



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 12:28 AM UTC

PDB ID : 9L2F / pdb_00009l2f
EMDB ID : EMD-62774
Title : Structure of SARM1 bound to M1 and 1AD in the active state
Authors : Huang, Y.; Zhang, J.; Zheng, S.; Wang, X.
Deposited on : 2024-12-17
Resolution : 3.55 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

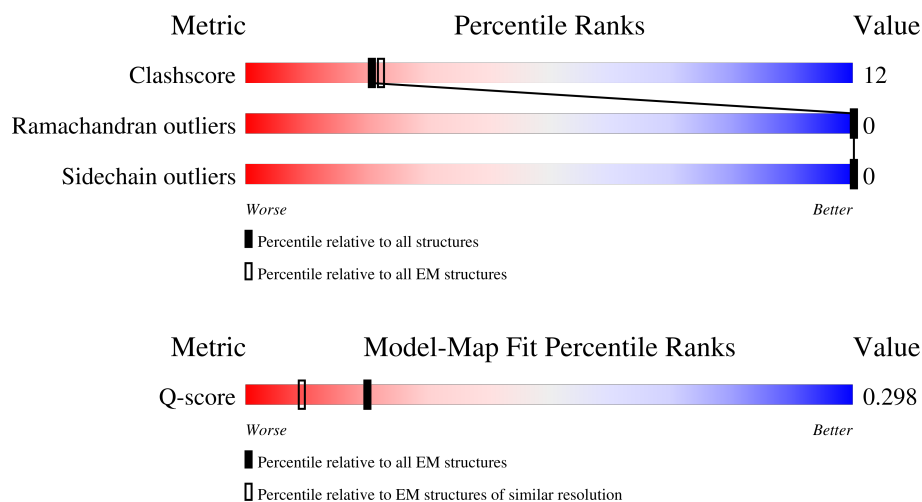
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.55 Å.

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



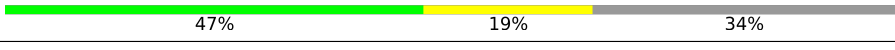
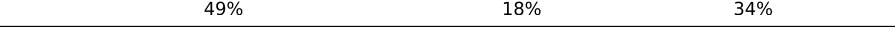
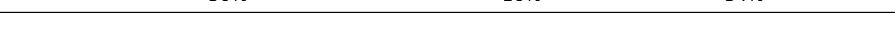
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12819 (3.05 - 4.05)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	732	
1	B	732	
1	C	732	
1	D	732	

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Mol	Chain	Length	Quality of chain
1	E	732	 47% 19% 34%
1	F	732	 47% 19% 34%
1	G	732	 49% 18% 34%
1	H	732	 50% 16% 34%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30320 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 NAD(+) hydrolase SARM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	485	Total	C	N	O	S	0	0
			3770	2365	690	698	17		
1	B	485	Total	C	N	O	S	0	0
			3770	2365	690	698	17		
1	C	485	Total	C	N	O	S	0	0
			3770	2365	690	698	17		
1	D	485	Total	C	N	O	S	0	0
			3770	2365	690	698	17		
1	E	485	Total	C	N	O	S	0	0
			3770	2365	690	698	17		
1	F	485	Total	C	N	O	S	0	0
			3770	2365	690	698	17		
1	G	485	Total	C	N	O	S	0	0
			3770	2365	690	698	17		
1	H	485	Total	C	N	O	S	0	0
			3770	2365	690	698	17		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	725	ASP	-	expression tag	UNP Q6SZW1
A	726	TYR	-	expression tag	UNP Q6SZW1
A	727	LYS	-	expression tag	UNP Q6SZW1
A	728	ASP	-	expression tag	UNP Q6SZW1
A	729	ASP	-	expression tag	UNP Q6SZW1
A	730	ASP	-	expression tag	UNP Q6SZW1
A	731	ASP	-	expression tag	UNP Q6SZW1
A	732	LYS	-	expression tag	UNP Q6SZW1
B	725	ASP	-	expression tag	UNP Q6SZW1
B	726	TYR	-	expression tag	UNP Q6SZW1
B	727	LYS	-	expression tag	UNP Q6SZW1
B	728	ASP	-	expression tag	UNP Q6SZW1
B	729	ASP	-	expression tag	UNP Q6SZW1
B	730	ASP	-	expression tag	UNP Q6SZW1

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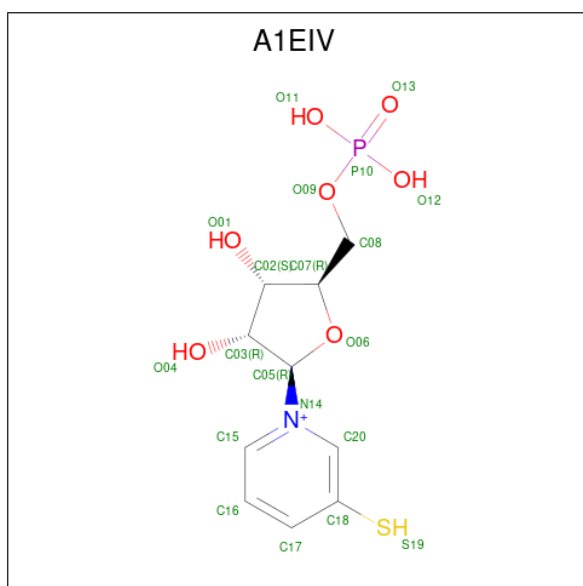
Chain	Residue	Modelled	Actual	Comment	Reference
B	731	ASP	-	expression tag	UNP Q6SZW1
B	732	LYS	-	expression tag	UNP Q6SZW1
C	725	ASP	-	expression tag	UNP Q6SZW1
C	726	TYR	-	expression tag	UNP Q6SZW1
C	727	LYS	-	expression tag	UNP Q6SZW1
C	728	ASP	-	expression tag	UNP Q6SZW1
C	729	ASP	-	expression tag	UNP Q6SZW1
C	730	ASP	-	expression tag	UNP Q6SZW1
C	731	ASP	-	expression tag	UNP Q6SZW1
C	732	LYS	-	expression tag	UNP Q6SZW1
D	725	ASP	-	expression tag	UNP Q6SZW1
D	726	TYR	-	expression tag	UNP Q6SZW1
D	727	LYS	-	expression tag	UNP Q6SZW1
D	728	ASP	-	expression tag	UNP Q6SZW1
D	729	ASP	-	expression tag	UNP Q6SZW1
D	730	ASP	-	expression tag	UNP Q6SZW1
D	731	ASP	-	expression tag	UNP Q6SZW1
D	732	LYS	-	expression tag	UNP Q6SZW1
E	725	ASP	-	expression tag	UNP Q6SZW1
E	726	TYR	-	expression tag	UNP Q6SZW1
E	727	LYS	-	expression tag	UNP Q6SZW1
E	728	ASP	-	expression tag	UNP Q6SZW1
E	729	ASP	-	expression tag	UNP Q6SZW1
E	730	ASP	-	expression tag	UNP Q6SZW1
E	731	ASP	-	expression tag	UNP Q6SZW1
E	732	LYS	-	expression tag	UNP Q6SZW1
F	725	ASP	-	expression tag	UNP Q6SZW1
F	726	TYR	-	expression tag	UNP Q6SZW1
F	727	LYS	-	expression tag	UNP Q6SZW1
F	728	ASP	-	expression tag	UNP Q6SZW1
F	729	ASP	-	expression tag	UNP Q6SZW1
F	730	ASP	-	expression tag	UNP Q6SZW1
F	731	ASP	-	expression tag	UNP Q6SZW1
F	732	LYS	-	expression tag	UNP Q6SZW1
G	725	ASP	-	expression tag	UNP Q6SZW1
G	726	TYR	-	expression tag	UNP Q6SZW1
G	727	LYS	-	expression tag	UNP Q6SZW1
G	728	ASP	-	expression tag	UNP Q6SZW1
G	729	ASP	-	expression tag	UNP Q6SZW1
G	730	ASP	-	expression tag	UNP Q6SZW1
G	731	ASP	-	expression tag	UNP Q6SZW1
G	732	LYS	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	725	ASP	-	expression tag	UNP Q6SZW1
H	726	TYR	-	expression tag	UNP Q6SZW1
H	727	LYS	-	expression tag	UNP Q6SZW1
H	728	ASP	-	expression tag	UNP Q6SZW1
H	729	ASP	-	expression tag	UNP Q6SZW1
H	730	ASP	-	expression tag	UNP Q6SZW1
H	731	ASP	-	expression tag	UNP Q6SZW1
H	732	LYS	-	expression tag	UNP Q6SZW1

- Molecule 2 is [(2 {R},3 {S},4 {R},5 {R})-3,4-bis(oxidanyl)-5-(3-sulfanylpurin-1-yl)oxolan-2-yl]methyl dihydrogen phosphate (CCD ID: A1EIV) (formula: C₁₀H₁₅NO₇PS) (labeled as "Ligand of Interest" by depositor).

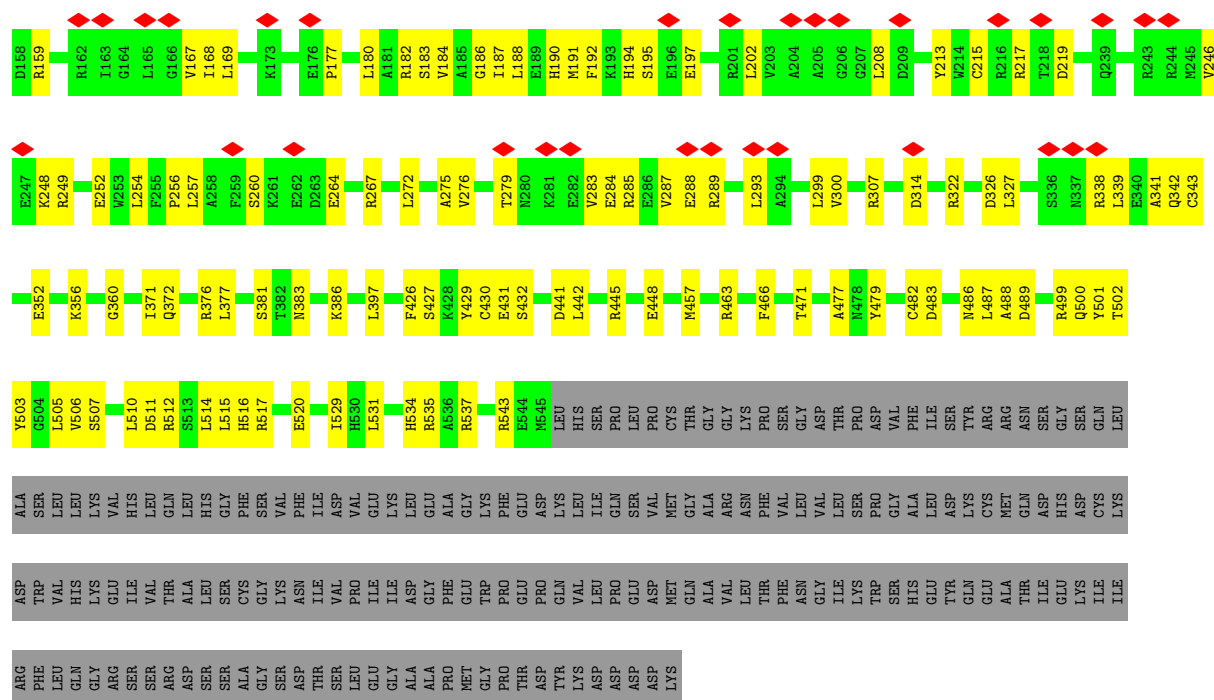


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 20	C 10	N 1	O 7	P 1	S 1	0
2	B	1	Total 20	C 10	N 1	O 7	P 1	S 1	0
2	C	1	Total 20	C 10	N 1	O 7	P 1	S 1	0
2	D	1	Total 20	C 10	N 1	O 7	P 1	S 1	0
2	E	1	Total 20	C 10	N 1	O 7	P 1	S 1	0
2	F	1	Total 20	C 10	N 1	O 7	P 1	S 1	0

