



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2024 – 09:42 PM EDT

PDB ID : 6NBB
EMDB ID : EMD-0406
Title : Horse liver alcohol dehydrogenase determined using single-particle cryo-EM at 200 keV
Authors : Herzik Jr., M.A.; Wu, M.; Lander, G.C.
Deposited on : 2018-12-06
Resolution : 2.90 Å(reported)
Based on initial model : 2JHF

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
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) : 2.39

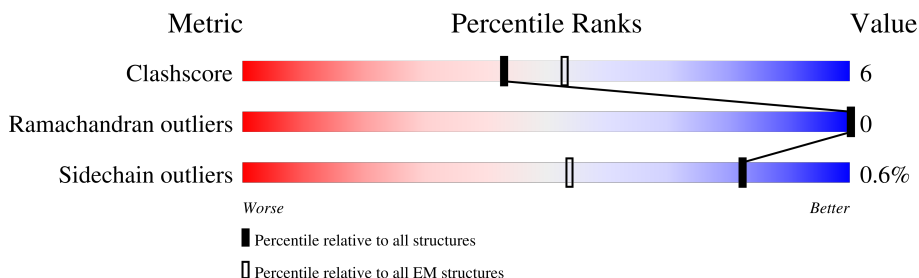
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1-A	374	85% 15%
1	1-B	374	86% 13%
1	10-A	374	78% 22%
1	10-B	374	81% 19%
1	2-A	374	84% 16%
1	2-B	374	82% 18%
1	3-A	374	83% 17%
1	3-B	374	85% 15%
1	4-A	374	83% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	4-B	374		84% 16%
1	5-A	374		83% 17%
1	5-B	374		83% 17%
1	6-A	374		81% 19%
1	6-B	374		83% 17%
1	7-A	374		82% 18%
1	7-B	374		83% 17%
1	8-A	374		81% 19%
1	8-B	374		81% 19%
1	9-A	374		79% 21%
1	9-B	374		82% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 56620 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 Alcohol dehydrogenase E chain.

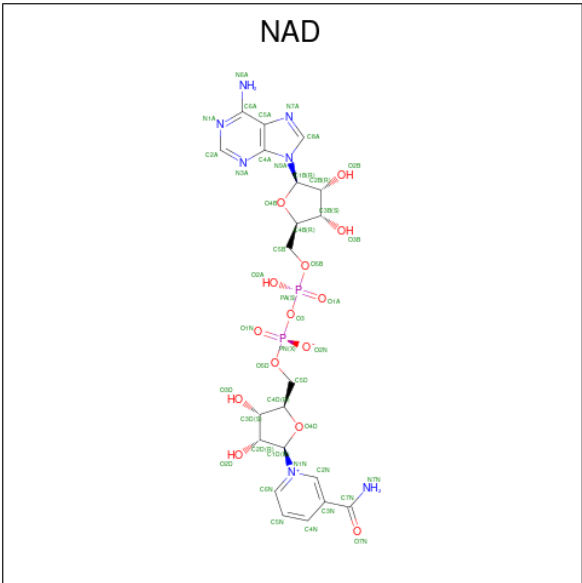
Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	2-A	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	3-A	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	4-A	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	5-A	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	6-A	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	7-A	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	8-A	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	9-A	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	10-A	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	1-B	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	2-B	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	3-B	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	4-B	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	5-B	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	6-B	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	7-B	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	8-B	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	9-B	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		
1	10-B	374	Total	C	N	O	S	0	0
			2785	1769	472	521	23		

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					AltConf
2	1-A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	2-A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	3-A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	4-A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	5-A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	6-A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	7-A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	8-A	1	Total	C	N	O	P	0
			44	21	7	14	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	9-A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	10-A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	1-B	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	2-B	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	3-B	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	4-B	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	5-B	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	6-B	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	7-B	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	8-B	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	9-B	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	10-B	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	1-A	2	Total	Zn	0
			2	2	
3	2-A	2	Total	Zn	0
			2	2	
3	3-A	2	Total	Zn	0
			2	2	
3	4-A	2	Total	Zn	0
			2	2	
3	5-A	2	Total	Zn	0
			2	2	
3	6-A	2	Total	Zn	0
			2	2	
3	7-A	2	Total	Zn	0
			2	2	

Continued on next page...

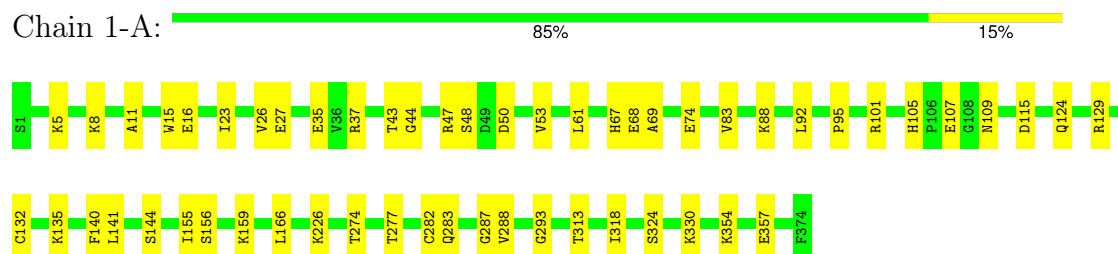
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
3	8-A	2	Total 2	Zn 2	0
3	9-A	2	Total 2	Zn 2	0
3	10-A	2	Total 2	Zn 2	0
3	1-B	2	Total 2	Zn 2	0
3	2-B	2	Total 2	Zn 2	0
3	3-B	2	Total 2	Zn 2	0
3	4-B	2	Total 2	Zn 2	0
3	5-B	2	Total 2	Zn 2	0
3	6-B	2	Total 2	Zn 2	0
3	7-B	2	Total 2	Zn 2	0
3	8-B	2	Total 2	Zn 2	0
3	9-B	2	Total 2	Zn 2	0
3	10-B	2	Total 2	Zn 2	0

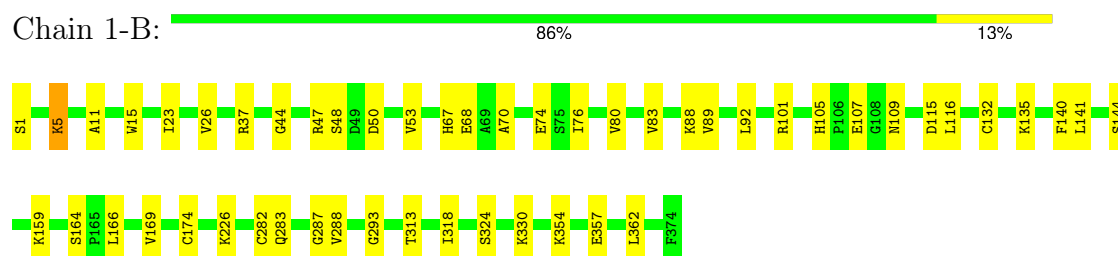
3 Residue-property plots

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. 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. 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.

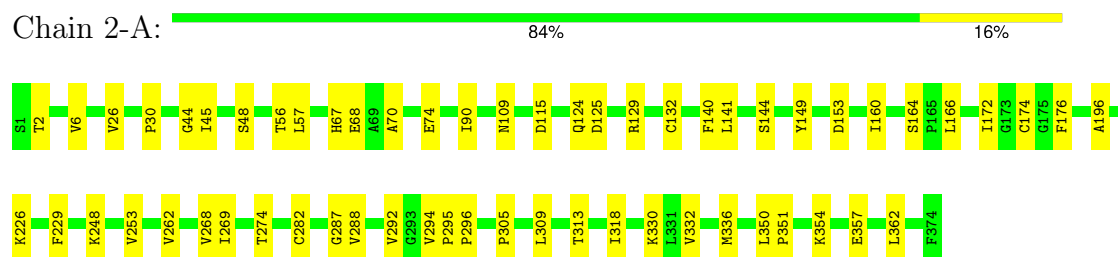
- Molecule 1: Alcohol dehydrogenase E chain



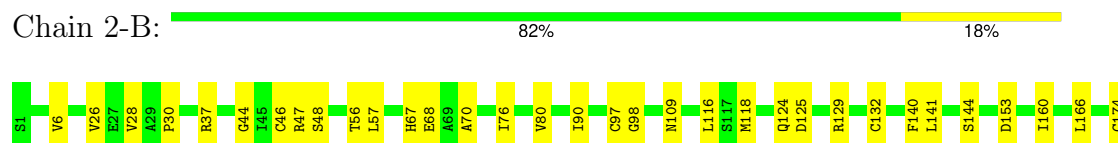
- Molecule 1: Alcohol dehydrogenase E chain

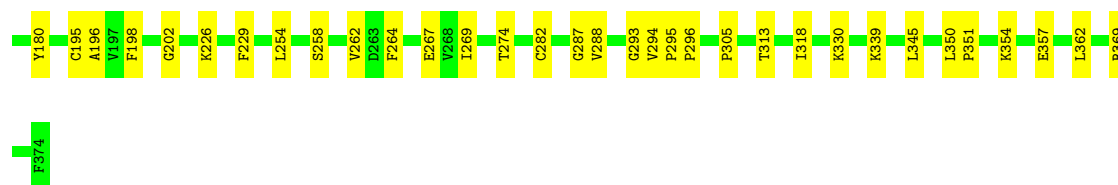


- Molecule 1: Alcohol dehydrogenase E chain



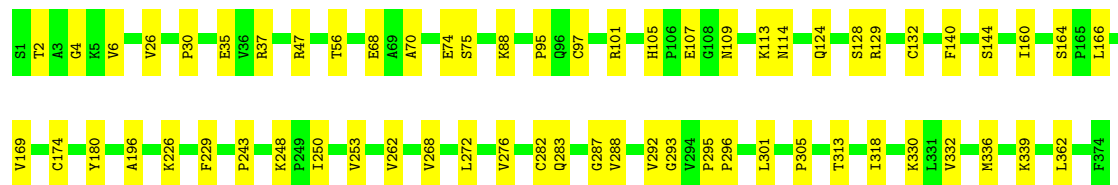
- Molecule 1: Alcohol dehydrogenase E chain





