WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Aug 3, 2021 – 06:59 pm BST

PDB ID	:	7P0M
EMDB ID	:	EMD-13148
Title	:	Human mitochondrial Lon protease with substrate in the ATPase and protease domains
Authors	:	Valentin Gese, G.; Shahzad, S.; Hallberg, B.M.
Deposited on	:	2021-06-30
Resolution	:	2.75 Å(reported)
Based on initial model	:	3M6A

This is a Full wwPDB EM Validation 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 following versions of software and data (see references (i)) were used in the production of this report:

|		
EMDB validation analysis	:	0.0.0.dev97
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)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.75 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		2.5%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
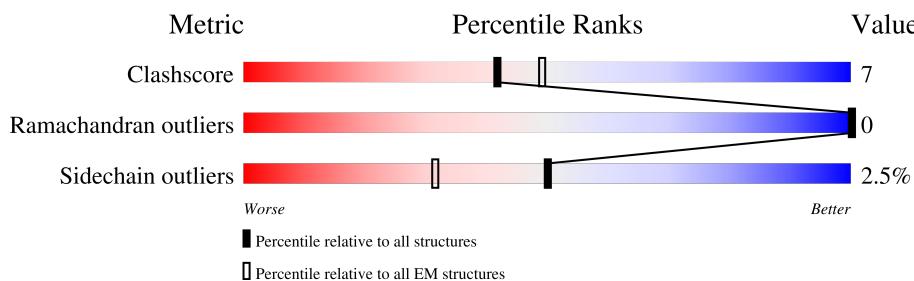
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	895	49% 11% 40%
1	B	895	50% 9% • 40%
1	C	895	50% 9% 41%
1	D	895	48% 11% 41%
1	E	895	48% 11% 41%
1	F	895	5% 45% 13% • 42%
2	G	11	18% 100%
2	H	11	27% 9% 64%
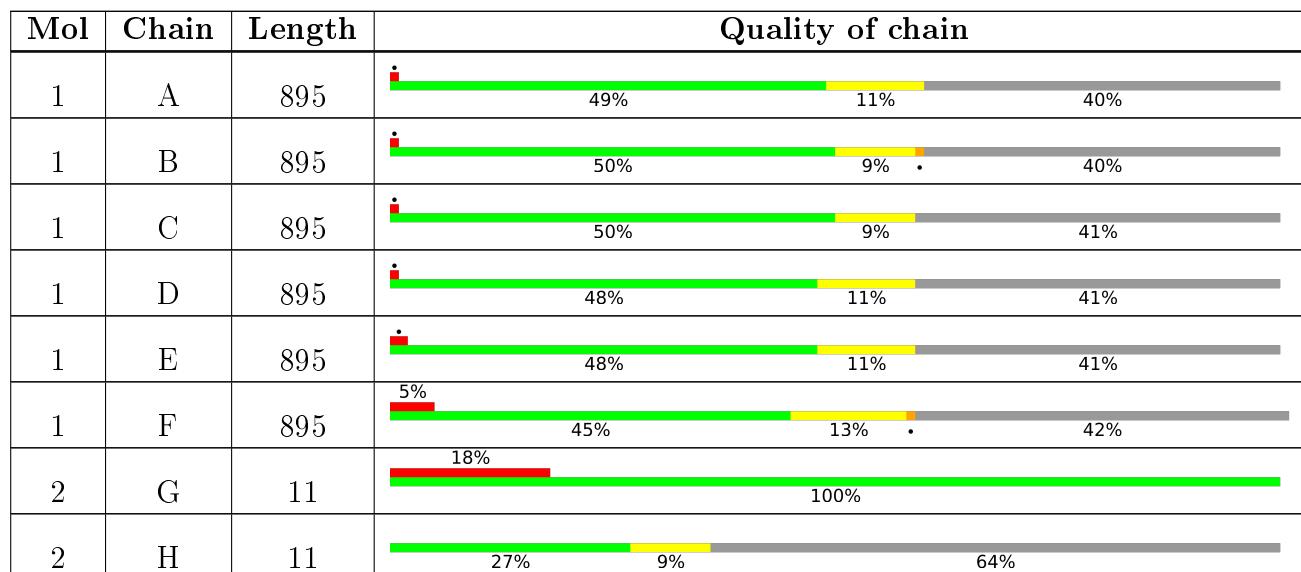
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Mol	Chain	Length	Quality of chain
2	I	11	27% 9% 64%
2	J	11	18% 18% 64%
2	K	11	18% / 27% 9% 64%
2	L	11	9% / 27% 9% 64%
2	M	11	27% 9% 64%
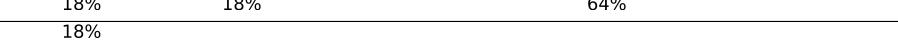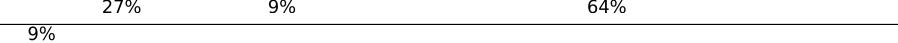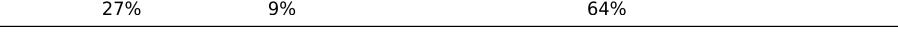
2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 25185 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 Lon protease homolog, mitochondrial.

| Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	534	Total	C	N	O	S	0	0
			4159	2637	712	790	20		
1	B	536	Total	C	N	O	S	0	0
			4181	2650	716	795	20		
1	C	532	Total	C	N	O	S	0	0
			4147	2631	710	786	20		
1	D	531	Total	C	N	O	S	0	0
			4140	2626	709	785	20		
1	E	532	Total	C	N	O	S	0	0
			4147	2631	710	786	20		
1	F	520	Total	C	N	O	S	0	0
			4054	2573	691	770	20		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	SER	-	expression tag	UNP P36776
A	66	MET	-	expression tag	UNP P36776
A	898	ALA	LYS	engineered mutation	UNP P36776
B	65	SER	-	expression tag	UNP P36776
B	66	MET	-	expression tag	UNP P36776
B	898	ALA	LYS	engineered mutation	UNP P36776
C	65	SER	-	expression tag	UNP P36776
C	66	MET	-	expression tag	UNP P36776
C	898	ALA	LYS	engineered mutation	UNP P36776
D	65	SER	-	expression tag	UNP P36776
D	66	MET	-	expression tag	UNP P36776
D	898	ALA	LYS	engineered mutation	UNP P36776
E	65	SER	-	expression tag	UNP P36776
E	66	MET	-	expression tag	UNP P36776
E	898	ALA	LYS	engineered mutation	UNP P36776
F	65	SER	-	expression tag	UNP P36776
F	66	MET	-	expression tag	UNP P36776
F	898	ALA	LYS	engineered mutation	UNP P36776

- Molecule 2 is a protein called Unknown peptide from human mitochondrial transcription factor A (TFAM).

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	11	Total	C	N	O	0	0
			55	33	11	11		
2	I	4	Total	C	N	O	0	0
			20	12	4	4		
2	J	4	Total	C	N	O	0	0
			20	12	4	4		
2	M	4	Total	C	N	O	0	0
			20	12	4	4		
2	H	4	Total	C	N	O	0	0
			20	12	4	4		
2	L	4	Total	C	N	O	0	0
			20	12	4	4		
2	K	4	Total	C	N	O	0	0
			20	12	4	4		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
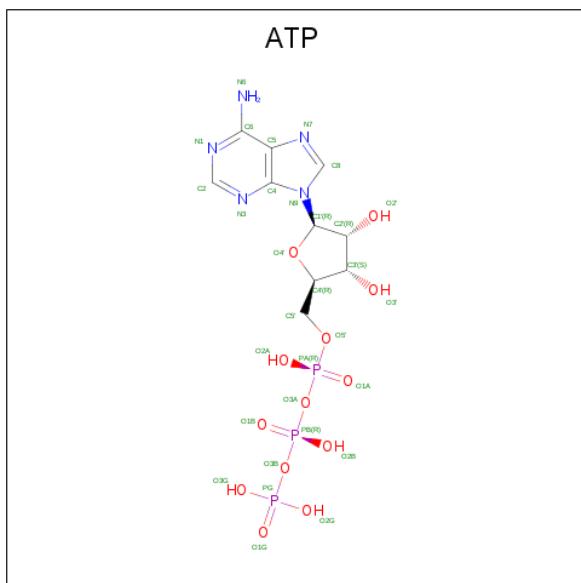
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	F	1	31	10	5	13	3	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	

- Molecule 5 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

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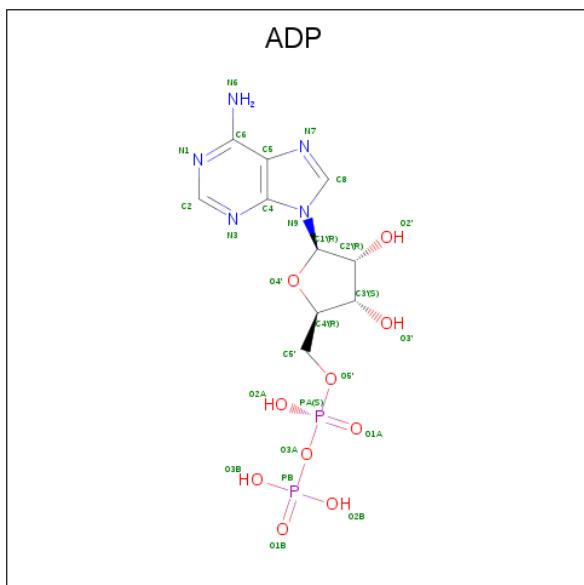
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	D	1	27	10	5	10	2	0
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, 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: Lon protease homolog, mitochondrial

Chain A: 49% 11% 40%

SER MET GLY PHE TRP GLU ALA SER SER ARG GLY GLY GLY ALA PHE SER GLY GLY GLU GLU ASP ALA SER GLU GLY GLY ALA GLU GLU GLY ALA GLY ALA GLY SER ALA GLY ALA GLU GLU PRO VAL ILE THR ALA LEU THR PRO MET THR ILE PRO ASP VAL PHE PRO HIS LEU

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

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

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

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

LEU LEU LYS LYS GLU PHE GLU LEU SER LYS LEU GLN GLN ARG LEU GLY ARG GLU VAL GLU GLU LYS ILE LYS GLN THR HIS ARG LYS TYR LEU LEU GLN GLU GLN LEU LYS ILE ILE LYS LYS GLU LEU GLY LEU **E410 K411 D412 D413 K414** E418 **F421 R422 E423 R424** L425 K426

M435 D439 L442 L445 Y461 T466 D490 H491 Y492 **D496** A537 R538 R546 T564 P570 I573 C576 **T580 K581 T582** P585 L586 D590 D593 K594 I595 P603 L608 E609 L610 L611 D612 Q615 Y623 L624 **D629** L630 S631

K632 V633 I636 V641 T642 D643 T644 L649 R650 D651 R652 K666 I669 A670 L674 R679 **L684 D685** A689 E706 N711 L712 T738 P739 E740 N741 L742 Q743 R755 M756 Y757 V765 L768 A769 G775 L778 T782 S783 L784 P787 GLN

ASP LYS ASP ALA LYS **G794** V802 T803 G804 Q805 E808 S813 I816 L825 M826 Q827 L835 S838 H841 L842 P850 K851 D852 S855 T862 L867 V873 N876 L885 V892 A898 R904 F926 I927 D949 GLU GLN ALA GLU ALA

LEU ALA VAL GLU ARG

- Molecule 1: Lon protease homolog, mitochondrial

Chain B: 50% 9% 40%

• Molecule 1: Lon protease homolog, mitochondrial

Chain C:

50% 9% 41%

I645 L649 R650 M655 A670 L674 R679 L684 D685 E686 A689 L699 R721 E736 V737 T738 N741 D744 F745 V746 T752 R755 V764 V765 L768 T771 G775 F779 V780 E781 L784 P787 GLN ASP LYS ASP ALA LYS

GLY ASP K796 T803 G804 Q805 L806 M810 K811 E812 F820 V836 T837 H841 L842 H843 V844 P845 S855 T862 R871 P872 V873 N876 E882 L885 L890 A898 D919 L931 D949 GLU GLN ALA GLU LEU ALA VAL GLU ARG

- Molecule 1: Lon protease homolog, mitochondrial

Chain D:

48% 11% 41%

SER MET GLY PHE TRP GLU ALA SER SER ARG GLY GLY ALA PHE SER GLY GLU GLU ASP ALA SER GLU GLY ALA GLU GLY ALA GLY GLY ALA GLY GLU GLY SER ALA GLY LEU GLU GLY MET THR PRO MET THR ILE PRO ASP VAL PHE PRO HIS LEU

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

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

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

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

LEU LEU LYS LYS GLU PHE GLU LEU SER LYS LEU GLN GLN ARG LEU GLY ARG GLU VAL GLU GLU LYS ILE LYS GLN THR HIS ARG LYS TYR LEU LEU GLN GLU GLN LEU LYS ILE ILE LYS LYS GLU LEU GLY LEU E410 K411 D412 D413 K414 E418 E419 K420 R424 L425 P431

