



## Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 06:36 pm GMT

PDB ID : 6ZJL  
EMDB ID : EMD-11235  
Title : Respiratory complex I from *Thermus thermophilus*, NAD<sup>+</sup> dataset, major state  
Authors : Kaszuba, K.; Tambalo, M.; Gallagher, G.T.; Sazanov, L.A.  
Deposited on : 2020-06-29  
Resolution : 4.30 Å (reported)  
Based on initial model : 6Y11

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

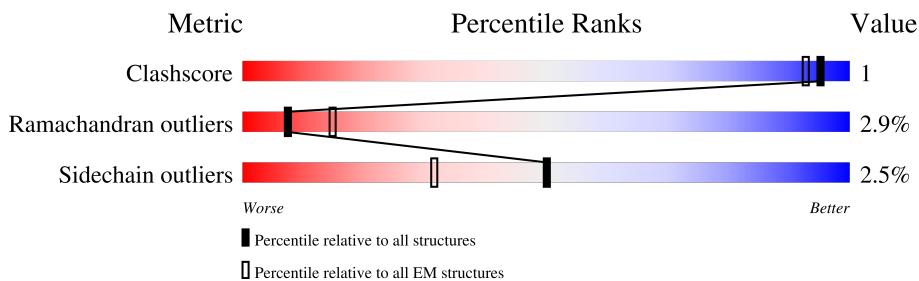
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	438	28% 88% 11%
2	2	181	25% 90% 8% ..
3	3	783	24% 86% 10% ..
4	4	409	17% 83% 10% • 6%
5	5	207	19% 87% 7% 5%
6	6	181	19% 81% 8% • 8%
7	9	182	10% 85% 13% ..
8	7	129	27% 88% 10% ..

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Mol	Chain	Length	Quality of chain
9	A	119	
10	J	176	
11	K	95	
12	L	606	
13	M	469	
14	N	427	
15	H	365	

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
17	FMN	1	502	-	-	X	-

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 36057 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-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	437	3417	2180	595	624	18	0	0

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	178	1406	895	238	265	8	0	0

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	754	5876	3740	1055	1050	31	0	0

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	384	3067	1975	522	559	11	0	0

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	196	1607	1043	273	288	3	0	0

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	166	1289	815	235	226	13	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	9	180	1388	890	232	255	11	0	0

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	127	1031	664	183	181	3	0	0

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	117	910	624	138	144	4	0	0

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	160	1183	806	183	191	3	0	0

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	95	703	456	118	126	3	0	0

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	605	4604	3089	740	756	19	0	0

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	467	3489	2363	546	572	8	0	0

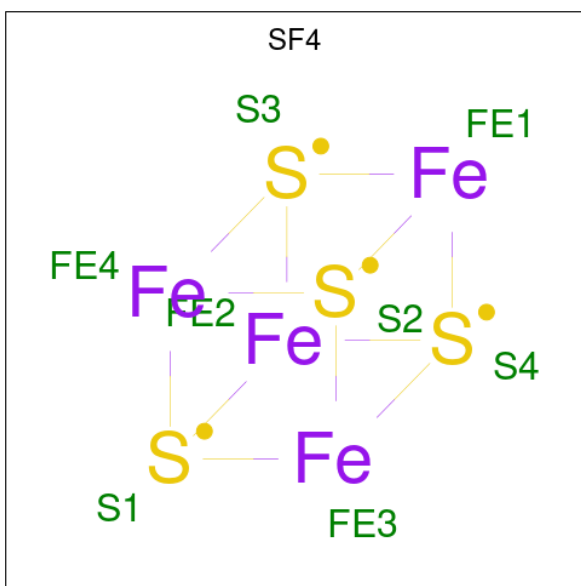
- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	427	3154	2125	505	518	6	0	0

- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	H	353	2838	1943	431	457	7	0	0

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
16	1	1	8	4	4	0
16	3	1	24	12	12	0
16	3	1	24	12	12	0
16	3	1	24	12	12	0
16	6	1	8	4	4	0
16	9	1	16	8	8	0
16	9	1	16	8	8	0

- Molecule 17 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	1	1	31	17	4	9	1	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

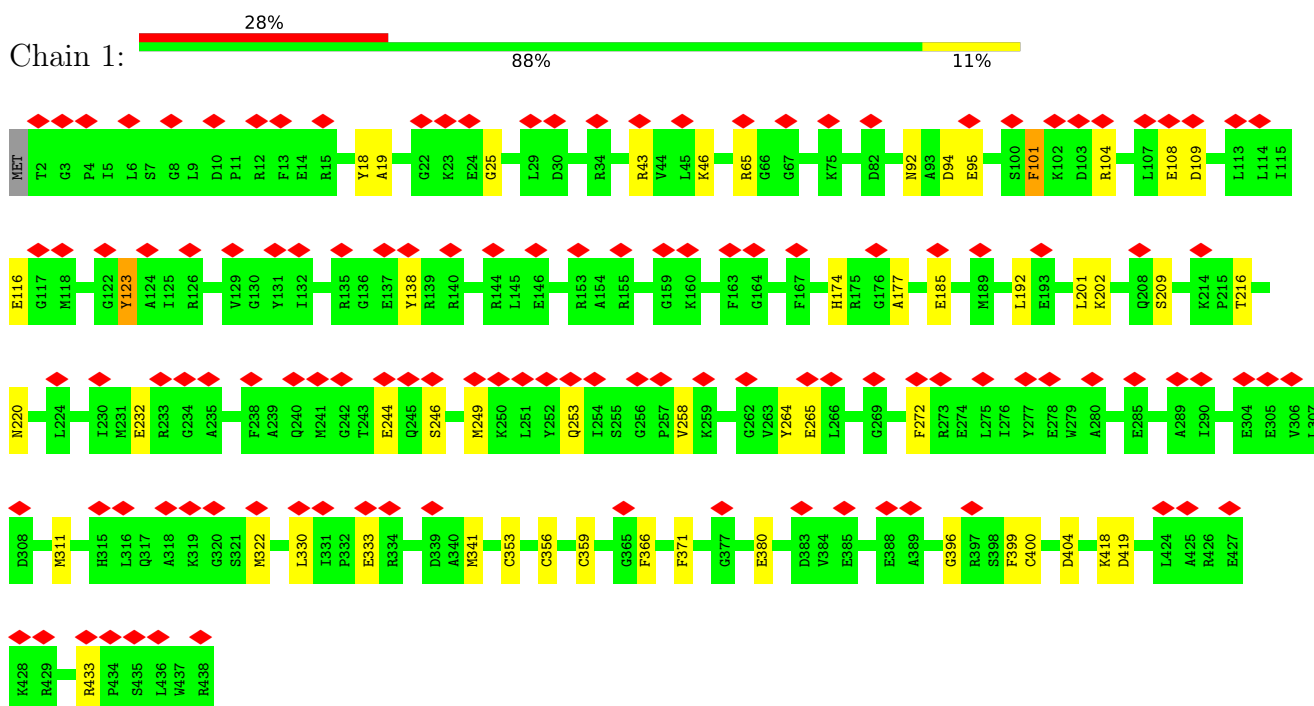


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	2	1	4	2	2	0
18	3	1	4	2	2	0

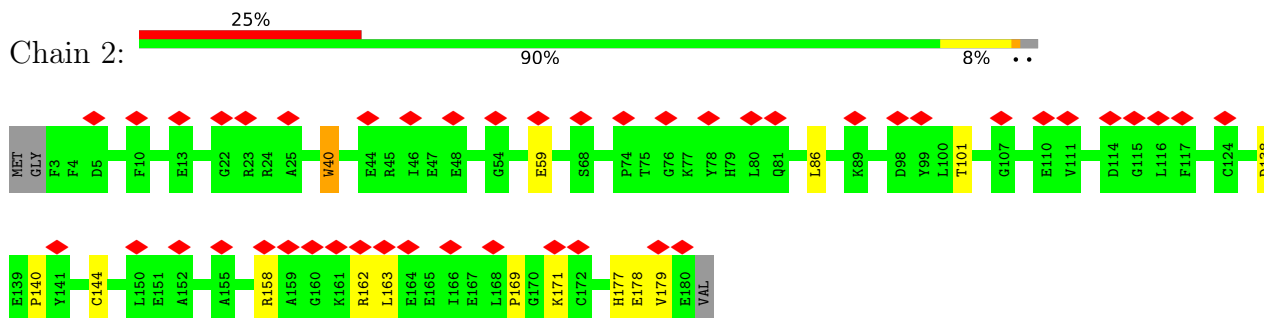
### 3 Residue-property plots

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 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.

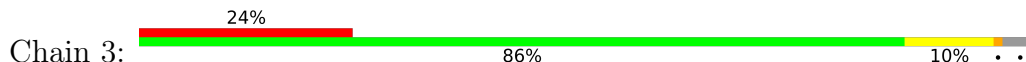
- Molecule 1: NADH-quinone oxidoreductase subunit 1



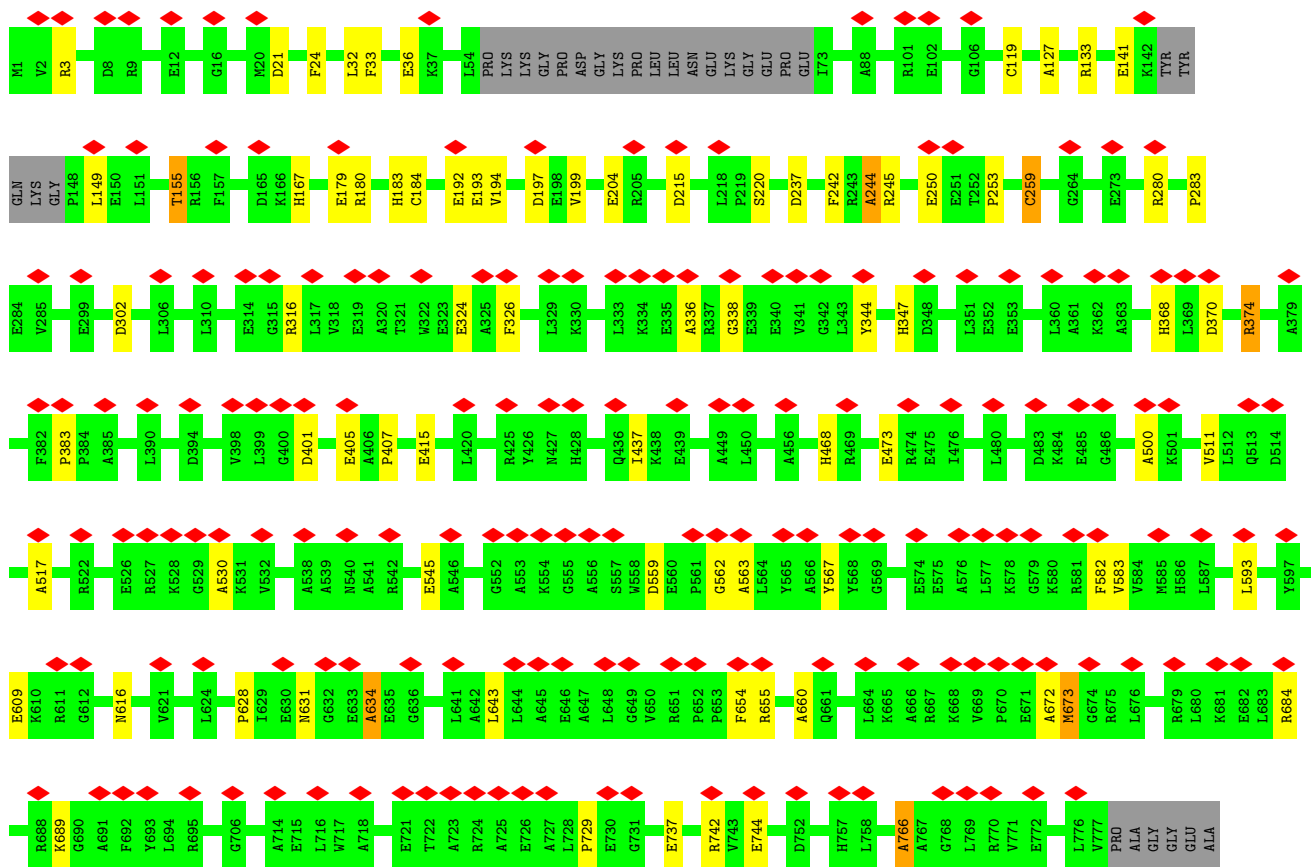
- Molecule 2: NADH-quinone oxidoreductase subunit 2



