wwPDB EM Validation Summary Report

Aug 5, 2026 – 03:29 AM EDT

PDB ID	:	9MQX / pdb_00009mqx
EMDB ID	:	EMD-48543
Title	:	Electron-bifurcating Tungstopyranopterin-containing aldehyde oxidoreductase with NADH
Authors	:	Feng, X.; Li, H.
Deposited on	:	2025-01-06
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:

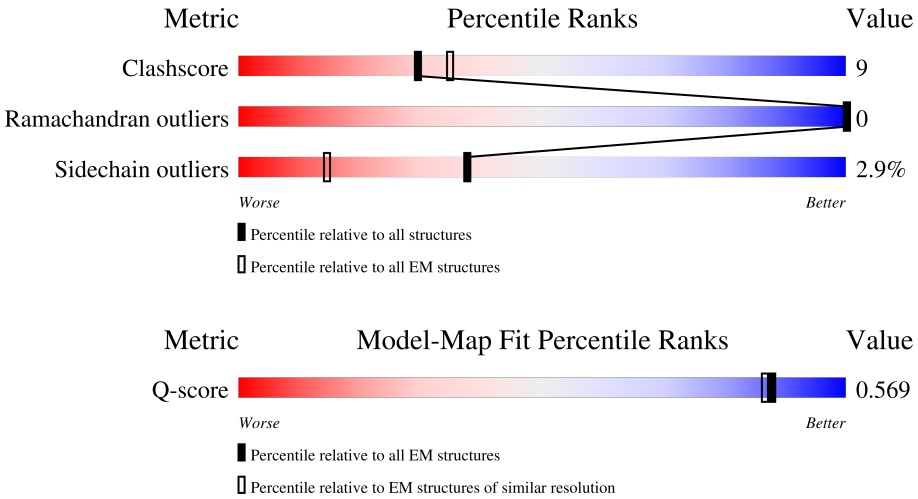
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 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.



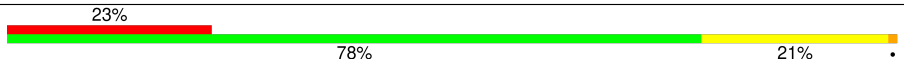
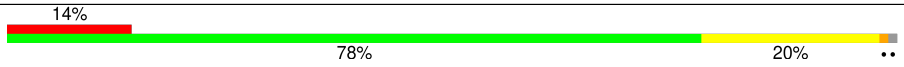
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	247	77% 21%
2	B	622	11% 81% 18%
3	C	159	13% 82% 16%
4	D	604	78% 21%

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Mol	Chain	Length	Quality of chain
4	F	604	
4	H	604	
5	E	152	
5	G	152	
5	I	152	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SF4	D	701	-	-	X	-
6	SF4	F	701	-	-	X	-
6	SF4	H	701	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 25410 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 NADH:ubiquinone oxidoreductase chain G-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	247	1924	1204	346	351	23	0	0

- Molecule 2 is a protein called NADH:ubiquinone oxidoreductase, NADH-binding (51 kD) subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	622	4743	2997	815	892	39	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase 24 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	159	1224	778	207	229	10	0	0

- Molecule 4 is a protein called Aldehyde:ferredoxin oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	604	4572	2902	782	862	26	0	0
4	F	604	4572	2902	782	862	26	0	0
4	H	604	4572	2902	782	862	26	0	0

- Molecule 5 is a protein called Fe-S-cluster-containing hydrogenase subunit.

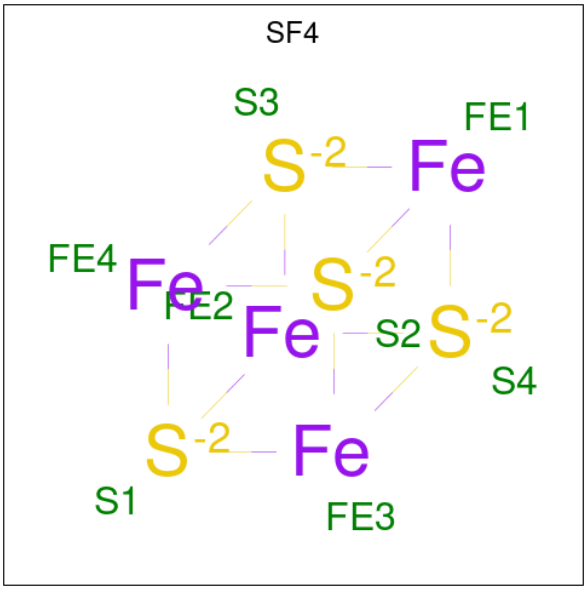
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	152	1142	707	195	218	22	0	0
5	G	150	1125	695	192	216	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	150	Total	C	N	O	S	0	0
			1125	695	192	216	22		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



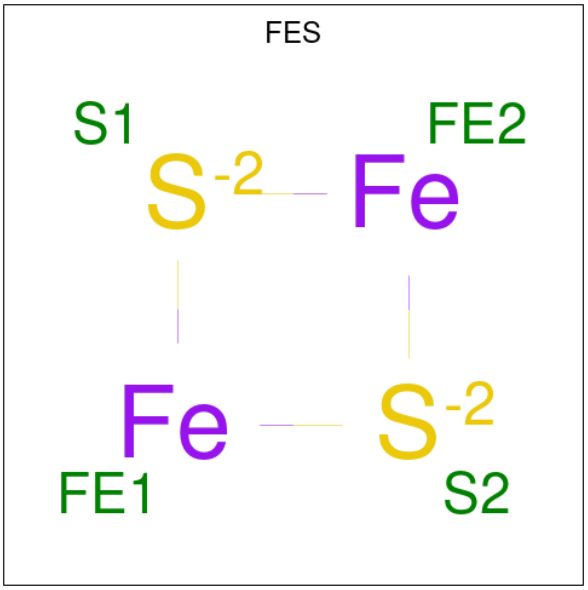
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	Fe	S		0
			8	4	4		
6	A	1	Total	Fe	S		0
			8	4	4		
6	B	1	Total	Fe	S		0
			8	4	4		
6	B	1	Total	Fe	S		0
			8	4	4		
6	B	1	Total	Fe	S		0
			8	4	4		
6	D	1	Total	Fe	S		0
			8	4	4		
6	E	1	Total	Fe	S		0
			8	4	4		
6	E	1	Total	Fe	S		0
			8	4	4		
6	E	1	Total	Fe	S		0
			8	4	4		
6	E	1	Total	Fe	S		0
			8	4	4		

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Mol	Chain	Residues	Atoms	AltConf
6	F	1	Total Fe S 8 4 4	0
6	G	1	Total Fe S 8 4 4	0
6	G	1	Total Fe S 8 4 4	0
6	G	1	Total Fe S 8 4 4	0
6	G	1	Total Fe S 8 4 4	0
6	H	1	Total Fe S 8 4 4	0
6	I	1	Total Fe S 8 4 4	0
6	I	1	Total Fe S 8 4 4	0
6	I	1	Total Fe S 8 4 4	0
6	I	1	Total Fe S 8 4 4	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total Fe S 4 2 2	0

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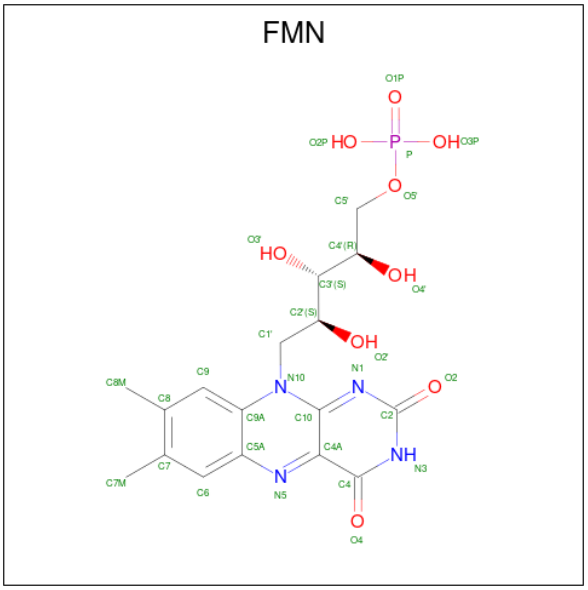
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Mol	Chain	Residues	Atoms	AltConf
7	B	1	Total Fe S 4 2 2	0
7	C	1	Total Fe S 4 2 2	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

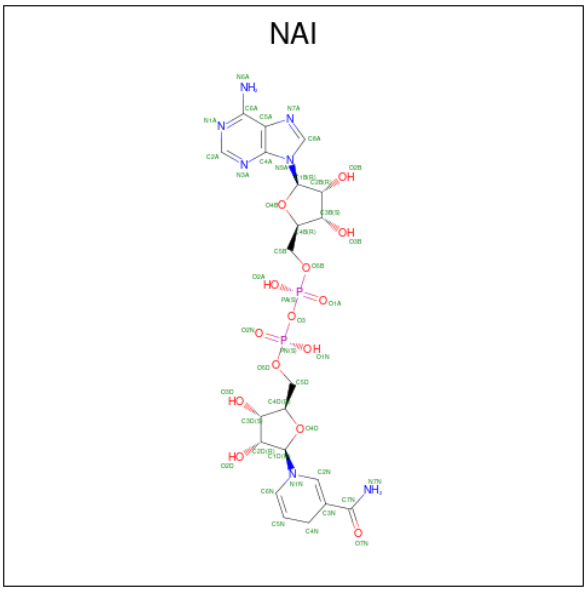
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total Zn 1 1	0
8	B	1	Total Zn 1 1	0

- Molecule 9 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
9	B	1	Total C N O P 31 17 4 9 1	0

- Molecule 10 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

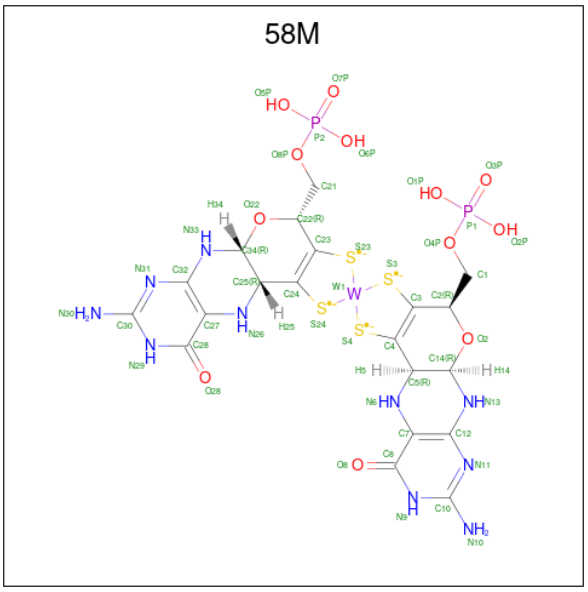


Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	D	3	Total	Mg	0
			3	3	
11	F	3	Total	Mg	0
			3	3	
11	H	3	Total	Mg	0
			3	3	

- Molecule 12 is TUNGSTOPTERIN COFACTOR (CCD ID: 58M) (formula: $C_{20}H_{24}N_{10}O_{12}P_2S_4W$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
12	D	1	Total	C	N	O	P	S	W	0
			49	20	10	12	2	4	1	
12	F	1	Total	C	N	O	P	S	W	0
			49	20	10	12	2	4	1	
12	H	1	Total	C	N	O	P	S	W	0
			49	20	10	12	2	4	1	

- Molecule 13 is water.