M435 D436 V437 V438 E441 L442 L445 L448 H451 E454 F455 T458 Y461 L465 T466 P469 W470 G471 K472 N477 L478 D479 L480 A481 R482 Y492 E503 Q509 F521 P524 G528 K529 F545 R546 T553 K572 I573 K579 P585

L588 I589 D590 D593 K594 Q600 P603 L610 L611 D612 P613 E614 Q615 N616 L624 D625 L630 V633 A639 N640 V641 T642 D643 R652 I656 V662 A663 Q664 K666 A670 L674 L691 G708 V709 R710 R721 E733 R755 M756 Y757

V765 M766 T771 A772 F779 V780 E781 L784 R785 R786 PRO GLN ASP LYS ASP ALA LYS GLY ASP K796 S799 T803 G804 Q805 L806 G807 E812 S813 I816 L825 L835 S838 H841 P845 E846 K851 S855 T862 V873 N876 E882

L885 L890 K896 E897 D949 GLU GLN ALA GLU LEU ALA VAL GLU ARG

- Molecule 1: Lon protease homolog, mitochondrial

Chain E:

48% 11% 41%

SER MET GLY PHE TRP GLU ALA SER SER ARG GLY GLY ALA PHE SER GLY GLU GLU ASP ALA SER GLU GLY ALA GLU GLY ALA GLY GLY ALA GLY GLU GLY SER ALA GLY LEU GLU GLY MET THR PRO MET THR ILE PRO ASP VAL PHE PRO HIS LEU

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

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

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

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

LEU LEU LYS LYS LYS GLU PHE GLU LEU SER LYS LEU GLN GLN ARG LEU GLY ARG GLU VAL GLU VAL LYS ILE LYS LYS GLU GLY LEU **E410 K411 D412 D413 K414** I417 E418 **R422 E423 R424 L425 K426 E427**

L428 V429 K432 V438 D439 L442 G446 L447 L448 H451 N460 Y461 L462 L465 T466 S467 **W470** E476 L480 Y492 E503 **Q515 G516 K517 I518 L519** V527 **G528 K529** R542 R546 **H561 R562 R563** A568 M569 P570 I574 K578

K581 P585 L588 V592 **R597 Q600** L607 L608 E609 **L610 L611** Q615 **D621 H622** Y623 **L624 D625** V633 I636 **C637** P648 L649 M655 V658 **Q664 E665 K666** L667 **A670 E671** R672 Y673 L674 **D685** K688 V695 Q702 R705 E706

R710 I727 **V728 T738 P739 E740 D744 P749 V750 F751** E754 **R755 M756 Y757** V765 L784 **R785 R786 P787** GLN ASP LYS ASP ALA LYS GLY ASP **K796** V802 **T803** E812 **S813** I816 D833 V836 **T837 S838** L842 E846 **T849 P850** K851 S855

T862 V873 E882 L890 I895 L912 D919 L931 E937 **D949** GLU GLN ALA GLU ALA LEU ALA VAL GLU ARG

• Molecule 1: Lon protease homolog, mitochondrial

Chain F:
5%
45% 13% • 42%

SER MET GLY PHE TRP GLU ALA SER SER ARG GLY GLY ALA PHE SER GLY GLU ASP ALA SER GLU GLY GLY ALA GLU GLY GLY ALA GLY GLY ALA GLY GLY SER ALA GLY GLU GLU PRO VAL ILE THR ALA LEU THR PRO MET THR ILE PRO ASP VAL PHE PRO HIS LEU

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

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

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

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

LEU LEU LYS LYS LYS GLU PHE GLU LEU SER LYS LEU GLN GLN ARG LEU GLY ARG GLU VAL GLU VAL LYS ILE LYS LYS GLU GLY LEU **E410 K411 D412 D413 K414 D415 E423 R424 L425 K426 E427 L428 V429 V430**

P431 **K432 H433 V434 M435 D436 E440** L445 **G446 L447 L448 D449 N450 H451 S452 S453 E454** F455 N456 V457 T458 R459 T466 **W470 G471** K472 Y473 **S474 N475** E476 N477 **L478** D479 L480 A481 **R482 A483 Q484** E488 **Y492 G493 M494 E495 D496 V497** R500 I501 L502 L510 S513 T514

• Molecule 2: Unknown peptide from human mitochondrial transcription factor A (TFAM)

Chain G:

• Molecule 2: Unknown peptide from human mitochondrial transcription factor A (TFAM)

Chain I:

• Molecule 2: Unknown peptide from human mitochondrial transcription factor A (TFAM)

Chain J:

• Molecule 2: Unknown peptide from human mitochondrial transcription factor A (TFAM)

Chain M:

• Molecule 2: Unknown peptide from human mitochondrial transcription factor A (TFAM)

Chain H:

• Molecule 2: Unknown peptide from human mitochondrial transcription factor A (TFAM)

Chain L:

Chain K:

- Molecule 2: Unknown peptide from human mitochondrial transcription factor A (TFAM)

4　Experimental information　ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	278511	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.466	Depositor
Minimum map value	-0.216	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	392.4, 392.4, 392.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.654, 0.654, 0.654	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: ATP, MG, 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	0.24	0/4234	0.45	0/5728
1	B	0.24	0/4256	0.44	0/5757
1	C	0.24	0/4222	0.45	0/5712
1	D	0.24	0/4214	0.44	0/5700
1	E	0.24	0/4222	0.45	0/5712
1	F	0.25	0/4125	0.46	0/5579
All	All	0.24	0/25273	0.45	0/34188

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4159	0	4202	60	0
1	B	4181	0	4224	52	0
1	C	4147	0	4195	58	0
1	D	4140	0	4189	68	0
1	E	4147	0	4196	69	0
1	F	4054	0	4103	76	0
2	G	55	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	20	0	6	4	0
2	I	20	0	7	7	0
2	J	20	0	6	7	0
2	K	20	0	6	6	0
2	L	20	0	6	6	0
2	M	20	0	6	5	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
3	C	31	0	12	2	0
3	F	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
5	D	27	0	12	3	0
5	E	27	0	12	2	0
All	All	25185	0	25232	366	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 7.