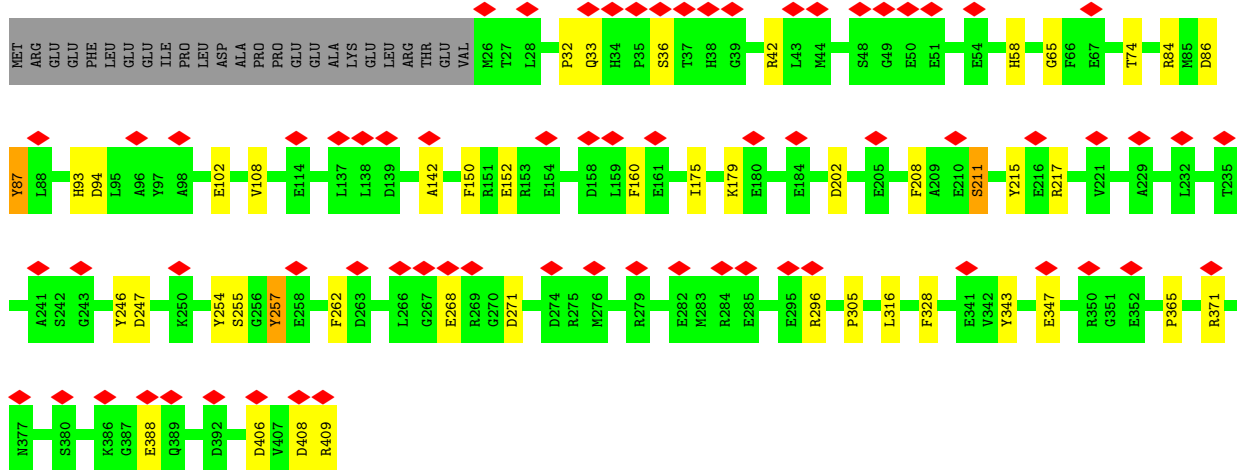
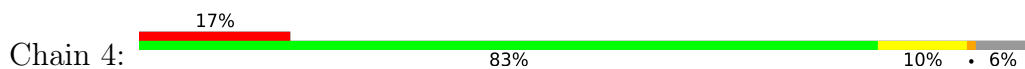
- Molecule 3: NADH-quinone oxidoreductase subunit 3



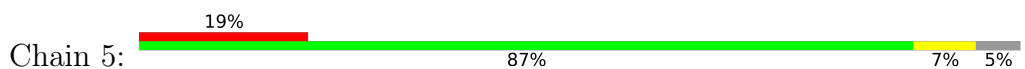


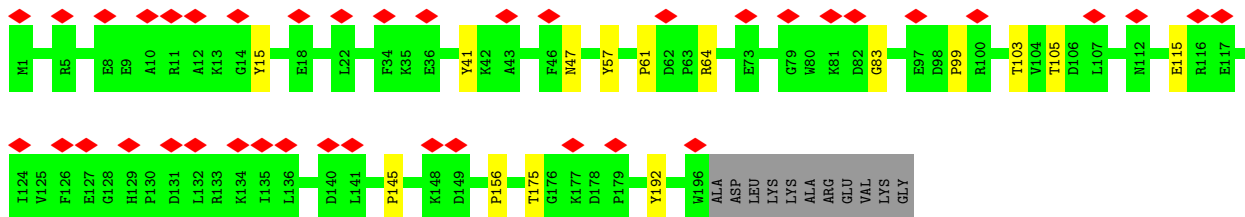


• Molecule 4: NADH-quinone oxidoreductase subunit 4

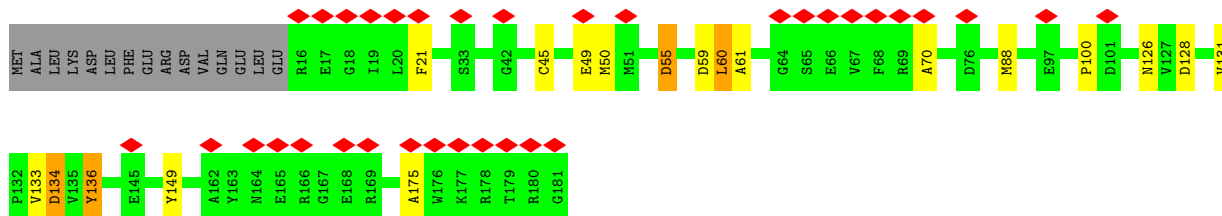
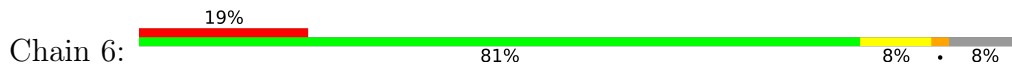


• Molecule 5: NADH-quinone oxidoreductase subunit 5

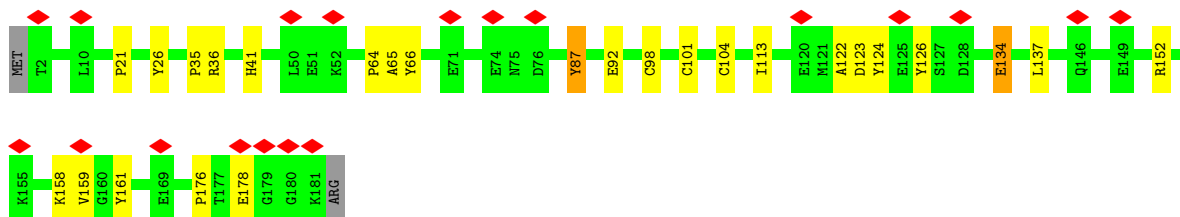
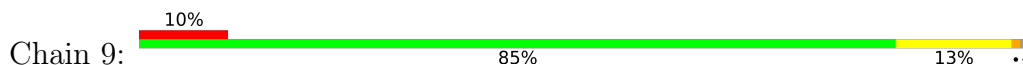




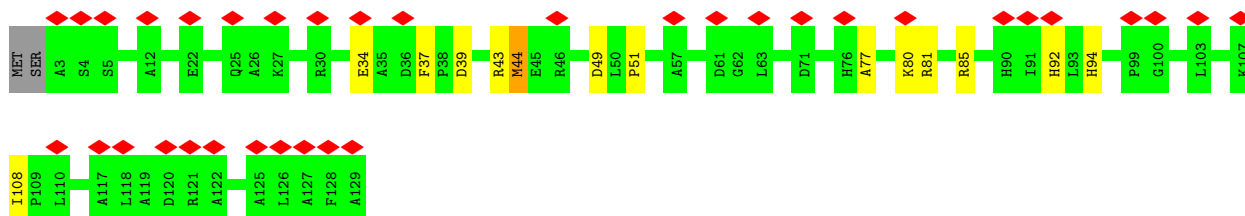
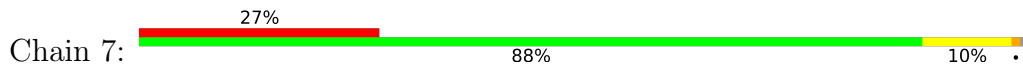
• Molecule 6: NADH-quinone oxidoreductase subunit 6



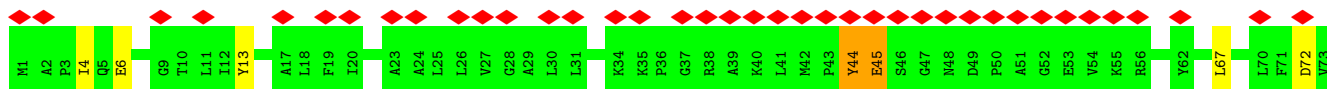
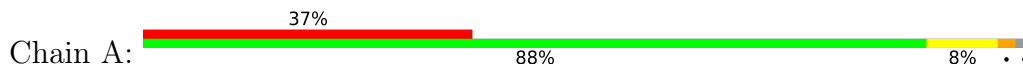
• Molecule 7: NADH-quinone oxidoreductase subunit 9

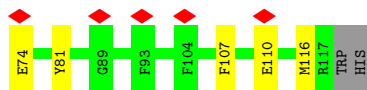


• Molecule 8: NADH-quinone oxidoreductase subunit 15

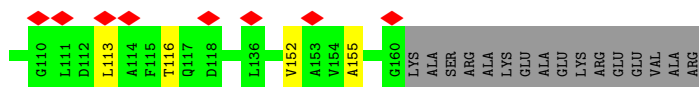
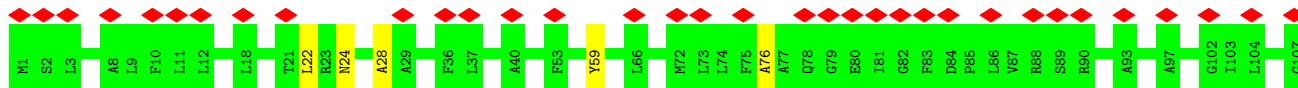
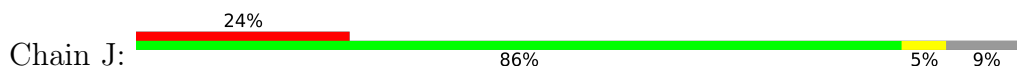


• Molecule 9: NADH-quinone oxidoreductase subunit 7

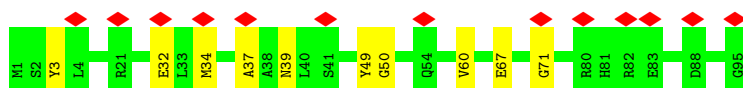
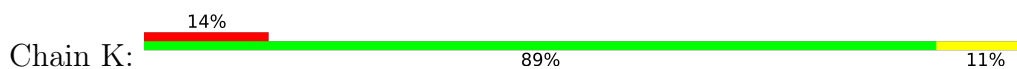