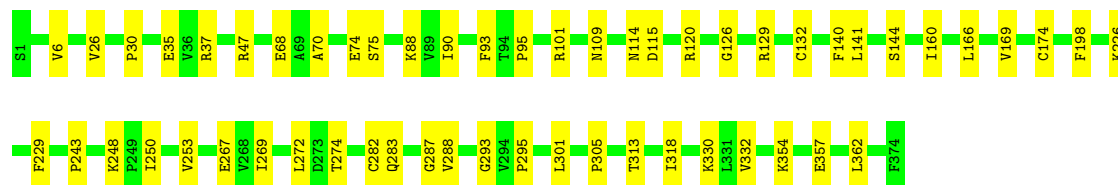
- Molecule 1: Alcohol dehydrogenase E chain

Chain 3-A: 83% 17%



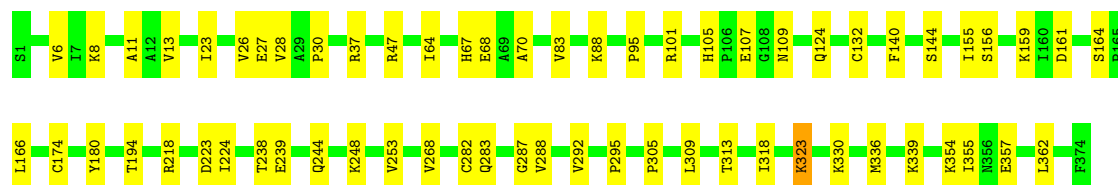
- Molecule 1: Alcohol dehydrogenase E chain

Chain 3-B: 85% 15%



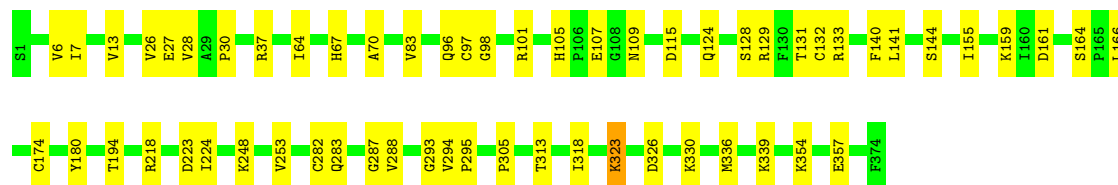
- Molecule 1: Alcohol dehydrogenase E chain

Chain 4-A: 83% 16%



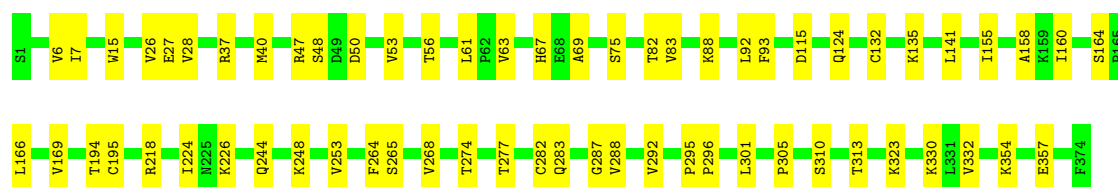
- Molecule 1: Alcohol dehydrogenase E chain

Chain 4-B: 84% 16%



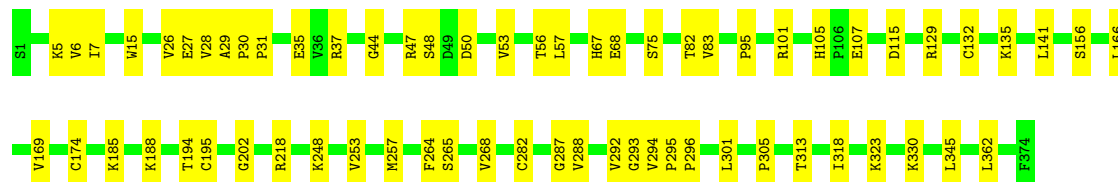
- Molecule 1: Alcohol dehydrogenase E chain

Chain 5-A: 83% 17%



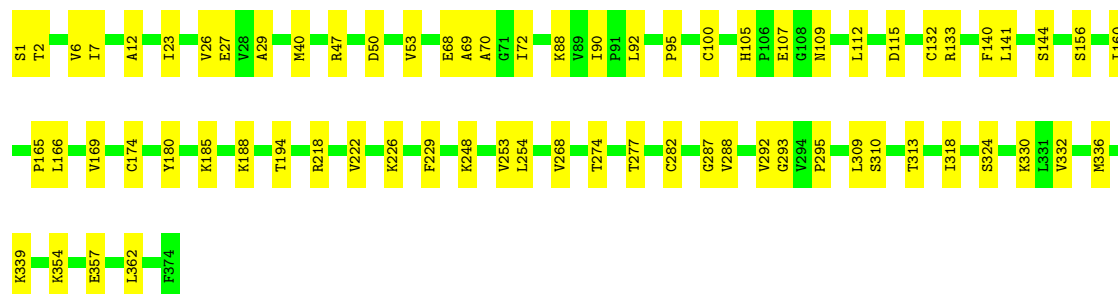
- Molecule 1: Alcohol dehydrogenase E chain

Chain 5-B: 83% 17%



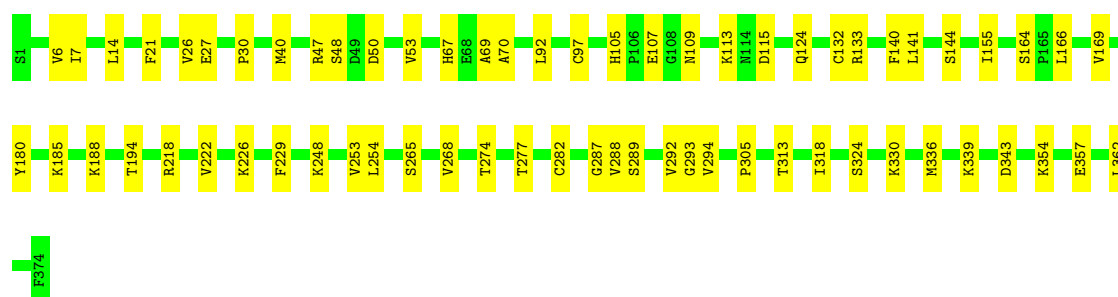
- Molecule 1: Alcohol dehydrogenase E chain

Chain 6-A: 81% 19%



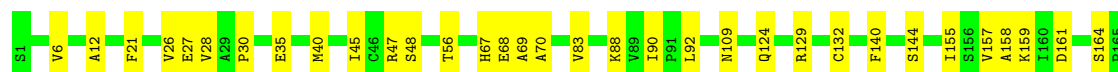
- Molecule 1: Alcohol dehydrogenase E chain

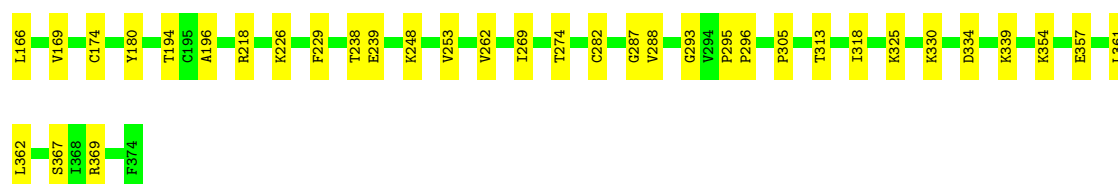
Chain 6-B: 83% 17%



- Molecule 1: Alcohol dehydrogenase E chain

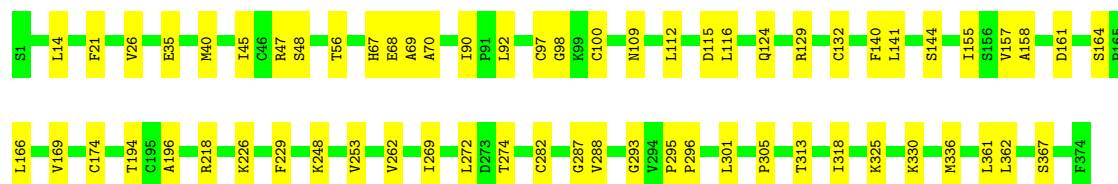
Chain 7-A: 82% 18%





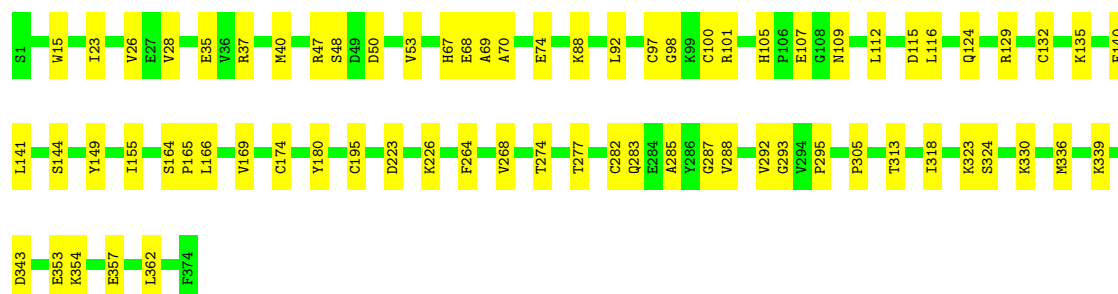
- Molecule 1: Alcohol dehydrogenase E chain

