



# wwPDB EM Validation Summary Report ⓘ

Apr 3, 2024 – 02:11 am BST

PDB ID : 8OKA  
EMDB ID : EMD-16923  
Title : Human Mitochondrial Lon Y394F Mutant ADP Bound  
Authors : Kereiche, S.; Bauer, J.A.; Matyas, P.; Novacek, J.; Kutejova, E.  
Deposited on : 2023-03-28  
Resolution : 3.89 Å (reported)  
Based on initial model : 7NFY

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev92  
Mogul : 1.8.4, 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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

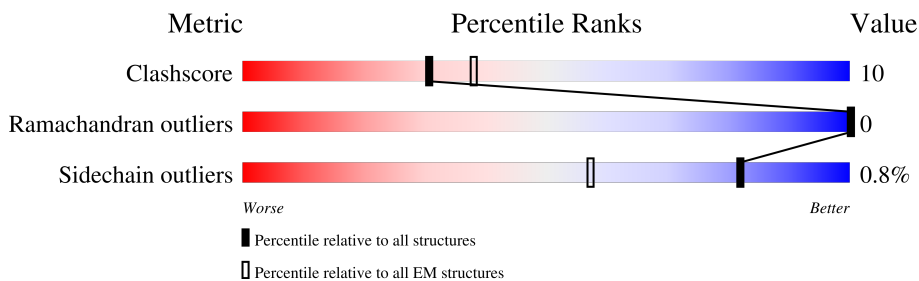
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.89 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  $\geq 3$ , 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	869	
1	B	869	
1	C	869	
1	D	869	
1	E	869	
1	F	869	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 74878 atoms, of which 37822 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
			Total	C	H	N	O	S		
1	A	777	12441	3901	6292	1067	1154	27	0	0
1	B	777	12441	3901	6292	1067	1154	27	0	0
1	C	777	12441	3901	6292	1067	1154	27	0	0
1	D	777	12441	3901	6292	1067	1154	27	0	0
1	E	777	12441	3901	6292	1067	1154	27	0	0
1	F	777	12439	3901	6290	1067	1154	27	0	0

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	MET	-	initiating methionine	UNP P36776
A	92	GLY	-	expression tag	UNP P36776
A	93	HIS	-	expression tag	UNP P36776
A	94	HIS	-	expression tag	UNP P36776
A	95	HIS	-	expression tag	UNP P36776
A	96	HIS	-	expression tag	UNP P36776
A	97	HIS	-	expression tag	UNP P36776
A	98	HIS	-	expression tag	UNP P36776
A	99	ASP	-	expression tag	UNP P36776
A	100	TYR	-	expression tag	UNP P36776
A	101	ASP	-	expression tag	UNP P36776
A	102	ILE	-	expression tag	UNP P36776
A	103	PRO	-	expression tag	UNP P36776
A	104	THR	-	expression tag	UNP P36776
A	105	THR	-	expression tag	UNP P36776
A	106	GLU	-	expression tag	UNP P36776
A	107	ASN	-	expression tag	UNP P36776
A	108	LEU	-	expression tag	UNP P36776

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	TYR	-	expression tag	UNP P36776
A	110	PHE	-	expression tag	UNP P36776
A	111	GLN	-	expression tag	UNP P36776
A	112	GLY	-	expression tag	UNP P36776
A	113	ALA	-	expression tag	UNP P36776
A	114	HIS	-	expression tag	UNP P36776
A	394	PHE	TYR	engineered mutation	UNP P36776
B	91	MET	-	initiating methionine	UNP P36776
B	92	GLY	-	expression tag	UNP P36776
B	93	HIS	-	expression tag	UNP P36776
B	94	HIS	-	expression tag	UNP P36776
B	95	HIS	-	expression tag	UNP P36776
B	96	HIS	-	expression tag	UNP P36776
B	97	HIS	-	expression tag	UNP P36776
B	98	HIS	-	expression tag	UNP P36776
B	99	ASP	-	expression tag	UNP P36776
B	100	TYR	-	expression tag	UNP P36776
B	101	ASP	-	expression tag	UNP P36776
B	102	ILE	-	expression tag	UNP P36776
B	103	PRO	-	expression tag	UNP P36776
B	104	THR	-	expression tag	UNP P36776
B	105	THR	-	expression tag	UNP P36776
B	106	GLU	-	expression tag	UNP P36776
B	107	ASN	-	expression tag	UNP P36776
B	108	LEU	-	expression tag	UNP P36776
B	109	TYR	-	expression tag	UNP P36776
B	110	PHE	-	expression tag	UNP P36776
B	111	GLN	-	expression tag	UNP P36776
B	112	GLY	-	expression tag	UNP P36776
B	113	ALA	-	expression tag	UNP P36776
B	114	HIS	-	expression tag	UNP P36776
B	394	PHE	TYR	engineered mutation	UNP P36776
C	91	MET	-	initiating methionine	UNP P36776
C	92	GLY	-	expression tag	UNP P36776
C	93	HIS	-	expression tag	UNP P36776
C	94	HIS	-	expression tag	UNP P36776
C	95	HIS	-	expression tag	UNP P36776
C	96	HIS	-	expression tag	UNP P36776
C	97	HIS	-	expression tag	UNP P36776
C	98	HIS	-	expression tag	UNP P36776
C	99	ASP	-	expression tag	UNP P36776
C	100	TYR	-	expression tag	UNP P36776

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	101	ASP	-	expression tag	UNP P36776
C	102	ILE	-	expression tag	UNP P36776
C	103	PRO	-	expression tag	UNP P36776
C	104	THR	-	expression tag	UNP P36776
C	105	THR	-	expression tag	UNP P36776
C	106	GLU	-	expression tag	UNP P36776
C	107	ASN	-	expression tag	UNP P36776
C	108	LEU	-	expression tag	UNP P36776
C	109	TYR	-	expression tag	UNP P36776
C	110	PHE	-	expression tag	UNP P36776
C	111	GLN	-	expression tag	UNP P36776
C	112	GLY	-	expression tag	UNP P36776
C	113	ALA	-	expression tag	UNP P36776
C	114	HIS	-	expression tag	UNP P36776
C	394	PHE	TYR	engineered mutation	UNP P36776
D	91	MET	-	initiating methionine	UNP P36776
D	92	GLY	-	expression tag	UNP P36776
D	93	HIS	-	expression tag	UNP P36776
D	94	HIS	-	expression tag	UNP P36776
D	95	HIS	-	expression tag	UNP P36776
D	96	HIS	-	expression tag	UNP P36776
D	97	HIS	-	expression tag	UNP P36776
D	98	HIS	-	expression tag	UNP P36776
D	99	ASP	-	expression tag	UNP P36776
D	100	TYR	-	expression tag	UNP P36776
D	101	ASP	-	expression tag	UNP P36776
D	102	ILE	-	expression tag	UNP P36776
D	103	PRO	-	expression tag	UNP P36776
D	104	THR	-	expression tag	UNP P36776
D	105	THR	-	expression tag	UNP P36776
D	106	GLU	-	expression tag	UNP P36776
D	107	ASN	-	expression tag	UNP P36776
D	108	LEU	-	expression tag	UNP P36776
D	109	TYR	-	expression tag	UNP P36776
D	110	PHE	-	expression tag	UNP P36776
D	111	GLN	-	expression tag	UNP P36776
D	112	GLY	-	expression tag	UNP P36776
D	113	ALA	-	expression tag	UNP P36776
D	114	HIS	-	expression tag	UNP P36776
D	394	PHE	TYR	engineered mutation	UNP P36776
E	91	MET	-	initiating methionine	UNP P36776
E	92	GLY	-	expression tag	UNP P36776

*Continued on next page...*

*Continued from previous page...*

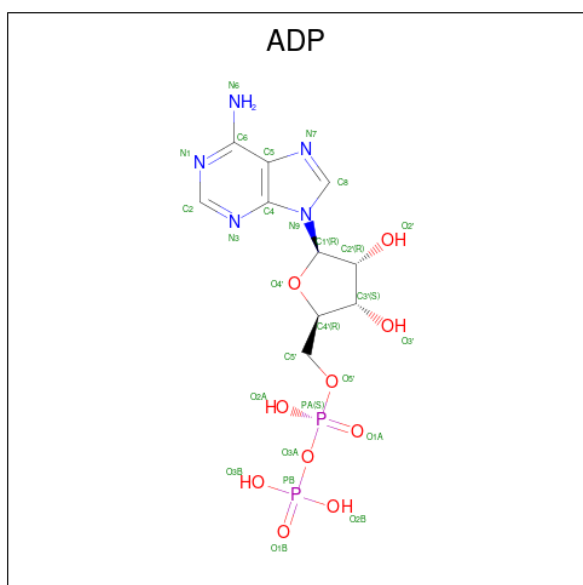
Chain	Residue	Modelled	Actual	Comment	Reference
E	93	HIS	-	expression tag	UNP P36776
E	94	HIS	-	expression tag	UNP P36776
E	95	HIS	-	expression tag	UNP P36776
E	96	HIS	-	expression tag	UNP P36776
E	97	HIS	-	expression tag	UNP P36776
E	98	HIS	-	expression tag	UNP P36776
E	99	ASP	-	expression tag	UNP P36776
E	100	TYR	-	expression tag	UNP P36776
E	101	ASP	-	expression tag	UNP P36776
E	102	ILE	-	expression tag	UNP P36776
E	103	PRO	-	expression tag	UNP P36776
E	104	THR	-	expression tag	UNP P36776
E	105	THR	-	expression tag	UNP P36776
E	106	GLU	-	expression tag	UNP P36776
E	107	ASN	-	expression tag	UNP P36776
E	108	LEU	-	expression tag	UNP P36776
E	109	TYR	-	expression tag	UNP P36776
E	110	PHE	-	expression tag	UNP P36776
E	111	GLN	-	expression tag	UNP P36776
E	112	GLY	-	expression tag	UNP P36776
E	113	ALA	-	expression tag	UNP P36776
E	114	HIS	-	expression tag	UNP P36776
E	394	PHE	TYR	engineered mutation	UNP P36776
F	91	MET	-	initiating methionine	UNP P36776
F	92	GLY	-	expression tag	UNP P36776
F	93	HIS	-	expression tag	UNP P36776
F	94	HIS	-	expression tag	UNP P36776
F	95	HIS	-	expression tag	UNP P36776
F	96	HIS	-	expression tag	UNP P36776
F	97	HIS	-	expression tag	UNP P36776
F	98	HIS	-	expression tag	UNP P36776
F	99	ASP	-	expression tag	UNP P36776
F	100	TYR	-	expression tag	UNP P36776
F	101	ASP	-	expression tag	UNP P36776
F	102	ILE	-	expression tag	UNP P36776
F	103	PRO	-	expression tag	UNP P36776
F	104	THR	-	expression tag	UNP P36776
F	105	THR	-	expression tag	UNP P36776
F	106	GLU	-	expression tag	UNP P36776
F	107	ASN	-	expression tag	UNP P36776
F	108	LEU	-	expression tag	UNP P36776
F	109	TYR	-	expression tag	UNP P36776

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	110	PHE	-	expression tag	UNP P36776
F	111	GLN	-	expression tag	UNP P36776
F	112	GLY	-	expression tag	UNP P36776
F	113	ALA	-	expression tag	UNP P36776
F	114	HIS	-	expression tag	UNP P36776
F	394	PHE	TYR	engineered mutation	UNP P36776

