wwPDB EM Validation Summary Report (i)

Sep 8, 2026 – 02:03 am BST

PDB ID	:	7P5H / pdb_00007p5h
EMDB ID	:	EMD-13199
Title	:	TmHydABC- D2 map
Authors	:	Furlan, C.; Chongdar, N.; Gupta, P.; Lubitz, W.; Ogata, H.; Blaza, J.N.; Birrell, J.A.
Deposited on	:	2021-07-14
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

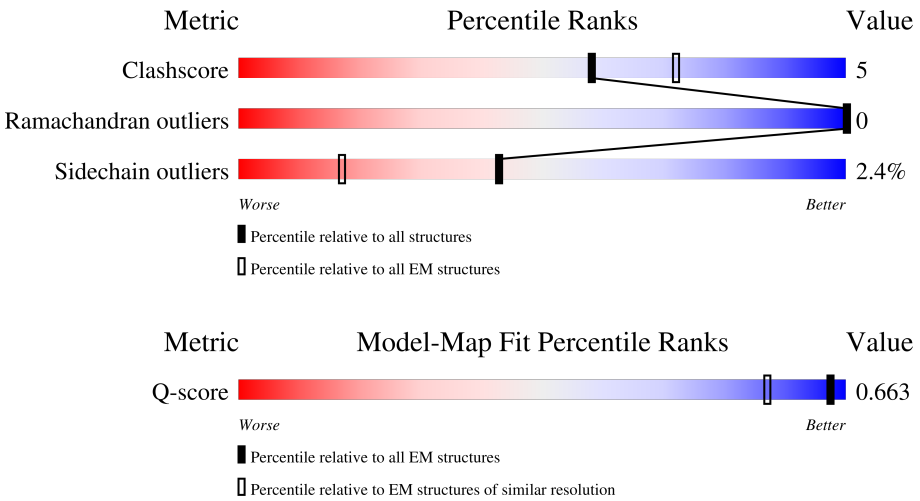
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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 <=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	645	78% 8% 14%
1	D	645	78% 8% 14%
1	a	645	78% 7% 14%
1	d	645	78% 7% 14%

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Mol	Chain	Length	Quality of chain
2	B	626	12% 75% 14% 11%
2	E	626	12% 75% 13% 11%
2	b	626	12% 74% 14% 11%
2	e	626	12% 74% 14% 11%
3	C	189	7% 70% 11% • 17%
3	F	189	7% 70% 12% • 17%
3	c	189	7% 71% 11% • 17%
3	f	189	7% 71% 11% • 17%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 80468 atoms, of which 40000 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 Fe-hydrogenase, subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	554	8791	2765	4415	753	826	32	2	0
1	D	554	8791	2765	4415	753	826	32	2	0
1	a	554	8791	2765	4415	753	826	32	2	0
1	d	554	8791	2765	4415	753	826	32	2	0

- Molecule 2 is a protein called Fe-hydrogenase, subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	555	8600	2723	4321	720	805	31	1	0
2	E	555	8600	2723	4321	720	805	31	1	0
2	b	555	8600	2723	4321	720	805	31	1	0
2	e	555	8600	2723	4321	720	805	31	1	0

- Molecule 3 is a protein called Fe-hydrogenase, subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	156	2463	784	1245	195	230	9	0	0
3	F	156	2463	784	1245	195	230	9	0	0
3	c	156	2463	784	1245	195	230	9	0	0
3	f	156	2463	784	1245	195	230	9	0	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-27	MET	-	initiating methionine	UNP Q9S5X7
C	-26	ALA	-	linker	UNP Q9S5X7
C	-25	SER	-	linker	UNP Q9S5X7
C	-24	TRP	-	expression tag	UNP Q9S5X7
C	-23	SER	-	expression tag	UNP Q9S5X7
C	-22	HIS	-	expression tag	UNP Q9S5X7
C	-21	PRO	-	expression tag	UNP Q9S5X7
C	-20	GLN	-	expression tag	UNP Q9S5X7
C	-19	PHE	-	expression tag	UNP Q9S5X7
C	-18	GLU	-	expression tag	UNP Q9S5X7
C	-17	LYS	-	expression tag	UNP Q9S5X7
C	-16	SER	-	linker	UNP Q9S5X7
C	-15	GLY	-	linker	UNP Q9S5X7
C	-14	GLY	-	linker	UNP Q9S5X7
C	-13	GLY	-	linker	UNP Q9S5X7
C	-12	GLY	-	linker	UNP Q9S5X7
C	-11	GLY	-	linker	UNP Q9S5X7
C	-10	GLU	-	expression tag	UNP Q9S5X7
C	-9	ASN	-	expression tag	UNP Q9S5X7
C	-8	LEU	-	expression tag	UNP Q9S5X7
C	-7	TYR	-	expression tag	UNP Q9S5X7
C	-6	PHE	-	expression tag	UNP Q9S5X7
C	-5	GLN	-	expression tag	UNP Q9S5X7
C	-4	GLY	-	expression tag	UNP Q9S5X7
C	-3	ALA	-	expression tag	UNP Q9S5X7
C	-2	VAL	-	expression tag	UNP Q9S5X7
F	-27	MET	-	initiating methionine	UNP Q9S5X7
F	-26	ALA	-	linker	UNP Q9S5X7
F	-25	SER	-	linker	UNP Q9S5X7
F	-24	TRP	-	expression tag	UNP Q9S5X7
F	-23	SER	-	expression tag	UNP Q9S5X7
F	-22	HIS	-	expression tag	UNP Q9S5X7
F	-21	PRO	-	expression tag	UNP Q9S5X7
F	-20	GLN	-	expression tag	UNP Q9S5X7
F	-19	PHE	-	expression tag	UNP Q9S5X7
F	-18	GLU	-	expression tag	UNP Q9S5X7
F	-17	LYS	-	expression tag	UNP Q9S5X7
F	-16	SER	-	linker	UNP Q9S5X7
F	-15	GLY	-	linker	UNP Q9S5X7
F	-14	GLY	-	linker	UNP Q9S5X7
F	-13	GLY	-	linker	UNP Q9S5X7
F	-12	GLY	-	linker	UNP Q9S5X7
F	-11	GLY	-	linker	UNP Q9S5X7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	GLU	-	expression tag	UNP Q9S5X7
F	-9	ASN	-	expression tag	UNP Q9S5X7
F	-8	LEU	-	expression tag	UNP Q9S5X7
F	-7	TYR	-	expression tag	UNP Q9S5X7
F	-6	PHE	-	expression tag	UNP Q9S5X7
F	-5	GLN	-	expression tag	UNP Q9S5X7
F	-4	GLY	-	expression tag	UNP Q9S5X7
F	-3	ALA	-	expression tag	UNP Q9S5X7
F	-2	VAL	-	expression tag	UNP Q9S5X7
c	-27	MET	-	initiating methionine	UNP Q9S5X7
c	-26	ALA	-	linker	UNP Q9S5X7
c	-25	SER	-	linker	UNP Q9S5X7
c	-24	TRP	-	expression tag	UNP Q9S5X7
c	-23	SER	-	expression tag	UNP Q9S5X7
c	-22	HIS	-	expression tag	UNP Q9S5X7
c	-21	PRO	-	expression tag	UNP Q9S5X7
c	-20	GLN	-	expression tag	UNP Q9S5X7
c	-19	PHE	-	expression tag	UNP Q9S5X7
c	-18	GLU	-	expression tag	UNP Q9S5X7
c	-17	LYS	-	expression tag	UNP Q9S5X7
c	-16	SER	-	linker	UNP Q9S5X7
c	-15	GLY	-	linker	UNP Q9S5X7
c	-14	GLY	-	linker	UNP Q9S5X7
c	-13	GLY	-	linker	UNP Q9S5X7
c	-12	GLY	-	linker	UNP Q9S5X7
c	-11	GLY	-	linker	UNP Q9S5X7
c	-10	GLU	-	expression tag	UNP Q9S5X7
c	-9	ASN	-	expression tag	UNP Q9S5X7
c	-8	LEU	-	expression tag	UNP Q9S5X7
c	-7	TYR	-	expression tag	UNP Q9S5X7
c	-6	PHE	-	expression tag	UNP Q9S5X7
c	-5	GLN	-	expression tag	UNP Q9S5X7
c	-4	GLY	-	expression tag	UNP Q9S5X7
c	-3	ALA	-	expression tag	UNP Q9S5X7
c	-2	VAL	-	expression tag	UNP Q9S5X7
f	-27	MET	-	initiating methionine	UNP Q9S5X7
f	-26	ALA	-	linker	UNP Q9S5X7
f	-25	SER	-	linker	UNP Q9S5X7
f	-24	TRP	-	expression tag	UNP Q9S5X7
f	-23	SER	-	expression tag	UNP Q9S5X7
f	-22	HIS	-	expression tag	UNP Q9S5X7
f	-21	PRO	-	expression tag	UNP Q9S5X7

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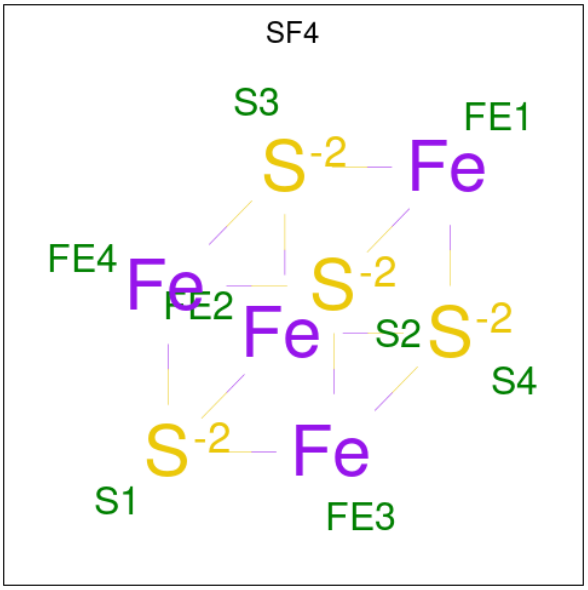
Chain	Residue	Modelled	Actual	Comment	Reference
f	-20	GLN	-	expression tag	UNP Q9S5X7
f	-19	PHE	-	expression tag	UNP Q9S5X7
f	-18	GLU	-	expression tag	UNP Q9S5X7
f	-17	LYS	-	expression tag	UNP Q9S5X7
f	-16	SER	-	linker	UNP Q9S5X7
f	-15	GLY	-	linker	UNP Q9S5X7
f	-14	GLY	-	linker	UNP Q9S5X7
f	-13	GLY	-	linker	UNP Q9S5X7
f	-12	GLY	-	linker	UNP Q9S5X7
f	-11	GLY	-	linker	UNP Q9S5X7
f	-10	GLU	-	expression tag	UNP Q9S5X7
f	-9	ASN	-	expression tag	UNP Q9S5X7
f	-8	LEU	-	expression tag	UNP Q9S5X7
f	-7	TYR	-	expression tag	UNP Q9S5X7
f	-6	PHE	-	expression tag	UNP Q9S5X7
f	-5	GLN	-	expression tag	UNP Q9S5X7
f	-4	GLY	-	expression tag	UNP Q9S5X7
f	-3	ALA	-	expression tag	UNP Q9S5X7
f	-2	VAL	-	expression tag	UNP Q9S5X7

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
4	A	1	8	4	4	0
			Total	Fe	S	
4	A	1	8	4	4	0