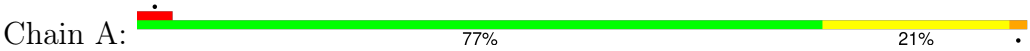
Mol	Chain	Residues	Atoms		AltConf
13	D	2	Total	O	0
			2	2	
13	F	2	Total	O	0
			2	2	
13	H	2	Total	O	0
			2	2	

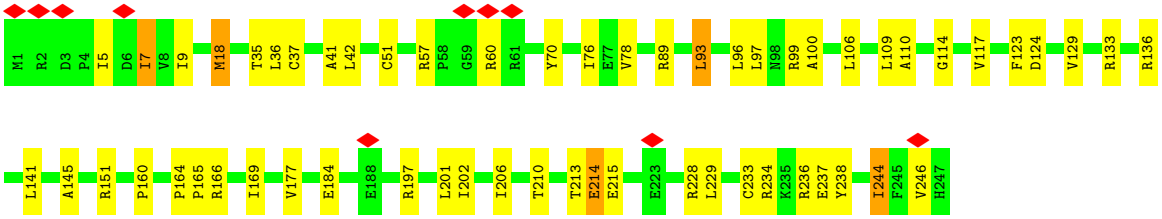
3 Residue-property plots (i)

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: NADH:ubiquinone oxidoreductase chain G-like protein

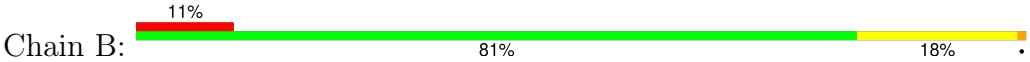
Chain A:

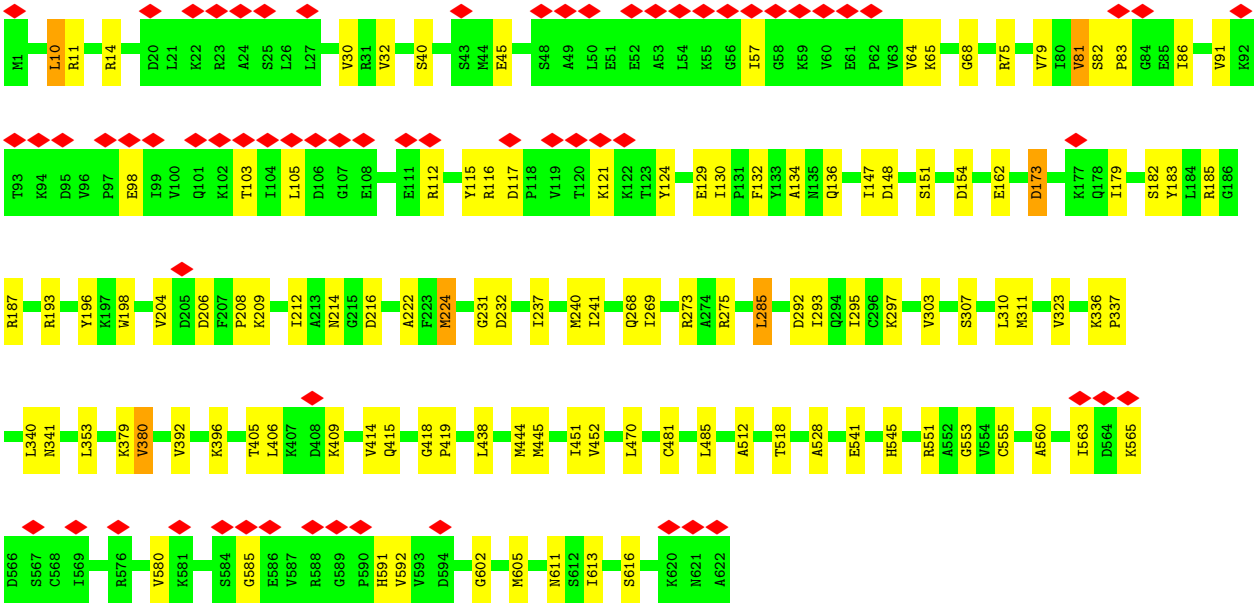




• Molecule 2: NADH:ubiquinone oxidoreductase, NADH-binding (51 kD) subunit

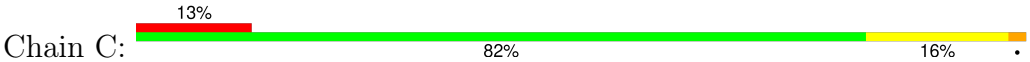
Chain B:

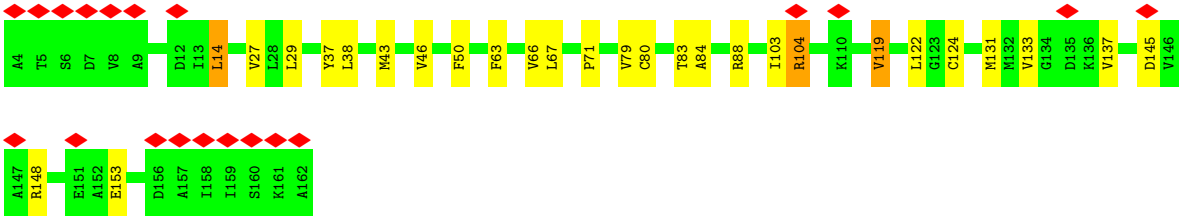




• Molecule 3: NADH:ubiquinone oxidoreductase 24 kD subunit

Chain C:

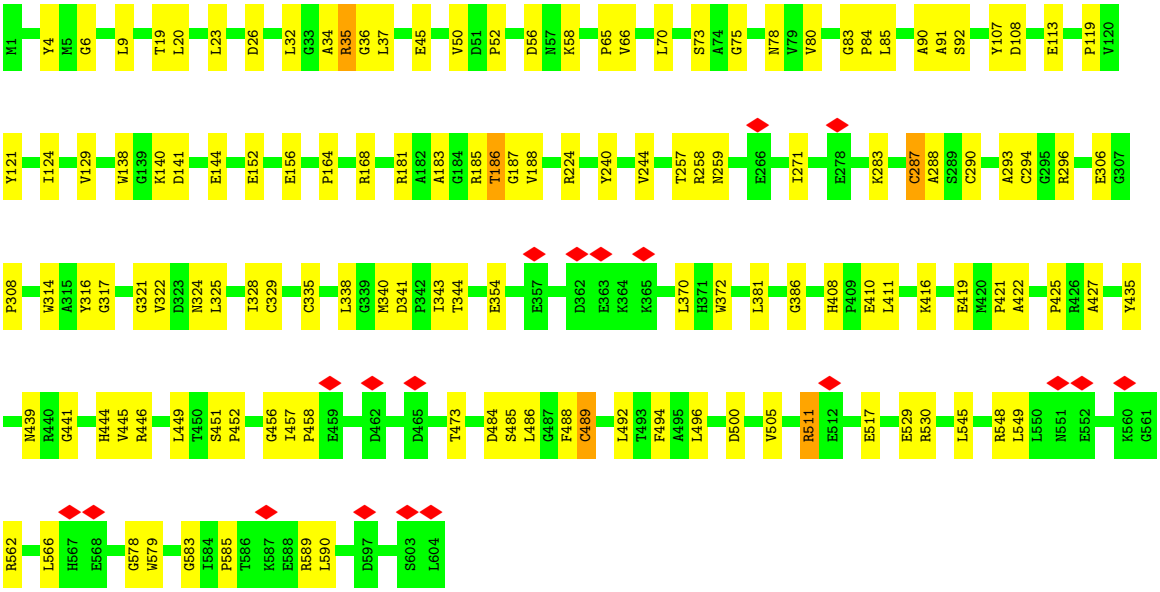




• Molecule 4: Aldehyde:ferredoxin oxidoreductase

Chain D:

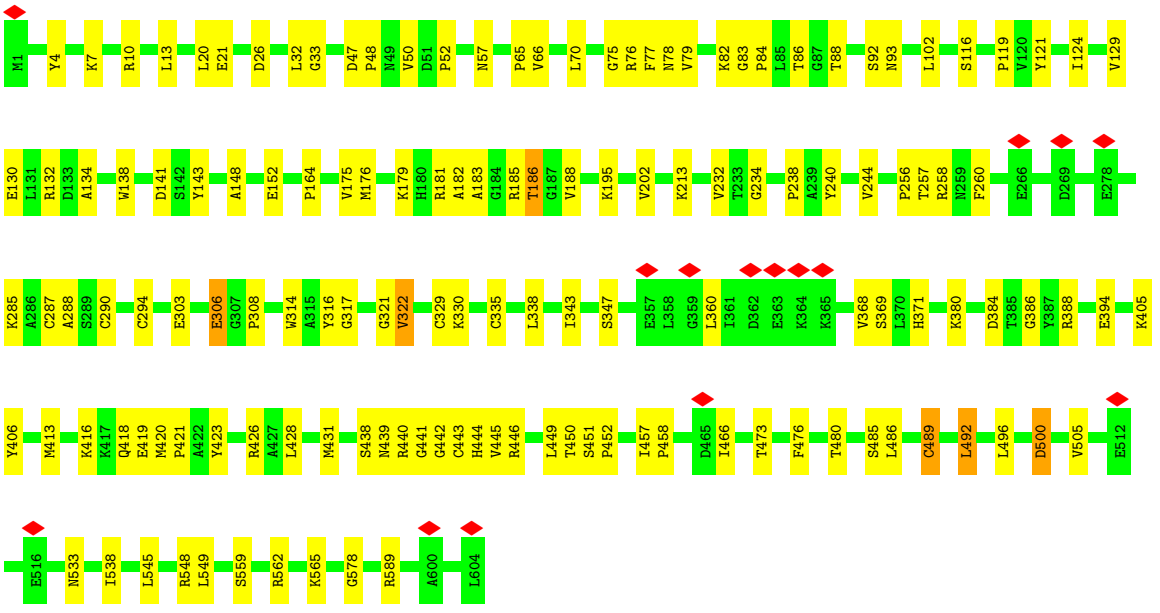




• Molecule 4: Aldehyde:ferredoxin oxidoreductase

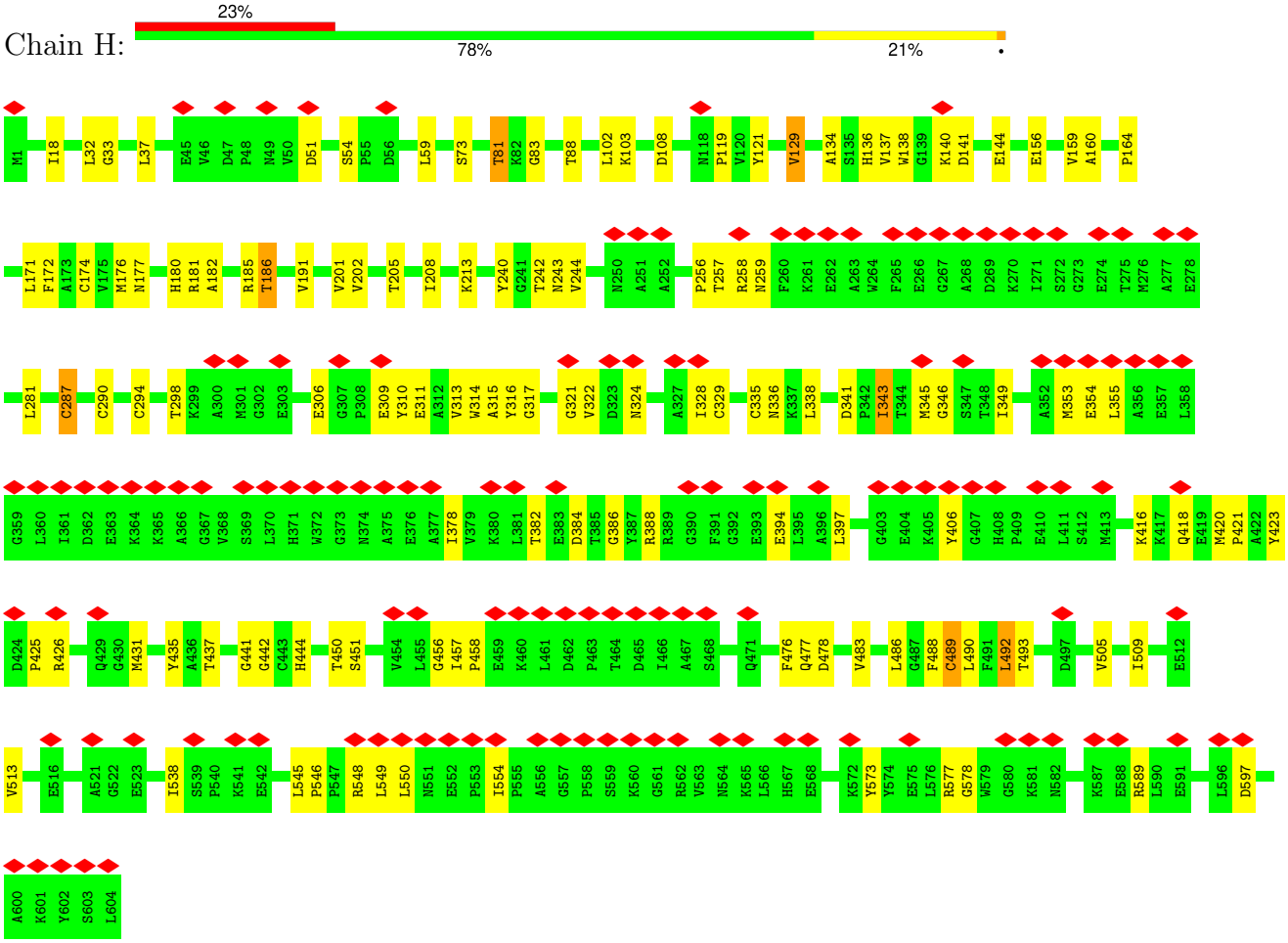
Chain F:





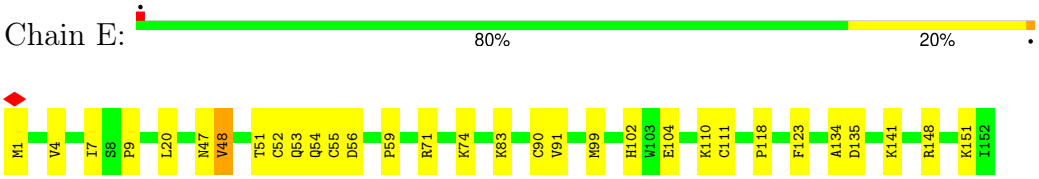
• Molecule 4: Aldehyde:ferredoxin oxidoreductase

Chain H:



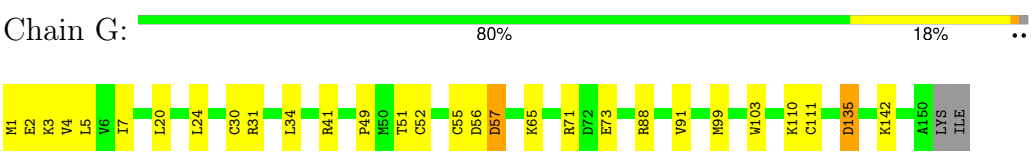
• Molecule 5: Fe-S-cluster-containing hydrogenase subunit

Chain E:



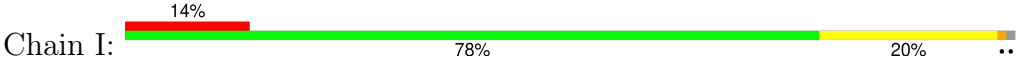
• Molecule 5: Fe-S-cluster-containing hydrogenase subunit

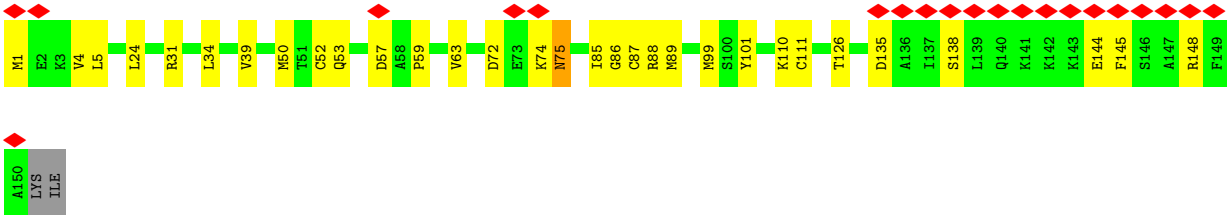
Chain G:



• Molecule 5: Fe-S-cluster-containing hydrogenase subunit

Chain I:




M1
E2
K3
V4
L5
L24
R31
L34
V39
M50
T51
C52
Q53
D57
A58
P59
V63
D72
E73
K74
N75
I85
G86
C87
R88
M89
M99
S100
Y101
K110
C111
T126
D135
A136
I137
S138
L139
Q140
K141
K142
K143
E144
F145
S146
A147
R148
F149
A150
LYS
ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	737000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	59	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	58.549	Depositor
Minimum map value	-32.908	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.243	Depositor
Recommended contour level	5.3	Depositor
Map size (Å)	298.08002, 298.08002, 298.08002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82800007, 0.82800007, 0.82800007	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, SF4, 58M, FMN, MG, ZN, FES

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	0.11	0/1964	0.28	0/2662
2	B	0.11	0/4829	0.26	0/6516
3	C	0.13	0/1240	0.27	0/1672
4	D	0.11	0/4666	0.29	0/6316
4	F	0.12	0/4666	0.30	0/6316
4	H	0.13	0/4666	0.30	0/6316
5	E	0.10	0/1161	0.26	0/1564
5	G	0.11	0/1144	0.26	0/1542
5	I	0.10	0/1144	0.27	0/1542
All	All	0.12	0/25480	0.28	0/34446

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

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	1924	0	1918	35	0
2	B	4743	0	4767	67	0
3	C	1224	0	1265	14	0
4	D	4572	0	4591	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	4572	0	4591	101	0
4	H	4572	0	4591	95	0
5	E	1142	0	1117	24	0
5	G	1125	0	1093	27	0
5	I	1125	0	1095	20	0
6	A	16	0	0	0	0
6	B	24	0	0	1	0
6	D	8	0	0	15	0
6	E	32	0	0	2	0
6	F	8	0	0	18	0
6	G	32	0	0	0	0
6	H	8	0	0	17	0
6	I	32	0	0	1	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
7	C	4	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	B	31	0	19	0	0
10	B	44	0	27	1	0
11	D	3	0	0	0	0
11	F	3	0	0	0	0
11	H	3	0	0	0	0
12	D	49	0	0	0	0
12	F	49	0	0	3	0
12	H	49	0	0	2	0
13	D	2	0	0	0	0
13	F	2	0	0	0	0
13	H	2	0	0	0	0
All	All	25410	0	25074	462	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 9.

The worst 5 of 462 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)
4:F:294:CYS:SG	6:F:701:SF4:FE3	1.08	1.44
4:D:294:CYS:SG	6:D:701:SF4:FE3	1.10	1.43
4:H:294:CYS:SG	6:H:701:SF4:FE3	1.10	1.40
4:F:287:CYS:SG	6:F:701:SF4:FE1	1.16	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:287:CYS:SG	6:D:701:SF4:FE1	1.18	1.33

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	245/247 (99%)	237 (97%)	8 (3%)	0	100	100
2	B	620/622 (100%)	604 (97%)	16 (3%)	0	100	100
3	C	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
4	D	602/604 (100%)	582 (97%)	20 (3%)	0	100	100
4	F	602/604 (100%)	582 (97%)	20 (3%)	0	100	100
4	H	602/604 (100%)	589 (98%)	13 (2%)	0	100	100
5	E	150/152 (99%)	149 (99%)	1 (1%)	0	100	100
5	G	148/152 (97%)	145 (98%)	3 (2%)	0	100	100
5	I	148/152 (97%)	146 (99%)	2 (1%)	0	100	100
All	All	3274/3296 (99%)	3188 (97%)	86 (3%)	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	213/213 (100%)	203 (95%)	10 (5%)	23	58
2	B	513/513 (100%)	494 (96%)	19 (4%)	30	64
3	C	134/134 (100%)	128 (96%)	6 (4%)	24	59
4	D	472/472 (100%)	462 (98%)	10 (2%)	47	75
4	F	472/472 (100%)	465 (98%)	7 (2%)	57	80
4	H	472/472 (100%)	460 (98%)	12 (2%)	42	72
5	E	129/129 (100%)	125 (97%)	4 (3%)	35	68
5	G	127/129 (98%)	124 (98%)	3 (2%)	43	73
5	I	127/129 (98%)	121 (95%)	6 (5%)	23	58
All	All	2659/2663 (100%)	2582 (97%)	77 (3%)	38	70