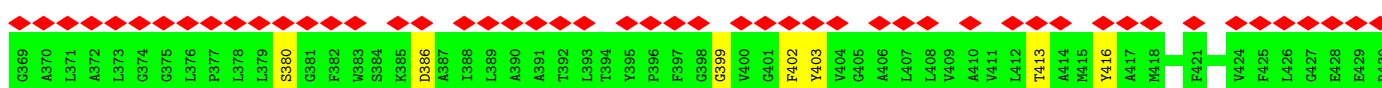
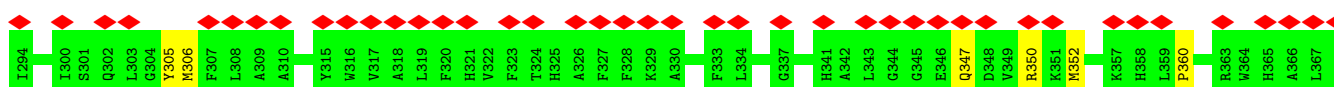
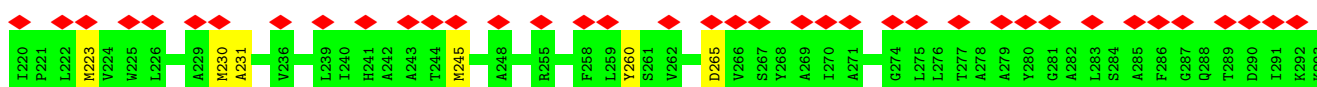
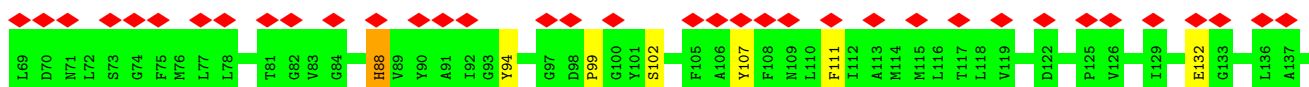
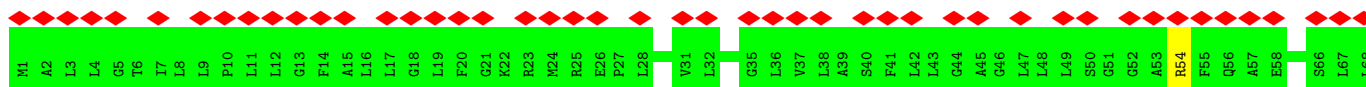
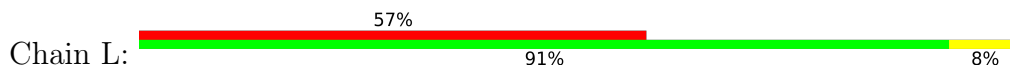
- Molecule 10: NADH-quinone oxidoreductase subunit 10

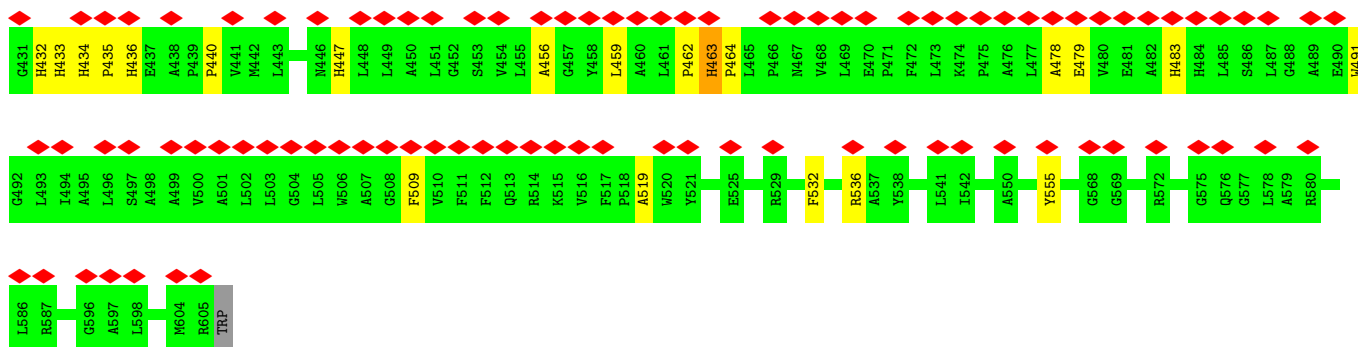


- Molecule 11: NADH-quinone oxidoreductase subunit 11



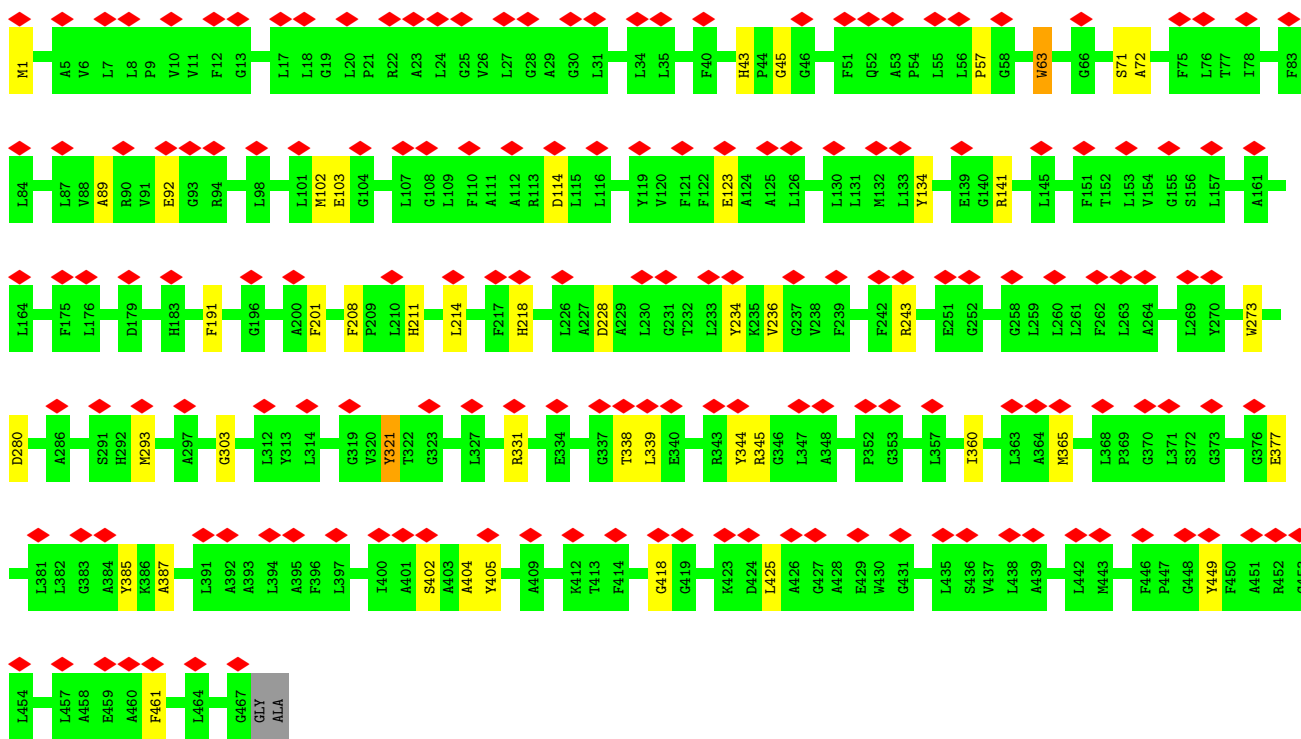
- Molecule 12: NADH-quinone oxidoreductase subunit 12





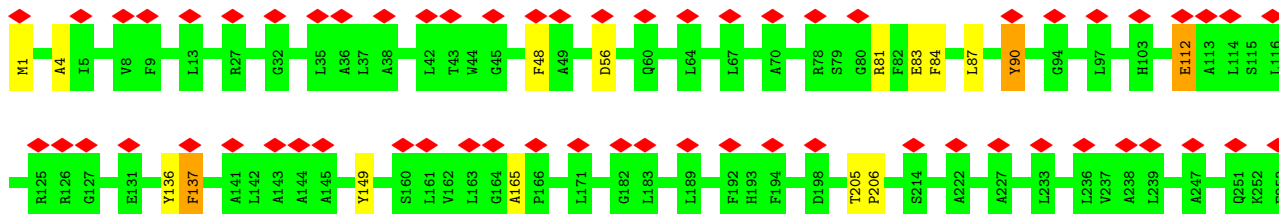
- Molecule 13: NADH-quinone oxidoreductase subunit 13

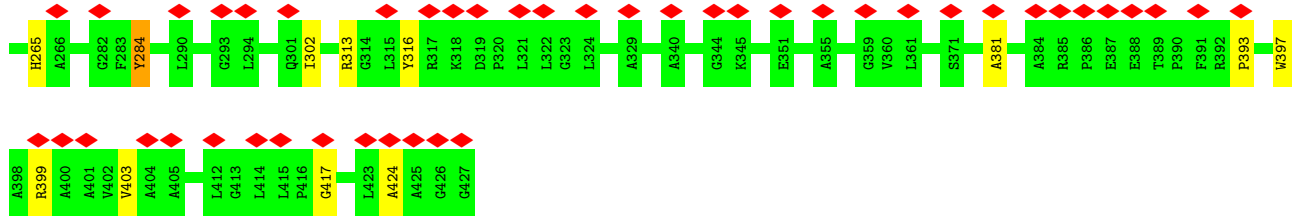
Chain M: 35% 90% 10%



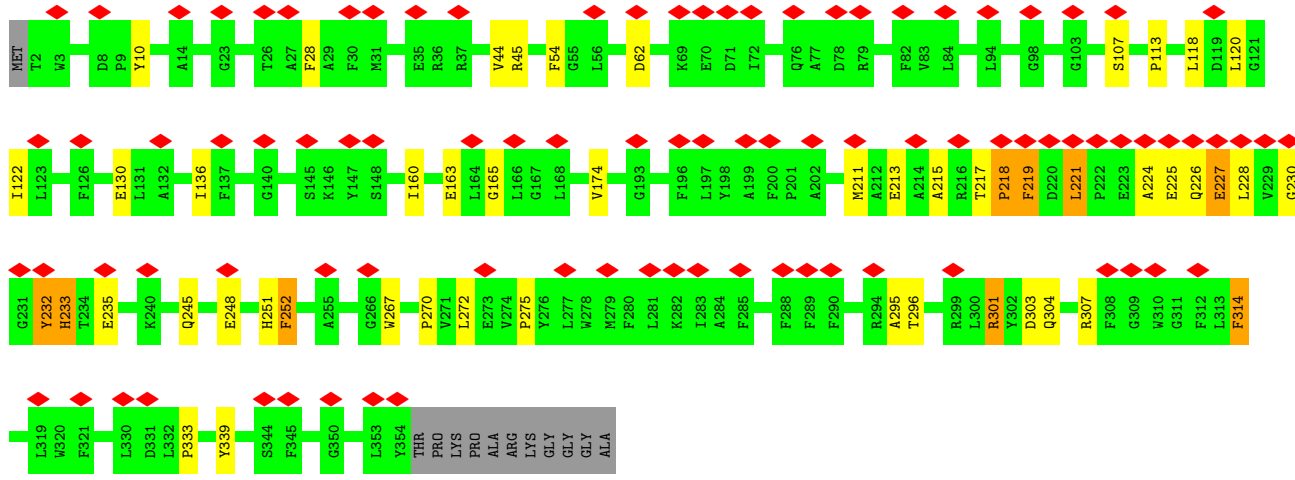
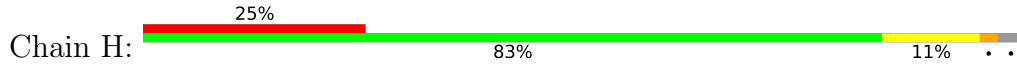
- Molecule 14: NADH-quinone oxidoreductase subunit 14

Chain N: 25% 93% 6%





• Molecule 15: NADH-quinone oxidoreductase subunit 8



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	34	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.713	Depositor
Minimum map value	-0.715	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	880.64, 880.64, 880.64	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.72, 1.72, 1.72	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: SF4, FES, 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	1	1.11	6/3506 (0.2%)	1.16	12/4745 (0.3%)
2	2	1.01	1/1439 (0.1%)	1.12	1/1953 (0.1%)
3	3	1.18	16/6014 (0.3%)	1.22	21/8155 (0.3%)
4	4	1.15	8/3150 (0.3%)	1.22	11/4284 (0.3%)
5	5	1.12	1/1656 (0.1%)	1.16	0/2246
6	6	1.20	4/1319 (0.3%)	1.27	8/1786 (0.4%)
7	9	1.11	1/1423 (0.1%)	1.17	1/1933 (0.1%)
8	7	1.13	1/1059 (0.1%)	1.14	2/1429 (0.1%)
9	A	1.28	5/940 (0.5%)	1.22	4/1280 (0.3%)
10	J	0.92	0/1206	1.08	0/1649
11	K	1.21	2/710 (0.3%)	1.11	0/962
12	L	0.95	2/4741 (0.0%)	1.06	13/6460 (0.2%)
13	M	1.05	6/3591 (0.2%)	1.10	12/4896 (0.2%)
14	N	0.98	1/3238 (0.0%)	1.07	8/4434 (0.2%)
15	H	1.18	9/2935 (0.3%)	1.18	10/4014 (0.2%)
All	All	1.10	63/36927 (0.2%)	1.15	103/50226 (0.2%)

