



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2024 – 05:15 PM JST

PDB ID : 7Y4W
EMDB ID : EMD-33608
Title : The cryo-EM structure of human ERAD retro-translocation complex
Authors : Cao, Y.; Rao, B.; Wang, Q.; Yao, D.; Xia, Y.; Li, W.; Li, S.; Shen, Y.
Deposited on : 2022-06-16
Resolution : 3.67 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

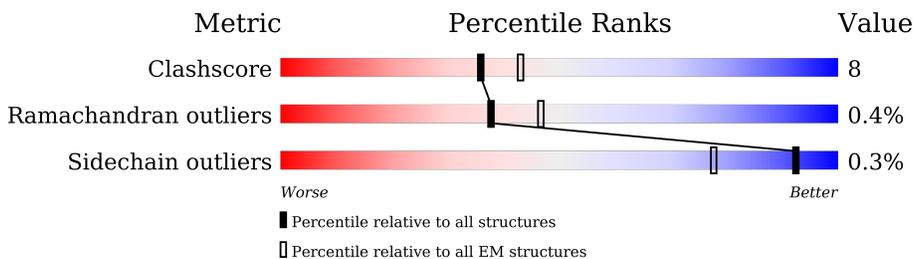
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	W	226	
1	X	226	
1	Y	226	
1	Z	226	
2	A	787	
2	B	787	
2	C	787	
2	D	787	

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Mol	Chain	Length	Quality of chain
2	E	787	
2	F	787	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 42776 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 Derlin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	W	225	1870	1267	297	295	11	0	0
1	X	225	1870	1267	297	295	11	0	0
1	Y	225	1870	1267	297	295	11	0	0
1	Z	225	1870	1267	297	295	11	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	?	-	ARG	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	VAL	deletion	UNP Q9BUN8
W	?	-	SER	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	PHE	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	VAL	deletion	UNP Q9BUN8
W	?	-	PRO	deletion	UNP Q9BUN8
W	?	-	PRO	deletion	UNP Q9BUN8
W	?	-	ALA	deletion	UNP Q9BUN8
W	?	-	SER	deletion	UNP Q9BUN8
W	?	-	MET	deletion	UNP Q9BUN8
W	?	-	ARG	deletion	UNP Q9BUN8
W	?	-	ARG	deletion	UNP Q9BUN8
W	?	-	ALA	deletion	UNP Q9BUN8
W	?	-	ALA	deletion	UNP Q9BUN8
W	?	-	ASP	deletion	UNP Q9BUN8
W	?	-	GLN	deletion	UNP Q9BUN8
W	?	-	ASN	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8

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Chain	Residue	Modelled	Actual	Comment	Reference
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	ARG	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	VAL	deletion	UNP Q9BUN8
X	?	-	SER	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	PHE	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	VAL	deletion	UNP Q9BUN8
X	?	-	PRO	deletion	UNP Q9BUN8
X	?	-	PRO	deletion	UNP Q9BUN8
X	?	-	ALA	deletion	UNP Q9BUN8
X	?	-	SER	deletion	UNP Q9BUN8
X	?	-	MET	deletion	UNP Q9BUN8
X	?	-	ARG	deletion	UNP Q9BUN8
X	?	-	ARG	deletion	UNP Q9BUN8
X	?	-	ALA	deletion	UNP Q9BUN8
X	?	-	ALA	deletion	UNP Q9BUN8
X	?	-	ASP	deletion	UNP Q9BUN8
X	?	-	GLN	deletion	UNP Q9BUN8
X	?	-	ASN	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	ARG	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	VAL	deletion	UNP Q9BUN8
Y	?	-	SER	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	PHE	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	VAL	deletion	UNP Q9BUN8
Y	?	-	PRO	deletion	UNP Q9BUN8
Y	?	-	PRO	deletion	UNP Q9BUN8
Y	?	-	ALA	deletion	UNP Q9BUN8
Y	?	-	SER	deletion	UNP Q9BUN8
Y	?	-	MET	deletion	UNP Q9BUN8

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	?	-	ARG	deletion	UNP Q9BUN8
Y	?	-	ARG	deletion	UNP Q9BUN8
Y	?	-	ALA	deletion	UNP Q9BUN8
Y	?	-	ALA	deletion	UNP Q9BUN8
Y	?	-	ASP	deletion	UNP Q9BUN8
Y	?	-	GLN	deletion	UNP Q9BUN8
Y	?	-	ASN	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	ARG	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	VAL	deletion	UNP Q9BUN8
Z	?	-	SER	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	PHE	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	VAL	deletion	UNP Q9BUN8
Z	?	-	PRO	deletion	UNP Q9BUN8
Z	?	-	PRO	deletion	UNP Q9BUN8
Z	?	-	ALA	deletion	UNP Q9BUN8
Z	?	-	SER	deletion	UNP Q9BUN8
Z	?	-	MET	deletion	UNP Q9BUN8
Z	?	-	ARG	deletion	UNP Q9BUN8
Z	?	-	ARG	deletion	UNP Q9BUN8
Z	?	-	ALA	deletion	UNP Q9BUN8
Z	?	-	ALA	deletion	UNP Q9BUN8
Z	?	-	ASP	deletion	UNP Q9BUN8
Z	?	-	GLN	deletion	UNP Q9BUN8
Z	?	-	ASN	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8

- Molecule 2 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	745	5846	3667	1035	1113	31	0	0

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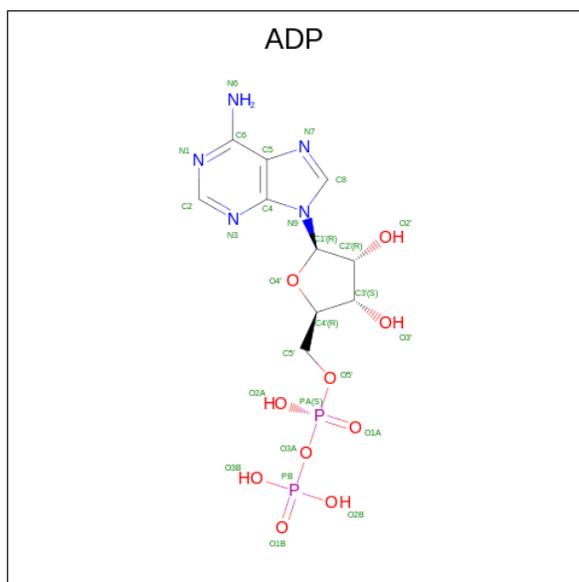
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	745	Total	C	N	O	S	0	0
			5846	3667	1035	1113	31		
2	C	744	Total	C	N	O	S	0	0
			5835	3661	1031	1112	31		
2	D	743	Total	C	N	O	S	0	0
			5829	3658	1030	1110	31		
2	E	753	Total	C	N	O	S	0	0
			5911	3712	1046	1122	31		
2	F	755	Total	C	N	O	S	0	0
			5921	3717	1048	1125	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP P55072
B	20	MET	-	initiating methionine	UNP P55072
C	20	MET	-	initiating methionine	UNP P55072
D	20	MET	-	initiating methionine	UNP P55072
E	20	MET	-	initiating methionine	UNP P55072
F	20	MET	-	initiating methionine	UNP P55072

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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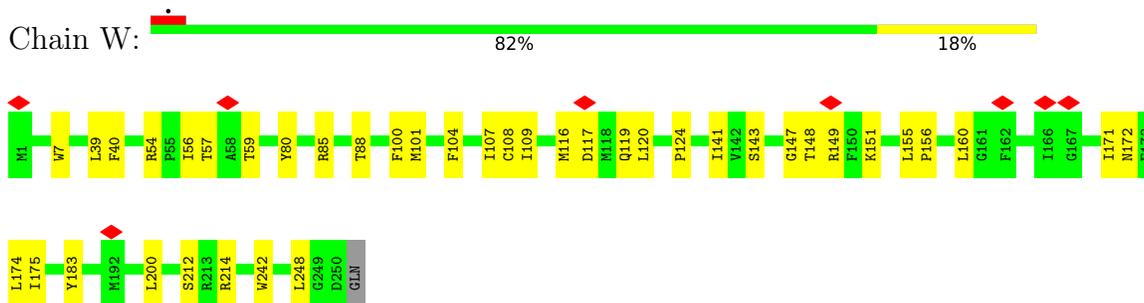
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	B	1	Total 27	10	5	10	2	0
3	E	1	Total 27	10	5	10	2	0
3	F	1	Total 27	10	5	10	2	0

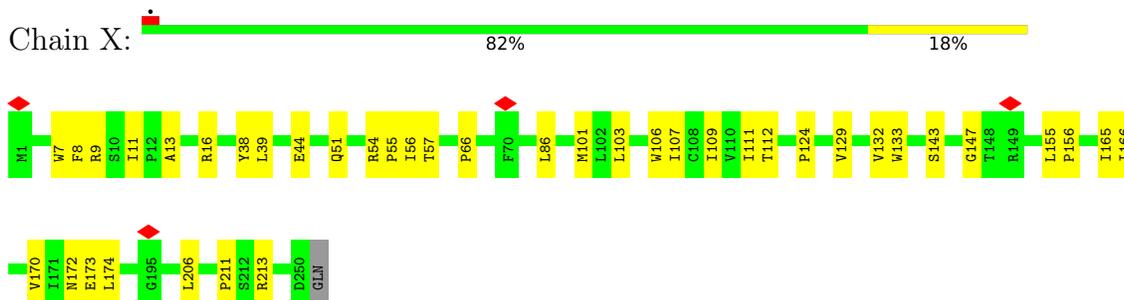
3 Residue-property plots

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.