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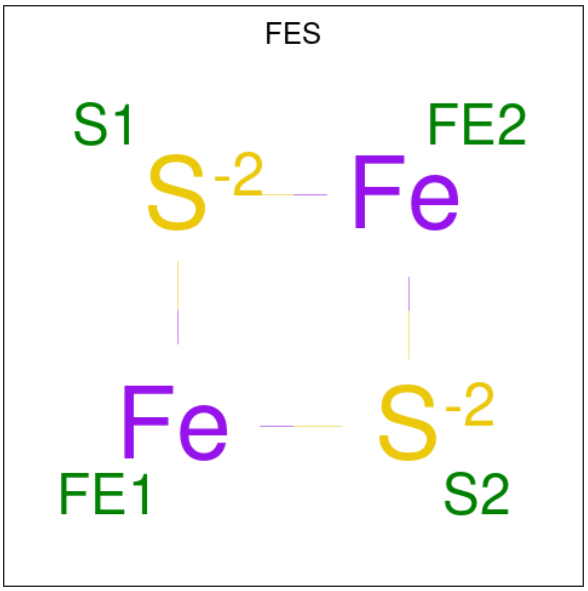
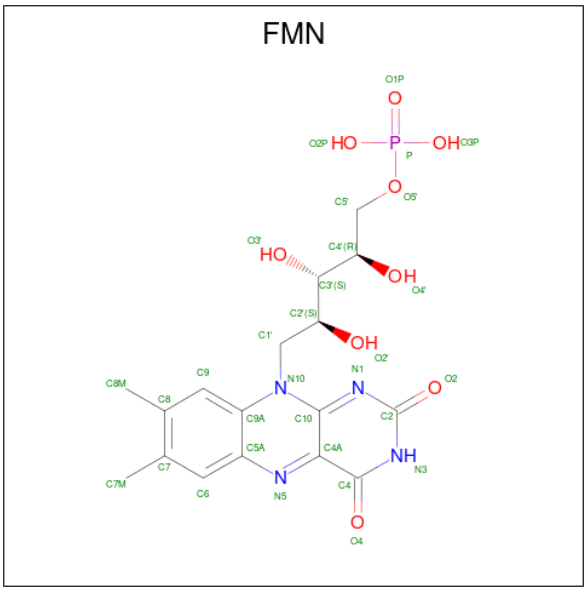
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
4	A	1	8	4	4	0
4	A	1	8	4	4	0
4	B	1	8	4	4	0
4	D	1	8	4	4	0
4	D	1	8	4	4	0
4	D	1	8	4	4	0
4	D	1	8	4	4	0
4	E	1	8	4	4	0
4	a	1	8	4	4	0
4	a	1	8	4	4	0
4	a	1	8	4	4	0
4	a	1	8	4	4	0
4	b	1	8	4	4	0
4	d	1	8	4	4	0
4	d	1	8	4	4	0
4	d	1	8	4	4	0
4	d	1	8	4	4	0
4	e	1	8	4	4	0

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
5	A	1	4	2	2	0
5	B	1	4	2	2	0
5	C	1	4	2	2	0
5	D	1	4	2	2	0
5	E	1	4	2	2	0
5	F	1	4	2	2	0
5	a	1	4	2	2	0
5	b	1	4	2	2	0
5	c	1	4	2	2	0
5	d	1	4	2	2	0
5	e	1	4	2	2	0
5	f	1	4	2	2	0

- Molecule 6 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
6	B	1	50	17	19	4	9	1	0
6	E	1	50	17	19	4	9	1	0
6	b	1	50	17	19	4	9	1	0
6	e	1	50	17	19	4	9	1	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
7	B	1	1	1	0
7	E	1	1	1	0
7	b	1	1	1	0
7	e	1	1	1	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
8	A	135	135	135	0

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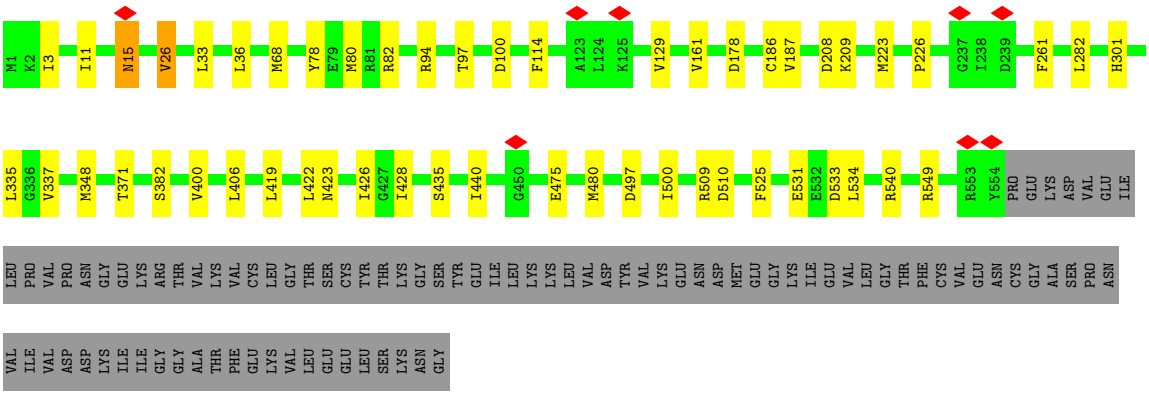
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
8	B	21	21	21	0
			Total	O	
8	C	4	4	4	0
			Total	O	
8	D	135	135	135	0
			Total	O	
8	E	21	21	21	0
			Total	O	
8	F	4	4	4	0
			Total	O	
8	a	135	135	135	0
			Total	O	
8	b	21	21	21	0
			Total	O	
8	c	4	4	4	0
			Total	O	
8	d	135	135	135	0
			Total	O	
8	e	21	21	21	0
			Total	O	
8	f	4	4	4	0

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.

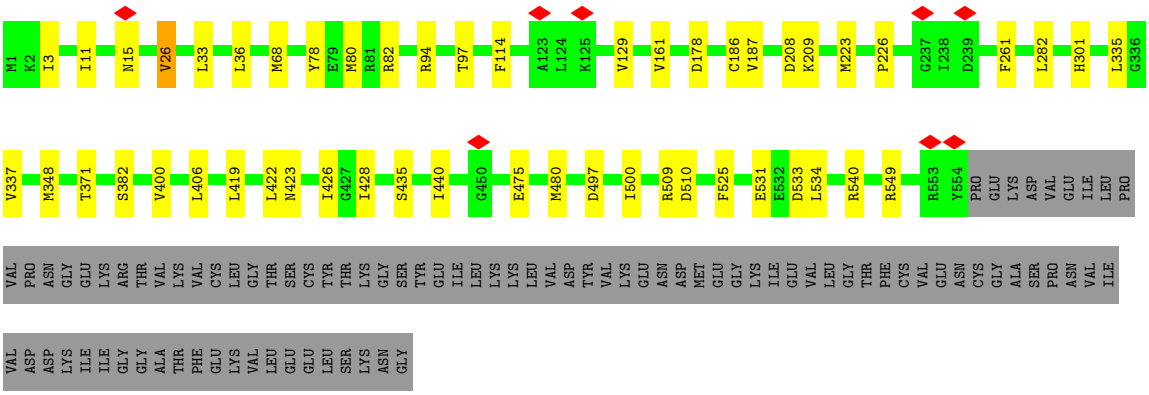
• Molecule 1: Fe-hydrogenase, subunit alpha

Chain A:



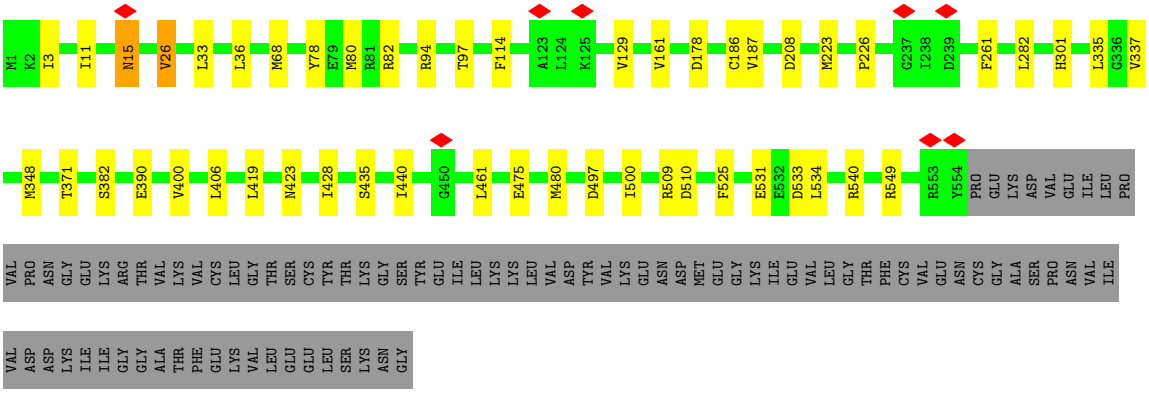
• Molecule 1: Fe-hydrogenase, subunit alpha

Chain D:



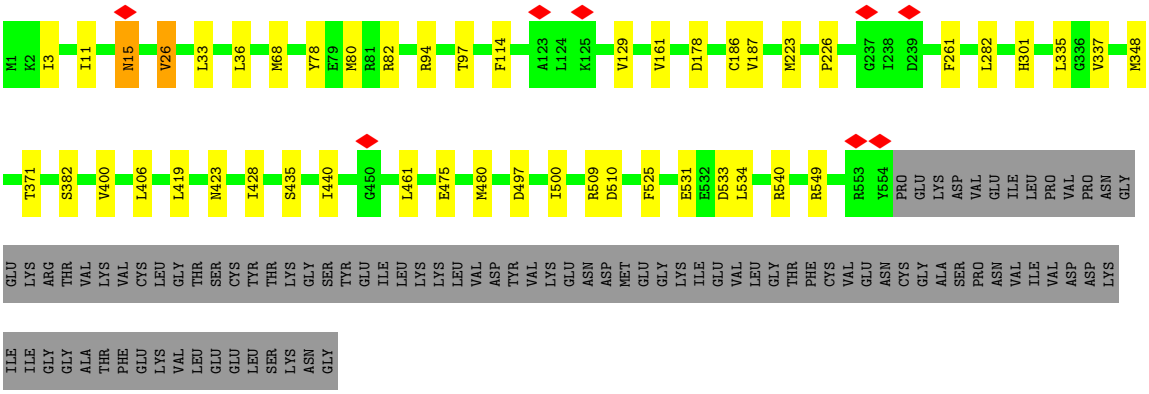
• Molecule 1: Fe-hydrogenase, subunit alpha

Chain a:



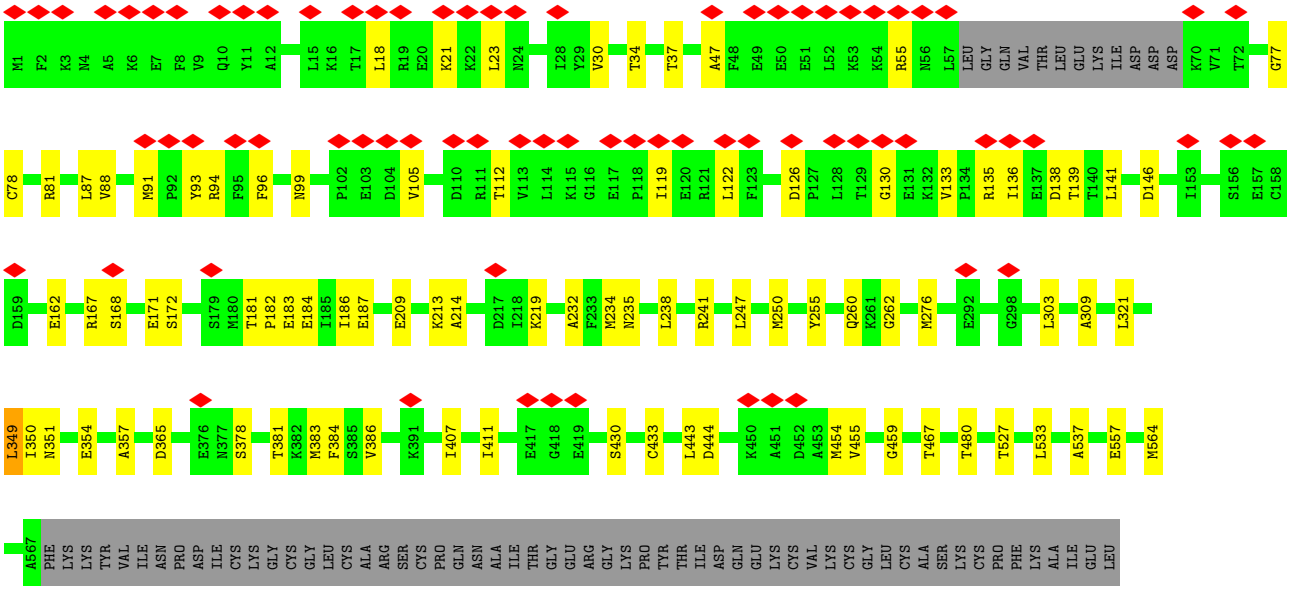
- Molecule 1: Fe-hydrogenase, subunit alpha

Chain d:



- Molecule 2: Fe-hydrogenase, subunit beta

Chain B:



VAL

• Molecule 2: Fe-hydrogenase, subunit beta

Chain E: 12% 75% 13% 11%

M1 F2 K3 N4 A5 K6 E7 F8 V9 Q10 Y11 A12 L15 K16 T17 L18 R19 E20 K21 K22 L23 N24 I28 Y29 V30 T34 T37 A47 F48 E49 E50 E51 L52 K53 K54 R55 N56 L57 LEU GLY GLN VAL THR LEU GLU LYS ILE ASP ASP ASP K70 V71 T72 G77