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	1	0	6
2	2	0	1
3	3	0	7
4	4	0	10
5	5	0	4
6	6	0	4
7	9	0	8
9	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	3
12	L	0	8
13	M	0	8
14	N	0	4
15	H	0	11
All	All	0	75

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	227	GLU	CD-OE2	13.03	1.40	1.25
7	9	92	GLU	CD-OE2	12.95	1.39	1.25
9	A	110	GLU	CD-OE2	12.86	1.39	1.25
3	3	415	GLU	CD-OE2	12.81	1.39	1.25
3	3	179	GLU	CD-OE2	12.71	1.39	1.25
14	N	112	GLU	CD-OE2	12.69	1.39	1.25
3	3	192	GLU	CD-OE2	12.68	1.39	1.25
3	3	36	GLU	CD-OE2	12.65	1.39	1.25
15	H	235	GLU	CD-OE2	12.65	1.39	1.25
3	3	609	GLU	CD-OE2	12.63	1.39	1.25
8	7	34	GLU	CD-OE2	12.59	1.39	1.25
4	4	347	GLU	CD-OE2	12.56	1.39	1.25
11	K	67	GLU	CD-OE2	12.52	1.39	1.25
6	6	49	GLU	CD-OE2	12.51	1.39	1.25
9	A	74	GLU	CD-OE2	12.50	1.39	1.25
11	K	32	GLU	CD-OE2	12.50	1.39	1.25
1	1	116	GLU	CD-OE2	12.48	1.39	1.25
13	M	377	GLU	CD-OE2	12.48	1.39	1.25
3	3	473	GLU	CD-OE2	12.46	1.39	1.25
4	4	152	GLU	CD-OE2	12.41	1.39	1.25
12	L	132	GLU	CD-OE2	12.38	1.39	1.25
13	M	92	GLU	CD-OE2	12.37	1.39	1.25
4	4	388	GLU	CD-OE2	12.35	1.39	1.25
9	A	6	GLU	CD-OE2	12.32	1.39	1.25
15	H	130	GLU	CD-OE2	12.28	1.39	1.25
15	H	248	GLU	CD-OE2	12.27	1.39	1.25
15	H	213	GLU	CD-OE2	12.26	1.39	1.25
13	M	103	GLU	CD-OE2	12.19	1.39	1.25
1	1	265	GLU	CD-OE2	12.17	1.39	1.25
1	1	108	GLU	CD-OE2	12.16	1.39	1.25
3	3	545	GLU	CD-OE2	12.11	1.39	1.25
15	H	163	GLU	CD-OE2	12.10	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	250	GLU	CD-OE2	12.07	1.39	1.25
3	3	405	GLU	CD-OE2	12.02	1.38	1.25
4	4	102	GLU	CD-OE2	11.81	1.38	1.25
1	1	95	GLU	CD-OE2	11.81	1.38	1.25
5	5	115	GLU	CD-OE2	11.74	1.38	1.25
3	3	193	GLU	CD-OE2	11.67	1.38	1.25
9	A	45	GLU	CD-OE2	11.51	1.38	1.25
15	H	225	GLU	CD-OE2	11.41	1.38	1.25
2	2	59	GLU	CD-OE2	11.28	1.38	1.25
13	M	123	GLU	CD-OE2	11.21	1.38	1.25
12	L	386	ASP	CG-OD2	6.31	1.39	1.25
4	4	408	ASP	CG-OD2	6.25	1.39	1.25
4	4	94	ASP	CG-OD2	6.20	1.39	1.25
13	M	114	ASP	CG-OD2	6.17	1.39	1.25
15	H	62	ASP	CG-OD2	6.14	1.39	1.25
6	6	55	ASP	CG-OD2	6.05	1.39	1.25
3	3	302	ASP	CG-OD2	6.05	1.39	1.25
4	4	271	ASP	CG-OD2	6.04	1.39	1.25
3	3	237	ASP	CG-OD2	6.03	1.39	1.25
15	H	303	ASP	CG-OD2	6.01	1.39	1.25
9	A	72	ASP	CG-OD2	5.97	1.39	1.25
4	4	406	ASP	CG-OD2	5.94	1.39	1.25
1	1	404	ASP	CG-OD2	5.94	1.39	1.25
3	3	370	ASP	CG-OD2	5.94	1.39	1.25
1	1	94	ASP	CG-OD2	5.92	1.39	1.25
3	3	401	ASP	CG-OD2	5.87	1.38	1.25
3	3	197	ASP	CG-OD2	5.79	1.38	1.25
13	M	228	ASP	CG-OD2	5.77	1.38	1.25
6	6	134	ASP	CG-OD2	5.68	1.38	1.25
3	3	21	ASP	CG-OD2	5.62	1.38	1.25
6	6	59	ASP	CG-OD2	5.52	1.38	1.25

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	13	TYR	CB-CG-CD2	-9.81	115.12	121.00
3	3	237	ASP	CB-CG-OD1	9.24	126.61	118.30
12	L	386	ASP	CB-CG-OD1	9.11	126.50	118.30
9	A	13	TYR	CB-CG-CD1	8.78	126.27	121.00
3	3	302	ASP	CB-CG-OD1	8.76	126.19	118.30
15	H	303	ASP	CB-CG-OD1	8.76	126.18	118.30
6	6	134	ASP	CB-CG-OD1	8.40	125.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	242	PHE	CB-CG-CD2	-8.30	114.99	120.80
3	3	242	PHE	CB-CG-CD1	8.26	126.58	120.80
15	H	303	ASP	CB-CG-OD2	-8.09	111.02	118.30
3	3	237	ASP	CB-CG-OD2	-8.06	111.04	118.30
4	4	406	ASP	CB-CG-OD1	8.01	125.51	118.30
13	M	114	ASP	CB-CG-OD1	7.88	125.39	118.30
3	3	21	ASP	CB-CG-OD1	7.83	125.35	118.30
3	3	370	ASP	CB-CG-OD1	7.75	125.27	118.30
9	A	72	ASP	CB-CG-OD1	7.73	125.26	118.30
6	6	134	ASP	CB-CG-OD2	-7.71	111.36	118.30
15	H	62	ASP	CB-CG-OD1	7.67	125.21	118.30
12	L	107	TYR	CB-CG-CD2	-7.66	116.41	121.00
13	M	228	ASP	CB-CG-OD1	7.66	125.19	118.30
1	1	404	ASP	CB-CG-OD1	7.66	125.19	118.30
4	4	94	ASP	CB-CG-OD1	7.63	125.17	118.30
3	3	197	ASP	CB-CG-OD1	7.53	125.08	118.30
6	6	55	ASP	CB-CG-OD1	7.29	124.86	118.30
4	4	208	PHE	CB-CG-CD1	-7.27	115.71	120.80
4	4	408	ASP	CB-CG-OD1	7.25	124.82	118.30
1	1	138	TYR	CB-CG-CD1	-7.19	116.69	121.00
1	1	94	ASP	CB-CG-OD1	7.18	124.76	118.30
3	3	21	ASP	CB-CG-OD2	-7.15	111.86	118.30
4	4	208	PHE	CB-CG-CD2	7.11	125.78	120.80
13	M	228	ASP	CB-CG-OD2	-6.95	112.05	118.30
3	3	401	ASP	CB-CG-OD1	6.88	124.49	118.30
15	H	252	PHE	CB-CG-CD2	-6.75	116.08	120.80
12	L	386	ASP	CB-CG-OD2	-6.73	112.25	118.30
4	4	406	ASP	CB-CG-OD2	-6.70	112.27	118.30
6	6	59	ASP	CB-CG-OD1	6.70	124.33	118.30
12	L	107	TYR	CB-CG-CD1	6.69	125.01	121.00
15	H	10	TYR	CB-CG-CD1	6.61	124.97	121.00
15	H	10	TYR	CB-CG-CD2	-6.60	117.04	121.00
14	N	90	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	1	366	PHE	CB-CG-CD2	-6.52	116.24	120.80
4	4	257	TYR	CB-CG-CD2	-6.51	117.09	121.00
3	3	302	ASP	CB-CG-OD2	-6.46	112.49	118.30
14	N	84	PHE	CB-CG-CD1	6.41	125.29	120.80
4	4	271	ASP	CB-CG-OD1	6.40	124.06	118.30
13	M	114	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	1	138	TYR	CB-CG-CD2	6.34	124.81	121.00
13	M	191	PHE	CB-CG-CD2	-6.32	116.37	120.80
12	L	402	PHE	CB-CG-CD2	-6.31	116.38	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	72	ASP	CB-CG-OD2	-6.30	112.63	118.30
14	N	136	TYR	CB-CG-CD2	-6.24	117.26	121.00
12	L	555	TYR	CB-CG-CD2	6.23	124.74	121.00
12	L	509	PHE	CB-CG-CD1	-6.19	116.47	120.80
6	6	60	LEU	N-CA-CB	6.12	122.65	110.40
14	N	84	PHE	CB-CG-CD2	-6.01	116.59	120.80
12	L	555	TYR	CB-CG-CD1	-5.97	117.42	121.00
15	H	252	PHE	CB-CG-CD1	5.95	124.96	120.80
15	H	307	ARG	CB-CA-C	-5.91	98.58	110.40
8	7	94	HIS	CB-CA-C	-5.88	98.63	110.40
13	M	134	TYR	CB-CG-CD2	-5.82	117.51	121.00
3	3	401	ASP	CB-CG-OD2	-5.80	113.08	118.30
3	3	197	ASP	CB-CG-OD2	-5.77	113.11	118.30
6	6	55	ASP	CB-CG-OD2	-5.75	113.13	118.30
4	4	262	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	1	366	PHE	CB-CG-CD1	5.72	124.80	120.80
1	1	404	ASP	CB-CG-OD2	-5.71	113.16	118.30
3	3	244	ALA	N-CA-CB	5.66	118.03	110.10
12	L	402	PHE	CB-CG-CD1	5.64	124.75	120.80
14	N	284	TYR	CB-CG-CD2	-5.63	117.62	121.00
13	M	461	PHE	CB-CG-CD1	5.61	124.72	120.80
15	H	62	ASP	CB-CG-OD2	-5.59	113.27	118.30
3	3	370	ASP	CB-CG-OD2	-5.54	113.32	118.30
4	4	94	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	1	94	ASP	CB-CG-OD2	-5.50	113.35	118.30
3	3	24	PHE	CB-CG-CD1	-5.44	116.99	120.80
7	9	87	TYR	CB-CG-CD1	-5.37	117.78	121.00
12	L	509	PHE	CB-CG-CD2	5.37	124.56	120.80
14	N	136	TYR	CB-CG-CD1	5.37	124.22	121.00
12	L	532	PHE	CB-CG-CD1	-5.36	117.05	120.80
13	M	191	PHE	CB-CG-CD1	5.36	124.55	120.80
3	3	634	ALA	N-CA-CB	5.34	117.57	110.10
6	6	59	ASP	CB-CG-OD2	-5.33	113.50	118.30
14	N	265	HIS	CA-CB-CG	-5.29	104.60	113.60
3	3	33	PHE	CB-CA-C	-5.22	99.95	110.40
1	1	322	MET	CG-SD-CE	-5.19	91.90	100.20
1	1	18	TYR	CB-CG-CD1	-5.14	117.91	121.00
1	1	25	GLY	N-CA-C	-5.13	100.27	113.10
13	M	63	TRP	CA-CB-CG	5.13	123.45	113.70
3	3	141	GLU	N-CA-C	-5.12	97.17	111.00
1	1	123	TYR	CB-CG-CD2	-5.10	117.94	121.00
8	7	37	PHE	CB-CA-C	-5.10	100.21	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6	88	MET	CG-SD-CE	-5.09	92.05	100.20
12	L	532	PHE	CB-CG-CD2	5.08	124.36	120.80
13	M	201	PHE	CB-CG-CD2	-5.08	117.24	120.80
14	N	149	TYR	CB-CG-CD1	-5.08	117.95	121.00
13	M	234	TYR	CB-CG-CD2	-5.06	117.96	121.00
13	M	102	MET	CG-SD-CE	-5.04	92.14	100.20
4	4	211	SER	N-CA-CB	5.03	118.05	110.50
2	2	40	TRP	N-CA-CB	5.02	119.64	110.60
3	3	673	MET	N-CA-CB	5.02	119.64	110.60
15	H	120	LEU	N-CA-C	-5.01	97.46	111.00
3	3	766	ALA	N-CA-CB	5.01	117.11	110.10
12	L	459	LEU	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	104	ARG	Sidechain
1	1	123	TYR	Sidechain
1	1	264	TYR	Sidechain
1	1	371	PHE	Sidechain
1	1	396	GLY	Peptide
1	1	433	ARG	Sidechain
2	2	158	ARG	Sidechain
3	3	180	ARG	Sidechain
3	3	183	HIS	Peptide
3	3	215	ASP	Peptide
3	3	245	ARG	Sidechain
3	3	344	TYR	Sidechain
3	3	374	ARG	Sidechain
3	3	567	TYR	Sidechain
4	4	142	ALA	Peptide
4	4	217	ARG	Sidechain
4	4	254	TYR	Sidechain
4	4	257	TYR	Sidechain
4	4	296	ARG	Sidechain
4	4	343	TYR	Sidechain
4	4	36	SER	Peptide
4	4	409	ARG	Sidechain
4	4	84	ARG	Sidechain
4	4	87	TYR	Sidechain
5	5	15	TYR	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
5	5	192	TYR	Sidechain
5	5	41	TYR	Sidechain
5	5	47	ASN	Peptide
6	6	100	PRO	Peptide
6	6	136	TYR	Sidechain
6	6	149	TYR	Sidechain
6	6	55	ASP	Peptide
7	9	124	TYR	Sidechain
7	9	126	TYR	Sidechain
7	9	152	ARG	Sidechain
7	9	161	TYR	Sidechain
7	9	21	PRO	Peptide
7	9	26	TYR	Sidechain
7	9	66	TYR	Sidechain
7	9	87	TYR	Sidechain
9	A	81	TYR	Sidechain
15	H	218	PRO	Peptide
15	H	219	PHE	Peptide
15	H	221	LEU	Peptide
15	H	227	GLU	Peptide
15	H	232	TYR	Sidechain
15	H	295	ALA	Peptide
15	H	301	ARG	Sidechain
15	H	314	PHE	Sidechain
15	H	339	TYR	Sidechain
15	H	45	ARG	Sidechain
15	H	54	PHE	Sidechain
11	K	3	TYR	Sidechain
11	K	49	TYR	Sidechain
11	K	50	GLY	Peptide
12	L	163	ARG	Sidechain
12	L	260	TYR	Sidechain
12	L	403	TYR	Sidechain
12	L	462	PRO	Peptide
12	L	536	ARG	Sidechain
12	L	54	ARG	Sidechain
12	L	88	HIS	Sidechain
12	L	94	TYR	Sidechain
13	M	208	PHE	Sidechain
13	M	243	ARG	Sidechain
13	M	321	TYR	Sidechain
13	M	331	ARG	Sidechain