All (366) 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:D:855:SER:HB2	2:L:390:UNK:C	1.35	1.55
1:B:855:SER:HB2	2:H:390:UNK:C	1.10	1.54
1:F:855:SER:HB3	2:J:390:UNK:C	1.33	1.51
1:B:855:SER:CB	2:H:390:UNK:C	1.85	1.48
1:E:855:SER:CB	2:K:390:UNK:C	1.96	1.44
1:F:855:SER:CB	2:J:390:UNK:C	1.95	1.43
1:E:855:SER:HB2	2:K:390:UNK:C	1.49	1.42
1:D:855:SER:CB	2:L:390:UNK:C	1.99	1.41
1:A:855:SER:CB	2:I:390:UNK:C	2.09	1.31
1:E:855:SER:OG	2:K:390:UNK:C	1.80	1.27
1:A:855:SER:OG	2:I:390:UNK:C	1.83	1.26
1:A:855:SER:HG	2:I:390:UNK:C	1.48	1.25
1:A:855:SER:HB2	2:I:390:UNK:C	1.65	1.24
1:C:855:SER:OG	2:M:390:UNK:C	1.90	1.20
1:D:855:SER:HG	2:L:390:UNK:C	1.58	1.17
1:C:855:SER:CB	2:M:390:UNK:C	2.22	1.16
1:C:855:SER:HG	2:M:390:UNK:C	1.60	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:855:SER:HB2	2:M:390:UNK:C	1.79	1.12
1:E:855:SER:HG	2:K:390:UNK:C	1.60	1.08
1:D:855:SER:OG	2:L:390:UNK:C	2.07	1.01
1:B:855:SER:OG	2:H:390:UNK:C	2.19	0.90
1:D:855:SER:OG	2:L:390:UNK:O	1.90	0.83
1:F:855:SER:OG	2:J:390:UNK:C	2.33	0.77
1:C:600:GLN:HE22	1:D:600:GLN:HG3	1.50	0.76
1:F:518:ILE:HG13	1:F:611:LEU:HD12	1.67	0.76
1:A:855:SER:OG	2:I:390:UNK:O	1.87	0.75
1:F:855:SER:HB2	2:J:390:UNK:C	2.15	0.75
1:B:479:ASP:HB3	1:B:482:ARG:HG2	1.70	0.73
1:C:582:THR:HG22	1:C:584:ASN:H	1.52	0.73
1:D:765:VAL:HG22	1:D:873:VAL:HG21	1.74	0.70
1:B:855:SER:HG	2:H:390:UNK:C	2.02	0.70
1:C:765:VAL:HG22	1:C:873:VAL:HG21	1.73	0.70
1:A:803:THR:OG1	1:A:841:HIS:NE2	2.26	0.69
1:E:855:SER:OG	2:K:390:UNK:O	1.85	0.69
1:F:500:ARG:NH2	1:F:654:GLU:OE1	2.26	0.69
1:D:438:VAL:HG12	1:D:465:LEU:HD13	1.76	0.68
1:E:418:GLU:HG2	1:E:442:LEU:HD22	1.77	0.67
1:E:414:LYS:HD2	1:E:446:GLY:HA2	1.76	0.67
1:C:670:ALA:HA	1:C:674:LEU:HB2	1.77	0.66
1:F:855:SER:CB	2:J:390:UNK:O	2.42	0.66
1:A:769:ALA:HB2	1:A:778:LEU:HD23	1.78	0.66
1:E:765:VAL:HG22	1:E:873:VAL:HG21	1.77	0.66
1:B:803:THR:OG1	1:B:841:HIS:NE2	2.28	0.65
1:C:803:THR:OG1	1:C:841:HIS:NE2	2.29	0.65
1:E:727:ILE:HD11	1:F:510:LEU:HD11	1.79	0.64
1:E:670:ALA:HA	1:E:674:LEU:HB2	1.79	0.64
1:D:855:SER:HB2	2:L:390:UNK:CA	2.25	0.64
1:A:765:VAL:HG22	1:A:873:VAL:HG21	1.80	0.64
1:A:411:LYS:NZ	1:A:412:ASP:O	2.31	0.63
1:D:573:ILE:HG13	1:D:610:LEU:HD11	1.81	0.63
1:A:580:THR:HG22	1:A:582:THR:H	1.64	0.62
1:D:803:THR:OG1	1:D:841:HIS:NE2	2.29	0.62
1:D:805:GLN:NE2	1:E:812:GLU:OE1	2.32	0.62
1:B:765:VAL:HG22	1:B:873:VAL:HG21	1.82	0.61
1:C:418:GLU:HG2	1:C:442:LEU:HD22	1.82	0.61
1:A:670:ALA:HA	1:A:674:LEU:HB2	1.81	0.61
1:A:784:LEU:HD11	1:A:838:SER:HB3	1.82	0.61
1:A:611:LEU:HD12	1:A:649:LEU:HD22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:585:PRO:HD2	1:C:633:VAL:HG22	1.83	0.61
1:C:843:HIS:HB3	1:D:885:LEU:HD22	1.83	0.61
1:B:611:LEU:HD12	1:B:649:LEU:HD11	1.84	0.60
1:E:438:VAL:HG13	1:E:462:LEU:HD21	1.84	0.60
1:B:769:ALA:HB2	1:B:778:LEU:HD23	1.84	0.60
1:D:524:PRO:O	1:D:529:LYS:NZ	2.35	0.60
1:F:765:VAL:HG22	1:F:873:VAL:HG21	1.82	0.60
1:F:555:VAL:HA	1:F:559:LYS:HB2	1.84	0.59
1:F:484:GLN:HB2	1:F:502:LEU:HD11	1.85	0.59
1:E:685:ASP:OD2	1:E:688:LYS:NZ	2.34	0.59
1:D:478:LEU:O	1:D:509:GLN:NE2	2.36	0.59
1:F:662:VAL:N	1:F:665:GLU:OE2	2.36	0.59
1:C:781:GLU:HG3	1:D:885:LEU:HD21	1.85	0.59
1:B:461:TYR:HB2	1:B:563:ARG:HD3	1.84	0.59
1:B:425:LEU:HD12	1:B:428:LEU:HD12	1.86	0.58
1:F:573:ILE:HG21	1:F:630:LEU:HD21	1.84	0.58
1:B:871:ARG:NH2	1:B:949:ASP:O	2.36	0.58
1:F:537:ALA:HB2	1:F:586:LEU:HD23	1.84	0.58
1:B:496:ASP:OD1	1:B:497:VAL:N	2.35	0.58
1:C:478:LEU:O	1:C:509:GLN:NE2	2.36	0.58
1:A:629:ASP:OD1	1:A:631:SER:OG	2.22	0.58
1:A:612:ASP:OD2	1:A:615:GLN:NE2	2.37	0.57
1:C:478:LEU:HD12	1:C:509:GLN:HG3	1.87	0.57
1:F:414:LYS:HD3	1:F:445:LEU:HG	1.87	0.57
1:B:670:ALA:HA	1:B:674:LEU:HB2	1.86	0.57
1:E:836:VAL:HG23	1:E:837:THR:HG23	1.86	0.57
1:A:679:ARG:NH2	1:A:689:ALA:O	2.37	0.57
1:F:473:TYR:HB3	1:F:583:GLU:HB2	1.87	0.57
1:B:813:SER:HA	1:B:816:ILE:HD12	1.87	0.56
1:A:666:LYS:NZ	1:A:706:GLU:O	2.37	0.56
1:A:738:THR:OG1	1:A:741:ASN:ND2	2.37	0.56
1:B:582:THR:HG22	1:B:584:ASN:H	1.69	0.56
1:F:666:LYS:NZ	1:F:706:GLU:O	2.35	0.56
1:D:616:ASN:HD22	1:D:630:LEU:HB3	1.70	0.56
1:C:492:TYR:H	3:C:1001:ATP:HN62	1.53	0.56
1:F:679:ARG:NH1	1:F:689:ALA:O	2.38	0.56
1:B:836:VAL:HG23	1:B:837:THR:HG23	1.88	0.55
1:C:611:LEU:HD12	1:C:649:LEU:HD11	1.87	0.55
1:C:645:ILE:O	1:C:650:ARG:NH2	2.39	0.55
1:C:836:VAL:HG23	1:C:837:THR:HG23	1.87	0.55
1:B:783:SER:HB3	1:C:885:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:611:LEU:HD12	1:E:649:LEU:HD22	1.87	0.55
1:B:591:GLU:HB2	1:B:594:LYS:HB2	1.87	0.55
1:E:855:SER:HB2	2:K:390:UNK:CA	2.32	0.55
1:D:670:ALA:HA	1:D:674:LEU:HB2	1.87	0.55
1:F:552:MET:HB3	1:F:603:PRO:HD2	1.88	0.55
1:C:855:SER:OG	2:M:390:UNK:O	2.04	0.55
1:E:710:ARG:NH2	5:E:1001:ADP:O3B	2.40	0.55
1:A:740:GLU:O	1:A:743:GLN:NE2	2.40	0.55
1:F:455:PHE:O	1:F:458:THR:OG1	2.25	0.55
1:A:422:ARG:NH2	1:A:439:ASP:OD1	2.39	0.54
1:F:710:ARG:NH2	3:F:1001:ATP:O3G	2.40	0.54
1:C:806:LEU:HD13	1:C:810:MET:HG2	1.88	0.54
1:E:563:ARG:NH2	1:E:625:ASP:OD2	2.41	0.54
1:C:417:ILE:HA	1:C:420:LYS:HE2	1.88	0.54
1:F:494:MET:HB3	1:F:497:VAL:HB	1.89	0.54
1:C:721:ARG:HG2	1:D:503:GLU:HB3	1.91	0.53
1:E:784:LEU:HD11	1:E:838:SER:HB3	1.90	0.53
1:D:666:LYS:NZ	1:D:708:GLY:O	2.36	0.53
1:F:479:ASP:HB3	1:F:482:ARG:HG2	1.89	0.53
1:F:492:TYR:HB3	1:F:669:ILE:HG12	1.91	0.53
1:E:467:SER:HB2	1:E:578:LYS:HG3	1.91	0.53
1:F:452:SER:HB3	1:F:455:PHE:CG	2.44	0.53
1:F:662:VAL:HG13	1:F:664:GLN:H	1.74	0.53
1:A:805:GLN:HB3	1:A:850:PRO:HA	1.90	0.53
1:E:813:SER:HA	1:E:816:ILE:HD12	1.90	0.53
3:C:1001:ATP:O3G	1:D:652:ARG:NH2	2.42	0.52
1:A:537:ALA:HB2	1:A:586:LEU:HD22	1.92	0.52
1:B:805:GLN:NE2	1:C:812:GLU:OE1	2.42	0.52
1:E:519:LEU:HB2	1:E:636:ILE:HD13	1.91	0.52
1:B:882:GLU:HB3	1:B:890:LEU:HB2	1.92	0.52
1:F:670:ALA:HA	1:F:674:LEU:HB2	1.90	0.52
1:F:813:SER:HA	1:F:816:ILE:HD12	1.91	0.52
1:F:496:ASP:N	1:F:496:ASP:OD1	2.42	0.52
1:D:755:ARG:NH1	1:D:876:ASN:OD1	2.37	0.52
1:E:414:LYS:HA	1:E:417:ILE:HD12	1.92	0.52
1:F:456:ASN:OD1	1:F:459:ARG:NH2	2.42	0.52
1:E:546:ARG:HG3	1:E:588:LEU:HD23	1.91	0.52
1:A:490:ASP:OD1	1:A:538:ARG:NH2	2.43	0.51
1:A:706:GLU:OE1	1:A:711:ASN:ND2	2.38	0.51
1:C:738:THR:OG1	1:C:741:ASN:OD1	2.29	0.51
1:E:609:GLU:HG2	1:E:615:GLN:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ASP:OD2	1:B:538:ARG:NH1	2.43	0.51
1:E:585:PRO:HD2	1:E:633:VAL:HG22	1.91	0.51
1:E:621:ASP:OD2	1:E:624:LEU:N	2.38	0.51
1:B:467:SER:HB3	1:B:578:LYS:HG3	1.93	0.51
1:E:428:LEU:HD22	1:E:470:TRP:H	1.76	0.50
1:F:855:SER:HB2	2:J:390:UNK:O	2.07	0.50
1:E:738:THR:HG23	1:E:740:GLU:H	1.75	0.50
1:E:476:GLU:OE1	1:E:542:ARG:NE	2.40	0.50
1:A:768:LEU:HD13	1:A:898:ALA:HB1	1.93	0.50
1:A:782:THR:HB	1:A:867:LEU:HD22	1.93	0.50
1:D:546:ARG:NH2	1:D:590:ASP:OD2	2.45	0.50
1:F:428:LEU:HD12	1:F:470:TRP:HB2	1.94	0.50
1:B:566:VAL:HG21	1:C:453:SER:HB3	1.94	0.50
1:D:641:VAL:HG22	1:D:643:ASP:H	1.77	0.50
1:B:679:ARG:NH2	1:B:689:ALA:O	2.45	0.50
1:F:585:PRO:HD2	1:F:633:VAL:HG22	1.93	0.50
1:F:836:VAL:HG23	1:F:837:THR:HG23	1.93	0.49
1:B:586:LEU:HD21	1:B:636:ILE:HD12	1.95	0.49
1:E:529:LYS:HG2	1:E:658:VAL:HG21	1.95	0.49
1:C:461:TYR:HE1	1:C:624:LEU:HA	1.76	0.49
1:D:662:VAL:HG13	1:D:664:GLN:H	1.78	0.49
1:E:757:TYR:OH	1:F:886:THR:OG1	2.24	0.49
1:E:849:THR:O	1:E:851:LYS:NZ	2.43	0.49
1:D:896:LYS:H	1:D:896:LYS:HD3	1.78	0.49
1:B:695:VAL:HG22	1:B:739:PRO:HD3	1.95	0.48
1:F:643:ASP:OD1	1:F:644:THR:N	2.45	0.48
1:A:852:ASP:O	2:I:390:UNK:N	2.46	0.48
1:D:807:GLY:N	1:D:851:LYS:O	2.44	0.48
1:A:670:ALA:HB2	1:A:712:LEU:HD21	1.94	0.48
1:D:418:GLU:HG2	1:D:442:LEU:HD22	1.96	0.48
1:A:423:GLU:HA	1:A:426:LYS:HD2	1.95	0.48
1:C:572:LYS:NZ	1:D:625:ASP:OD1	2.47	0.48
1:F:475:ASN:OD1	1:F:541:ASN:ND2	2.43	0.48
1:A:461:TYR:HE1	1:A:624:LEU:HA	1.78	0.48
1:D:425:LEU:HD21	1:D:466:THR:HG22	1.95	0.48
1:E:527:VAL:HG11	1:E:658:VAL:HB	1.96	0.48
1:A:608:LEU:HA	1:A:649:LEU:HD21	1.95	0.47
1:A:641:VAL:HG22	1:A:643:ASP:H	1.78	0.47
1:B:686:GLU:HB3	1:B:690:LYS:HE2	1.95	0.47
1:D:469:PRO:HB2	1:D:472:LYS:HB2	1.96	0.47
1:A:414:LYS:HD2	1:A:445:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:TYR:H	5:D:1001:ADP:HN62	1.62	0.47
1:A:418:GLU:HG2	1:A:442:LEU:HD22	1.95	0.47
1:B:825:LEU:HD22	1:B:835:LEU:HD12	1.96	0.47
1:F:692:SER:HB3	1:F:695:VAL:HG13	1.96	0.47
1:B:492:TYR:HB3	1:B:669:ILE:HG12	1.96	0.47
1:C:820:PHE:HB2	1:C:885:LEU:HA	1.95	0.47
1:D:593:ASP:OD1	1:D:593:ASP:N	2.46	0.47
1:B:744:ASP:N	1:B:744:ASP:OD1	2.45	0.47
1:B:785:ARG:NH2	1:B:799:SER:OG	2.47	0.47
1:C:543:GLU:HG3	1:C:580:THR:HG23	1.97	0.47
1:C:546:ARG:HG3	1:C:588:LEU:HD23	1.96	0.47
1:F:554:ASP:HA	1:F:603:PRO:HB3	1.96	0.47
1:B:903:LYS:NZ	1:B:929:GLU:O	2.44	0.47
1:E:608:LEU:HD21	1:E:648:PRO:HB2	1.97	0.47
1:E:561:HIS:HB2	1:E:568:ALA:HB1	1.97	0.47
1:F:588:LEU:HD11	1:F:638:THR:HG23	1.97	0.47
1:E:608:LEU:HD11	1:E:648:PRO:HB2	1.97	0.46
1:A:421:PHE:HA	1:A:424:ARG:HD3	1.98	0.46
1:A:546:ARG:NE	1:A:590:ASP:OD1	2.48	0.46
1:D:757:TYR:OH	1:D:781:GLU:OE2	2.25	0.46
1:A:802:VAL:HG12	1:A:842:LEU:HD22	1.98	0.46
1:C:679:ARG:NH2	1:C:689:ALA:O	2.49	0.46
1:D:545:PHE:HE2	1:D:579:LYS:HD3	1.80	0.46
1:F:547:PHE:HB3	1:F:589:ILE:HA	1.98	0.46
1:A:593:ASP:HB2	1:A:644:THR:OG1	2.15	0.46
1:C:882:GLU:HB3	1:C:890:LEU:HB2	1.96	0.46
1:D:765:VAL:HG21	1:D:862:THR:HB	1.98	0.46
1:F:593:ASP:OD2	1:F:593:ASP:N	2.49	0.46
1:F:768:LEU:HD13	1:F:898:ALA:HB1	1.96	0.46
1:D:771:THR:OG1	1:D:772:ALA:N	2.48	0.46
1:D:785:ARG:NH2	1:D:799:SER:OG	2.49	0.46
1:C:593:ASP:O	1:C:597:ARG:NH2	2.49	0.45
1:F:652:ARG:HD2	1:F:652:ARG:HA	1.80	0.45
1:C:755:ARG:NH1	1:C:876:ASN:OD1	2.49	0.45
1:F:414:LYS:NZ	1:F:450:ASN:HB2	2.31	0.45
1:B:478:LEU:O	1:B:509:GLN:NE2	2.49	0.45
1:B:557:GLU:HA	1:C:562:ARG:HH21	1.81	0.45
1:B:475:ASN:O	1:B:541:ASN:ND2	2.39	0.45
1:E:802:VAL:HG12	1:E:842:LEU:HD22	1.98	0.45
1:A:757:TYR:OH	1:B:886:THR:OG1	2.25	0.45
1:A:755:ARG:NH1	1:A:876:ASN:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LYS:HA	1:B:414:LYS:HD3	1.79	0.44
1:C:593:ASP:OD1	1:C:593:ASP:N	2.50	0.44
1:D:528:GLY:H	5:D:1001:ADP:H5'1	1.81	0.44
1:E:517:LYS:HE2	1:E:517:LYS:HB2	1.70	0.44
1:D:521:PHE:HE1	1:D:656:ILE:HD12	1.83	0.44
1:E:882:GLU:HB3	1:E:890:LEU:HB2	2.00	0.44
1:F:414:LYS:HB2	1:F:414:LYS:HE3	1.77	0.44
1:A:813:SER:HA	1:A:816:ILE:HD12	1.98	0.44
1:B:492:TYR:H	3:B:1001:ATP:HN62	1.65	0.44
1:D:424:ARG:HD3	1:D:466:THR:HB	2.00	0.44
1:E:705:ARG:HH21	1:E:751:PHE:HB3	1.83	0.44
1:F:846:GLU:O	1:F:851:LYS:NZ	2.51	0.44
1:D:441:GLU:O	1:D:445:LEU:HD23	2.17	0.44
1:E:702:GLN:HB3	1:E:749:PRO:HB3	1.99	0.44
1:A:808:GLU:HG3	1:F:805:GLN:HE22	1.83	0.44
1:D:612:ASP:HB3	1:D:615:GLN:HB2	1.98	0.44
1:E:666:LYS:NZ	1:E:706:GLU:O	2.45	0.44
1:F:764:VAL:HG22	1:F:781:GLU:HB3	1.99	0.44
1:A:424:ARG:NH2	1:A:466:THR:OG1	2.50	0.44
1:B:608:LEU:HD21	1:B:648:PRO:HB2	1.99	0.44
1:D:431:PRO:HD3	1:D:470:TRP:HB3	2.00	0.44
1:E:784:LEU:HD12	1:E:784:LEU:HA	1.84	0.44
1:A:573:ILE:HG13	1:A:610:LEU:HD11	2.00	0.44
1:B:684:LEU:HD23	1:B:684:LEU:HA	1.85	0.44
1:D:479:ASP:HB3	1:D:482:ARG:HB2	1.99	0.44
1:D:813:SER:HA	1:D:816:ILE:HD12	2.00	0.44
1:D:435:MET:HA	1:D:438:VAL:HG22	1.99	0.43
1:E:412:ASP:OD1	1:E:412:ASP:N	2.51	0.43
1:F:527:VAL:HG23	1:F:529:LYS:HG3	2.00	0.43
1:F:619:PHE:HB3	1:F:628:VAL:HG23	1.99	0.43
1:D:448:LEU:HD23	1:D:448:LEU:HA	1.86	0.43
1:E:765:VAL:HG21	1:E:862:THR:HB	2.01	0.43
1:F:882:GLU:HB3	1:F:890:LEU:HB2	2.00	0.43
1:B:590:ASP:N	1:B:590:ASP:OD2	2.51	0.43
1:E:465:LEU:HD13	1:E:624:LEU:HD12	2.00	0.43
1:A:585:PRO:HD2	1:A:633:VAL:HG22	2.00	0.43
1:A:651:ASP:OD1	1:A:652:ARG:N	2.52	0.43
1:F:448:LEU:HD22	1:F:455:PHE:CE1	2.53	0.43
1:F:521:PHE:O	1:F:639:ALA:N	2.44	0.43
1:F:771:THR:OG1	1:F:774:GLY:O	2.25	0.43
1:B:445:LEU:HD13	1:B:462:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:LEU:HD22	1:A:835:LEU:HD12	2.01	0.43
1:C:461:TYR:HB2	1:C:563:ARG:HD2	2.01	0.43
1:D:545:PHE:CE2	1:D:579:LYS:HD3	2.53	0.43
1:D:882:GLU:HB3	1:D:890:LEU:HB2	2.00	0.43
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.90	0.43
1:D:448:LEU:HB3	1:D:455:PHE:HD1	1.84	0.43
1:D:454:GLU:O	1:D:458:THR:HG22	2.19	0.43
1:E:429:VAL:N	1:E:470:TRP:O	2.51	0.43
1:E:492:TYR:H	5:E:1001:ADP:HN62	1.67	0.43
1:E:895:ILE:HD12	1:E:912:LEU:HD22	2.01	0.43
1:F:589:ILE:HG13	1:F:637:CYS:HA	2.01	0.43
1:A:570:PRO:HG3	1:A:623:TYR:CD2	2.54	0.43
1:A:586:LEU:HD21	1:A:636:ILE:HD12	2.00	0.43
1:B:435:MET:HE3	1:B:438:VAL:HB	2.00	0.43
1:B:608:LEU:HD12	1:B:649:LEU:HD13	2.00	0.43
1:F:425:LEU:HD13	1:F:466:THR:HG22	2.01	0.43
1:F:432:LYS:HA	1:F:435:MET:HG2	2.01	0.43
1:D:420:LYS:O	1:D:424:ARG:HG3	2.19	0.42
1:E:574:ILE:HG21	1:E:624:LEU:HD23	2.01	0.42
1:A:784:LEU:HD12	1:A:784:LEU:HA	1.84	0.42
1:C:765:VAL:HG21	1:C:862:THR:HB	2.00	0.42
1:E:833:ASP:OD1	1:E:833:ASP:N	2.51	0.42
1:F:612:ASP:HB3	1:F:615:GLN:HG3	2.00	0.42
1:C:478:LEU:HD13	1:C:505:ILE:HG23	2.00	0.42
1:B:768:LEU:HD13	1:B:898:ALA:HB1	2.00	0.42
1:C:699:LEU:HD21	1:C:746:VAL:HG21	2.01	0.42
1:D:480:LEU:HD23	1:D:480:LEU:HA	1.90	0.42
1:D:585:PRO:HD2	1:D:633:VAL:HG22	2.01	0.42
1:D:896:LYS:HG2	1:D:897:GLU:N	2.35	0.42
1:F:433:HIS:NE2	1:F:626:VAL:HG12	2.35	0.42
1:F:771:THR:HG22	2:J:388:UNK:HA	2.00	0.42
1:C:435:MET:HE3	1:C:438:VAL:HB	2.01	0.42
1:A:855:SER:HB2	2:I:390:UNK:CA	2.39	0.42
1:E:672:ARG:NH1	1:E:673:TYR:OH	2.52	0.42
1:F:662:VAL:HG12	1:F:665:GLU:HG3	2.01	0.42
1:D:594:LYS:HE3	1:D:594:LYS:HB3	1.86	0.42
1:D:825:LEU:HD22	1:D:835:LEU:HD12	2.02	0.42
1:E:425:LEU:HG	1:E:466:THR:HG22	2.02	0.42
1:E:705:ARG:HA	1:E:705:ARG:HD3	1.88	0.42
1:F:425:LEU:HG	1:F:430:VAL:HG21	2.01	0.42
1:F:699:LEU:HD12	1:F:742:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:871:ARG:HE	1:C:871:ARG:HB3	1.69	0.42
1:E:738:THR:HG23	1:E:740:GLU:N	2.35	0.41
1:F:450:ASN:HA	1:F:455:PHE:HB3	2.02	0.41
1:F:514:THR:HB	1:F:542:ARG:HH22	1.85	0.41
1:B:660:GLY:HA3	1:B:707:SER:HB3	2.01	0.41
1:D:461:TYR:HE1	1:D:624:LEU:HA	1.85	0.41
1:E:607:LEU:HD23	1:E:607:LEU:HA	1.95	0.41
1:A:413:ASP:N	1:A:413:ASP:OD1	2.53	0.41
1:A:684:LEU:HD23	1:A:684:LEU:HA	1.89	0.41
1:C:764:VAL:HG22	1:C:781:GLU:HB3	2.03	0.41
1:D:593:ASP:HB3	1:D:639:ALA:HB1	2.03	0.41
1:F:519:LEU:HD22	1:F:656:ILE:HD11	2.02	0.41
1:E:931:LEU:HD23	1:E:931:LEU:HA	1.93	0.41
1:F:452:SER:OG	1:F:453:SER:N	2.53	0.41
1:A:816:ILE:HG23	1:A:885:LEU:HB3	2.03	0.41
1:C:655:MET:HA	1:C:655:MET:HE3	2.03	0.41
1:C:768:LEU:HD13	1:C:898:ALA:HB1	2.01	0.41
1:D:846:GLU:O	1:D:851:LYS:NZ	2.41	0.41
1:E:744:ASP:OD1	1:E:744:ASP:N	2.54	0.41
1:F:529:LYS:HG2	1:F:658:VAL:HG21	2.01	0.41
1:F:714:LYS:HA	1:F:714:LYS:HD3	1.89	0.41
1:E:728:VAL:HG12	1:F:480:LEU:HD22	2.03	0.41
1:F:694:ASP:OD1	1:F:694:ASP:N	2.53	0.41
1:B:461:TYR:HE1	1:B:624:LEU:HA	1.85	0.41
1:A:765:VAL:HG21	1:A:862:THR:HB	2.03	0.41
1:A:855:SER:HA	1:A:892:VAL:HG11	2.02	0.41
1:C:416:ALA:HA	1:C:419:GLU:HG2	2.02	0.41
1:C:744:ASP:N	1:C:744:ASP:OD1	2.53	0.41
1:A:595:ILE:HD11	1:A:603:PRO:HB2	2.03	0.41
1:A:775:GLY:O	1:A:904:ARG:NH2	2.47	0.41
1:A:926:PHE:CD1	1:A:927:ILE:HG23	2.56	0.41
1:B:585:PRO:HG2	1:B:587:ILE:HD11	2.02	0.41
1:C:784:LEU:HD23	1:C:784:LEU:HA	1.91	0.41
1:C:805:GLN:NE2	1:D:812:GLU:OE1	2.45	0.41
1:D:779:PHE:O	1:D:845:PRO:HD2	2.21	0.41
1:E:424:ARG:NH2	1:E:466:THR:OG1	2.54	0.41
1:E:784:LEU:HG	1:E:786:ARG:O	2.21	0.41
1:F:785:ARG:NH2	1:F:799:SER:OG	2.48	0.41
1:D:785:ARG:HG3	1:D:841:HIS:HB2	2.02	0.41
1:E:592:VAL:HG21	1:E:637:CYS:HB2	2.02	0.41
1:B:607:LEU:HD13	1:B:607:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:LEU:HD21	1:C:466:THR:HG22	2.01	0.40
1:D:784:LEU:HD21	1:D:838:SER:HB3	2.02	0.40
1:E:597:ARG:HE	1:E:597:ARG:N	2.19	0.40
1:A:492:TYR:HB3	1:A:669:ILE:HG12	2.02	0.40
1:C:480:LEU:HD23	1:C:480:LEU:HA	1.90	0.40
1:C:771:THR:H	1:C:775:GLY:HA2	1.86	0.40
1:D:553:THR:HA	1:D:603:PRO:HG3	2.04	0.40
1:B:766:MET:HG3	1:B:779:PHE:CZ	2.56	0.40
1:C:600:GLN:H	1:C:600:GLN:CD	2.24	0.40
1:C:684:LEU:HD12	1:C:684:LEU:HA	1.91	0.40
1:D:528:GLY:N	5:D:1001:ADP:O2A	2.53	0.40
1:E:754:GLU:HG3	1:E:755:ARG:HG2	2.03	0.40
1:F:484:GLN:O	1:F:488:GLU:HG2	2.22	0.40
1:C:779:PHE:O	1:C:845:PRO:HD2	2.21	0.40
1:D:721:ARG:HG2	1:E:503:GLU:HB3	2.04	0.40
1:E:578:LYS:O	1:E:581:LYS:NZ	2.51	0.40
1:F:670:ALA:HB2	1:F:712:LEU:HD21	2.03	0.40
1:B:630:LEU:HD23	1:B:630:LEU:HA	1.89	0.40
1:E:480:LEU:HD23	1:E:480:LEU:HA	1.90	0.40
1:E:570:PRO:HG3	1:E:623:TYR:CD2	2.57	0.40
1:F:547:PHE:HB3	1:F:589:ILE:HG22	2.04	0.40