C78 R81 L87 V88 M91 P92 Y93 R94 F95 F96 N99 P102 E103 D104 V105 D110 R111 T112 V113 L114 K115 G116 E117 P118 I119 E120 R121 L122 F123 D126 P127 L128 T129 G130 E131 K132 V133 P134 R135 I136 E137 D138 T139 T140 L141 D146 I153 S156 E157 C158

D159 E162 R167 S168 E171 S172 S179 M180 T181 P182 E183 E184 I185 I186 E187 E209 K213 A214 D217 I218 K219 A232 F233 M234 N235 L238 R241 L247 M250 Y255 Q260 K261 G262 M276 E292 G298 L303 A309 L321

L349 I350 N351 E354 D365 E376 N377 S378 T381 K382 M383 K391 I407 I411 E417 G418 E419 S430 C433 D444 K450 A451 D452 A453 M454 V455 G459 T467 T480 E503 T527 L533 A537 E557 M564 A567 PHE LYS

LYS TYR VAL ILE ASN PRO ASP ILE CYS LYS GLY CYS GLY LEU CYS ALA ARG SER CYS PRO GLN ASN ALA ILE THR GLY GLU ARG GLY LYS PRO TYR THR ILE ASP GLN GLU LYS CYS VAL LYS CYS GLY LEU CYS ALA SER LYS CYS PRO PHE LYS ALA ILE GLU LEU VAL

• Molecule 2: Fe-hydrogenase, subunit beta

Chain b: 12% 74% 14% 11%

M1 F2 K3 N4 A5 K6 E7 F8 V9 Q10 Y11 A12 L15 K16 T17 L18 R19 E20 K21 K22 L23 N24 I28 Y29 V30 T34 T37 Y45 S46 A47 F48 E49 E50 E51 L52 K53 K54 R55 N56 L57 LEU GLY GLN VAL THR LEU GLU LYS ILE ASP ASP ASP K70 V71 T72

R75 T76 G77 C78 R81 L87 V88 M91 P92 Y93 R94 F95 F96 N99 P102 E103 D104 V105 D110 R111 T112 V113 L114 K115 G116 E117 P118 I119 E120 R121 L122 F123 D126 P127 L128 T129 G130 E131 K132 V133 P134 R135 I136 E137 D138 T139 T140 L141 D146 I153

S156 E157 C158 D159 E162 R167 S168 E171 S172 S179 M180 T181 P182 E183 E184 I185 I186 E187 E209 K213 A214 D217 I218 K219 A232 F233 M234 N235 L238 R241 L247 M250 Y255 Q260 K261 G262 M276 E292 N293 I294 L295 G298

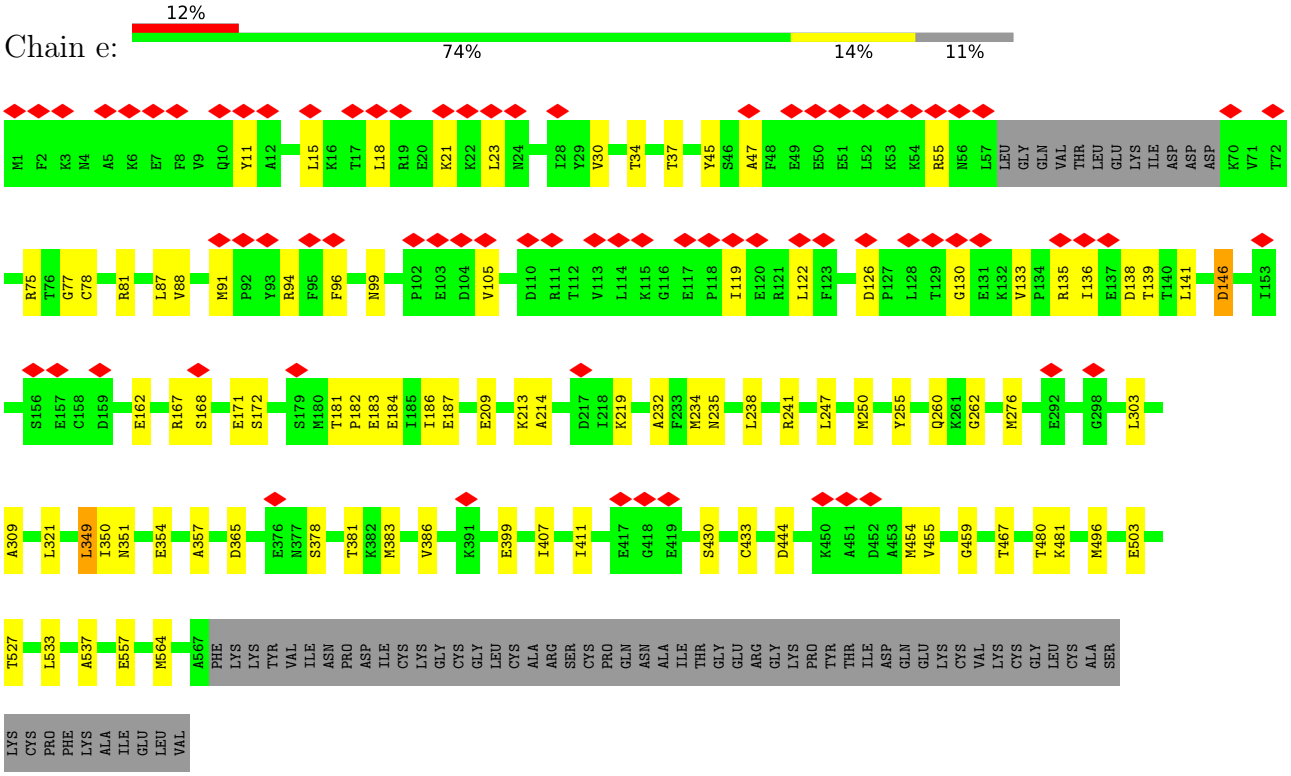
L303 A309 L321 L349 I350 N351 E354 D365 E376 N377 S378 T381 K382 M383 K391 I407 I411 E417 G418 E419 S430 C433 D444 K450 A451 D452 A453 M454 V455 G459 T467 T480 K481 M496 E503 T527 L533

A537 E557 M564 A567 PHE LYS LYS TYR VAL ILE ASN PRO ASP ILE CYS LYS GLY CYS GLY LEU CYS ALA ARG SER CYS PRO GLN ASN ALA ILE THR GLY GLU ARG GLY LYS PRO TYR THR ILE ASP GLN GLU LYS CYS VAL LYS CYS GLY LEU CYS ALA SER LYS CYS PRO

PHE LYS ALA ILE GLU LEU VAL

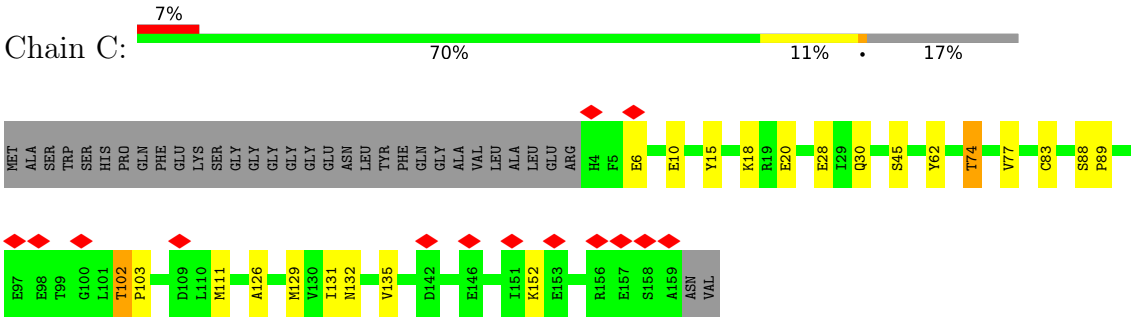
• Molecule 2: Fe-hydrogenase, subunit beta

Chain e:



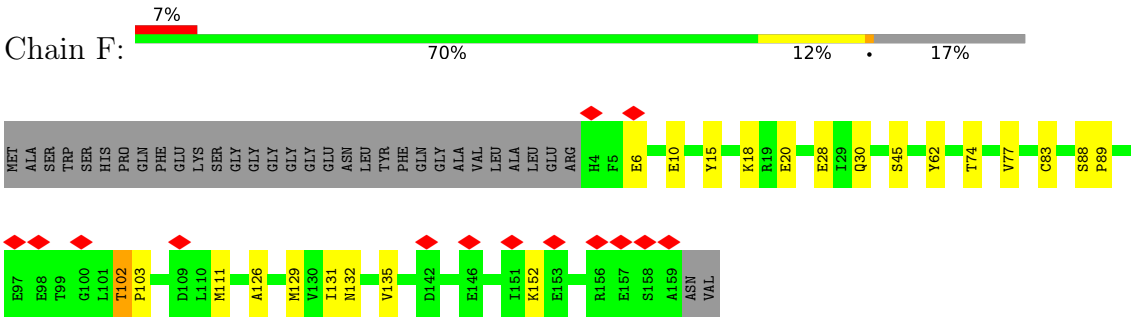
- Molecule 3: Fe-hydrogenase, subunit gamma

Chain C:



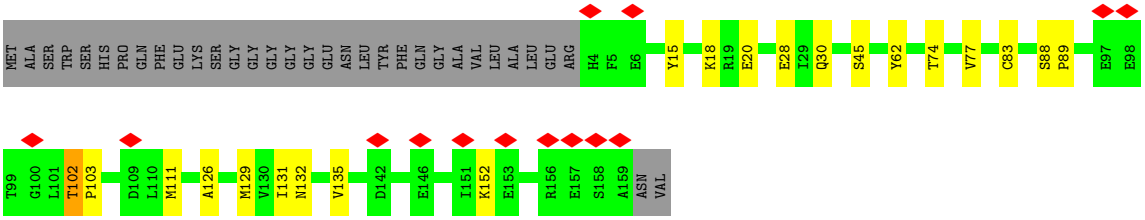
- Molecule 3: Fe-hydrogenase, subunit gamma

Chain F:



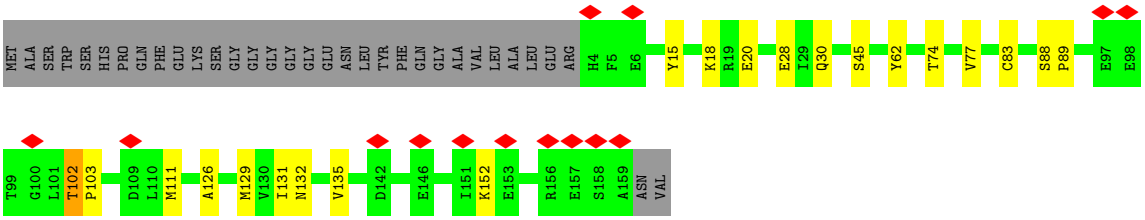
- Molecule 3: Fe-hydrogenase, subunit gamma

Chain c:



• Molecule 3: Fe-hydrogenase, subunit gamma

Chain f:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	278793	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 ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60700	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.327	Depositor
Minimum map value	-0.189	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	270.272, 270.272, 270.272	wwPDB
Map dimensions	328, 328, 328	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	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: FES, SF4, ZN, FMN

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	0.20	0/4456	0.34	0/6006
1	D	0.20	0/4456	0.34	0/6006
1	a	0.20	0/4456	0.34	0/6006
1	d	0.20	0/4456	0.34	0/6006
2	B	0.17	0/4362	0.34	0/5873
2	E	0.17	0/4362	0.34	0/5873
2	b	0.17	0/4362	0.34	0/5873
2	e	0.17	0/4362	0.34	0/5873
3	C	0.17	0/1239	0.34	0/1671
3	F	0.17	0/1239	0.34	0/1671
3	c	0.17	0/1239	0.34	0/1671
3	f	0.17	0/1239	0.34	0/1671
All	All	0.18	0/40228	0.34	0/54200

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	4376	4415	4410	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4376	4415	4410	29	0
1	a	4376	4415	4410	28	0
1	d	4376	4415	4410	27	0
2	B	4279	4321	4321	59	0
2	E	4279	4321	4321	57	0
2	b	4279	4321	4321	61	0
2	e	4279	4321	4321	63	0
3	C	1218	1245	1245	12	0
3	F	1218	1245	1245	12	0
3	c	1218	1245	1245	11	0
3	f	1218	1245	1245	11	0
4	A	32	0	0	1	0
4	B	8	0	0	0	0
4	D	32	0	0	1	0
4	E	8	0	0	0	0
4	a	32	0	0	1	0
4	b	8	0	0	0	0
4	d	32	0	0	1	0
4	e	8	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
5	a	4	0	0	0	0
5	b	4	0	0	0	0
5	c	4	0	0	0	0
5	d	4	0	0	0	0
5	e	4	0	0	0	0
5	f	4	0	0	0	0
6	B	31	19	19	0	0
6	E	31	19	19	0	0
6	b	31	19	19	0	0
6	e	31	19	19	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	b	1	0	0	0	0
7	e	1	0	0	0	0
8	A	135	0	0	1	0
8	B	21	0	0	0	0
8	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	135	0	0	1	0
8	E	21	0	0	0	0
8	F	4	0	0	0	0
8	a	135	0	0	0	0
8	b	21	0	0	0	0
8	c	4	0	0	0	0
8	d	135	0	0	0	0
8	e	21	0	0	0	0
8	f	4	0	0	0	0
All	All	40468	40000	39980	378	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 5.