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Mol	Chain	Res	Type	Group
13	M	344	TYR	Sidechain
13	M	385	TYR	Sidechain
13	M	449	TYR	Sidechain
13	M	71	SER	Peptide
14	N	137	PHE	Sidechain
14	N	316	TYR	Sidechain
14	N	399	ARG	Sidechain
14	N	90	TYR	Sidechain

## 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	1	3417	0	3388	14	0
2	2	1406	0	1373	3	0
3	3	5876	0	5914	9	0
4	4	3067	0	3049	4	0
5	5	1607	0	1574	2	0
6	6	1289	0	1298	2	0
7	9	1388	0	1383	2	0
8	7	1031	0	1029	3	0
9	A	910	0	939	0	0
10	J	1183	0	1286	2	0
11	K	703	0	747	3	0
12	L	4604	0	4734	9	0
13	M	3489	0	3606	7	0
14	N	3154	0	3343	6	0
15	H	2838	0	2903	7	0
16	1	8	0	0	0	0
16	3	24	0	0	1	0
16	6	8	0	0	0	0
16	9	16	0	0	0	0
17	1	31	0	19	11	0
18	2	4	0	0	0	0
18	3	4	0	0	0	0
All	All	36057	0	36585	71	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 1.

All (71) 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)
1:1:92:ASN:OD1	17:1:502:FMN:C2	1.88	1.20
1:1:220:ASN:HB2	17:1:502:FMN:O2P	1.51	1.10
1:1:65:ARG:N	17:1:502:FMN:O1P	1.94	0.98
1:1:92:ASN:OD1	17:1:502:FMN:O2	1.91	0.88
1:1:220:ASN:CB	17:1:502:FMN:O2P	2.26	0.83
1:1:92:ASN:OD1	17:1:502:FMN:N3	2.17	0.77
4:4:42:ARG:HH21	4:4:58:HIS:CD2	2.17	0.62
12:L:380:SER:HB3	12:L:456:ALA:HB3	1.82	0.61
12:L:433:HIS:H	12:L:433:HIS:CD2	2.21	0.58
13:M:425:LEU:HD23	13:M:425:LEU:H	1.70	0.57
13:M:43:HIS:CD2	13:M:45:GLY:H	2.23	0.55
17:1:502:FMN:H2'	17:1:502:FMN:N1	2.21	0.55
13:M:214:LEU:HD11	13:M:218:HIS:CE1	2.41	0.54
2:2:101:THR:HG22	8:7:108:ILE:HD11	1.89	0.54
15:H:219:PHE:C	15:H:221:LEU:H	2.12	0.53
3:3:167:HIS:CD2	3:3:167:HIS:O	2.62	0.53
1:1:356:CYS:SG	1:1:399:PHE:HB3	2.49	0.52
15:H:301:ARG:HE	15:H:304:GLN:HE21	1.56	0.52
8:7:85:ARG:HE	8:7:92:HIS:CE1	2.28	0.52
1:1:101:PHE:H	1:1:253:GLN:HE21	1.57	0.52
3:3:654:PHE:CE2	3:3:660:ALA:HB2	2.45	0.51
12:L:479:GLU:H	12:L:479:GLU:CD	2.14	0.51
1:1:43:ARG:HH22	1:1:232:GLU:HA	1.75	0.51
12:L:380:SER:CB	12:L:456:ALA:HB3	2.41	0.50
1:1:220:ASN:ND2	17:1:502:FMN:O2	2.45	0.49
12:L:413:THR:HA	12:L:416:TYR:CE2	2.49	0.48
6:6:133:VAL:HG12	6:6:134:ASP:N	2.29	0.48
12:L:463:HIS:H	12:L:463:HIS:CD2	2.32	0.48
17:1:502:FMN:O2P	17:1:502:FMN:O4'	2.16	0.47
3:3:259:CYS:HB3	16:3:803:SF4:S3	2.55	0.47
4:4:86:ASP:HB2	4:4:93:HIS:CE1	2.50	0.47
15:H:211:MET:O	15:H:215:ALA:HB3	2.15	0.46
3:3:511:VAL:HG13	3:3:517:ALA:HB1	1.98	0.46
13:M:214:LEU:HD11	13:M:218:HIS:HE1	1.81	0.46
11:K:39:ASN:HD21	11:K:60:VAL:HB	1.81	0.46
5:5:57:TYR:CD1	5:5:64:ARG:HG3	2.51	0.46
7:9:41:HIS:CD2	7:9:113:ILE:HD11	2.51	0.46
17:1:502:FMN:H9	17:1:502:FMN:H1'1	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:71:GLY:HA3	14:N:137:PHE:CZ	2.51	0.45
14:N:313:ARG:HG2	14:N:381:ALA:HB1	1.98	0.45
6:6:133:VAL:HG11	6:6:136:TYR:CE1	2.52	0.45
8:7:108:ILE:H	8:7:108:ILE:HD12	1.81	0.44
10:J:155:ALA:HB2	14:N:83:GLU:HG2	1.99	0.44
15:H:224:ALA:HA	15:H:230:GLY:H	1.81	0.44
3:3:468:HIS:CD2	3:3:468:HIS:H	2.35	0.44
3:3:326:PHE:CE1	3:3:643:LEU:HD22	2.53	0.43
3:3:253:PRO:HB3	3:3:280:ARG:HH11	1.83	0.43
4:4:42:ARG:HH21	4:4:58:HIS:CG	2.35	0.43
14:N:1:MET:HB2	14:N:4:ALA:H	1.83	0.43
12:L:432:HIS:HD2	12:L:434:HIS:CE1	2.37	0.43
13:M:338:THR:HG22	13:M:339:LEU:H	1.84	0.42
1:1:185:GLU:HB3	17:1:502:FMN:O2'	2.19	0.42
1:1:258:VAL:HB	1:1:330:LEU:HD12	2.02	0.42
5:5:103:THR:HB	5:5:105:THR:H	1.85	0.42
15:H:296:THR:HG22	15:H:296:THR:O	2.19	0.42
1:1:272:PHE:CZ	1:1:311:MET:HG2	2.54	0.42
10:J:152:VAL:HG22	14:N:87:LEU:HD22	2.01	0.42
3:3:119:CYS:HB3	4:4:328:PHE:CD1	2.55	0.42
1:1:174:HIS:CD2	1:1:192:LEU:HD22	2.55	0.41
12:L:464:PRO:HG2	12:L:491:TRP:CZ2	2.55	0.41
11:K:34:MET:O	11:K:37:ALA:HB3	2.21	0.41
14:N:205:THR:HB	14:N:206:PRO:HD3	2.03	0.41
15:H:122:ILE:HD13	15:H:174:VAL:HG21	2.02	0.41
15:H:165:GLY:HA3	15:H:314:PHE:CE1	2.55	0.41
7:9:134:GLU:CD	7:9:134:GLU:H	2.23	0.41
3:3:368:HIS:CE1	3:3:563:ALA:HB2	2.56	0.41
2:2:177:HIS:CG	2:2:178:GLU:H	2.39	0.41
13:M:402:SER:HA	13:M:405:TYR:CE2	2.55	0.41
2:2:171:LYS:O	2:2:177:HIS:CE1	2.73	0.41
12:L:88:HIS:O	12:L:88:HIS:CD2	2.73	0.41
13:M:321:TYR:CE1	13:M:365:MET:HA	2.56	0.40