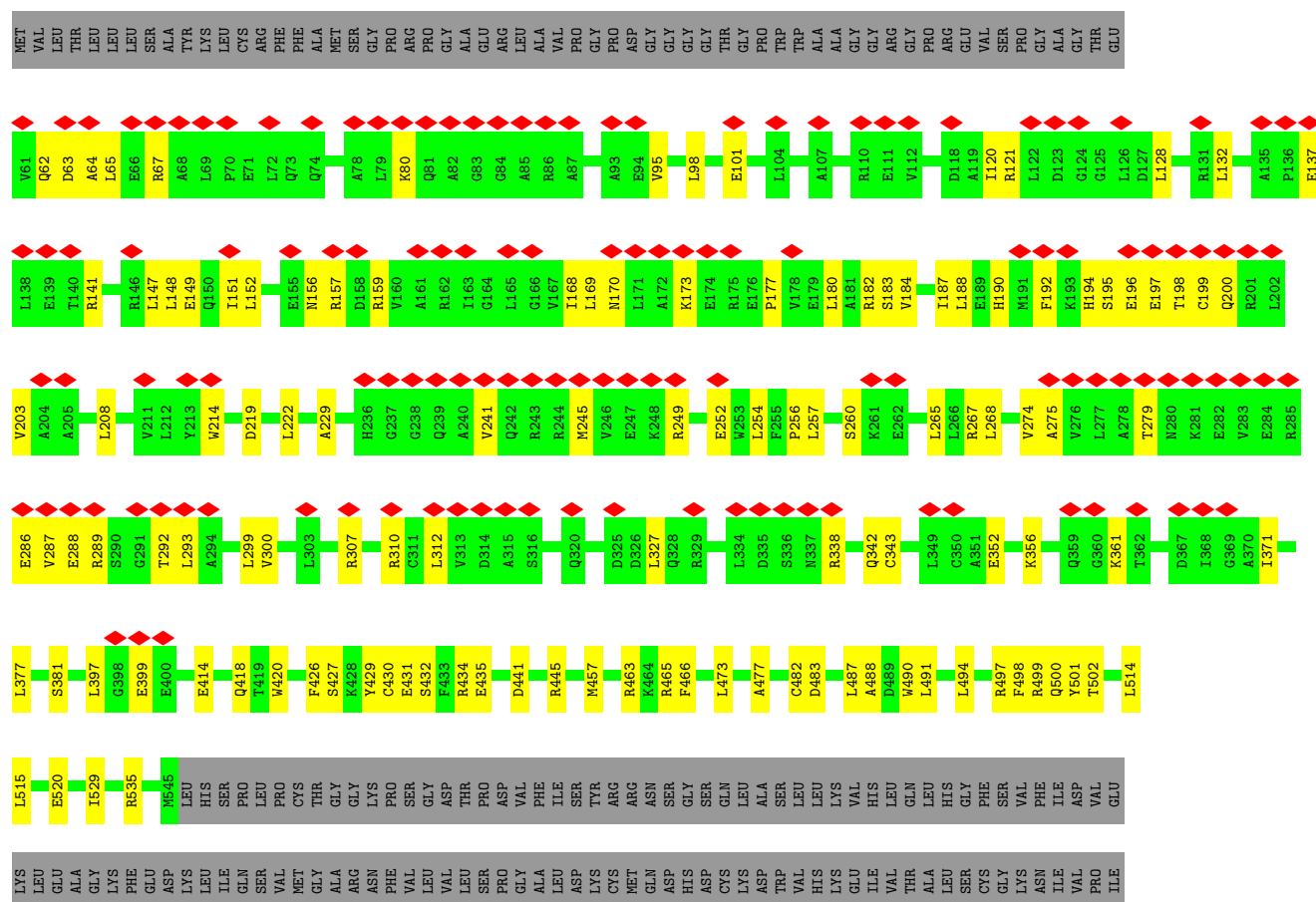
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Mol	Chain	Residues	Atoms						AltConf
2	G	1	Total	C	N	O	P	S	0
			20	10	1	7	1	1	
2	H	1	Total	C	N	O	P	S	0
			20	10	1	7	1	1	

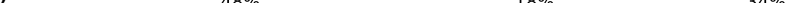


• Molecule 1: NAD(+) hydrolase SARM1



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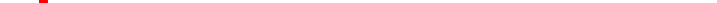
- Molecule 1: NAD(+) hydrolase SARM1

Chain D: 

MET	VAL	LEU	THR	LEU	LEU	SER	ALA	TYR	LYS	CYS	ARG	PHE	PHE	ALA	MET	SER	GLY	GLY	ARG	PRO	ARG	PRO	GLY	ALA	ALA	VAL	PRO	GLY	GLY	ASP	GLY	GLY	GLY	GLY	THR	PRO	TRP	TRP	ALA	ALA	GLY	GLY	GLY	ARG	GLY	PRO	ARG	GLU	VAL	SER	PRO	GLY	ALA	ALA	GLY	GLY	THR	GLU
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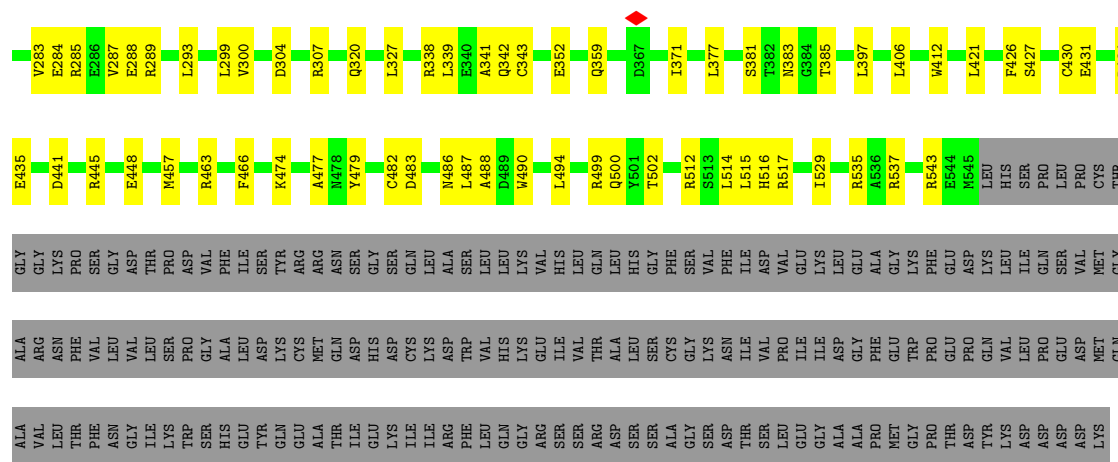
ASP	GLU	SER	LEU	F433	E262	H170	V61
ASP	ASP	VAL	PRO	R434	L266	L171	Q62
LYS	MET	MET	CYS	E435	L272	R175	D63
	GLN	GLY	THR	D441	L276	E176	A64
	ALA	ARG	GLY	L442	V277	P177	L66
	VAL	ASN	LYS	R445	L277	L180	E66
	LEU	PHE	PRO	M457	K281	A181	R67
	THR	VAL	SER	E457	E282	R182	Q81
	PHE	LEU	GLY	R463	V283	A82	G83
	ASN	VAL	ASP	R468	E284	A185	
	GLY	SER	PRO	L473	R285	G186	R86
	TRP	GLY	ASP	A477	E287	I187	A87
	SER	ALA	PHE	L494	E288	H190	V95
	HIS	LEU	ILE	R499	R289	M191	
	GLU	LEU	LYS	M486	L293	F192	L98
	THR	ASP	TYR	L487	E300	H194	V99
	ALA	MET	CYS	A488	A301	S195	E100
	ALA	GLN	ARG	D489	L302	E196	E101
	ILE	ASP	ASN	M490	L303	E197	A102
	ILE	HIS	GLY	L494	D304	T198	W103
	GLU	ASP	SER	R499	R307	C199	L104
	LYS	CYS	GLN	T502	L312	Q200	P106
	ILE	LYS	LEU	Y503	V313	R201	A107
	ARG	GLU	ALA	G504	D314	L202	V108
	GLY	ILE	VAL	L505	R329	V203	G109
	SER	THR	HIS	L510	K337	A204	R110
	SER	VAL	LEU	D511	R338	D219	L123
	ARG	THR	GLN	R512	L339	A229	L126
	ASP	ALA	LEU	S513	Q342	C233	L129
	SER	LEU	HIS	L514	C343	A234	L130
	SER	SER	GLY	L515	Y348	L235	L133
	ALA	CYS	PHE	H516	R367	R248	Q134
	GLY	GLY	SER	E520	K383	R249	A135
	SER	LYS	VAL	T529	E414	E252	E137
	ASP	ASN	ASP	H530	Q418	L254	
	THR	ILE	VAL	L531	R419	R257	R141
	LEU	GLU	VAL	R534	L420	M245	L147
	GLY	ILE	LYS	R535	W426	E149	L148
	ALA	ASP	LEU	E436	K428	Q150	L149
	ALA	GLY	PHE	R537	L429	I151	
	MET	GLU	GLY	R543	W429	N156	
	PRO	TRP	LYS	E544	W420	R157	
	GLY	PRO	PHE	M545	S427	V253	
	PRO	ASP	GLU	R545	L428	L254	
	THR	GLU	GLU	HIS	Y429	L257	
	ASP	VAL	LEU	SER	C430		
	LYS	LEU	ILE	PRO	E431		
	ASP	PRO	GLN		S432		

- Molecule 1: NAD(+) hydrolase SARM1

Chain E:  47% 19% 34%

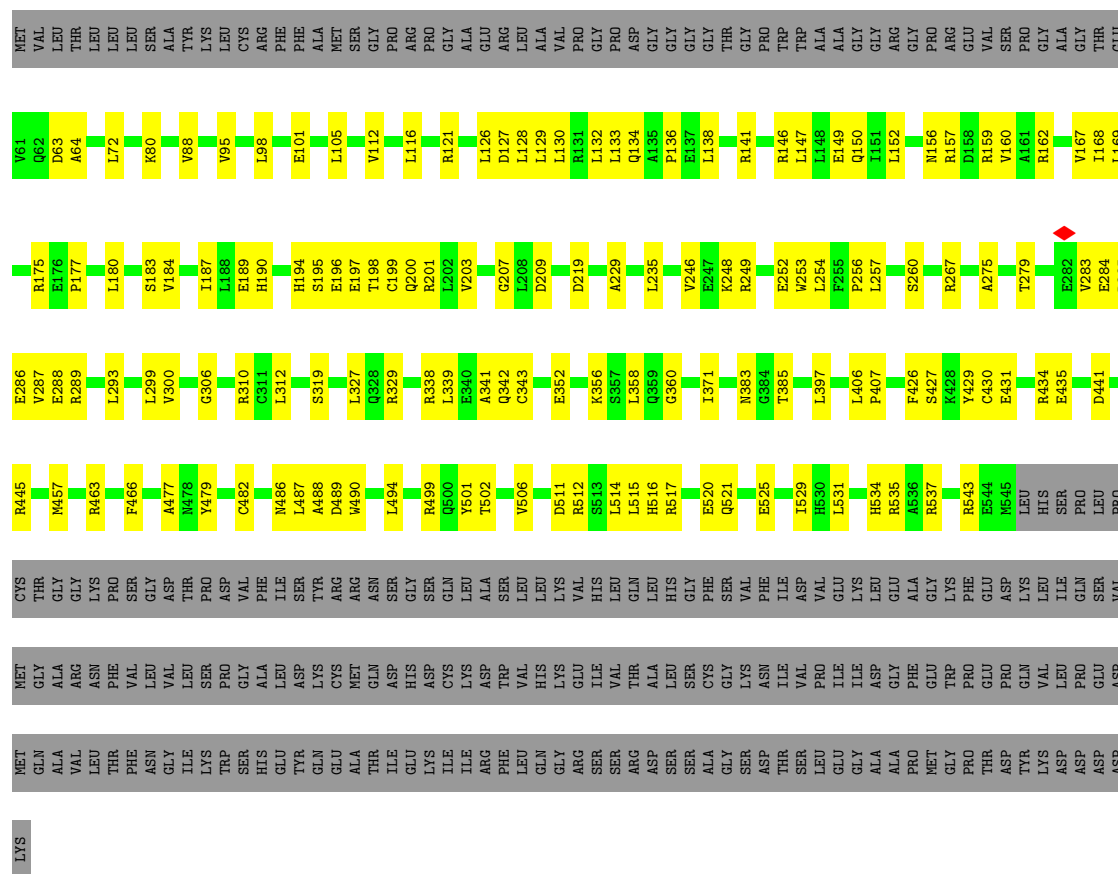
MET	VAL	LEU	LEU	THR	LEU	LEU	LEU	SER	ALA	ALA	TYR	LYS	LEU	CYS	ARG	PHE	PHE	ARG	PRO	PRO	PRO	GLY	ALA	ALA	LEU	VAL	PRO	GLY	GLY	ASP	ASP	GLY	GLY	GLY	GLY	THR	PRO	TRP	TRP	ALA	ALA	GLY	GLY	GLY	ARG	GLY	PRO	PRO	SER	THR	GLY	ALA	GLY	THR
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[illegible]