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	G	57	ASP
5	I	5	LEU
4	H	81	THR
4	H	287	CYS
5	I	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	128	HIS
4	F	471	GLN
4	H	49	ASN
5	G	53	GLN
4	D	439	ASN

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 39 ligands modelled in this entry, 11 are monoatomic - leaving 28 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	$\#\|Z\| > 2$
7	FES	B	704	2	0,4,4	-	-	-		
12	58M	H	705	11	46,56,56	1.66	8 (17%)	44,90,90	2.05	15 (34%)
9	FMN	B	702	-	33,33,33	1.02	2 (6%)	48,50,50	1.21	6 (12%)
7	FES	C	201	3	0,4,4	-	-	-		
6	SF4	E	203	5	0,12,12	-	-	-		
6	SF4	G	204	5	0,12,12	-	-	-		
7	FES	A	303	1	0,4,4	-	-	-		
6	SF4	A	302	1	0,12,12	-	-	-		
6	SF4	E	204	5	0,12,12	-	-	-		
12	58M	D	705	11	46,56,56	1.68	8 (17%)	44,90,90	1.79	11 (25%)
6	SF4	E	201	5	0,12,12	-	-	-		
6	SF4	I	202	5	0,12,12	-	-	-		
10	NAI	B	703	-	47,48,48	0.50	0	64,73,73	0.53	1 (1%)
6	SF4	E	202	5	0,12,12	-	-	-		
6	SF4	G	201	5	0,12,12	-	-	-		
6	SF4	G	203	5	0,12,12	-	-	-		
6	SF4	D	701	-	0,12,12	-	-	-		
6	SF4	B	707	2	0,12,12	-	-	-		
12	58M	F	705	11	46,56,56	1.72	9 (19%)	44,90,90	2.08	14 (31%)
6	SF4	G	202	5	0,12,12	-	-	-		
6	SF4	H	701	-	0,12,12	-	-	-		
6	SF4	B	706	2	0,12,12	-	-	-		
6	SF4	F	701	-	0,12,12	-	-	-		
6	SF4	I	203	5	0,12,12	-	-	-		
6	SF4	I	201	5	0,12,12	-	-	-		
6	SF4	A	301	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SF4	I	204	5	0,12,12	-	-	-		
6	SF4	B	701	2	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
12	58M	H	705	11	-	0/12/88/88	0/8/8/8
7	FES	B	704	2	-	-	0/1/1/1
9	FMN	B	702	-	-	2/18/18/18	0/3/3/3
7	FES	C	201	3	-	-	0/1/1/1
6	SF4	E	203	5	-	-	0/6/5/5
6	SF4	G	204	5	-	-	0/6/5/5
7	FES	A	303	1	-	-	0/1/1/1
6	SF4	A	302	1	-	-	0/6/5/5
6	SF4	E	204	5	-	-	0/6/5/5
12	58M	D	705	11	-	5/12/88/88	0/8/8/8
6	SF4	E	201	5	-	-	0/6/5/5
6	SF4	I	202	5	-	-	0/6/5/5
10	NAI	B	703	-	-	7/29/72/72	0/5/5/5
6	SF4	E	202	5	-	-	0/6/5/5
6	SF4	G	201	5	-	-	0/6/5/5
6	SF4	G	203	5	-	-	0/6/5/5
12	58M	F	705	11	-	4/12/88/88	0/8/8/8
6	SF4	B	707	2	-	-	0/6/5/5
6	SF4	D	701	-	-	-	0/6/5/5
6	SF4	G	202	5	-	-	0/6/5/5
6	SF4	H	701	-	-	-	0/6/5/5
6	SF4	B	706	2	-	-	0/6/5/5
6	SF4	F	701	-	-	-	0/6/5/5
6	SF4	I	203	5	-	-	0/6/5/5
6	SF4	I	201	5	-	-	0/6/5/5
6	SF4	A	301	1	-	-	0/6/5/5
6	SF4	I	204	5	-	-	0/6/5/5
6	SF4	B	701	2	-	-	0/6/5/5

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	705	58M	C7-C12	4.82	1.46	1.38
12	F	705	58M	C27-C32	4.68	1.46	1.38
12	H	705	58M	C7-C12	4.58	1.46	1.38
12	H	705	58M	C27-C32	4.50	1.46	1.38
12	D	705	58M	C27-C32	4.46	1.46	1.38

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	705	58M	C4-C3-S3	-5.99	110.93	119.62
12	F	705	58M	C30-N31-C32	4.76	121.77	113.36
12	F	705	58M	C10-N11-C12	4.74	121.73	113.36
12	D	705	58M	C30-N31-C32	4.70	121.65	113.36
12	D	705	58M	C10-N11-C12	4.59	121.46	113.36

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	702	FMN	N10-C1'-C2'-O2'
9	B	702	FMN	N10-C1'-C2'-C3'
10	B	703	NAI	PA-O3-PN-O5D
12	D	705	58M	O4P-C1-C2-O2
12	D	705	58M	C1-O4P-P1-O1P

There are no ring outliers.

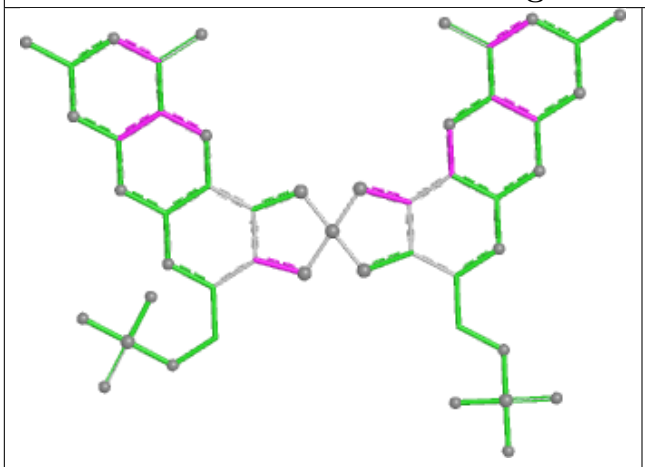
10 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	705	58M	2	0
6	E	204	SF4	1	0
6	E	201	SF4	1	0
10	B	703	NAI	1	0
6	D	701	SF4	15	0
12	F	705	58M	3	0
6	H	701	SF4	17	0
6	F	701	SF4	18	0
6	I	201	SF4	1	0
6	B	701	SF4	1	0

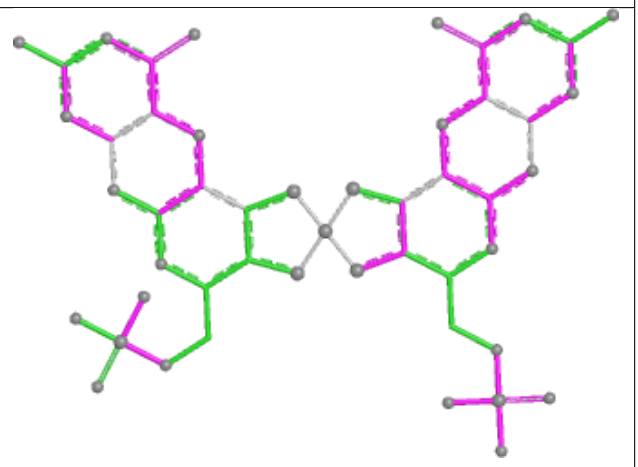
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