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	435/438 (99%)	377 (87%)	50 (12%)	8 (2%)	8	42
2	2	176/181 (97%)	154 (88%)	14 (8%)	8 (4%)	2	24
3	3	748/783 (96%)	640 (86%)	81 (11%)	27 (4%)	3	28
4	4	382/409 (93%)	328 (86%)	42 (11%)	12 (3%)	4	31
5	5	194/207 (94%)	173 (89%)	16 (8%)	5 (3%)	5	35
6	6	164/181 (91%)	140 (85%)	17 (10%)	7 (4%)	2	25
7	9	178/182 (98%)	152 (85%)	17 (10%)	9 (5%)	2	22
8	7	125/129 (97%)	112 (90%)	8 (6%)	5 (4%)	3	26
9	A	115/119 (97%)	102 (89%)	11 (10%)	2 (2%)	9	43
10	J	158/176 (90%)	138 (87%)	15 (10%)	5 (3%)	4	30
11	K	93/95 (98%)	82 (88%)	11 (12%)	0	100	100
12	L	603/606 (100%)	547 (91%)	42 (7%)	14 (2%)	6	37
13	M	465/469 (99%)	412 (89%)	44 (10%)	9 (2%)	8	41
14	N	425/427 (100%)	380 (89%)	39 (9%)	6 (1%)	11	47
15	H	351/365 (96%)	302 (86%)	34 (10%)	15 (4%)	2	25
All	All	4612/4767 (97%)	4039 (88%)	441 (10%)	132 (3%)	7	32

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	19	ALA
1	1	177	ALA
2	2	138	ASP
2	2	179	VAL
3	3	149	LEU
3	3	220	SER
3	3	244	ALA
3	3	336	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	3	374	ARG
3	3	616	ASN
3	3	628	PRO
3	3	655	ARG
3	3	673	MET
3	3	766	ALA
4	4	316	LEU
6	6	21	PHE
6	6	60	LEU
6	6	61	ALA
6	6	70	ALA
6	6	175	ALA
7	9	64	PRO
7	9	98	CYS
9	A	45	GLU
12	L	435	PRO
12	L	436	HIS
13	M	72	ALA
14	N	165	ALA
15	H	217	THR
15	H	218	PRO
2	2	162	ARG
3	3	500	ALA
3	3	689	LYS
3	3	729	PRO
4	4	108	VAL
4	4	211	SER
4	4	255	SER
5	5	83	GLY
5	5	99	PRO
6	6	128	ASP
7	9	36	ARG
7	9	65	ALA
7	9	122	ALA
7	9	137	LEU
7	9	176	PRO
10	J	22	LEU
10	J	76	ALA
12	L	99	PRO
13	M	89	ALA
15	H	233	HIS
15	H	267	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	209	SER
1	1	246	SER
2	2	40	TRP
2	2	86	LEU
2	2	140	PRO
3	3	155	THR
3	3	283	PRO
3	3	530	ALA
3	3	634	ALA
4	4	74	THR
4	4	175	ILE
4	4	305	PRO
6	6	126	ASN
8	7	44	MET
8	7	77	ALA
9	A	44	TYR
10	J	116	THR
12	L	231	ALA
12	L	399	GLY
12	L	478	ALA
12	L	519	ALA
13	M	303	GLY
13	M	418	GLY
15	H	118	LEU
15	H	272	LEU
15	H	275	PRO
1	1	101	PHE
1	1	201	LEU
2	2	144	CYS
3	3	32	LEU
3	3	562	GLY
3	3	593	LEU
4	4	33	GLN
5	5	61	PRO
7	9	35	PRO
7	9	178	GLU
8	7	39	ASP
8	7	80	LYS
10	J	24	ASN
12	L	245	MET
12	L	347	GLN
12	L	350	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	M	387	ALA
13	M	404	ALA
14	N	393	PRO
14	N	417	GLY
14	N	424	ALA
15	H	113	PRO
15	H	333	PRO
3	3	127	ALA
3	3	194	VAL
3	3	204	GLU
3	3	407	PRO
3	3	672	ALA
4	4	65	GLY
4	4	246	TYR
4	4	365	PRO
12	L	102	SER
12	L	440	PRO
14	N	397	TRP
15	H	107	SER
15	H	226	GLN
15	H	232	TYR
15	H	270	PRO
1	1	418	LYS
5	5	145	PRO
5	5	175	THR
10	J	28	ALA
12	L	360	PRO
14	N	302	ILE
15	H	44	VAL
3	3	199	VAL
13	M	57	PRO
1	1	202	LYS
2	2	169	PRO
3	3	338	GLY
4	4	32	PRO
13	M	236	VAL
12	L	185	ILE
13	M	360	ILE
15	H	136	ILE
8	7	51	PRO

### 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	1	355/356 (100%)	343 (97%)	12 (3%)	37	61
2	2	150/152 (99%)	149 (99%)	1 (1%)	84	90
3	3	607/628 (97%)	589 (97%)	18 (3%)	41	64
4	4	332/355 (94%)	323 (97%)	9 (3%)	44	66
5	5	167/175 (95%)	166 (99%)	1 (1%)	86	92
6	6	135/149 (91%)	132 (98%)	3 (2%)	52	71
7	9	148/150 (99%)	142 (96%)	6 (4%)	30	56
8	7	104/106 (98%)	100 (96%)	4 (4%)	33	58
9	A	90/92 (98%)	85 (94%)	5 (6%)	21	48
10	J	118/130 (91%)	116 (98%)	2 (2%)	60	78
11	K	71/71 (100%)	71 (100%)	0	100	100
12	L	453/454 (100%)	442 (98%)	11 (2%)	49	69
13	M	332/332 (100%)	324 (98%)	8 (2%)	49	69
14	N	302/302 (100%)	296 (98%)	6 (2%)	55	73
15	H	293/300 (98%)	286 (98%)	7 (2%)	49	69
All	All	3657/3752 (98%)	3564 (98%)	93 (2%)	50	68

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	46	LYS
1	1	109	ASP
1	1	216	THR
1	1	244	GLU
1	1	249	MET
1	1	333	GLU
1	1	341	MET
1	1	353	CYS
1	1	359	CYS
1	1	380	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	400	CYS
1	1	419	ASP
2	2	163	LEU
3	3	3	ARG
3	3	133	ARG
3	3	155	THR
3	3	184	CYS
3	3	259	CYS
3	3	316	ARG
3	3	324	GLU
3	3	347	HIS
3	3	383	PRO
3	3	437	ILE
3	3	559	ASP
3	3	582	PHE
3	3	583	VAL
3	3	631	ASN
3	3	684	ARG
3	3	737	GLU
3	3	742	ARG
3	3	744	GLU
4	4	87	TYR
4	4	150	PHE
4	4	160	PHE
4	4	179	LYS
4	4	202	ASP
4	4	215	TYR
4	4	247	ASP
4	4	268	GLU
4	4	371	ARG
5	5	156	PRO
6	6	45	CYS
6	6	50	MET
6	6	131	VAL
7	9	101	CYS
7	9	104	CYS
7	9	123	ASP
7	9	134	GLU
7	9	158	LYS
7	9	159	VAL
8	7	43	ARG
8	7	44	MET

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Mol	Chain	Res	Type
8	7	49	ASP
8	7	81	ARG
9	A	4	ILE
9	A	44	TYR
9	A	67	LEU
9	A	107	PHE
9	A	116	MET
10	J	59	TYR
10	J	113	LEU
12	L	111	PHE
12	L	173	MET
12	L	223	MET
12	L	230	MET
12	L	265	ASP
12	L	305	TYR
12	L	306	MET
12	L	352	MET
12	L	447	HIS
12	L	463	HIS
12	L	483	HIS
13	M	1	MET
13	M	63	TRP
13	M	141	ARG
13	M	211	HIS
13	M	273	TRP
13	M	280	ASP
13	M	293	MET
13	M	345	ARG
14	N	48	PHE
14	N	56	ASP
14	N	81	ARG
14	N	112	GLU
14	N	284	TYR
14	N	403	VAL
15	H	28	PHE
15	H	160	ILE
15	H	228	LEU
15	H	233	HIS
15	H	245	GLN
15	H	251	HIS
15	H	252	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46)

such sidechains are listed below:

Mol	Chain	Res	Type
1	1	174	HIS
1	1	208	GLN
1	1	219	ASN
1	1	315	HIS
1	1	343	ASN
2	2	120	GLN
2	2	174	HIS
3	3	25	HIS
3	3	38	HIS
3	3	163	HIS
3	3	167	HIS
3	3	298	HIS
3	3	347	HIS
3	3	368	HIS
3	3	372	GLN
3	3	465	HIS
3	3	468	HIS
3	3	661	GLN
4	4	58	HIS
4	4	63	HIS
4	4	93	HIS
4	4	315	HIS
4	4	379	GLN
5	5	20	ASN
6	6	34	ASN
6	6	58	ASN
7	9	41	HIS
8	7	92	HIS
11	K	36	ASN
11	K	39	ASN
12	L	150	GLN
12	L	321	HIS
12	L	432	HIS
12	L	433	HIS
12	L	434	HIS
12	L	463	HIS
12	L	483	HIS
13	M	43	HIS
13	M	183	HIS
13	M	211	HIS
13	M	218	HIS
13	M	292	HIS

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Mol	Chain	Res	Type
14	N	193	HIS
14	N	245	ASN
15	H	192	HIS
15	H	304	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	SF4	3	801	3	0,12,12	-	-	-		
17	FMN	1	502	-	33,33,33	1.44	4 (12%)	48,50,50	1.21	6 (12%)
16	SF4	6	201	6	0,12,12	-	-	-		
16	SF4	9	201	7	0,12,12	-	-	-		
16	SF4	9	202	7	0,12,12	-	-	-		
16	SF4	1	501	1	0,12,12	-	-	-		
18	FES	2	201	2	0,4,4	-	-	-		
18	FES	3	804	3	0,4,4	-	-	-		
16	SF4	3	802	3	0,12,12	-	-	-		
16	SF4	3	803	3	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
16	SF4	3	801	3	-	-	0/6/5/5
17	FMN	1	502	-	-	7/18/18/18	0/3/3/3
16	SF4	6	201	6	-	-	0/6/5/5
16	SF4	9	201	7	-	-	0/6/5/5
16	SF4	9	202	7	-	-	0/6/5/5
16	SF4	1	501	1	-	-	0/6/5/5
18	FES	2	201	2	-	-	0/1/1/1
18	FES	3	804	3	-	-	0/1/1/1
16	SF4	3	802	3	-	-	0/6/5/5
16	SF4	3	803	3	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	502	FMN	C9A-C5A	5.04	1.49	1.41
17	1	502	FMN	C8-C7	3.34	1.49	1.40
17	1	502	FMN	C4A-N5	2.54	1.35	1.30
17	1	502	FMN	C4-N3	-2.46	1.34	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	502	FMN	C4-C4A-N5	2.73	122.12	118.23
17	1	502	FMN	C4A-C10-N1	-2.66	118.57	124.73
17	1	502	FMN	C10-N1-C2	2.27	121.43	116.90
17	1	502	FMN	O4-C4-C4A	-2.20	120.78	126.60
17	1	502	FMN	C4A-C4-N3	2.06	118.43	113.19
17	1	502	FMN	C4A-C10-N10	2.04	119.47	116.48

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	502	FMN	C5'-O5'-P-O3P
17	1	502	FMN	C4'-C5'-O5'-P
17	1	502	FMN	C2'-C1'-N10-C10
17	1	502	FMN	C5'-O5'-P-O2P