The worst 5 of 378 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)
2:e:238:LEU:HD13	2:e:383:MET:HE2	1.62	0.80
2:B:238:LEU:HD13	2:B:383:MET:HE2	1.62	0.79
2:E:467:THR:HA	2:E:564:MET:HE3	1.70	0.74
2:B:467:THR:HA	2:B:564:MET:HE3	1.70	0.73
2:e:467:THR:HA	2:e:564:MET:HE3	1.70	0.71

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	554/645 (86%)	544 (98%)	10 (2%)	0	100	100
1	D	554/645 (86%)	544 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	554/645 (86%)	544 (98%)	10 (2%)	0	100	100
1	d	554/645 (86%)	544 (98%)	10 (2%)	0	100	100
2	B	552/626 (88%)	518 (94%)	34 (6%)	0	100	100
2	E	552/626 (88%)	518 (94%)	34 (6%)	0	100	100
2	b	552/626 (88%)	519 (94%)	33 (6%)	0	100	100
2	e	552/626 (88%)	518 (94%)	34 (6%)	0	100	100
3	C	154/189 (82%)	152 (99%)	2 (1%)	0	100	100
3	F	154/189 (82%)	152 (99%)	2 (1%)	0	100	100
3	c	154/189 (82%)	152 (99%)	2 (1%)	0	100	100
3	f	154/189 (82%)	152 (99%)	2 (1%)	0	100	100
All	All	5040/5840 (86%)	4857 (96%)	183 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/561 (86%)	474 (98%)	9 (2%)	50	69
1	D	483/561 (86%)	475 (98%)	8 (2%)	53	72
1	a	483/561 (86%)	475 (98%)	8 (2%)	53	72
1	d	483/561 (86%)	476 (99%)	7 (1%)	59	76
2	B	458/518 (88%)	446 (97%)	12 (3%)	40	59
2	E	458/518 (88%)	446 (97%)	12 (3%)	40	59
2	b	458/518 (88%)	446 (97%)	12 (3%)	40	59
2	e	458/518 (88%)	445 (97%)	13 (3%)	38	56
3	C	132/156 (85%)	126 (96%)	6 (4%)	24	37
3	F	132/156 (85%)	127 (96%)	5 (4%)	29	44
3	c	132/156 (85%)	127 (96%)	5 (4%)	29	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	f	132/156 (85%)	127 (96%)	5 (4%)	29	44
All	All	4292/4940 (87%)	4190 (98%)	102 (2%)	43	62

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	440	ILE
2	b	503	GLU
3	f	77	VAL
1	a	533	ASP
2	b	354	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	403	GLN
1	d	13	ASN
3	c	138	ASN
1	d	320	GLN
1	D	321	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)

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 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	$\#\|Z\| > 2$
6	FMN	b	702	-	33,33,33	1.04	2 (6%)	48,50,50	1.25	6 (12%)
5	FES	b	703	2	0,4,4	-	-	-		
5	FES	a	705	1	0,4,4	-	-	-		
4	SF4	d	704	1	0,12,12	-	-	-		
4	SF4	D	701	1	0,12,12	-	-	-		
4	SF4	e	701	2	0,12,12	-	-	-		
4	SF4	a	701	1	0,12,12	-	-	-		
6	FMN	e	702	-	33,33,33	1.04	2 (6%)	48,50,50	1.25	6 (12%)
4	SF4	A	702	1	0,12,12	-	-	-		
6	FMN	E	702	-	33,33,33	1.04	2 (6%)	48,50,50	1.25	6 (12%)
4	SF4	D	702	1	0,12,12	-	-	-		
4	SF4	B	701	2	0,12,12	-	-	-		
4	SF4	d	702	1	0,12,12	-	-	-		
4	SF4	d	703	1	0,12,12	-	-	-		
5	FES	e	703	2	0,4,4	-	-	-		
4	SF4	D	703	1	0,12,12	-	-	-		
5	FES	B	703	2	0,4,4	-	-	-		
5	FES	C	201	3	0,4,4	-	-	-		
5	FES	A	705	1	0,4,4	-	-	-		
6	FMN	B	702	-	33,33,33	1.04	2 (6%)	48,50,50	1.25	6 (12%)
4	SF4	E	701	2	0,12,12	-	-	-		
4	SF4	d	701	1	0,12,12	-	-	-		
5	FES	f	201	3	0,4,4	-	-	-		
4	SF4	A	704	1	0,12,12	-	-	-		
4	SF4	A	703	1	0,12,12	-	-	-		
5	FES	d	705	1	0,4,4	-	-	-		
5	FES	E	703	2	0,4,4	-	-	-		
4	SF4	D	704	1	0,12,12	-	-	-		
4	SF4	b	701	2	0,12,12	-	-	-		
5	FES	F	201	3	0,4,4	-	-	-		
4	SF4	A	701	1	0,12,12	-	-	-		
4	SF4	a	704	1	0,12,12	-	-	-		
5	FES	D	705	1	0,4,4	-	-	-		
5	FES	c	201	3	0,4,4	-	-	-		
4	SF4	a	702	1	0,12,12	-	-	-		
4	SF4	a	703	1	0,12,12	-	-	-		

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
6	FMN	b	702	-	-	5/18/18/18	0/3/3/3
5	FES	b	703	2	-	-	0/1/1/1
5	FES	a	705	1	-	-	0/1/1/1
4	SF4	d	704	1	-	-	0/6/5/5
4	SF4	D	701	1	-	-	0/6/5/5
4	SF4	e	701	2	-	-	0/6/5/5
4	SF4	a	701	1	-	-	0/6/5/5
6	FMN	e	702	-	-	5/18/18/18	0/3/3/3
6	FMN	E	702	-	-	5/18/18/18	0/3/3/3
4	SF4	A	702	1	-	-	0/6/5/5
4	SF4	D	702	1	-	-	0/6/5/5
4	SF4	B	701	2	-	-	0/6/5/5
4	SF4	d	702	1	-	-	0/6/5/5
4	SF4	d	703	1	-	-	0/6/5/5
5	FES	e	703	2	-	-	0/1/1/1
4	SF4	D	703	1	-	-	0/6/5/5
5	FES	B	703	2	-	-	0/1/1/1
5	FES	C	201	3	-	-	0/1/1/1
5	FES	A	705	1	-	-	0/1/1/1
6	FMN	B	702	-	-	5/18/18/18	0/3/3/3
4	SF4	E	701	2	-	-	0/6/5/5
4	SF4	d	701	1	-	-	0/6/5/5
5	FES	f	201	3	-	-	0/1/1/1
4	SF4	A	704	1	-	-	0/6/5/5
4	SF4	A	703	1	-	-	0/6/5/5
5	FES	d	705	1	-	-	0/1/1/1
5	FES	E	703	2	-	-	0/1/1/1
4	SF4	D	704	1	-	-	0/6/5/5
4	SF4	b	701	2	-	-	0/6/5/5
5	FES	F	201	3	-	-	0/1/1/1
4	SF4	A	701	1	-	-	0/6/5/5
4	SF4	a	704	1	-	-	0/6/5/5
5	FES	D	705	1	-	-	0/1/1/1
5	FES	c	201	3	-	-	0/1/1/1
4	SF4	a	702	1	-	-	0/6/5/5
4	SF4	a	703	1	-	-	0/6/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	702	FMN	C4A-N5	3.55	1.37	1.30
6	E	702	FMN	C4A-N5	3.55	1.37	1.30
6	b	702	FMN	C4A-N5	3.55	1.37	1.30
6	e	702	FMN	C4A-N5	3.55	1.37	1.30
6	B	702	FMN	C10-N1	2.53	1.38	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	e	702	FMN	C4-N3-C2	-3.29	119.57	125.64
6	b	702	FMN	C4-N3-C2	-3.28	119.58	125.64
6	E	702	FMN	C4-N3-C2	-3.25	119.64	125.64
6	B	702	FMN	C4-N3-C2	-3.24	119.65	125.64
6	b	702	FMN	C4A-C4-N3	2.81	120.34	113.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	702	FMN	N10-C1'-C2'-O2'
6	B	702	FMN	N10-C1'-C2'-C3'
6	B	702	FMN	C5'-O5'-P-O1P
6	E	702	FMN	N10-C1'-C2'-O2'
6	E	702	FMN	N10-C1'-C2'-C3'

There are no ring outliers.

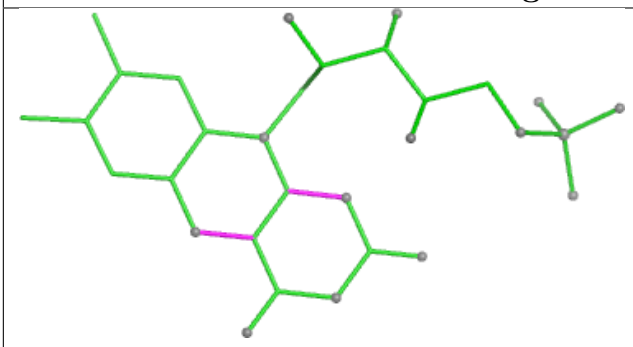
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	701	SF4	1	0
4	a	701	SF4	1	0
4	d	701	SF4	1	0
4	A	701	SF4	1	0

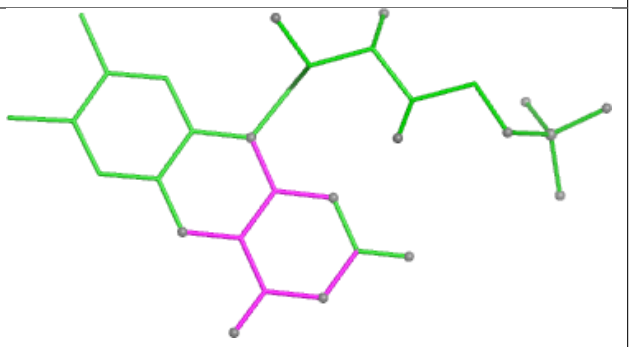
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

