



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2025 – 04:27 PM JST

PDB ID : 9J3E / pdb_00009j3e
EMDB ID : EMD-61115
Title : Cryo-EM structure of TMexCD1-TOprJ1 in complex with 1-(1-naphthylmet
hyl)piperazine
Authors : Shi, Y.; Feng, Y.
Deposited on : 2024-08-08
Resolution : 3.00 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.dev126
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

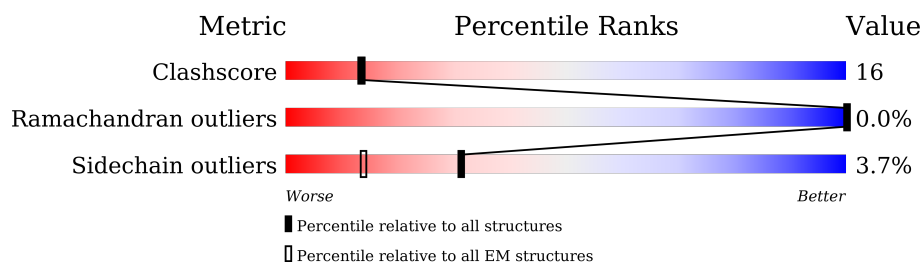
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	483	<div> <div>8%</div> <div>59%</div> <div>24%</div> <div>•</div> <div>17%</div> </div>
1	B	483	<div> <div>7%</div> <div>60%</div> <div>23%</div> <div>•</div> <div>17%</div> </div>
1	C	483	<div> <div>7%</div> <div>62%</div> <div>21%</div> <div>•</div> <div>17%</div> </div>
2	D	395	<div> <div>66%</div> <div>18%</div> <div>•</div> <div>14%</div> </div>
2	E	395	<div> <div>10%</div> <div>62%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>
2	F	395	<div> <div>66%</div> <div>19%</div> <div>•</div> <div>14%</div> </div>
2	G	395	<div> <div>10%</div> <div>59%</div> <div>26%</div> <div>•</div> <div>14%</div> </div>
2	H	395	<div> <div>67%</div> <div>18%</div> <div>•</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	395	<div><div></div><div>10%</div><div>60%</div><div>26%</div><div>14%</div></div>
3	J	1044	<div><div></div><div>56%</div><div>41%</div><div>..</div></div>
3	K	1044	<div><div></div><div>5%</div><div>57%</div><div>40%</div><div>..</div></div>
3	L	1044	<div><div></div><div>5%</div><div>59%</div><div>38%</div><div>..</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47916 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 RND efflux system, OprJ-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	402	Total	C	N	O	S	0	0
			3065	1876	576	609	4		
1	B	402	Total	C	N	O	S	0	0
			3065	1876	576	609	4		
1	C	402	Total	C	N	O	S	0	0
			3065	1876	576	609	4		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	478	HIS	-	expression tag	UNP A0A411AKN6
A	479	HIS	-	expression tag	UNP A0A411AKN6
A	480	HIS	-	expression tag	UNP A0A411AKN6
A	481	HIS	-	expression tag	UNP A0A411AKN6
A	482	HIS	-	expression tag	UNP A0A411AKN6
A	483	HIS	-	expression tag	UNP A0A411AKN6
B	478	HIS	-	expression tag	UNP A0A411AKN6
B	479	HIS	-	expression tag	UNP A0A411AKN6
B	480	HIS	-	expression tag	UNP A0A411AKN6
B	481	HIS	-	expression tag	UNP A0A411AKN6
B	482	HIS	-	expression tag	UNP A0A411AKN6
B	483	HIS	-	expression tag	UNP A0A411AKN6
C	478	HIS	-	expression tag	UNP A0A411AKN6
C	479	HIS	-	expression tag	UNP A0A411AKN6
C	480	HIS	-	expression tag	UNP A0A411AKN6
C	481	HIS	-	expression tag	UNP A0A411AKN6
C	482	HIS	-	expression tag	UNP A0A411AKN6
C	483	HIS	-	expression tag	UNP A0A411AKN6

- Molecule 2 is a protein called RND efflux system, MexC-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	338	Total 2543	C 1580	N 471	O 487	S 5	0	0
2	E	338	Total 2543	C 1580	N 471	O 487	S 5	0	0
2	F	338	Total 2543	C 1580	N 471	O 487	S 5	0	0
2	G	338	Total 2543	C 1580	N 471	O 487	S 5	0	0
2	H	338	Total 2543	C 1580	N 471	O 487	S 5	0	0
2	I	338	Total 2543	C 1580	N 471	O 487	S 5	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	388	TRP	-	expression tag	UNP A0A411AKL2
D	389	SER	-	expression tag	UNP A0A411AKL2
D	390	HIS	-	expression tag	UNP A0A411AKL2
D	391	PRO	-	expression tag	UNP A0A411AKL2
D	392	GLN	-	expression tag	UNP A0A411AKL2
D	393	PHE	-	expression tag	UNP A0A411AKL2
D	394	GLU	-	expression tag	UNP A0A411AKL2
D	395	LYS	-	expression tag	UNP A0A411AKL2
E	388	TRP	-	expression tag	UNP A0A411AKL2
E	389	SER	-	expression tag	UNP A0A411AKL2
E	390	HIS	-	expression tag	UNP A0A411AKL2
E	391	PRO	-	expression tag	UNP A0A411AKL2
E	392	GLN	-	expression tag	UNP A0A411AKL2
E	393	PHE	-	expression tag	UNP A0A411AKL2
E	394	GLU	-	expression tag	UNP A0A411AKL2
E	395	LYS	-	expression tag	UNP A0A411AKL2
F	388	TRP	-	expression tag	UNP A0A411AKL2
F	389	SER	-	expression tag	UNP A0A411AKL2
F	390	HIS	-	expression tag	UNP A0A411AKL2
F	391	PRO	-	expression tag	UNP A0A411AKL2
F	392	GLN	-	expression tag	UNP A0A411AKL2
F	393	PHE	-	expression tag	UNP A0A411AKL2
F	394	GLU	-	expression tag	UNP A0A411AKL2
F	395	LYS	-	expression tag	UNP A0A411AKL2
G	388	TRP	-	expression tag	UNP A0A411AKL2
G	389	SER	-	expression tag	UNP A0A411AKL2
G	390	HIS	-	expression tag	UNP A0A411AKL2
G	391	PRO	-	expression tag	UNP A0A411AKL2

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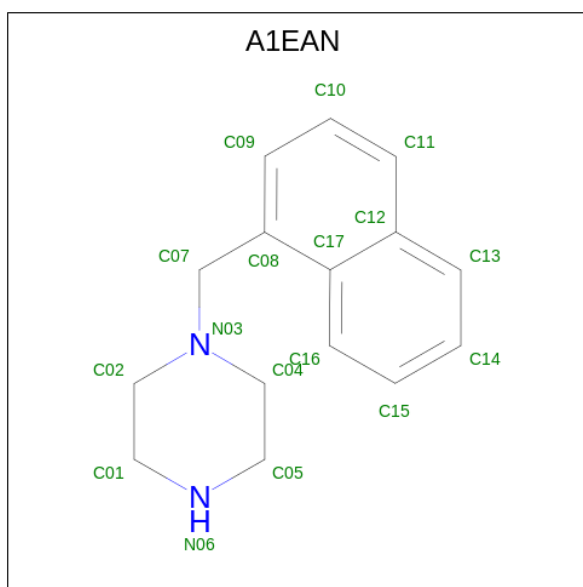
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	392	GLN	-	expression tag	UNP A0A411AKL2
G	393	PHE	-	expression tag	UNP A0A411AKL2
G	394	GLU	-	expression tag	UNP A0A411AKL2
G	395	LYS	-	expression tag	UNP A0A411AKL2
H	388	TRP	-	expression tag	UNP A0A411AKL2
H	389	SER	-	expression tag	UNP A0A411AKL2
H	390	HIS	-	expression tag	UNP A0A411AKL2
H	391	PRO	-	expression tag	UNP A0A411AKL2
H	392	GLN	-	expression tag	UNP A0A411AKL2
H	393	PHE	-	expression tag	UNP A0A411AKL2
H	394	GLU	-	expression tag	UNP A0A411AKL2
H	395	LYS	-	expression tag	UNP A0A411AKL2
I	388	TRP	-	expression tag	UNP A0A411AKL2
I	389	SER	-	expression tag	UNP A0A411AKL2
I	390	HIS	-	expression tag	UNP A0A411AKL2
I	391	PRO	-	expression tag	UNP A0A411AKL2
I	392	GLN	-	expression tag	UNP A0A411AKL2
I	393	PHE	-	expression tag	UNP A0A411AKL2
I	394	GLU	-	expression tag	UNP A0A411AKL2
I	395	LYS	-	expression tag	UNP A0A411AKL2

- Molecule 3 is a protein called Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	1032	Total	C	N	O	S	0	0
			7804	5030	1295	1445	34		
3	J	1032	Total	C	N	O	S	0	0
			7804	5030	1295	1445	34		
3	L	1032	Total	C	N	O	S	0	0
			7804	5030	1295	1445	34		

- Molecule 4 is 1-(naphthalen-1-ylmethyl)piperazine (CCD ID: A1EAN) (formula: C₁₅H₁₈N₂) (labeled as "Ligand of Interest" by depositor).

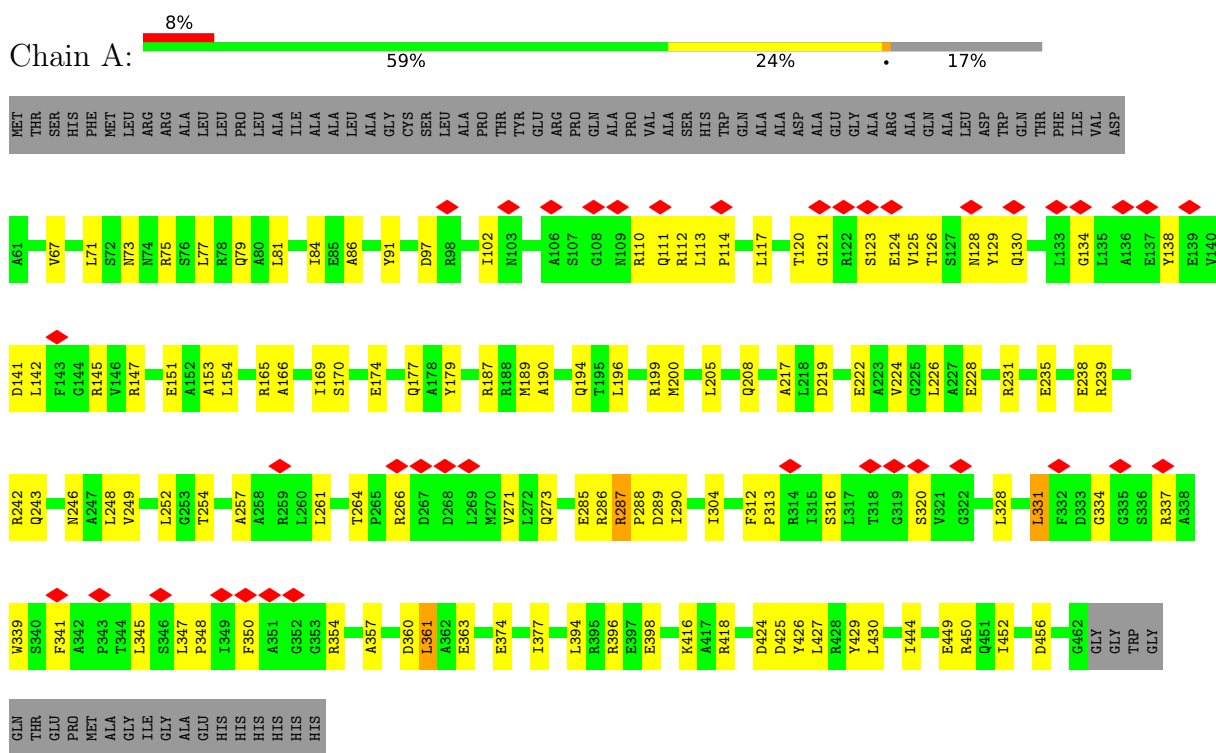


Mol	Chain	Residues	Atoms			AltConf
4	K	1	Total	C	N	0
			17	15	2	
4	J	1	Total	C	N	0
			17	15	2	
4	L	1	Total	C	N	0
			17	15	2	