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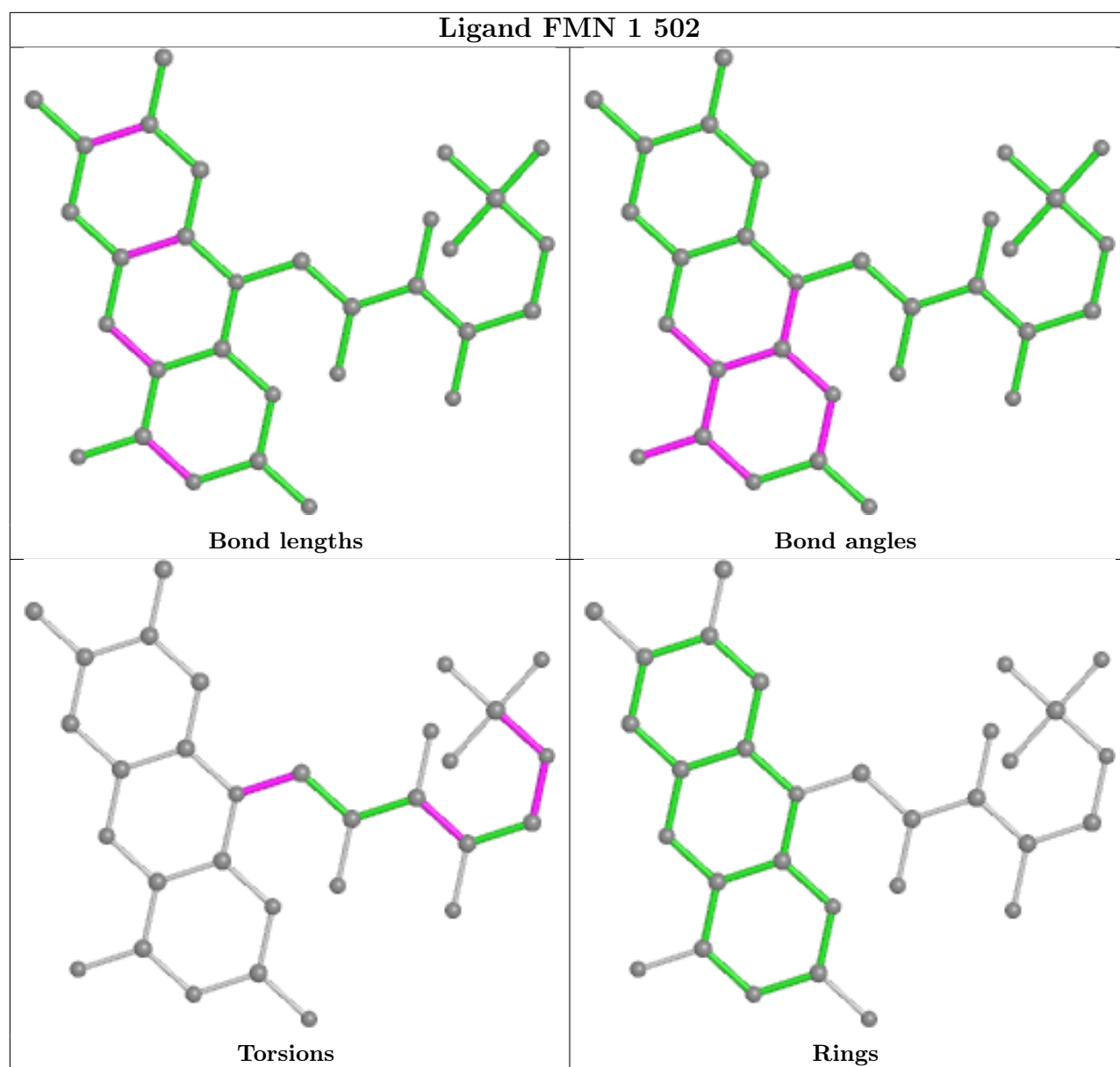
Mol	Chain	Res	Type	Atoms
17	1	502	FMN	C5'-O5'-P-O1P
17	1	502	FMN	C2'-C3'-C4'-O4'
17	1	502	FMN	O3'-C3'-C4'-C5'

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	1	502	FMN	11	0
16	3	803	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 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.

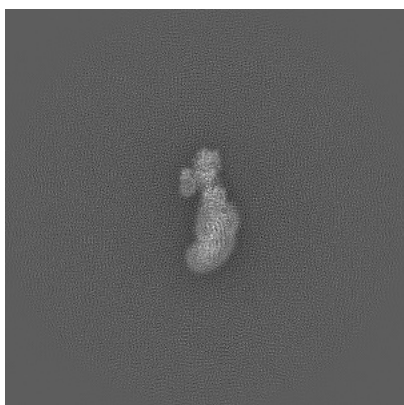
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11235. These allow visual inspection of the internal detail of the map and identification of artifacts.

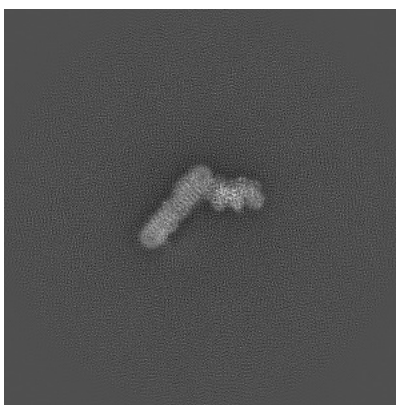
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

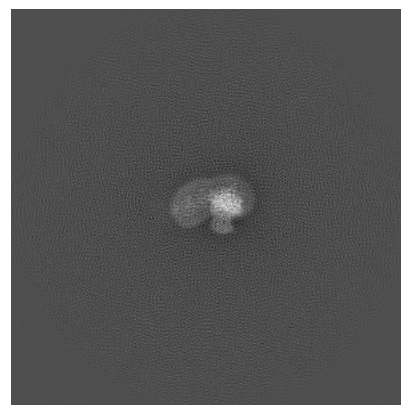
#### 6.1.1 Primary map



X



Y

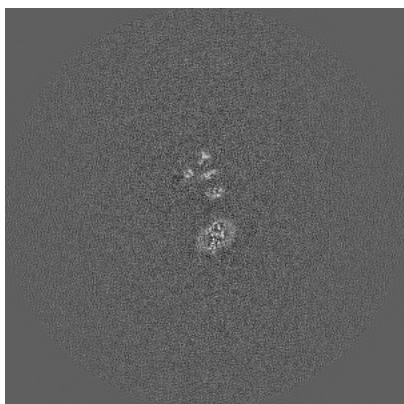


Z

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

### 6.2 Central slices [i](#)

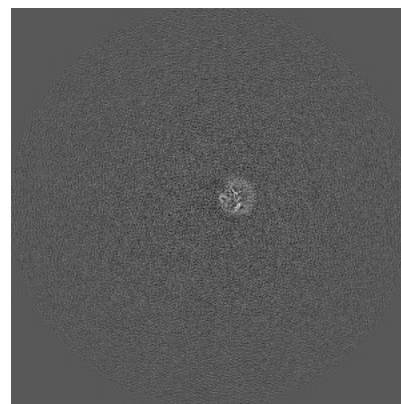
#### 6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

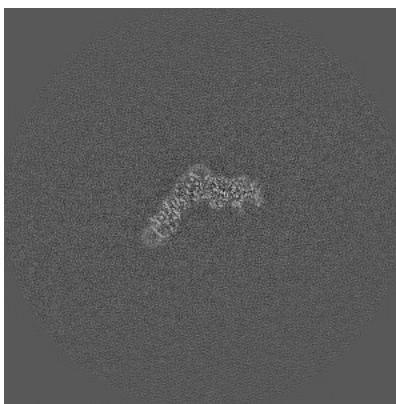
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

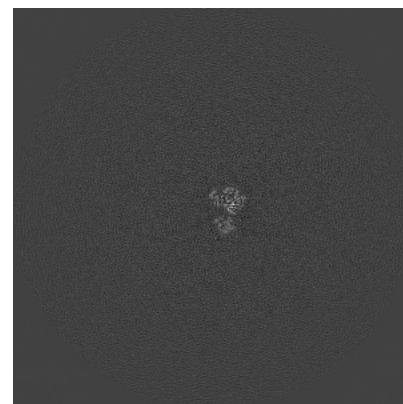
### 6.3.1 Primary map



X Index: 278



Y Index: 264



Z Index: 279

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

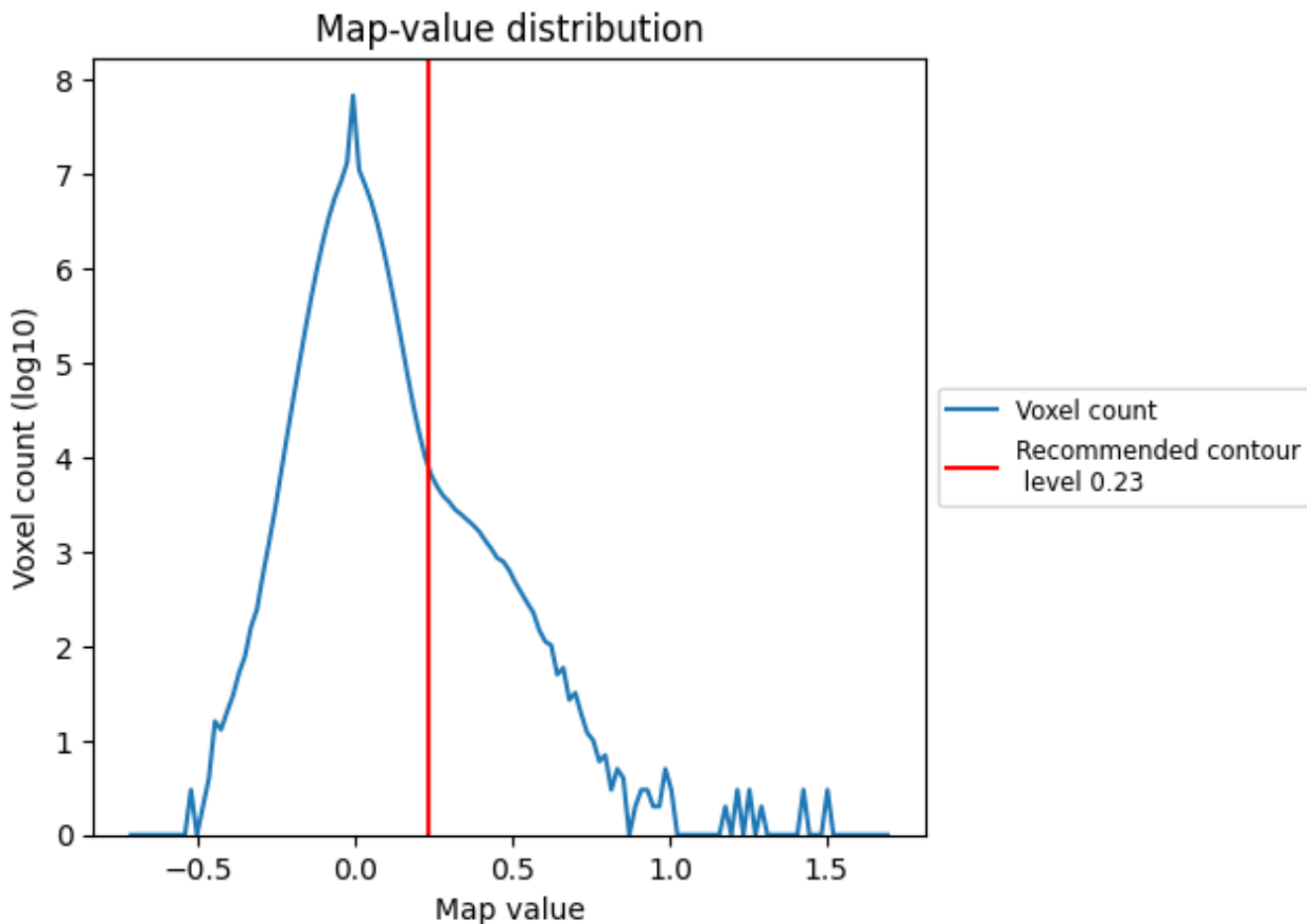
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