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



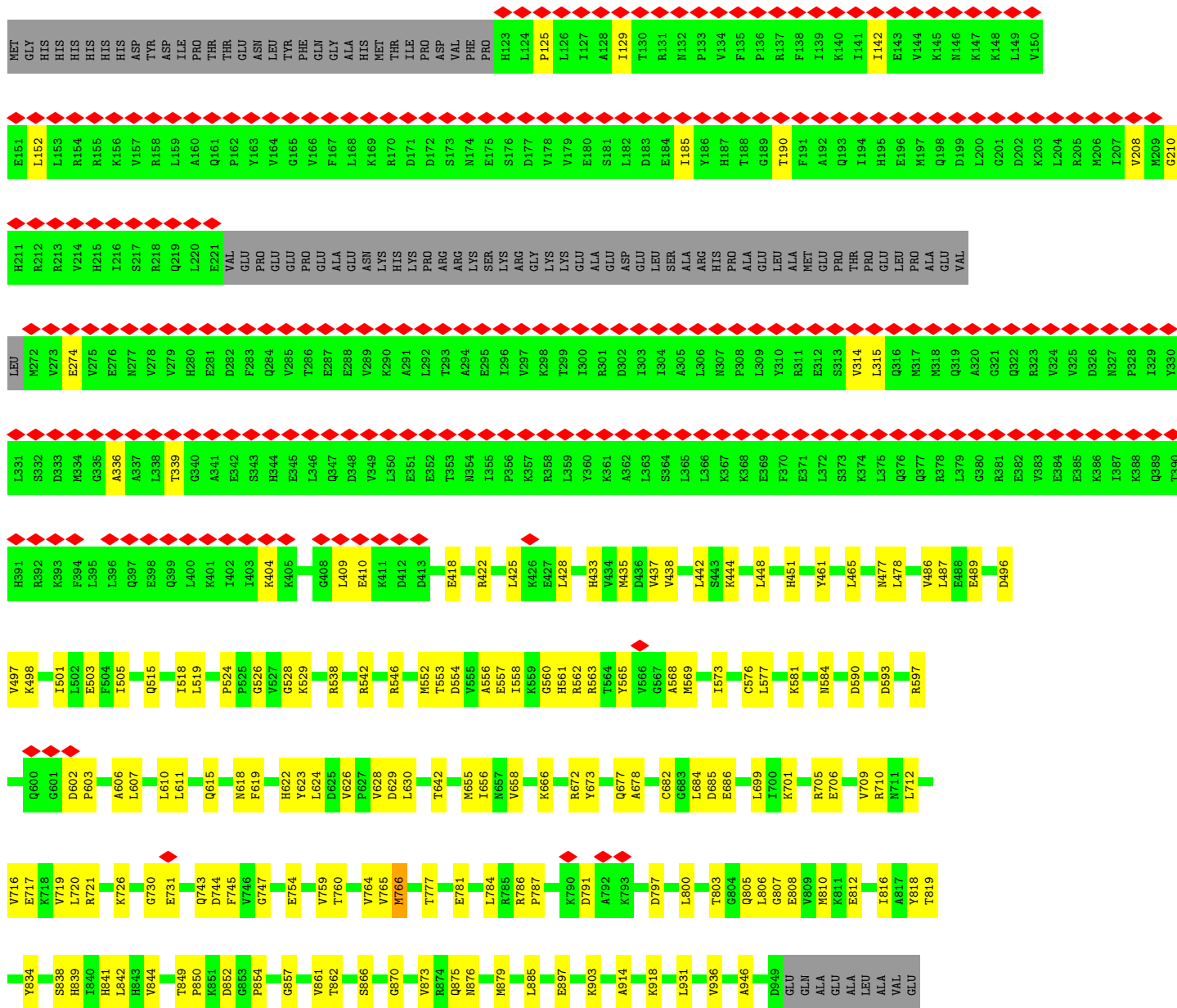
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
2	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	B	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	C	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	





GLU  
ALA  
LEU  
ALA  
VAL  
GLU  
ARG

• Molecule 1: Lon protease homolog, mitochondrial



ARG

• Molecule 1: Lon protease homolog, mitochondrial

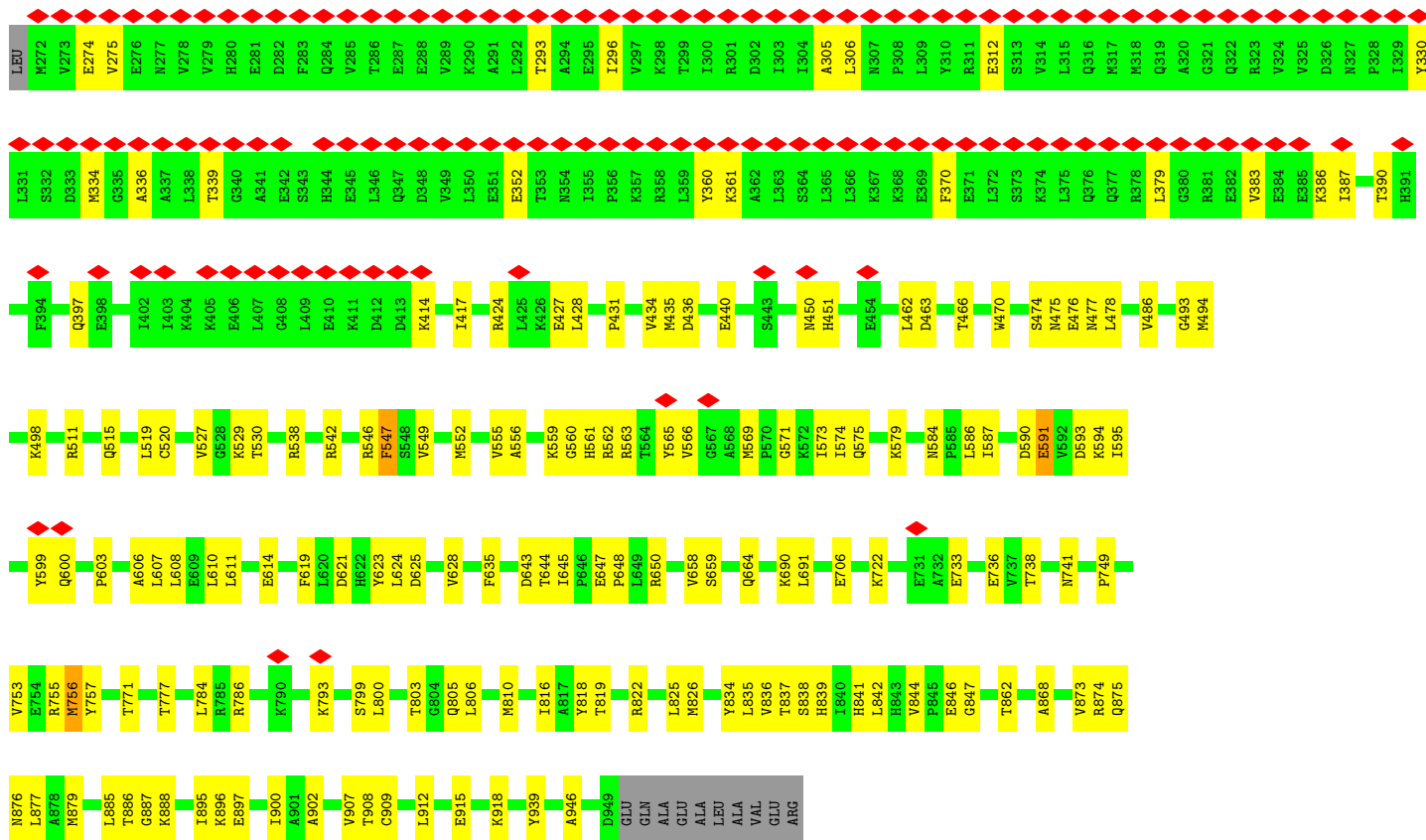


MET	GLY	HIS	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ASP	ILE	PRO	THR	THR	GLU	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	ALA	MET	THR	PRO	PRO	VAL	PHE	PRO	H123	L124	P125	L126	I127	A128	I129	T130	R131	N132	P133	V134	F135	P136	R137	F138	I139	K140	I141	I142	E143	V144	K145	N146	K147	K148	L149	V150
E151	L152	L153	R154	R155	K156	V157	R158	L159	A160	Q161	P162	Y163	V164	G165	V166	F167	L168	K169	R170	D171	D172	S173	N174	E175	S176	D177	V178	V179	E180	S181	L182	D183	E184	I185	Y186	H187	T188	G189	T190	F191	F191	A192	Q193	I194	H195	E196	M197	Q198	D199	L200	G201	D202	K203	L204	R205	M206	I207	V208	M209	G210
H211	R212	R213	V214	H215	I216	S217	R218	Q219	L220	E221	VAL	PRO	GLU	GLU	PRO	PRO	GLU	GLU	GLU	PRO	PRO	ARG	ARG	LYS	LYS	ARG	ARG	ASP	ASP	ALA	ALA	ASP	GLU	GLU	LEU	LEU	ALA	ALA	ARG	HIS	PRO	ALA	ALA	THR	PRO	PRO	THR	PRO	PRO	THR	PRO	GLU	VAL							
LEU	M272	V273	E274	V275	E276	N277	V278	V279	H280	E281	D282	F283	Q284	V285	T286	E287	E288	V289	K290	A291	L292	T293	E295	I296	V297	K298	T299	I300	R301	I303	I304	A305	L306	N307	P308	L309	Y310	R311	E312	S313	V314	L315	Q316	M317	M318	Q319	A320	G321	R323	V324	V325	D326	N327	I329	Y330					
L331	S332	D333	M334	G335	A336	A337	L338	T339	G340	A341	E342	S343	H344	E345	L346	Q347	D348	V349	L350	E351	E352	T353	N354	I355	P356	K357	R358	L359	Y360	K361	A362	L363	S364	L365	L366	K367	K368	E369	F370	E371	L372	S373	K374	L375	Q376	Q377	R378	L379	G380	R381	E382	V383	E384	E385	K386	I387	K388	Q389	T390	
H391	R392	K393	F394	L395	L396	Q397	E398	Q399	L400	K401	I402	K403	K404	K405	L406	L407	G408	E410	K411	D412	K414	D415	A416	E427	L428	V434	M435	D436	V437	V438	L442	S443	K444	L447	L448	L462	W470	A476	M477	L478	D479	L480	E495	D496	V497	L502	E503	F504												
I505	L510	L519	G526	A533	R542	F547	S548	V549	A556	E557	L558	K559	G560	H561	R562	R563	T564	Y565	V566	G567	L573	L574	P585	L588	L589	D590	Y699	Q600	D602	P603	A606	L607	L610	L611	N616	A617	L620	D621	H622	Y623	L624	B625	V626																	
P627	V628	D629	L630	F635	E647	P648	L649	M653	E654	V658	V662	A663	E671	G679	D795	K796	D797	E801	Y802	E808	V809	M810	K811	E812	L816	K817	Y818	R822	D833	Y834	L835	V836	T837	S838	L842	H843	V844	K851	C858	T862	A863	L864	L865	S866	Y759															
M669	G670	Q675	M676	L677	A678	S684	L685	M686	K688	A902	Y907	T908	C909	K918	T928	E937	H938	Y939	I942	D949	GLU	GLN	ALA	ALA	ALA	LEU	ALA	ALA	VAL	GLU	ARG	L742	Q743	D744	F745	V746	G747	K748	P749	V753	E754	R755	M756	Y759																

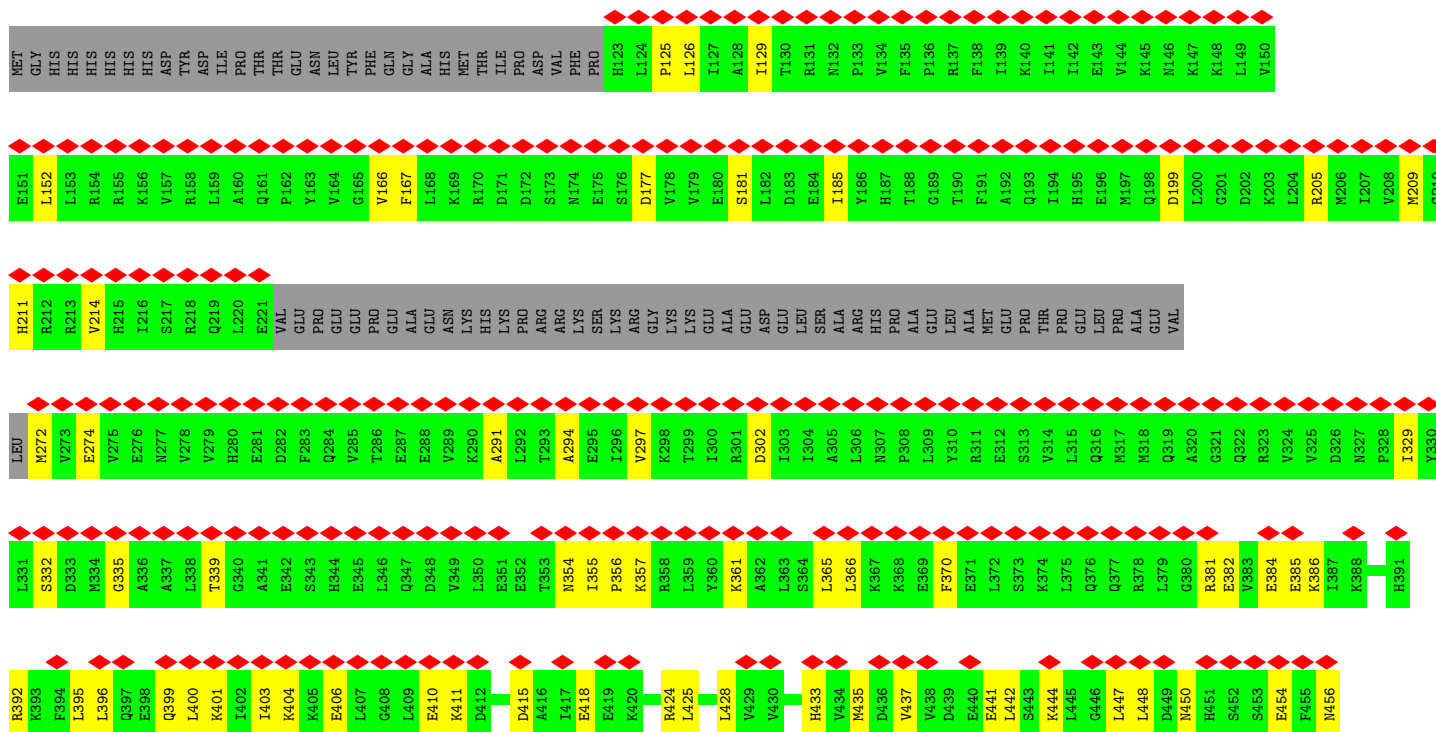
• Molecule 1: Lon protease homolog, mitochondrial