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	530/895 (59%)	523 (99%)	7 (1%)	0	100	100
1	B	532/895 (59%)	519 (98%)	13 (2%)	0	100	100
1	C	528/895 (59%)	518 (98%)	10 (2%)	0	100	100
1	D	527/895 (59%)	517 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	528/895 (59%)	522 (99%)	6 (1%)	0	100	100
1	F	512/895 (57%)	503 (98%)	9 (2%)	0	100	100
All	All	3157/5370 (59%)	3102 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	453/758 (60%)	445 (98%)	8 (2%)	59	75
1	B	456/758 (60%)	444 (97%)	12 (3%)	46	66
1	C	452/758 (60%)	440 (97%)	12 (3%)	44	65
1	D	451/758 (60%)	440 (98%)	11 (2%)	49	68
1	E	452/758 (60%)	439 (97%)	13 (3%)	42	62
1	F	444/758 (59%)	431 (97%)	13 (3%)	42	62
All	All	2708/4548 (60%)	2639 (98%)	69 (2%)	50	67

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	ARG
1	A	435	MET
1	A	564	THR
1	A	576	CYS
1	A	582	THR
1	A	803	THR
1	A	805	GLN
1	A	827	GLN
1	B	432	LYS
1	B	435	MET
1	B	451	HIS
1	B	576	CYS

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Mol	Chain	Res	Type
1	B	590	ASP
1	B	600	GLN
1	B	607	LEU
1	B	620	LEU
1	B	744	ASP
1	B	753	VAL
1	B	803	THR
1	B	949	ASP
1	C	435	MET
1	C	463	ASP
1	C	527	VAL
1	C	576	CYS
1	C	594	LYS
1	C	626	VAL
1	C	686	GLU
1	C	736	GLU
1	C	752	THR
1	C	803	THR
1	C	862	THR
1	C	919	ASP
1	D	435	MET
1	D	445	LEU
1	D	477	ASN
1	D	572	LYS
1	D	588	LEU
1	D	625	ASP
1	D	691	LEU
1	D	710	ARG
1	D	733	GLU
1	D	766	MET
1	D	896	LYS
1	E	414	LYS
1	E	515	GLN
1	E	569	MET
1	E	597	ARG
1	E	637	CYS
1	E	655	MET
1	E	664	GLN
1	E	667	LEU
1	E	695	VAL
1	E	803	THR
1	E	846	GLU