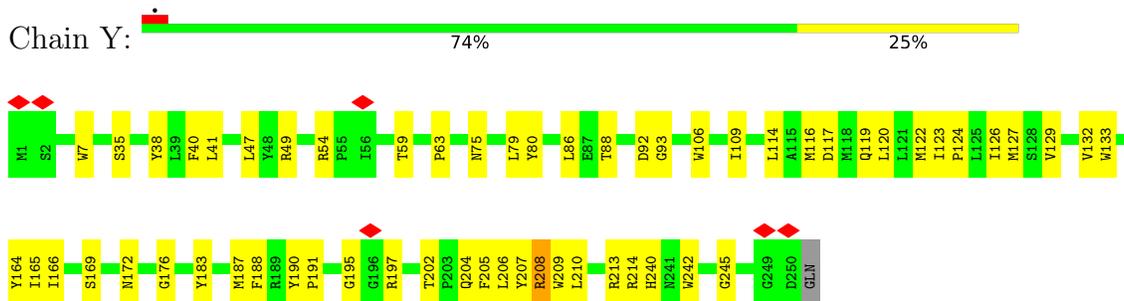
- Molecule 1: Derlin-1



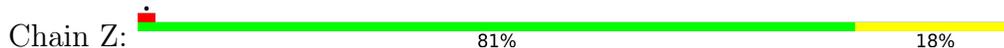
- Molecule 1: Derlin-1

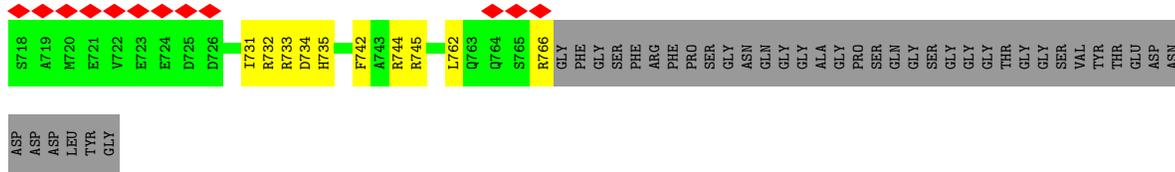


- Molecule 1: Derlin-1

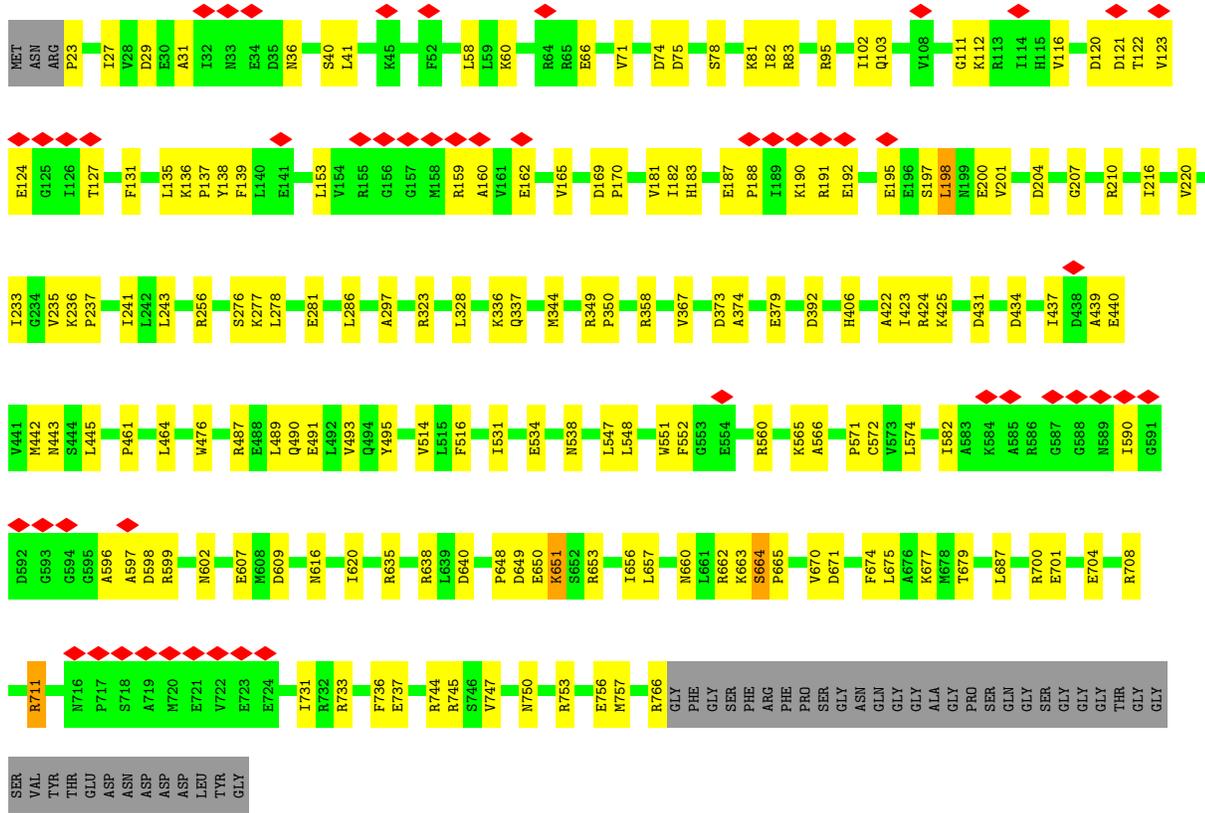
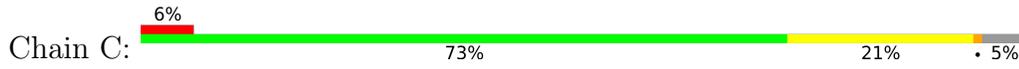


- Molecule 1: Derlin-1

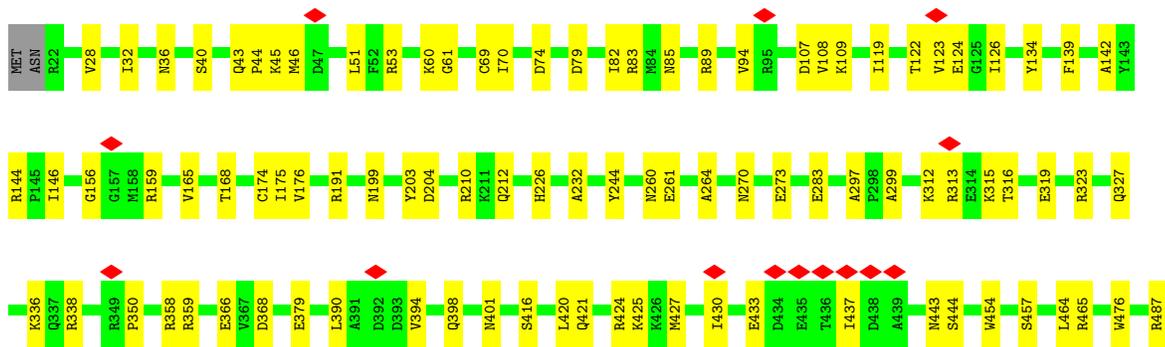


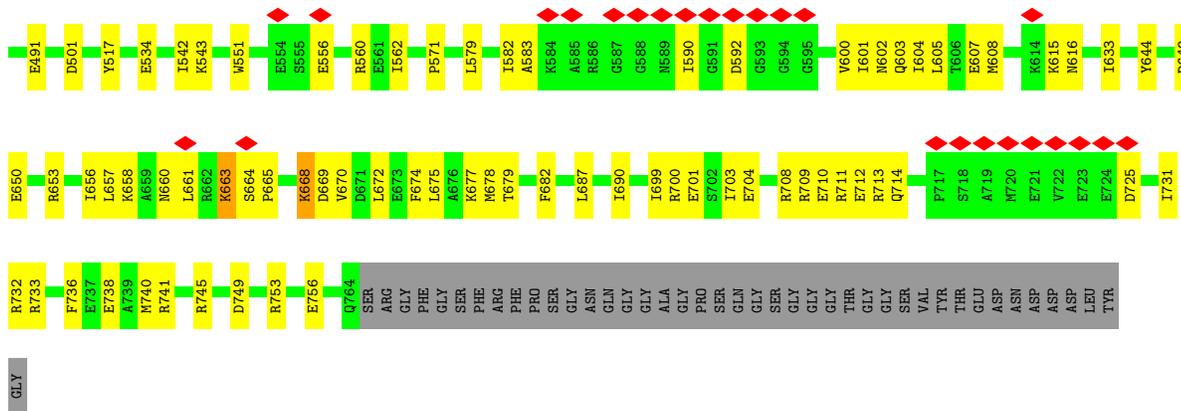


• Molecule 2: Transitional endoplasmic reticulum ATPase

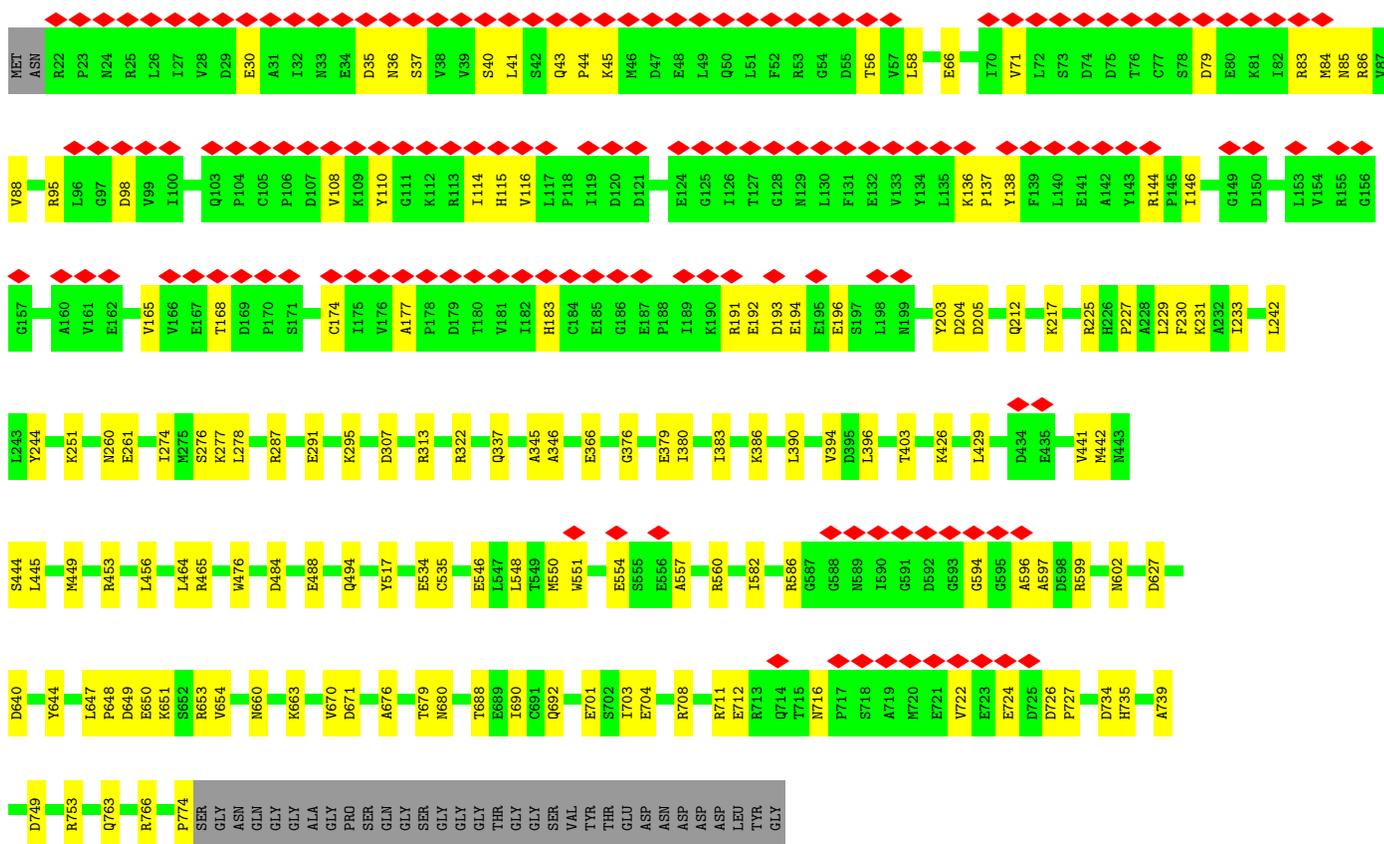
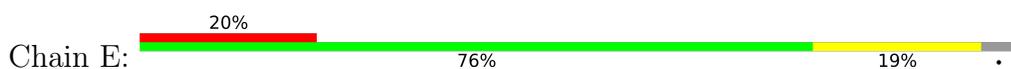