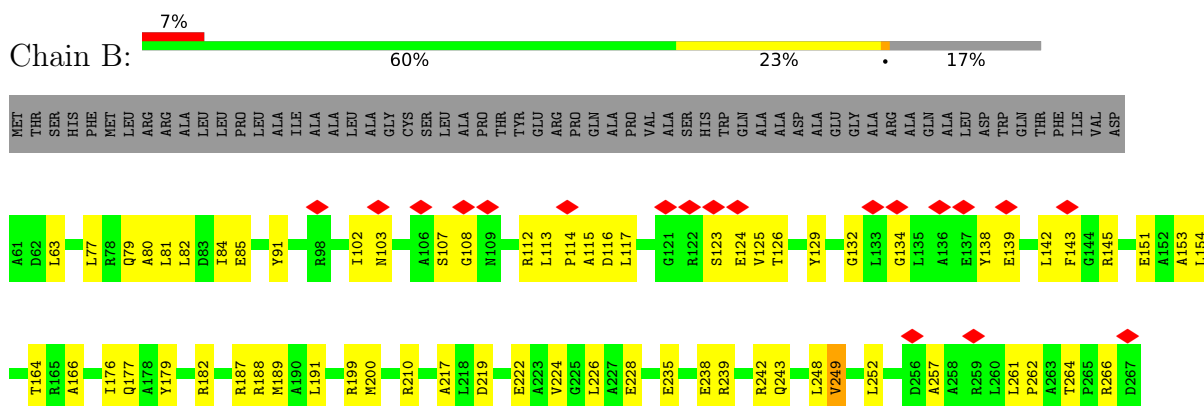
3 Residue-property plots [i](#)

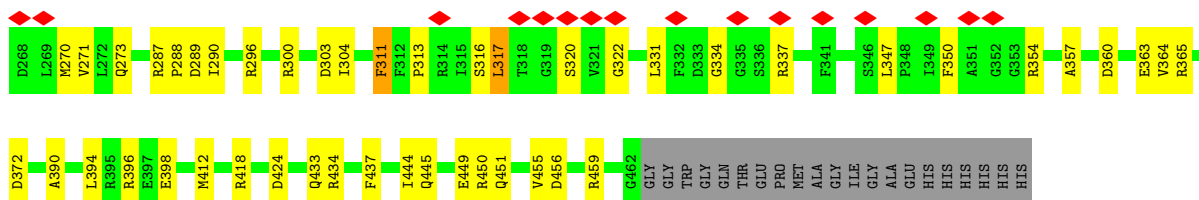
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RND efflux system, OprJ-like protein

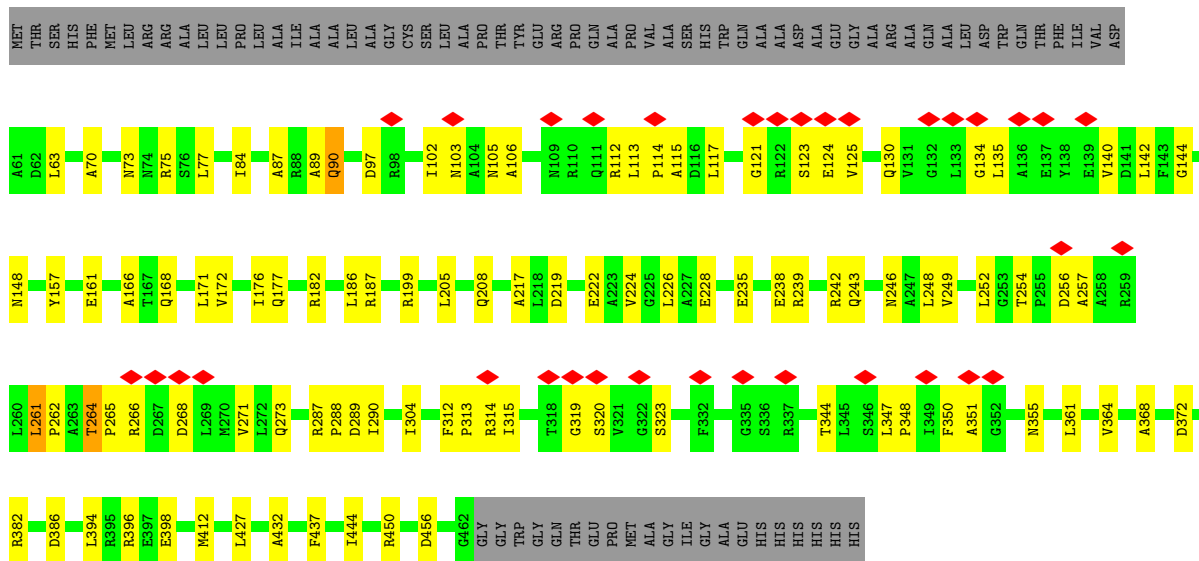


- Molecule 1: RND efflux system, OprJ-like protein

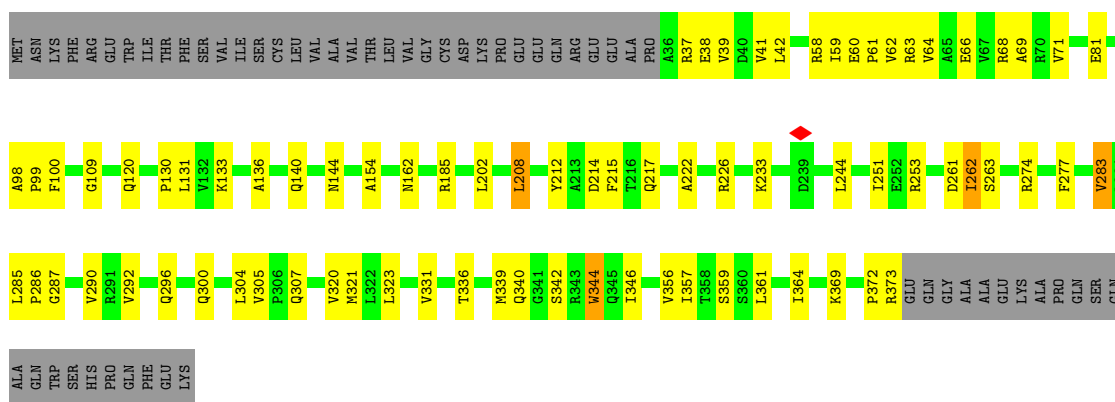




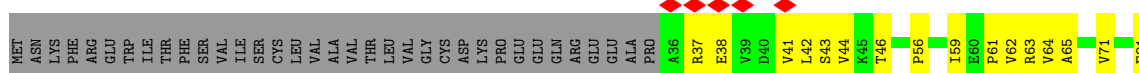
• Molecule 1: RND efflux system, OprJ-like protein

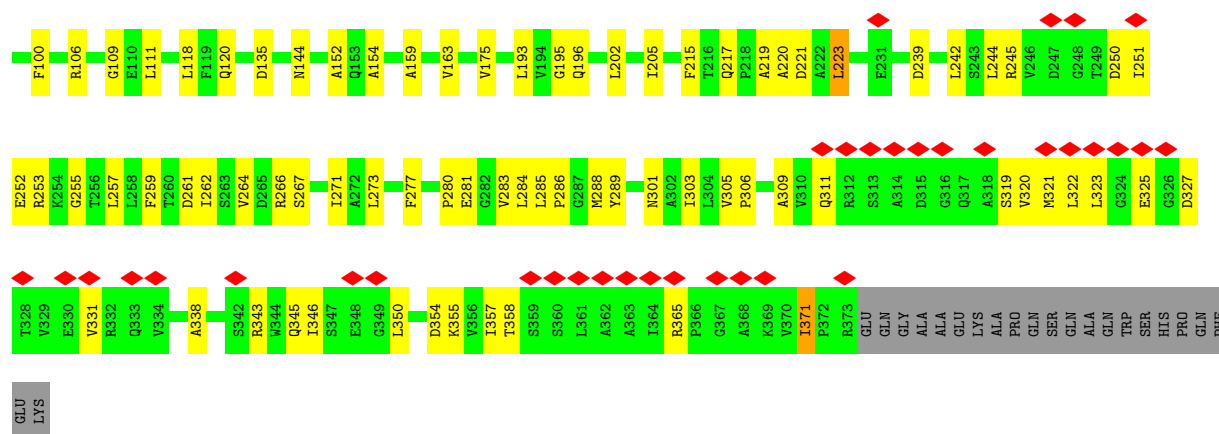


• Molecule 2: RND efflux system, MexC-like protein

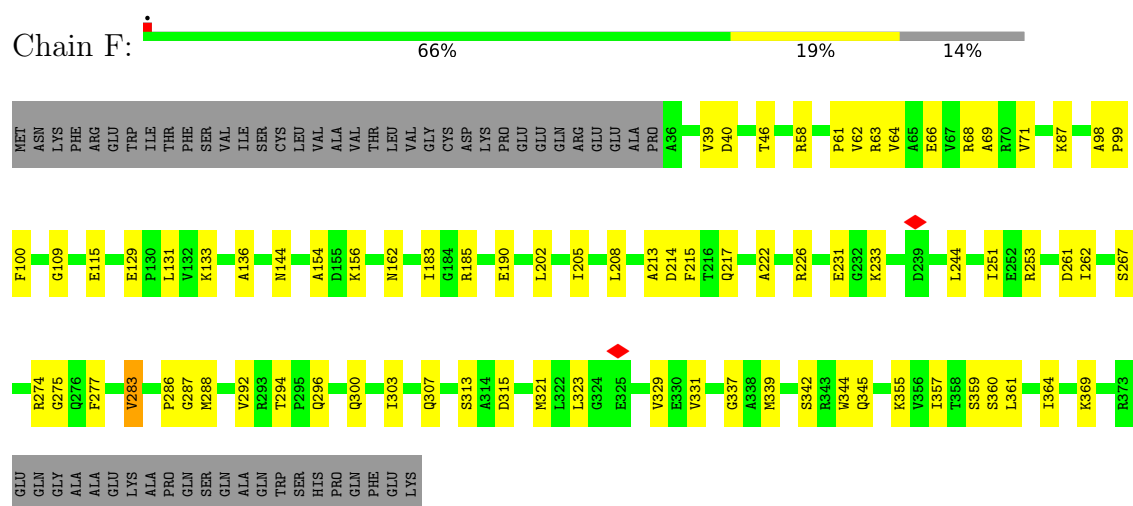


• Molecule 2: RND efflux system, MexC-like protein

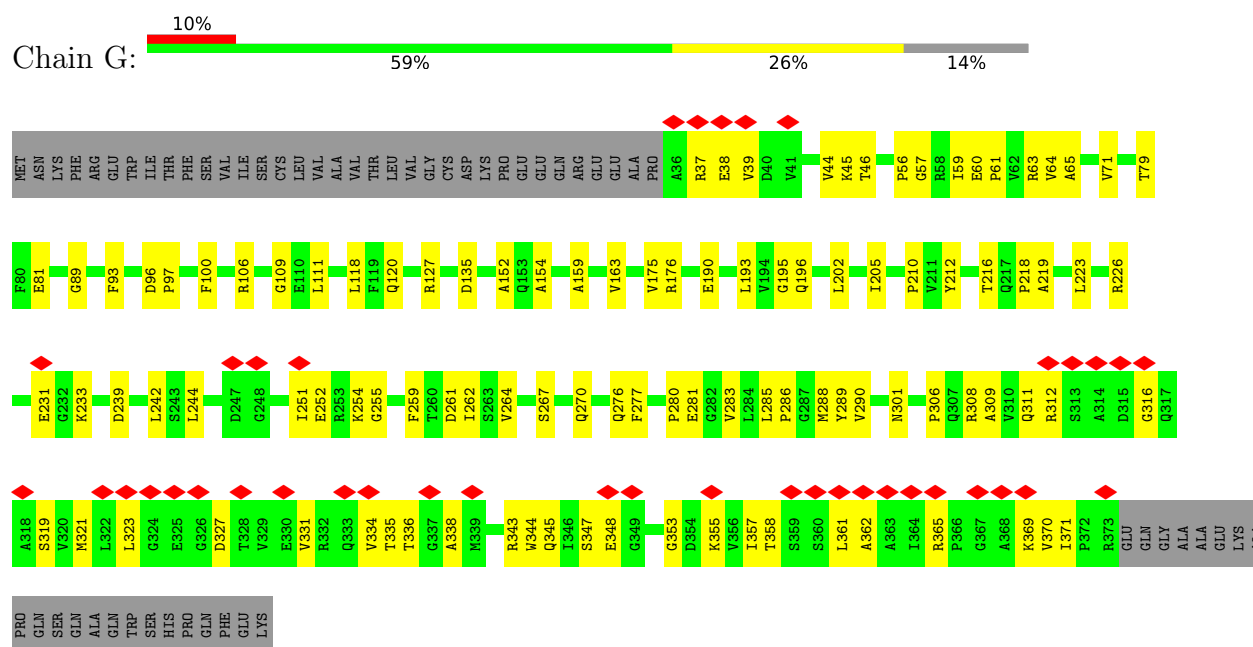




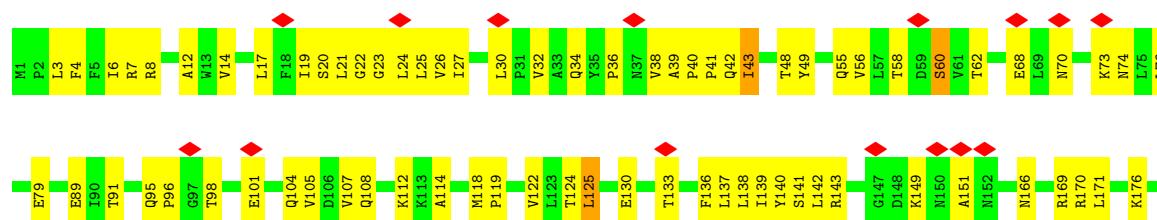
• Molecule 2: RND efflux system, MexC-like protein