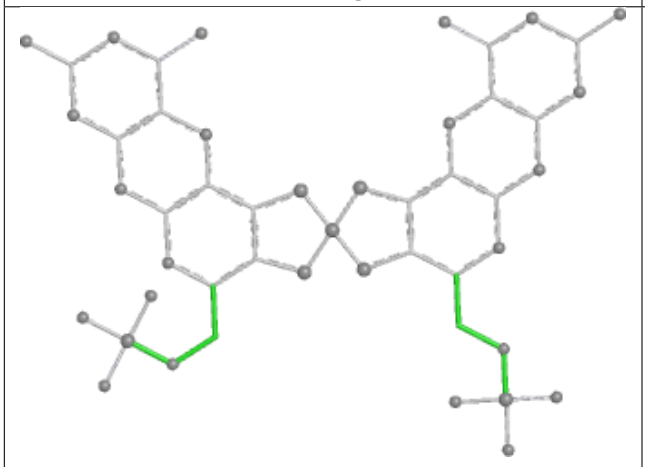
Ligand 58M H 705



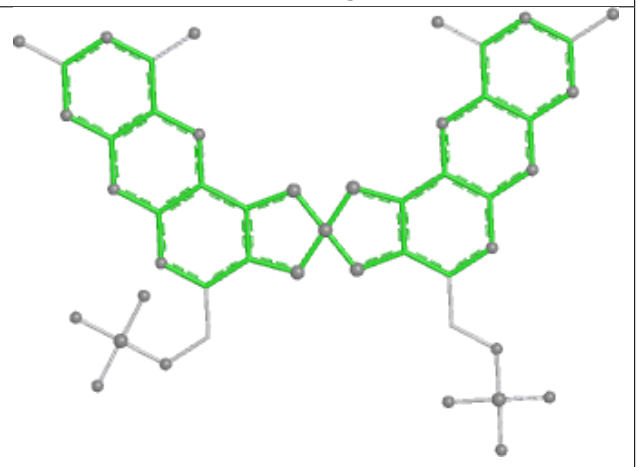
Bond lengths



Bond angles

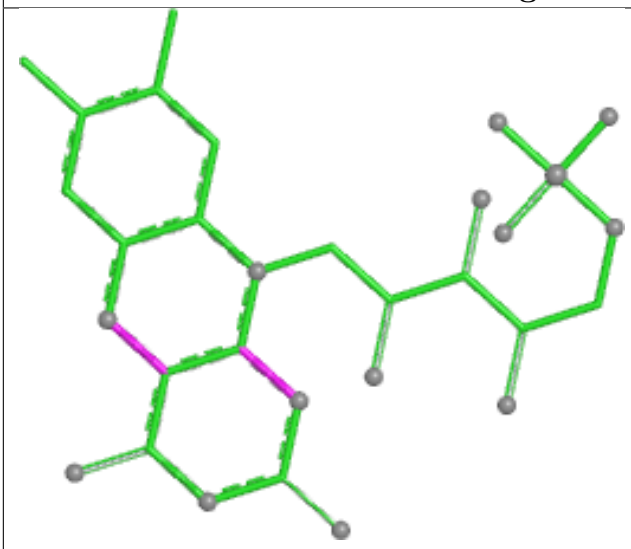


Torsions

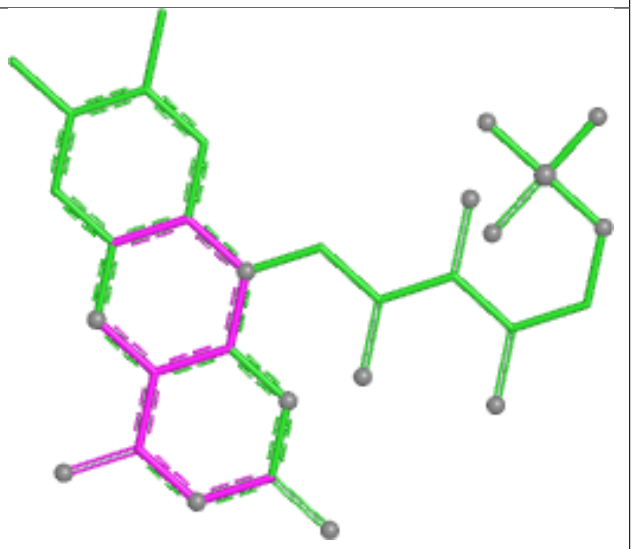


Rings

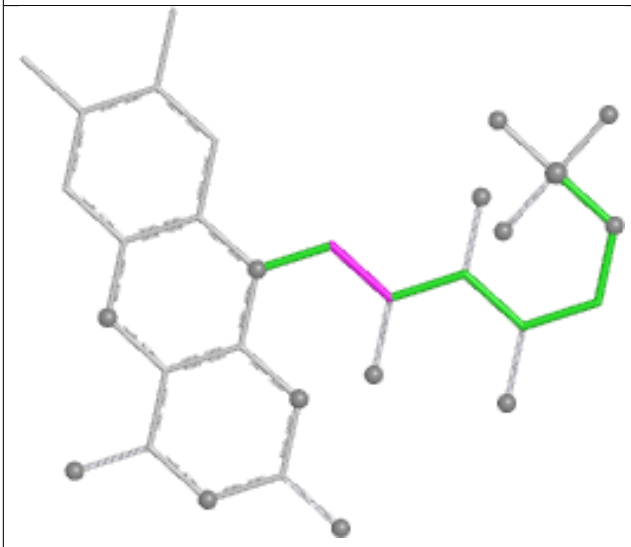
Ligand FMN B 702



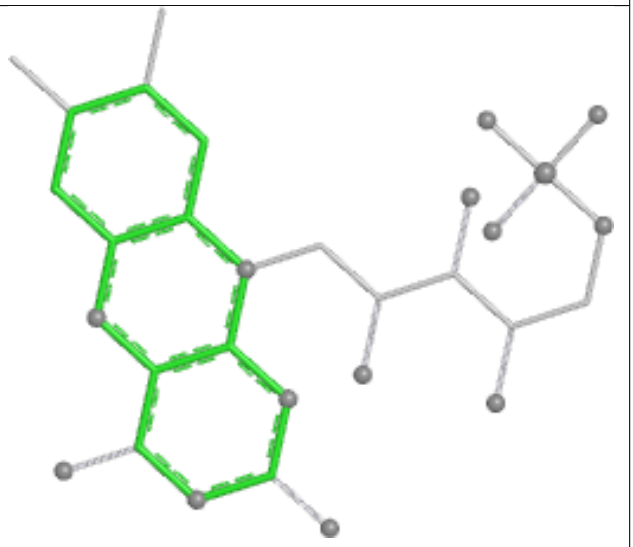
Bond lengths



Bond angles

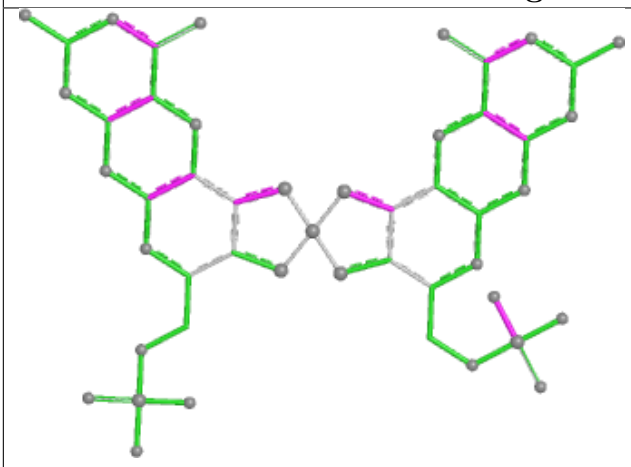


Torsions

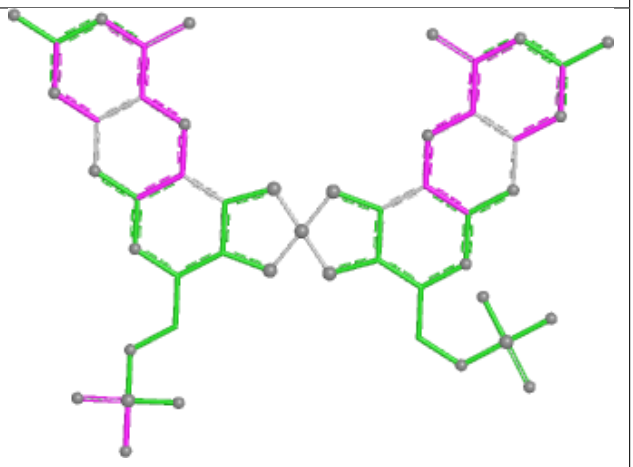


Rings

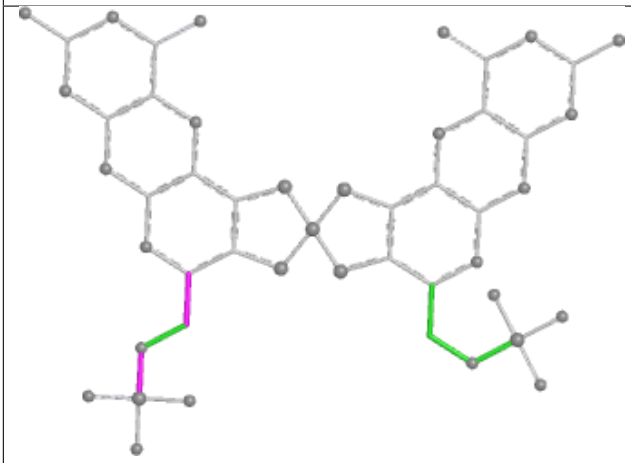
Ligand 58M D 705



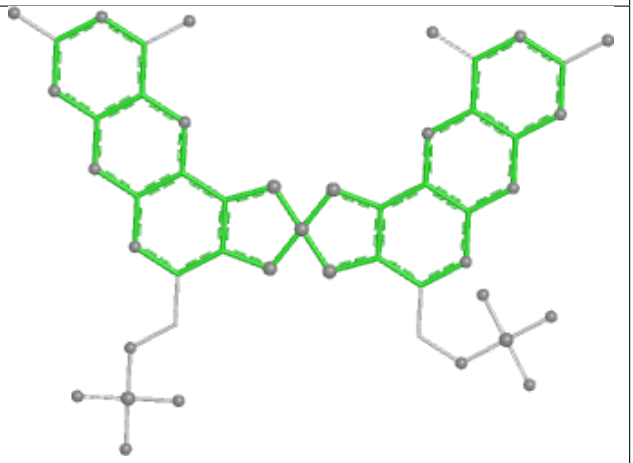
Bond lengths



Bond angles

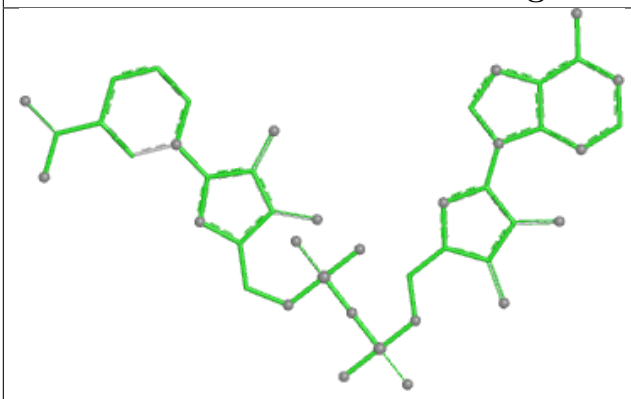


Torsions

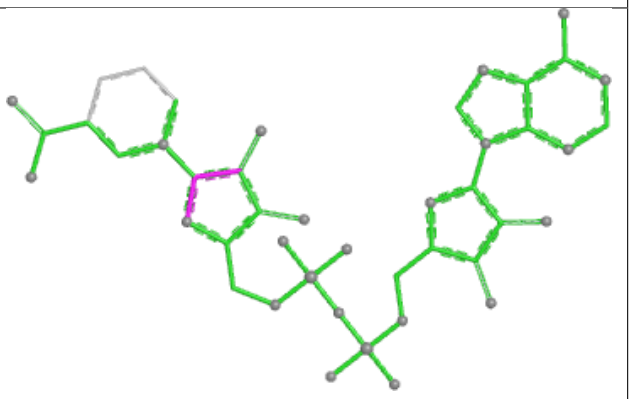


Rings

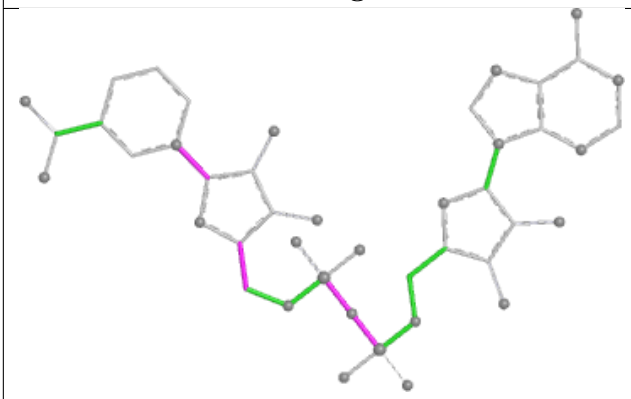
Ligand NAI B 703



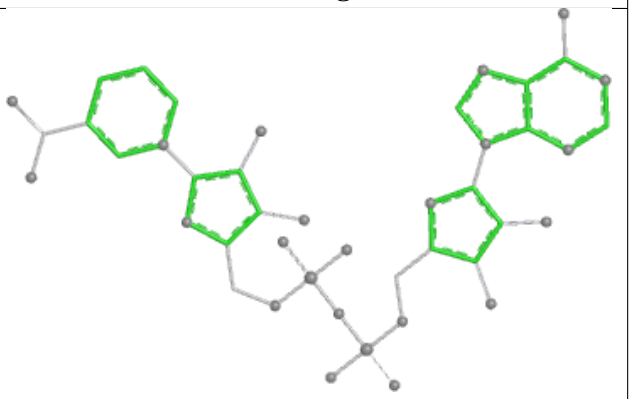
Bond lengths



Bond angles

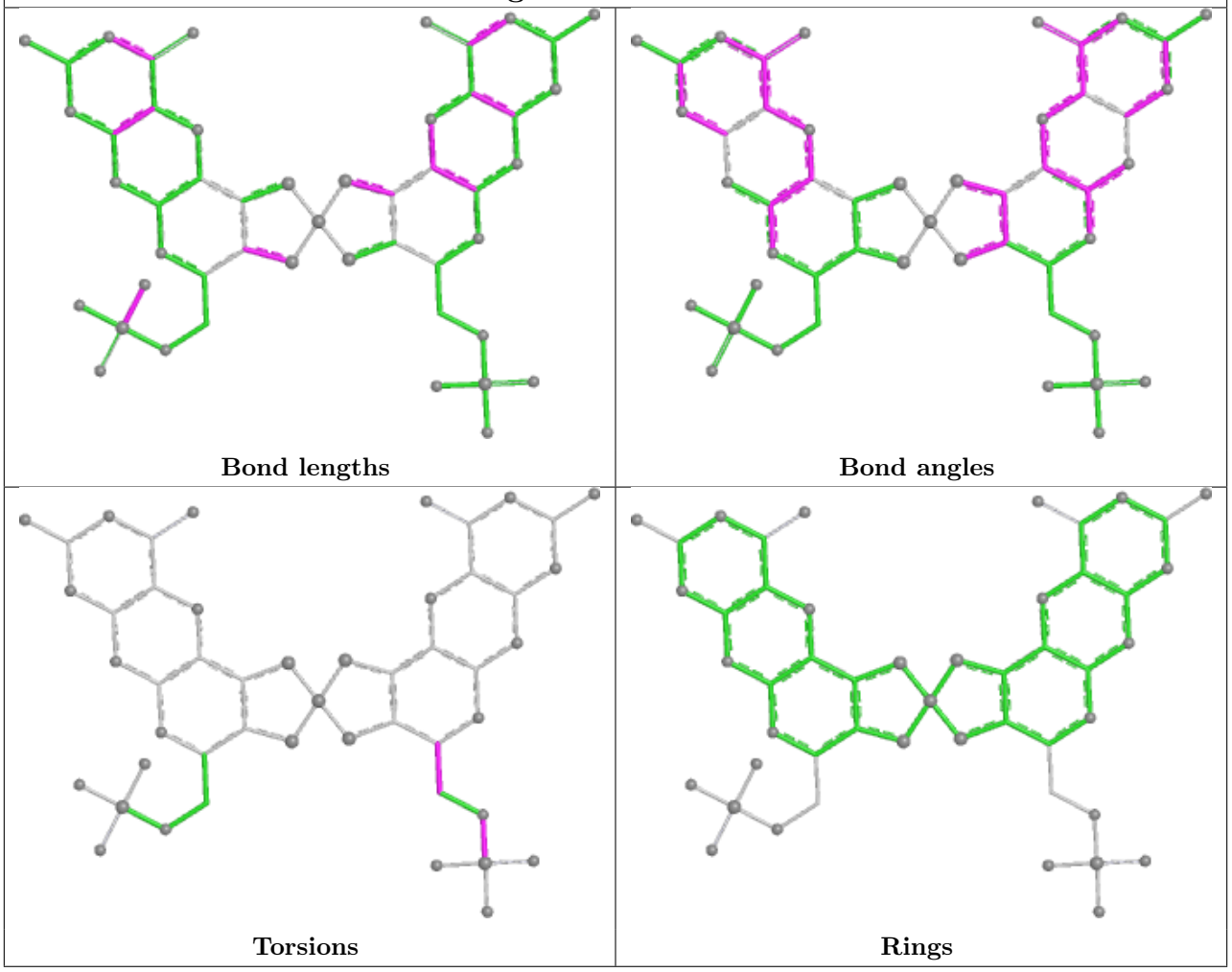


Torsions



Rings

Ligand 58M F 705



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.

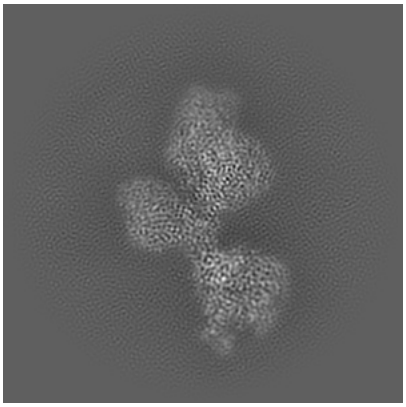