Chain 7-B: 83% 17%



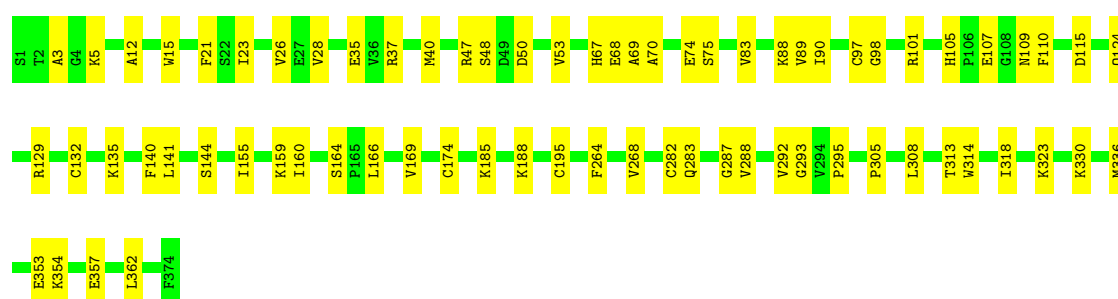
- Molecule 1: Alcohol dehydrogenase E chain

Chain 8-A: 81% 19%



- Molecule 1: Alcohol dehydrogenase E chain

Chain 8-B: 81% 19%



- Molecule 1: Alcohol dehydrogenase E chain

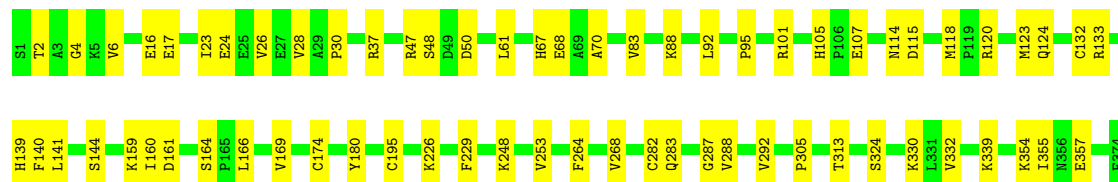
Chain 9-A: 79% 21%





- Molecule 1: Alcohol dehydrogenase E chain

Chain 9-B: 82% 18%



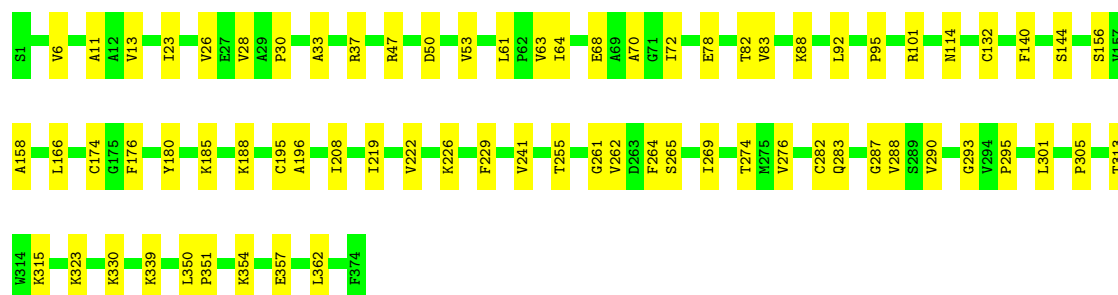
- Molecule 1: Alcohol dehydrogenase E chain

Chain 10-A: 78% 22%



- Molecule 1: Alcohol dehydrogenase E chain

Chain 10-B: 81% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	11672	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	69	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	16000	Depositor
Magnification	73000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.038	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	205.528, 205.528, 205.528	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5585, 0.5585, 0.5585	Depositor

5 Model quality

5.1 Standard geometry

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

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	1-A	0.39	0/2837	0.56	0/3834
1	1-B	0.38	0/2837	0.57	0/3834
1	2-A	0.32	0/2837	0.55	0/3834
1	2-B	0.32	0/2837	0.57	0/3834
1	3-A	0.44	0/2837	0.59	0/3834
1	3-B	0.43	0/2837	0.59	0/3834
1	4-A	0.48	0/2837	0.60	0/3834
1	4-B	0.48	0/2837	0.61	0/3834
1	5-A	0.33	0/2837	0.53	0/3834
1	5-B	0.33	0/2837	0.55	0/3834
1	6-A	0.49	0/2837	0.60	0/3834
1	6-B	0.49	0/2837	0.60	0/3834
1	7-A	0.40	0/2837	0.58	0/3834
1	7-B	0.39	0/2837	0.58	0/3834
1	8-A	0.39	0/2837	0.57	0/3834
1	8-B	0.39	0/2837	0.57	0/3834
1	9-A	0.40	0/2837	0.58	0/3834
1	9-B	0.40	0/2837	0.58	0/3834
1	10-A	0.32	0/2837	0.55	0/3834
1	10-B	0.32	0/2837	0.55	0/3834
All	All	0.40	0/56740	0.57	0/76680

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4-A	0	1
1	4-B	0	1
1	5-A	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5-B	0	1
1	8-A	0	1
1	8-B	0	1
1	10-A	0	1
1	10-B	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4-A	323	LYS	Peptide
1	4-B	323	LYS	Peptide
1	5-A	323	LYS	Peptide
1	5-B	323	LYS	Peptide
1	8-A	323	LYS	Peptide

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	1-A	2785	0	2848	29	0
1	1-B	2785	0	2848	30	0
1	2-A	2785	0	2848	33	0
1	2-B	2785	0	2848	36	0
1	3-A	2785	0	2848	40	0
1	3-B	2785	0	2848	34	0
1	4-A	2785	0	2848	40	0
1	4-B	2785	0	2848	35	0
1	5-A	2785	0	2848	36	0
1	5-B	2785	0	2848	42	0
1	6-A	2785	0	2848	37	0
1	6-B	2785	0	2848	37	0
1	7-A	2785	0	2848	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7-B	2785	0	2848	36	0
1	8-A	2785	0	2848	43	0
1	8-B	2785	0	2848	44	0
1	9-A	2785	0	2848	50	0
1	9-B	2785	0	2848	39	0
1	10-A	2785	0	2848	48	0
1	10-B	2785	0	2848	44	0
2	1-A	44	0	24	1	0
2	1-B	44	0	24	2	0
2	2-A	44	0	24	0	0
2	2-B	44	0	24	2	0
2	3-A	44	0	24	2	0
2	3-B	44	0	24	2	0
2	4-A	44	0	24	2	0
2	4-B	44	0	24	2	0
2	5-A	44	0	24	0	0
2	5-B	44	0	24	2	0
2	6-A	44	0	24	1	0
2	6-B	44	0	24	1	0
2	7-A	44	0	24	2	0
2	7-B	44	0	24	2	0
2	8-A	44	0	24	3	0
2	8-B	44	0	24	2	0
2	9-A	44	0	24	4	0
2	9-B	44	0	24	0	0
2	10-A	44	0	24	2	0
2	10-B	44	0	24	2	0
3	1-A	2	0	0	0	0
3	1-B	2	0	0	0	0
3	2-A	2	0	0	0	0
3	2-B	2	0	0	0	0
3	3-A	2	0	0	0	0
3	3-B	2	0	0	0	0
3	4-A	2	0	0	0	0
3	4-B	2	0	0	0	0
3	5-A	2	0	0	0	0
3	5-B	2	0	0	0	0
3	6-A	2	0	0	0	0
3	6-B	2	0	0	0	0
3	7-A	2	0	0	0	0
3	7-B	2	0	0	0	0
3	8-A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8-B	2	0	0	0	0
3	9-A	2	0	0	0	0
3	9-B	2	0	0	0	0
3	10-A	2	0	0	0	0
3	10-B	2	0	0	0	0
All	All	56620	0	57440	733	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 6.

The worst 5 of 733 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:B:48:SER:OG	1:B:67:HIS:CE1	2.37	0.78
1:A:48:SER:OG	1:A:67:HIS:CE1	2.37	0.77
1:B:68:GLU:HG2	1:B:174:CYS:HB3	1.66	0.76
1:B:68:GLU:HG2	1:B:174:CYS:HB3	1.68	0.75
1:B:68:GLU:HG2	1:B:174:CYS:HB3	1.68	0.75

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	1-A	372/374 (100%)	354 (95%)	18 (5%)	0	100	100
1	1-B	372/374 (100%)	358 (96%)	14 (4%)	0	100	100
1	2-A	372/374 (100%)	359 (96%)	13 (4%)	0	100	100
1	2-B	372/374 (100%)	356 (96%)	16 (4%)	0	100	100
1	3-A	372/374 (100%)	354 (95%)	18 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-B	372/374 (100%)	352 (95%)	20 (5%)	0	100	100
1	4-A	372/374 (100%)	359 (96%)	13 (4%)	0	100	100
1	4-B	372/374 (100%)	352 (95%)	20 (5%)	0	100	100
1	5-A	372/374 (100%)	356 (96%)	16 (4%)	0	100	100
1	5-B	372/374 (100%)	356 (96%)	16 (4%)	0	100	100
1	6-A	372/374 (100%)	356 (96%)	16 (4%)	0	100	100
1	6-B	372/374 (100%)	350 (94%)	22 (6%)	0	100	100
1	7-A	372/374 (100%)	354 (95%)	18 (5%)	0	100	100
1	7-B	372/374 (100%)	355 (95%)	17 (5%)	0	100	100
1	8-A	372/374 (100%)	354 (95%)	18 (5%)	0	100	100
1	8-B	372/374 (100%)	357 (96%)	15 (4%)	0	100	100
1	9-A	372/374 (100%)	356 (96%)	16 (4%)	0	100	100
1	9-B	372/374 (100%)	358 (96%)	14 (4%)	0	100	100
1	10-A	372/374 (100%)	357 (96%)	15 (4%)	0	100	100
1	10-B	372/374 (100%)	351 (94%)	21 (6%)	0	100	100
All	All	7440/7480 (100%)	7104 (96%)	336 (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	1-A	308/308 (100%)	305 (99%)	3 (1%)	73	91
1	1-B	308/308 (100%)	305 (99%)	3 (1%)	73	91
1	2-A	308/308 (100%)	307 (100%)	1 (0%)	91	97
1	2-B	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	3-A	308/308 (100%)	307 (100%)	1 (0%)	91	97
1	3-B	308/308 (100%)	306 (99%)	2 (1%)	84	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4-A	308/308 (100%)	307 (100%)	1 (0%)	91	97
1	4-B	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	5-A	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	5-B	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	6-A	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	6-B	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	7-A	308/308 (100%)	307 (100%)	1 (0%)	91	97
1	7-B	308/308 (100%)	307 (100%)	1 (0%)	91	97
1	8-A	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	8-B	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	9-A	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	9-B	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	10-A	308/308 (100%)	306 (99%)	2 (1%)	84	95
1	10-B	308/308 (100%)	307 (100%)	1 (0%)	91	97
All	All	6160/6160 (100%)	6124 (99%)	36 (1%)	82	95