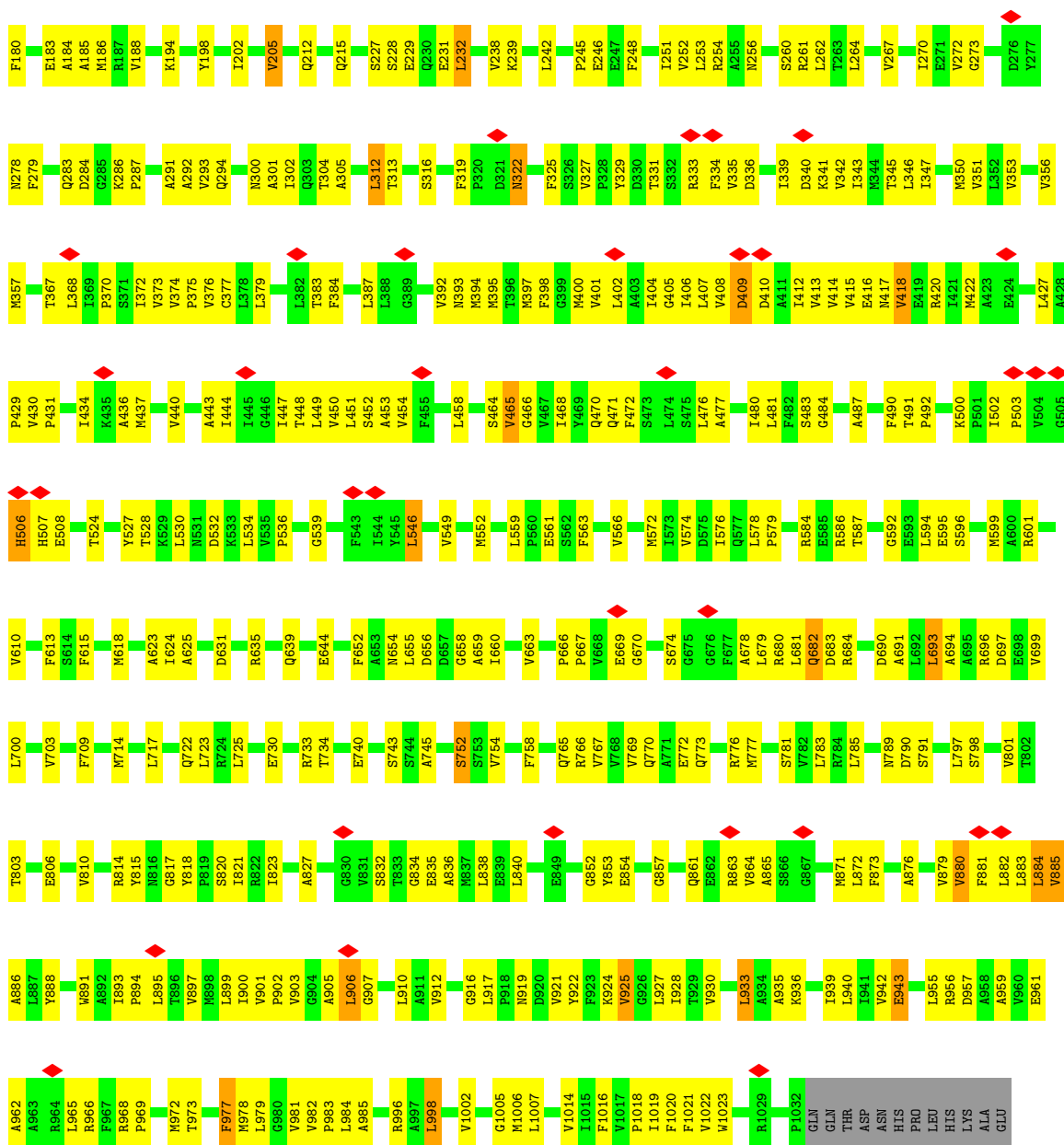


• Molecule 2: RND efflux system, MexC-like protein



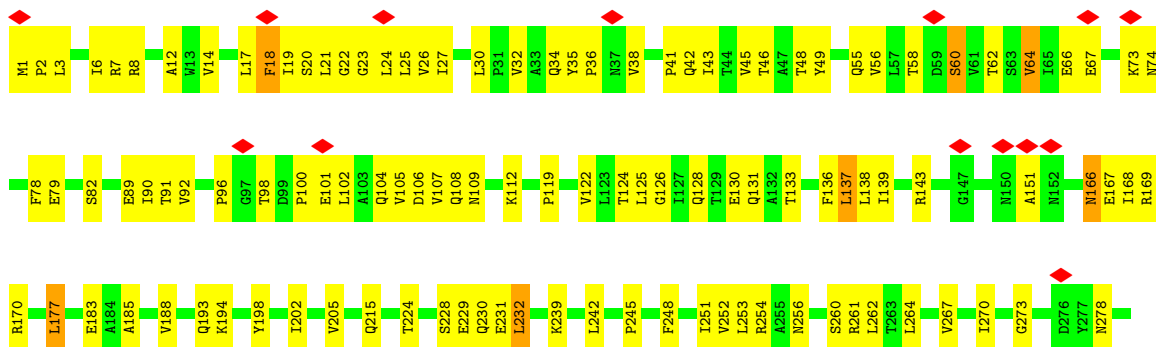
- Chain H:  67% 18% 14%

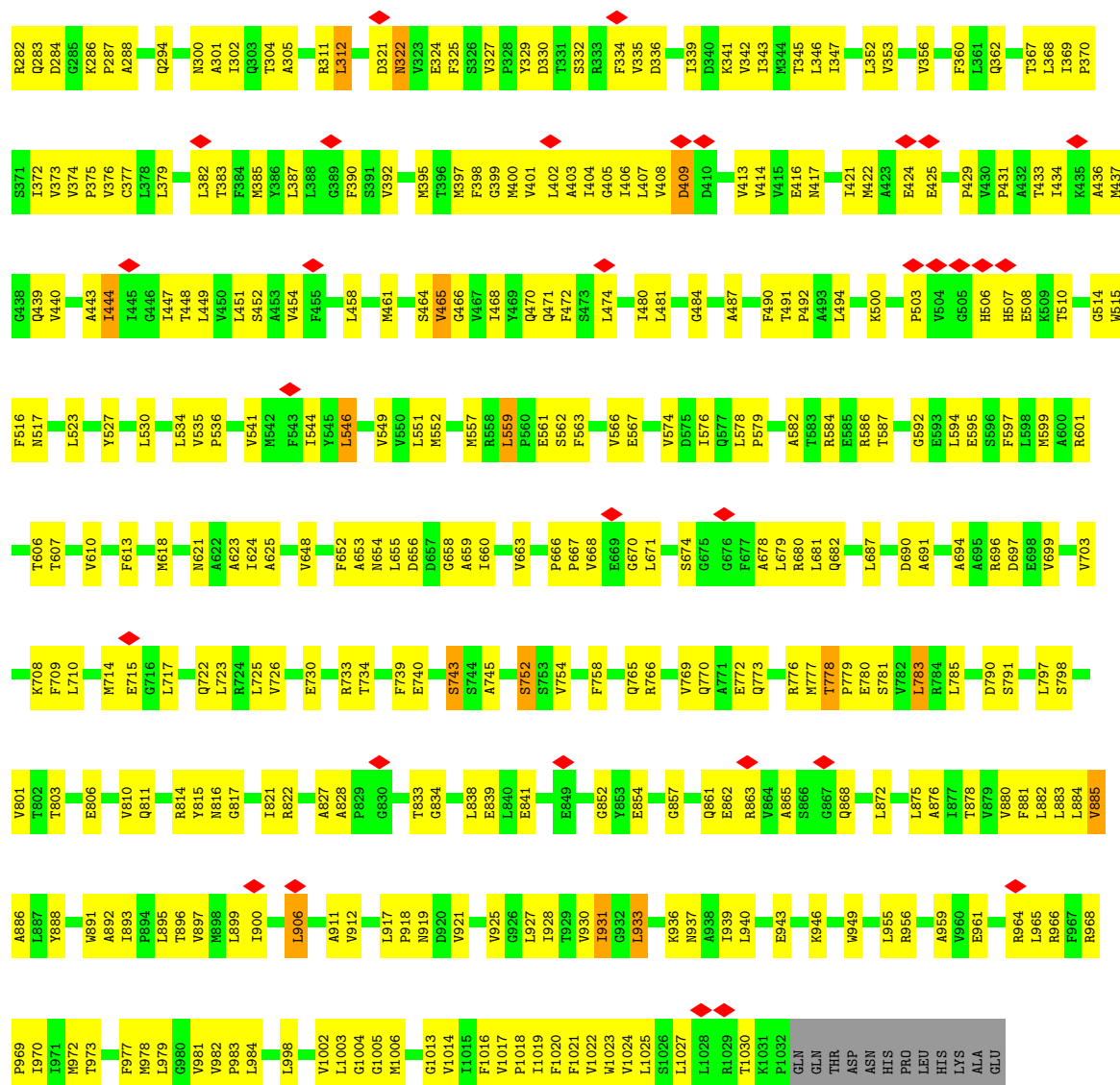




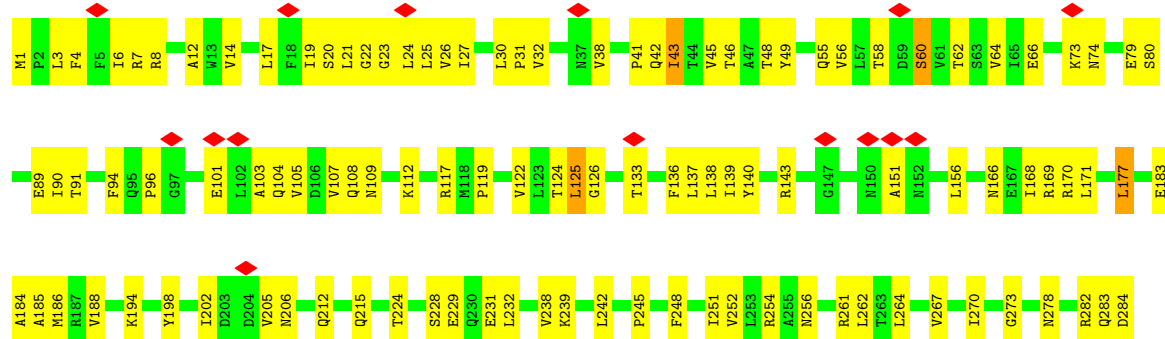
• Molecule 3: Efflux pump membrane transporter