• Molecule 1: NAD(+) hydrolase SARM1

Chain F: 47% 19% 34%



• Molecule 1: NAD(+) hydrolase SARM1

Chain G: 49% 18% 34%



VAL	R463	L327	I187	Q62
PHE	F466	Q328	L188	D63
ILE	SER	R329	M191	A64
TYR	L473	L333	F192	L65
CYS	K474	L333	K193	E66
MET	ARG	ARG	H194	L72
ASN	Y479	S336	S195	L22
SER	ASN	R337	S195	L22
GLY	GLY	R338	V203	V95
ASP	SER	D483	L208	L98
CYS	GLN	A341	L208	L98
LEU	LEU	Q342	W214	E101
ASP	ALA	A488	W214	E101
TRP	SER	D489	D219	L116
VAL	LEU	W490	D219	L116
HIS	LEU	L494	L222	R121
LYS	VAL	L494	L222	R121
GLU	VAL	L494	L222	R121
ILE	HIS	R497	A229	G125
VAL	LEU	R497	A229	L126
THR	GLN	Q500	L235	L126
ALA	LEU	Y501	L235	L126
LEU	HIS	T502	V246	L129
SER	GLY	T502	V246	L129
CYS	PHE	R512	K248	L130
GLY	SER	S513	R249	L130
LYS	VAL	L514	I371	L133
ASN	PHE	L514	E282	Q134
ILE	ILE	R516	W253	A135
VAL	ASP	R517	K254	P136
PRO	VAL	E520	L254	E137
ILE	GLU	E520	L257	R141
ILE	LYS	L531	L257	R141
ASP	LEU	L531	L265	L147
GLY	GLU	V409	L266	L148
PHE	ALA	H534	R267	E149
GLU	GLY	R535	L268	Q150
TRP	LYS	L535	W412	I151
PRO	PHE	R543	K413	L51
GLU	GLU	E544	E414	N156
PRO	ASP	M545	Q418	R157
GLN	LYS	LEU	T279	D158
VAL	VAL	HIS	W420	R159
ILE	LEU	SER	E284	V160
PRO	GLN	PRO	F426	I168
ASP	SER	LEU	S427	L169
GLU	VAL	VAL	K428	N170
MET	MET	CYS	Y429	L171
GLN	GLY	THR	C430	A172
ALA	ALA	GLY	E431	L172
VAL	ARG	GLY	L293	K173
LEU	ASN	LYS	R434	P177
THR	PHE	PRO	L299	P177
ASN	VAL	SER	D441	L180
GLY	LEU	GLY	R445	A181
ILE	LEU	THR	M457	R182
LYS	PRO	ASP	M457	S183
TRP	PRO	ASP	M457	V194

SER	HIS	GLU	TYR	GLN	ALA	THR	ILE	LYS	ILE	ARG	PHE	TRP	VAL	HIS	GLN	GLY	ARG	SER	ILE	GLY	LEU	ASP	PRO	ILE	GLY	LEU	ASP	PRO	GLN	VAL	ALA	ARG	VAL	ASN	PHE	THR	VAL	LEU	GLY	ILE	LYS
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● Molecule 1: NAD(+) hydrolase SARM1



MET	VAL	LEU	THR	LEU	LEU	SER	ALA	TYR	LYS	LEU	CYS	ARG	PHE	PHE	ALA	MET	SER	GLY	PRO	ARG	ASP	GLY	LEU	ASP	PRO	GLY	THR	GLY	THR	GLY	PRO	TRP	ALA	ALA	GLY	GLY	ARG	VAL	SER	PRO	GLY	ALA	GLY	THR	GLU
V61	Q62	D63	A64	L72	G83	V95	L98	V99	E100	E101	G109	R110	E111	V112	A113	G115	L116	C117	R121	G125	L126	D127	L128	P136	E137	R141	L147	L148	E149	Q150	I151	L152	V153	N156	R157	D158	R159	R162	I168	L169	R175	E176	P177	V178	
E179	L180	A181	R182	S183	V184	I187	L188	E189	H190	M191	F192	K193	C311	L312	S195	C199	V203	A204	G207	L208	D209	A210	V211	L212	D219	A229	A240	R243	V246	E247	R249	E252	W253	L254	L257	L265	L268	A275	T279	V283	E284	R285	P177	E286	
V287	E288	R289	L293	V300	D304	R307	R310	C311	L312	V313	R338	A341	Q342	C343	F347	K356	K361	F426	S427	C430	E431	R434	E435	M457	R463	F466	K474	A477	N478	Y479	C482	N486	L487	A488	D489	W490	L494								
R499	Q500	T502	V506	R512	L515	H516	L531	H534	E543	E544	M545	LEU	HIS	SER	PRO	GLN	SER	LEU	PRO	MET	CYS	THR	GLY	ALA	ARG	GLY	LEU	SER	PRO	ASP	VAL	PHE	ILE	SER	GLY	HIS	ASP	LEU	ASP	GLN	VAL	THR	ALA		
HIS	GLY	PHE	SER	VAL	PHE	ILE	ASP	VAL	VAL	GLY	LYS	LEU	ALA	GLY	THR	GLY	ALA	ARG	ASN	VAL	LEU	VAL	LEU	LEU	THR	LEU	LEU	THR	PRO	ASP	GLY	ALA	PHE	ILE	ASP	GLY	THR	TRP	SER	LEU	ASP	GLN	VAL	THR	ALA
LEU	SER	CYS	GLY	LYS	ASN	ILE	VAL	PRO	ILE	ILE	GLY	ASP	PHE	GLY	TRP	PRO	GLU	GLU	ASP	MET	GLN	ALA	VAL	VAL	LEU	LEU	THR	THR	TRP	LYS	LEU	ALA	THR	ILE	GLU	LYS	ILE	ILE	ARG	PHE	LEU	GLN	GLY	ASP	
SER	SER	ALA	GLY	SER	ASP	THR	SER	LEU	GLY	GLY	PRO	THR	ASP	TYR	LYS	ASP	GLN	VAL	MET	GLN	ALA	VAL	LEU	THR	THR	THR	PHE	ASN	GLY	ILE	LYS	TRP	SER	LEU	ASP	PRO	GLN	VAL	ASN	PHE	THR	GLU	ASP		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65229	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	680	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.151	Depositor
Minimum map value	-0.439	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.226	Depositor
Map size (Å)	367.2, 367.2, 367.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: A1EIV

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	0.13	0/3824	0.30	0/5168
1	B	0.12	0/3824	0.29	0/5168
1	C	0.12	0/3824	0.29	0/5168
1	D	0.12	0/3824	0.30	0/5168
1	E	0.12	0/3824	0.29	0/5168
1	F	0.13	0/3824	0.30	0/5168
1	G	0.13	0/3824	0.30	0/5168
1	H	0.14	0/3824	0.31	0/5168
All	All	0.13	0/30592	0.30	0/41344

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	3770	0	3852	98	0
1	B	3770	0	3852	97	0
1	C	3770	0	3852	88	0
1	D	3770	0	3852	89	0
1	E	3770	0	3852	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3770	0	3852	99	0
1	G	3770	0	3852	83	0
1	H	3770	0	3852	88	0
2	A	20	0	0	2	0
2	B	20	0	0	1	0
2	C	20	0	0	2	0
2	D	20	0	0	2	0
2	E	20	0	0	2	0
2	F	20	0	0	2	0
2	G	20	0	0	1	0
2	H	20	0	0	2	0
All	All	30320	0	30816	732	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 12.

The worst 5 of 732 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:H:204:ALA:O	1:H:208:LEU:HB2	1.77	0.83
1:D:200:GLN:O	1:D:204:ALA:HB2	1.79	0.81
1:E:197:GLU:HB3	1:E:201:ARG:HH12	1.51	0.76
1:H:254:LEU:HD23	1:H:257:LEU:HD12	1.70	0.72
1:H:156:ASN:OD1	1:H:159:ARG:NH2	2.19	0.72

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	483/732 (66%)	467 (97%)	16 (3%)	0	100 100

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	483/732 (66%)	471 (98%)	12 (2%)	0	100	100
1	C	483/732 (66%)	463 (96%)	20 (4%)	0	100	100
1	D	483/732 (66%)	465 (96%)	18 (4%)	0	100	100
1	E	483/732 (66%)	468 (97%)	15 (3%)	0	100	100
1	F	483/732 (66%)	463 (96%)	20 (4%)	0	100	100
1	G	483/732 (66%)	468 (97%)	15 (3%)	0	100	100
1	H	483/732 (66%)	463 (96%)	20 (4%)	0	100	100
All	All	3864/5856 (66%)	3728 (96%)	136 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	396/598 (66%)	396 (100%)	0	100	100
1	B	396/598 (66%)	396 (100%)	0	100	100
1	C	396/598 (66%)	396 (100%)	0	100	100
1	D	396/598 (66%)	396 (100%)	0	100	100
1	E	396/598 (66%)	396 (100%)	0	100	100
1	F	396/598 (66%)	396 (100%)	0	100	100
1	G	396/598 (66%)	396 (100%)	0	100	100
1	H	396/598 (66%)	396 (100%)	0	100	100
All	All	3168/4784 (66%)	3168 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	359	GLN
1	H	134	GLN
1	E	200	GLN
1	G	134	GLN
1	E	134	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	A1EIV	G	801	-	19,21,21	2.64	5 (26%)	23,31,31	1.74	6 (26%)
2	A1EIV	H	801	-	19,21,21	2.58	5 (26%)	23,31,31	1.76	6 (26%)
2	A1EIV	A	801	-	19,21,21	2.63	5 (26%)	23,31,31	1.77	6 (26%)
2	A1EIV	C	801	-	19,21,21	2.64	5 (26%)	23,31,31	1.82	7 (30%)
2	A1EIV	D	801	-	19,21,21	2.64	5 (26%)	23,31,31	1.86	7 (30%)
2	A1EIV	F	801	-	19,21,21	2.57	5 (26%)	23,31,31	1.81	7 (30%)
2	A1EIV	B	801	-	19,21,21	2.64	5 (26%)	23,31,31	1.77	6 (26%)
2	A1EIV	E	801	-	19,21,21	2.65	5 (26%)	23,31,31	1.77	6 (26%)

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	A1EIV	G	801	-	-	3/10/26/26	0/2/2/2
2	A1EIV	H	801	-	-	4/10/26/26	0/2/2/2
2	A1EIV	A	801	-	-	5/10/26/26	0/2/2/2
2	A1EIV	C	801	-	-	4/10/26/26	0/2/2/2
2	A1EIV	D	801	-	-	1/10/26/26	0/2/2/2
2	A1EIV	F	801	-	-	3/10/26/26	0/2/2/2
2	A1EIV	B	801	-	-	2/10/26/26	0/2/2/2
2	A1EIV	E	801	-	-	0/10/26/26	0/2/2/2

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	A1EIV	P10-O09	9.11	1.89	1.60
2	D	801	A1EIV	P10-O09	9.09	1.89	1.60
2	B	801	A1EIV	P10-O09	9.01	1.88	1.60
2	A	801	A1EIV	P10-O09	8.98	1.88	1.60
2	E	801	A1EIV	P10-O09	8.95	1.88	1.60

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	801	A1EIV	O11-P10-O09	-4.27	95.52	106.67
2	A	801	A1EIV	O11-P10-O09	-4.26	95.56	106.67
2	H	801	A1EIV	O11-P10-O09	-4.22	95.67	106.67
2	G	801	A1EIV	O11-P10-O09	-4.20	95.73	106.67
2	B	801	A1EIV	O11-P10-O09	-4.18	95.76	106.67

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

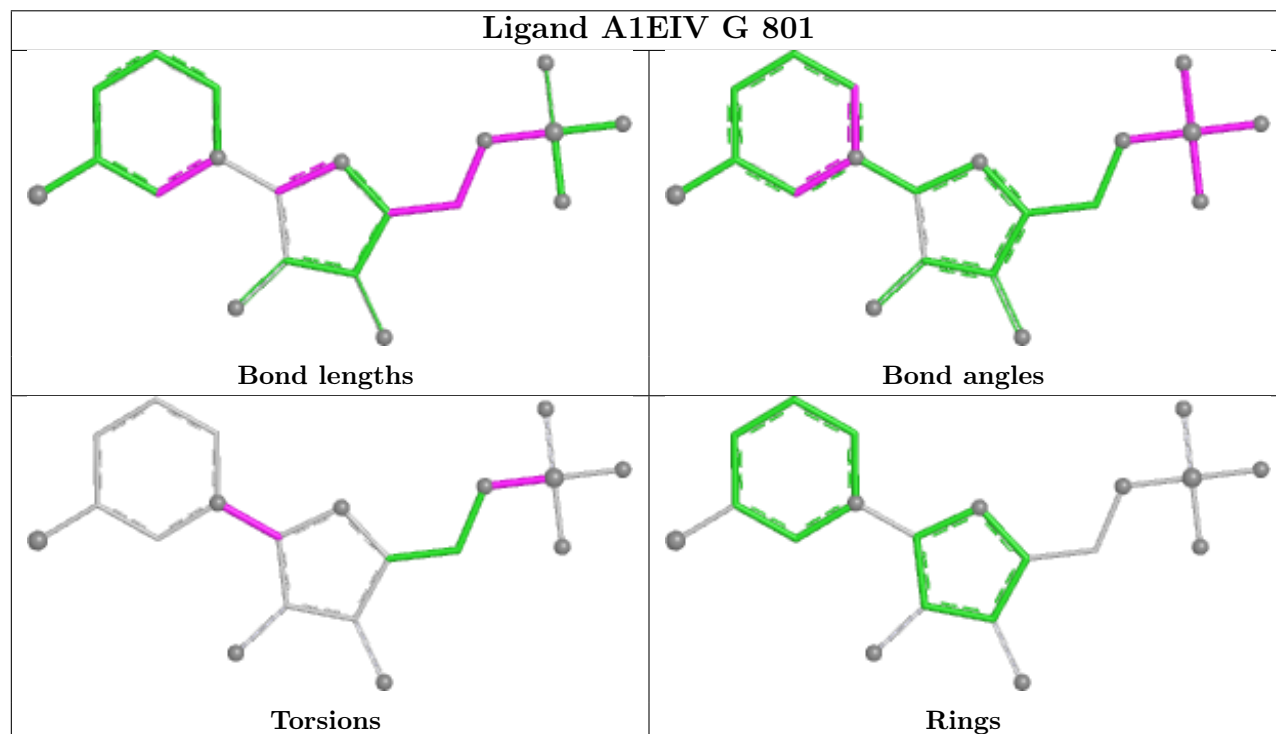
Mol	Chain	Res	Type	Atoms
2	A	801	A1EIV	O06-C07-C08-O09
2	A	801	A1EIV	C08-O09-P10-O11
2	A	801	A1EIV	C08-O09-P10-O12
2	B	801	A1EIV	C02-C07-C08-O09
2	B	801	A1EIV	O06-C07-C08-O09

There are no ring outliers.