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Mol	Chain	Res	Type
1	E	919	ASP
1	E	937	GLU
1	F	423	GLU
1	F	428	LEU
1	F	449	ASP
1	F	476	GLU
1	F	513	SER
1	F	552	MET
1	F	569	MET
1	F	593	ASP
1	F	628	VAL
1	F	746	VAL
1	F	781	GLU
1	F	803	THR
1	F	918	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	741	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)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	ATP	F	1001	4	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
3	ATP	A	1001	4	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
5	ADP	D	1001	-	24,29,29	0.97	1 (4%)	29,45,45	1.52	4 (13%)
3	ATP	C	1001	4	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
5	ADP	E	1001	-	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
3	ATP	B	1001	4	26,33,33	0.59	0	31,52,52	0.75	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	F	1001	4	-	7/18/38/38	0/3/3/3
3	ATP	A	1001	4	-	3/18/38/38	0/3/3/3
5	ADP	D	1001	-	-	3/12/32/32	0/3/3/3
3	ATP	C	1001	4	-	0/18/38/38	0/3/3/3
5	ADP	E	1001	-	-	4/12/32/32	0/3/3/3
3	ATP	B	1001	4	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1001	ADP	C5-C4	2.51	1.47	1.40
5	E	1001	ADP	C5-C4	2.43	1.47	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1001	ADP	PA-O3A-PB	-3.94	119.29	132.83
5	E	1001	ADP	PA-O3A-PB	-3.64	120.34	132.83
5	D	1001	ADP	C3'-C2'-C1'	3.51	106.26	100.98
5	E	1001	ADP	C3'-C2'-C1'	3.43	106.14	100.98
5	D	1001	ADP	N3-C2-N1	-3.12	123.80	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1001	ADP	N3-C2-N1	-3.08	123.86	128.68
5	E	1001	ADP	C4-C5-N7	-2.68	106.60	109.40
5	D	1001	ADP	C4-C5-N7	-2.65	106.63	109.40
3	A	1001	ATP	C5-C6-N6	2.29	123.84	120.35
3	F	1001	ATP	C5-C6-N6	2.29	123.83	120.35
3	B	1001	ATP	C5-C6-N6	2.27	123.81	120.35
3	C	1001	ATP	C5-C6-N6	2.27	123.80	120.35
3	A	1001	ATP	PB-O3B-PG	2.05	139.87	132.83
3	C	1001	ATP	PB-O3B-PG	2.04	139.82	132.83
3	F	1001	ATP	PB-O3B-PG	2.03	139.79	132.83
3	B	1001	ATP	PB-O3B-PG	2.02	139.77	132.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1001	ATP	C5'-O5'-PA-O1A
5	D	1001	ADP	C5'-O5'-PA-O3A
5	E	1001	ADP	C5'-O5'-PA-O1A
5	E	1001	ADP	C5'-O5'-PA-O2A
3	F	1001	ATP	O4'-C4'-C5'-O5'
3	F	1001	ATP	C3'-C4'-C5'-O5'
3	A	1001	ATP	PA-O3A-PB-O1B
3	A	1001	ATP	O4'-C4'-C5'-O5'
3	F	1001	ATP	C5'-O5'-PA-O2A
5	D	1001	ADP	C5'-O5'-PA-O1A
3	B	1001	ATP	PA-O3A-PB-O1B
3	B	1001	ATP	PA-O3A-PB-O2B
3	F	1001	ATP	PA-O3A-PB-O2B
3	A	1001	ATP	PA-O3A-PB-O2B
3	F	1001	ATP	C5'-O5'-PA-O3A
5	E	1001	ADP	C5'-O5'-PA-O3A
5	D	1001	ADP	O4'-C4'-C5'-O5'
3	F	1001	ATP	C4'-C5'-O5'-PA
5	E	1001	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1001	ATP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1001	ADP	3	0
3	C	1001	ATP	2	0
5	E	1001	ADP	2	0
3	B	1001	ATP	1	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 ATP F 1001

Bond lengths   Bond angles   Torsions   Rings

Ligand ATP A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 1001

Bond lengths

Bond angles

Torsions

Rings
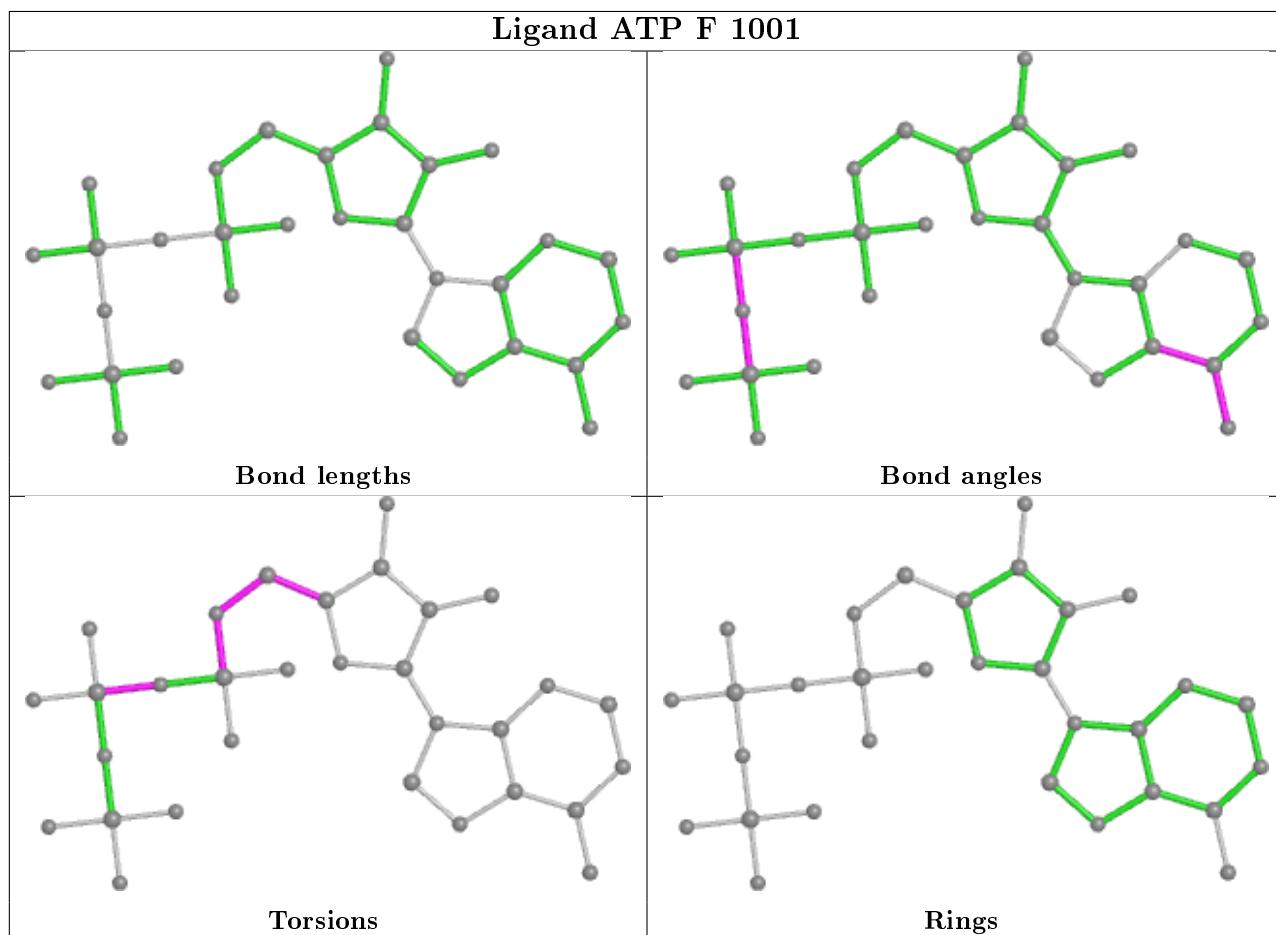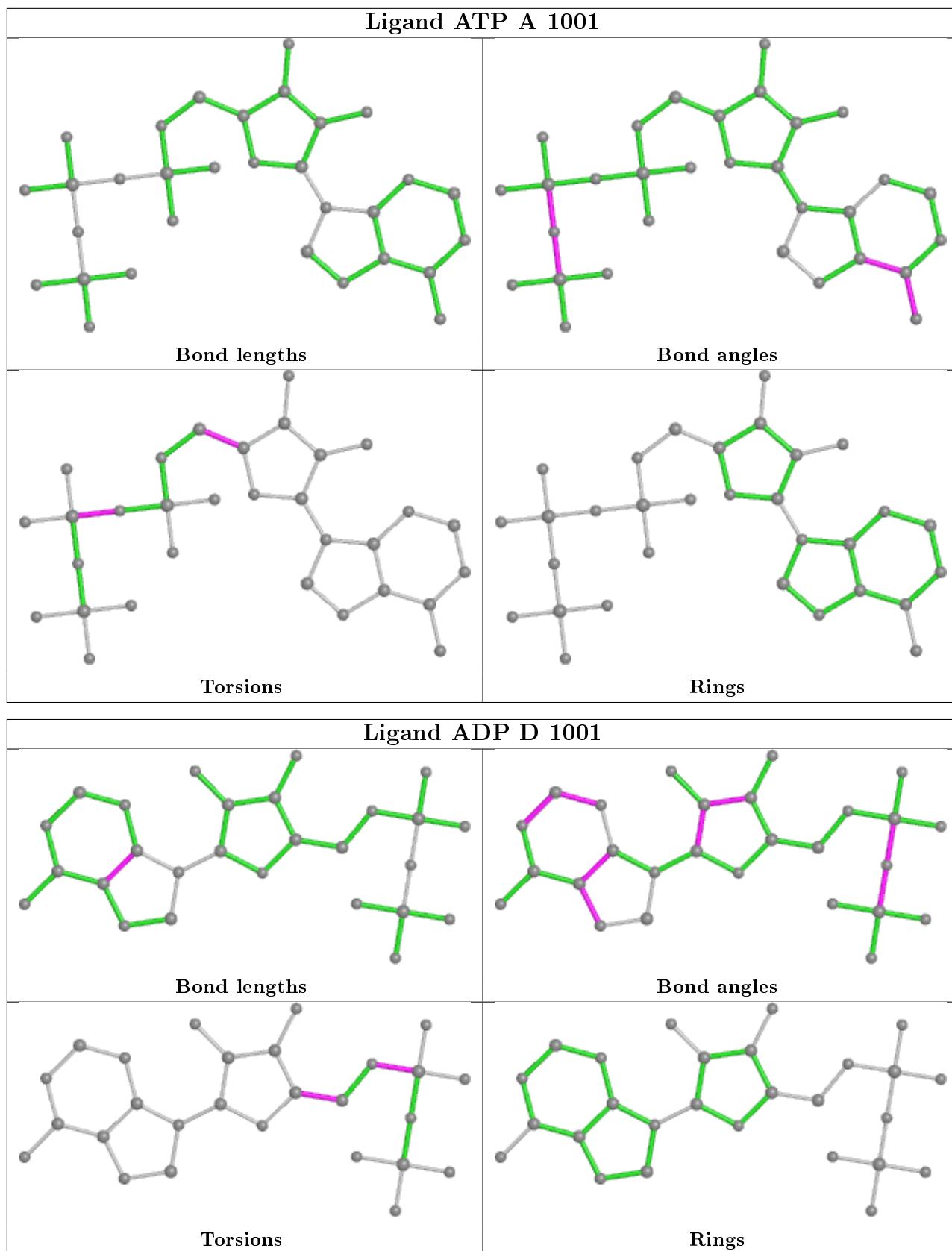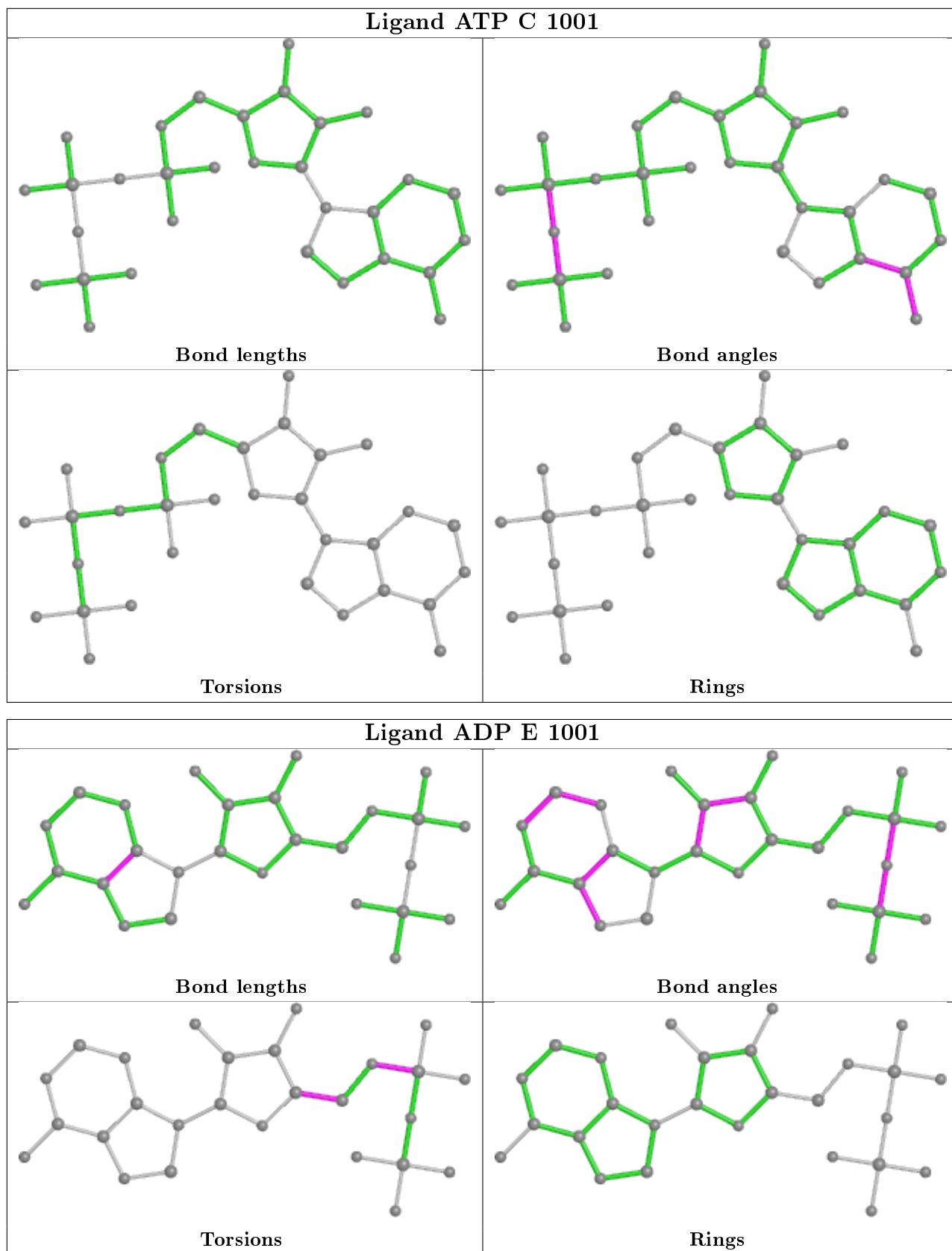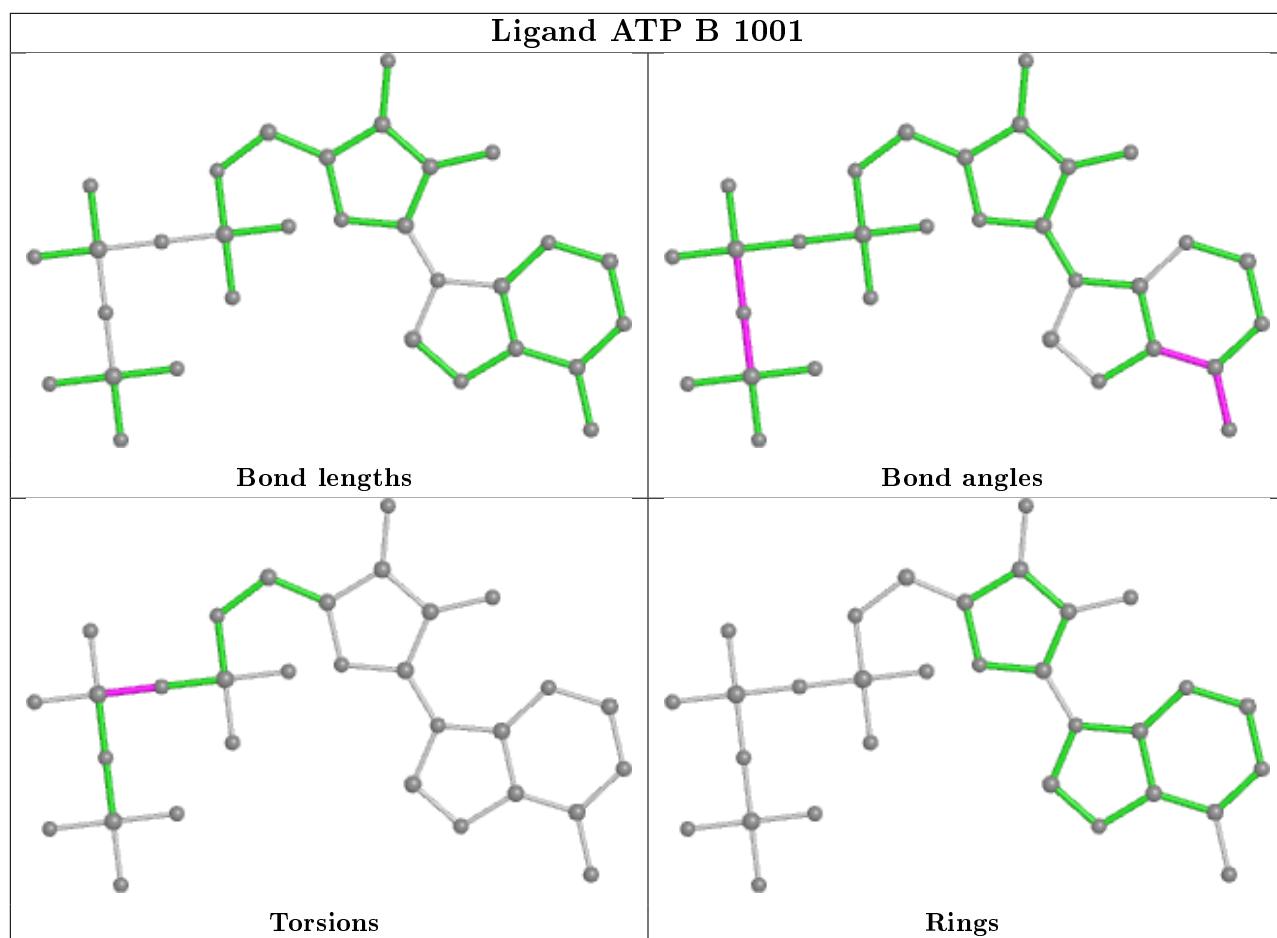
5.7 Other polymers (i)