Chain J: 56% 41%





• Molecule 3: Efflux pump membrane transporter



V1017	P1018	I1019	F1020	F1021	V1022	G926	E849	S743	L655	V535	M437	P370	G285
R1029	P1018	I1019	F1020	F1021	V1022	L927	G850	S744	D856	P536	V440	S371	K286
	P1018	I1019	F1020	F1021	V1022	T929	I851	A745	D657		V440	I372	P287
	P1018	I1019	F1020	F1021	V1022	V930	G852	T748	G658	M541	V374	V373	A291
	P1018	I1019	F1020	F1021	V1022	L933	Y853		A659	F543	A443	P375	A292
	P1018	I1019	F1020	F1021	V1022	A934	E854	S752	I660		I445	I444	Q294
F1032	P1018	I1019	F1020	F1021	V1022	A935	Y860	S753	P666	L546	I445	L378	A301
	P1018	I1019	F1020	F1021	V1022	K936	Q861	V754	P667	G547	G446	L379	I302
	P1018	I1019	F1020	F1021	V1022	N937	E862	F758	V668	G547	I447	L378	A301
	P1018	I1019	F1020	F1021	V1022	I938	R863		E669	V549	T448	L379	I302
	P1018	I1019	F1020	F1021	V1022	V939	V864	Q765	G670	M552	L451	L382	A305
G1032	P1018	I1019	F1020	F1021	V1022	L940	R864	R766	S674	L559	V454	L387	V308
	P1018	I1019	F1020	F1021	V1022	I941	G867	V767	G675	L559	F455	L388	V308
	P1018	I1019	F1020	F1021	V1022	V942	Q868	V768	F677	F563	L458	G389	L312
	P1018	I1019	F1020	F1021	V1022	E943	A869	V769	A678	V566	A459	V392	S316
	P1018	I1019	F1020	F1021	V1022	E950	T870	E772	L687	M572	F460	L402	F319
ALA	P1018	I1019	F1020	F1021	V1022	R956	M871	Q773	Q682	I573	S464	M395	P320
	P1018	I1019	F1020	F1021	V1022	L955	L875	R776	R680	V574	V465	T396	
	P1018	I1019	F1020	F1021	V1022	A959	A876	M777	L681	D575		M397	
	P1018	I1019	F1020	F1021	V1022	A959	V880	E780	G688	I576	S464	F398	
	P1018	I1019	F1020	F1021	V1022	V960	F881	S781	R689	Q577	Y469	G399	
GLU	P1018	I1019	F1020	F1021	V1022	A962	L882	V782	Q690	P579	Q471	V401	F325
	P1018	I1019	F1020	F1021	V1022	L965	L883	L783	D690		F472	L402	S326
	P1018	I1019	F1020	F1021	V1022	R966	L884	R784	A691	S473	S474	L402	V327
	P1018	I1019	F1020	F1021	V1022	P969	V885	L785	A694	L474	I404	Y329	
	P1018	I1019	F1020	F1021	V1022	I970	A866	L785	A695	S475	G405	D330	
V1014	P1018	I1019	F1020	F1021	V1022	P969	L887	S798	R696	T587	L406	T331	
	P1018	I1019	F1020	F1021	V1022	L971	V888		D697		I407	R333	
	P1018	I1019	F1020	F1021	V1022	N972	W891	T803	E698	G592	V408	F334	
	P1018	I1019	F1020	F1021	V1022	T973	A892	V810	V699	E593	D409	V335	
	P1018	I1019	F1020	F1021	V1022	F977	L893		L700	E595	D410	D336	
V1016	P1018	I1019	F1020	F1021	V1022	N978	P894	R814	V703	M599	L486	I412	T339
	P1018	I1019	F1020	F1021	V1022	L979	V897	Y815		A600	A487	V413	D340
	P1018	I1019	F1020	F1021	V1022	G980	M898	N816	F709	A600		V414	
	P1018	I1019	F1020	F1021	V1022	V981	G980	G817	L710	R601	V490	V415	K341
	P1018	I1019	F1020	F1021	V1022	V982	I900	Y818	Y711	A601		V415	V342
V1018	P1018	I1019	F1020	F1021	V1022	P983	I900	P819	A712	T607	L494	M417	H544
	P1018	I1019	F1020	F1021	V1022	I986	P902	S820	M713			V418	T345
	P1018	I1019	F1020	F1021	V1022	L998	V903	I821	M714	V610	I502	E419	L346
	P1018	I1019	F1020	F1021	V1022	G904	G904	R822	E715		P503	M422	L347
	P1018	I1019	F1020	F1021	V1022	L998	A905	I823	G716	M618		E348	
S1008	P1018	I1019	F1020	F1021	V1022	V1002	L906	D826	L717	A623	V504	A423	A349
	P1018	I1019	F1020	F1021	V1022	L1003	G907	A827	A718	G505	E424	E424	A349
	P1018	I1019	F1020	F1021	V1022	G1004			E719		G426	M350	V350
	P1018	I1019	F1020	F1021	V1022	M1006	V912	G830	L723	H506	L427	L352	V351
	P1018	I1019	F1020	F1021	V1022	S1008	V912	G830	L723	H507		L352	V351
V1016	P1018	I1019	F1020	F1021	V1022	L998	V912	G830	L723	D631	E508	L427	V356
	P1018	I1019	F1020	F1021	V1022	G916	G916	G834	E730			V430	
	P1018	I1019	F1020	F1021	V1022	L917	L917	E835		W515	V430	L361	
	P1018	I1019	F1020	F1021	V1022	P918	P918	E835		Y527	A432	L361	
	P1018	I1019	F1020	F1021	V1022	N919	N919	L838	T733	F652	T433	T367	
F1016	P1018	I1019	F1020	F1021	V1022	D920	D920	T734	T734	A653	L434	L368	
	P1018	I1019	F1020	F1021	V1022	V921	V921	E841	E740	N654	K435	L369	
	P1018	I1019	F1020	F1021	V1022	F1016							
	P1018	I1019	F1020	F1021	V1022								
	P1018	I1019	F1020	F1021	V1022								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52844	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 ($e^-/\text{\AA}^2$)	51.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.285	Depositor
Minimum map value	-0.778	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	558.0, 558.0, 558.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/3096	0.42	0/4192
1	B	0.24	0/3096	0.42	3/4192 (0.1%)
1	C	0.24	0/3096	0.42	0/4192
2	D	0.29	0/2574	0.37	0/3487
2	E	0.29	0/2574	0.42	0/3487
2	F	0.29	0/2574	0.36	0/3487
2	G	0.28	0/2574	0.43	0/3487
2	H	0.30	0/2574	0.39	0/3487
2	I	0.27	0/2574	0.43	0/3487
3	J	0.31	0/7960	0.53	0/10845
3	K	0.31	0/7960	0.53	0/10845
3	L	0.30	0/7960	0.51	2/10845 (0.0%)
All	All	0.29	0/48612	0.47	5/66033 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ASP	CB-CA-C	-5.56	110.17	116.63
3	L	817	GLY	CA-C-N	-5.36	111.21	123.15
3	L	817	GLY	C-N-CA	-5.36	111.21	123.15
1	B	189	MET	CB-CG-SD	-5.08	97.44	112.70
1	B	151	GLU	CA-CB-CG	5.04	124.19	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3065	0	3060	93	0
1	B	3065	0	3060	81	0
1	C	3065	0	3060	76	0
2	D	2543	0	2591	61	0
2	E	2543	0	2591	70	0
2	F	2543	0	2591	55	0
2	G	2543	0	2591	77	0
2	H	2543	0	2591	60	0
2	I	2543	0	2591	71	0
3	J	7804	0	7946	353	0
3	K	7804	0	7946	330	0
3	L	7804	0	7946	318	0
4	J	17	0	0	0	0
4	K	17	0	0	0	0
4	L	17	0	0	0	0
All	All	47916	0	48564	1527	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 16.

The worst 5 of 1527 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)
3:J:2:PRO:HB3	3:J:437:MET:HE2	1.40	1.03
3:K:112:LYS:HZ1	3:L:112:LYS:HE2	1.32	0.95
2:G:46:THR:HG23	2:G:301:ASN:HA	1.53	0.87
2:I:46:THR:HG23	2:I:301:ASN:HA	1.57	0.87
1:C:84:ILE:HD11	1:C:161:GLU:HA	1.61	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	400/483 (83%)	392 (98%)	8 (2%)	0	100	100
1	B	400/483 (83%)	390 (98%)	10 (2%)	0	100	100
1	C	400/483 (83%)	393 (98%)	7 (2%)	0	100	100
2	D	336/395 (85%)	332 (99%)	4 (1%)	0	100	100
2	E	336/395 (85%)	330 (98%)	6 (2%)	0	100	100
2	F	336/395 (85%)	331 (98%)	5 (2%)	0	100	100
2	G	336/395 (85%)	327 (97%)	9 (3%)	0	100	100
2	H	336/395 (85%)	332 (99%)	4 (1%)	0	100	100
2	I	336/395 (85%)	328 (98%)	8 (2%)	0	100	100
3	J	1030/1044 (99%)	993 (96%)	36 (4%)	1 (0%)	48	81
3	K	1030/1044 (99%)	994 (96%)	35 (3%)	1 (0%)	48	81
3	L	1030/1044 (99%)	989 (96%)	40 (4%)	1 (0%)	48	81
All	All	6306/6951 (91%)	6131 (97%)	172 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	752	SER
3	K	752	SER
3	J	752	SER

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	310/368 (84%)	304 (98%)	6 (2%)	52	79
1	B	310/368 (84%)	300 (97%)	10 (3%)	34	67
1	C	310/368 (84%)	303 (98%)	7 (2%)	45	75
2	D	259/308 (84%)	254 (98%)	5 (2%)	52	79
2	E	259/308 (84%)	256 (99%)	3 (1%)	67	86
2	F	259/308 (84%)	256 (99%)	3 (1%)	67	86
2	G	259/308 (84%)	252 (97%)	7 (3%)	40	71
2	H	259/308 (84%)	254 (98%)	5 (2%)	52	79
2	I	259/308 (84%)	256 (99%)	3 (1%)	67	86
3	J	828/839 (99%)	789 (95%)	39 (5%)	22	56
3	K	828/839 (99%)	779 (94%)	49 (6%)	16	47
3	L	828/839 (99%)	781 (94%)	47 (6%)	17	49
All	All	4968/5469 (91%)	4784 (96%)	184 (4%)	31	63

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	327	VAL
3	L	125	LEU
3	J	444	ILE
3	J	781	SER
3	L	350	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
3	K	811	GLN
3	L	83	ASN
3	K	995	GLN
3	J	206	ASN
3	L	128	GLN

5.3.3 RNA ⓘ

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](#)

3 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$
4	A1EAN	J	1101	-	19,19,19	3.28	4 (21%)	25,25,25	1.25	3 (12%)
4	A1EAN	L	1101	-	19,19,19	3.27	4 (21%)	25,25,25	1.26	3 (12%)
4	A1EAN	K	1101	-	19,19,19	3.27	4 (21%)	25,25,25	1.21	3 (12%)

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
4	A1EAN	J	1101	-	-	4/4/12/12	0/3/3/3
4	A1EAN	L	1101	-	-	4/4/12/12	0/3/3/3
4	A1EAN	K	1101	-	-	4/4/12/12	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1101	A1EAN	C07-N03	-12.35	1.23	1.47
4	J	1101	A1EAN	C07-N03	-12.34	1.23	1.47
4	L	1101	A1EAN	C07-N03	-12.30	1.23	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1101	A1EAN	C17-C12	-4.23	1.35	1.43
4	L	1101	A1EAN	C17-C12	-4.21	1.35	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1101	A1EAN	C01-C02-N03	3.36	115.76	110.94
4	L	1101	A1EAN	C01-C02-N03	3.29	115.66	110.94
4	K	1101	A1EAN	C08-C07-N03	-3.22	109.55	114.14
4	J	1101	A1EAN	C08-C07-N03	-3.09	109.74	114.14
4	L	1101	A1EAN	C08-C07-N03	-3.05	109.80	114.14

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

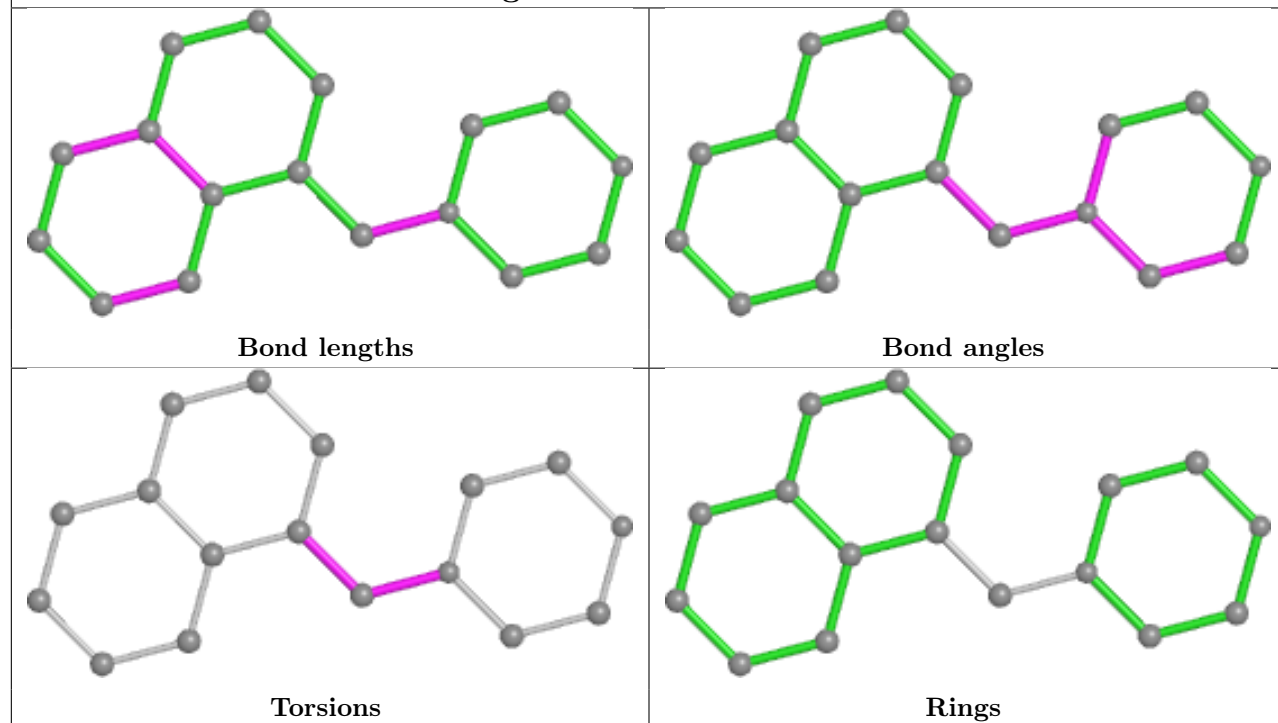
Mol	Chain	Res	Type	Atoms
4	L	1101	A1EAN	C08-C07-N03-C02
4	K	1101	A1EAN	C08-C07-N03-C02
4	K	1101	A1EAN	C08-C07-N03-C04
4	J	1101	A1EAN	C08-C07-N03-C02
4	J	1101	A1EAN	C08-C07-N03-C04

There are no ring outliers.