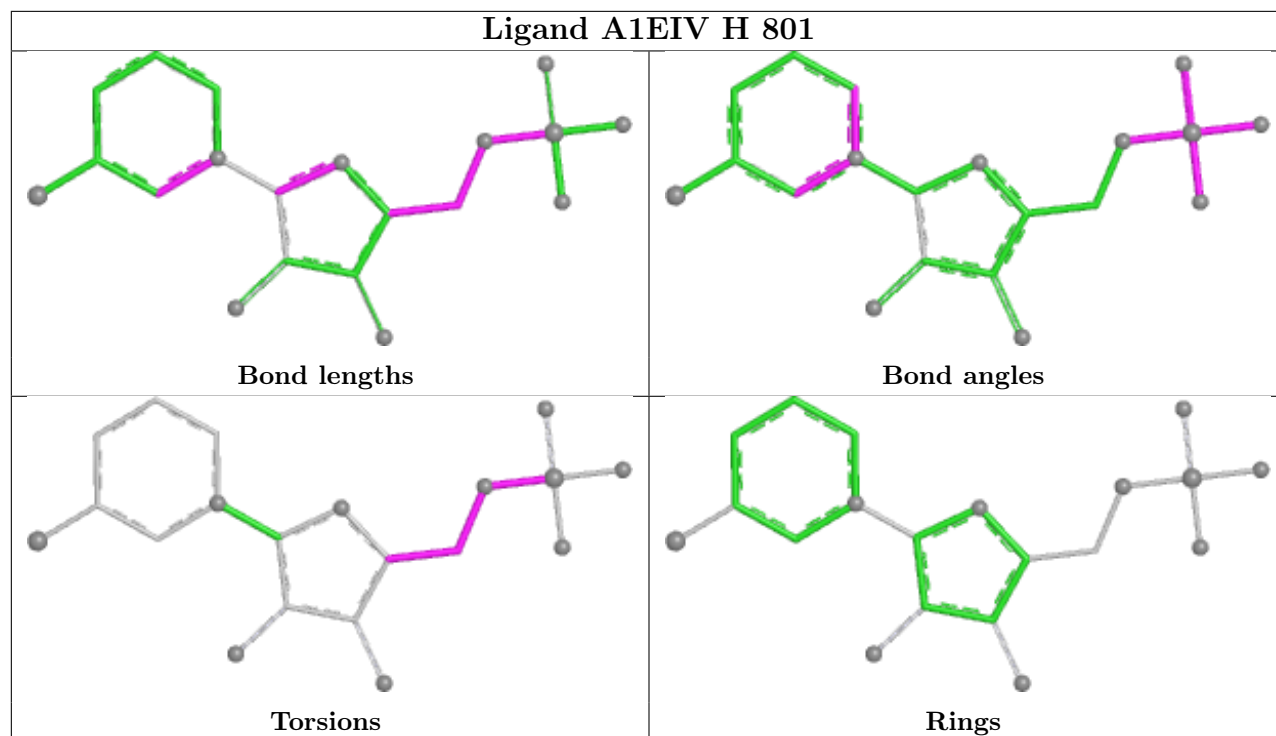
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	801	A1EIV	1	0
2	H	801	A1EIV	2	0
2	A	801	A1EIV	2	0
2	C	801	A1EIV	2	0
2	D	801	A1EIV	2	0
2	F	801	A1EIV	2	0
2	B	801	A1EIV	1	0
2	E	801	A1EIV	2	0

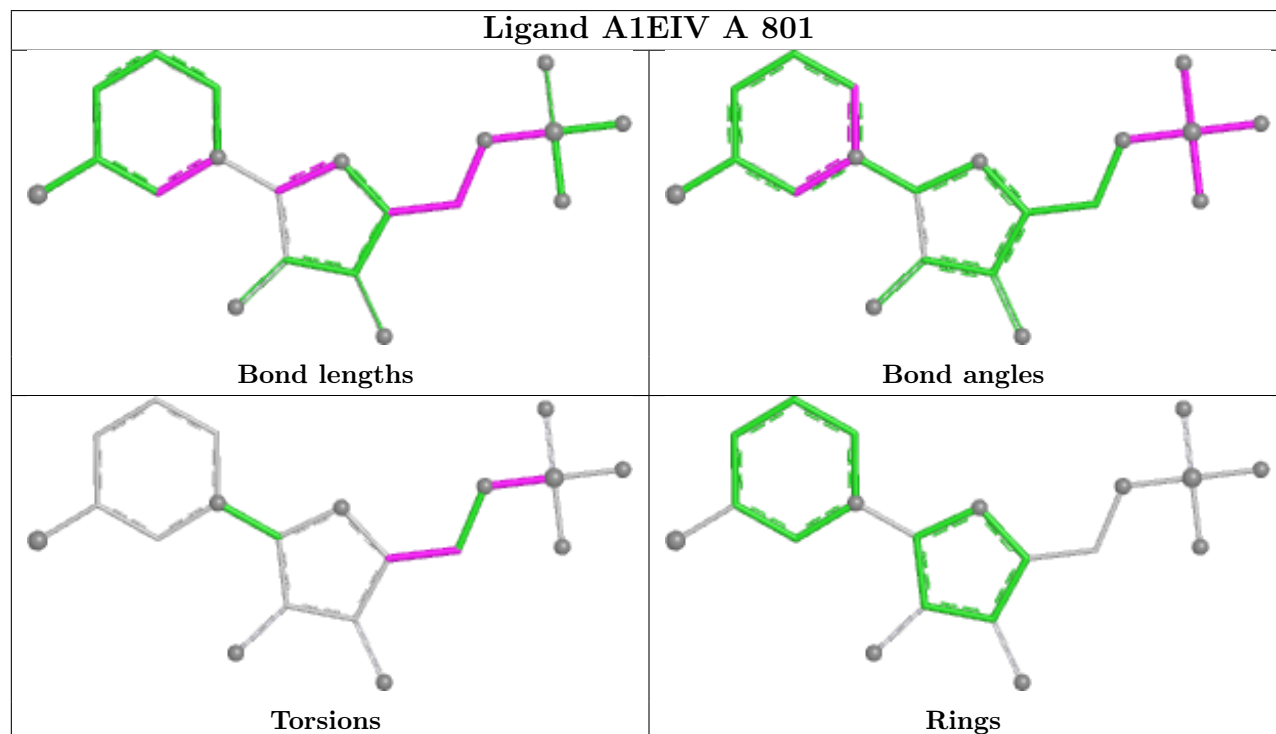
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

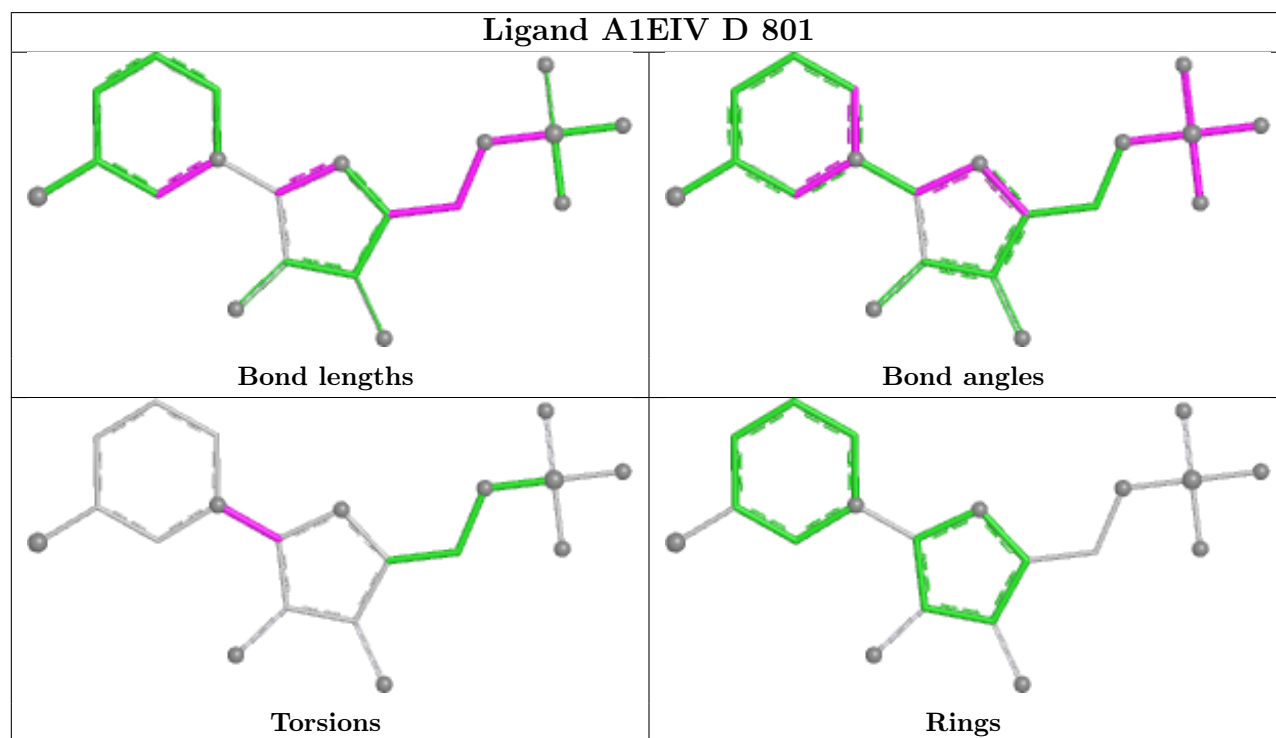
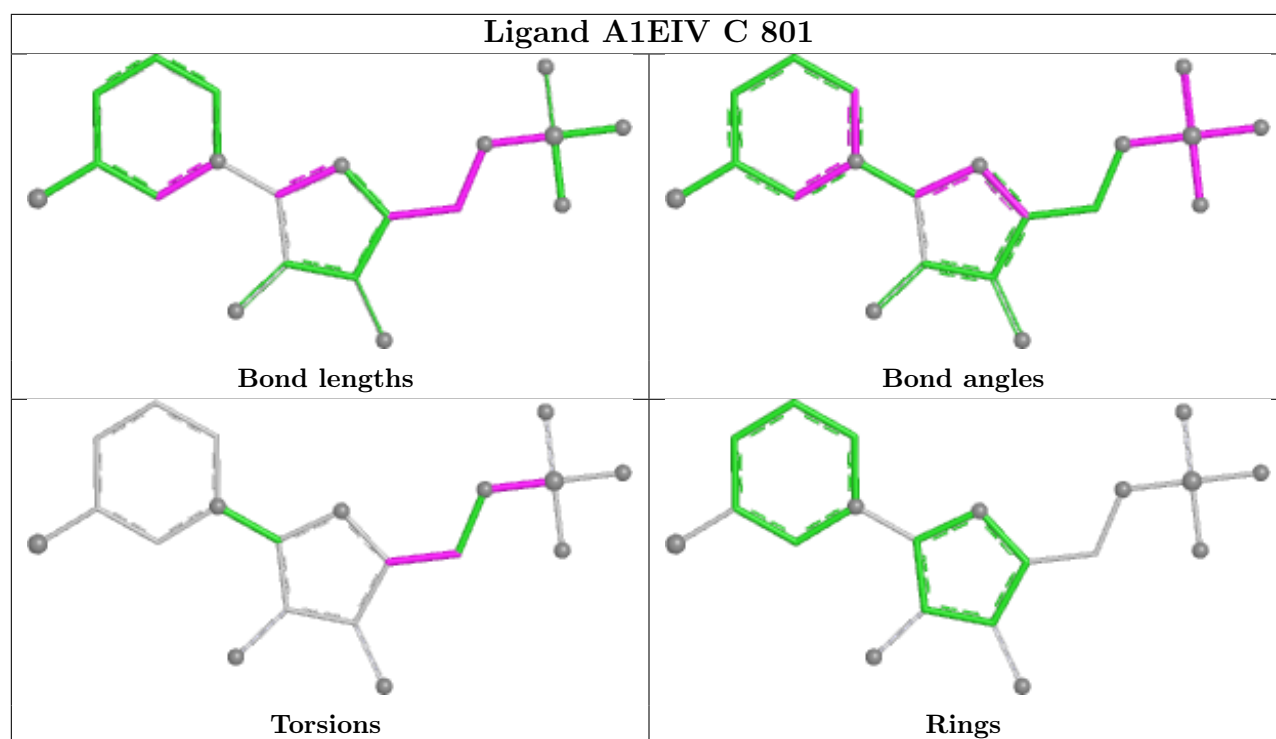