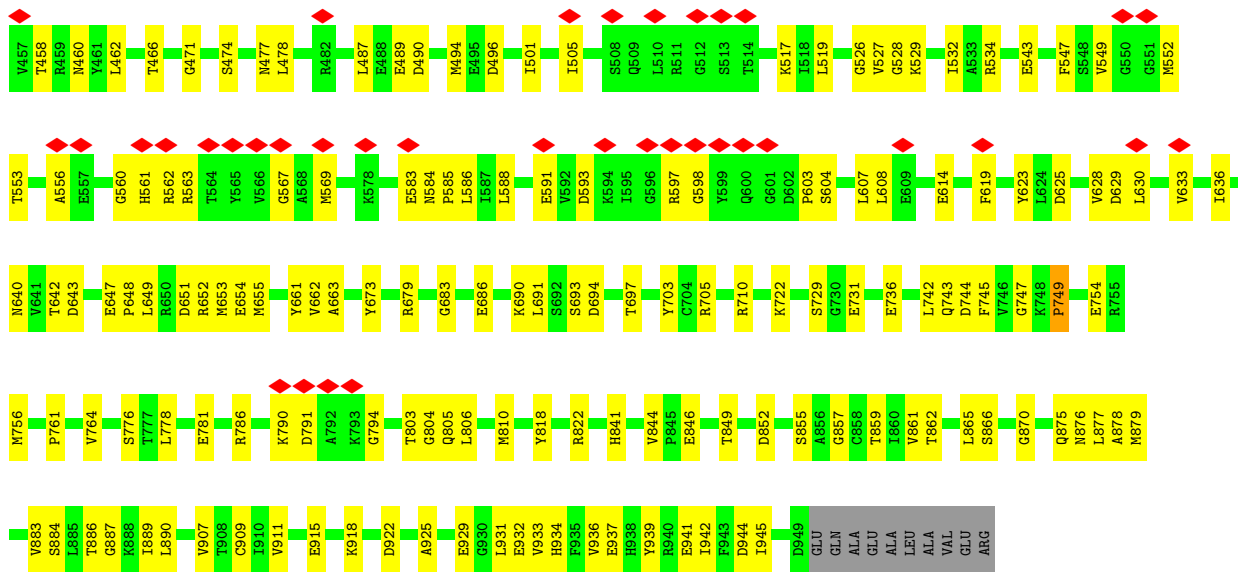


MET	GLY	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ASP	ILE	PRO	THR	THR	THR	GLU	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	ALA	MET	THR	PRO	PRO	VAL	PHE	PRO	H123	L124	P125	L126	I127	A128	I129	T130	R131	N132	P133	V134	F135	P136	R137	F138	I139	K140	I141	I142	E143	V144	K145	N146	K147	K148	L149	V150
E151	L152	L153	R154	R155	K156	V157	R158	L159	A160	Q161	P162	Y163	V164	G165	V166	F167	L168	K169	R170	D171	D172	S173	N174	E175	S176	D177	V178	V179	E180	S181	L182	D183	E184	I185	Y186	H187	T188	G189	T190	F191	F191	A192	Q193	I194	H195	E196	M197	Q198	D199	L200	G201	D202	K203	L204	R205	M206	I207	V208	M209	G210
H211	R212	R213	V214	H215	I216	S217	R218	Q219	L220	E221	VAL	PRO	GLU	GLU	PRO	PRO	GLU	GLU	PRO	PRO	ARG	ARG	LYS	LYS	ARG	ARG	ASP	ASP	ALA	ALA	ASP	GLU	GLU	LEU	LEU	ALA	ALA	ARG	HIS	PRO	ALA	ALA	THR	PRO	PRO	THR	PRO	PRO	THR	PRO	PRO	THR	PRO	GLU	VAL					

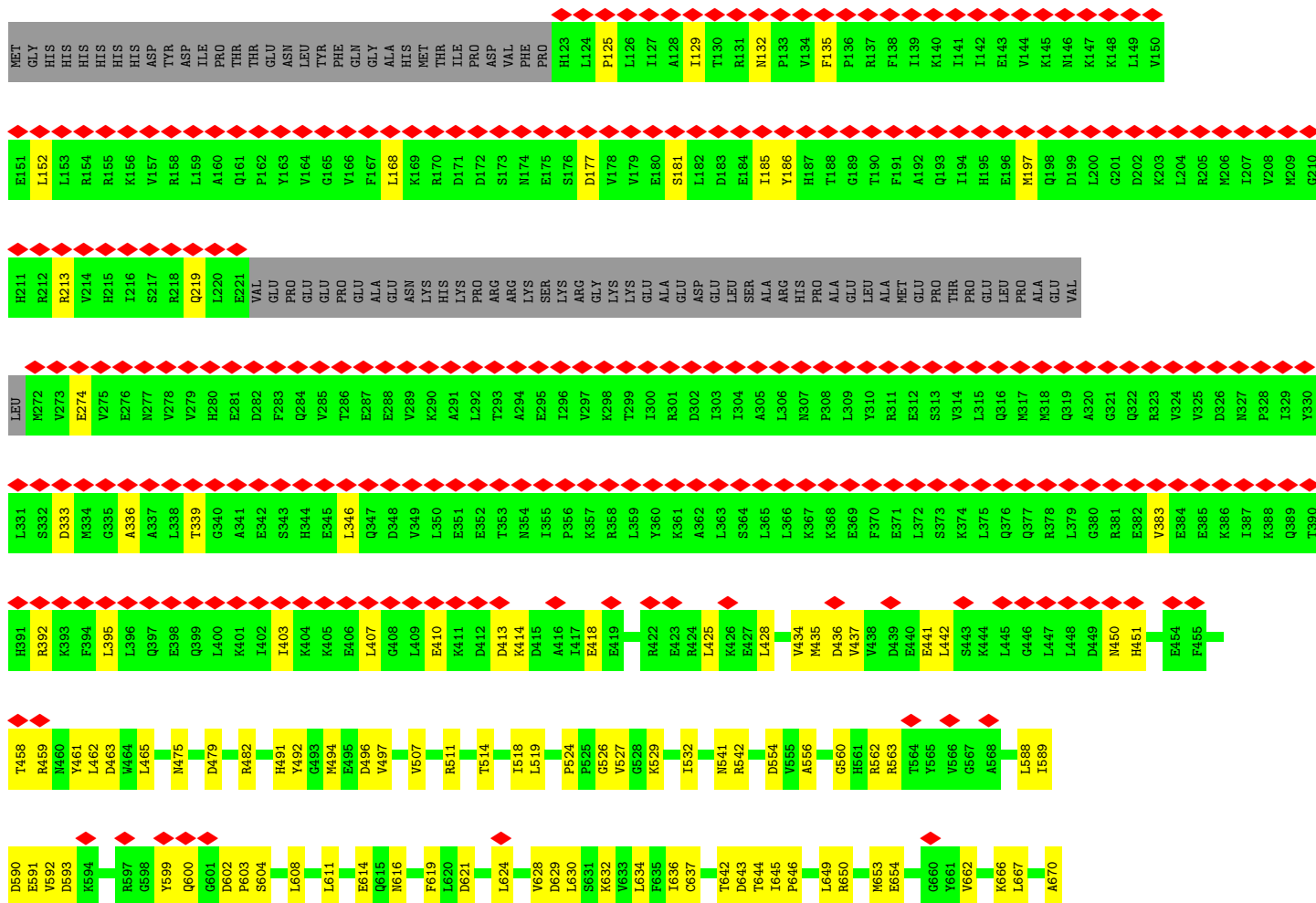


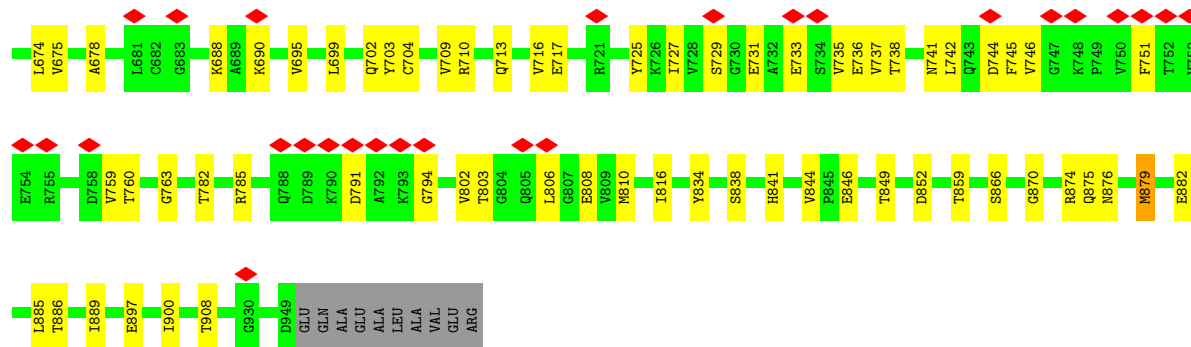
• Molecule 1: Lon protease homolog, mitochondrial





• Molecule 1: Lon protease homolog, mitochondrial





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34462	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.305	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.077	Depositor
Map size ( $\text{\AA}$ )	328.86, 328.86, 328.86	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.783, 0.783, 0.783	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	0.25	0/6251	0.49	0/8438
1	B	0.25	0/6251	0.48	0/8438
1	C	0.25	0/6251	0.49	0/8438
1	D	0.25	0/6251	0.49	0/8438
1	E	0.25	0/6251	0.49	0/8438
1	F	0.25	0/6251	0.48	0/8438
All	All	0.25	0/37506	0.49	0/50628

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	6149	6292	6290	112	0
1	B	6149	6292	6290	121	0
1	C	6149	6292	6290	130	0
1	D	6149	6292	6290	129	0
1	E	6149	6292	6290	160	0
1	F	6149	6290	6290	120	0
2	A	27	12	12	4	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	12	12	3	0
2	C	27	12	12	1	0
2	D	27	12	12	2	0
2	E	27	12	12	4	0
2	F	27	12	12	4	0
All	All	37056	37822	37812	737	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 10.