• Molecule 2: Transitional endoplasmic reticulum ATPase

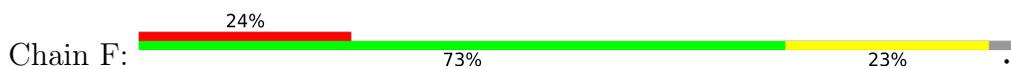




• Molecule 2: Transitional endoplasmic reticulum ATPase



• Molecule 2: Transitional endoplasmic reticulum ATPase



VAL	TYR	THR	GLU	ASP	ASN	ASP	ASP	ASP	ASP	LEU	TYR	GLY	R713	Q714	T715	N716	P717	S718	A719	M720	E721	V722	E723	E724	D725	D726	R733	D734	H735	F736	E737	E738	F742	A743	R744	R745	S748	D749	N750	D751	I752	R753	K754	L762	S770	F771	R772	G776	ASN	GLN	GLY	GLY	ALA	GLY	PRO	SER	GLN	GLY	SER	GLY	GLY	GLY	THR	GLY	GLY	SER	E748	M550	M551	F552	E556	A557	R560	E578	S581	G587	G588	N589	I590	G591	D592	G593	G594	G595	A596	A597	L605	T606	E607	M608	I619	D627	I628	I633	Y644	D649	E650	L657	S664	N680	L687	E701	S702	I703	E704	I707	R708	R709	T347	N348	D364	R365	E366	A374	R377	I380	D392	L420	I423	R424	K425	L429	I430	D434	E435	T436	V441	L445	W454	Q458	D484	E491	L492	Q494	Y495	D501	R502	F503	F506	G507	V514	Y517	C535	L547	L548	G202	Y203	D204	D205	I206	G207	R210	R211	Q212	L213	L224	L229	V235	R239	G240	Y244	L253	T269	K288	A289	E291	E294	A297	P298	I303	D304	E305	R313	E314	K315	T316	H317	G318	R322	L331	M332	D333	G334	L335	K336	Q337	R338	V343	C902	Y903	D904	I905	M906	N907	D908	L909	L910	L911	L912	L913	V914	R915	G916	G917	A918	V919	A920	T921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	R947	K948	G949	D950	I951	F952	L953	V954	R955	G956	G957	M958	R959	A960	V961	E962	F963	K964	V965	V966	E967	T968	D969	P970	S971	P972	Y973	C974	I975	V976	A977	P978	D979	T980	V981	I982	H983	C984	E985	E986	G987	E988	I989	I990	R991	E992	D993	E994	E995	E996	S997	L998	V201	K81	I82	R83	M84	N85	R86	V87	V88	R89	N90	N91	L92	R93	V94	R95	L96	G97	D98	V99	I100	S101	I102	Q103	P104	C105	P106	D107	V108	K109	Y110	G111	K112	R113	I114	H115	V116	L117	P118	I119	D120	D121	T122	V123	E124	G125	I126	T127	G128	N129	L130	F131	E132	V133	Y134	L135	K136	P137	Y138	F139	L140
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	183316	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.567	Depositor
Minimum map value	-0.666	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.25	Depositor
Map size (\AA)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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	W	0.26	0/1941	0.50	0/2647
1	X	0.26	0/1941	0.52	0/2647
1	Y	0.26	0/1941	0.51	0/2647
1	Z	0.26	0/1941	0.51	0/2647
2	A	0.25	0/5941	0.50	0/8023
2	B	0.25	0/5941	0.50	0/8023
2	C	0.25	0/5930	0.52	1/8008 (0.0%)
2	D	0.25	0/5924	0.52	0/8001
2	E	0.25	0/6010	0.52	0/8115
2	F	0.25	0/6020	0.52	0/8128
All	All	0.25	0/43530	0.51	1/58886 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	198	LEU	CA-CB-CG	5.88	128.83	115.30

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	W	1870	0	1856	29	0
1	X	1870	0	1856	31	0
1	Y	1870	0	1856	44	0
1	Z	1870	0	1856	24	0
2	A	5846	0	5905	96	0
2	B	5846	0	5905	91	0
2	C	5835	0	5893	118	0
2	D	5829	0	5887	129	0
2	E	5911	0	5963	101	0
2	F	5921	0	5971	119	0
3	A	27	0	12	2	0
3	B	27	0	12	2	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
All	All	42776	0	42996	728	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 8.

The worst 5 of 728 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:Y:7:TRP:HE1	1:Y:80:TYR:HH	0.97	0.91
2:F:43:GLN:HG2	2:F:44:PRO:HD3	1.61	0.81
2:C:111:GLY:HA2	2:C:170:PRO:HD2	1.65	0.79
2:A:709:ARG:HB3	2:A:713:ARG:HH12	1.48	0.78
2:E:596:ALA:O	2:E:599:ARG:HB2	1.85	0.76

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	W	223/226 (99%)	205 (92%)	18 (8%)	0	100	100
1	X	223/226 (99%)	203 (91%)	20 (9%)	0	100	100
1	Y	223/226 (99%)	202 (91%)	21 (9%)	0	100	100
1	Z	223/226 (99%)	202 (91%)	20 (9%)	1 (0%)	34	69
2	A	743/787 (94%)	678 (91%)	62 (8%)	3 (0%)	34	69
2	B	743/787 (94%)	685 (92%)	53 (7%)	5 (1%)	22	59
2	C	742/787 (94%)	679 (92%)	59 (8%)	4 (0%)	29	66
2	D	741/787 (94%)	678 (92%)	59 (8%)	4 (0%)	29	66
2	E	751/787 (95%)	683 (91%)	66 (9%)	2 (0%)	41	74
2	F	753/787 (96%)	691 (92%)	57 (8%)	5 (1%)	22	59
All	All	5365/5626 (95%)	4906 (91%)	435 (8%)	24 (0%)	38	69

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	663	LYS
2	E	337	GLN
2	F	298	PRO
2	F	434	ASP
2	F	770	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	193/194 (100%)	193 (100%)	0	100	100
1	X	193/194 (100%)	193 (100%)	0	100	100
1	Y	193/194 (100%)	191 (99%)	2 (1%)	76	86
1	Z	193/194 (100%)	192 (100%)	1 (0%)	88	94
2	A	636/664 (96%)	635 (100%)	1 (0%)	93	97
2	B	636/664 (96%)	634 (100%)	2 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	635/664 (96%)	631 (99%)	4 (1%)	86	93
2	D	634/664 (96%)	632 (100%)	2 (0%)	92	96
2	E	642/664 (97%)	642 (100%)	0	100	100
2	F	643/664 (97%)	641 (100%)	2 (0%)	92	96
All	All	4598/4760 (97%)	4584 (100%)	14 (0%)	92	96

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	651	LYS
2	C	711	ARG
2	F	772	ARG
2	D	713	ARG
2	F	155	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	36	ASN
2	C	443	ASN
2	C	660	ASN
2	D	714	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	901	-	24,29,29	0.93	1 (4%)	29,45,45	1.50	4 (13%)
3	ADP	E	901	-	24,29,29	0.94	1 (4%)	29,45,45	1.37	4 (13%)
3	ADP	F	901	-	24,29,29	0.94	1 (4%)	29,45,45	1.39	4 (13%)
3	ADP	B	901	-	24,29,29	0.94	1 (4%)	29,45,45	1.41	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
3	ADP	A	901	-	-	6/12/32/32	0/3/3/3
3	ADP	E	901	-	-	5/12/32/32	0/3/3/3
3	ADP	F	901	-	-	2/12/32/32	0/3/3/3
3	ADP	B	901	-	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	901	ADP	C5-C4	2.44	1.47	1.40
3	E	901	ADP	C5-C4	2.43	1.47	1.40
3	B	901	ADP	C5-C4	2.42	1.47	1.40
3	A	901	ADP	C5-C4	2.42	1.47	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ADP	PA-O3A-PB	-3.72	120.05	132.83
3	B	901	ADP	PA-O3A-PB	-3.63	120.38	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	901	ADP	PA-O3A-PB	-3.54	120.68	132.83
3	E	901	ADP	PA-O3A-PB	-3.36	121.31	132.83
3	A	901	ADP	C3'-C2'-C1'	3.35	106.02	100.98