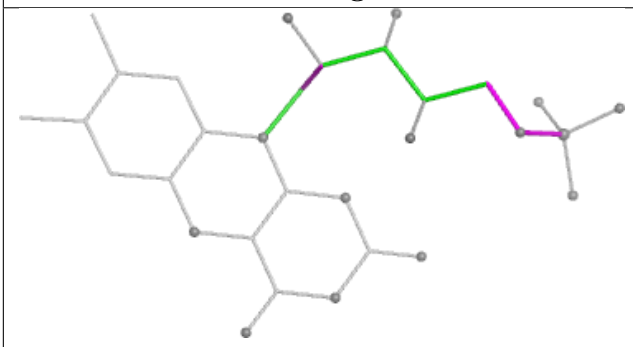
Ligand FMN b 702



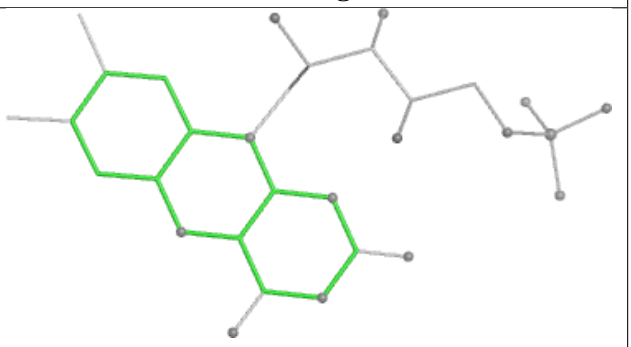
Bond lengths



Bond angles

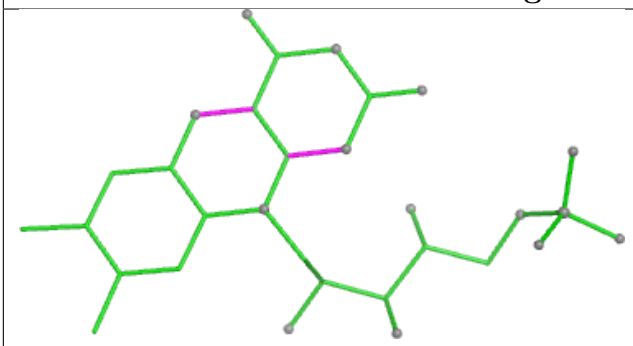


Torsions

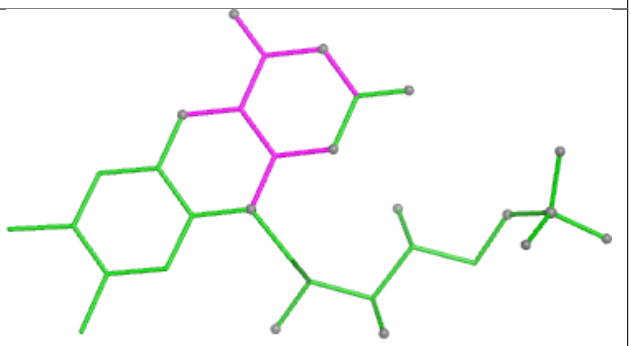


Rings

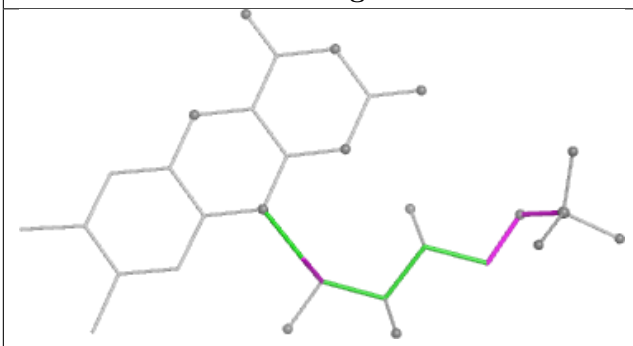
Ligand FMN e 702



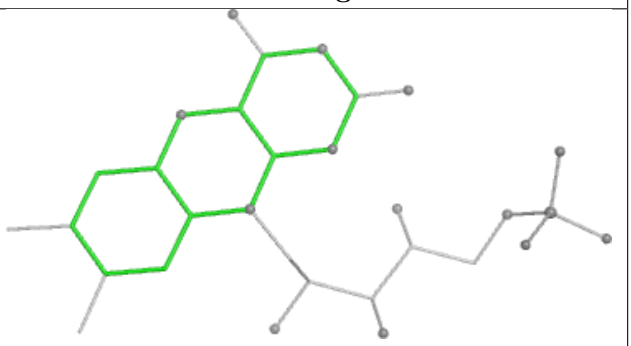
Bond lengths



Bond angles

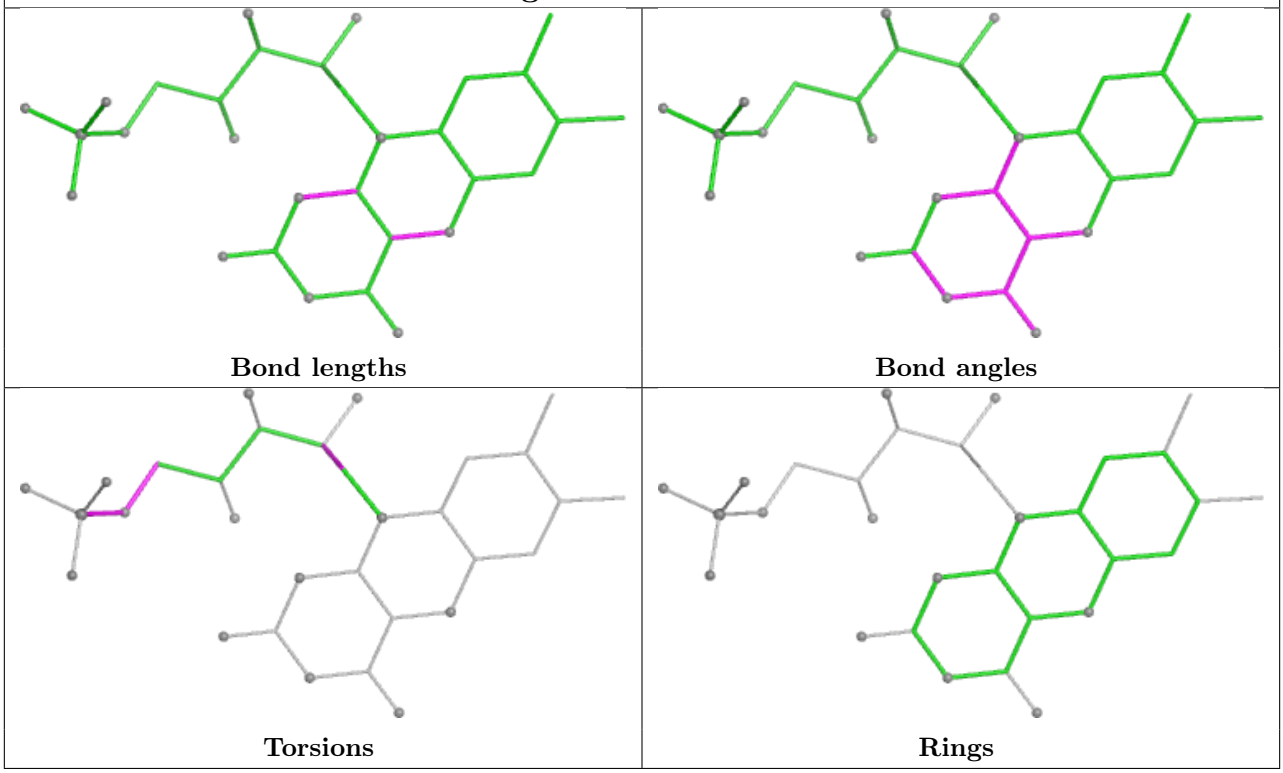


Torsions

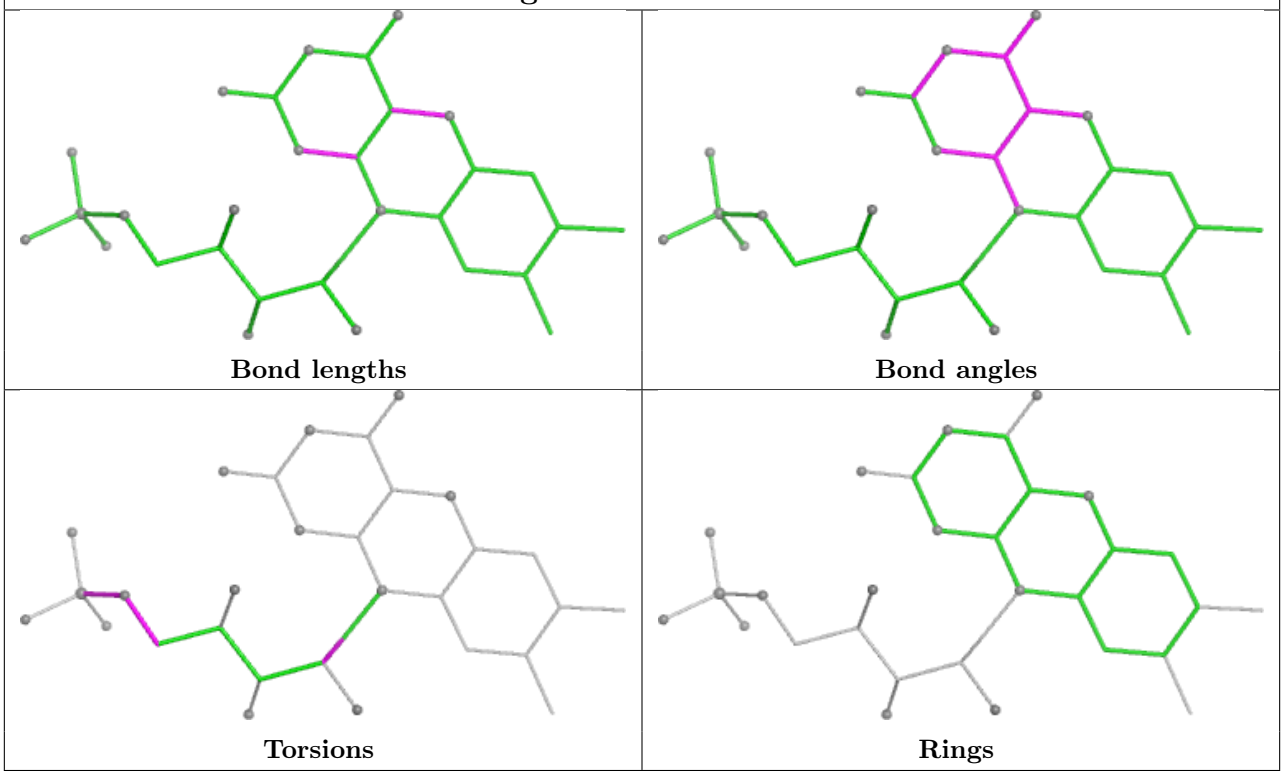


Rings

Ligand FMN E 702



Ligand FMN B 702



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.

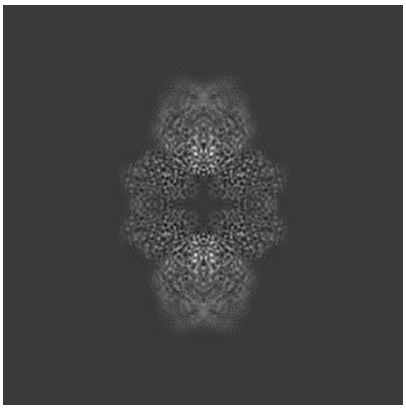
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13199. These allow visual inspection of the internal detail of the map and identification of artifacts.

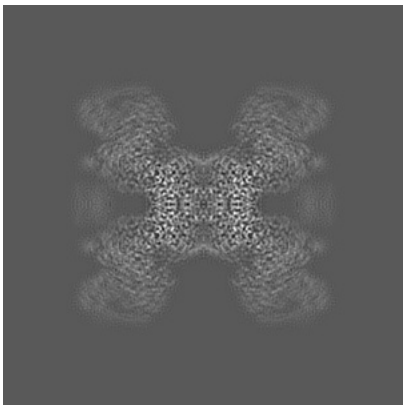
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

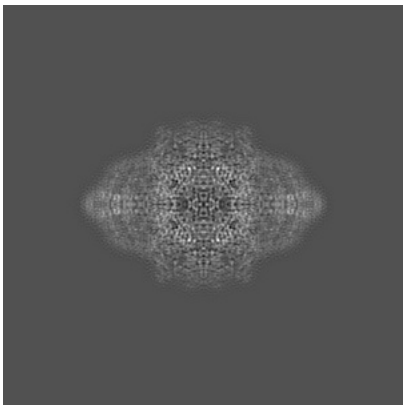
6.1.1 Primary map



X

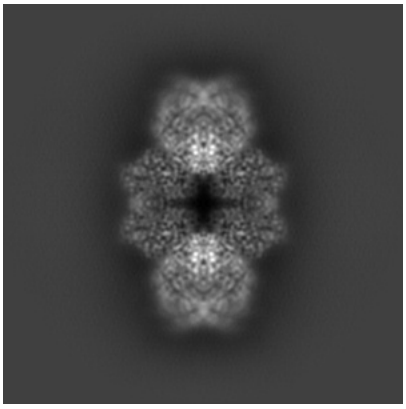


Y

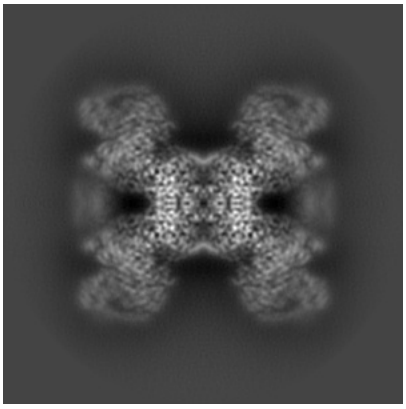


Z

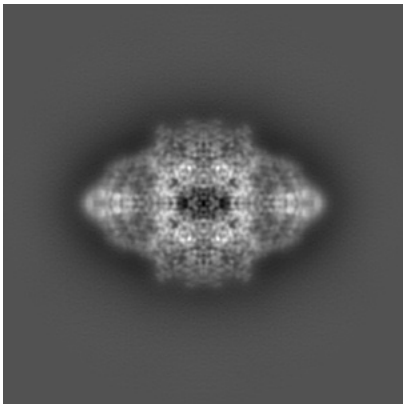
6.1.2 Raw map



X



Y

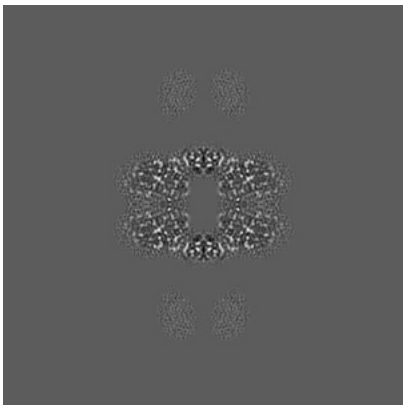


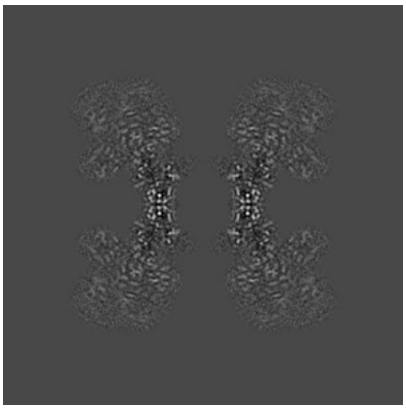
Z

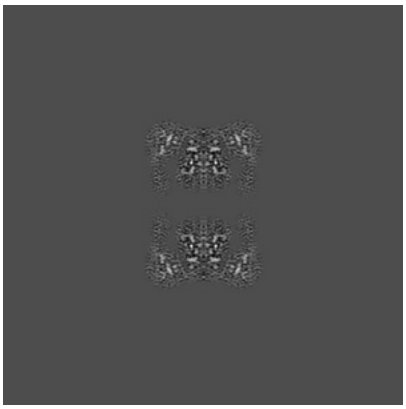
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