The worst 5 of 737 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:C:756:MET:O	1:D:888:LYS:NZ	1.94	1.00
1:F:803:THR:HG1	1:F:841:HIS:HE2	1.15	0.94
1:D:556:ALA:O	1:D:560:GLY:N	2.05	0.89
1:C:802:VAL:HG12	1:C:842:LEU:HD21	1.56	0.85
1:C:434:VAL:O	1:C:438:VAL:HG23	1.76	0.84

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	773/869 (89%)	748 (97%)	25 (3%)	0	100	100
1	B	773/869 (89%)	749 (97%)	24 (3%)	0	100	100
1	C	773/869 (89%)	743 (96%)	30 (4%)	0	100	100
1	D	773/869 (89%)	735 (95%)	38 (5%)	0	100	100
1	E	773/869 (89%)	734 (95%)	39 (5%)	0	100	100

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	773/869 (89%)	744 (96%)	29 (4%)	0	100	100
All	All	4638/5214 (89%)	4453 (96%)	185 (4%)	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	676/755 (90%)	673 (100%)	3 (0%)	91	94
1	B	676/755 (90%)	669 (99%)	7 (1%)	76	86
1	C	676/755 (90%)	673 (100%)	3 (0%)	91	94
1	D	676/755 (90%)	667 (99%)	9 (1%)	69	82
1	E	676/755 (90%)	670 (99%)	6 (1%)	78	87
1	F	676/755 (90%)	673 (100%)	3 (0%)	91	94
All	All	4056/4530 (90%)	4025 (99%)	31 (1%)	82	89

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	547	PHE
1	E	944	ASP
1	D	591	GLU
1	F	704	CYS
1	E	552	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	841	HIS
1	D	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	B	1001	-	24,29,29	0.93	1 (4%)	29,45,45	1.52	4 (13%)
2	ADP	C	1001	-	24,29,29	0.92	1 (4%)	29,45,45	1.51	4 (13%)
2	ADP	E	1001	-	24,29,29	0.96	1 (4%)	29,45,45	1.53	5 (17%)
2	ADP	F	1001	-	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
2	ADP	A	1001	-	24,29,29	0.92	1 (4%)	29,45,45	1.65	4 (13%)
2	ADP	D	1001	-	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	1001	-	-	1/12/32/32	0/3/3/3
2	ADP	C	1001	-	-	2/12/32/32	0/3/3/3

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	E	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	F	1001	-	-	3/12/32/32	0/3/3/3
2	ADP	A	1001	-	-	6/12/32/32	0/3/3/3
2	ADP	D	1001	-	-	1/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	ADP	C5-C4	2.40	1.47	1.40
2	F	1001	ADP	C5-C4	2.34	1.47	1.40
2	B	1001	ADP	C5-C4	2.31	1.47	1.40
2	A	1001	ADP	C5-C4	2.30	1.47	1.40
2	C	1001	ADP	C5-C4	2.28	1.47	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ADP	PA-O3A-PB	-4.84	116.22	132.83
2	F	1001	ADP	PA-O3A-PB	-4.07	118.85	132.83
2	D	1001	ADP	PA-O3A-PB	-3.88	119.53	132.83
2	C	1001	ADP	PA-O3A-PB	-3.66	120.28	132.83
2	E	1001	ADP	PA-O3A-PB	-3.65	120.30	132.83

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	C5'-O5'-PA-O1A
2	A	1001	ADP	C5'-O5'-PA-O2A
2	E	1001	ADP	C5'-O5'-PA-O2A
2	E	1001	ADP	C5'-O5'-PA-O3A
2	A	1001	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 18 short contacts:

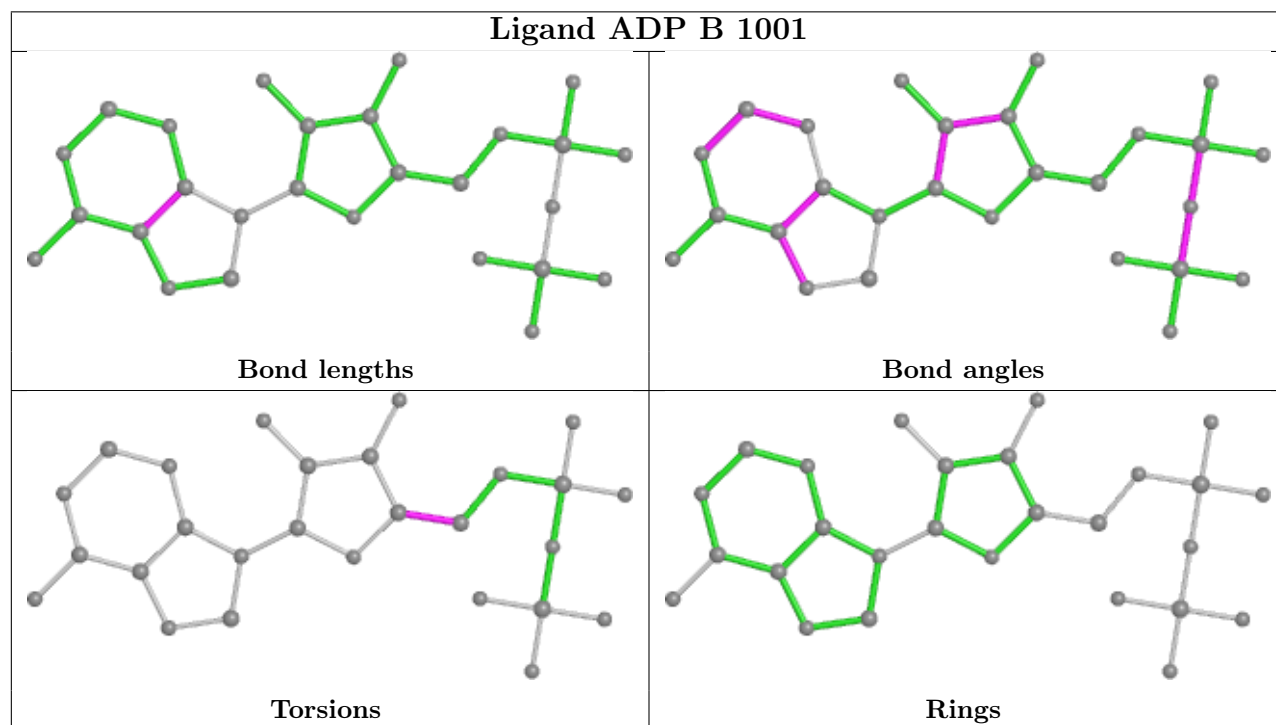
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	ADP	3	0
2	C	1001	ADP	1	0
2	E	1001	ADP	4	0

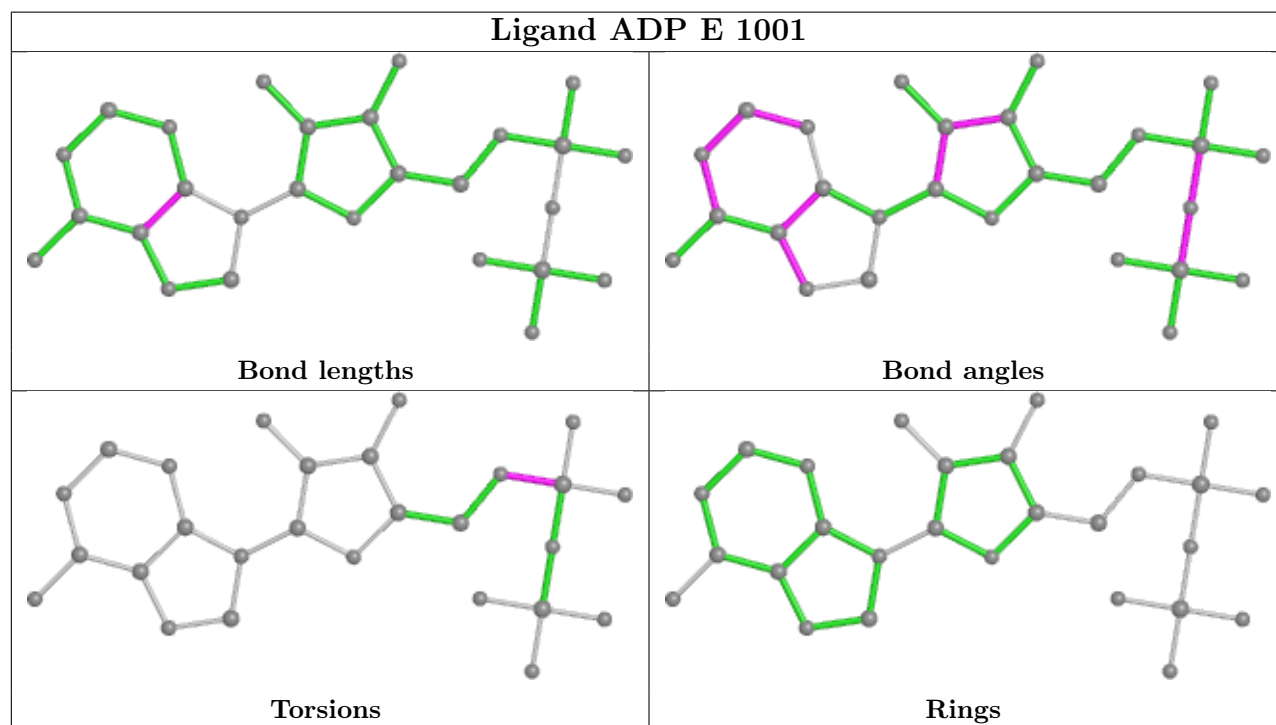
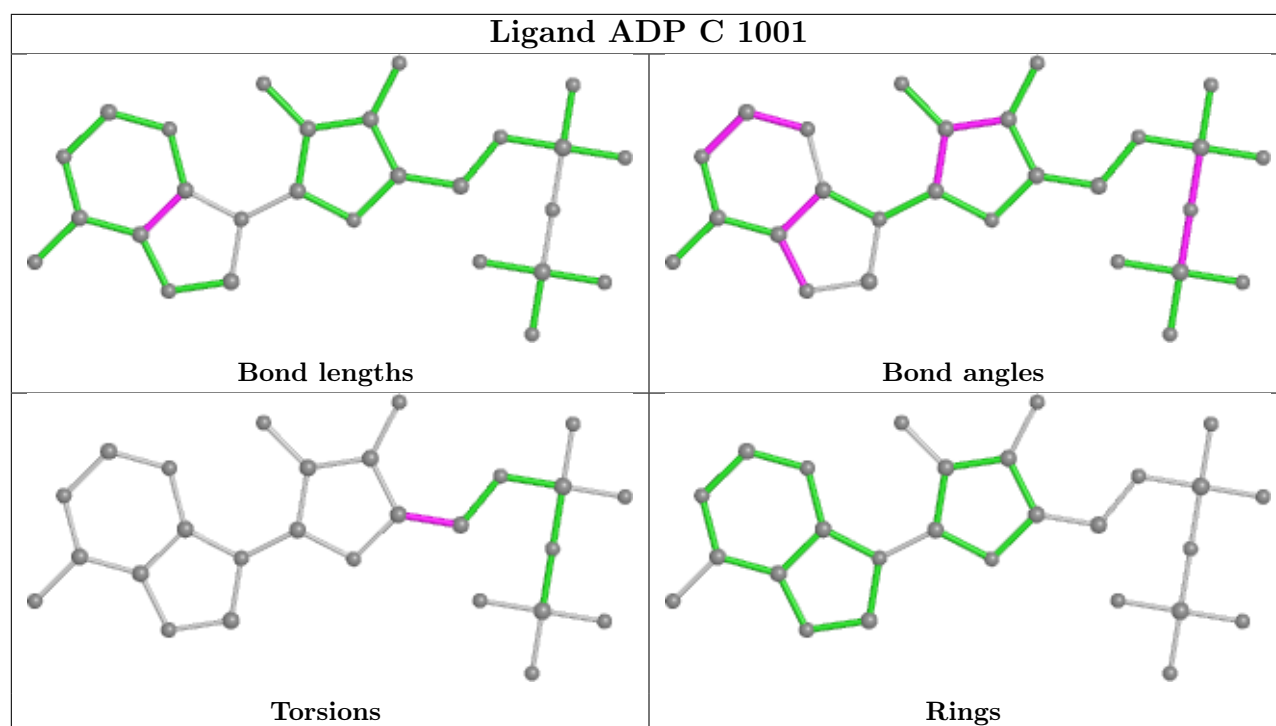
Continued on next page...