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48543. These allow visual inspection of the internal detail of the map and identification of artifacts.

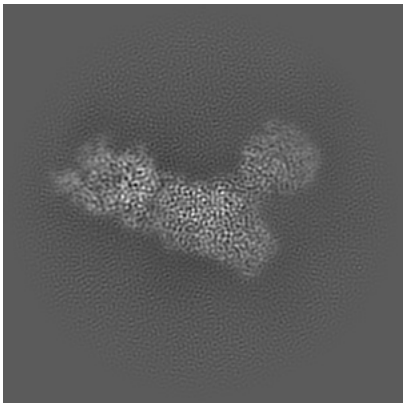
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

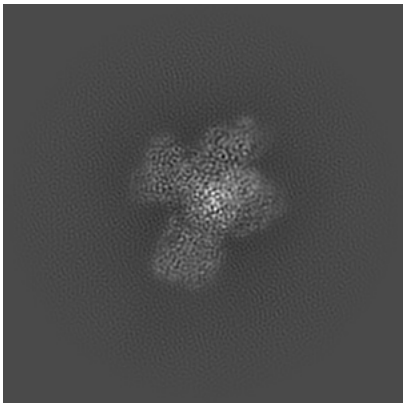
6.1.1 Primary map



X



Y

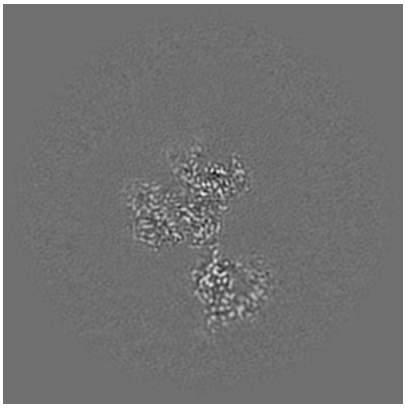


Z

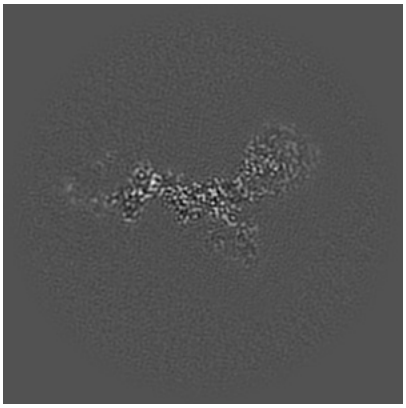
The images above show the map projected in three orthogonal directions.

6.2 Central slices

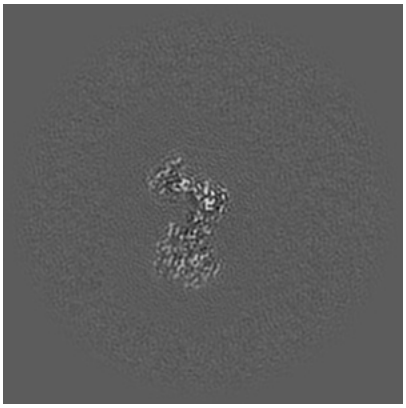
6.2.1 Primary map



X Index: 180



Y Index: 180

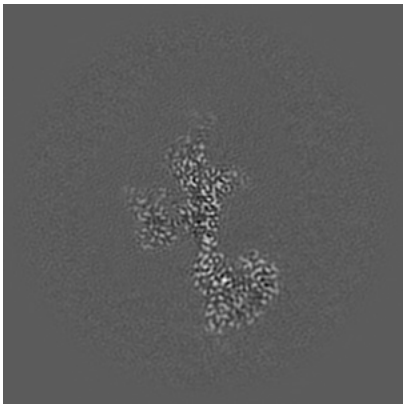


Z Index: 180

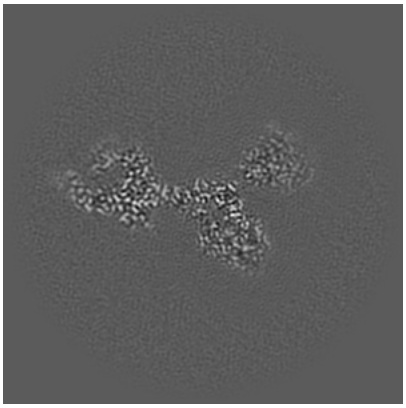
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

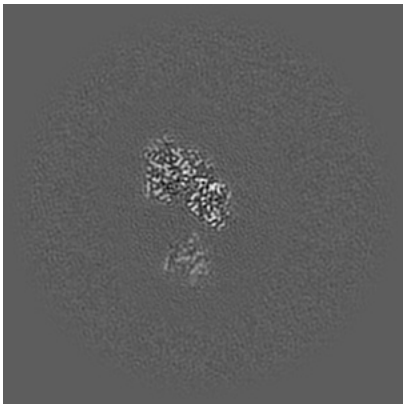
6.3.1 Primary map



X Index: 188



Y Index: 191

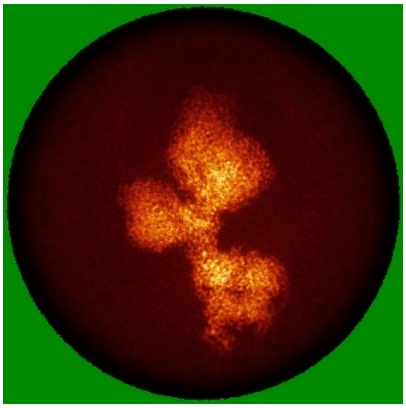


Z Index: 198

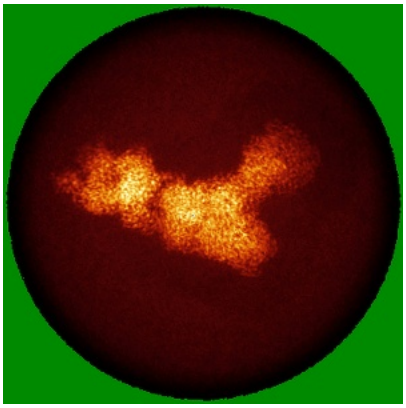
The images above show the largest variance slices of the map in three orthogonal directions.