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 ⓘ

This section contains visualisations of the EMDB entry EMD-13148. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1   Orthogonal projections ⓘ
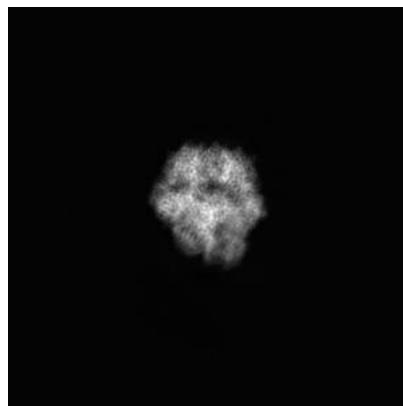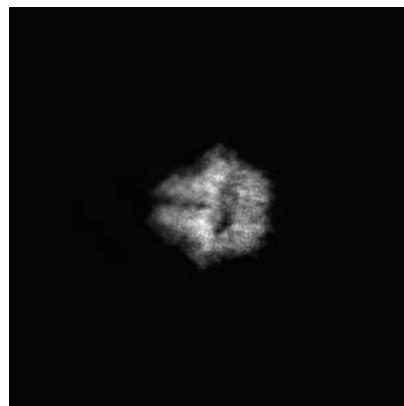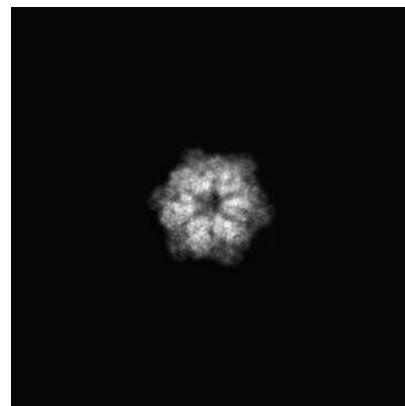
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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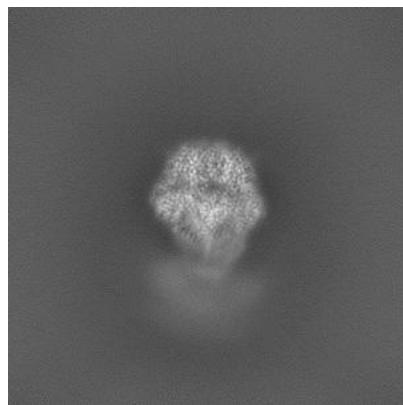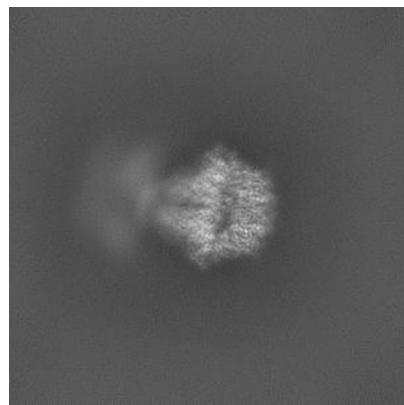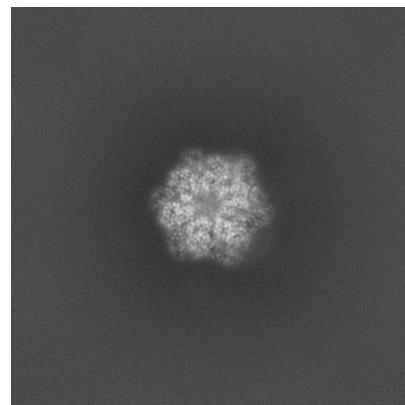
The images above show the map projected in three orthogonal directions.

6.2　Central slices ⓘ
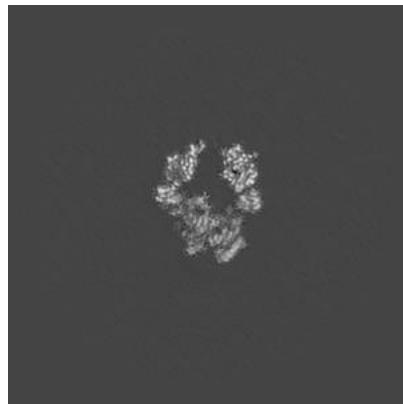
6.2.1　Primary map
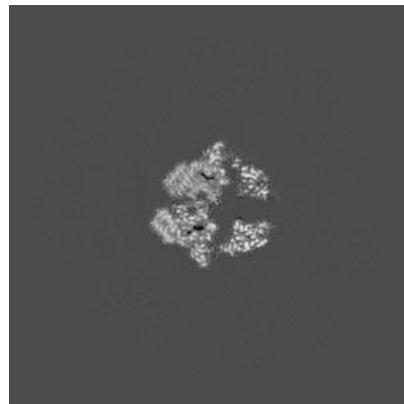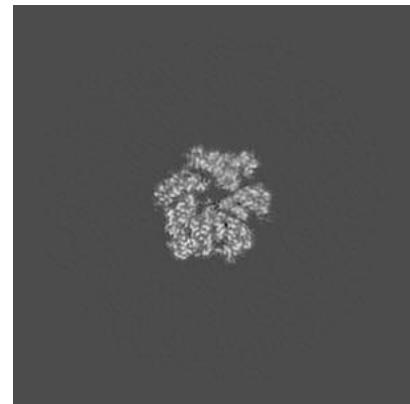
| X Index: 300 | Y Index: 300 | Z Index: 300 |

6.2.2　Raw map
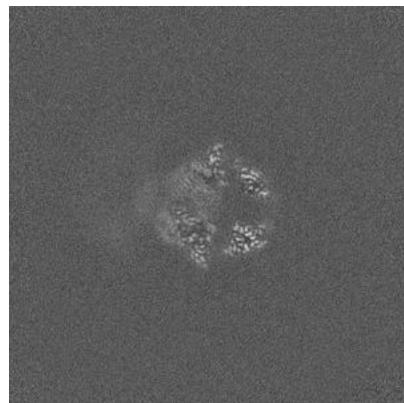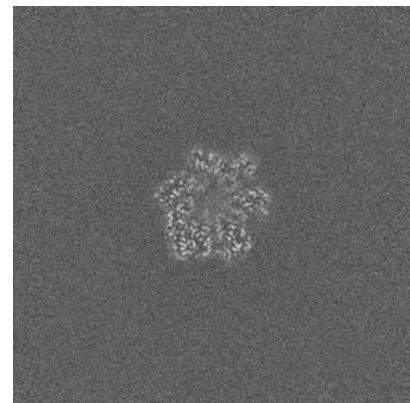
| X Index: 300 | Y Index: 300 | Z Index: 300 |