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

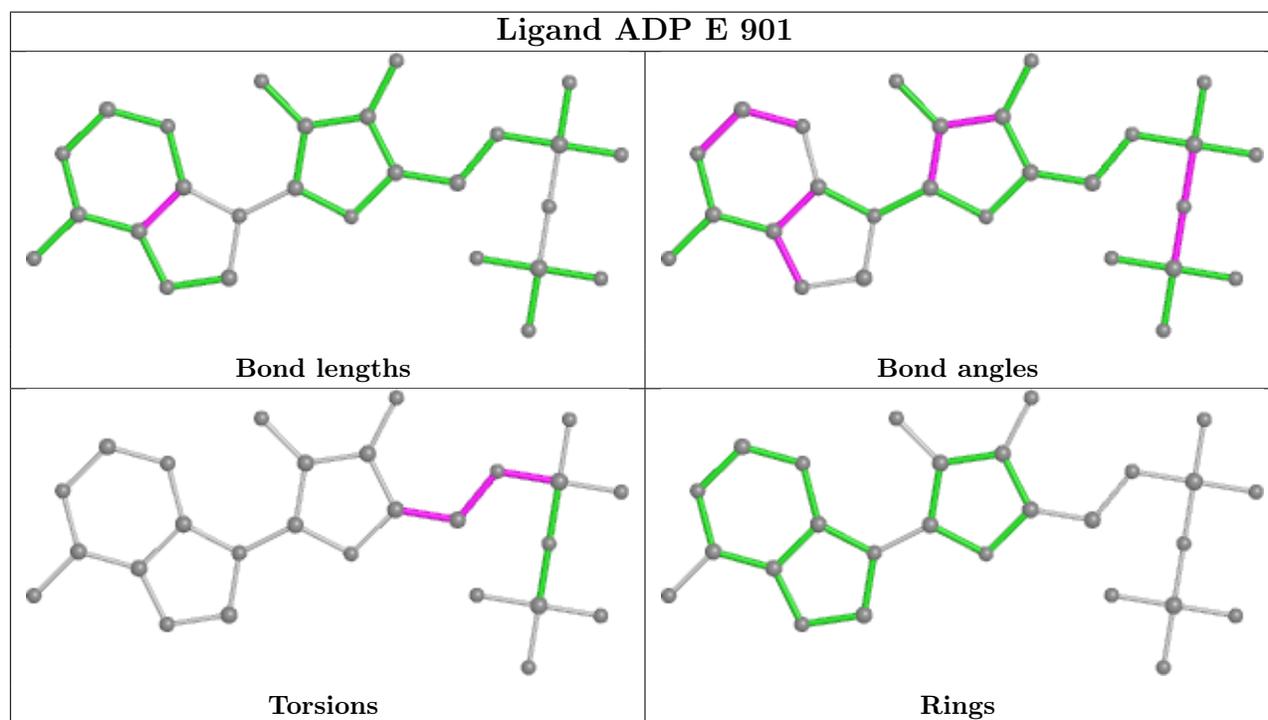
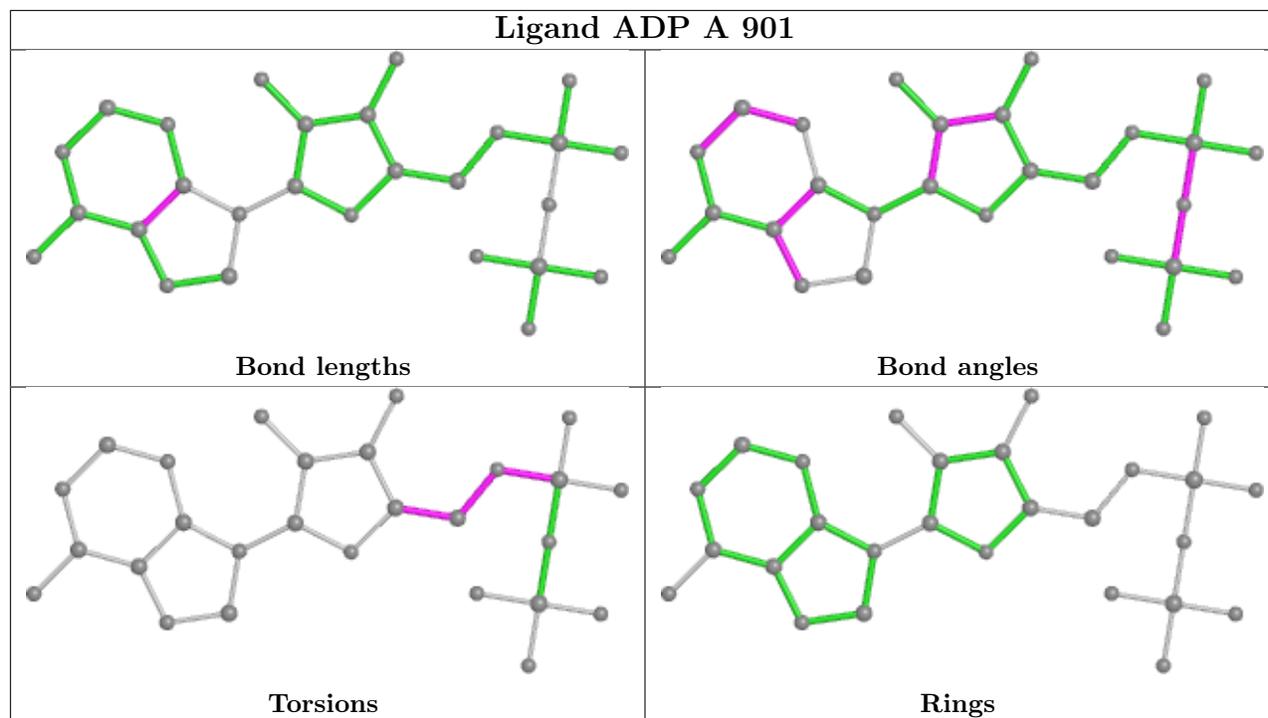
Mol	Chain	Res	Type	Atoms
3	A	901	ADP	C5'-O5'-PA-O1A
3	A	901	ADP	C5'-O5'-PA-O2A
3	A	901	ADP	O4'-C4'-C5'-O5'
3	E	901	ADP	C5'-O5'-PA-O3A
3	A	901	ADP	C3'-C4'-C5'-O5'

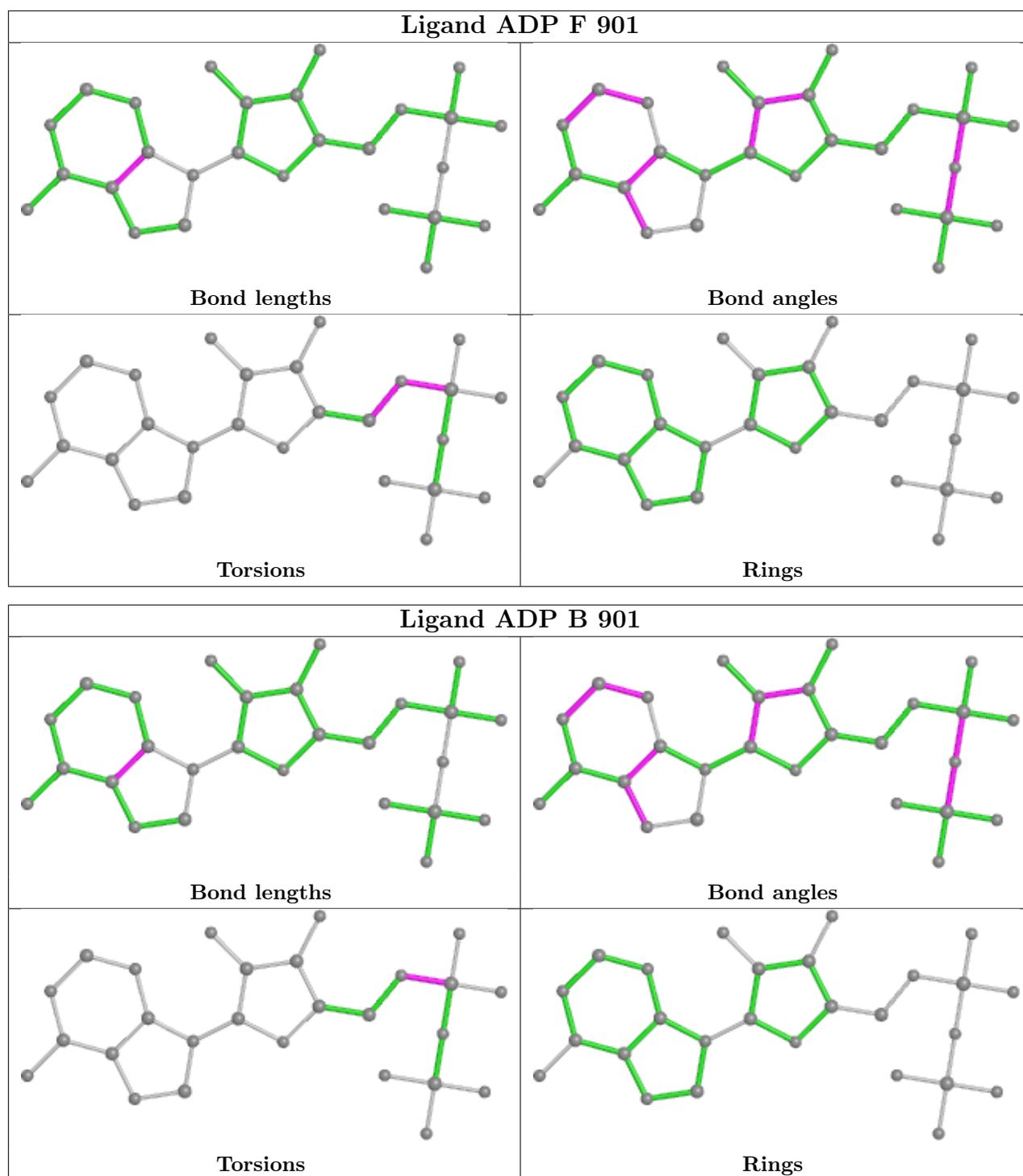
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	ADP	2	0
3	E	901	ADP	1	0
3	F	901	ADP	2	0
3	B	901	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

There are no chain breaks in this entry.

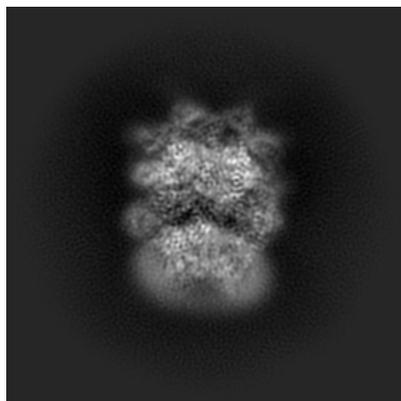
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33608. These allow visual inspection of the internal detail of the map and identification of artifacts.

