This section contains the results of statistical analysis of the map.

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.

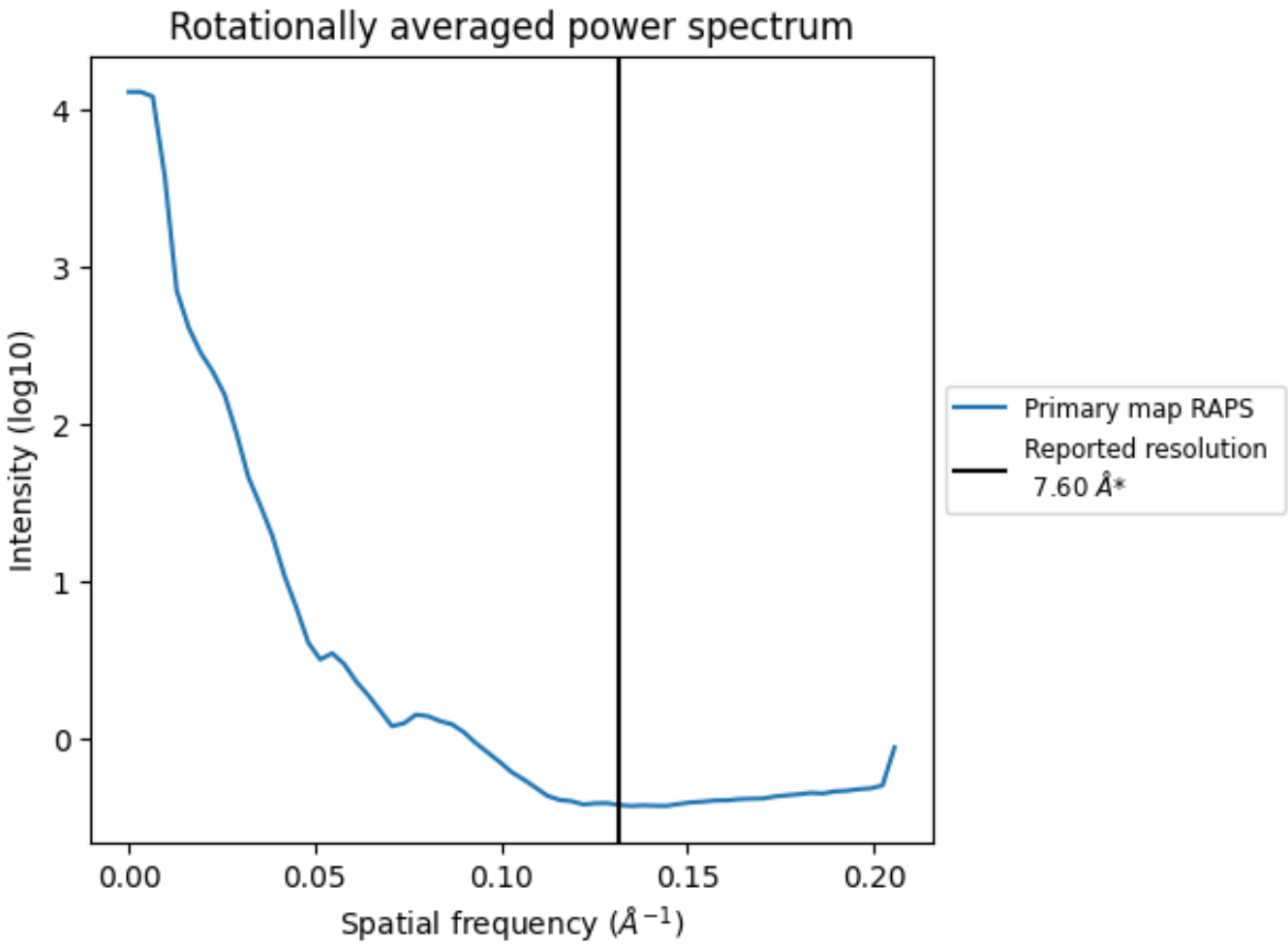
7.2 Volume estimate (i)



The volume at the recommended contour level is 239 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.132 Å^{-1}