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

6.3 Largest variance slices ⓘ
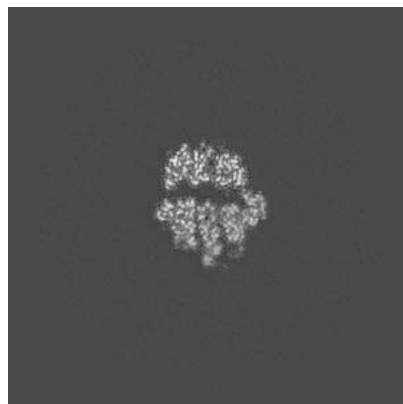
6.3.1 Primary map
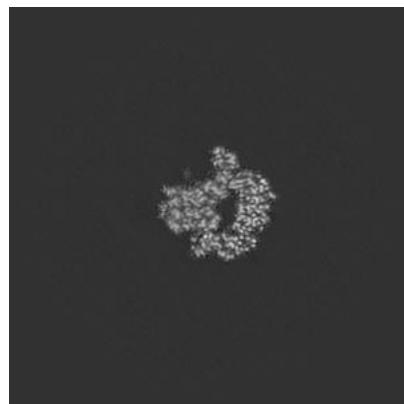
X Index: 271	Y Index: 275	Z Index: 297
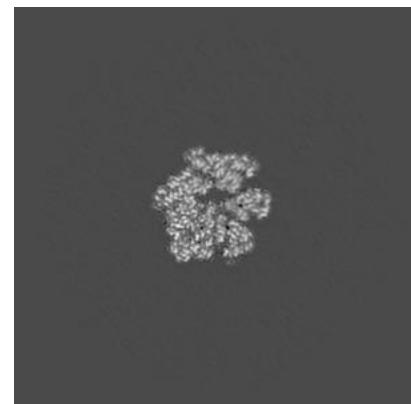
6.3.2 Raw map
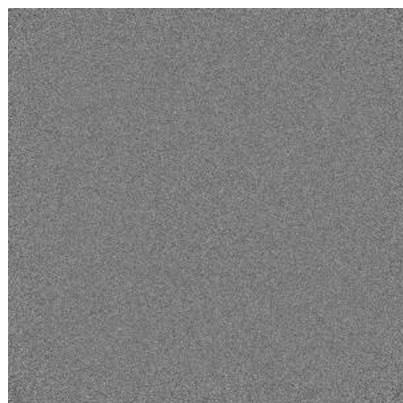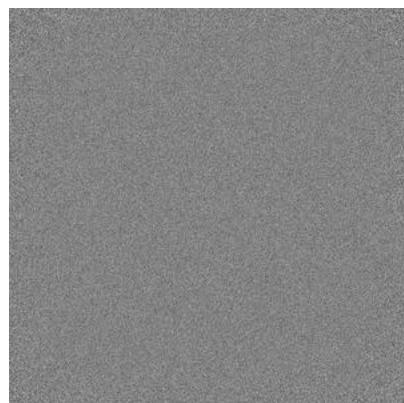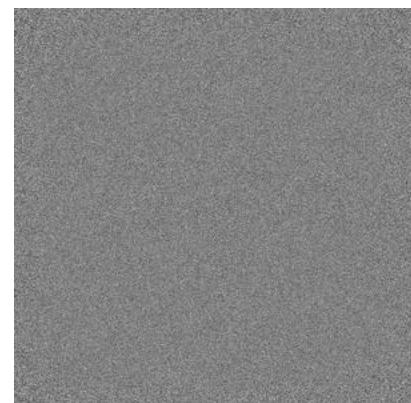
X Index: 0	Y Index: 0	Z Index: 0

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X   Y   Z
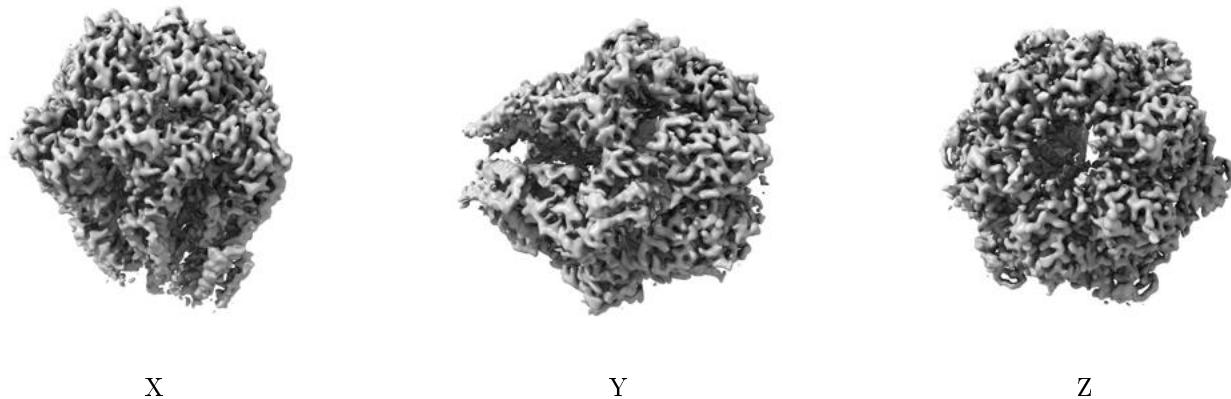
The images above show the 3D surface view of the map at the recommended contour level 0.15.
These images, in conjunction with the slice images, may facilitate assessment of whether an ap-
propriate contour level has been provided.

6.4.2 Raw map

X   Y   Z
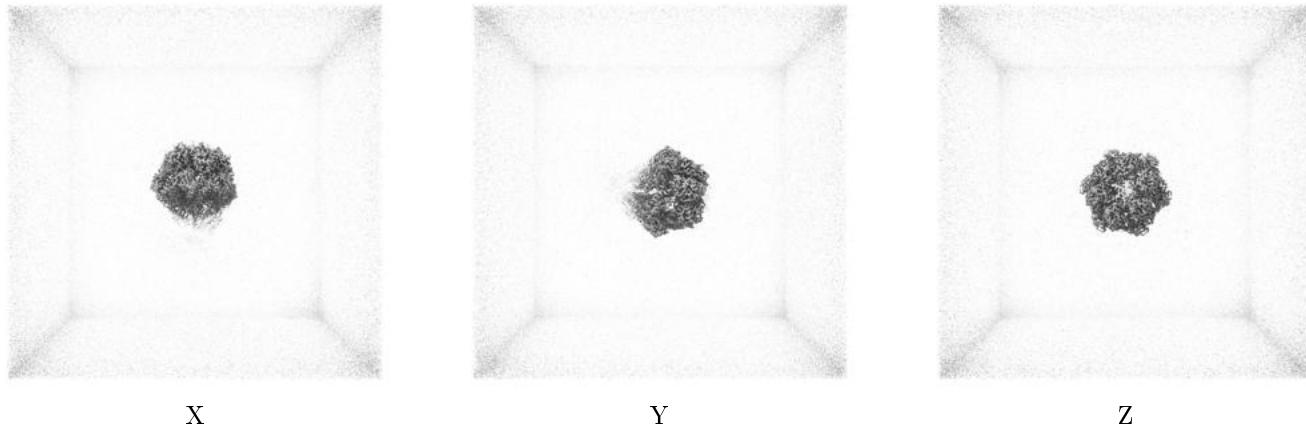
These images show the 3D surface of the raw map. The raw map's contour level was selected so
that its surface encloses the same volume as the primary map does at its recommended contour
level.

6.5 Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.5.1 emd_13148_msk_1.map ⓘ

X   Y   Z
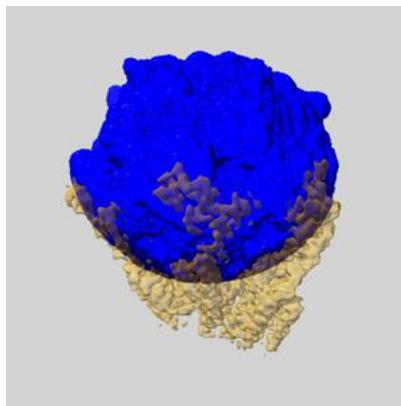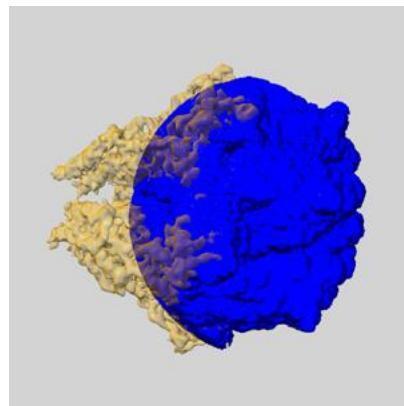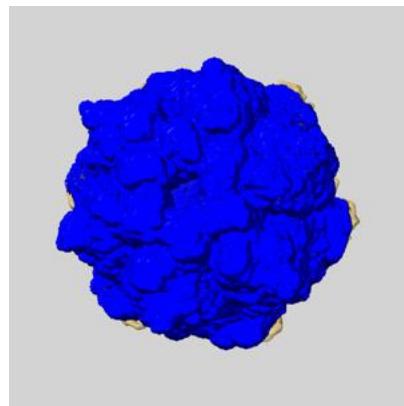
7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

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 ⓘ
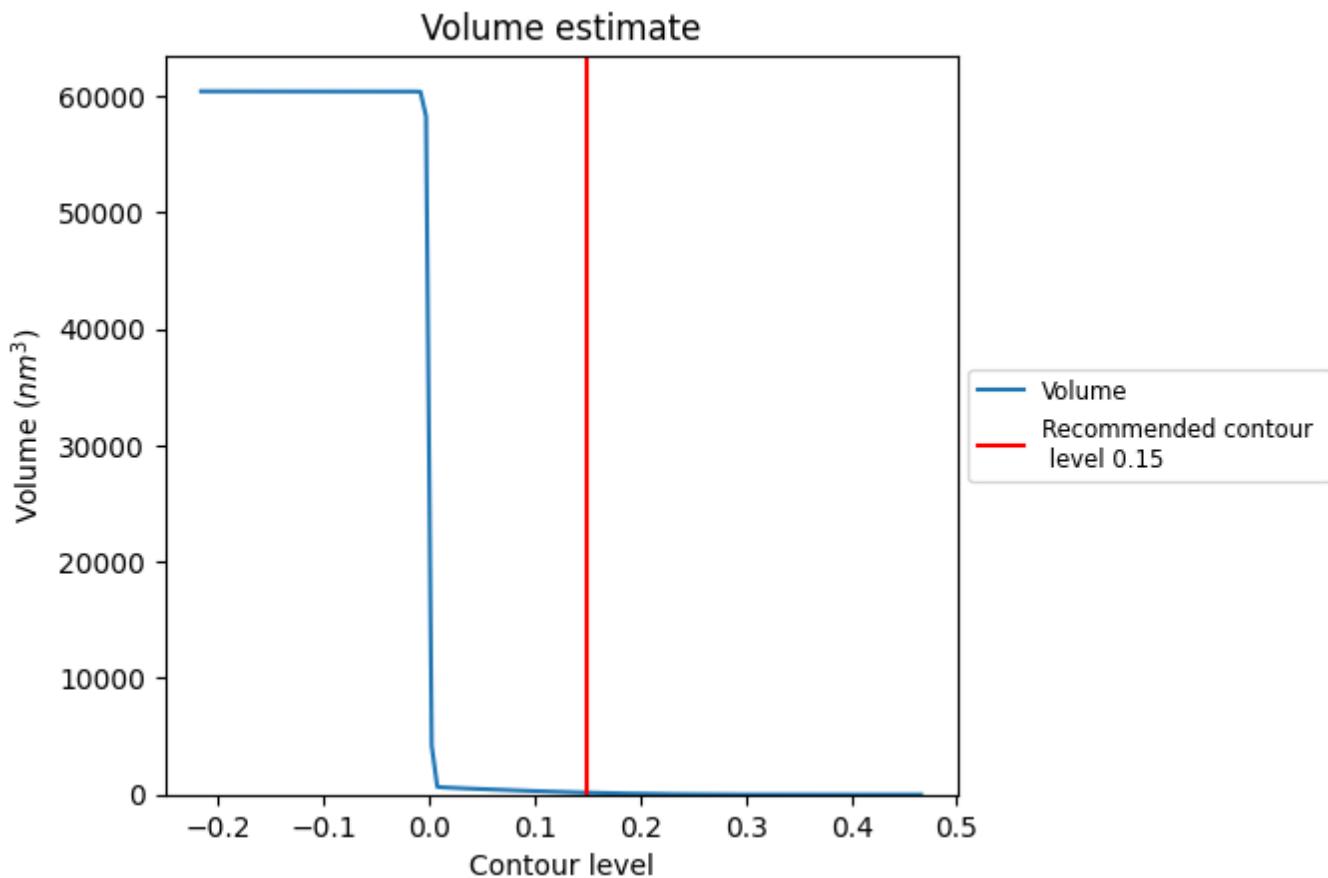
The volume at the recommended contour level is 161 nm^3; this corresponds to an approximate mass of 146 kDa.