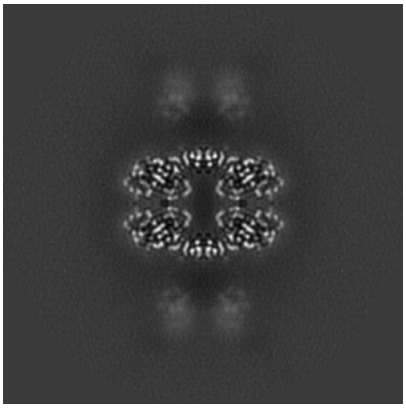
6.2.1 Primary map

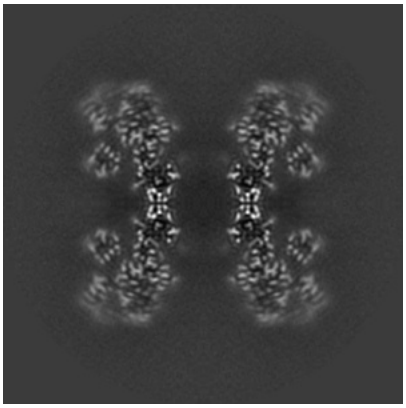

X Index: 164

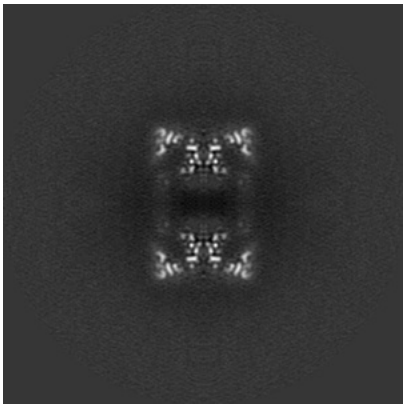

Y Index: 164


Z Index: 164

6.2.2 Raw map


X Index: 164

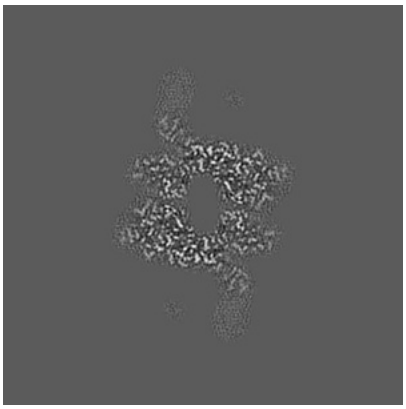

Y Index: 164


Z Index: 164

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

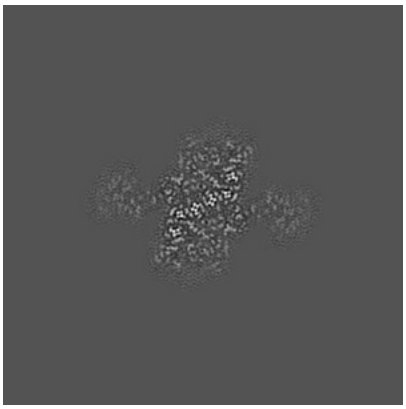
6.3 Largest variance slices (i)

6.3.1 Primary map



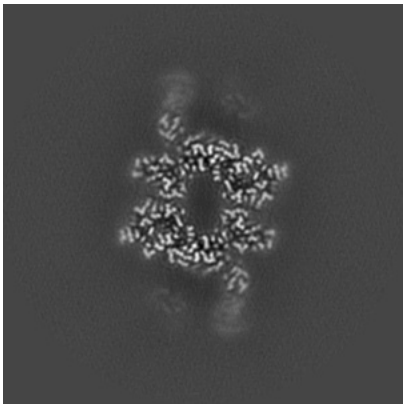
X Index: 176

Y Index: 171

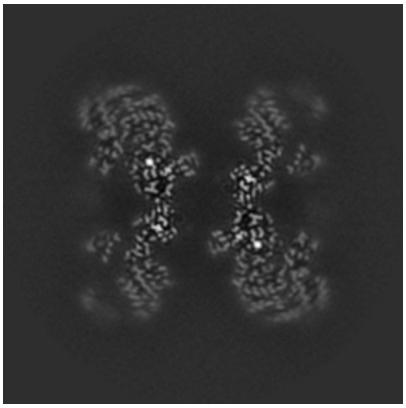


Z Index: 200

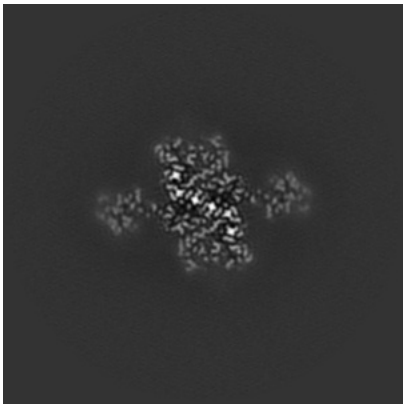
6.3.2 Raw map



X Index: 176



Y Index: 171

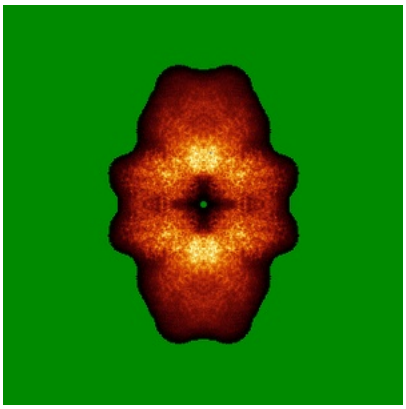


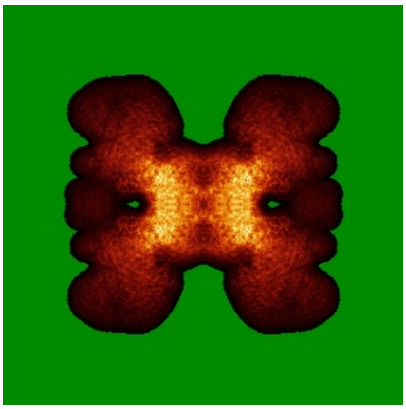
Z Index: 128

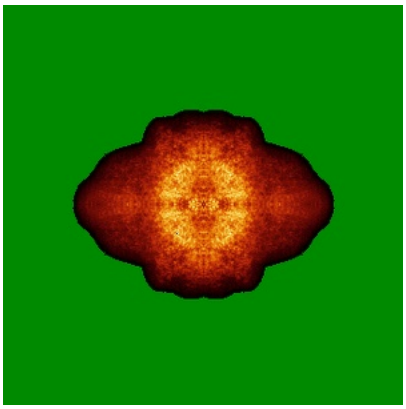
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

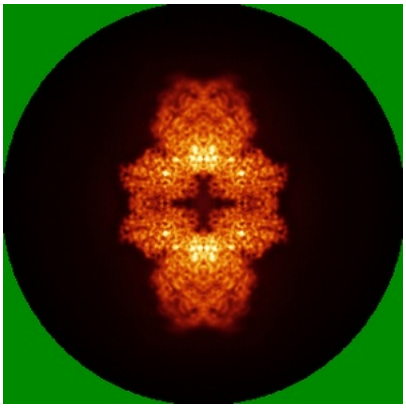
6.4.1 Primary map

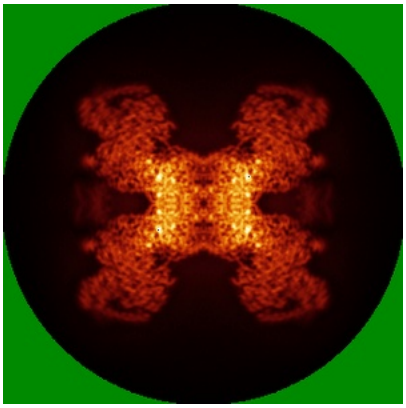

X

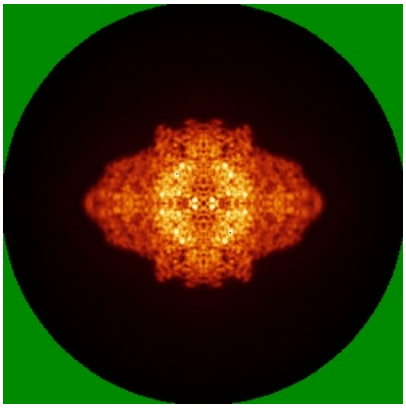

Y


Z

6.4.2 Raw map


X

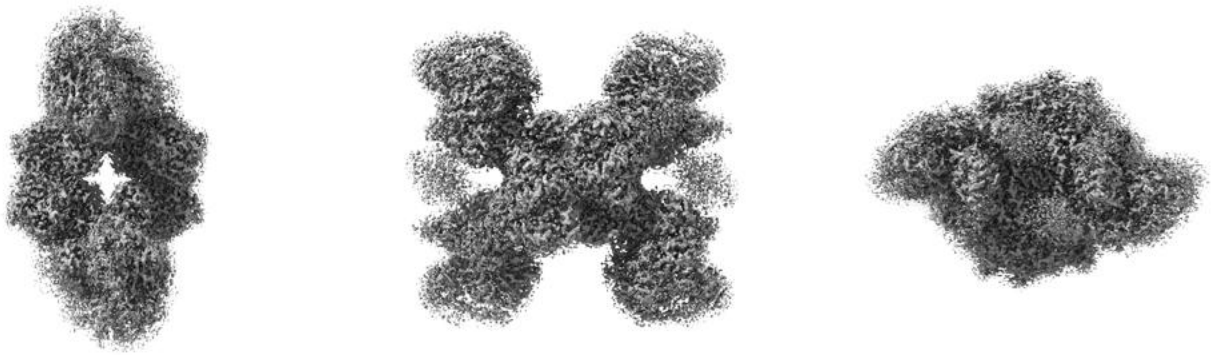

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. 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

X Y Z

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.