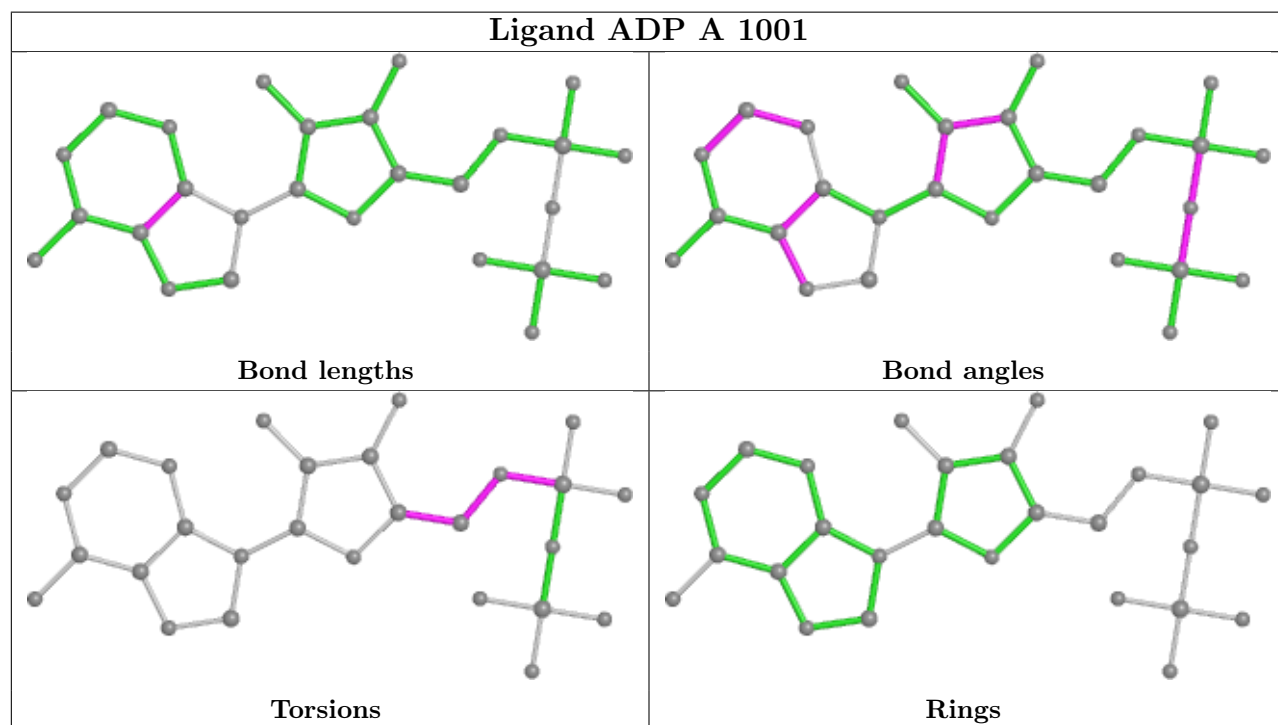
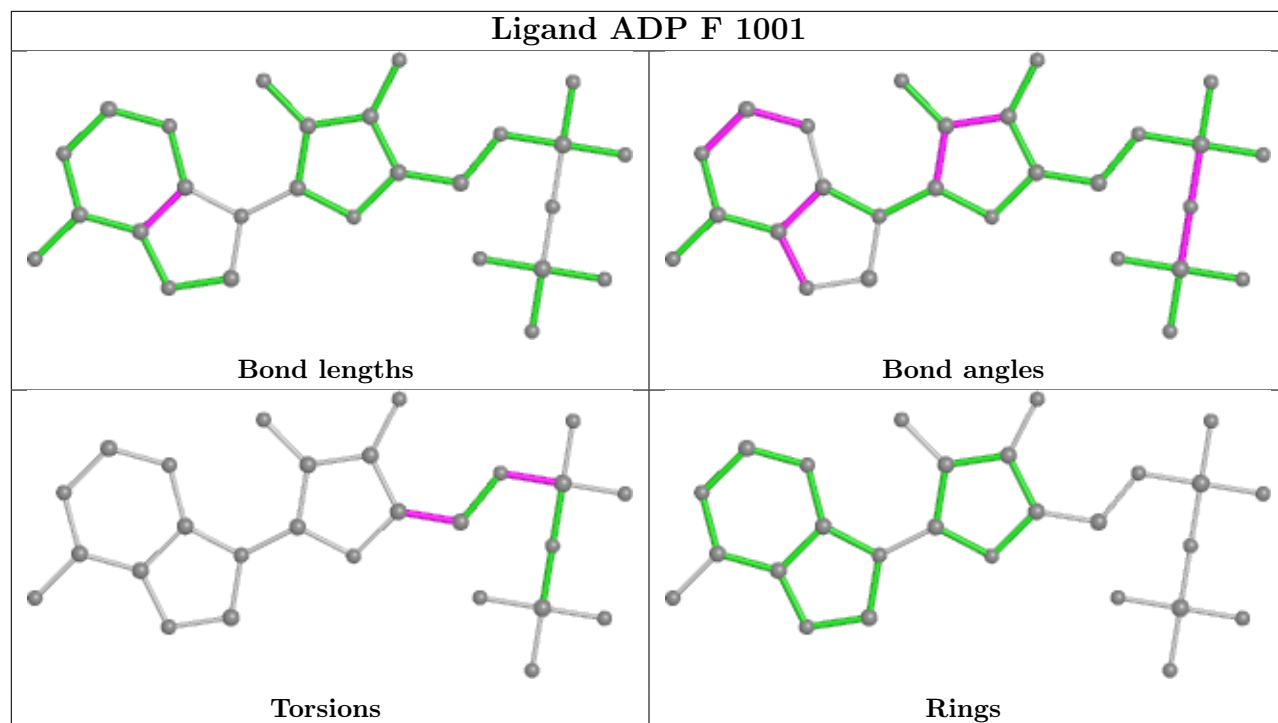
*Continued from previous page...*

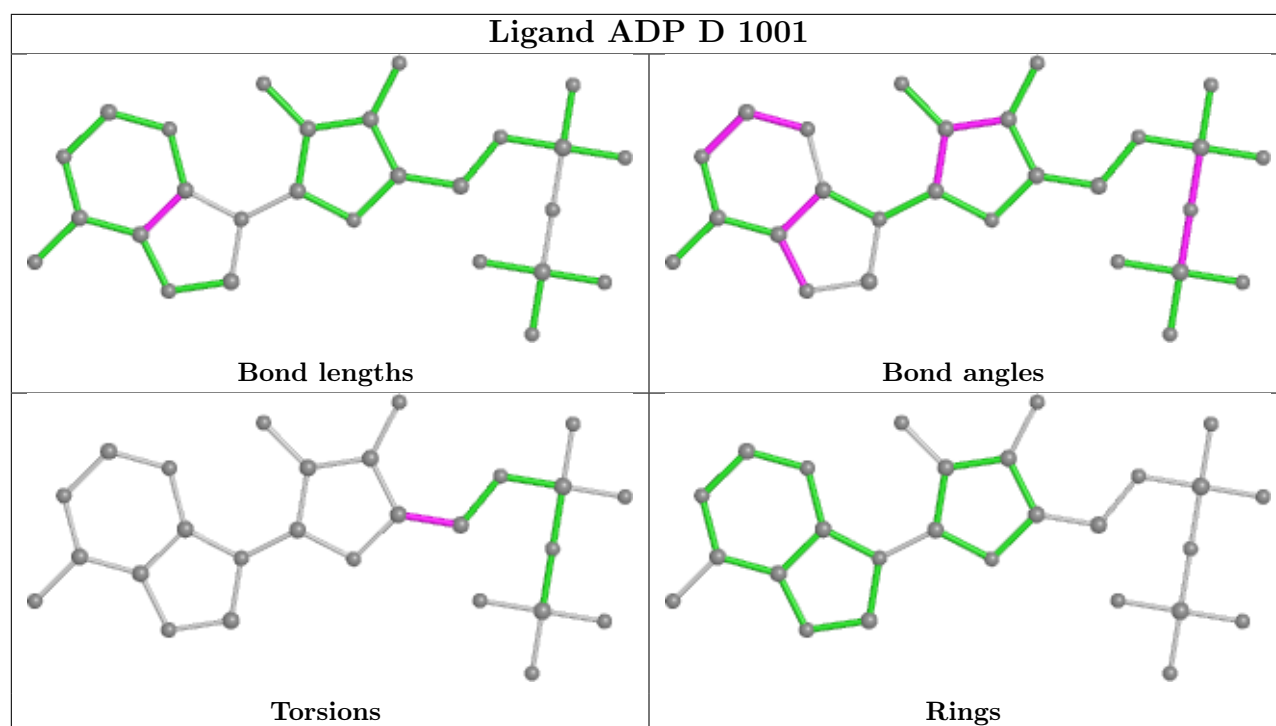
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1001	ADP	4	0
2	A	1001	ADP	4	0
2	D	1001	ADP	2	0

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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

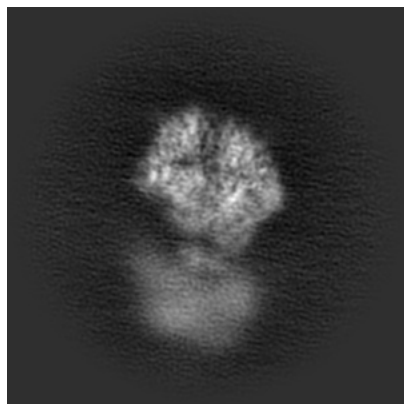
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16923. These allow visual inspection of the internal detail of the map and identification of artifacts.

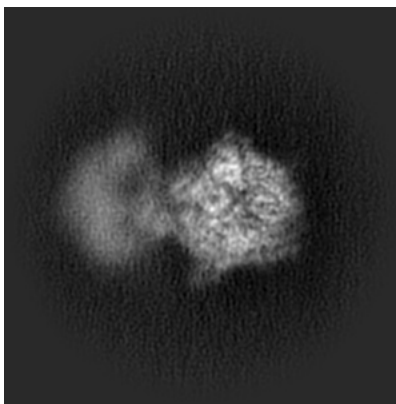
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