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 ⓘ
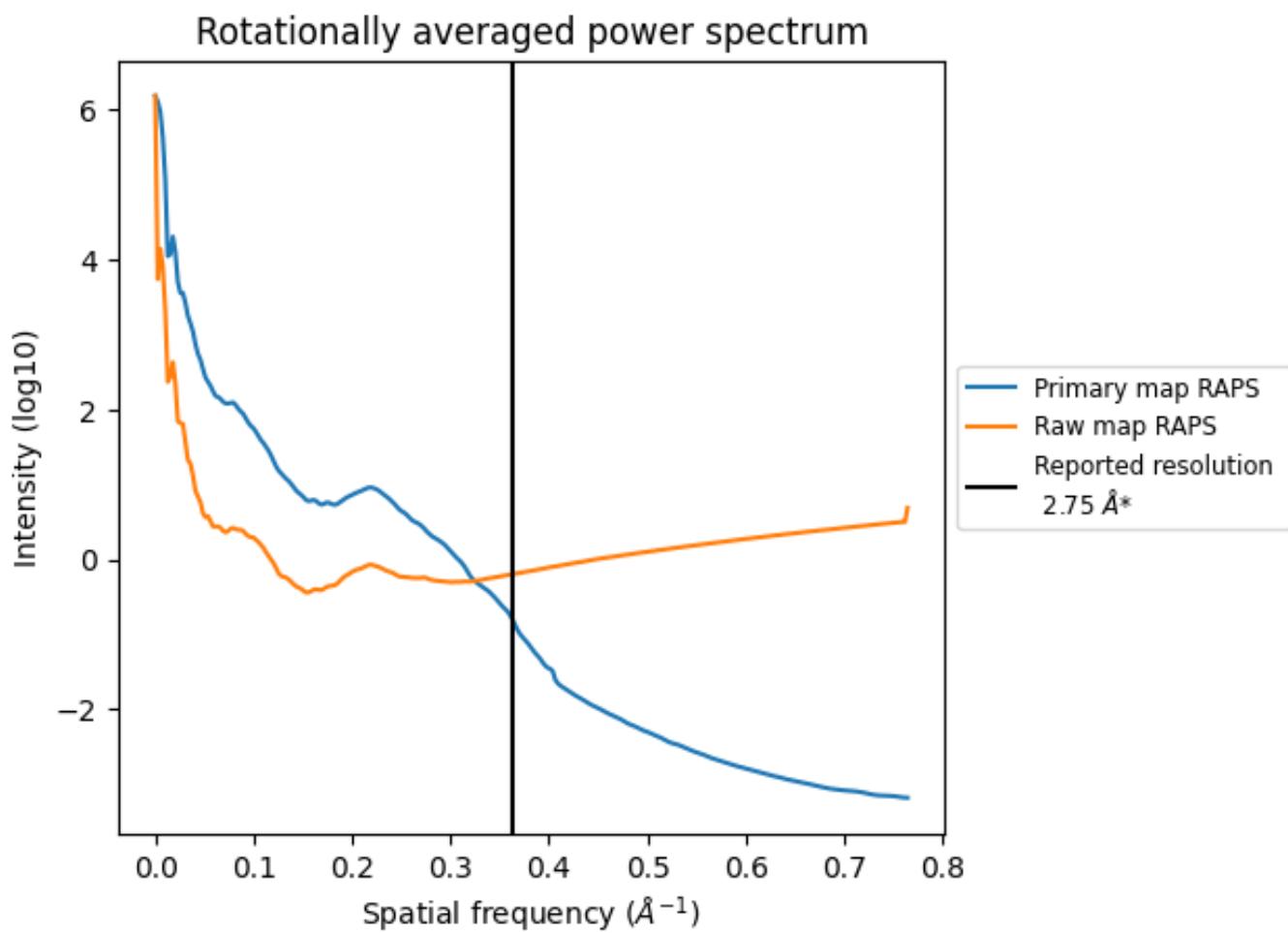
*Reported resolution corresponds to spatial frequency of 0.364 $Å^{-1}$

8   Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1   FSC (i)
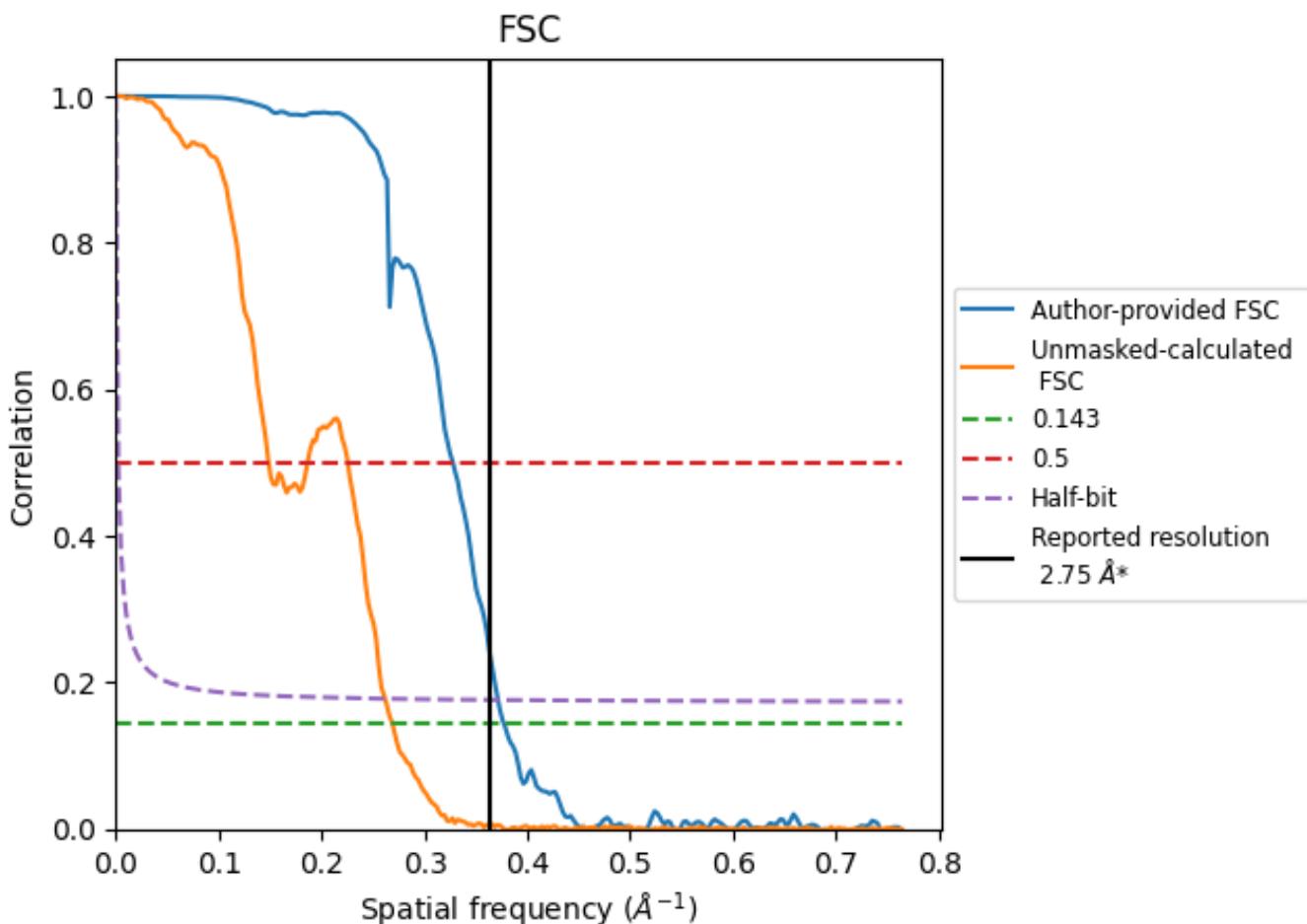
*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.65	3.05	2.69
Unmasked-calculated*	3.72	6.73	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.72 differs from the reported value 2.75 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13148 and PDB model 7P0M. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)

| X | Y | Z |
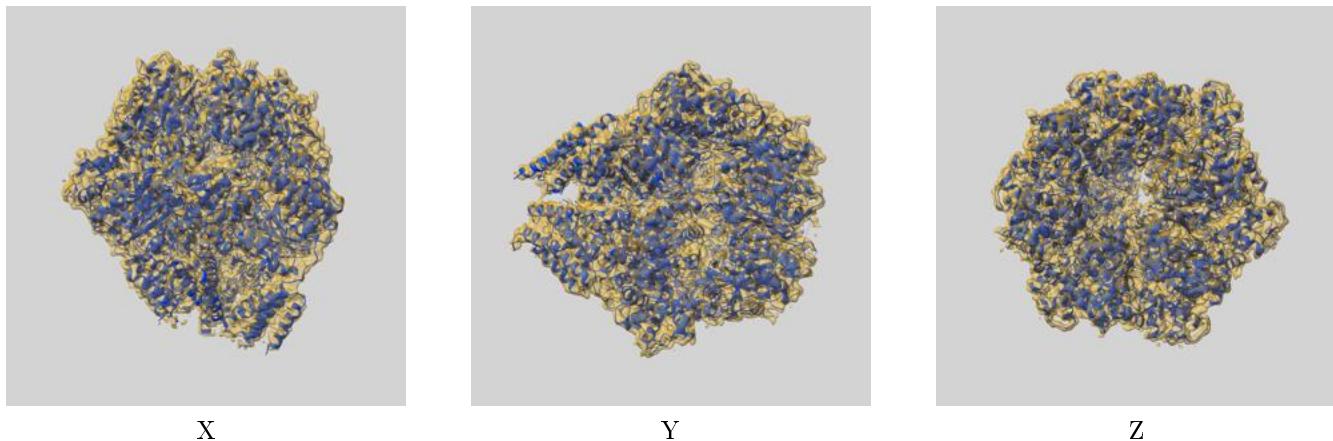
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)
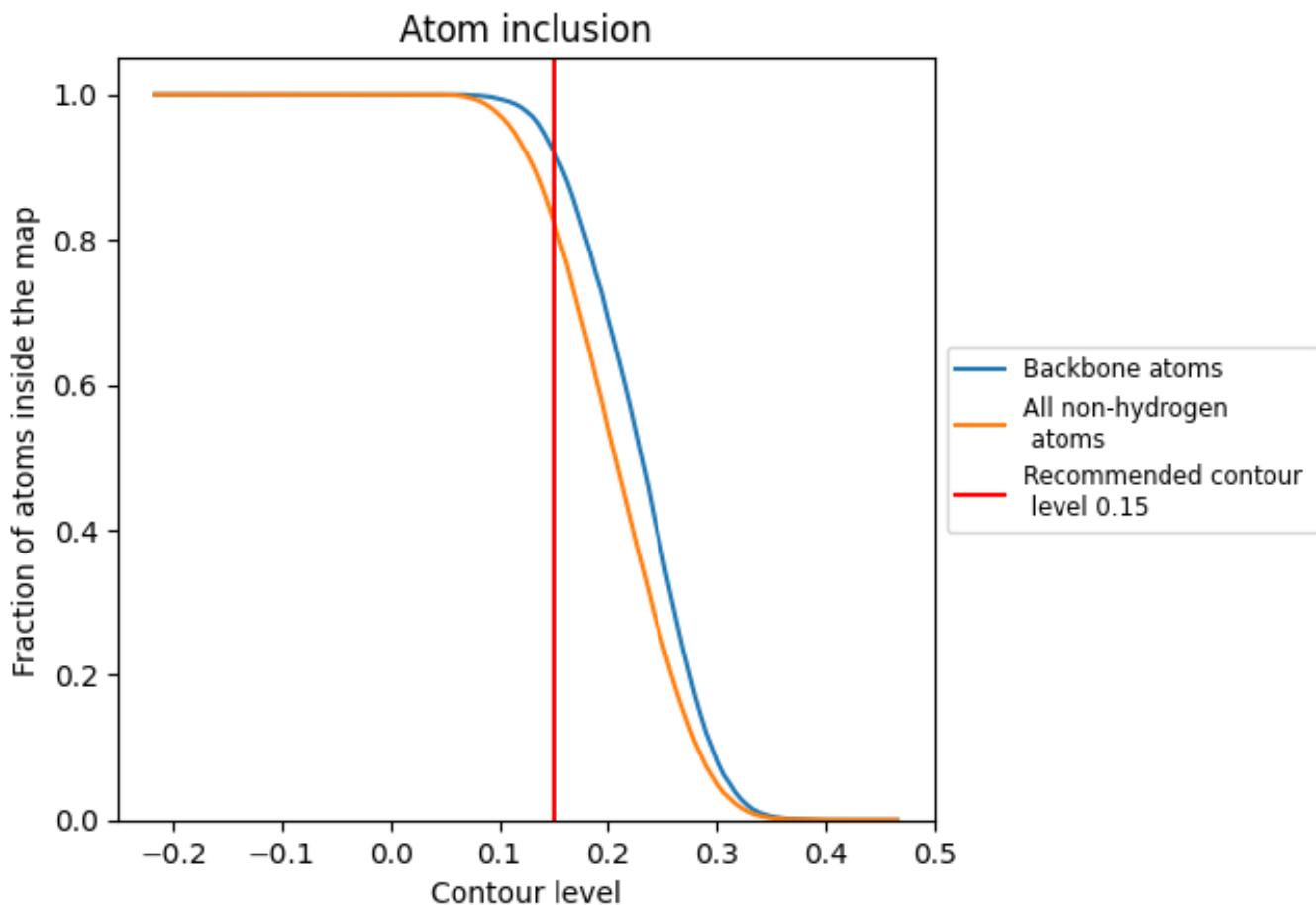
At the recommended contour level, 92% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.