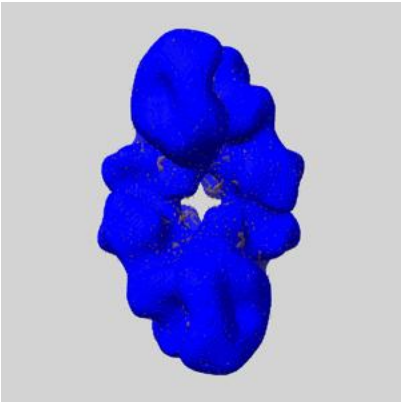
6.6 Mask visualisation (i)

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

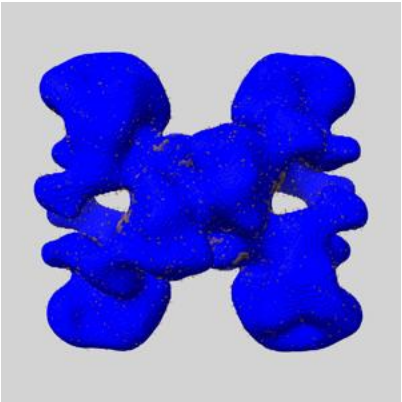
A mask typically either:

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

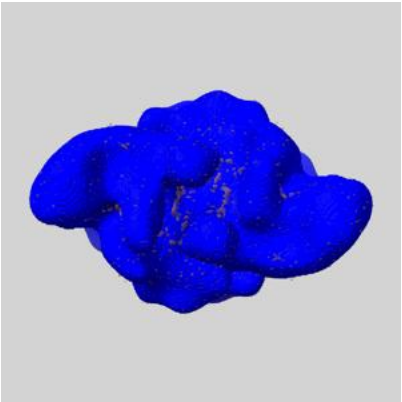
6.6.1 emd_13199_msk_1.map (i)



X



Y

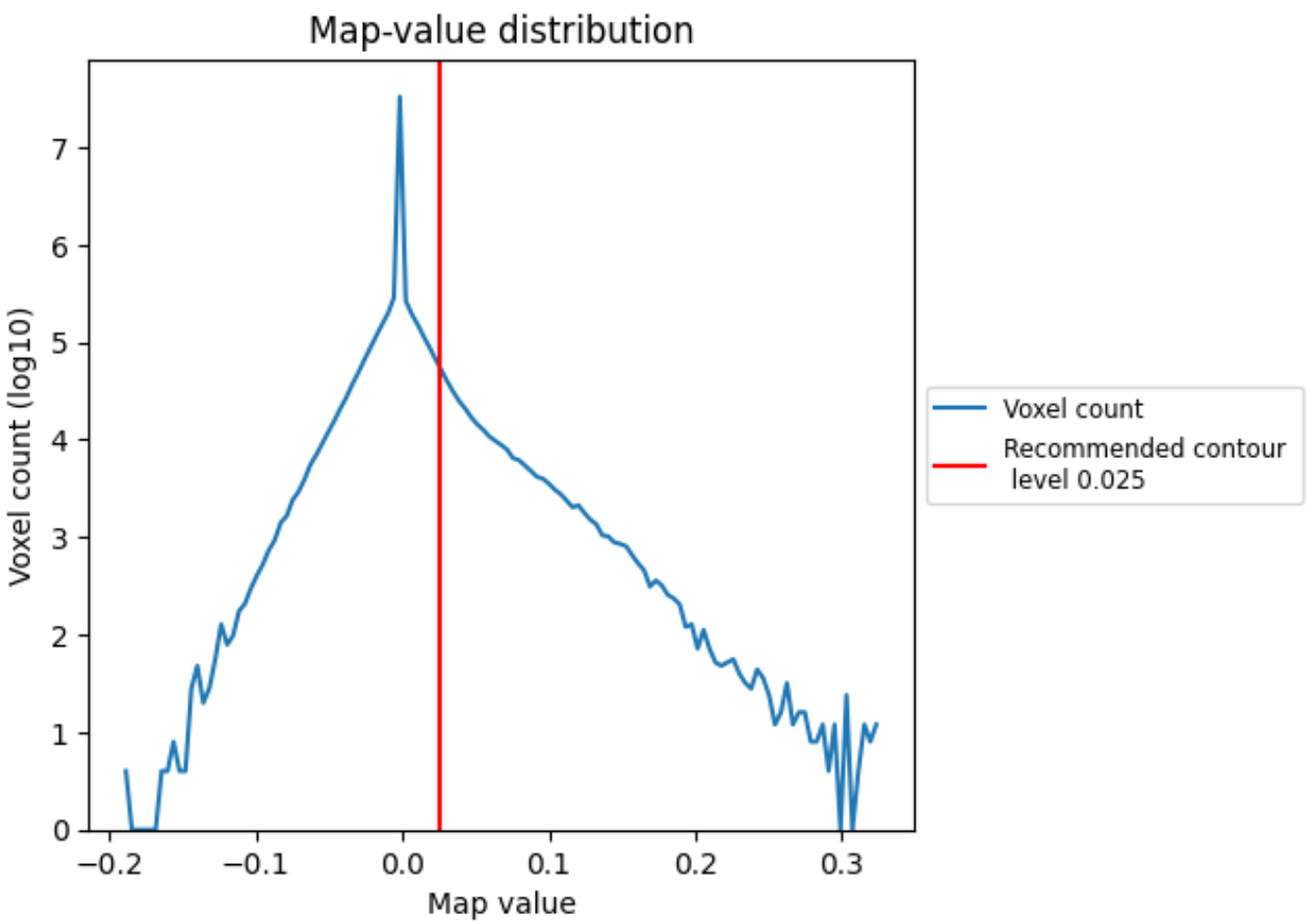


Z

7 Map analysis (i)

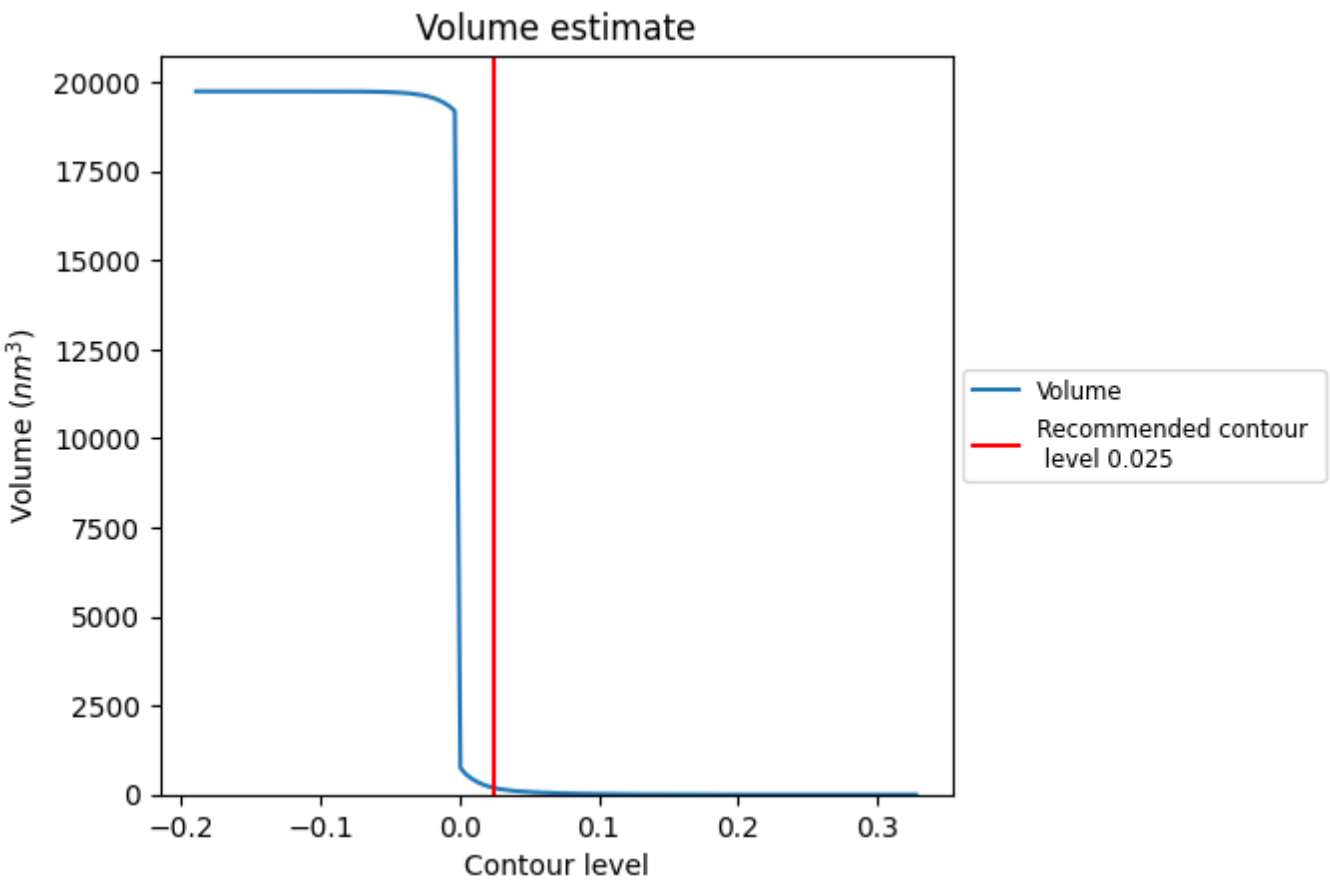
This section contains the results of statistical analysis of the map.

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.

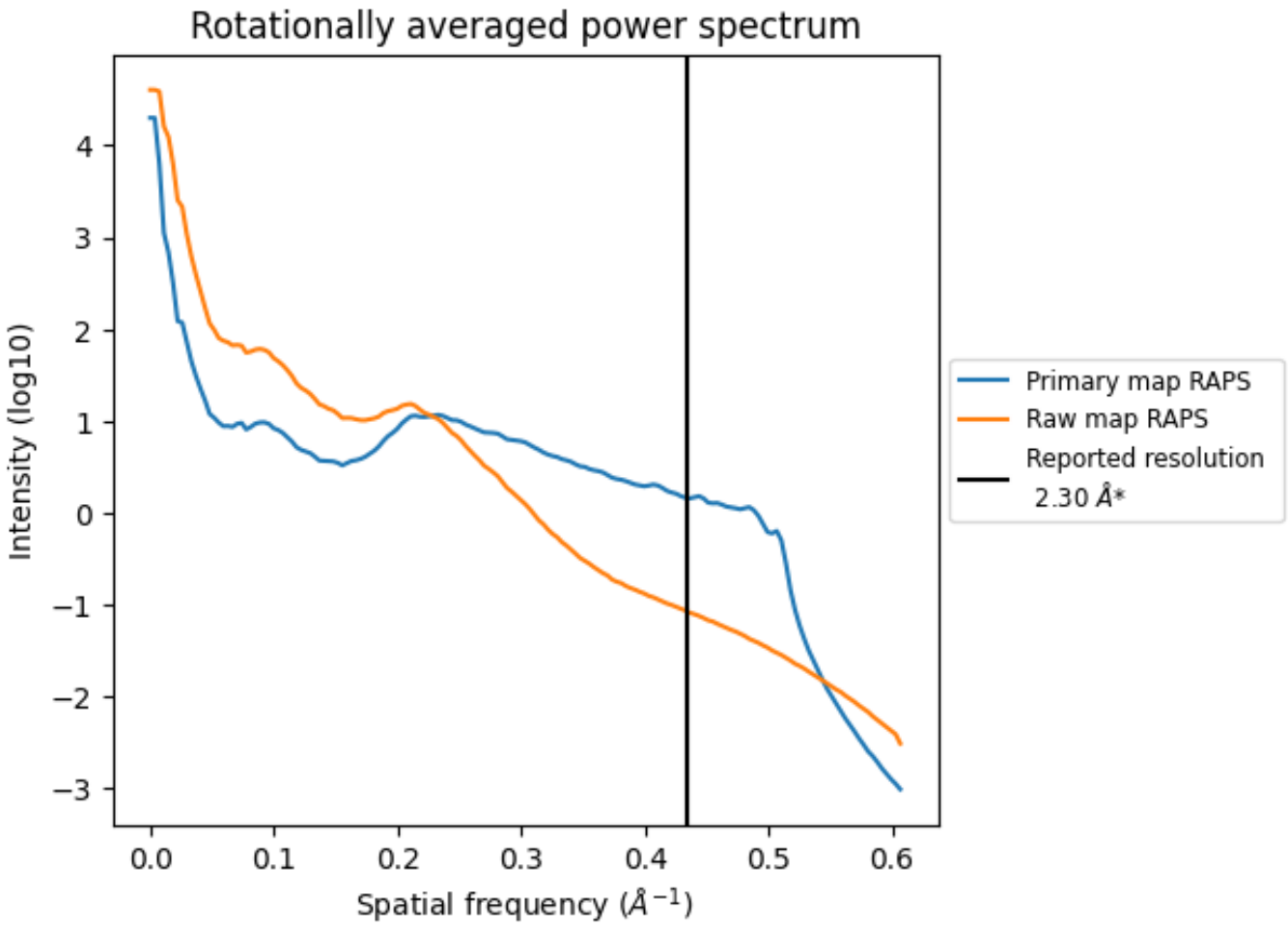
7.2 Volume estimate (i)



The volume at the recommended contour level is 187 nm^3; this corresponds to an approximate mass of 169 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)