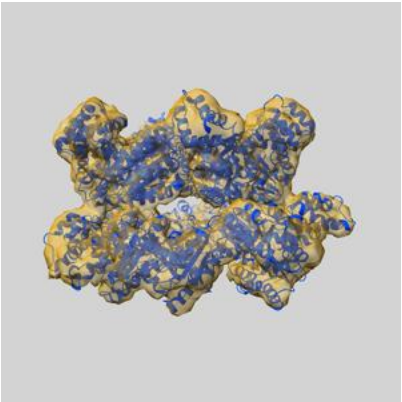
8 Fourier-Shell correlation (i)

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

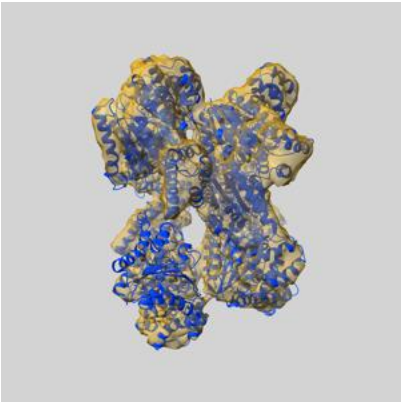
9 Map-model fit (i)

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.

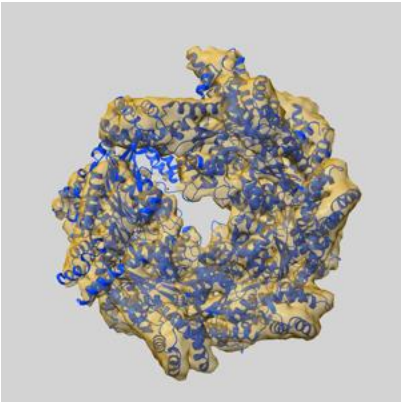
9.1 Map-model overlay (i)



X



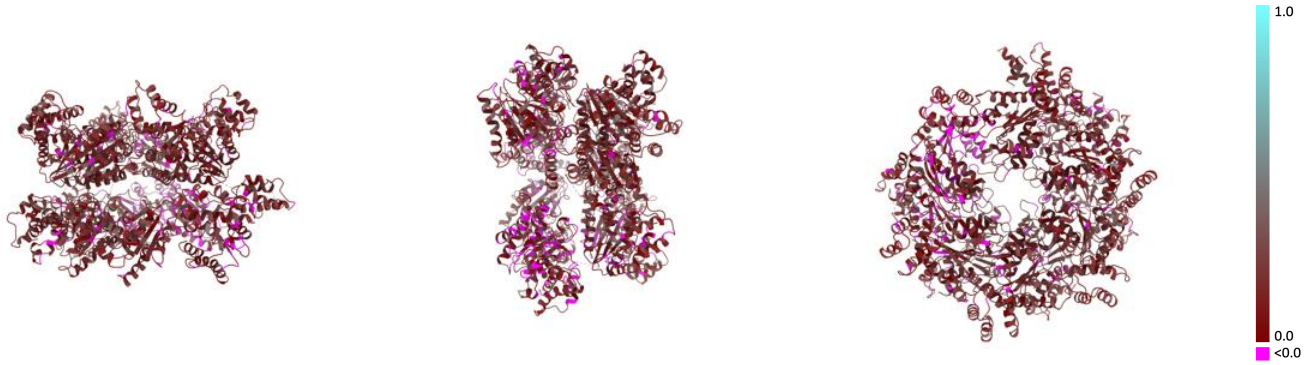
Y



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.

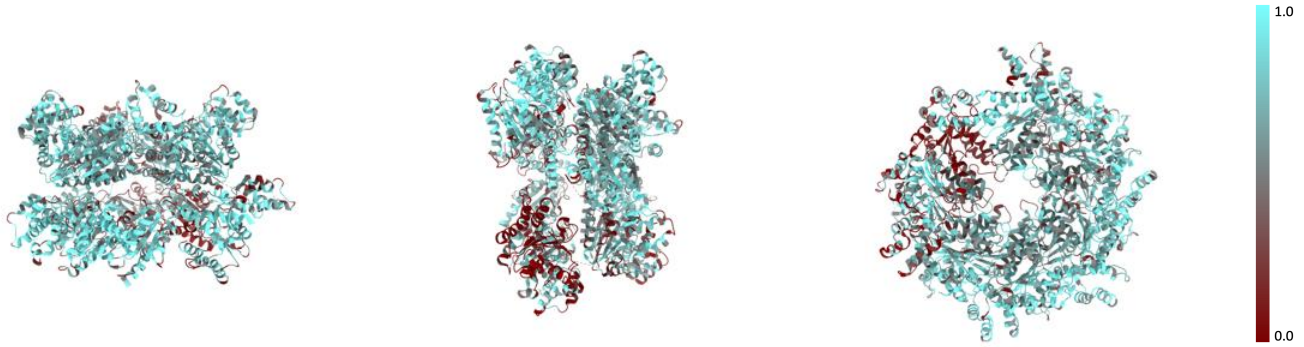
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