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	8-B	330	LYS
1	10-B	330	LYS
1	9-A	330	LYS
1	9-B	330	LYS
1	4-A	330	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	7-B	300	ASN
1	9-B	300	ASN
1	8-A	283	GLN
1	8-B	283	GLN
1	10-A	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 60 ligands modelled in this entry, 40 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	4-A	401	-	42,48,48	3.72	18 (42%)	50,73,73	2.88	9 (18%)
2	NAD	5-A	401	-	42,48,48	3.71	17 (40%)	50,73,73	2.71	7 (14%)
2	NAD	3-A	401	-	42,48,48	3.76	18 (42%)	50,73,73	2.94	7 (14%)
2	NAD	10-A	401	-	42,48,48	3.72	17 (40%)	50,73,73	2.81	7 (14%)
2	NAD	1-B	401	-	42,48,48	3.72	18 (42%)	50,73,73	2.86	7 (14%)
2	NAD	9-B	401	-	42,48,48	3.70	17 (40%)	50,73,73	2.77	7 (14%)
2	NAD	1-A	401	-	42,48,48	3.75	18 (42%)	50,73,73	2.92	7 (14%)
2	NAD	5-B	401	-	42,48,48	3.73	17 (40%)	50,73,73	2.84	7 (14%)
2	NAD	6-A	401	-	42,48,48	3.73	18 (42%)	50,73,73	2.84	8 (16%)
2	NAD	7-A	401	-	42,48,48	3.71	17 (40%)	50,73,73	2.86	7 (14%)
2	NAD	6-B	401	-	42,48,48	3.73	18 (42%)	50,73,73	2.84	8 (16%)
2	NAD	7-B	401	-	42,48,48	3.72	17 (40%)	50,73,73	2.85	7 (14%)
2	NAD	10-B	401	-	42,48,48	3.70	17 (40%)	50,73,73	2.80	7 (14%)
2	NAD	4-B	401	-	42,48,48	3.74	18 (42%)	50,73,73	2.89	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	2-A	401	-	42,48,48	3.71	17 (40%)	50,73,73	2.72	7 (14%)
2	NAD	8-A	401	-	42,48,48	3.68	17 (40%)	50,73,73	2.74	8 (16%)
2	NAD	3-B	401	-	42,48,48	3.72	17 (40%)	50,73,73	2.84	7 (14%)
2	NAD	9-A	401	-	42,48,48	3.73	18 (42%)	50,73,73	2.93	7 (14%)
2	NAD	2-B	401	-	42,48,48	3.71	17 (40%)	50,73,73	2.81	7 (14%)
2	NAD	8-B	401	-	42,48,48	3.74	17 (40%)	50,73,73	2.86	7 (14%)

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	NAD	4-A	401	-	-	18/26/62/62	0/5/5/5
2	NAD	5-A	401	-	-	10/26/62/62	0/5/5/5
2	NAD	3-A	401	-	-	12/26/62/62	0/5/5/5
2	NAD	10-A	401	-	-	11/26/62/62	0/5/5/5
2	NAD	1-B	401	-	-	18/26/62/62	0/5/5/5
2	NAD	9-B	401	-	-	12/26/62/62	0/5/5/5
2	NAD	1-A	401	-	-	9/26/62/62	0/5/5/5
2	NAD	5-B	401	-	-	12/26/62/62	0/5/5/5
2	NAD	6-A	401	-	-	13/26/62/62	0/5/5/5
2	NAD	7-A	401	-	-	14/26/62/62	0/5/5/5
2	NAD	6-B	401	-	-	12/26/62/62	0/5/5/5
2	NAD	7-B	401	-	-	14/26/62/62	0/5/5/5
2	NAD	10-B	401	-	-	12/26/62/62	0/5/5/5
2	NAD	4-B	401	-	-	14/26/62/62	0/5/5/5
2	NAD	2-A	401	-	-	11/26/62/62	0/5/5/5
2	NAD	8-A	401	-	-	13/26/62/62	0/5/5/5
2	NAD	3-B	401	-	-	9/26/62/62	0/5/5/5
2	NAD	9-A	401	-	-	10/26/62/62	0/5/5/5
2	NAD	2-B	401	-	-	8/26/62/62	0/5/5/5
2	NAD	8-B	401	-	-	12/26/62/62	0/5/5/5

The worst 5 of 348 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-B	401	NAD	C3D-C4D	-9.08	1.30	1.53
2	8-B	401	NAD	C3D-C4D	-9.06	1.30	1.53
2	6-A	401	NAD	C3D-C4D	-9.06	1.30	1.53
2	9-B	401	NAD	C3D-C4D	-9.03	1.30	1.53
2	8-A	401	NAD	C3D-C4D	-8.97	1.30	1.53

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-B	401	NAD	C5A-C6A-N6A	11.00	137.07	120.31
2	10-A	401	NAD	C5A-C6A-N6A	10.98	137.03	120.31
2	5-A	401	NAD	C5A-C6A-N6A	10.84	136.82	120.31
2	2-B	401	NAD	C5A-C6A-N6A	10.82	136.80	120.31
2	5-B	401	NAD	C5A-C6A-N6A	10.80	136.76	120.31

There are no chirality outliers.

5 of 244 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-A	401	NAD	C5B-O5B-PA-O2A
2	1-A	401	NAD	C5B-O5B-PA-O3
2	1-A	401	NAD	O4D-C1D-N1N-C6N
2	2-A	401	NAD	C5B-O5B-PA-O2A
2	2-A	401	NAD	C5B-O5B-PA-O3

There are no ring outliers.

17 monomers are involved in 34 short contacts:

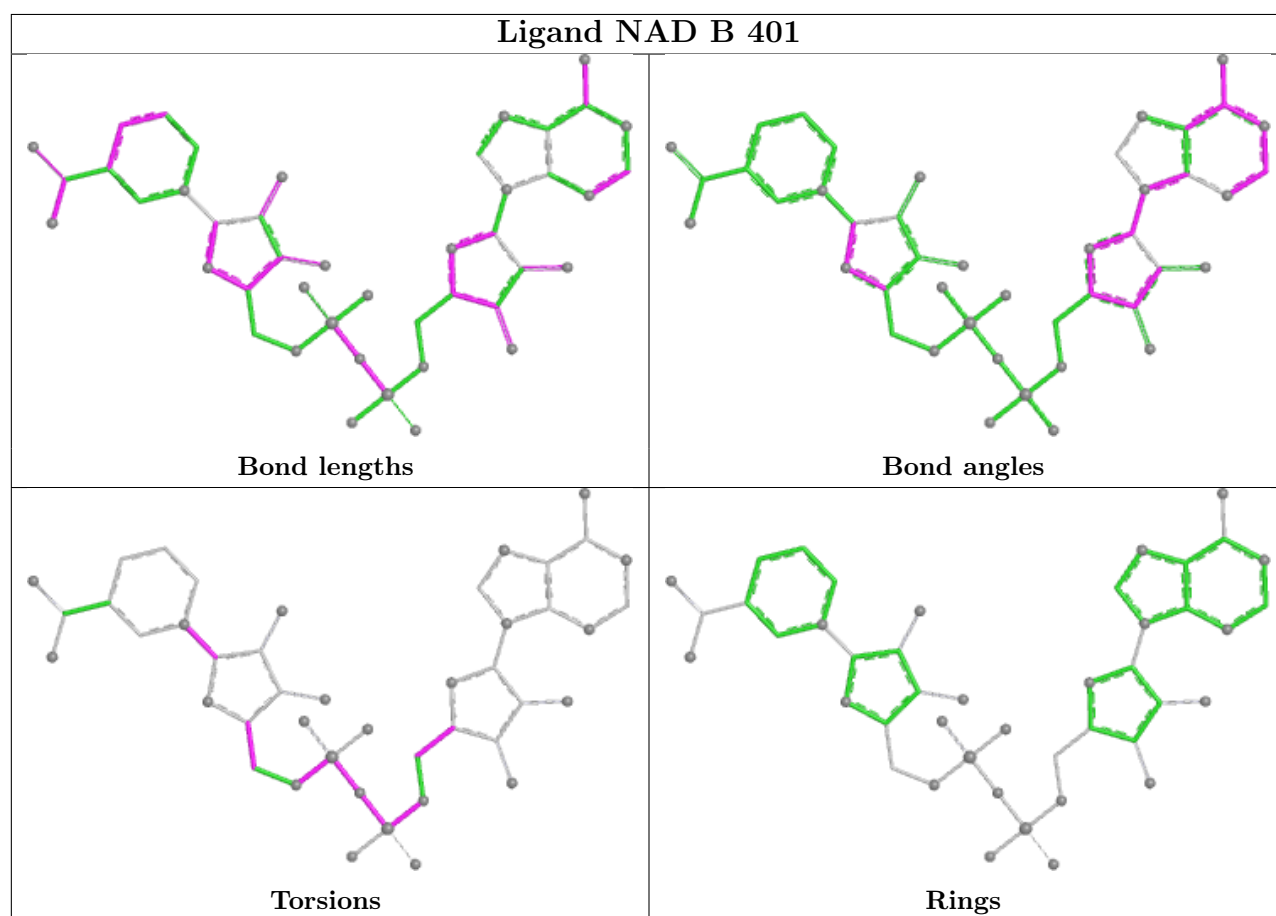
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	4-A	401	NAD	2	0
2	3-A	401	NAD	2	0
2	10-A	401	NAD	2	0
2	1-B	401	NAD	2	0
2	1-A	401	NAD	1	0
2	5-B	401	NAD	2	0
2	6-A	401	NAD	1	0
2	7-A	401	NAD	2	0
2	6-B	401	NAD	1	0
2	7-B	401	NAD	2	0
2	10-B	401	NAD	2	0
2	4-B	401	NAD	2	0
2	8-A	401	NAD	3	0