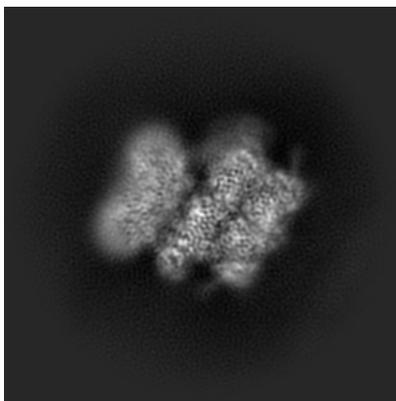
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

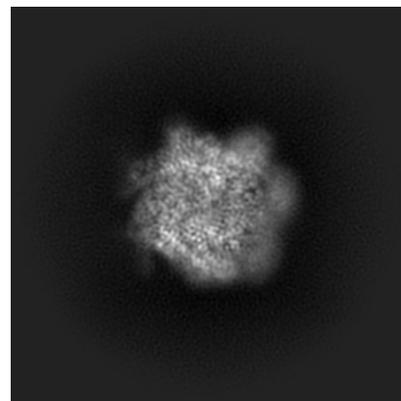
6.1.1 Primary map



X

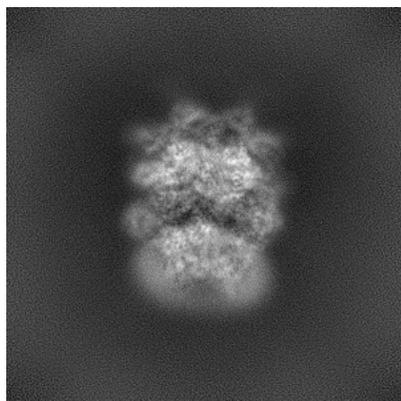


Y

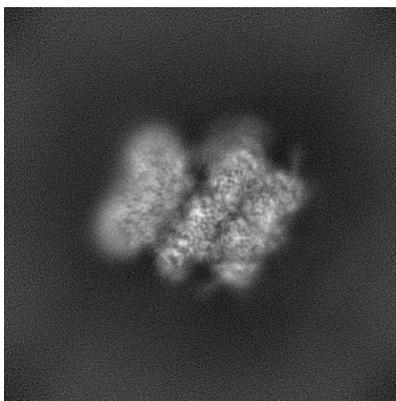


Z

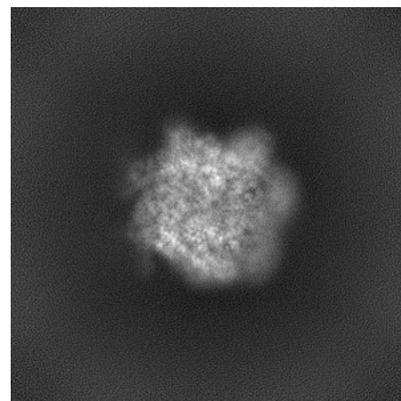
6.1.2 Raw map



X



Y

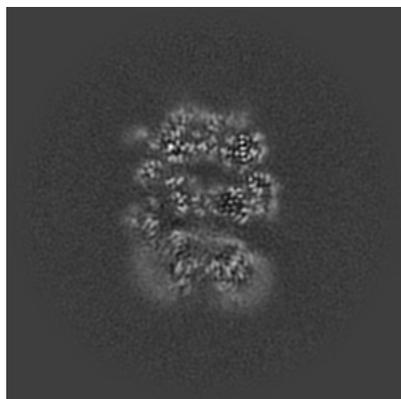


Z

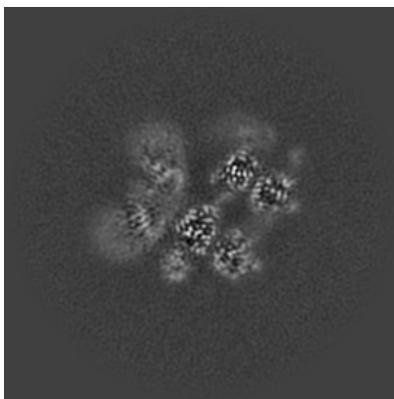
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

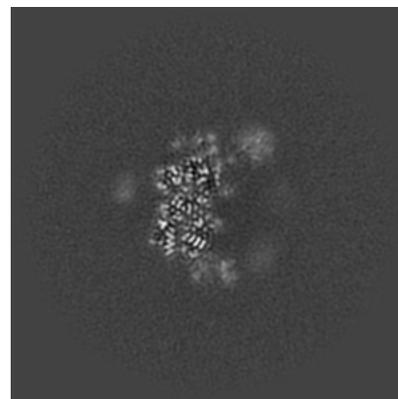
6.2.1 Primary map



X Index: 160

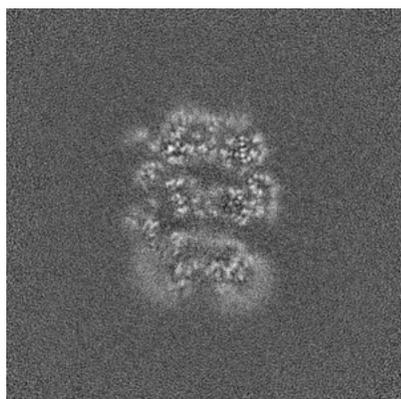


Y Index: 160

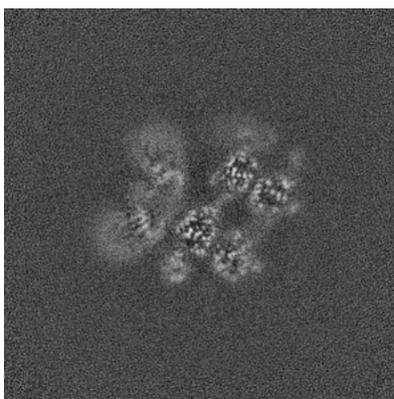


Z Index: 160

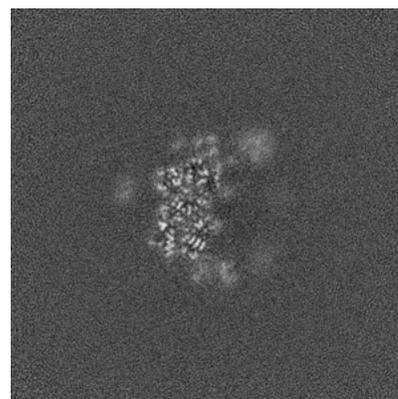
6.2.2 Raw map



X Index: 160



Y Index: 160

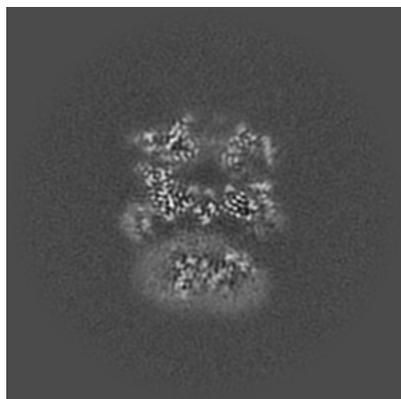


Z Index: 160

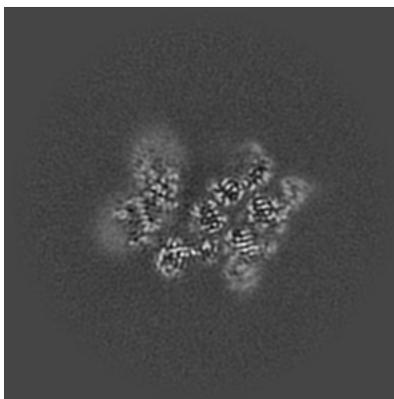
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

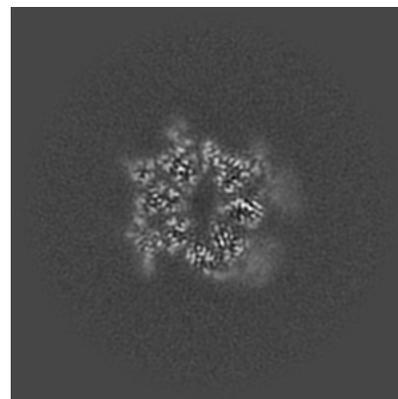
6.3.1 Primary map



X Index: 151

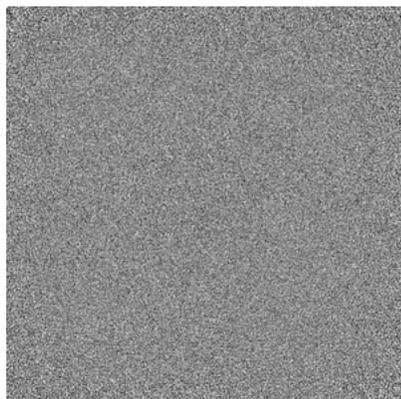


Y Index: 137

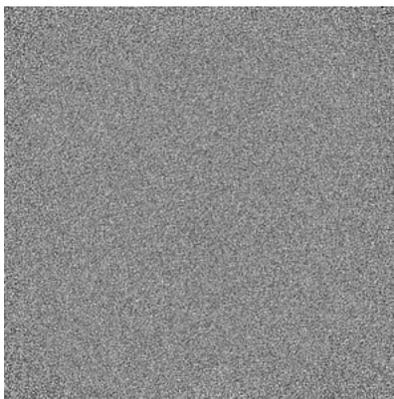


Z Index: 184

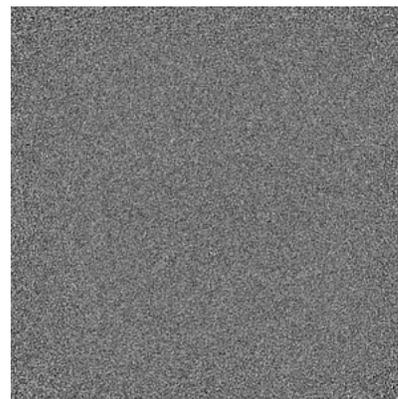
6.3.2 Raw map



X Index: 0



Y Index: 0

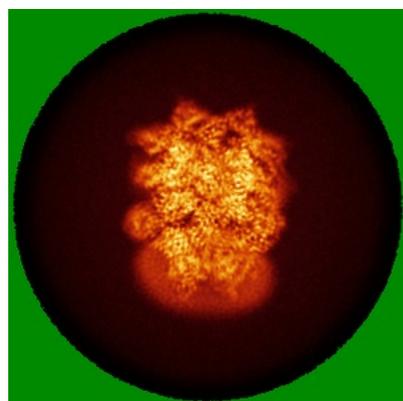


Z Index: 0

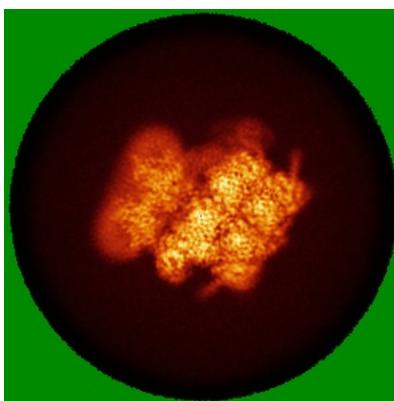
The images above show the largest variance slices of the map in three orthogonal directions.