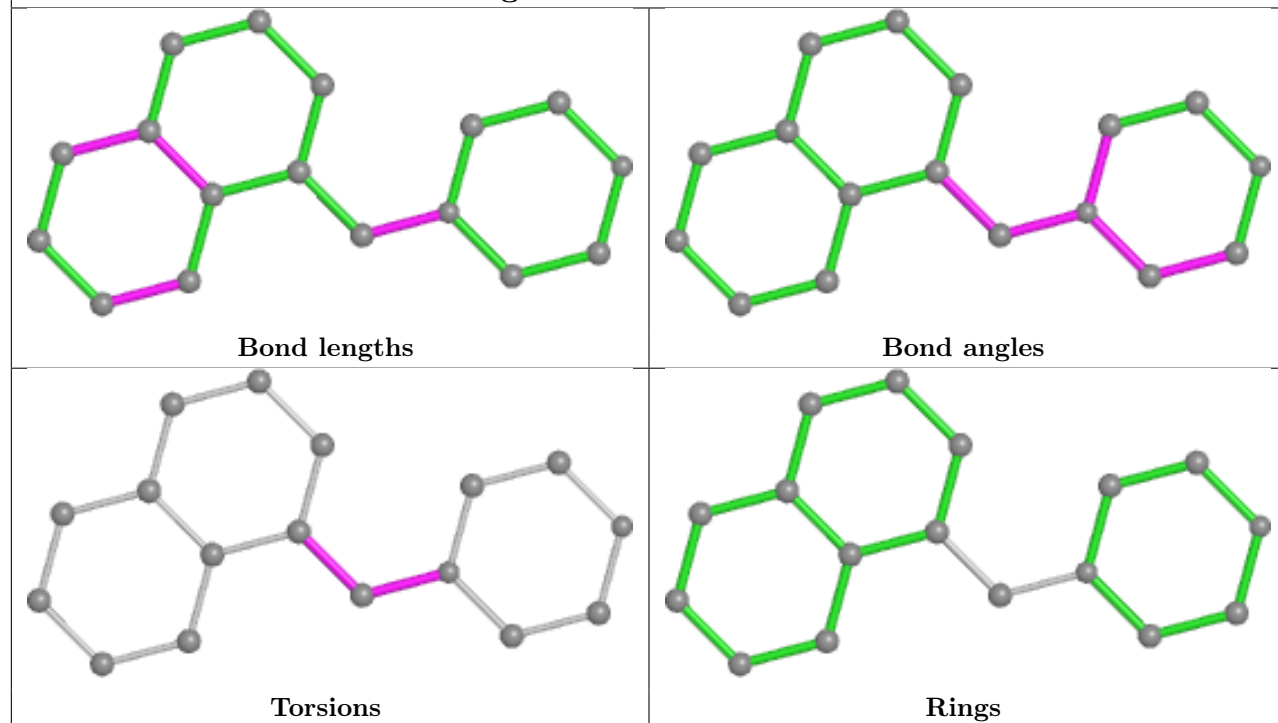
No monomer is involved in short contacts.

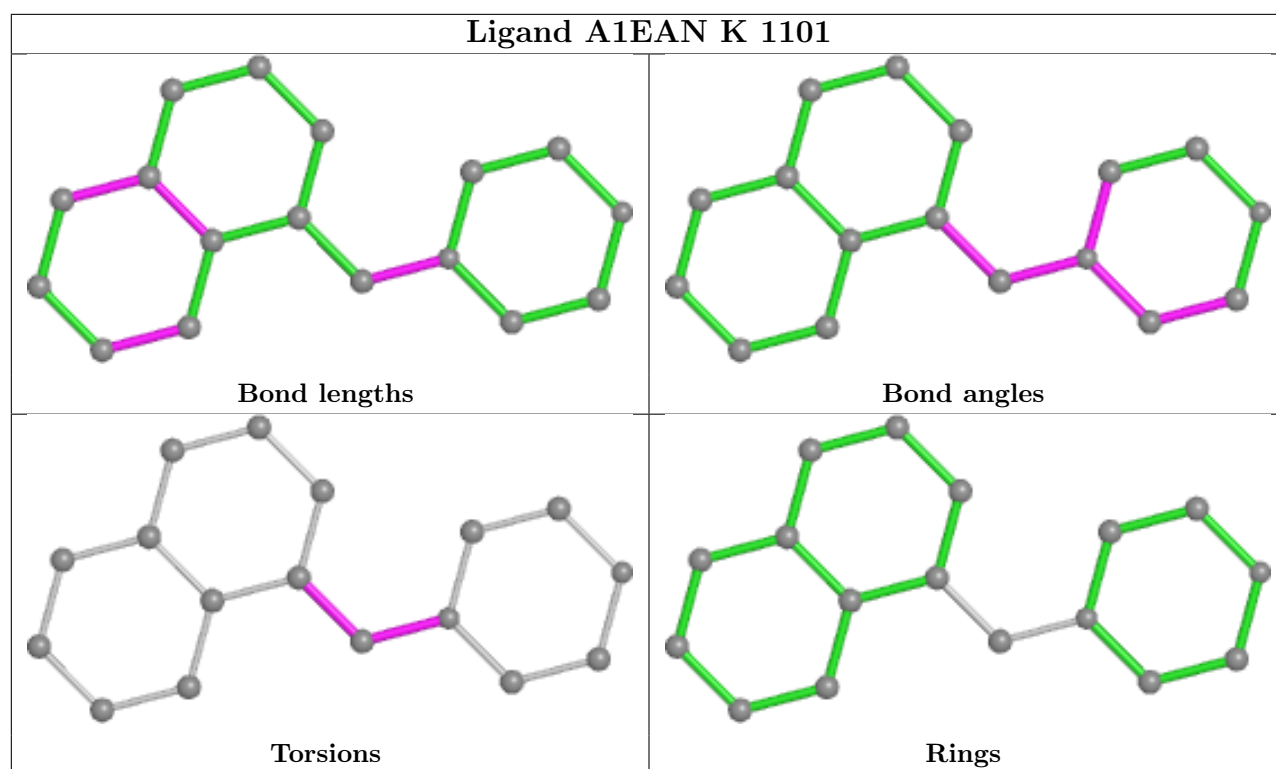
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A1EAN J 1101



Ligand A1EAN L 1101





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.

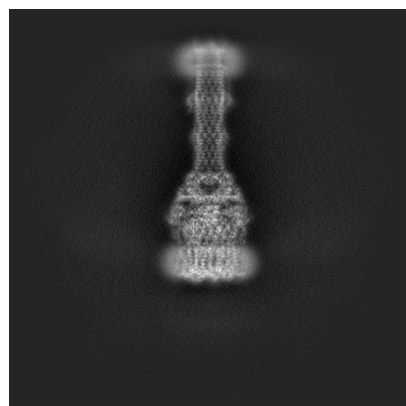
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61115. These allow visual inspection of the internal detail of the map and identification of artifacts.

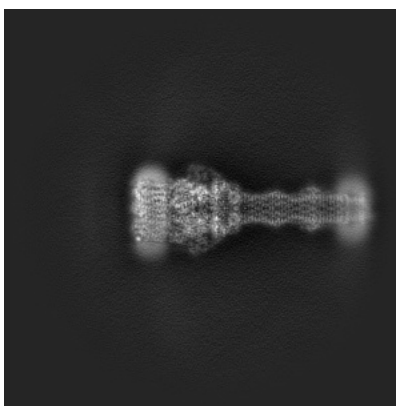
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

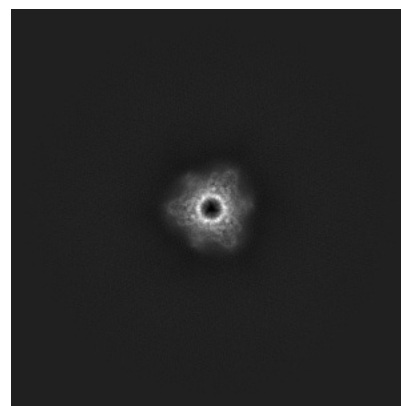
6.1.1 Primary map



X

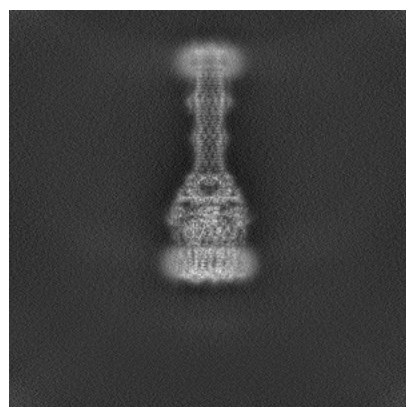


Y

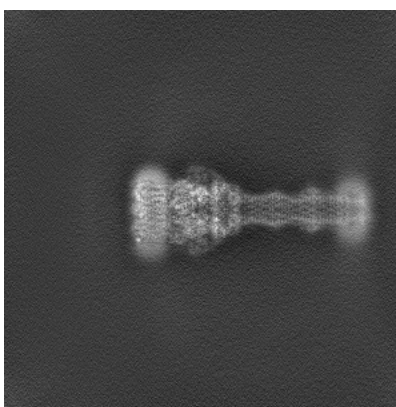


Z

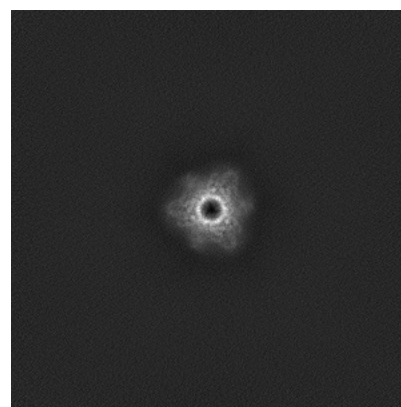
6.1.2 Raw map



X



Y

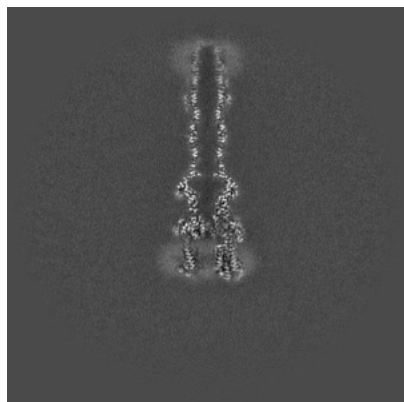


Z

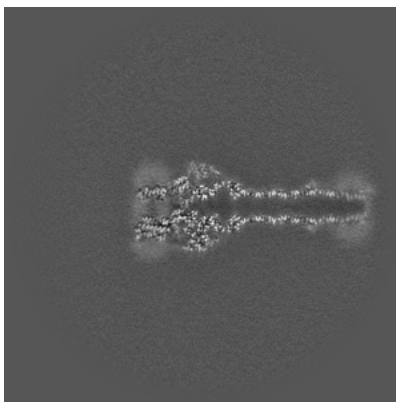
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