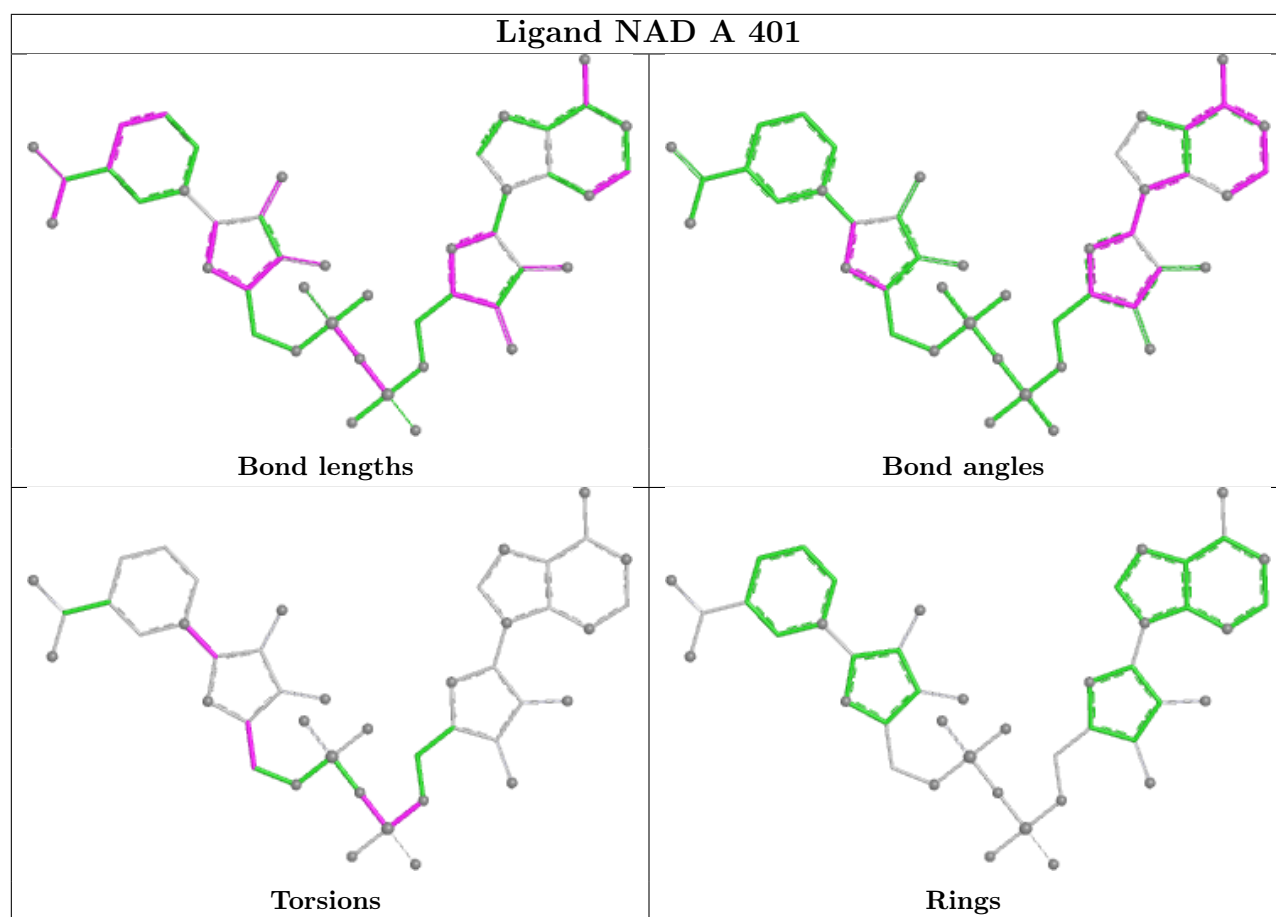
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	3-B	401	NAD	2	0
2	9-A	401	NAD	4	0
2	2-B	401	NAD	2	0
2	8-B	401	NAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

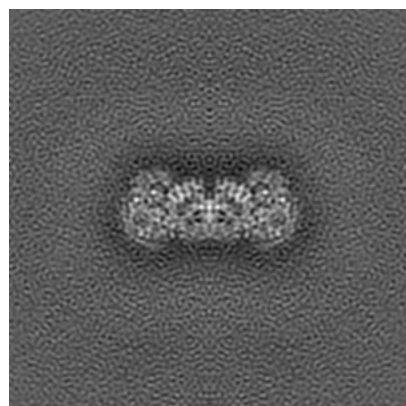
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0406. These allow visual inspection of the internal detail of the map and identification of artifacts.

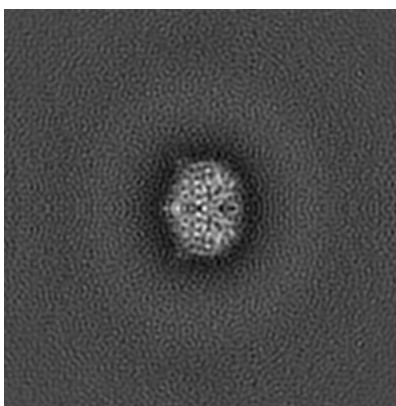
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

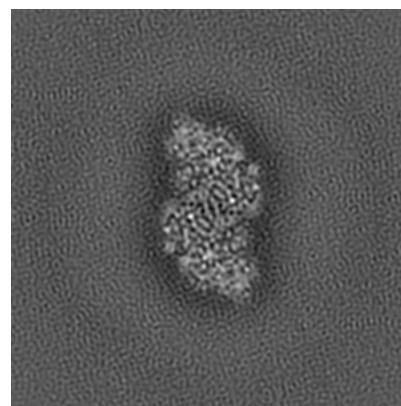
6.1.1 Primary map



X

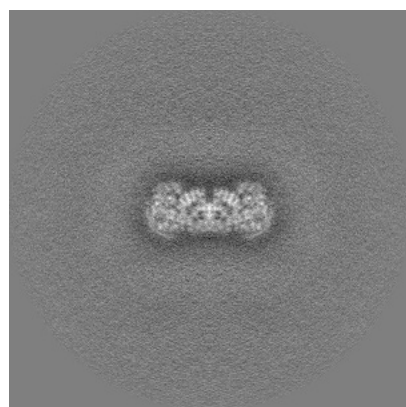


Y

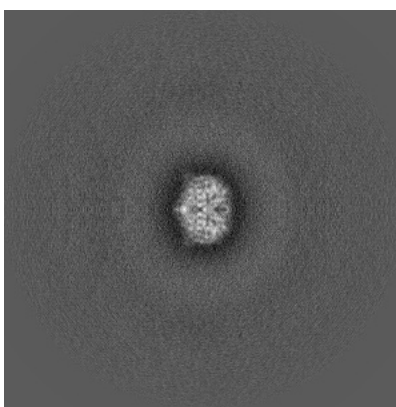


Z

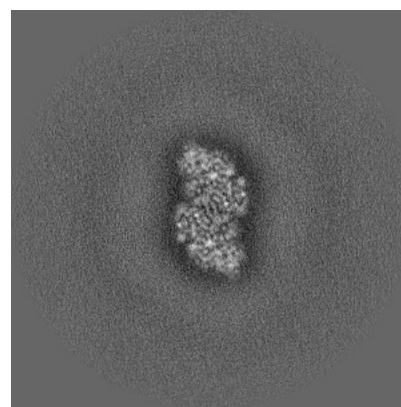
6.1.2 Raw map



X



Y



Z

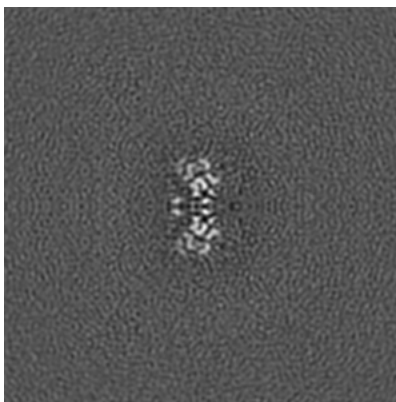
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