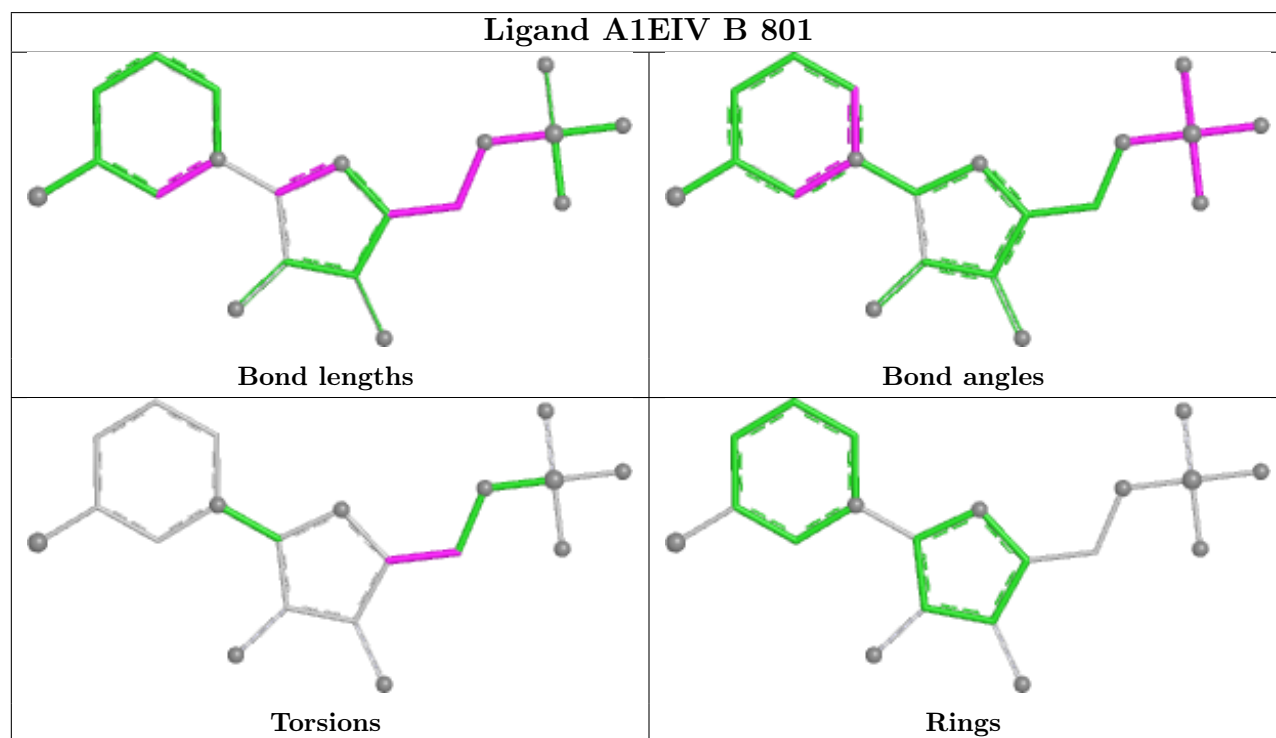
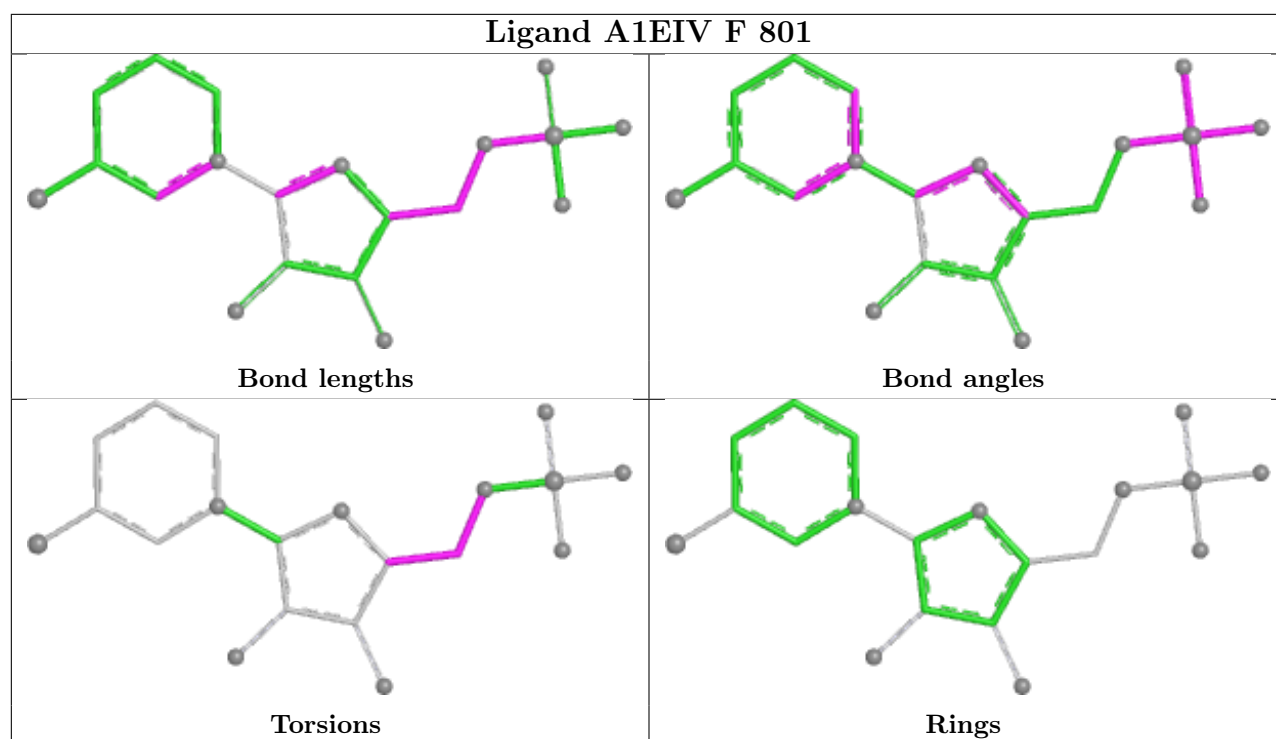
Ligand A1EIV H 801

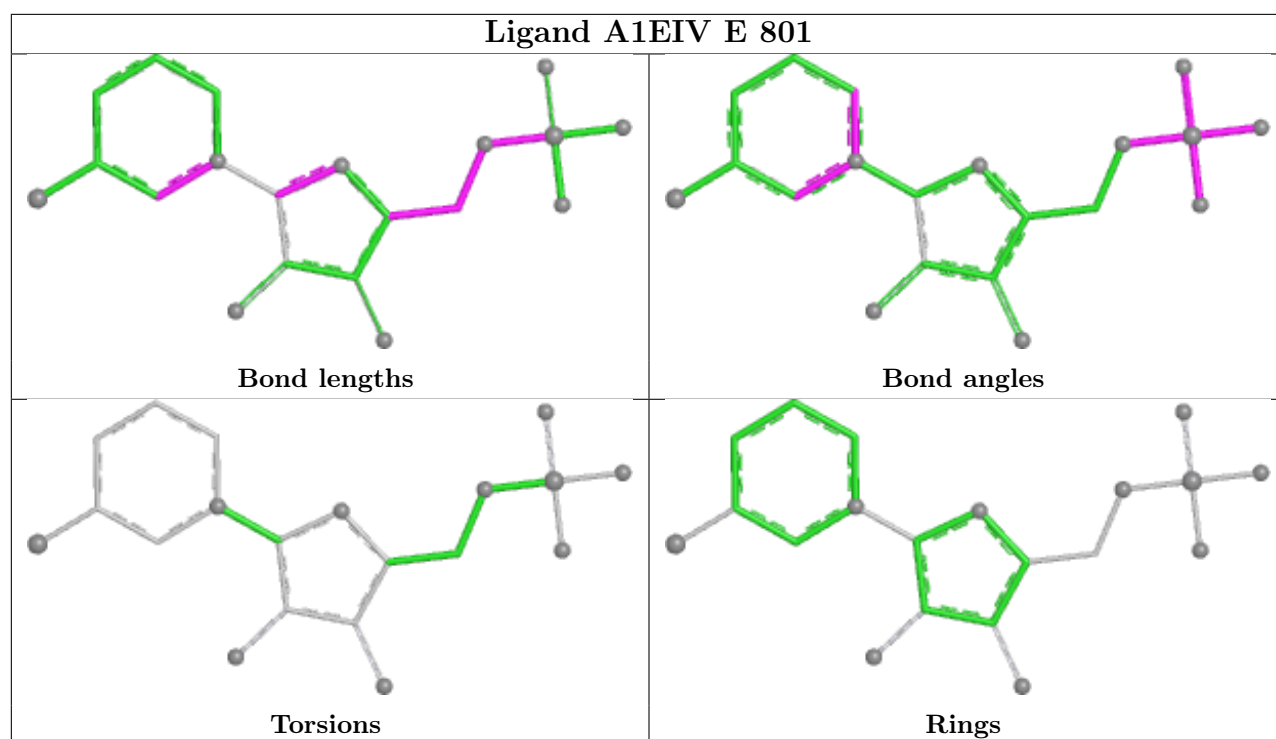


Ligand A1EIV A 801









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

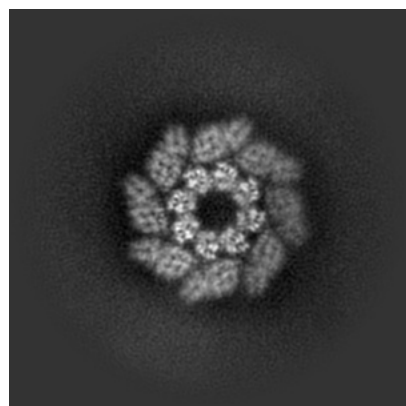
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62774. These allow visual inspection of the internal detail of the map and identification of artifacts.

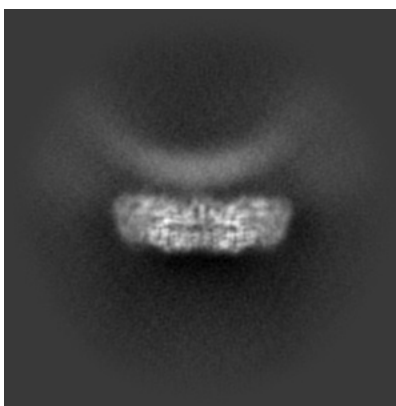
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

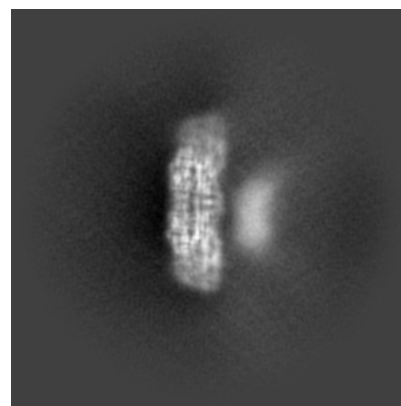
6.1.1 Primary map



X

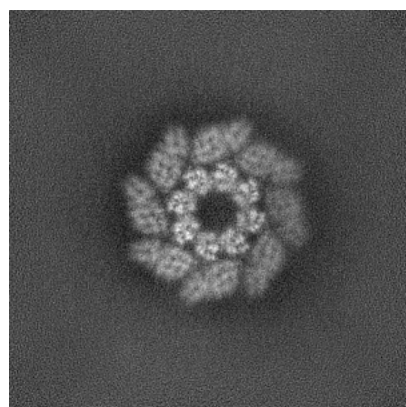


Y

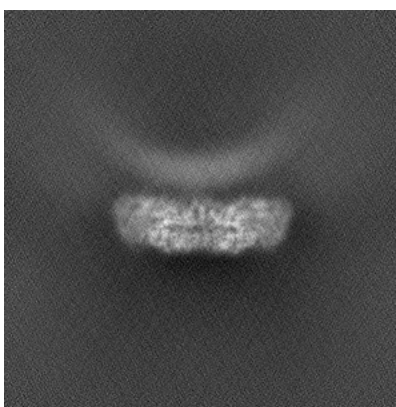


Z

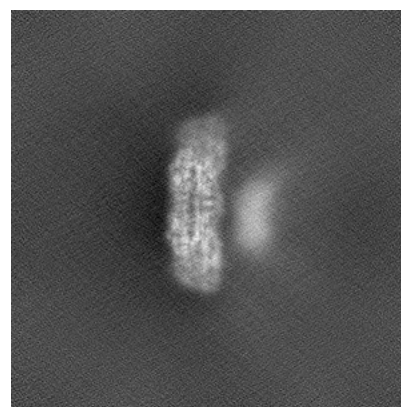
6.1.2 Raw map



X



Y

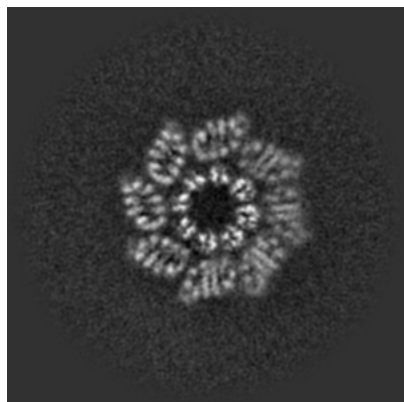


Z

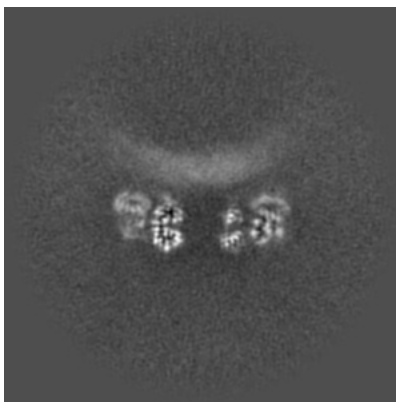
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