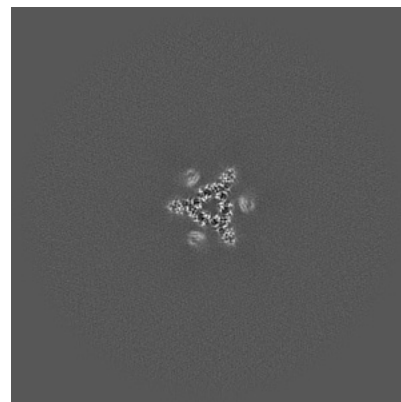
6.2.1 Primary map



X Index: 300

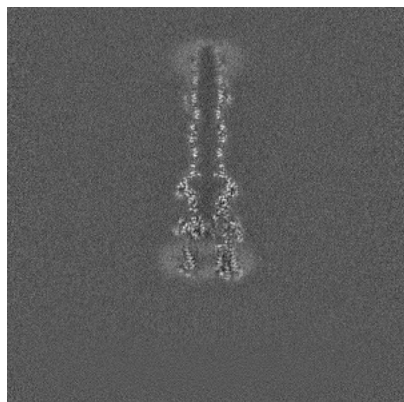


Y Index: 300

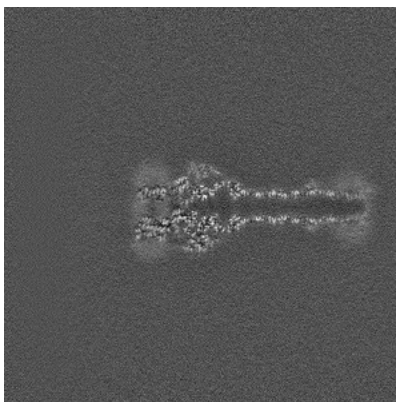


Z Index: 300

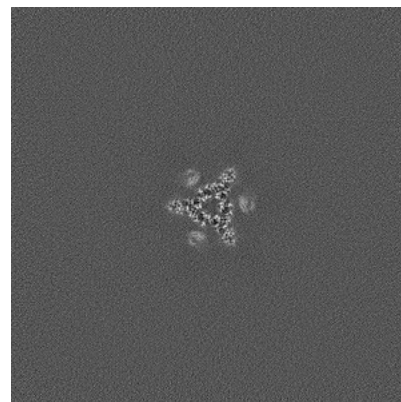
6.2.2 Raw map



X Index: 300



Y Index: 300

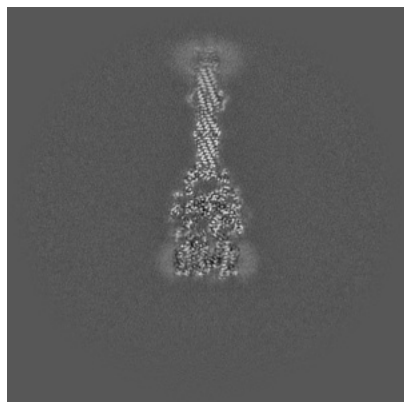


Z Index: 300

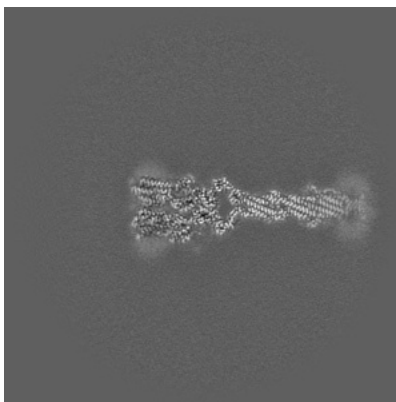
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

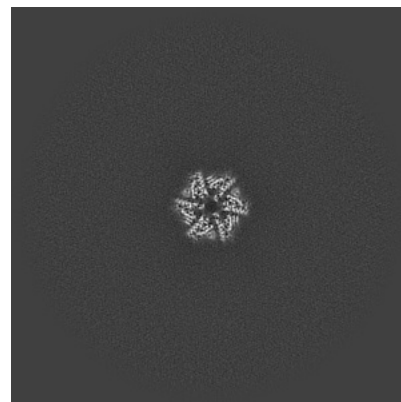
6.3.1 Primary map



X Index: 318

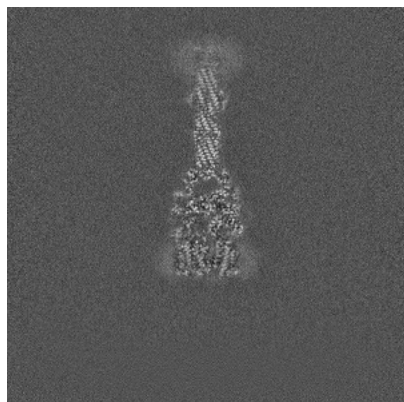


Y Index: 283

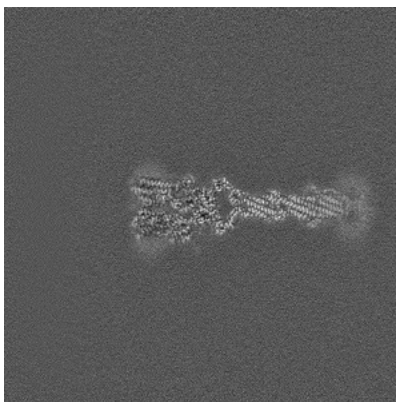


Z Index: 318

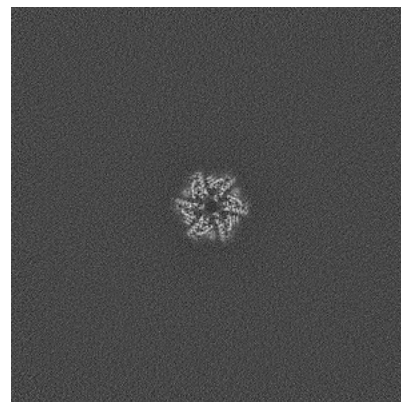
6.3.2 Raw map



X Index: 317



Y Index: 283

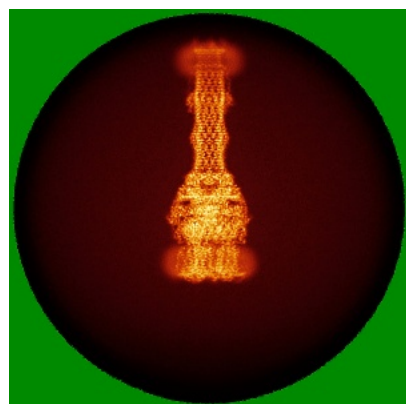


Z Index: 318

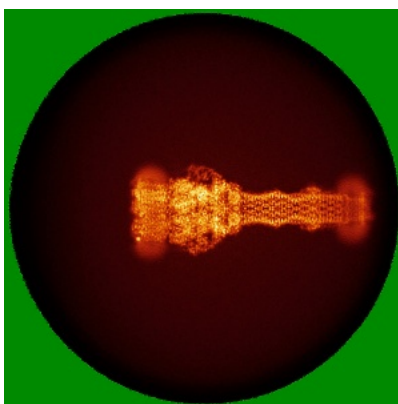
The images above show the largest variance slices of the map in three orthogonal directions.

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

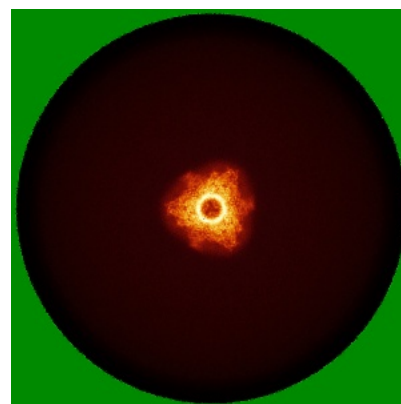
6.4.1 Primary map



X

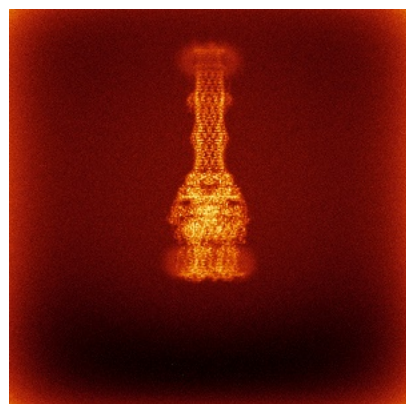


Y

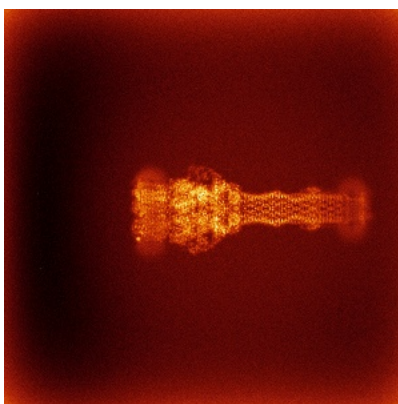


Z

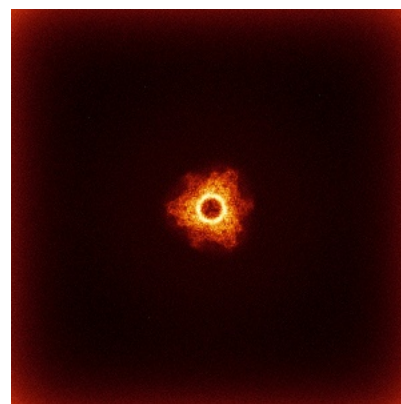
6.4.2 Raw map



X



Y

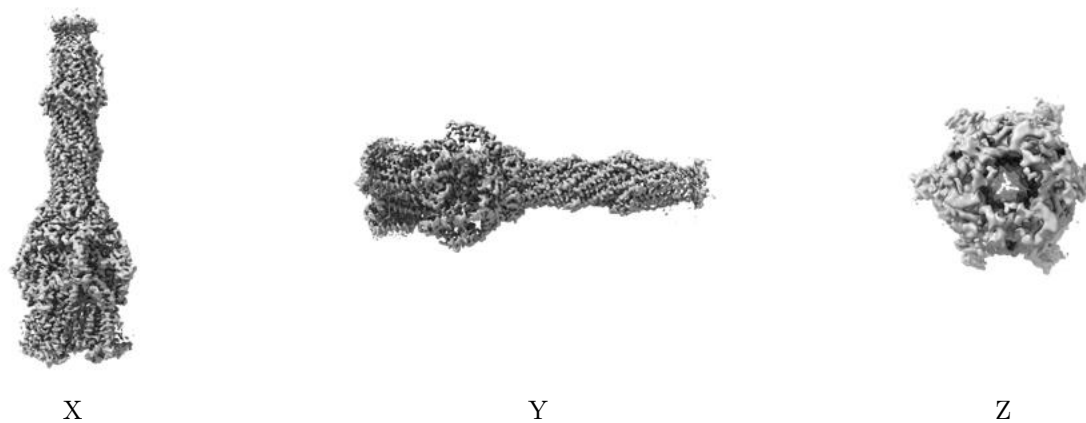


Z

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.

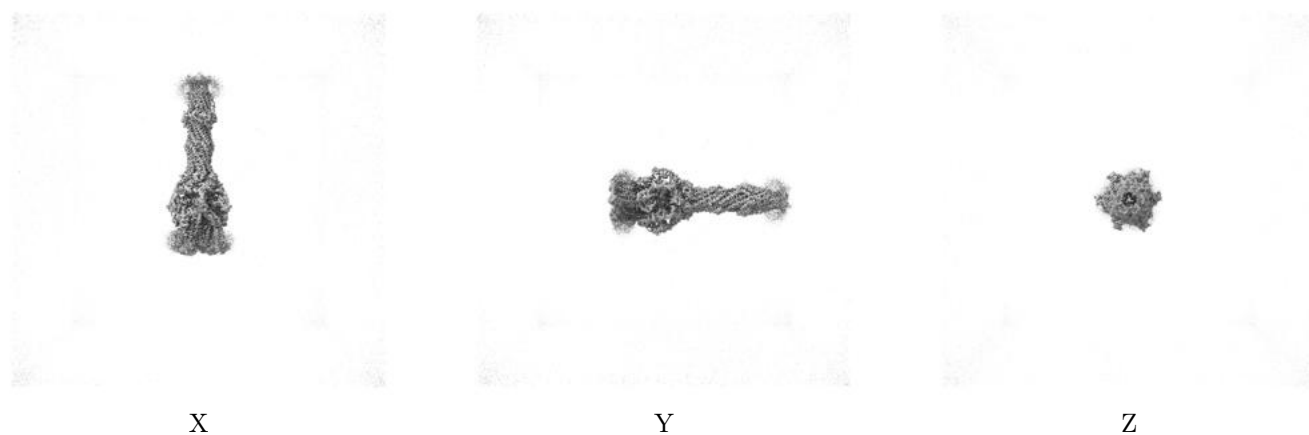
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