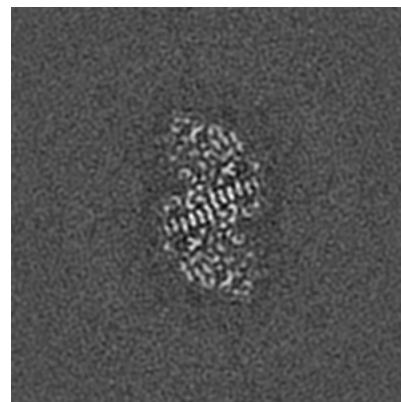
6.2.1 Primary map



X Index: 184

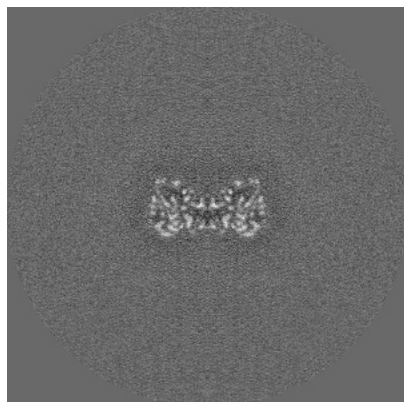


Y Index: 184

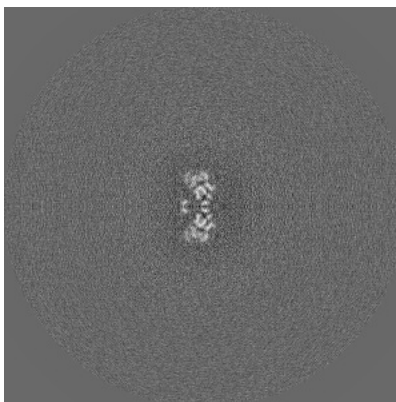


Z Index: 184

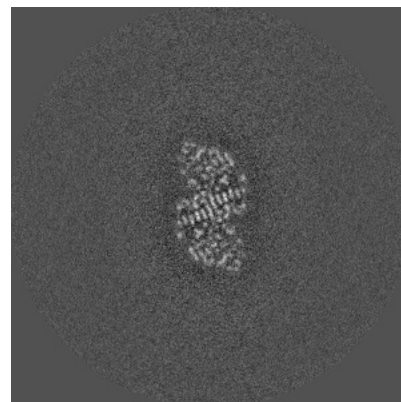
6.2.2 Raw map



X Index: 256



Y Index: 256

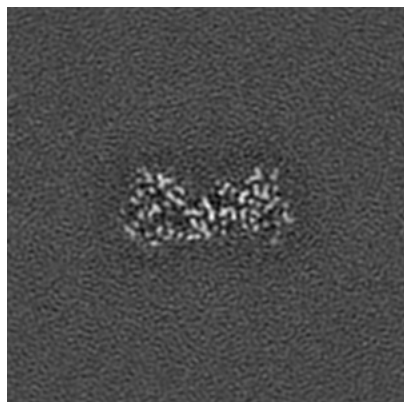


Z Index: 256

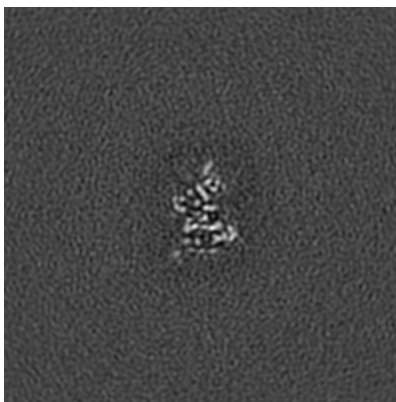
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

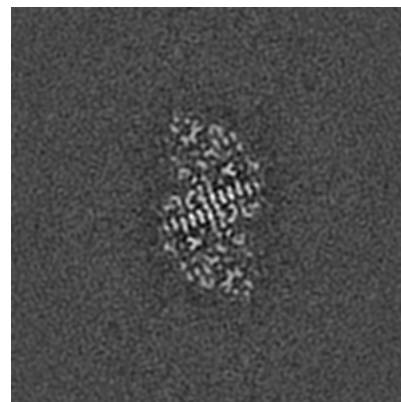
6.3.1 Primary map



X Index: 189

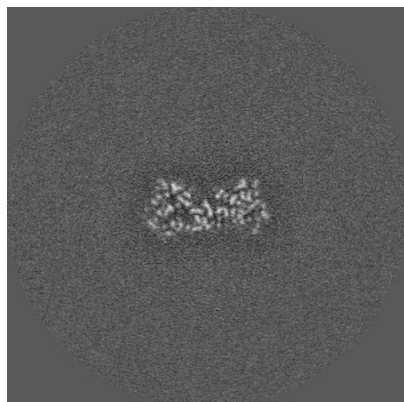


Y Index: 177

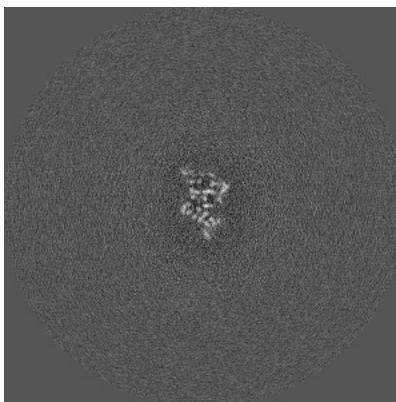


Z Index: 185

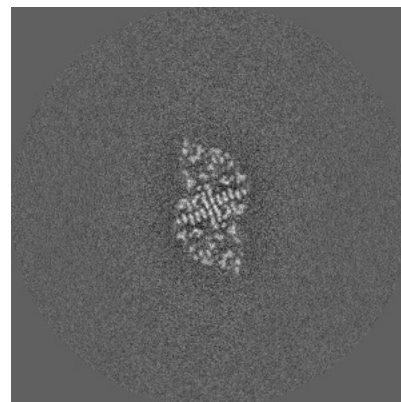
6.3.2 Raw map



X Index: 261



Y Index: 264

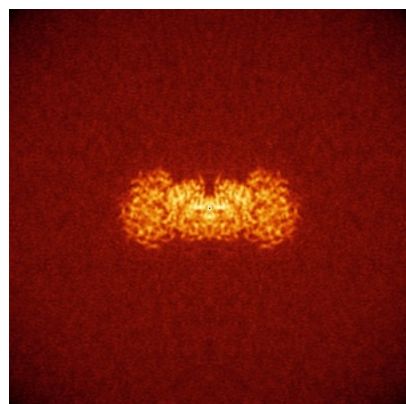


Z Index: 258

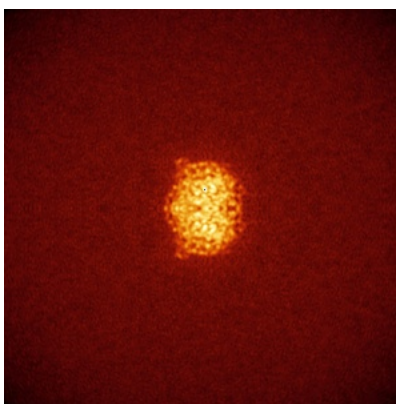
The images above show the largest variance slices of the map in three orthogonal directions.

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

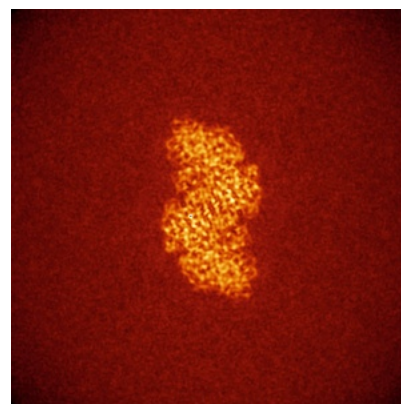
6.4.1 Primary map



X

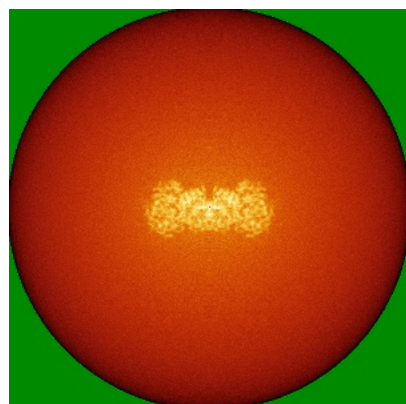


Y

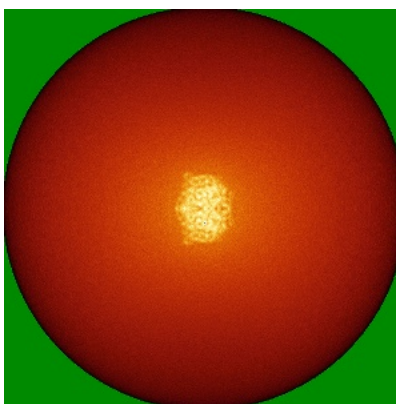


Z

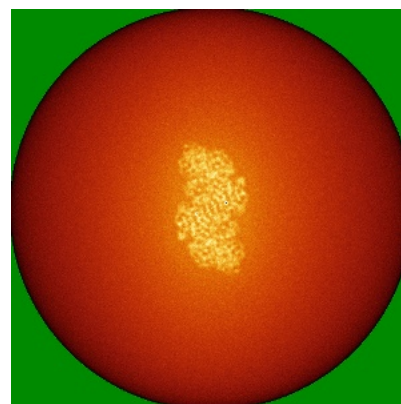
6.4.2 Raw map



X



Y

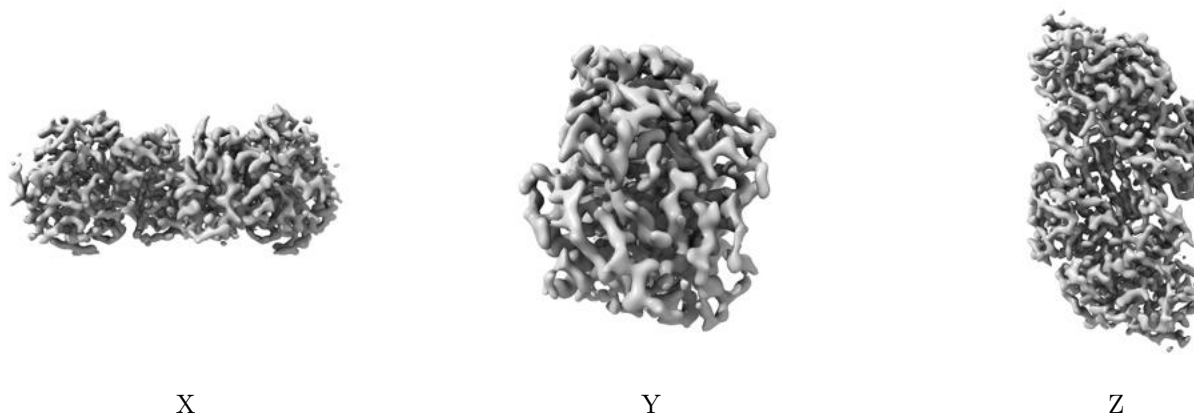


Z

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.