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

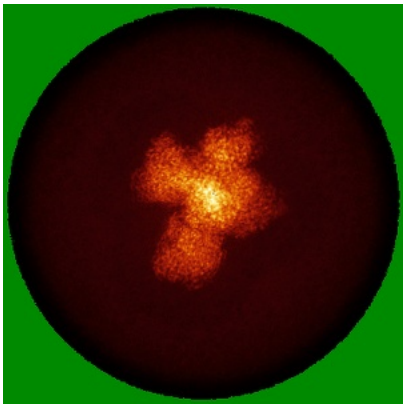
6.4.1 Primary map



X



Y

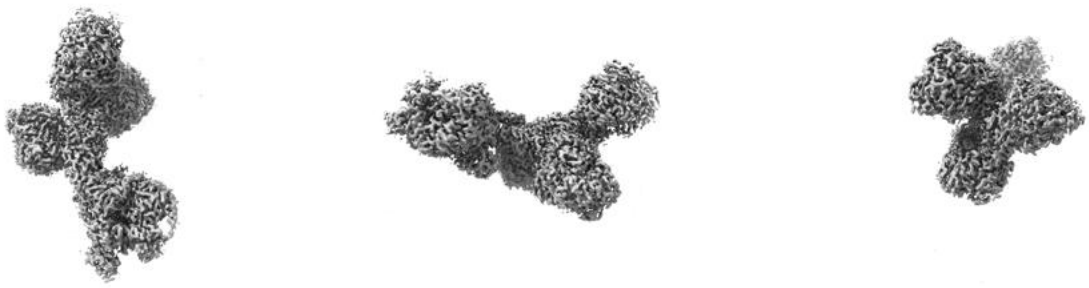


Z

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 5.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

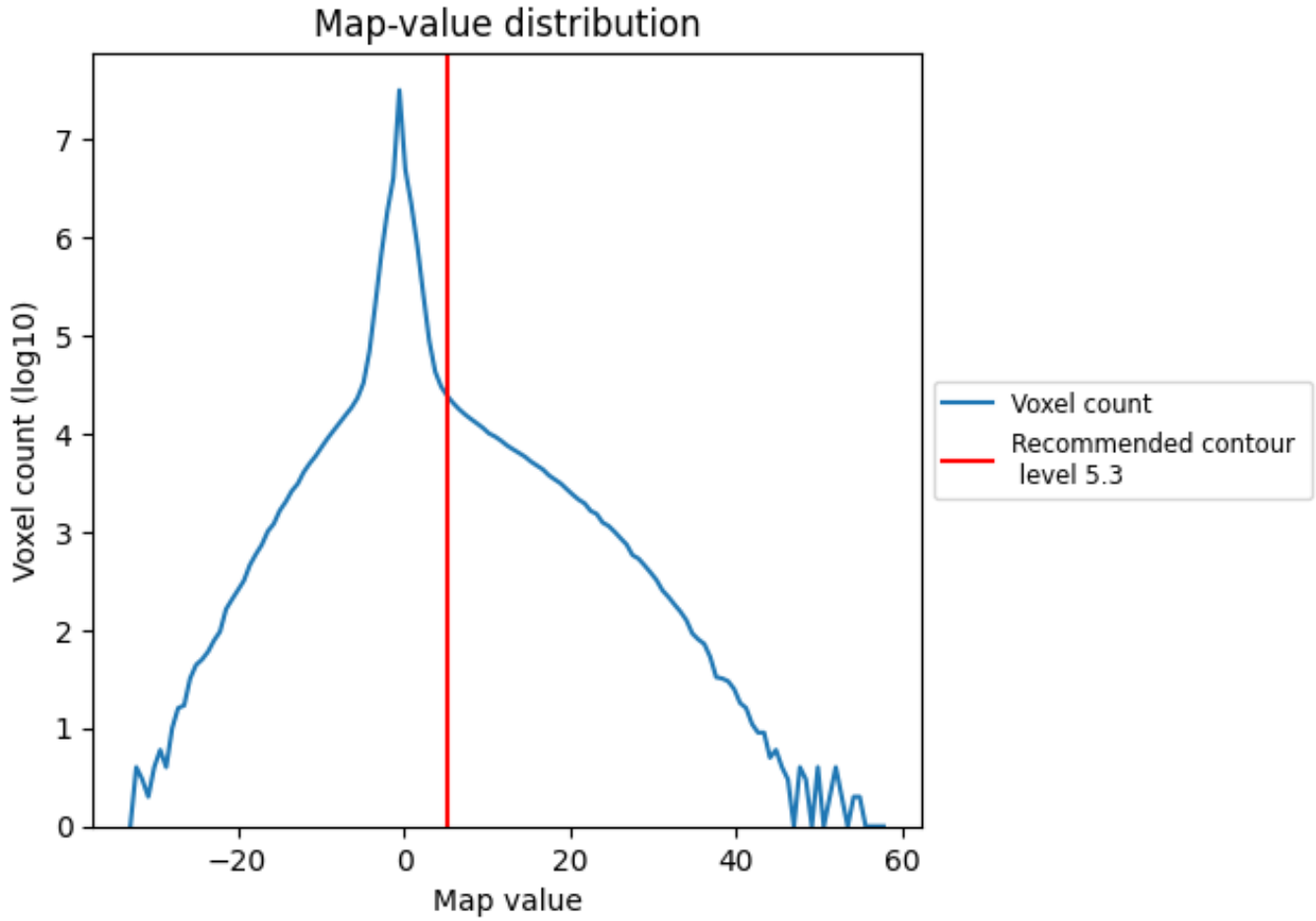
6.6 Mask visualisation (i)

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

7 Map analysis

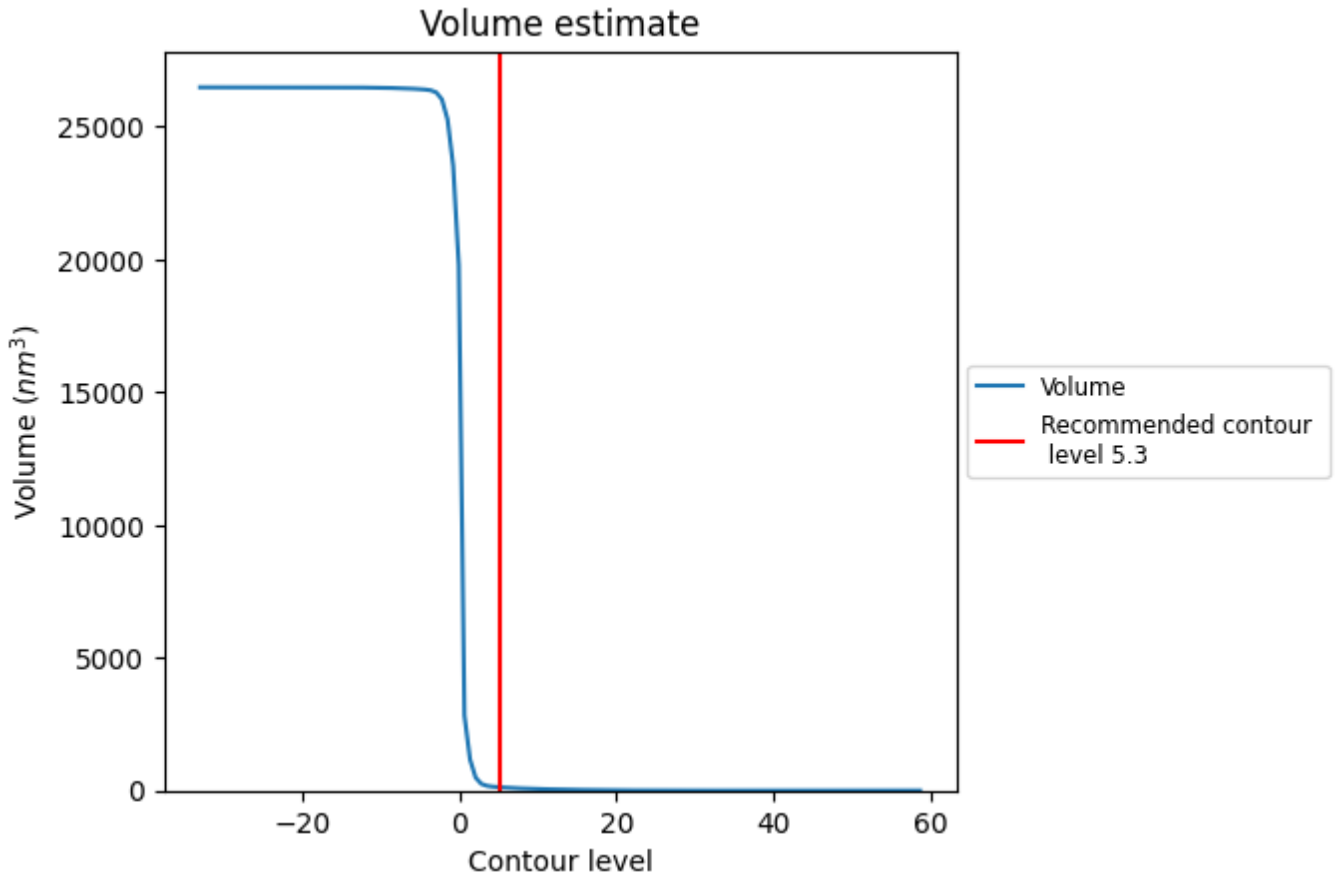
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

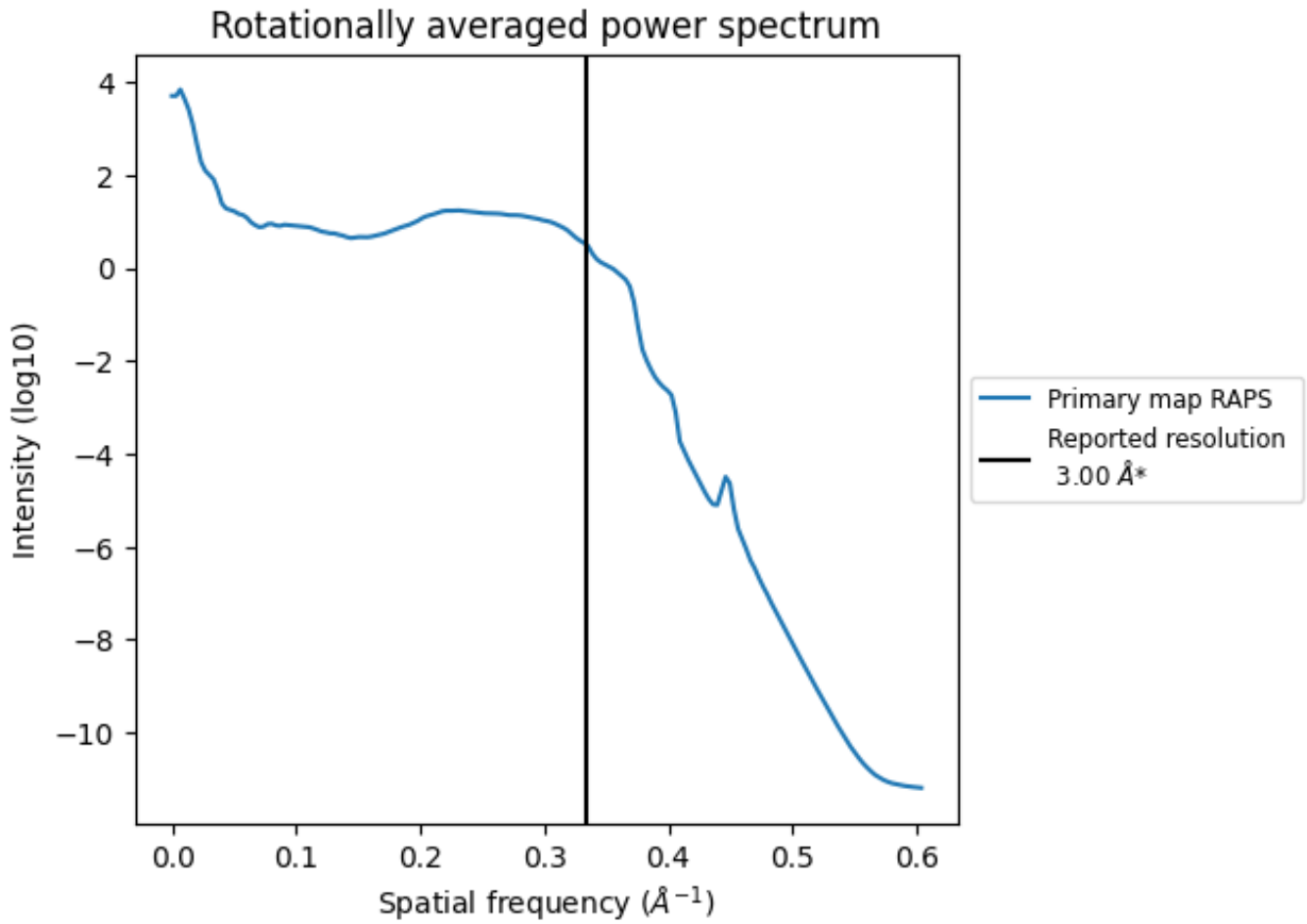
7.2 Volume estimate (i)