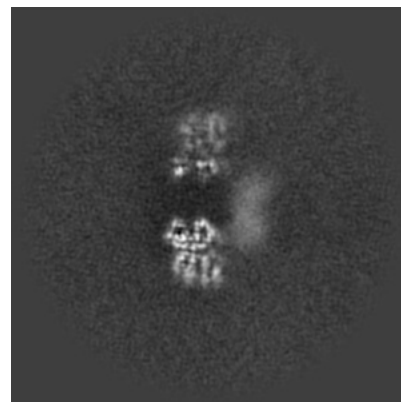
6.2.1 Primary map



X Index: 170

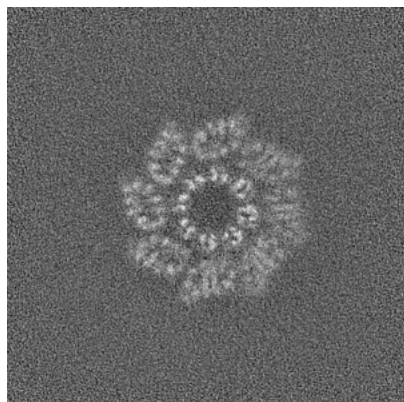


Y Index: 170

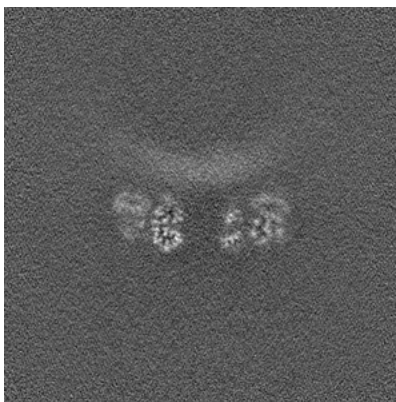


Z Index: 170

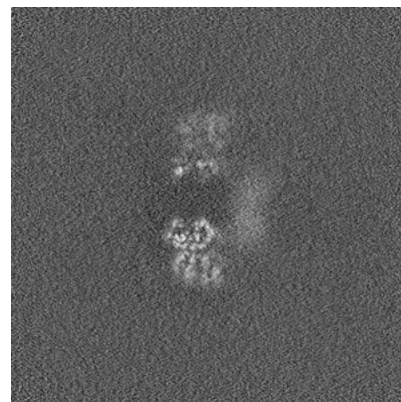
6.2.2 Raw map



X Index: 170



Y Index: 170

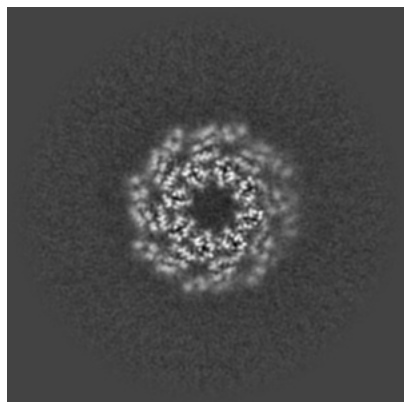


Z Index: 170

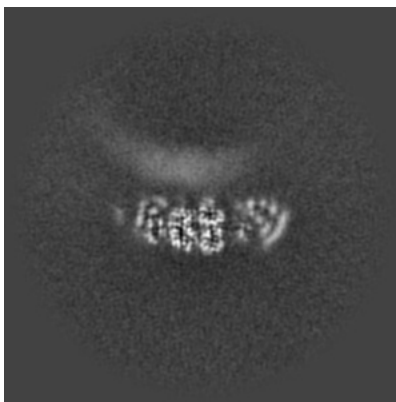
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

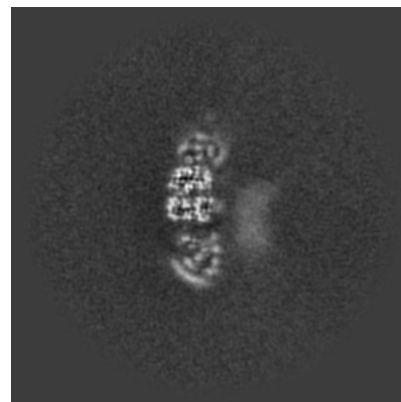
6.3.1 Primary map



X Index: 148

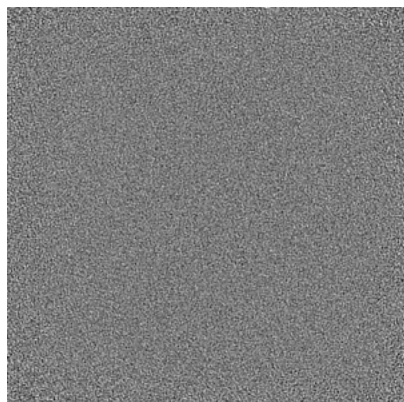


Y Index: 145

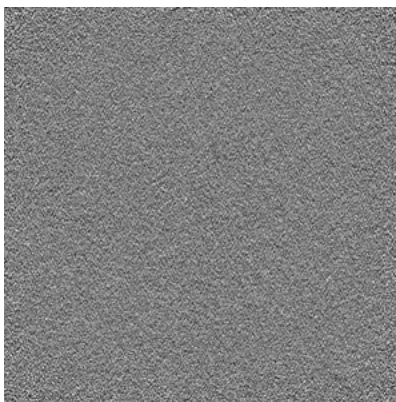


Z Index: 137

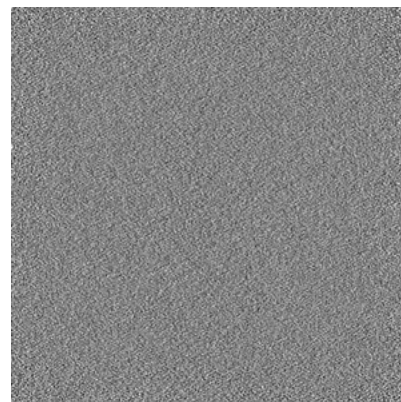
6.3.2 Raw map



X Index: 0



Y Index: 0

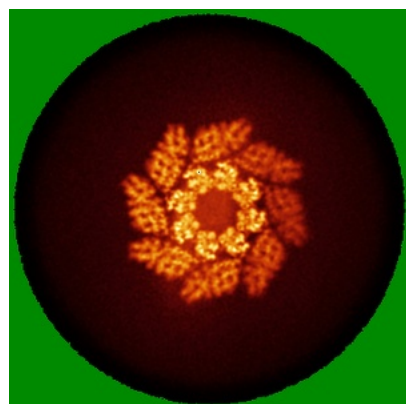


Z Index: 339

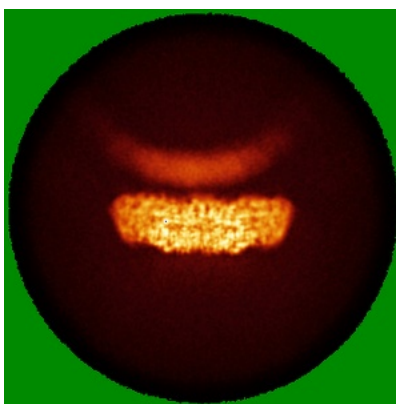
The images above show the largest variance slices of the map in three orthogonal directions.

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

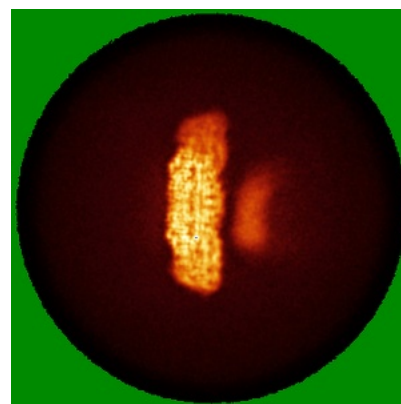
6.4.1 Primary map



X

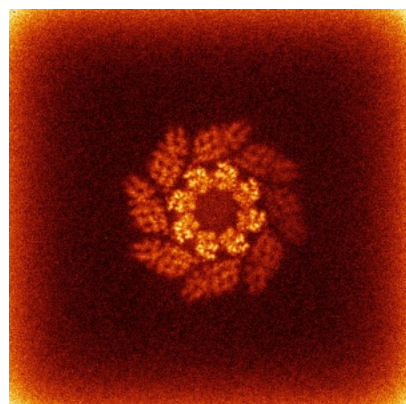


Y

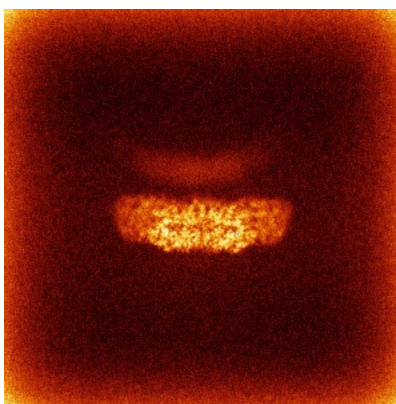


Z

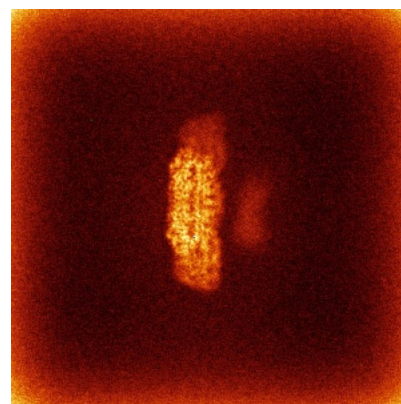
6.4.2 Raw map



X



Y

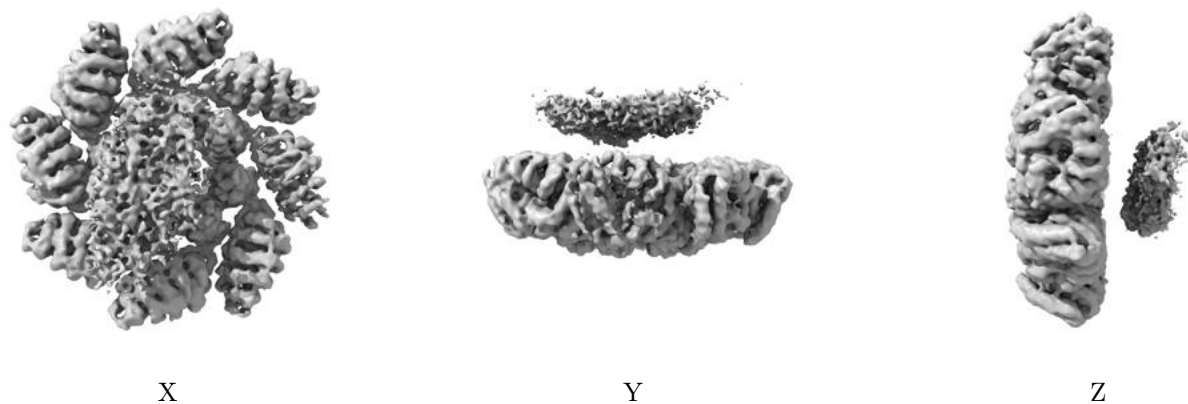


Z

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.