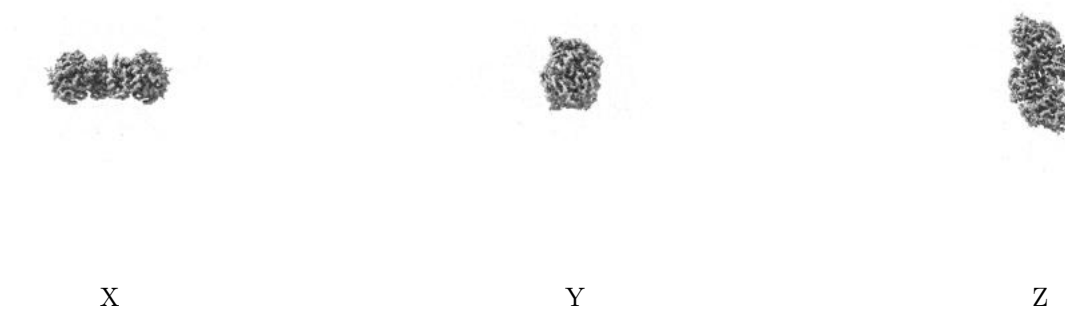
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

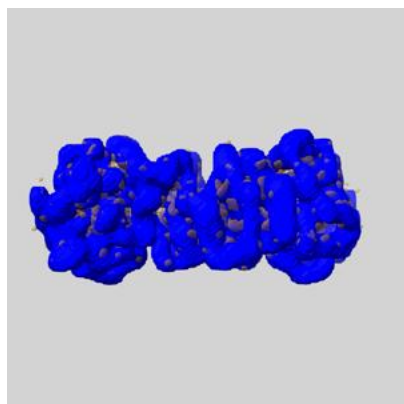
6.6 Mask visualisation [i](#)

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

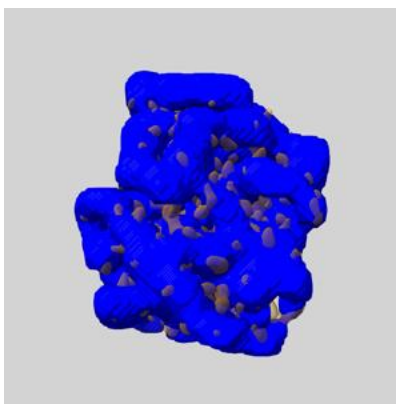
A mask typically either:

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

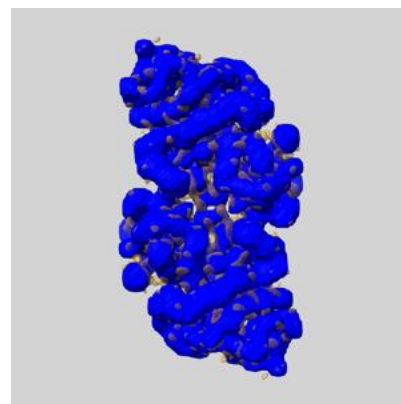
6.6.1 emd_0406_msk_1.map [i](#)



X



Y

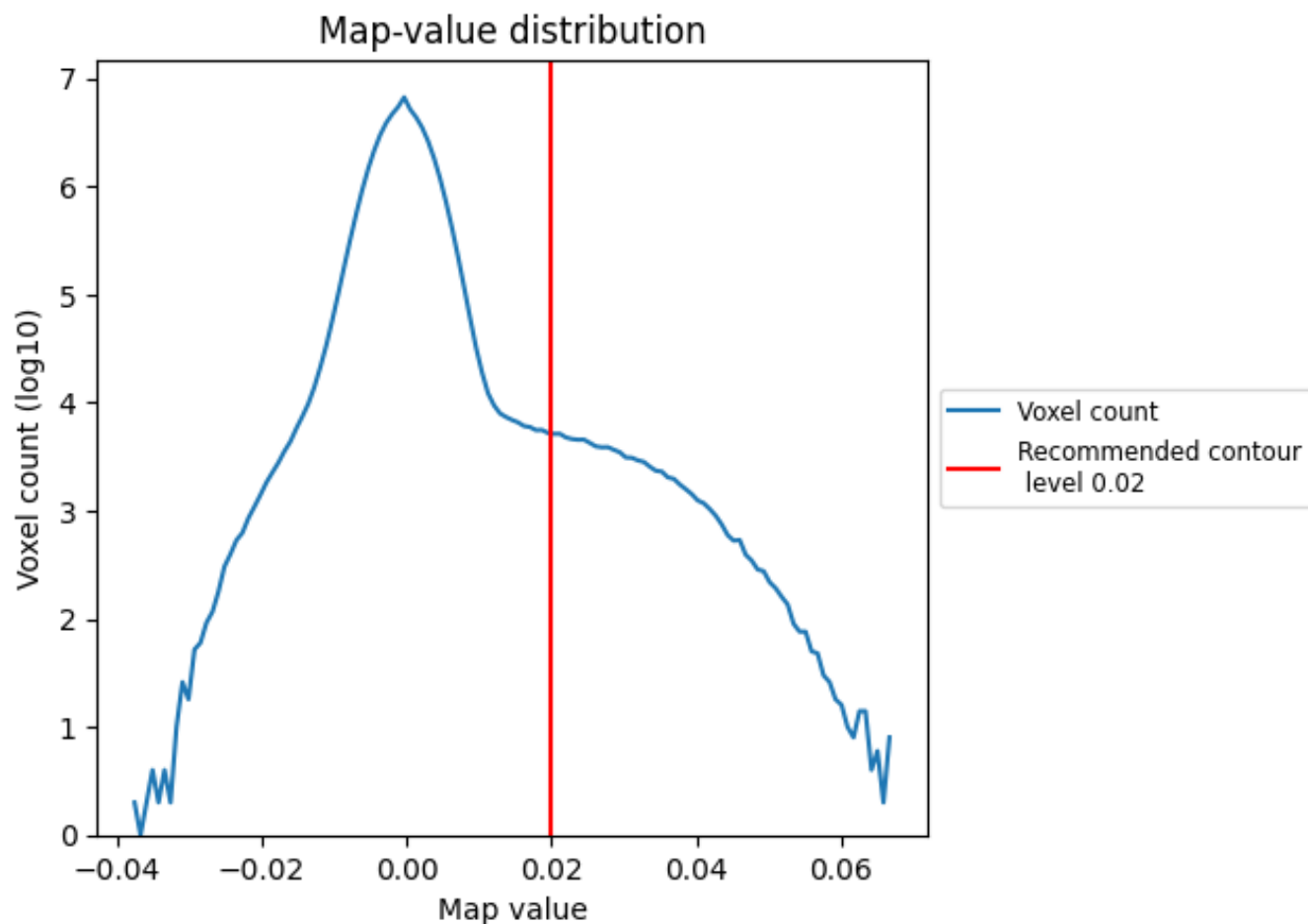


Z

7 Map analysis [i](#)

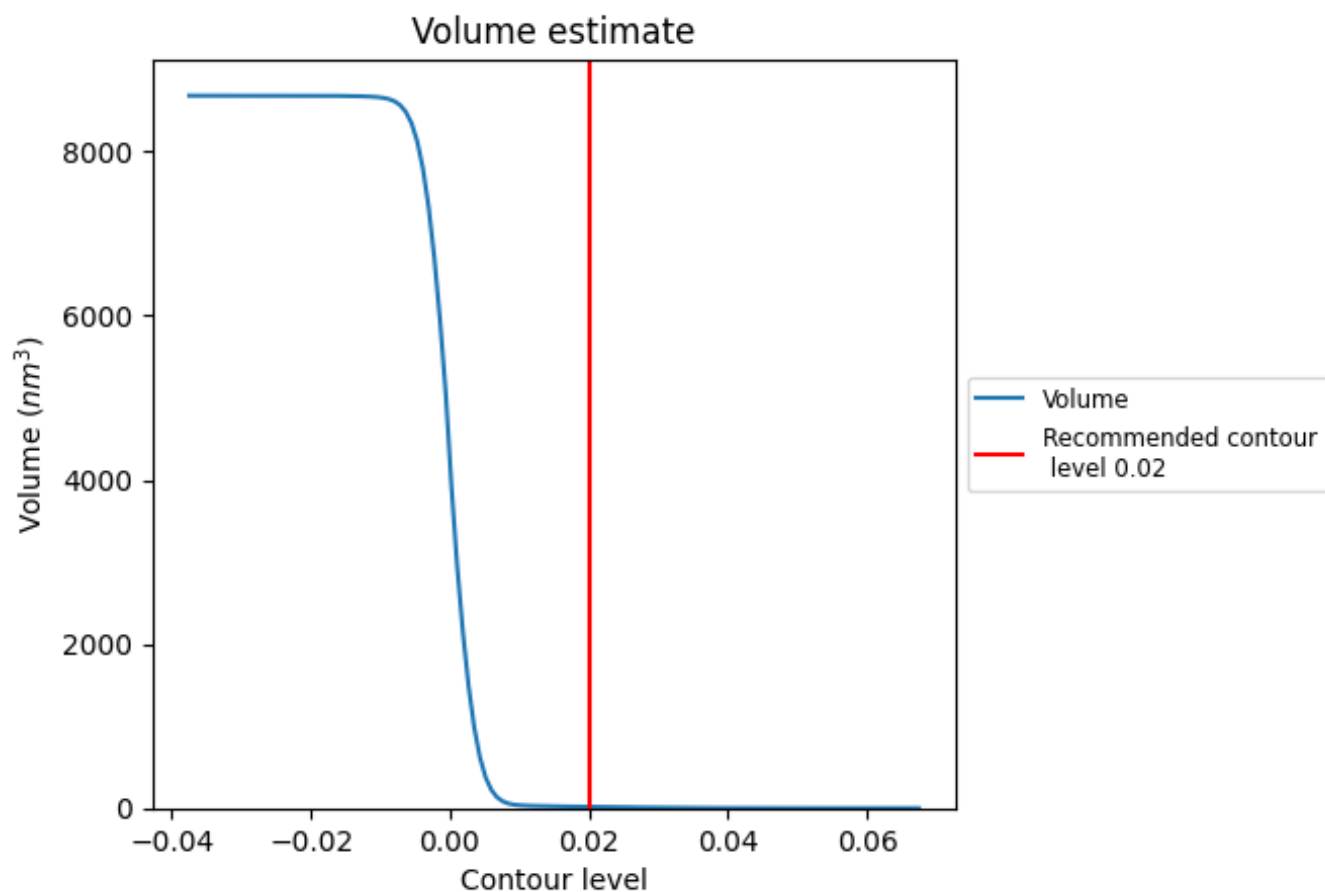
This section contains the results of statistical analysis of the map.