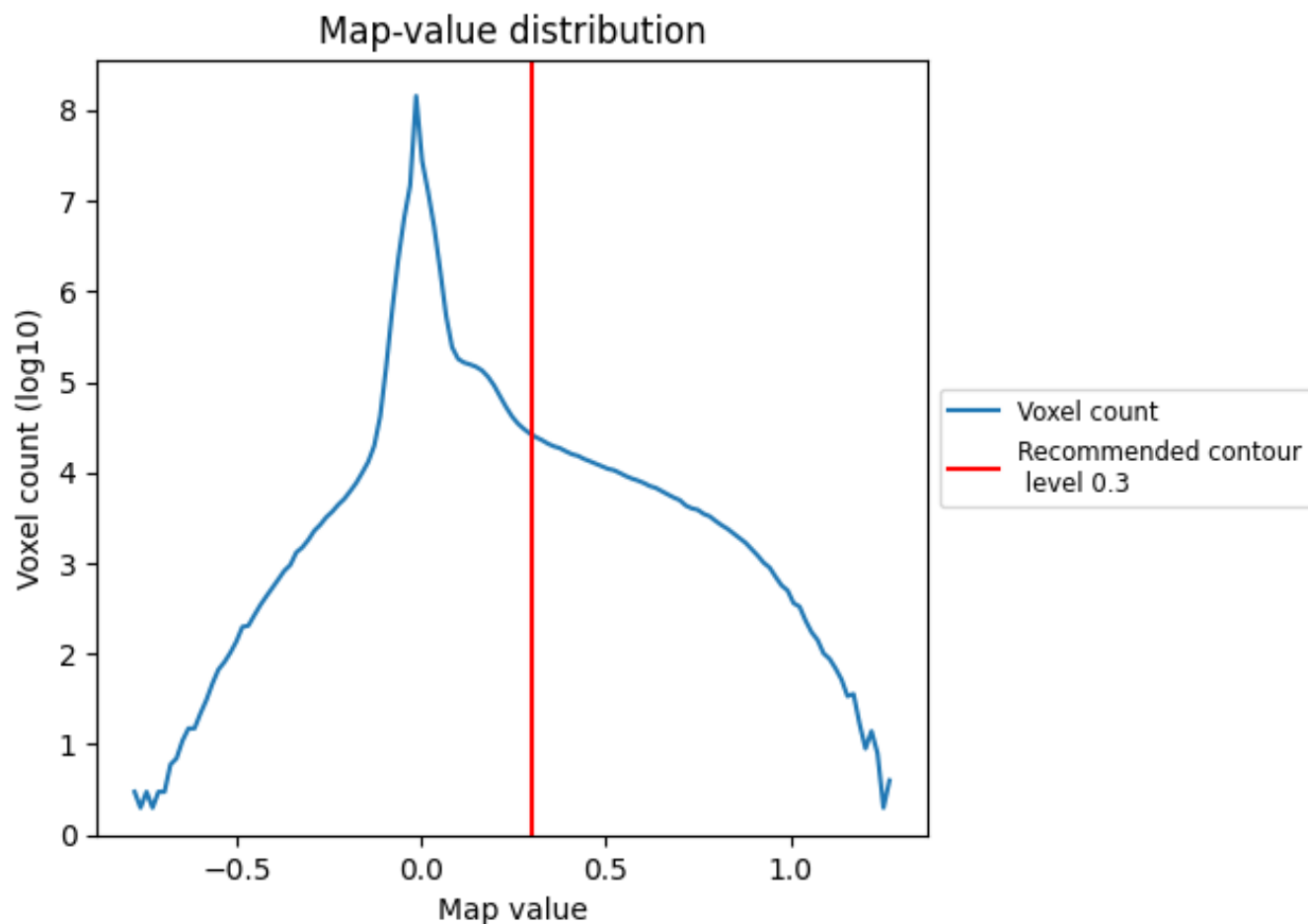
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

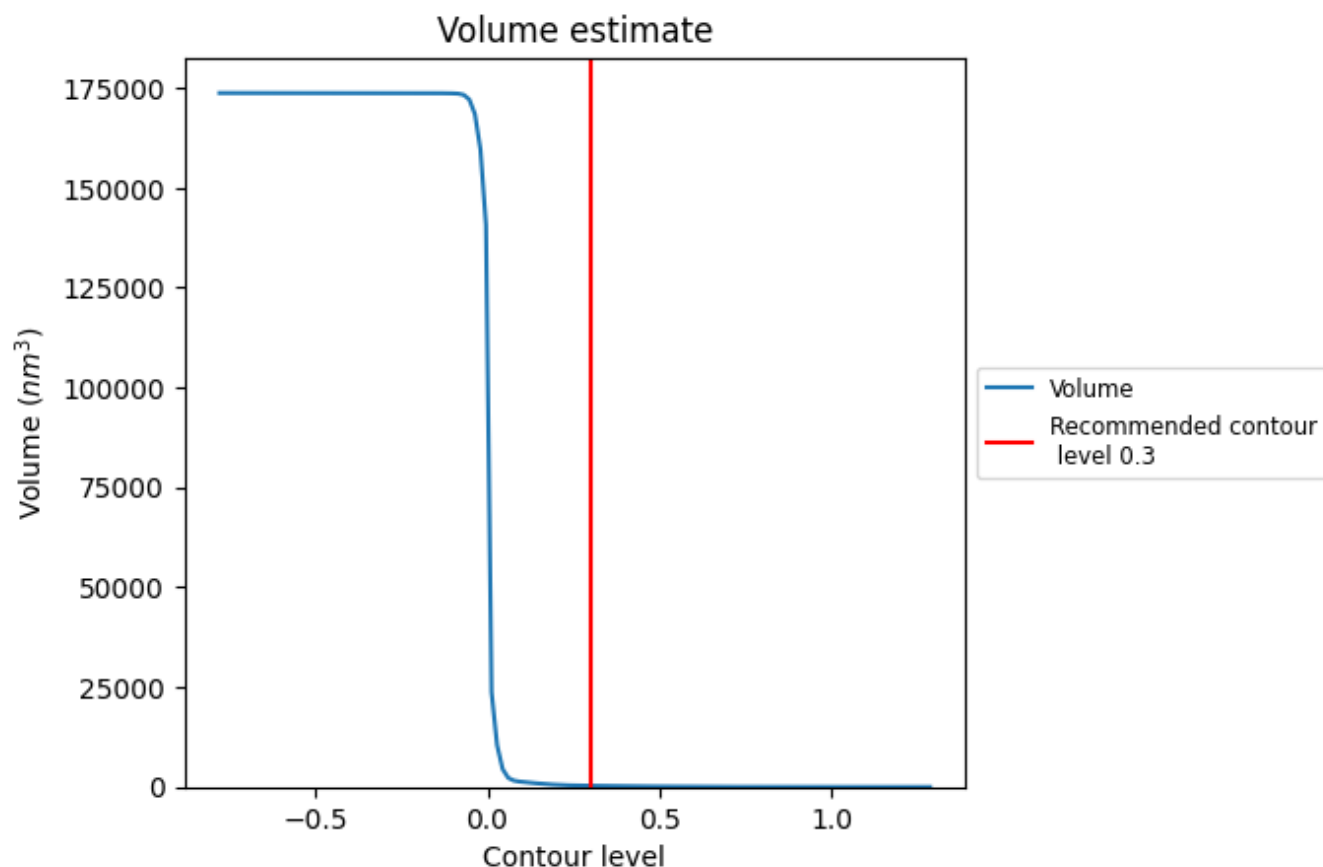
This section contains the results of statistical analysis of the map.

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.

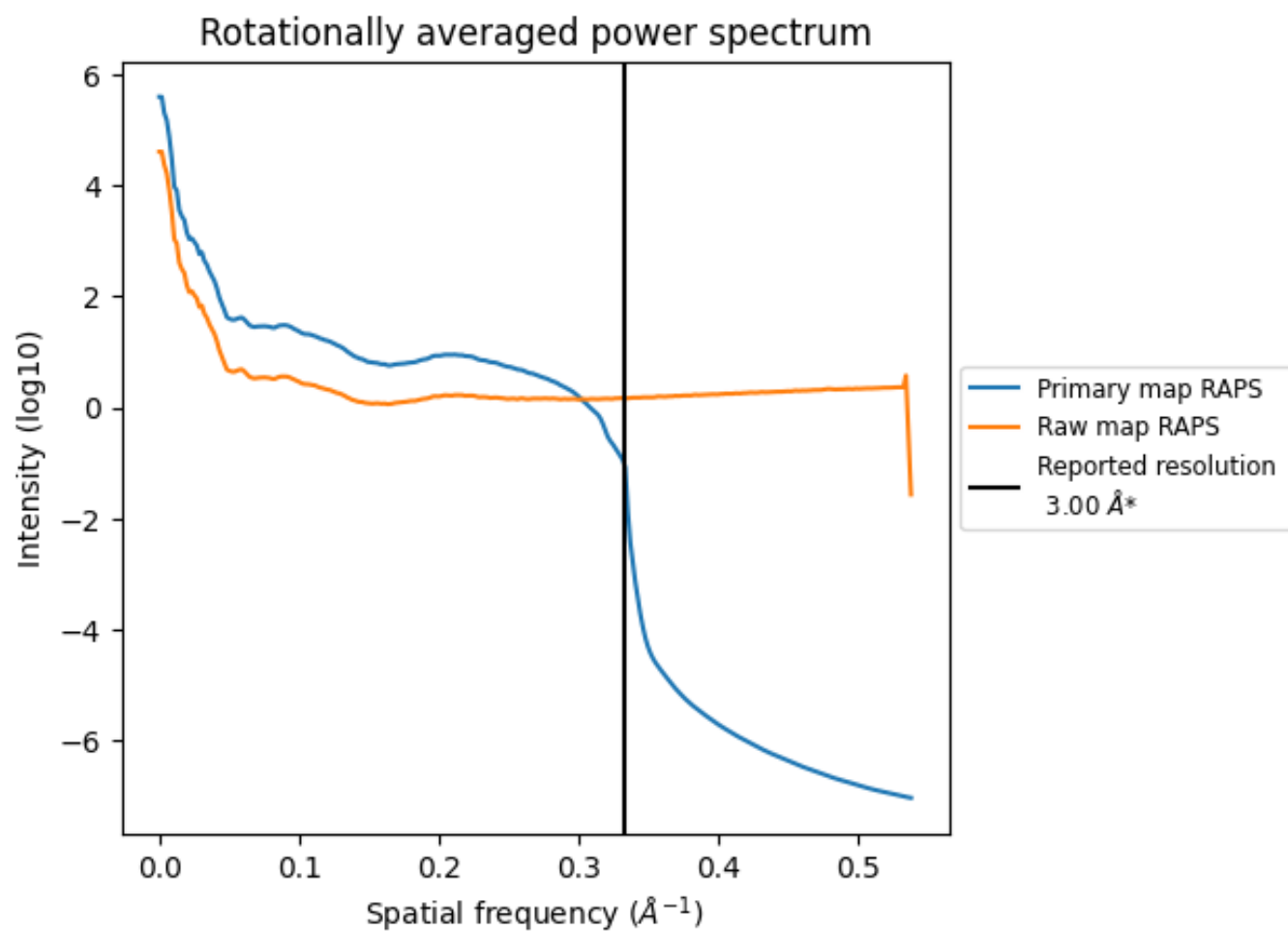
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 293 nm³; this corresponds to an approximate mass of 265 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 ⓘ