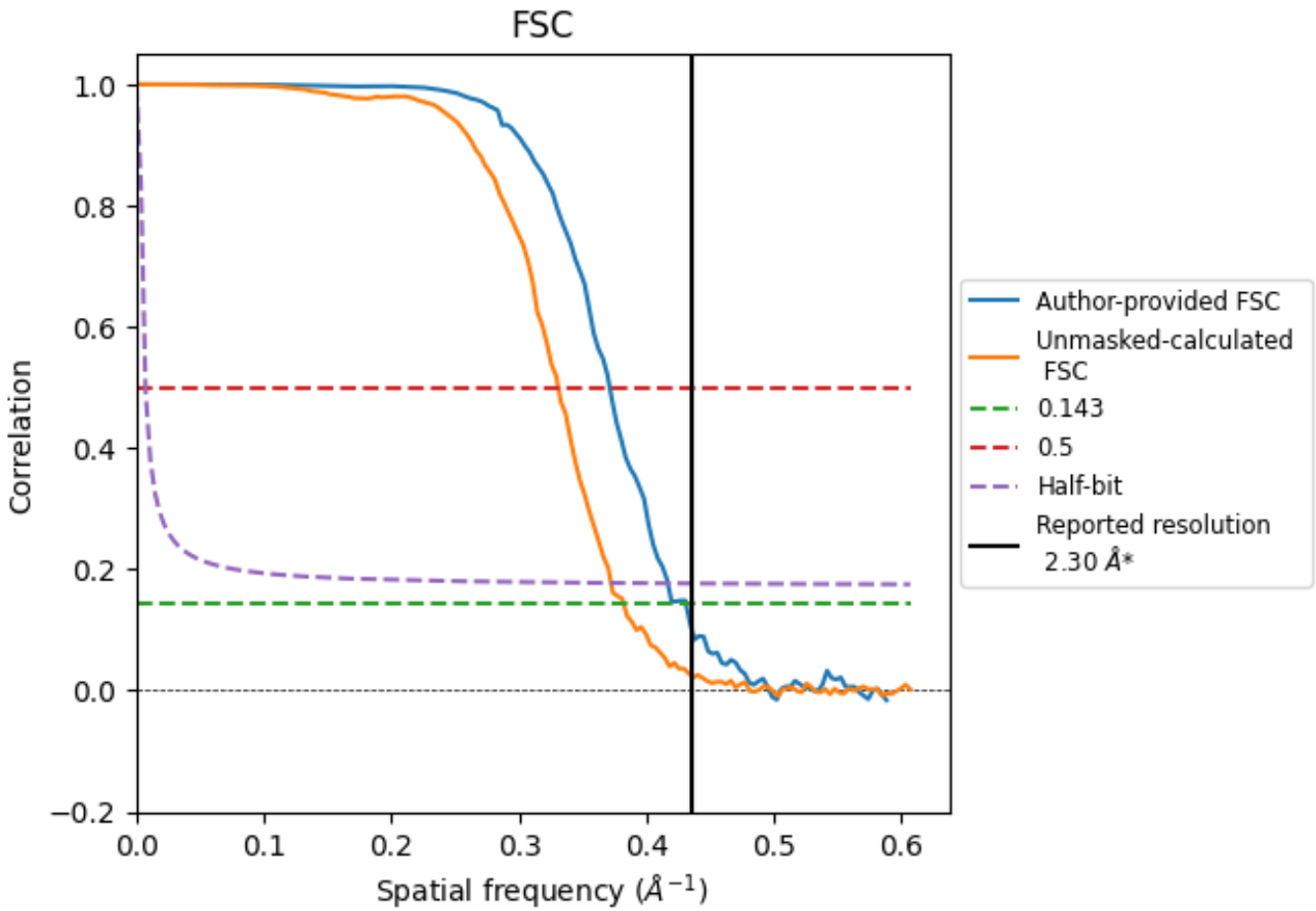


*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

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 0.435 Å^{-1}

8.2 Resolution estimates (i)

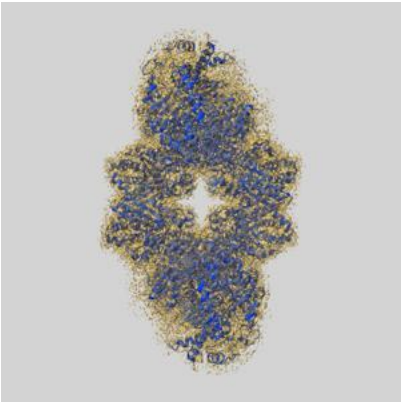
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.32	2.69	2.40
Unmasked-calculated*	2.62	3.02	2.69

*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 2.62 differs from the reported value 2.3 by more than 10 %

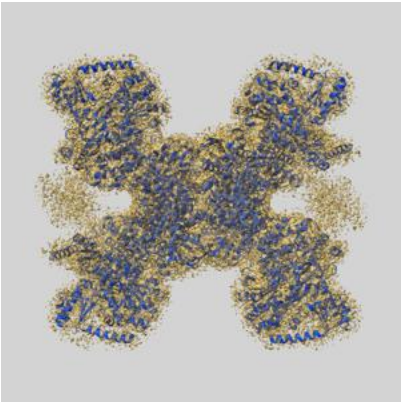
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13199 and PDB model 7P5H. Per-residue inclusion information can be found in section 3 on page 12.

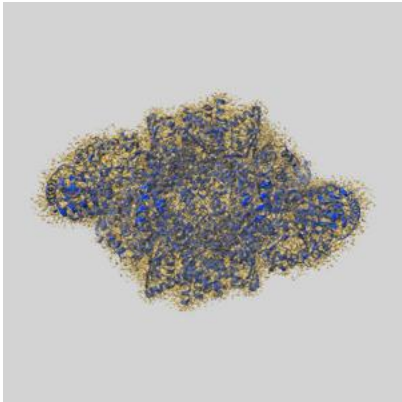
9.1 Map-model overlay (i)



X



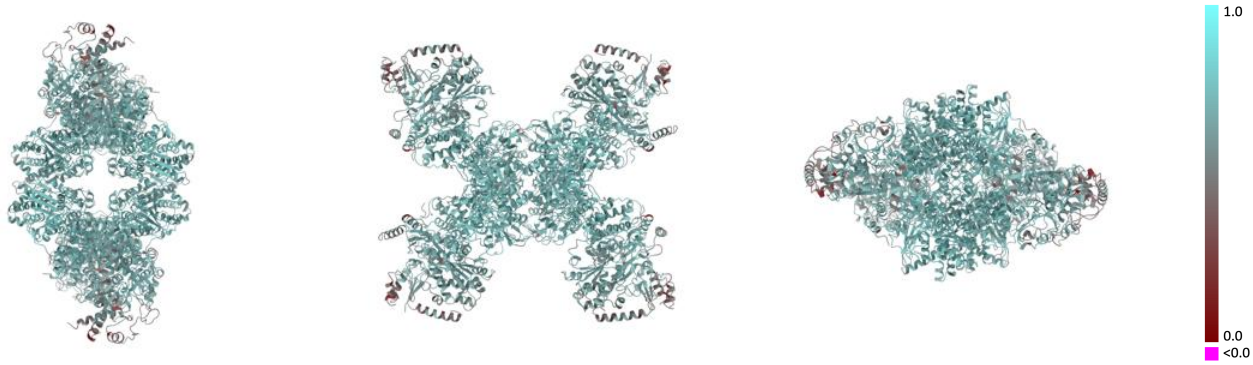
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

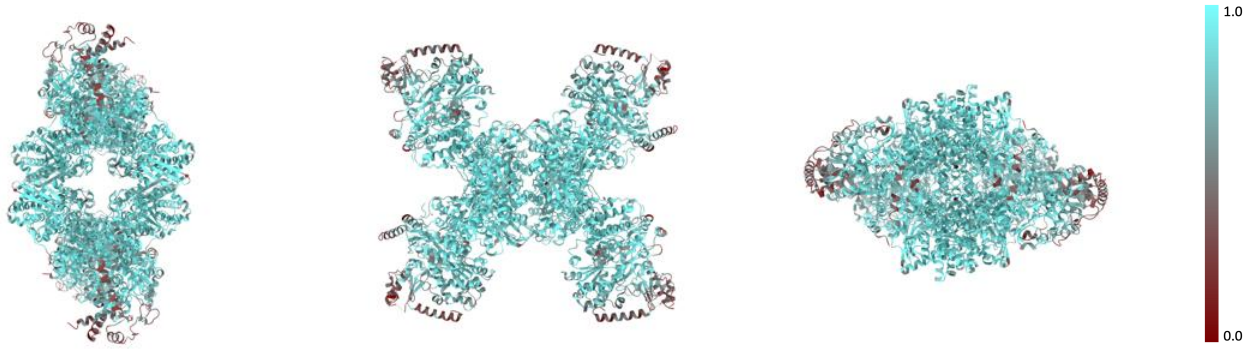
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

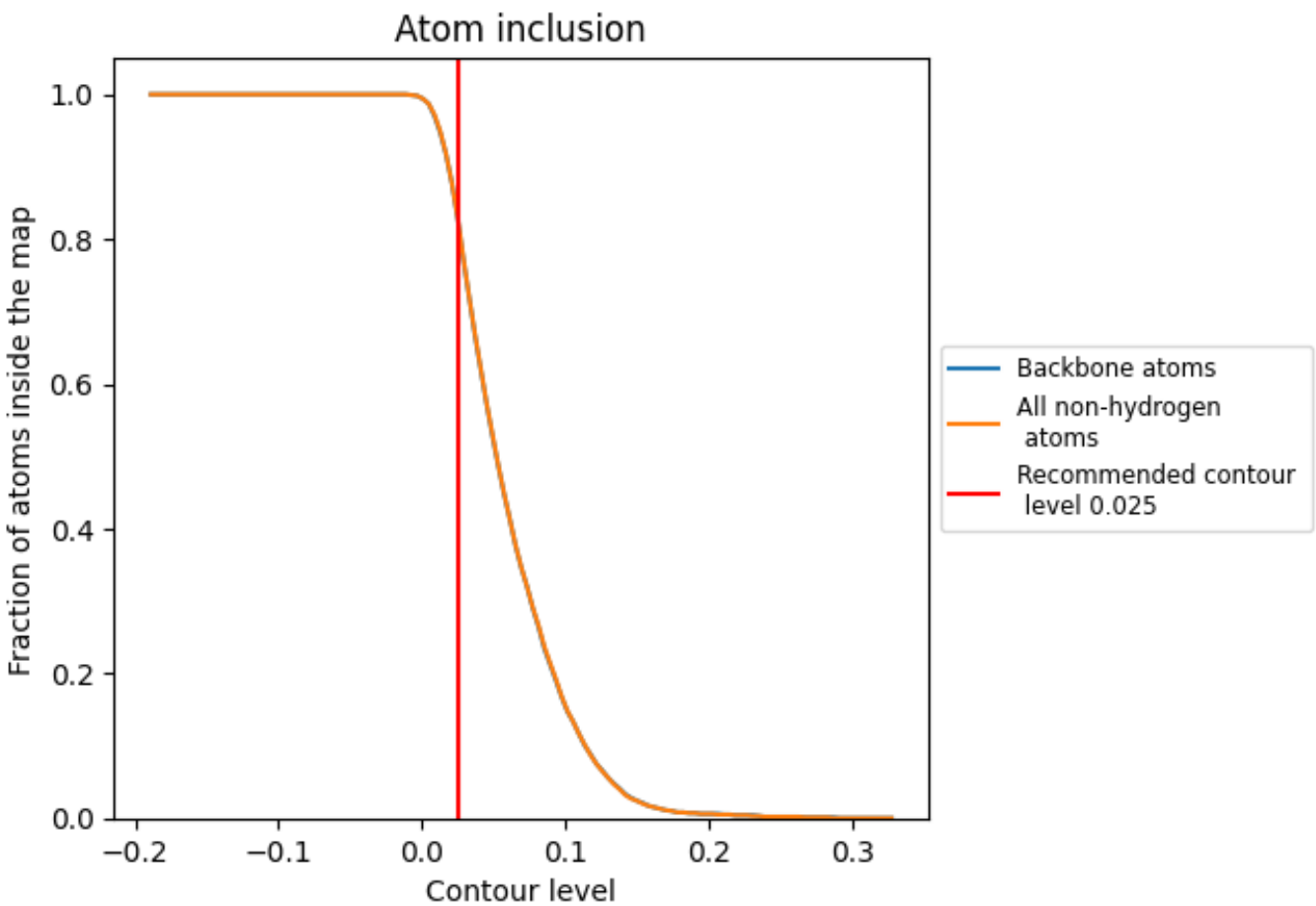
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.6630
A	0.9310	0.7220
B	0.7390	0.6120
C	0.7880	0.6340
D	0.9300	0.7210
E	0.7390	0.6110
F	0.7880	0.6310
a	0.9300	0.7220
b	0.7390	0.6110
c	0.7880	0.6300
d	0.9310	0.7220
e	0.7380	0.6120
f	0.7880	0.6330