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

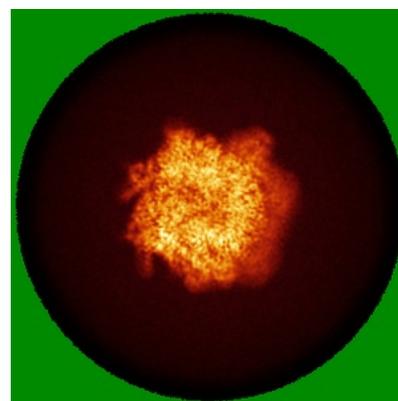
6.4.1 Primary map



X

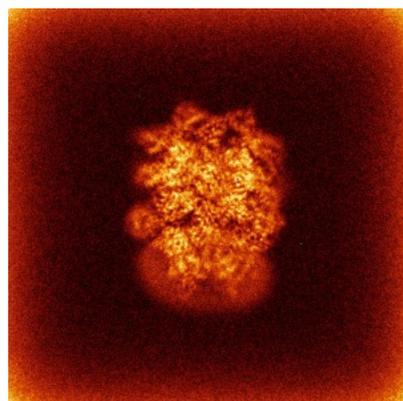


Y

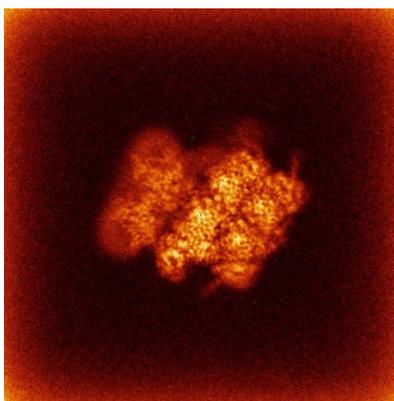


Z

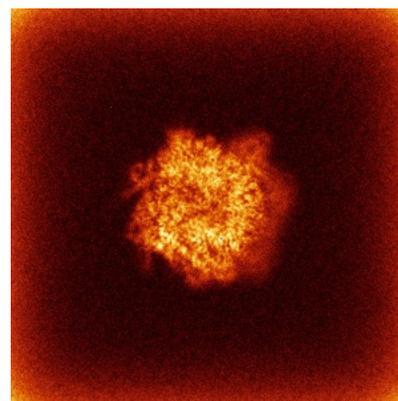
6.4.2 Raw map



X



Y

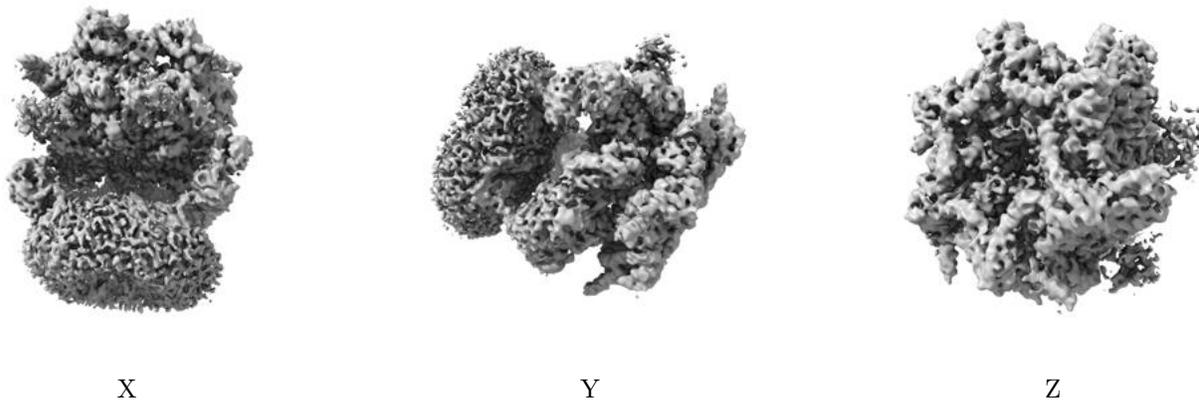


Z

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

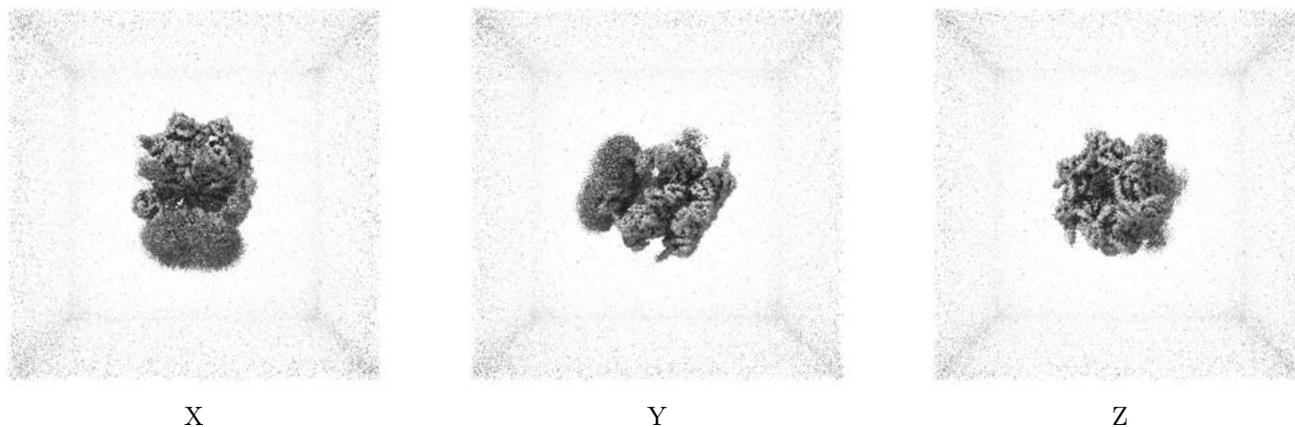
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

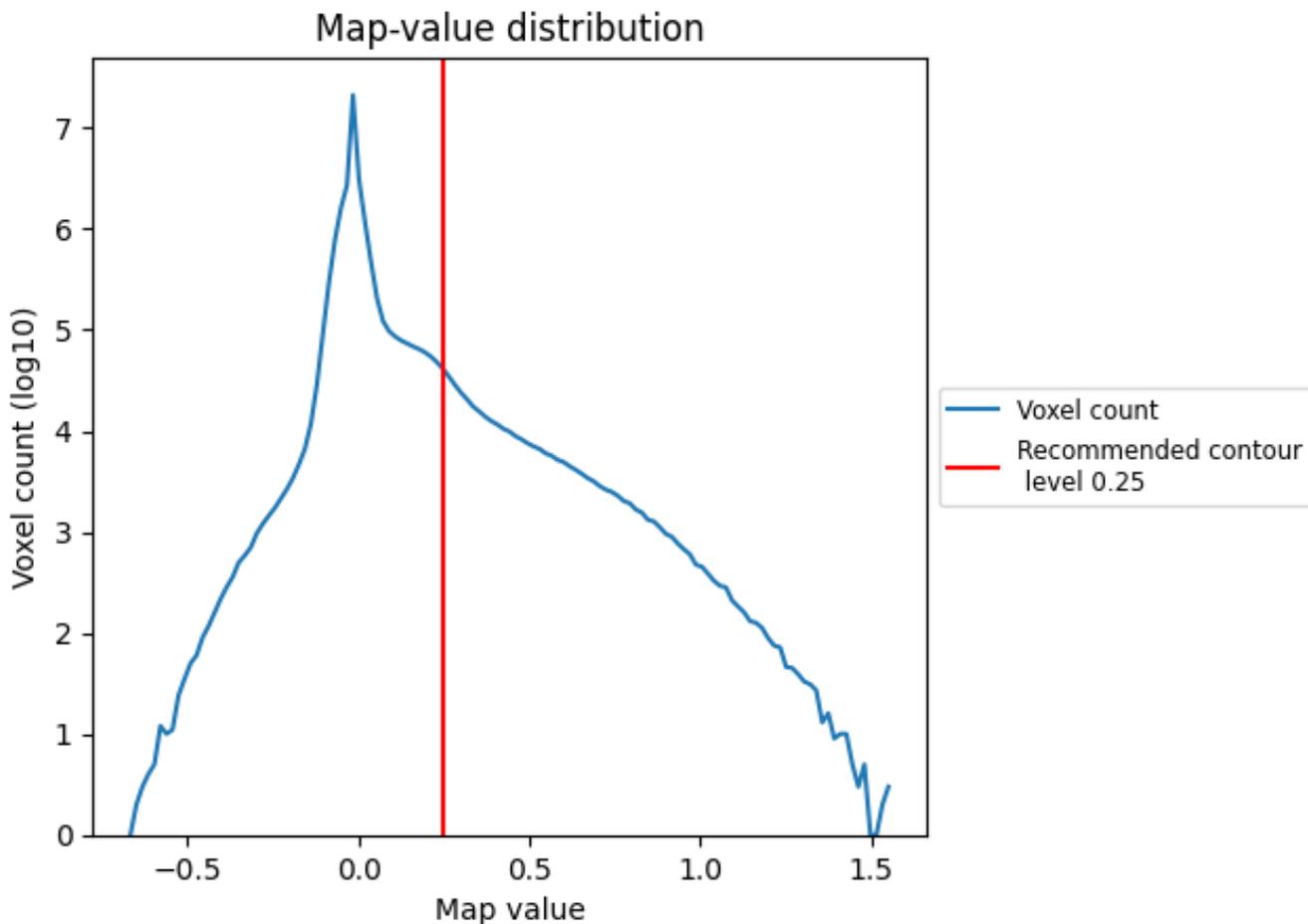
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