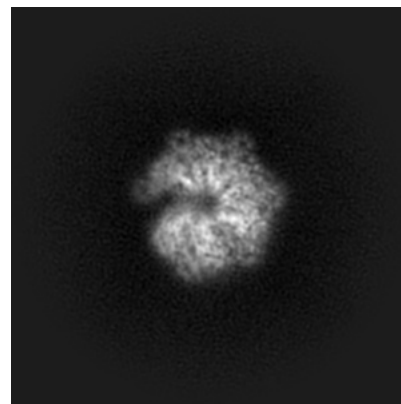
#### 6.1.1 Primary map



X

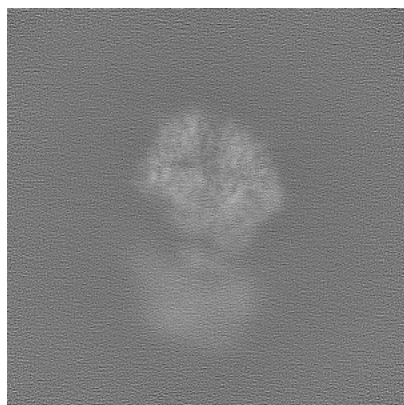


Y

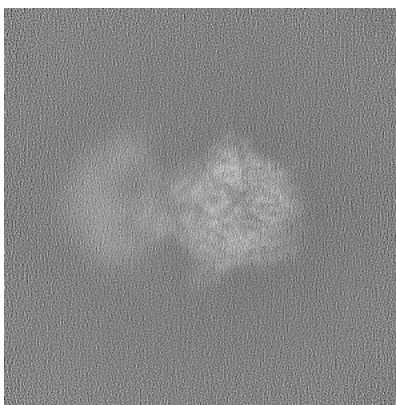


Z

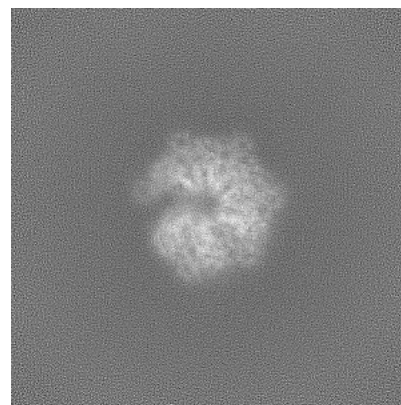
#### 6.1.2 Raw map



X



Y



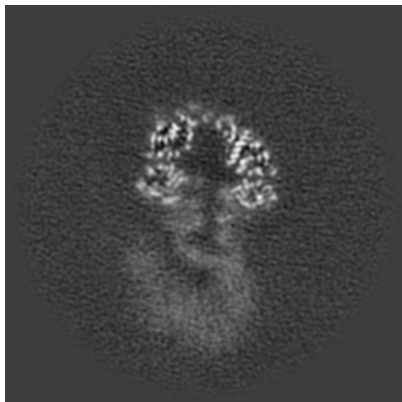
Z

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

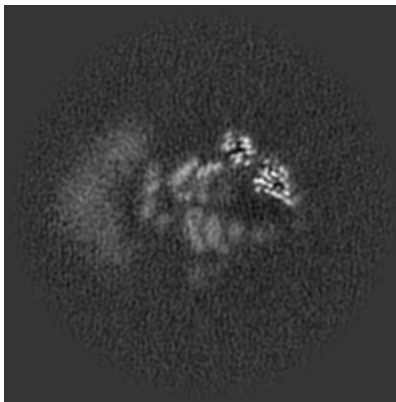


## 6.2 Central slices [i](#)

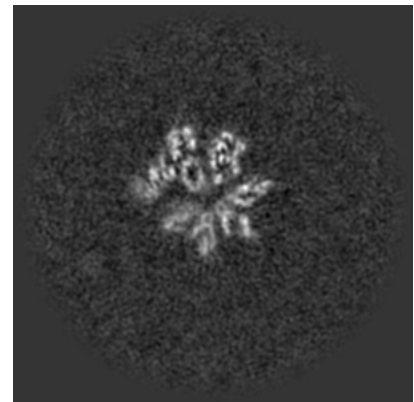
### 6.2.1 Primary map



X Index: 210

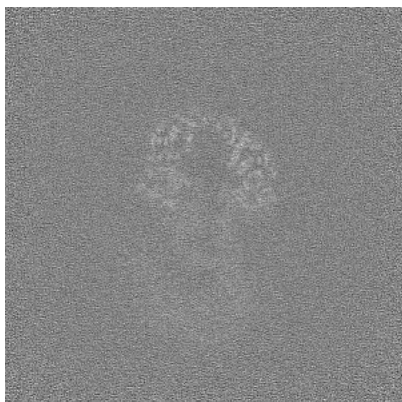


Y Index: 210



Z Index: 210

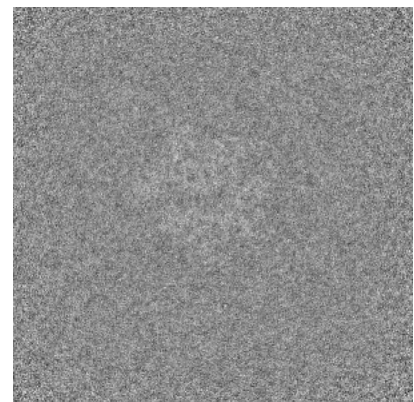
### 6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

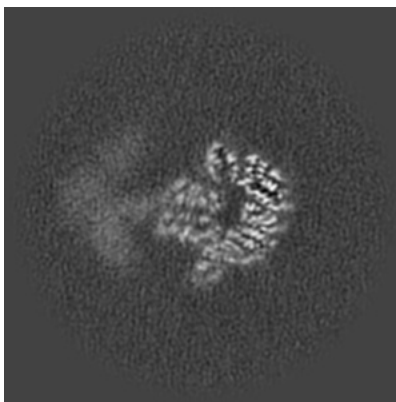
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

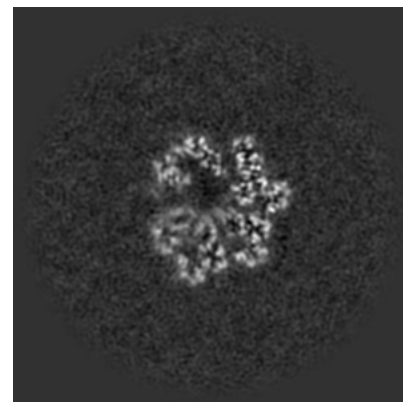
### 6.3.1 Primary map



X Index: 208

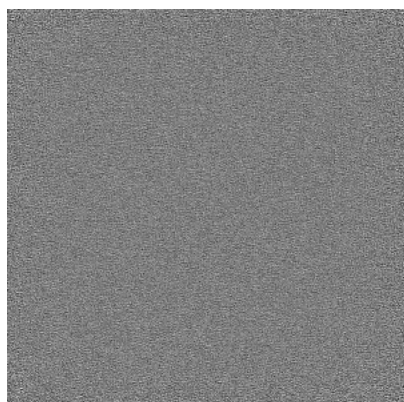


Y Index: 238

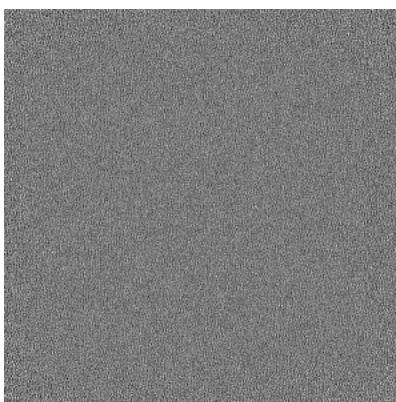


Z Index: 236

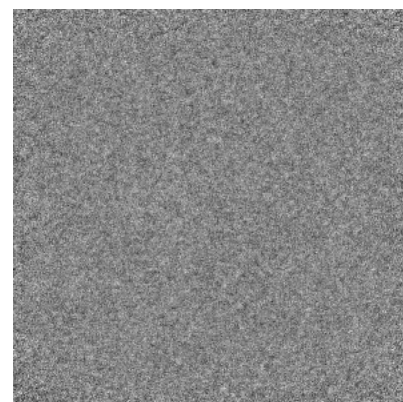
### 6.3.2 Raw map



X Index: 0



Y Index: 0

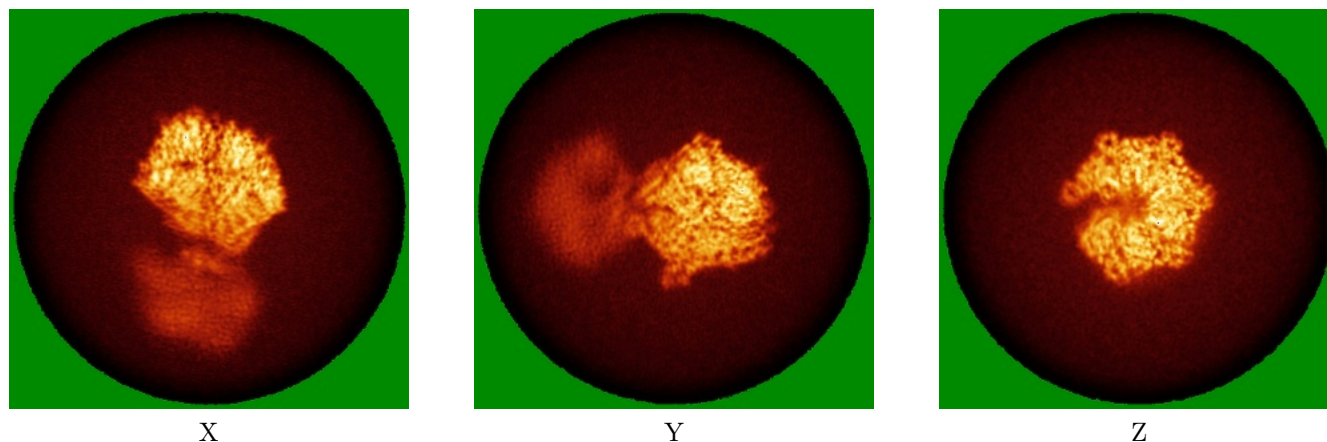


Z Index: 0

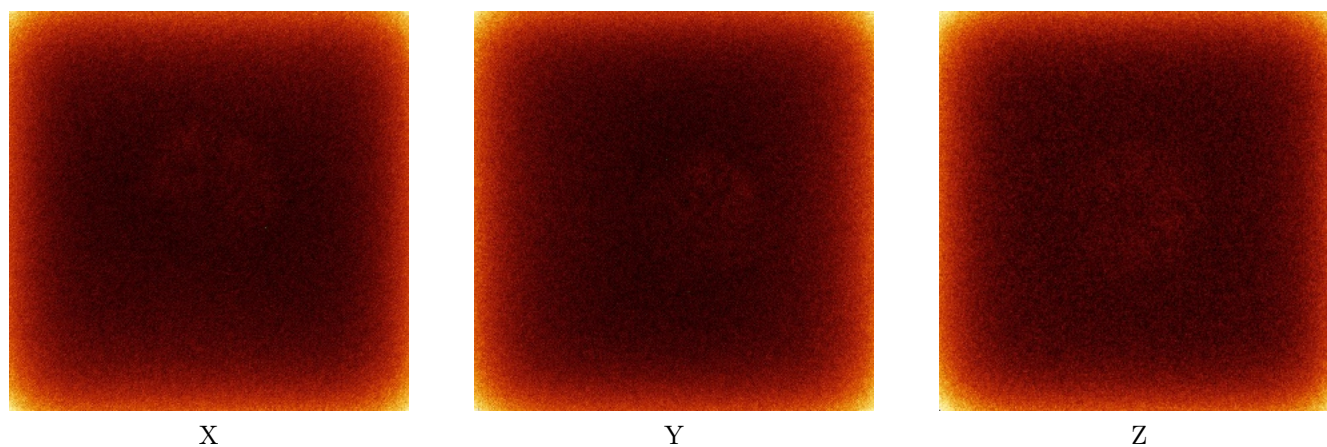
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



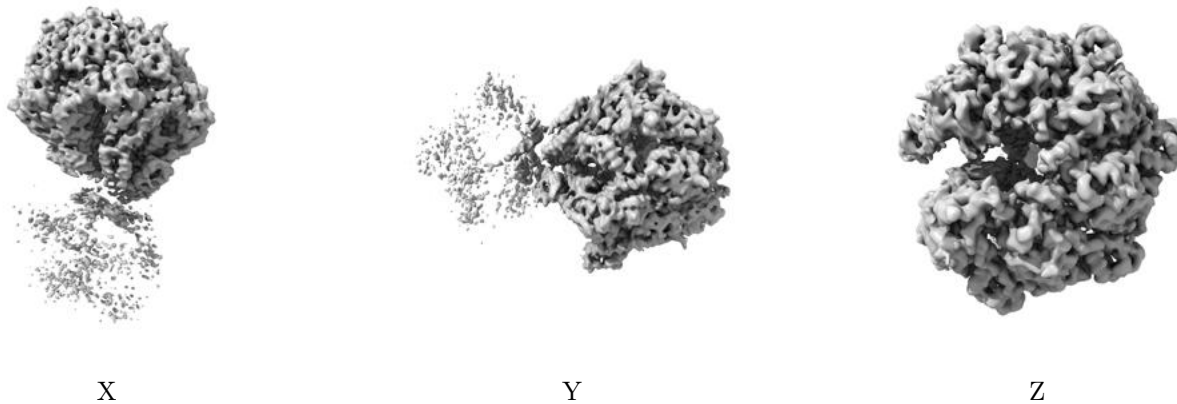
### 6.4.2 Raw map



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.

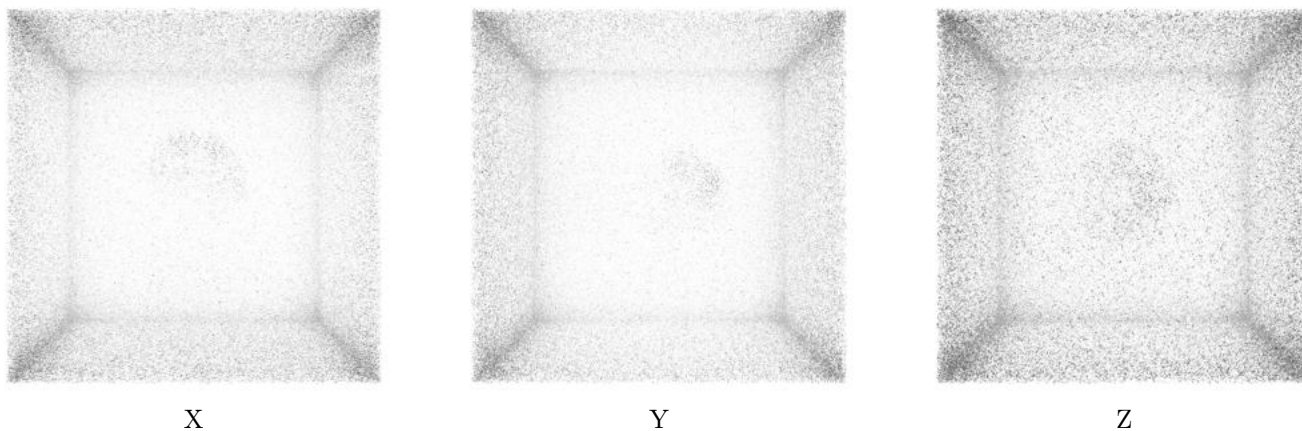
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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.