The volume at the recommended contour level is 122 nm^3; this corresponds to an approximate mass of 110 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 0.333 Å^{-1}

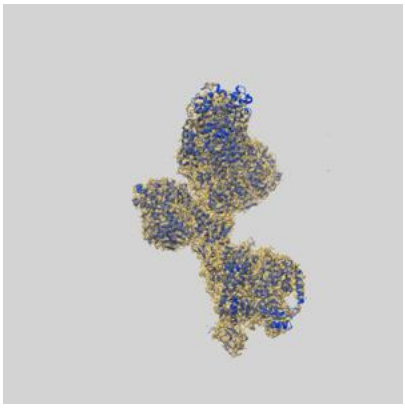
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

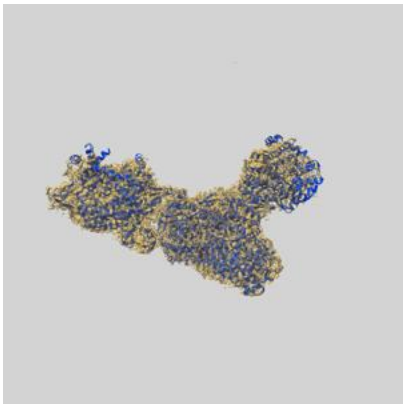
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48543 and PDB model 9MQX. Per-residue inclusion information can be found in section 3 on page 10.

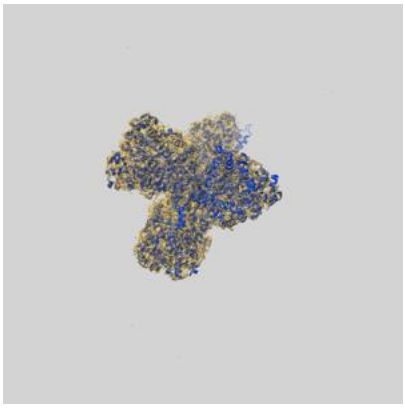
9.1 Map-model overlay



X



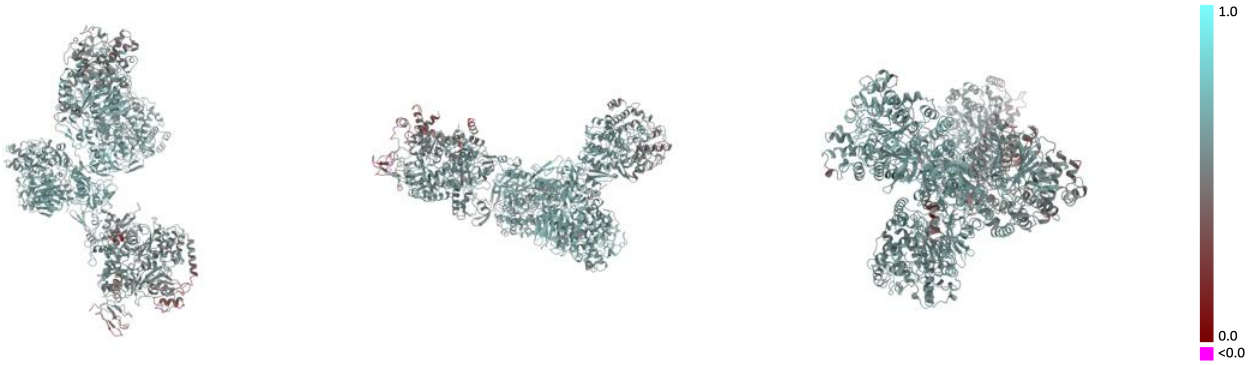
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.3 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.

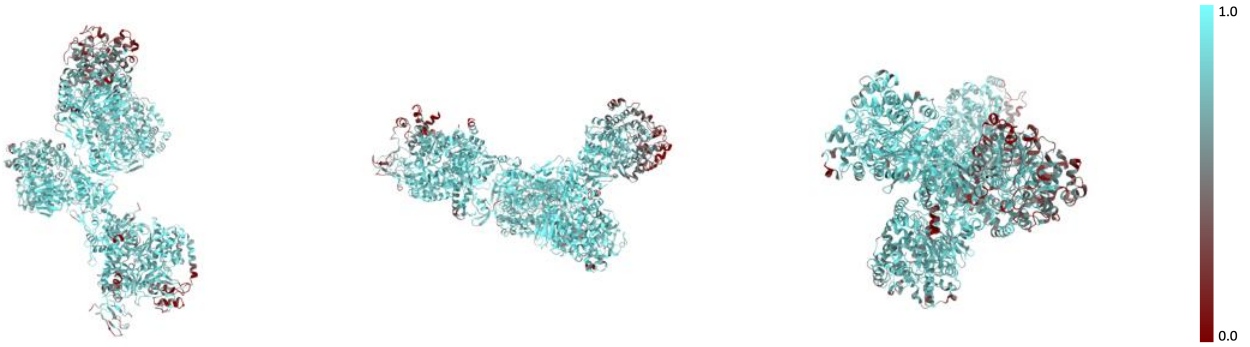
9.2 Q-score mapped to coordinate model (i)



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.

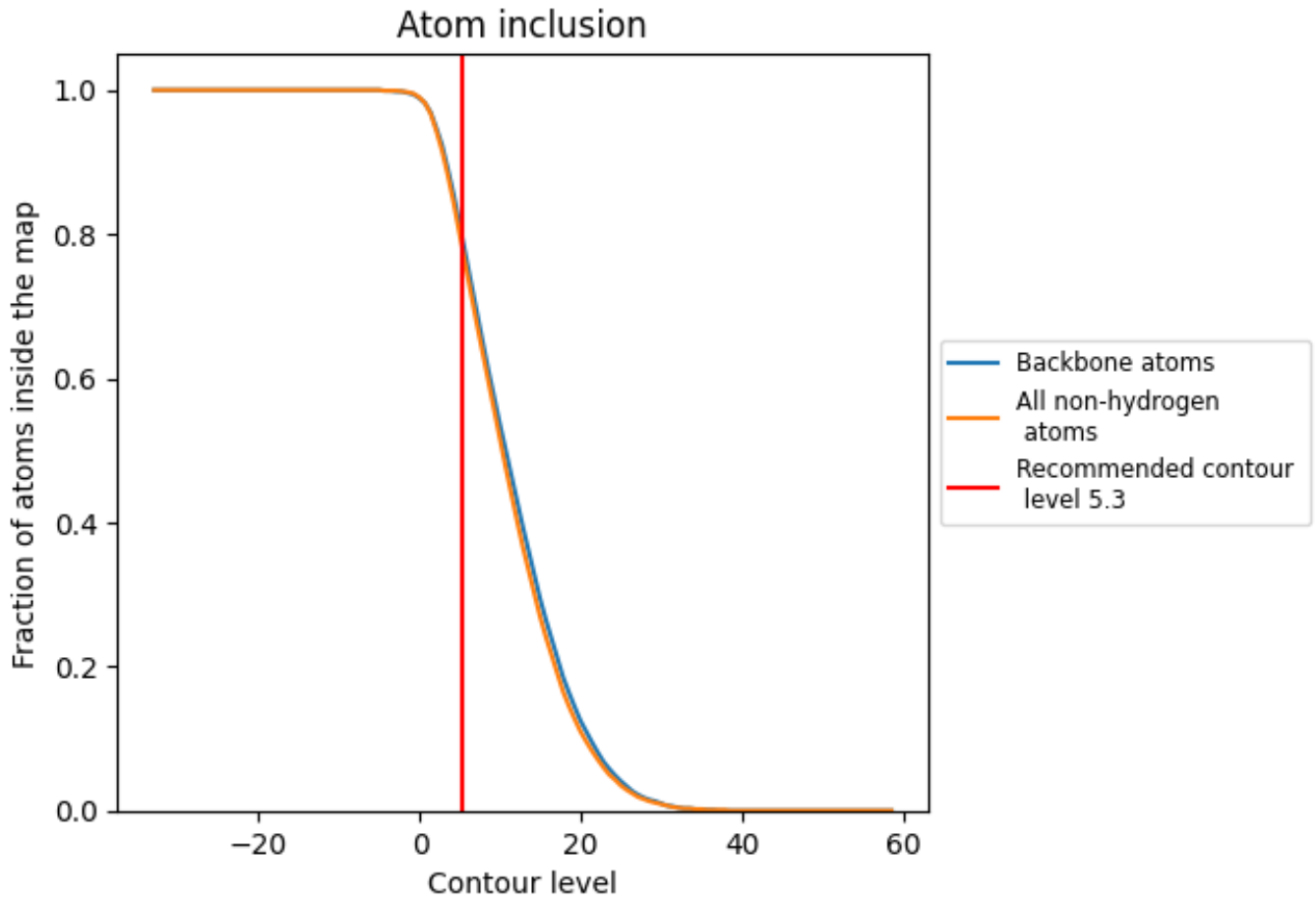
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.3).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 78% 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 (5.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.5690
A	0.8200	0.5520
B	0.7600	0.5170
C	0.7090	0.5110
D	0.8220	0.5970
E	0.9180	0.6320
F	0.8550	0.6100
G	0.9310	0.6360
H	0.6250	0.5450
I	0.7920	0.5670