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.

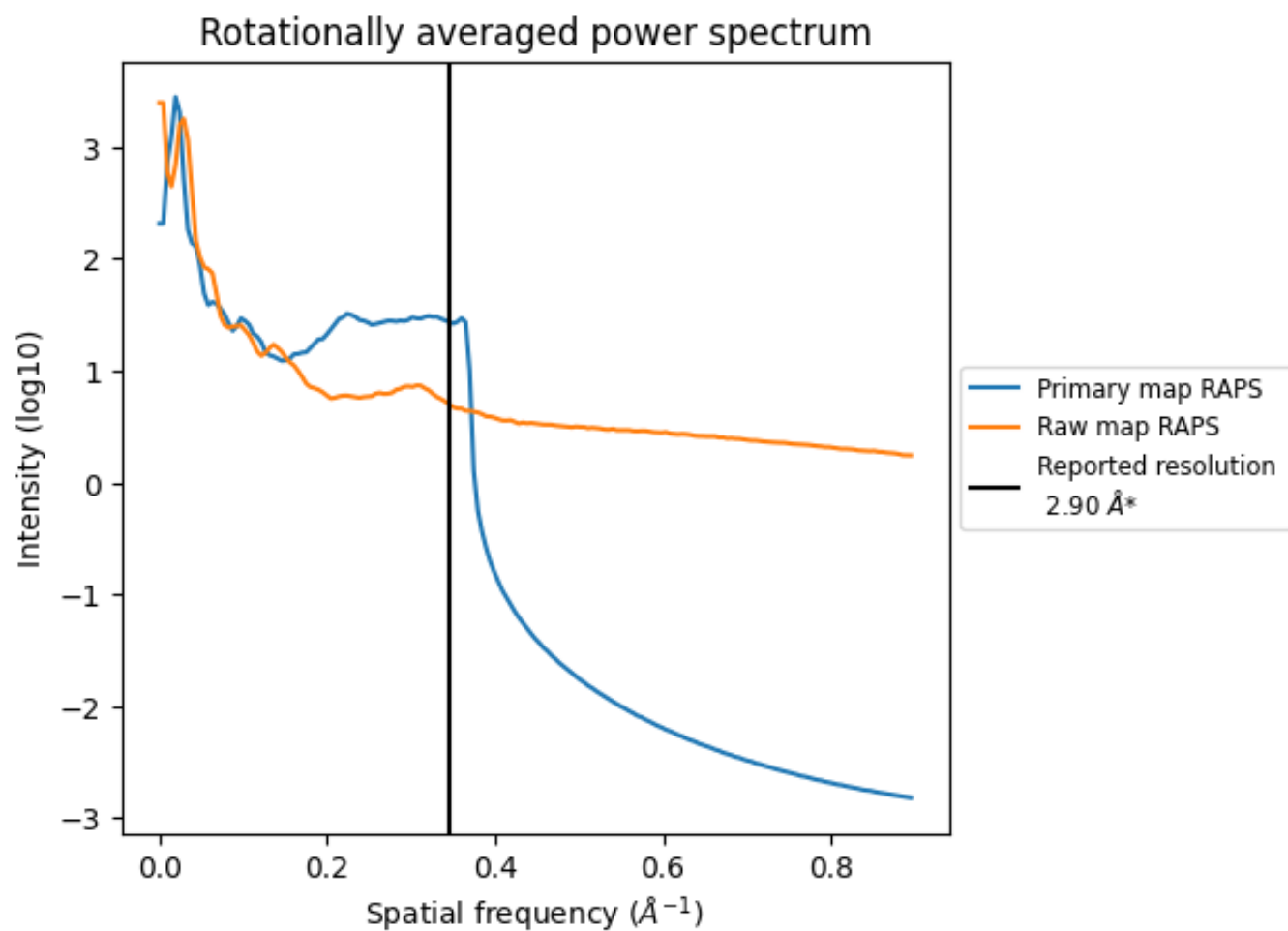
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 16 nm³; this corresponds to an approximate mass of 14 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](#)

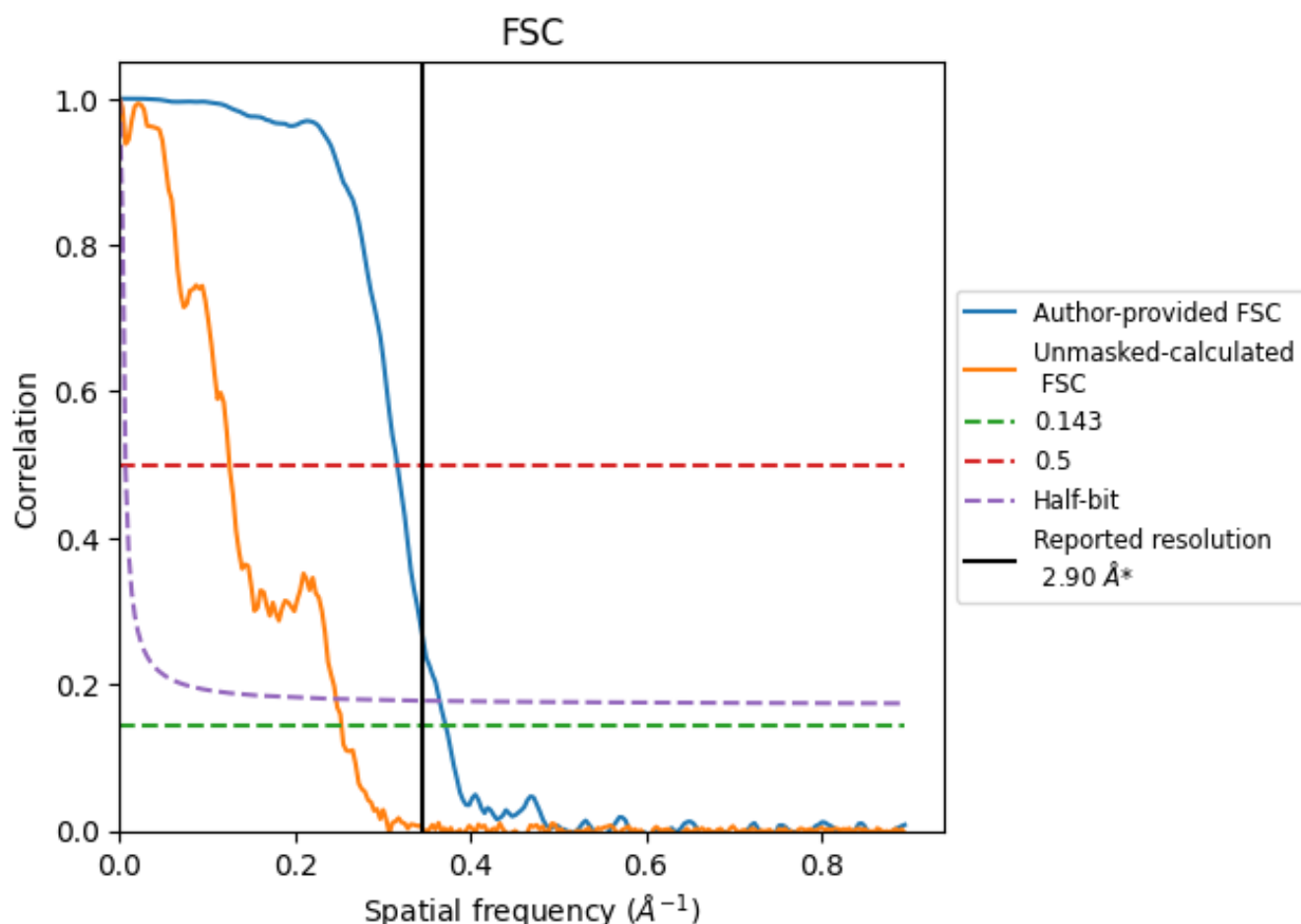


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.69	3.16	2.74
Unmasked-calculated*	3.95	7.97	4.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 2.9 by more than 10 %

9 Map-model fit

This section was not generated.