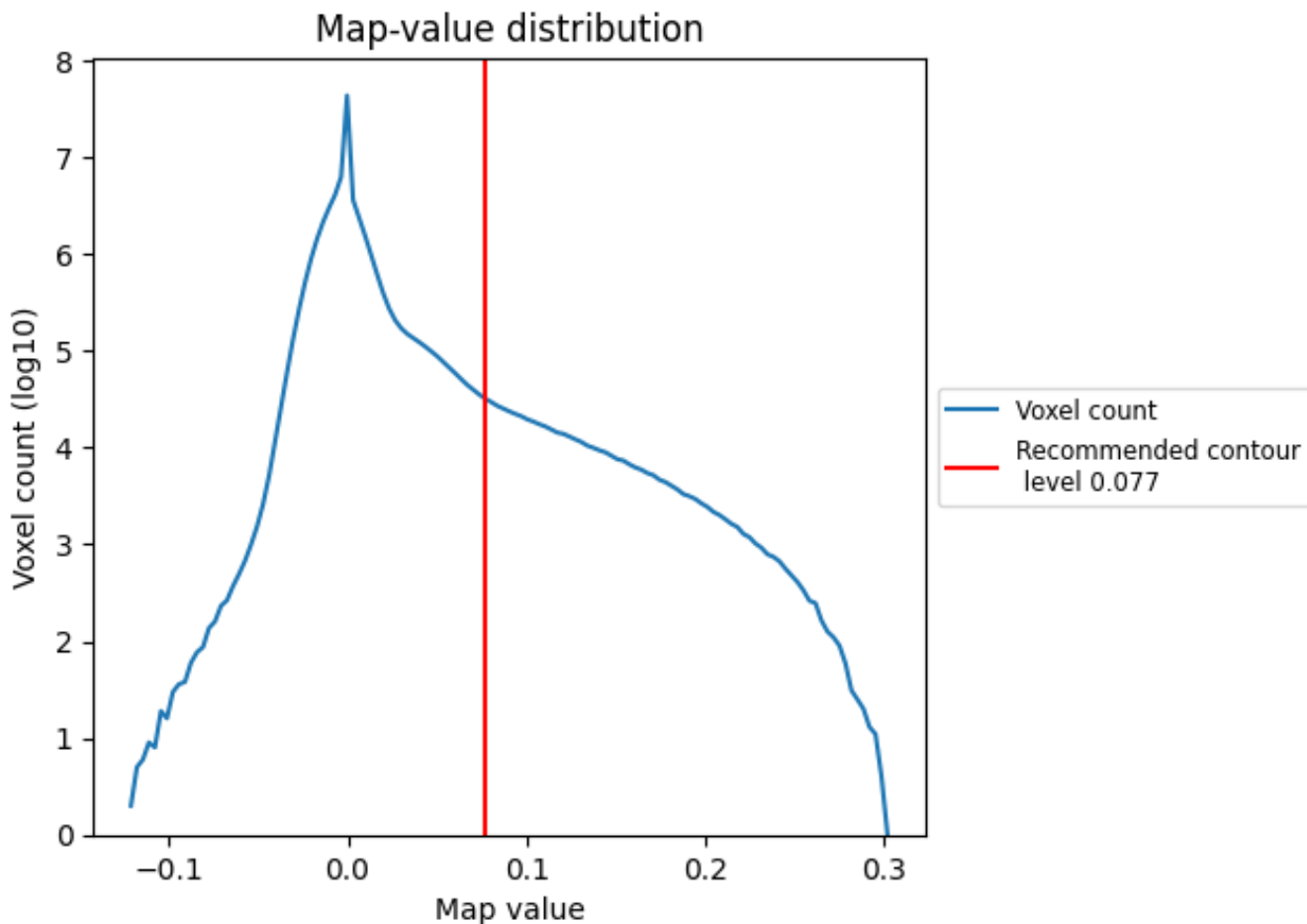
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

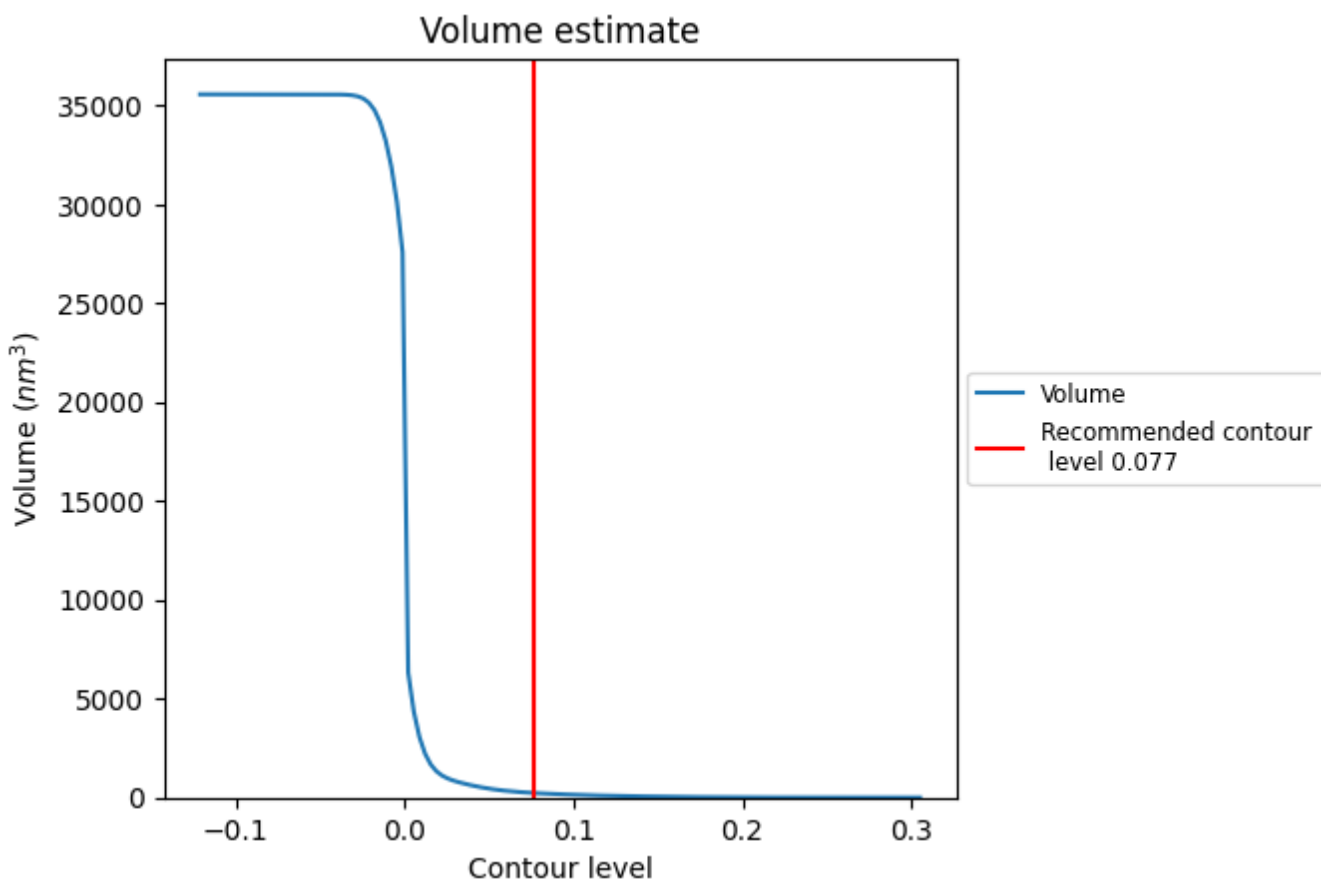
This section contains the results of statistical analysis of the map.

### 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.

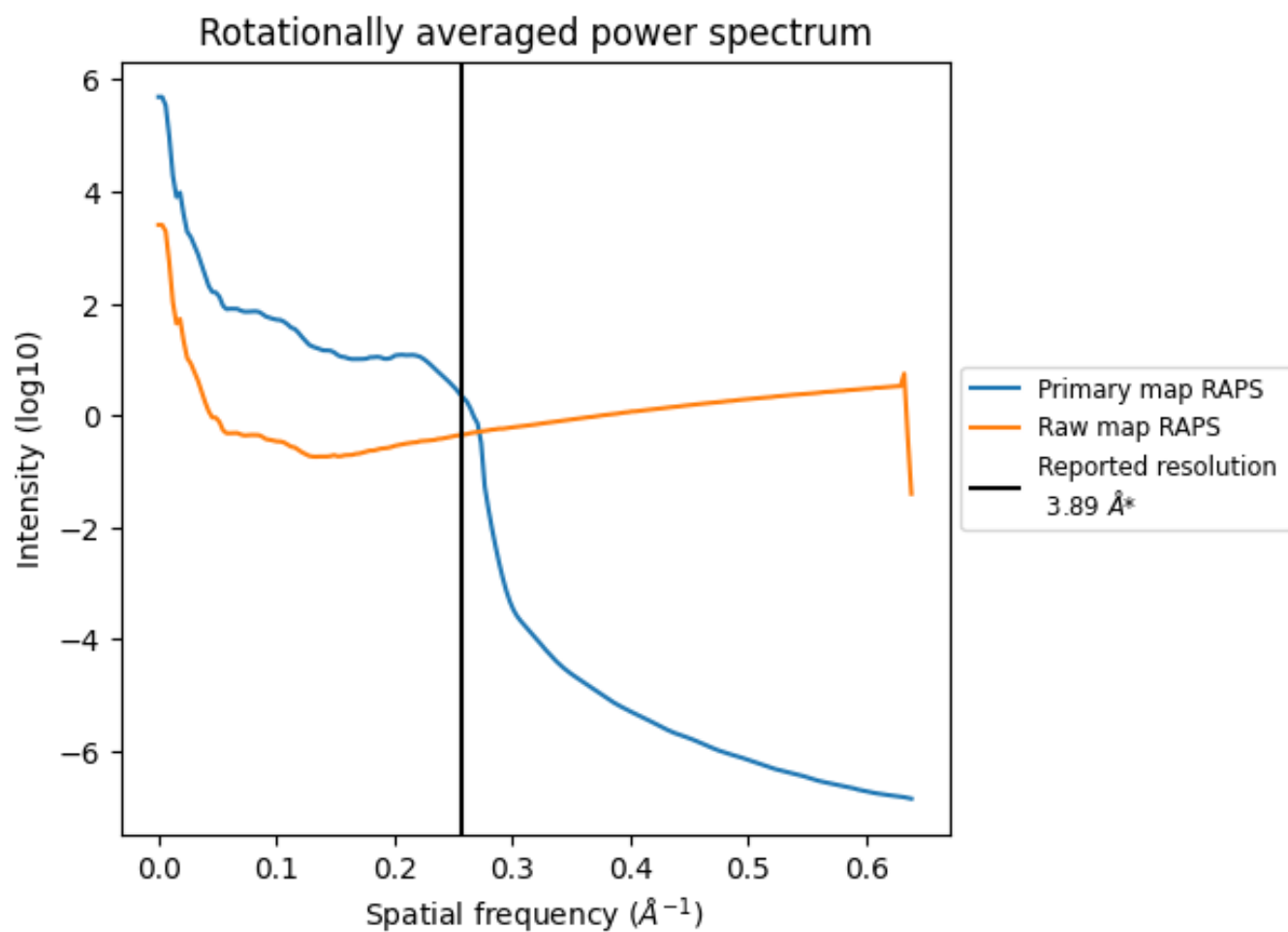
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 228 nm<sup>3</sup>; this corresponds to an approximate mass of 206 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