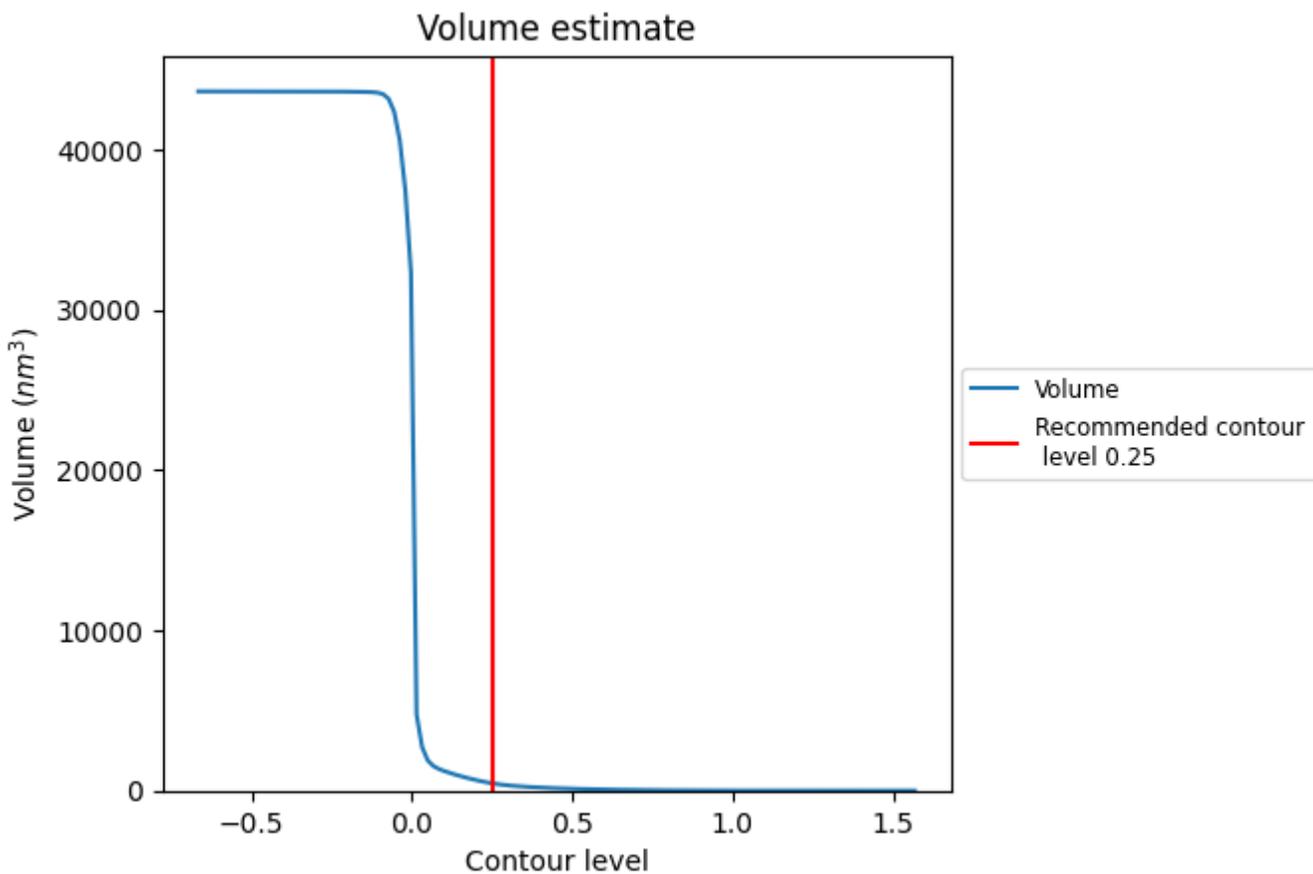
This section contains the results of statistical analysis of the map.

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.

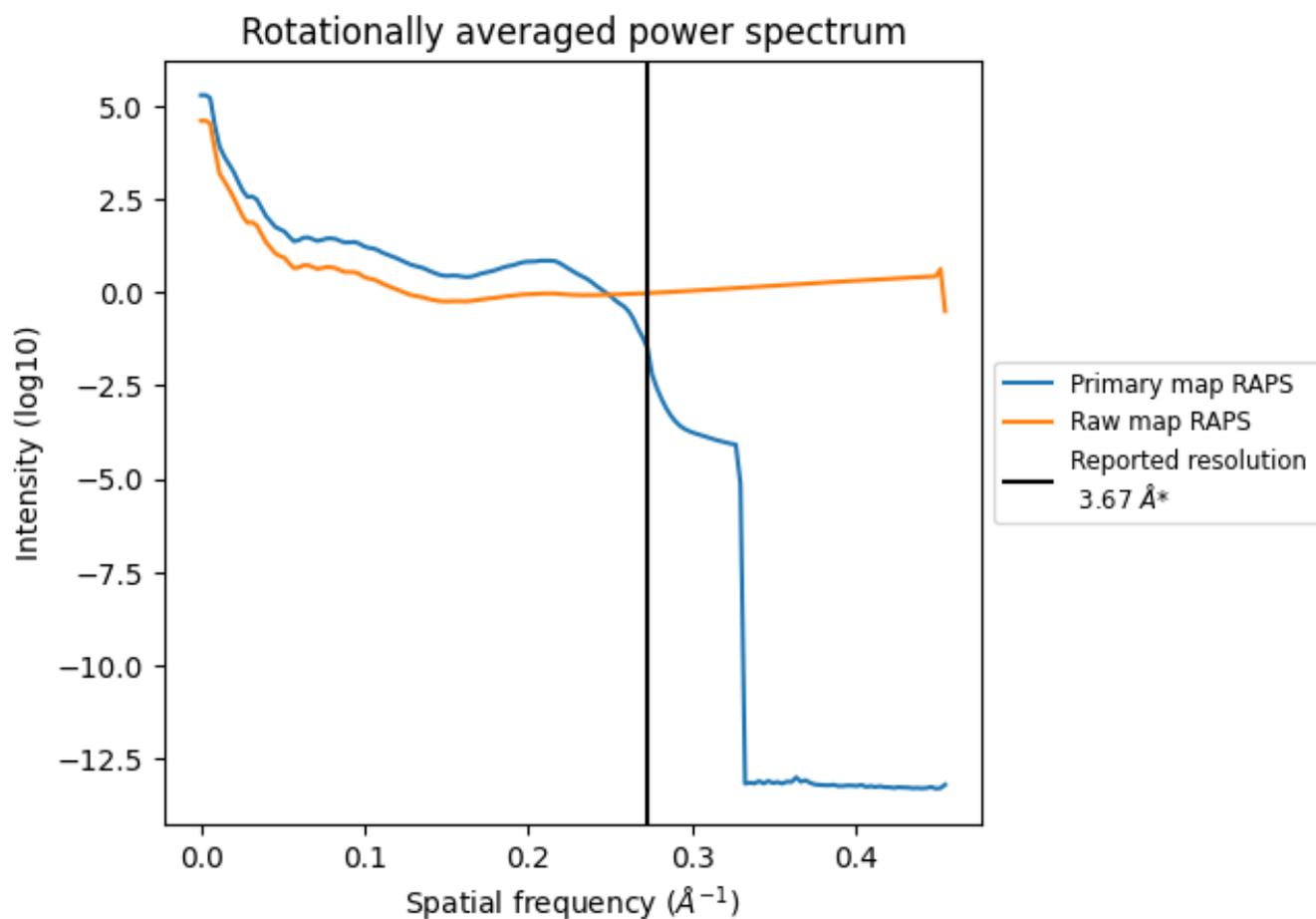
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 456 nm^3 ; this corresponds to an approximate mass of 412 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](#)