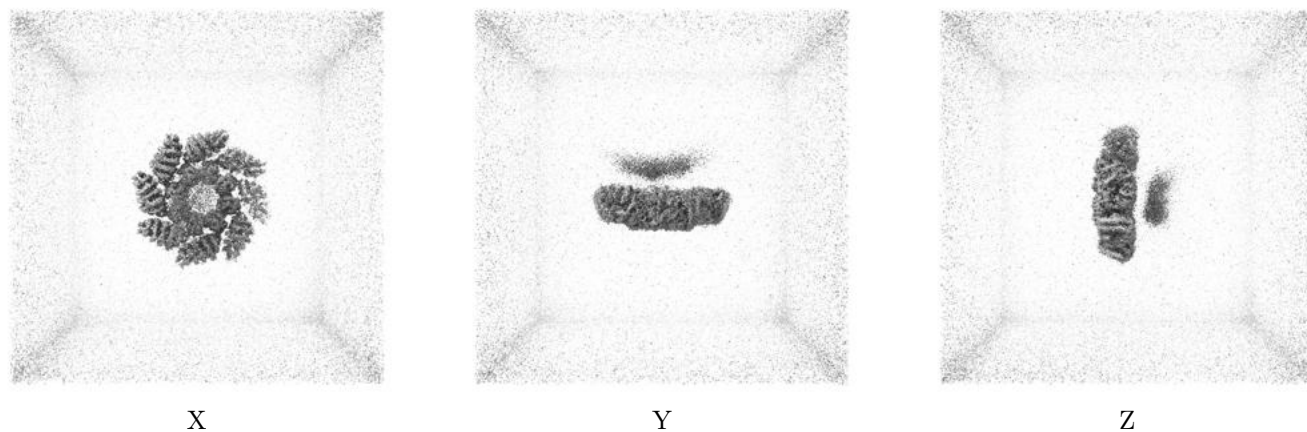
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.226. 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.

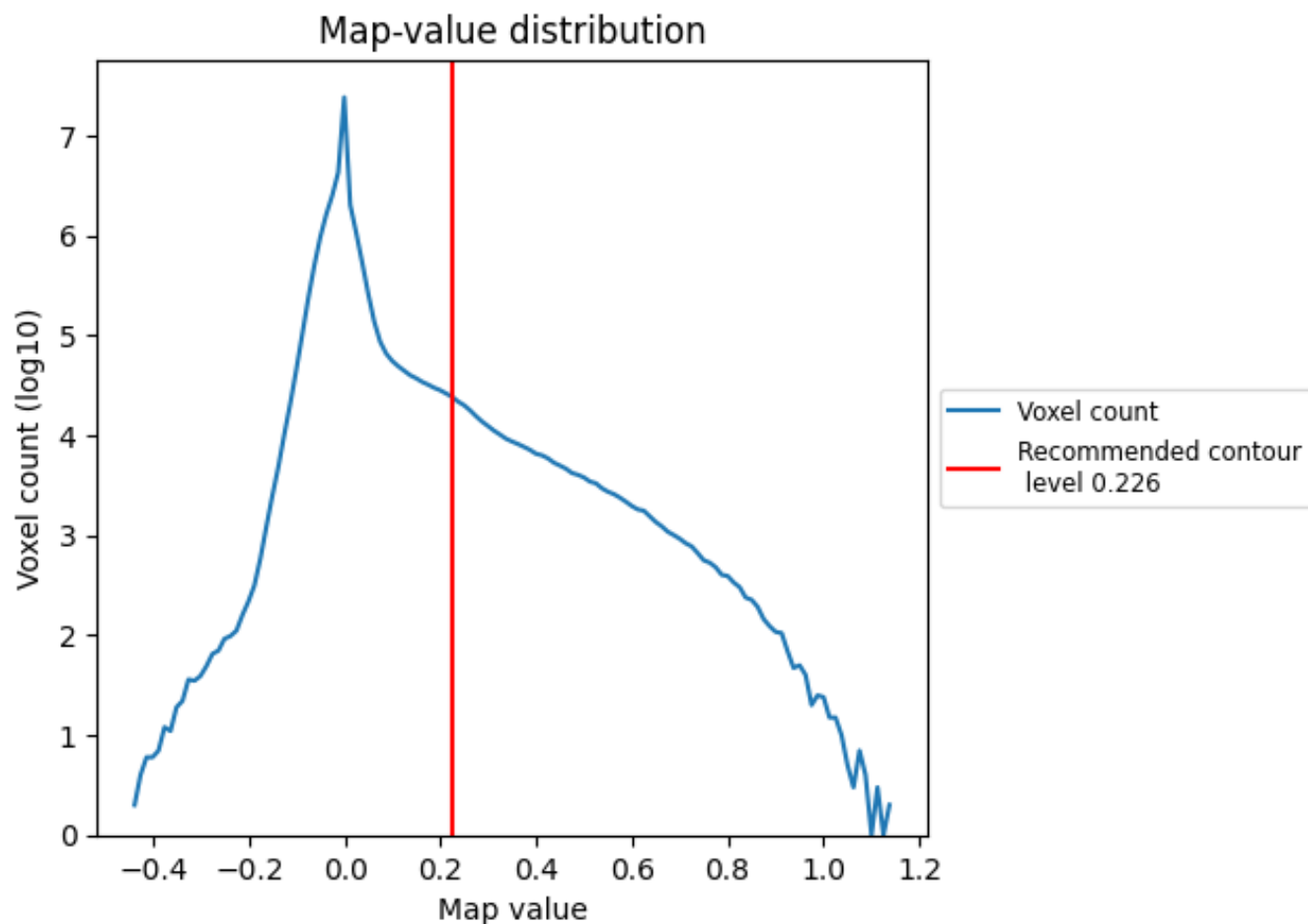
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

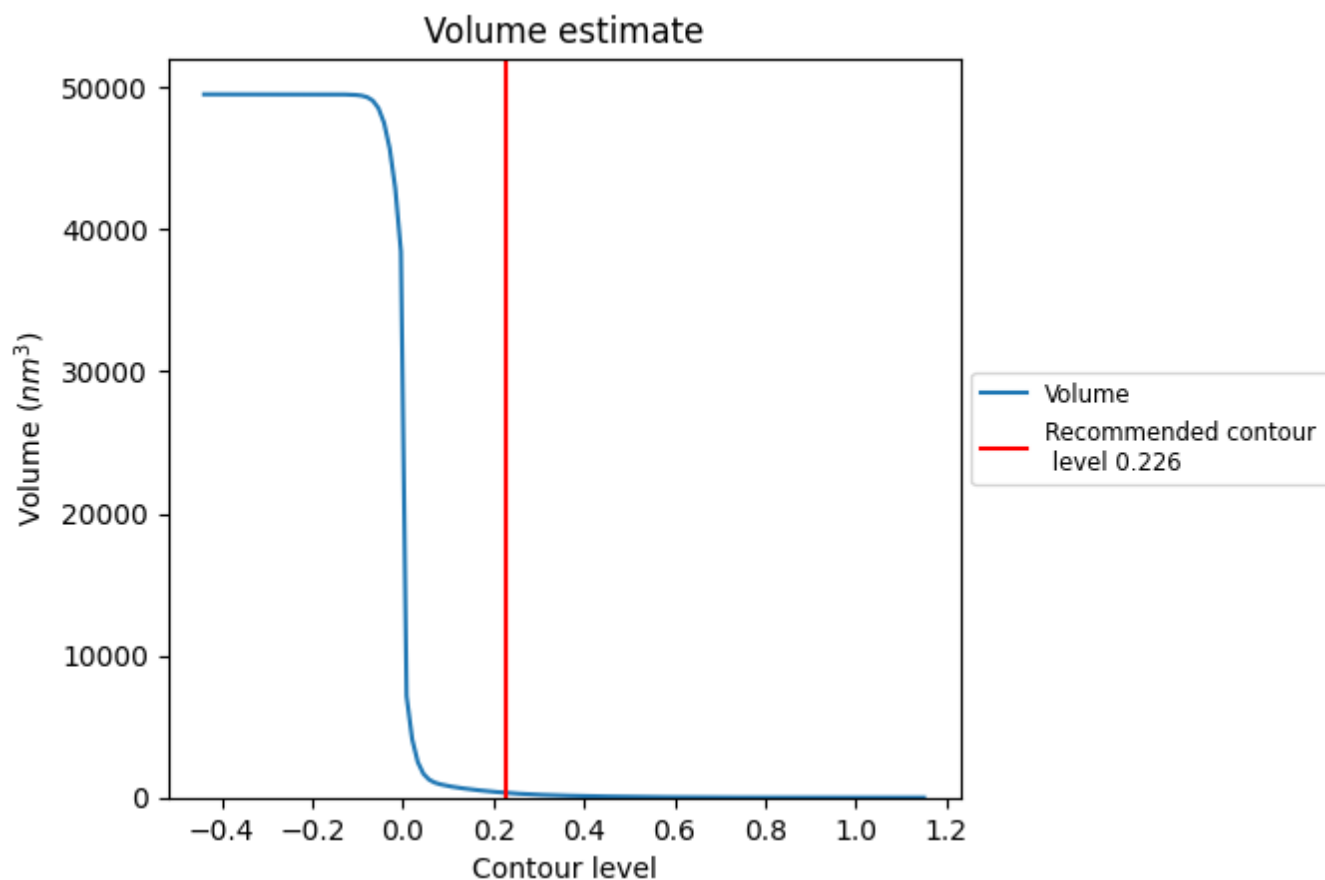
This section contains the results of statistical analysis of the map.

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.

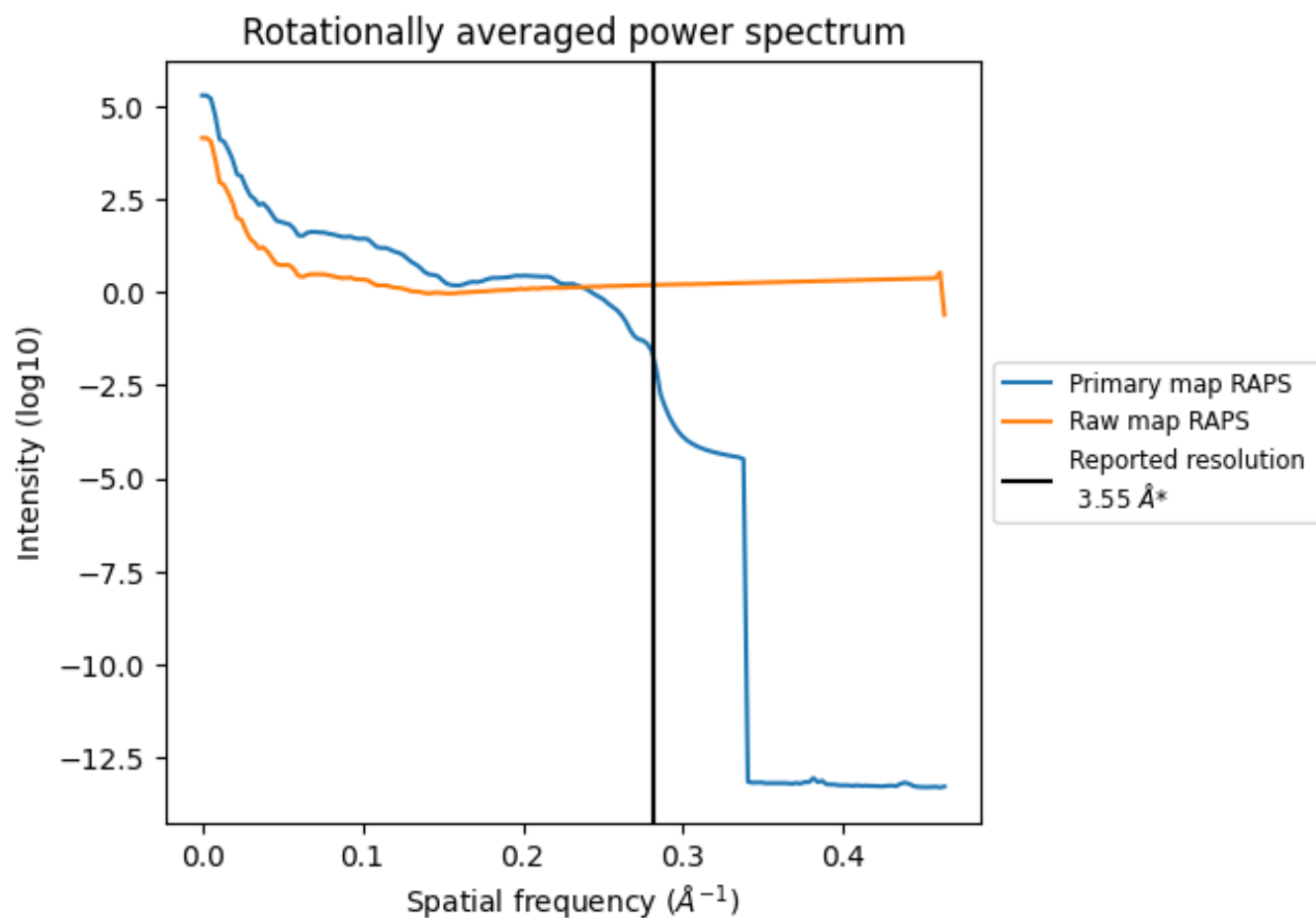
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm³; this corresponds to an approximate mass of 307 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 ⓘ