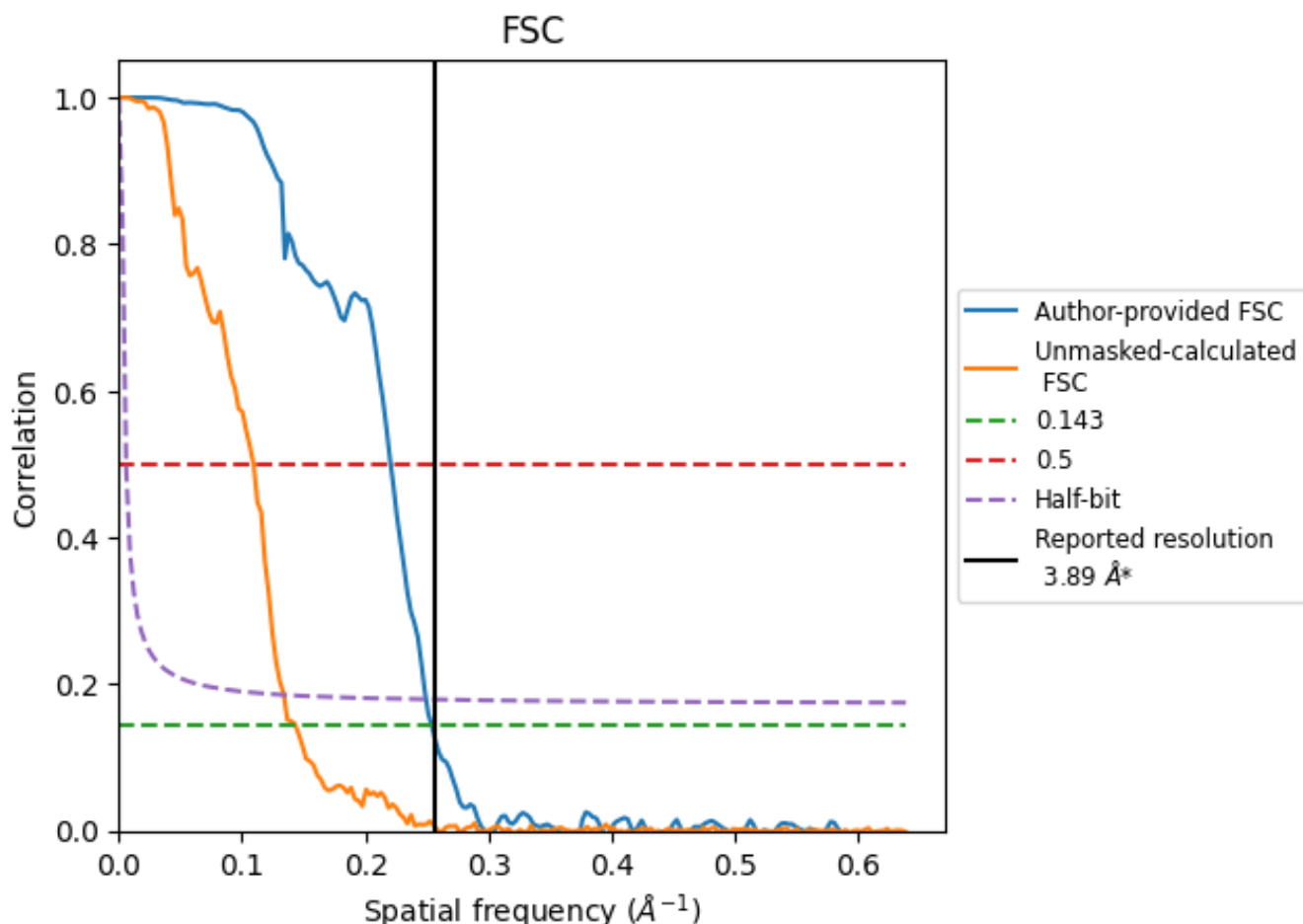


\*Reported resolution corresponds to spatial frequency of 0.257 Å<sup>-1</sup>

## 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 0.257 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

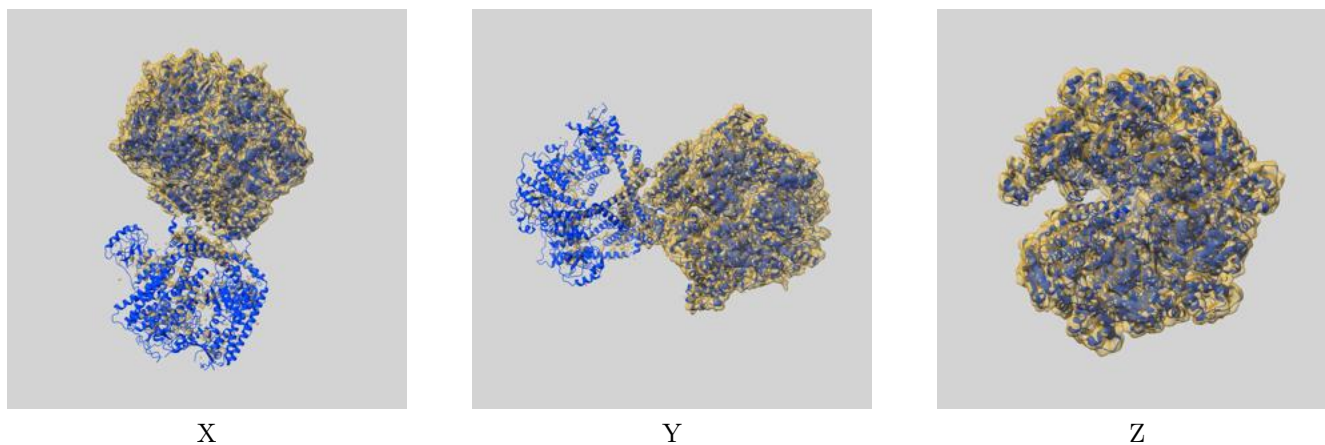
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	3.94	4.54	4.01
Unmasked-calculated*	6.97	9.15	7.47

\*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 6.97 differs from the reported value 3.89 by more than 10 %

## 9 Map-model fit [i](#)

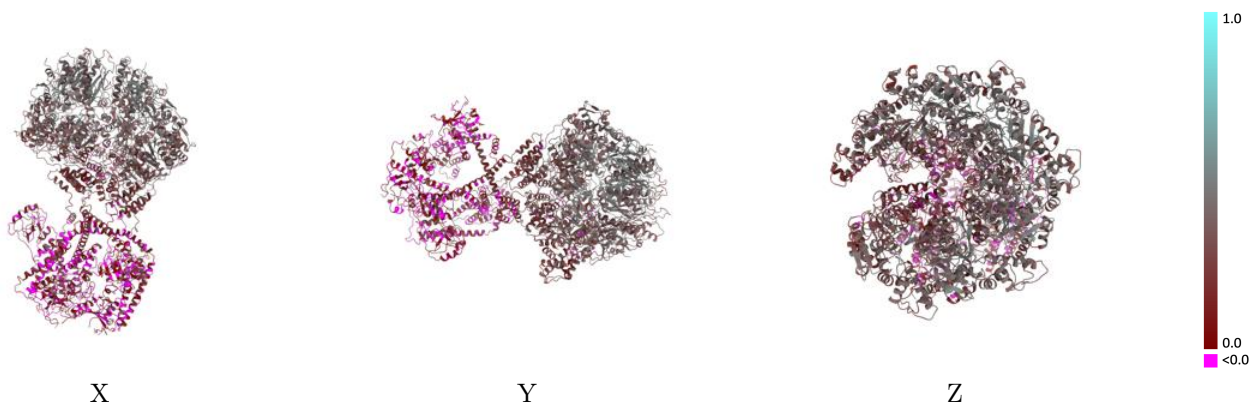
This section contains information regarding the fit between EMDB map EMD-16923 and PDB model 8OKA. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlay [i](#)



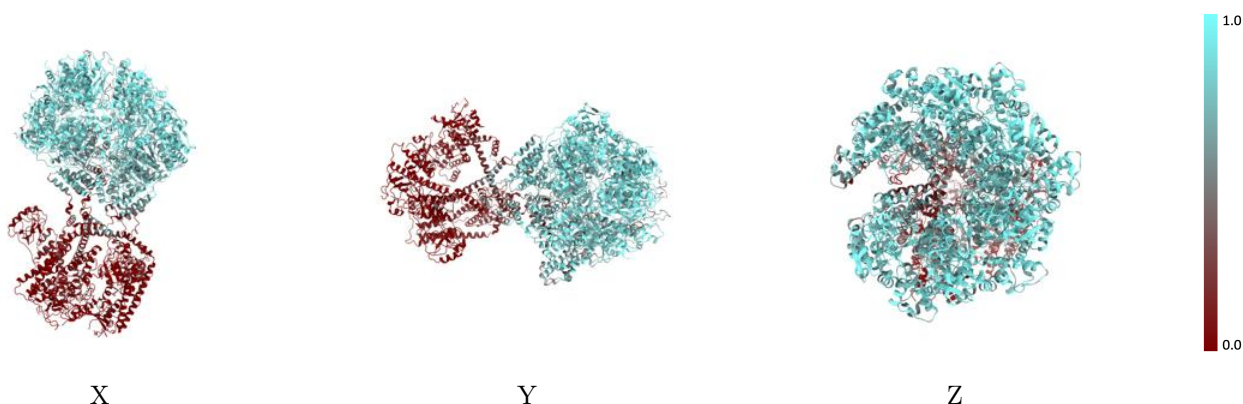
The images above show the 3D surface view of the map at the recommended contour level 0.077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



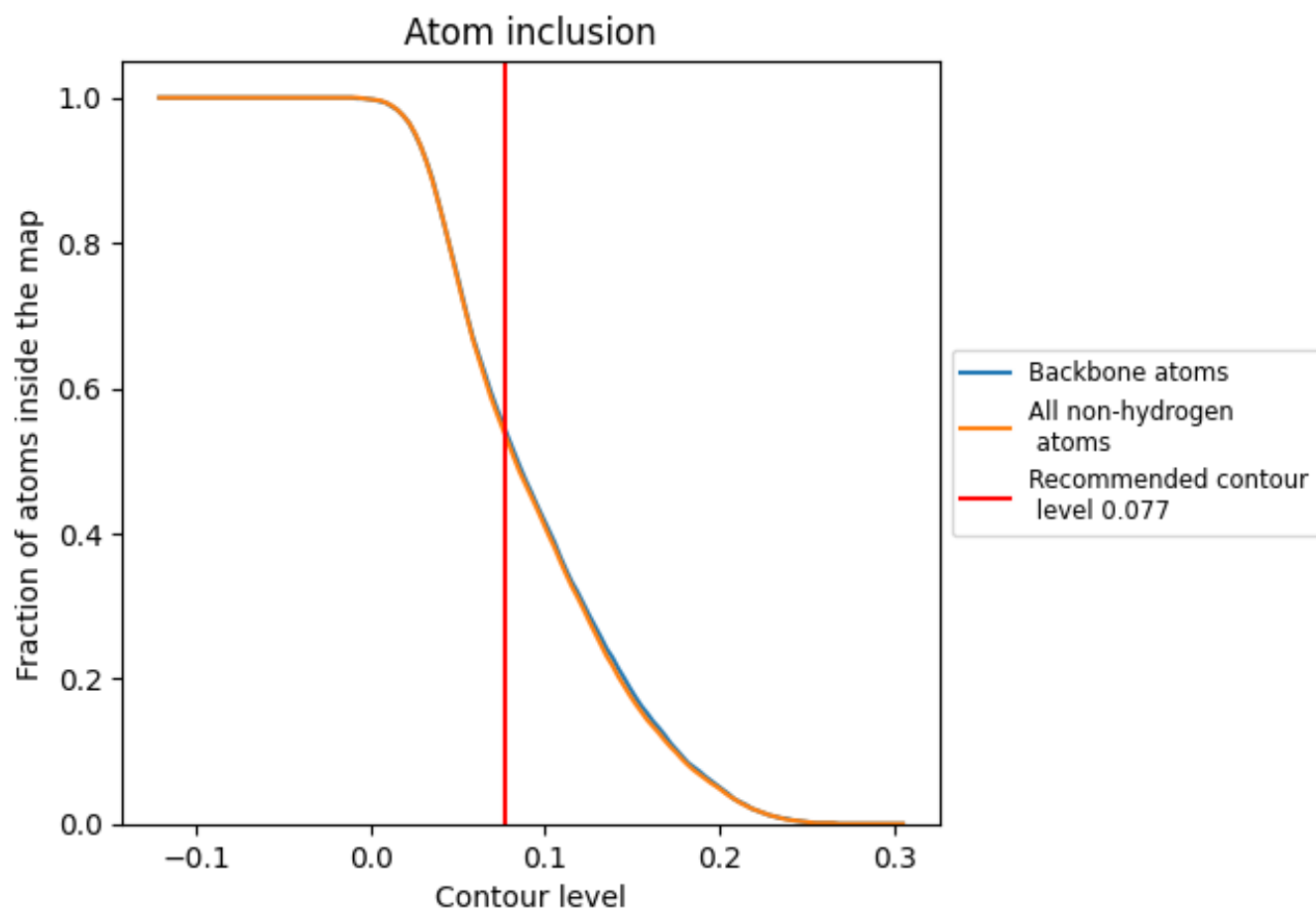
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.077).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (0.077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5360	 0.2810
A	 0.5670	 0.2960
B	 0.5730	 0.3010
C	 0.5540	 0.2920
D	 0.5770	 0.3050
E	 0.5040	 0.2470
F	 0.4860	 0.2440