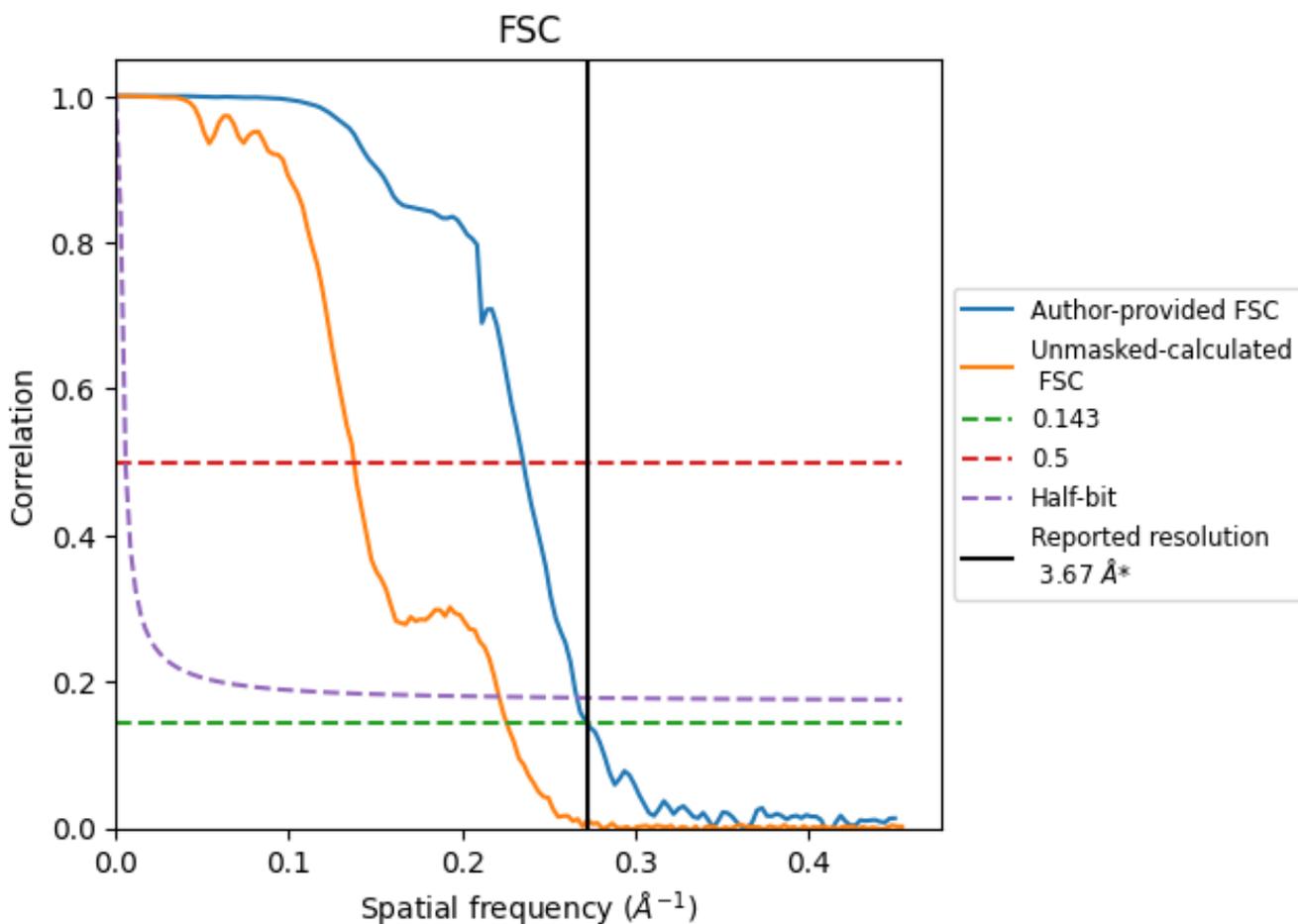


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 Å⁻¹

8.2 Resolution estimates [i](#)

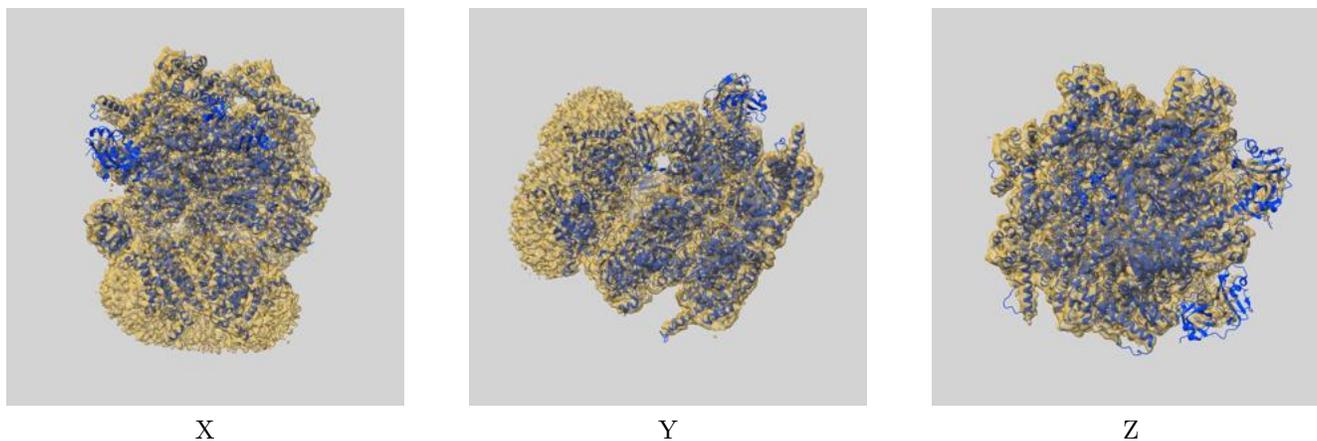
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.67	-	-
Author-provided FSC curve	3.67	4.25	3.75
Unmasked-calculated*	4.42	7.26	4.51

*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 4.42 differs from the reported value 3.67 by more than 10 %

9 Map-model fit [i](#)

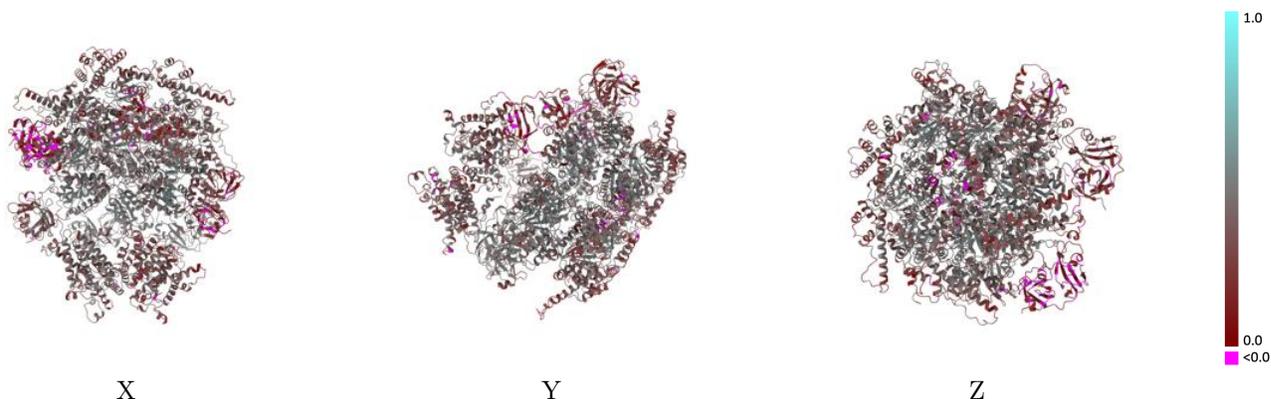
This section contains information regarding the fit between EMDB map EMD-33608 and PDB model 7Y4W. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



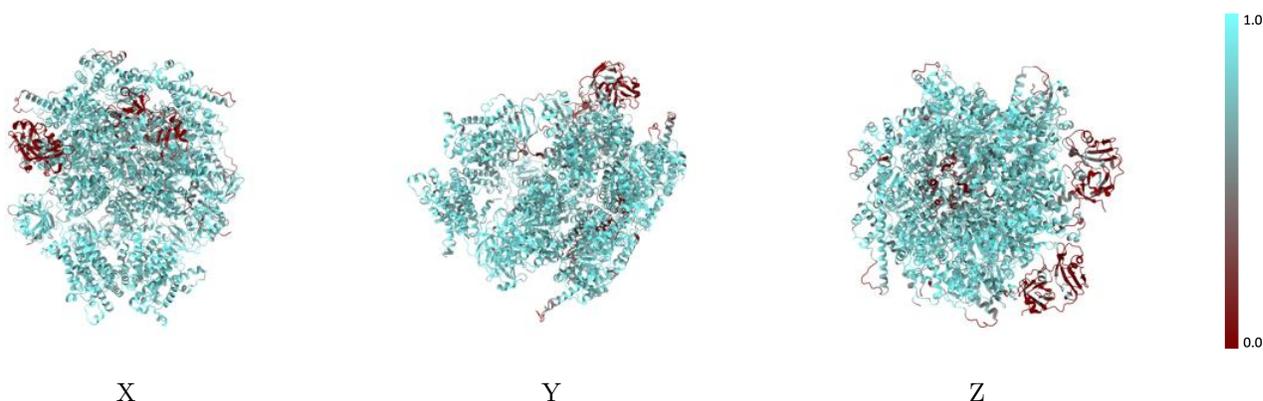
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



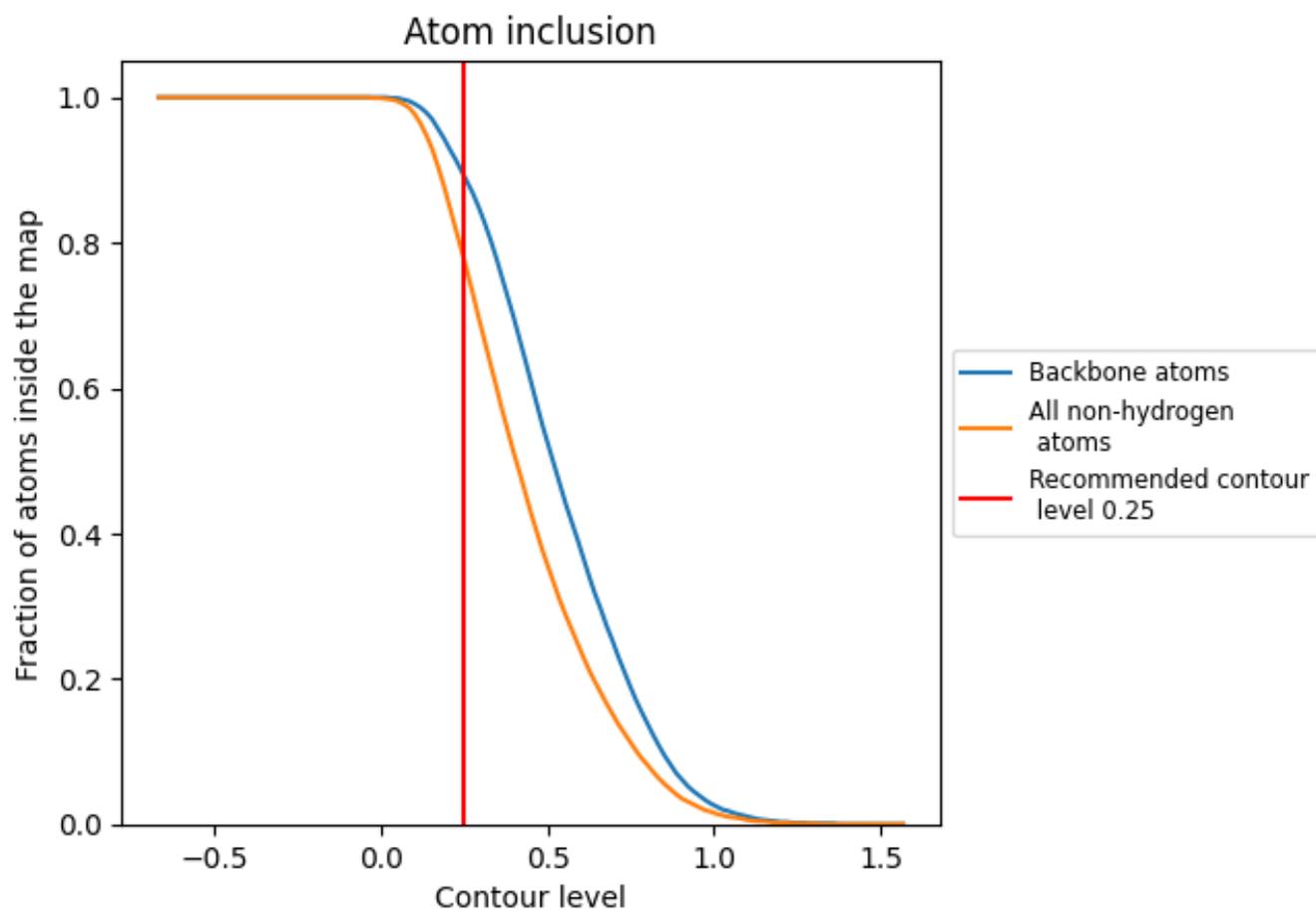
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 78% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7760	 0.3670
A	 0.8320	 0.4100
B	 0.8220	 0.4050
C	 0.7860	 0.3540
D	 0.8100	 0.3780
E	 0.6770	 0.3580
F	 0.6430	 0.3200
W	 0.8320	 0.3290
X	 0.8580	 0.3650
Y	 0.8310	 0.3280
Z	 0.8600	 0.3800