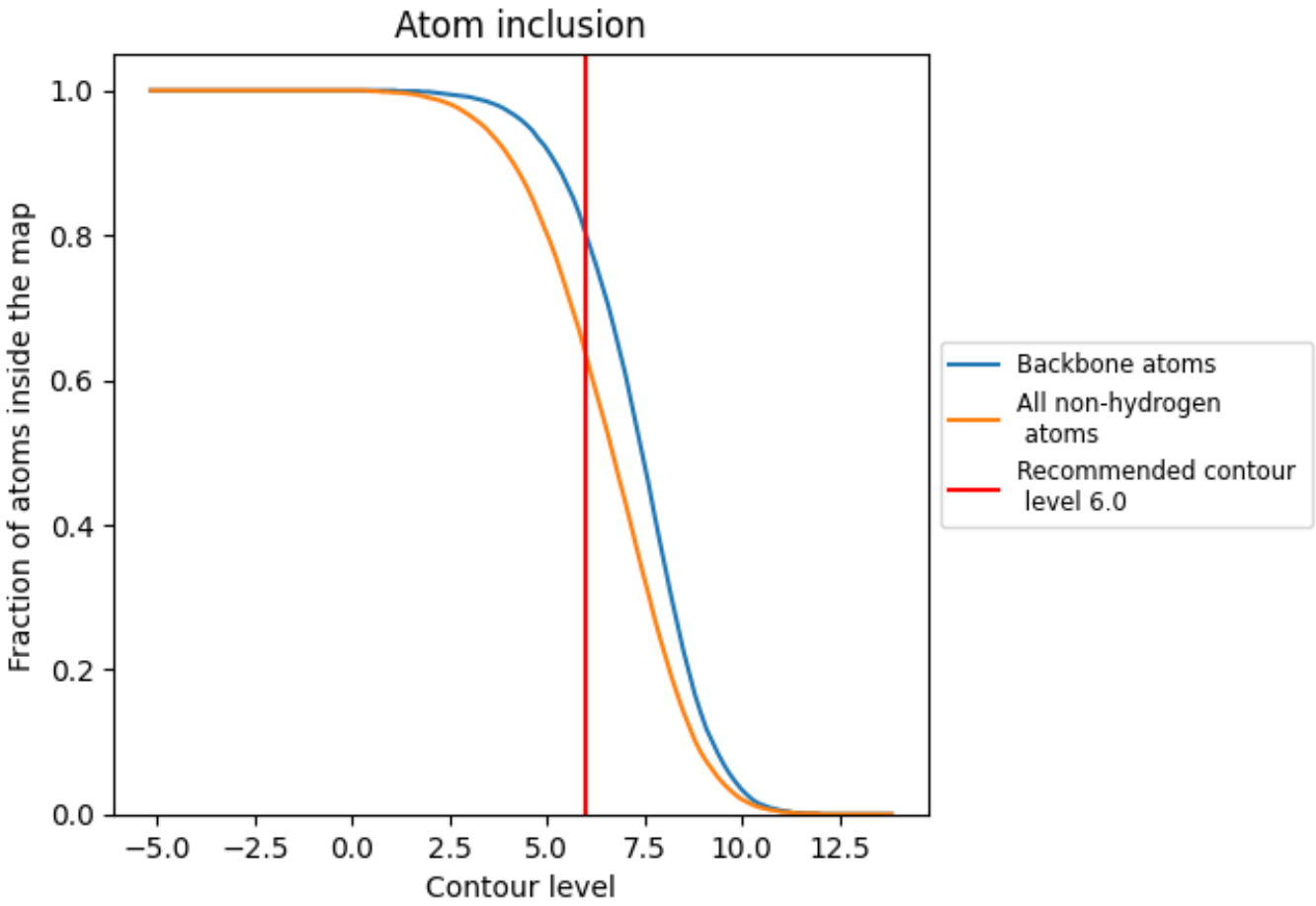
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (6.0).

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 (i)

The table lists the average atom inclusion at the recommended contour level (6.0) 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