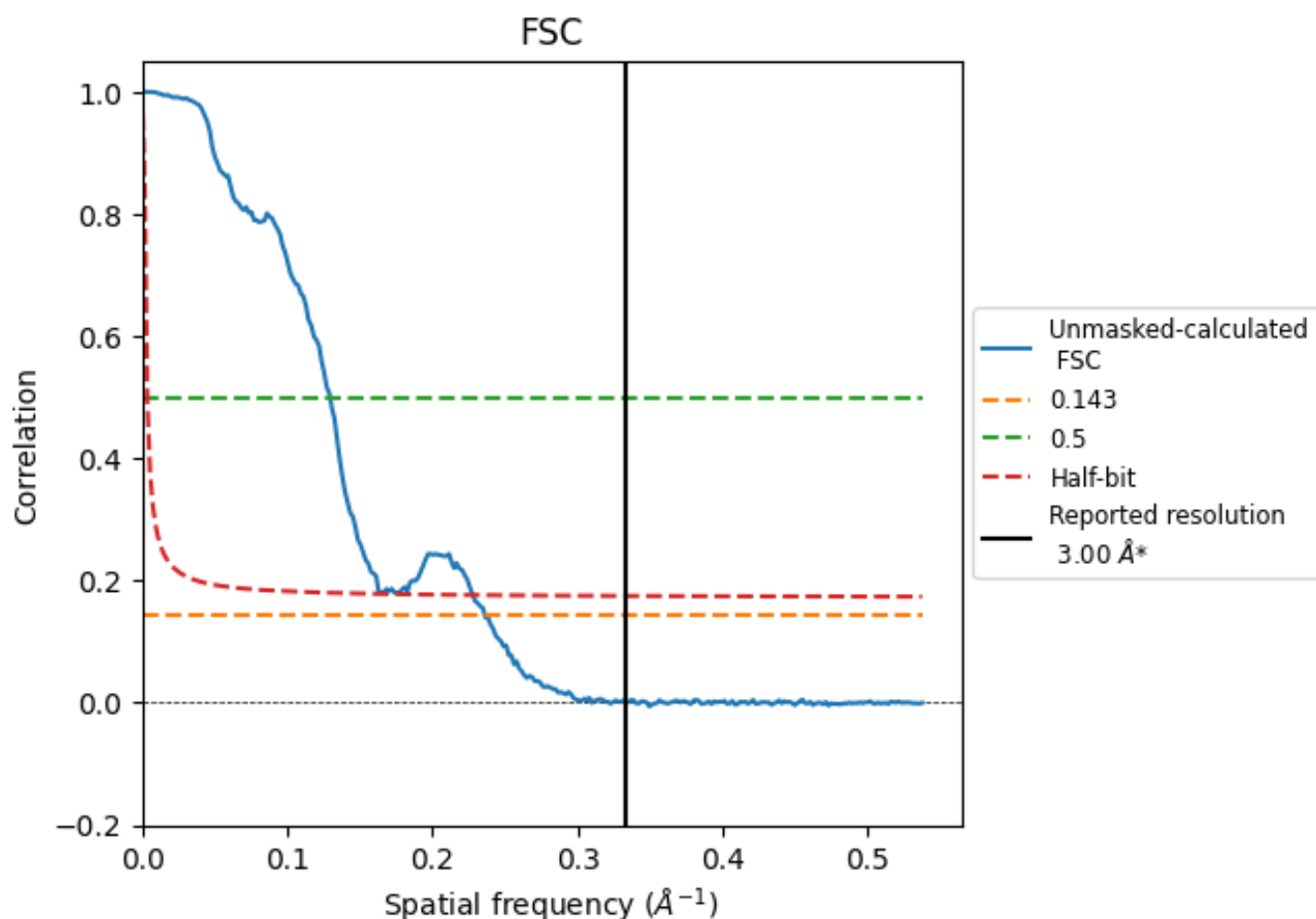


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

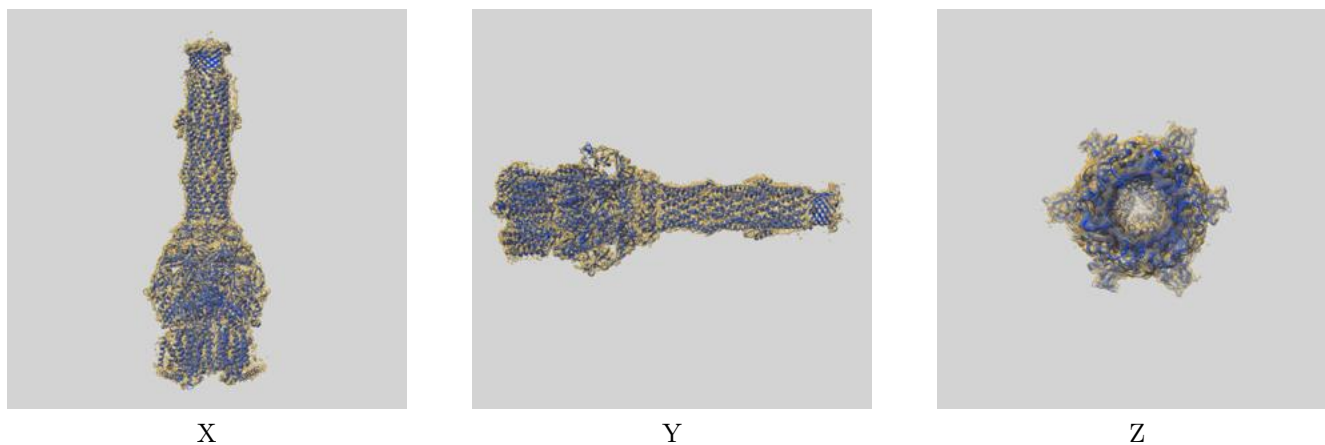
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.72	4.39

*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 4.24 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

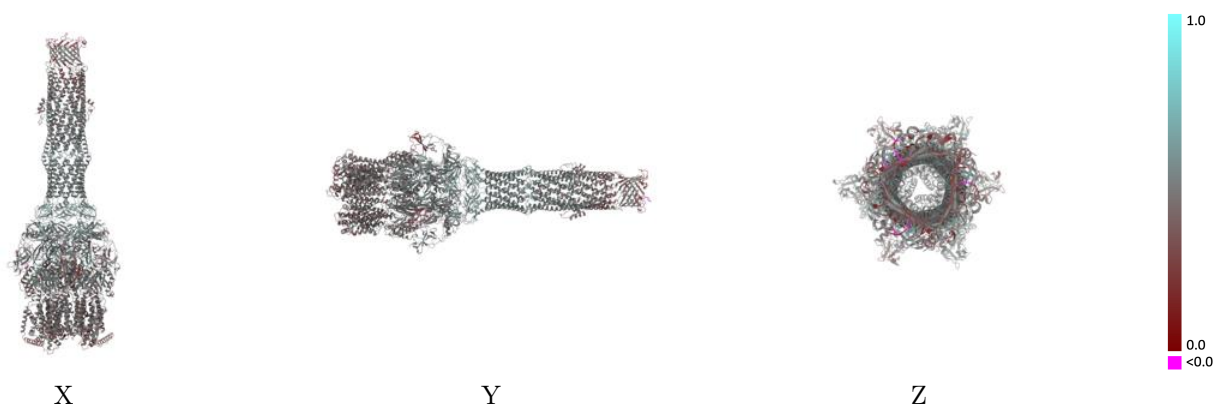
This section contains information regarding the fit between EMDB map EMD-61115 and PDB model 9J3E. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



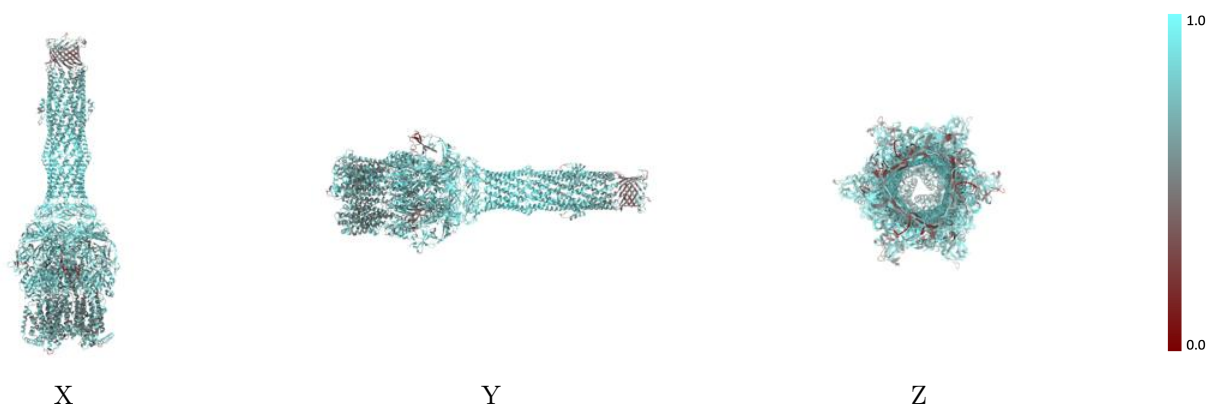
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



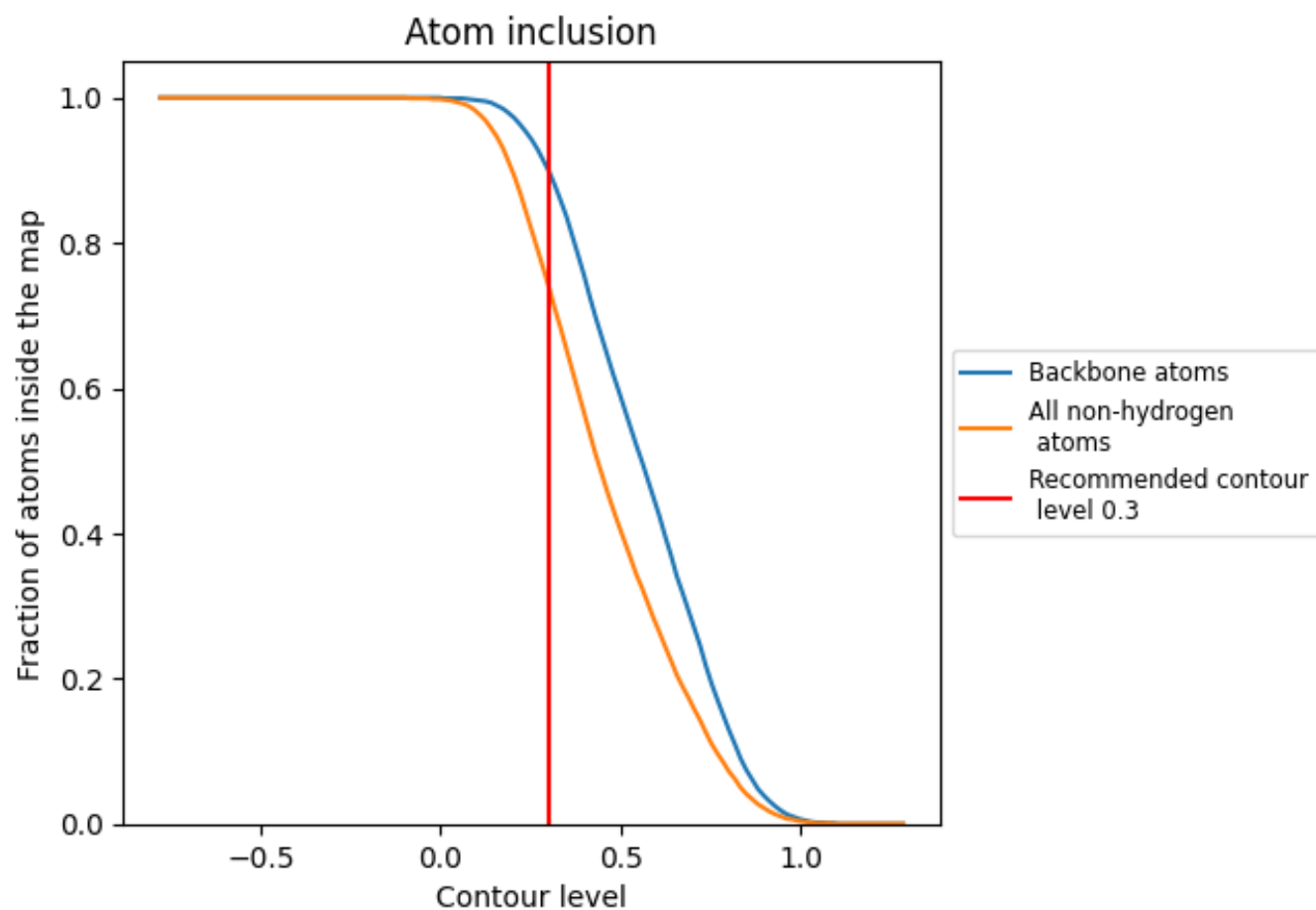
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 74% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7410</div>	<div><div></div>0.4680</div>
A	<div><div></div>0.7110</div>	<div><div></div>0.4440</div>
B	<div><div></div>0.7130</div>	<div><div></div>0.4450</div>
C	<div><div></div>0.7100</div>	<div><div></div>0.4460</div>
D	<div><div></div>0.8310</div>	<div><div></div>0.5120</div>
E	<div><div></div>0.7460</div>	<div><div></div>0.4690</div>
F	<div><div></div>0.8340</div>	<div><div></div>0.5100</div>
G	<div><div></div>0.7440</div>	<div><div></div>0.4690</div>
H	<div><div></div>0.8330</div>	<div><div></div>0.5120</div>
I	<div><div></div>0.7470</div>	<div><div></div>0.4700</div>
J	<div><div></div>0.7200</div>	<div><div></div>0.4620</div>
K	<div><div></div>0.7220</div>	<div><div></div>0.4620</div>
L	<div><div></div>0.7230</div>	<div><div></div>0.4640</div>

1.0

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