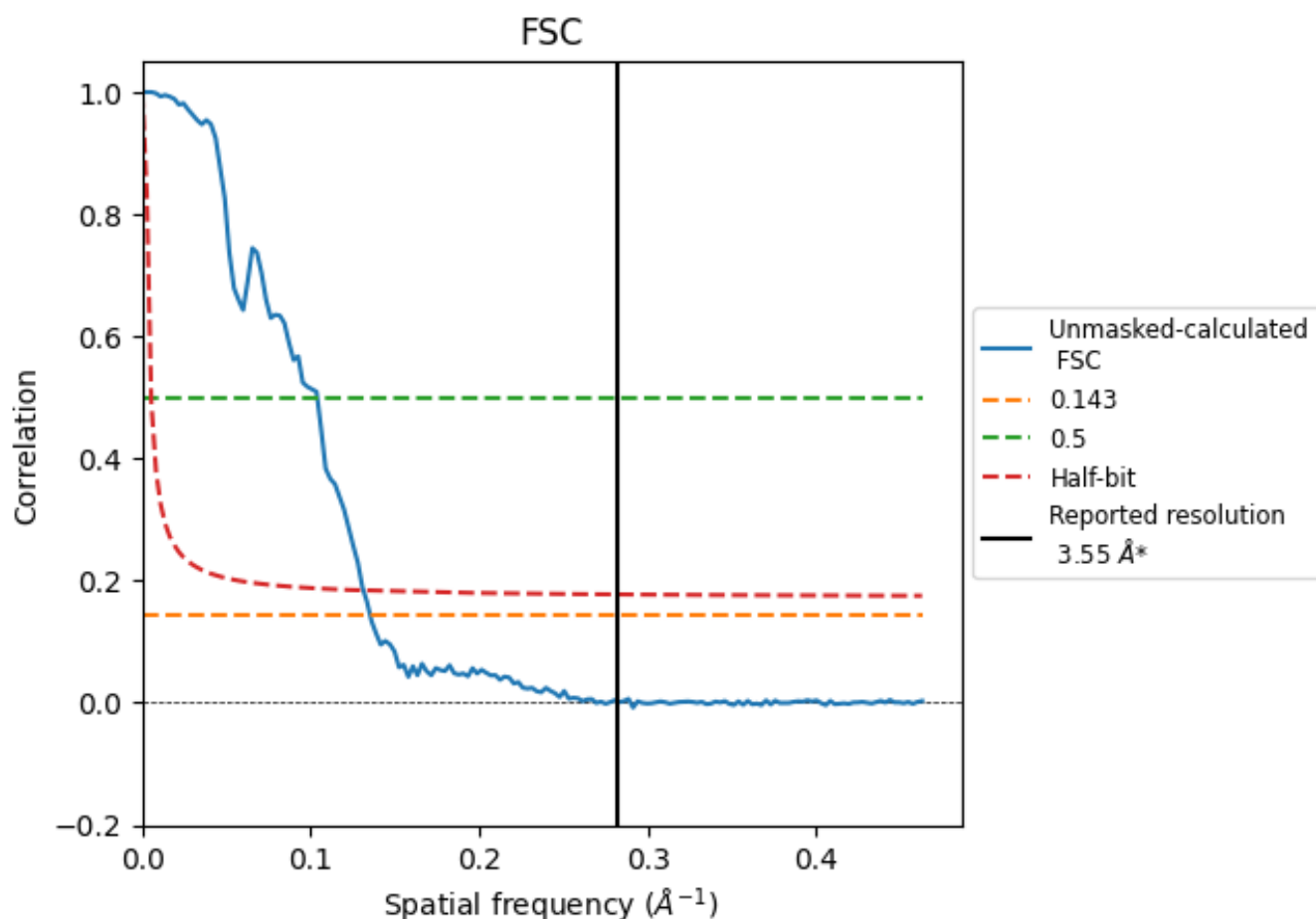


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

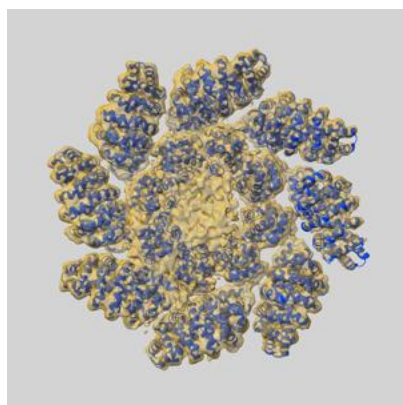
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.39	9.62	7.62

*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 7.39 differs from the reported value 3.55 by more than 10 %

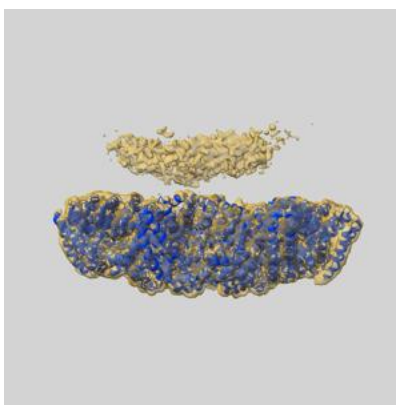
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62774 and PDB model 9L2F. Per-residue inclusion information can be found in section [3](#) on page [8](#).

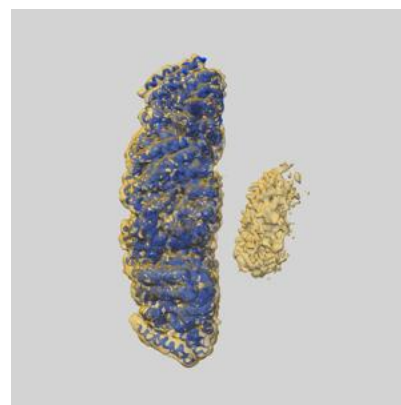
9.1 Map-model overlay [i](#)



X



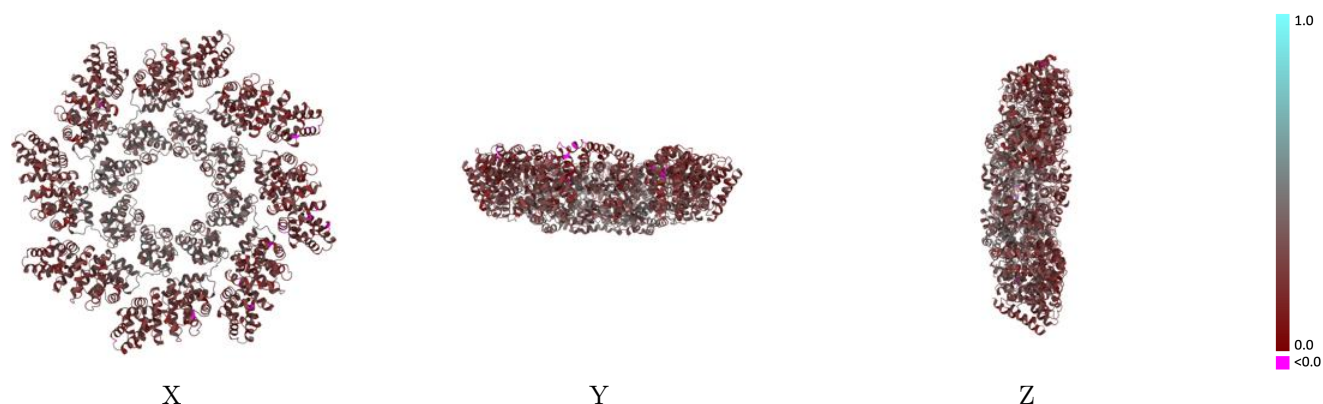
Y



Z

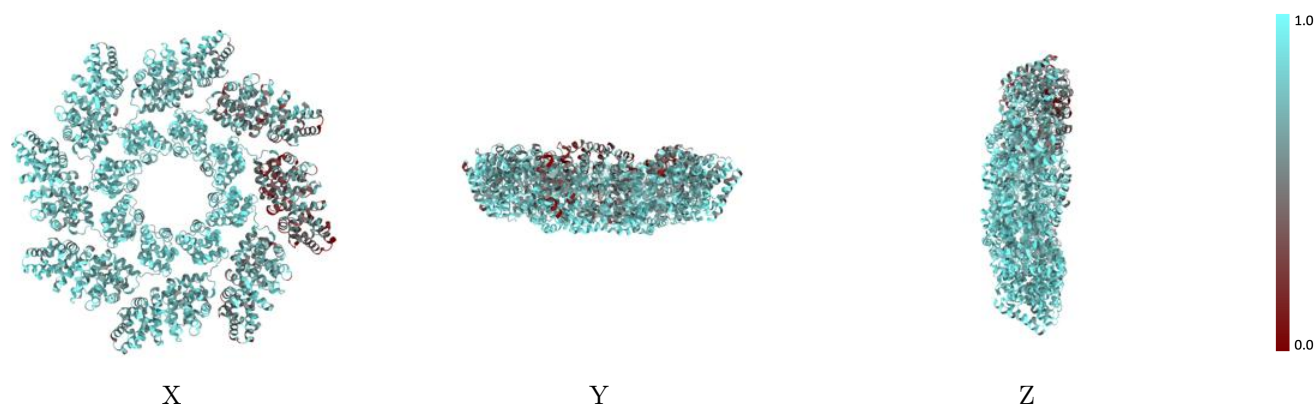
The images above show the 3D surface view of the map at the recommended contour level 0.226 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



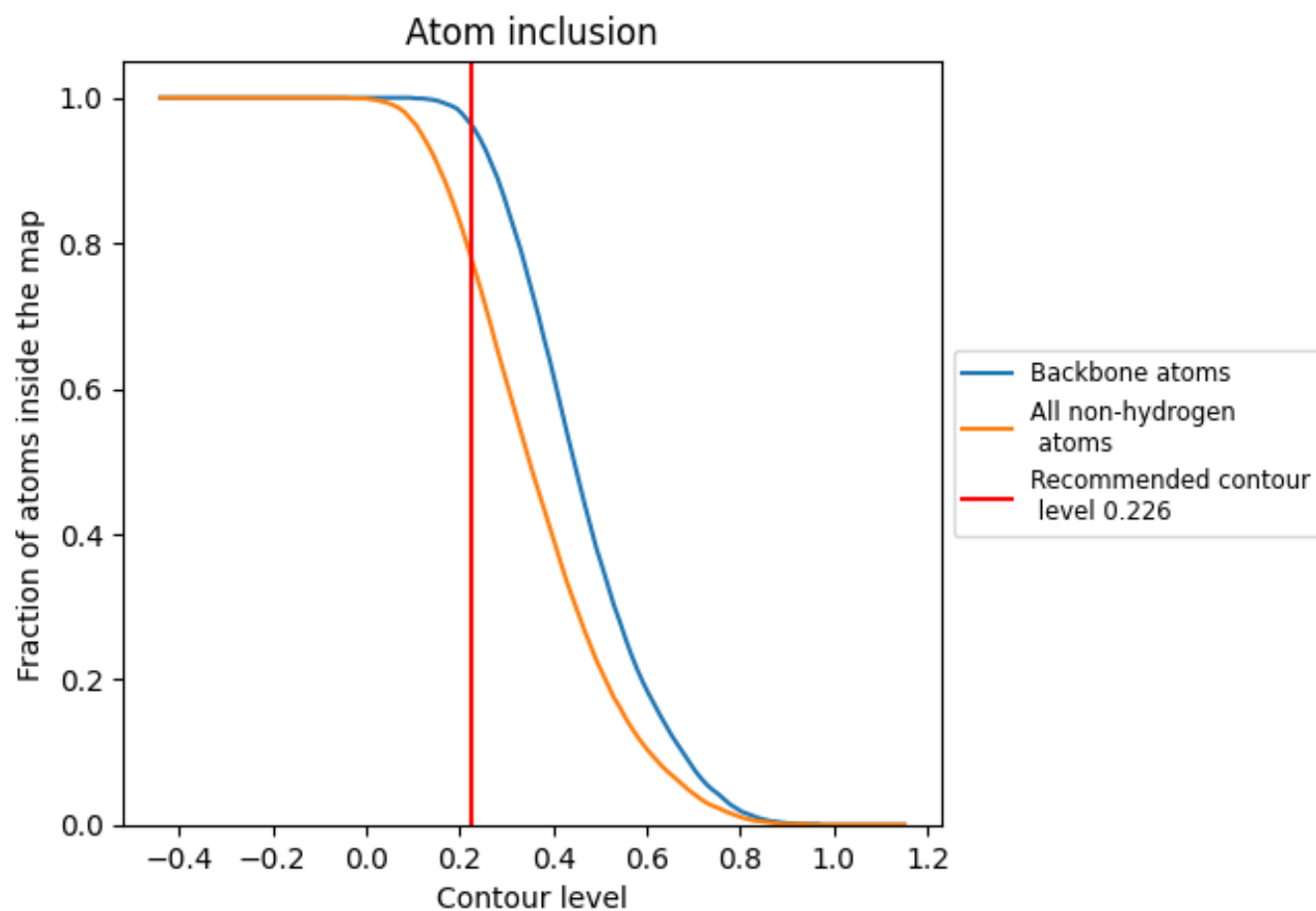
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.226).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (0.226) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7770	0.2980
A	0.8210	0.3010
B	0.7140	0.2840
C	0.5850	0.2750
D	0.7520	0.2900
E	0.8240	0.2970
F	0.8340	0.3100
G	0.8390	0.3140
H	0.8480	0.3130

1.0

0.0

<0.0