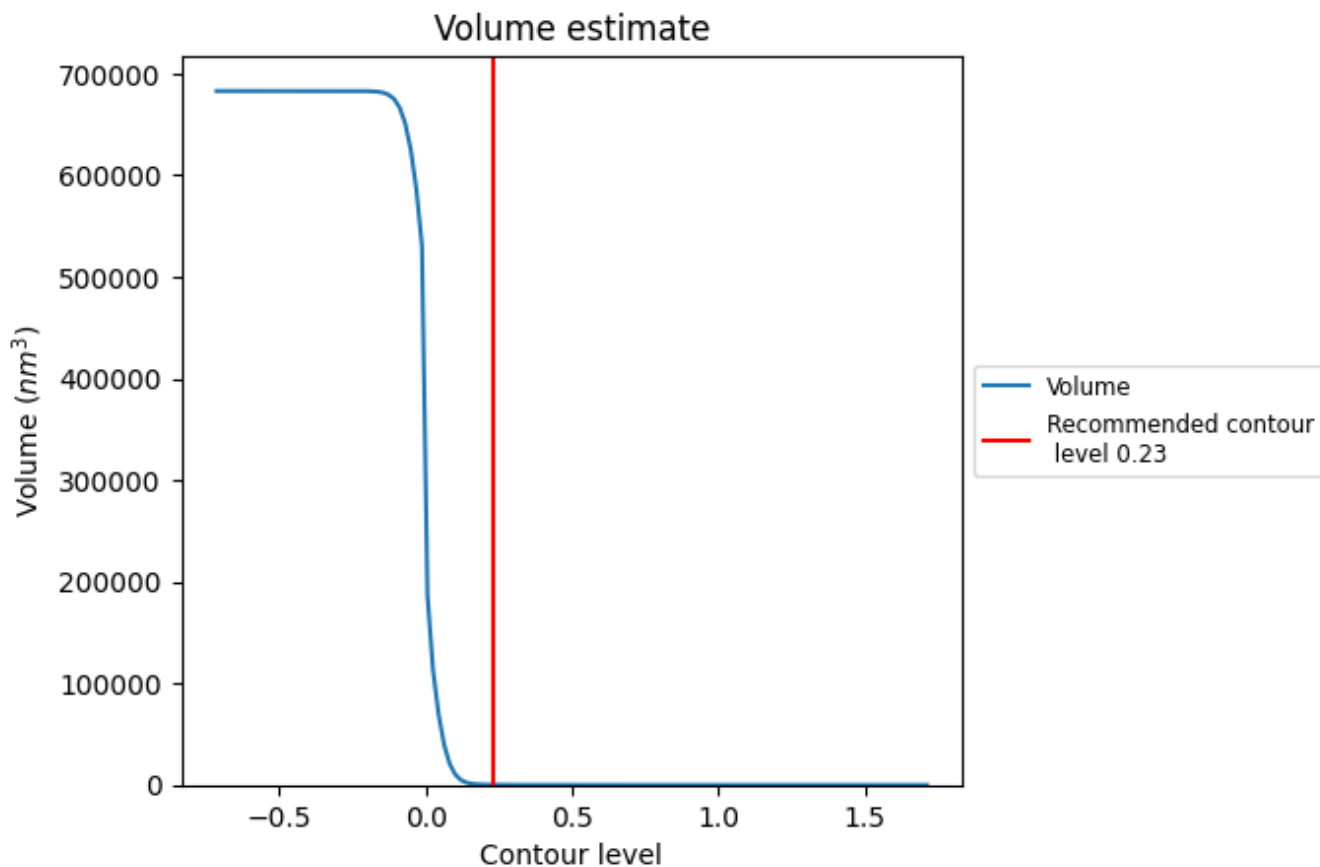
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



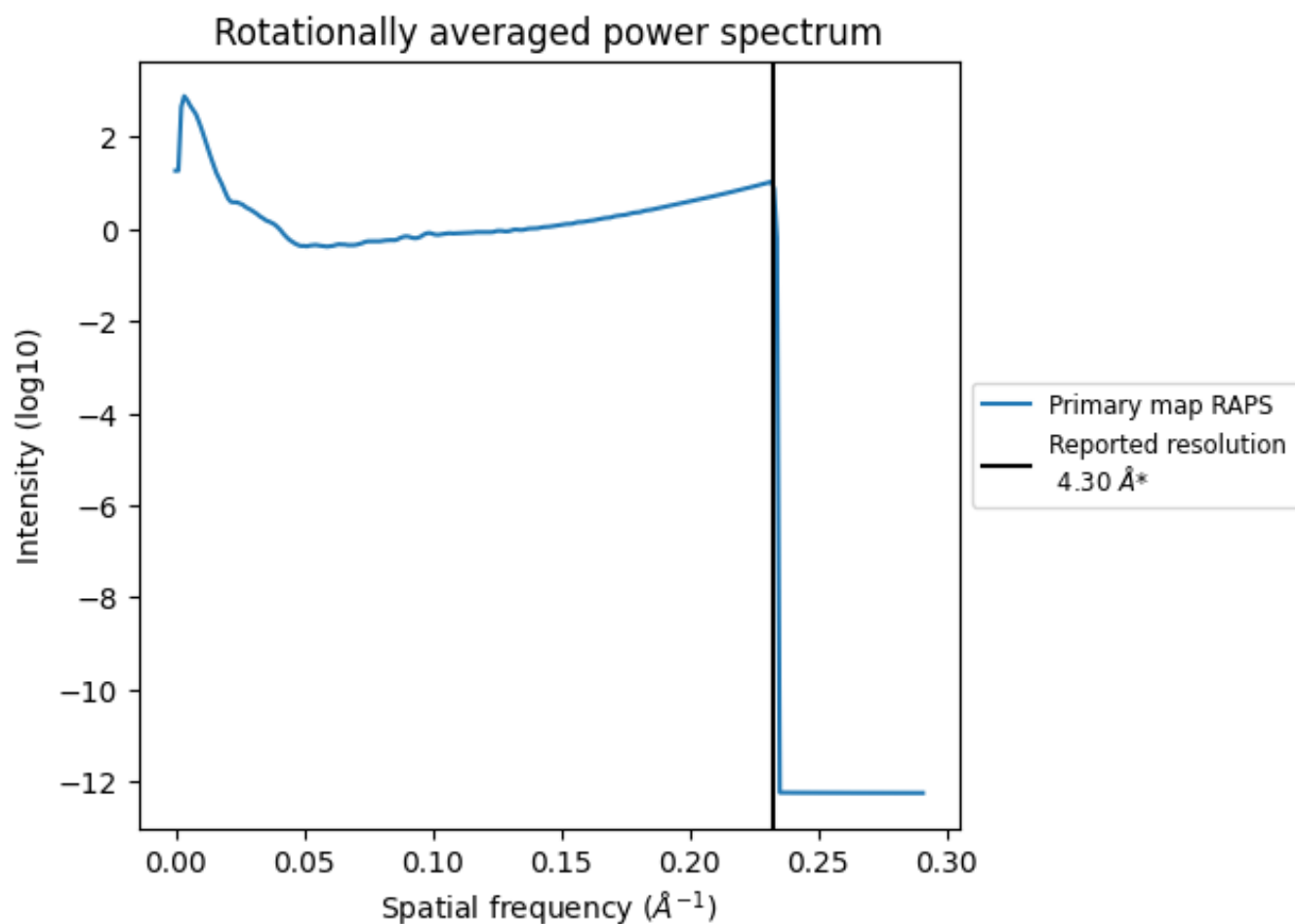
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 216  $\text{nm}^3$ ; this corresponds to an approximate mass of 195 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 [\(i\)](#)

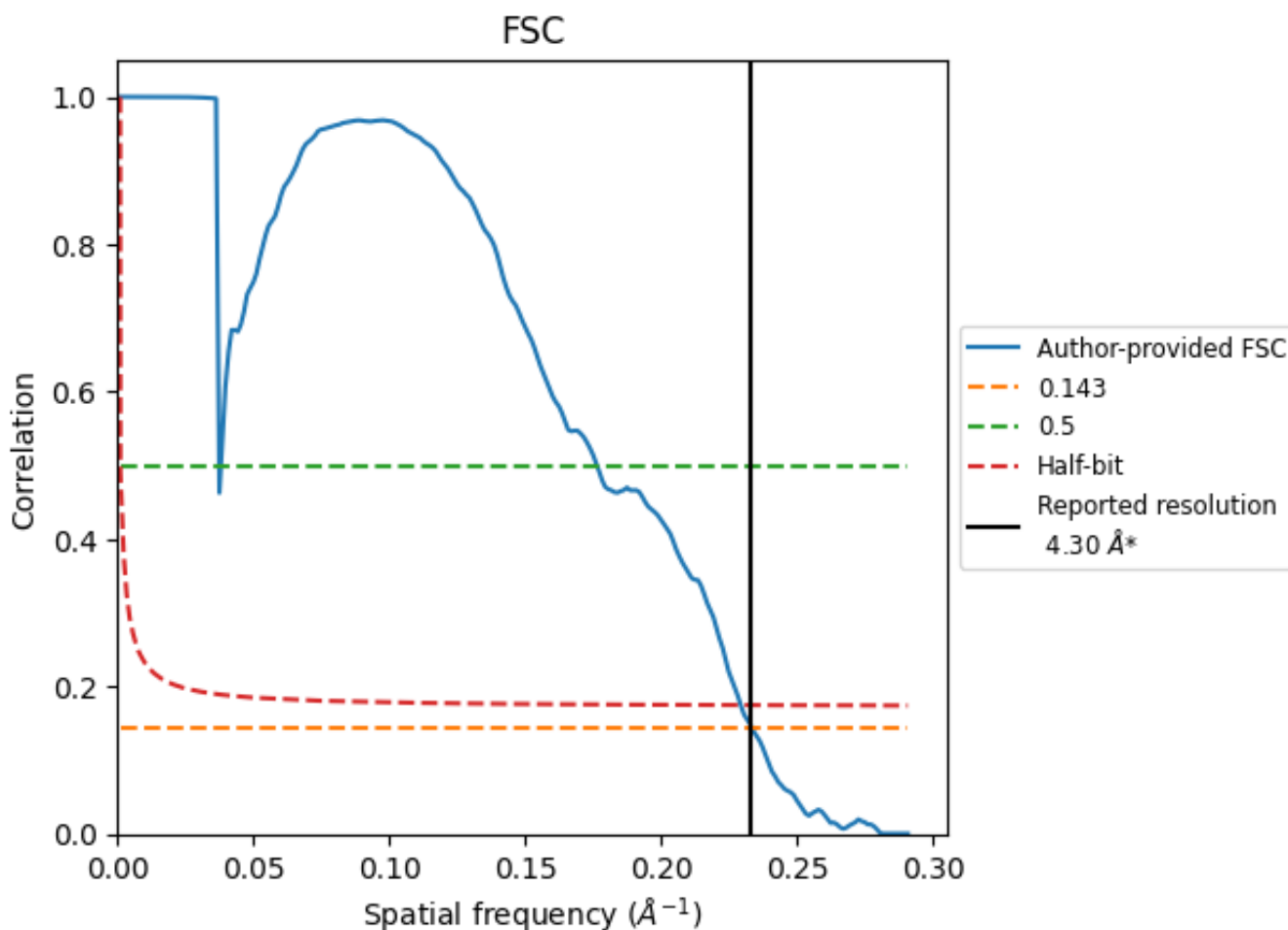


\*Reported resolution corresponds to spatial frequency of  $0.233 \text{\AA}^{-1}$

## 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 0.233 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

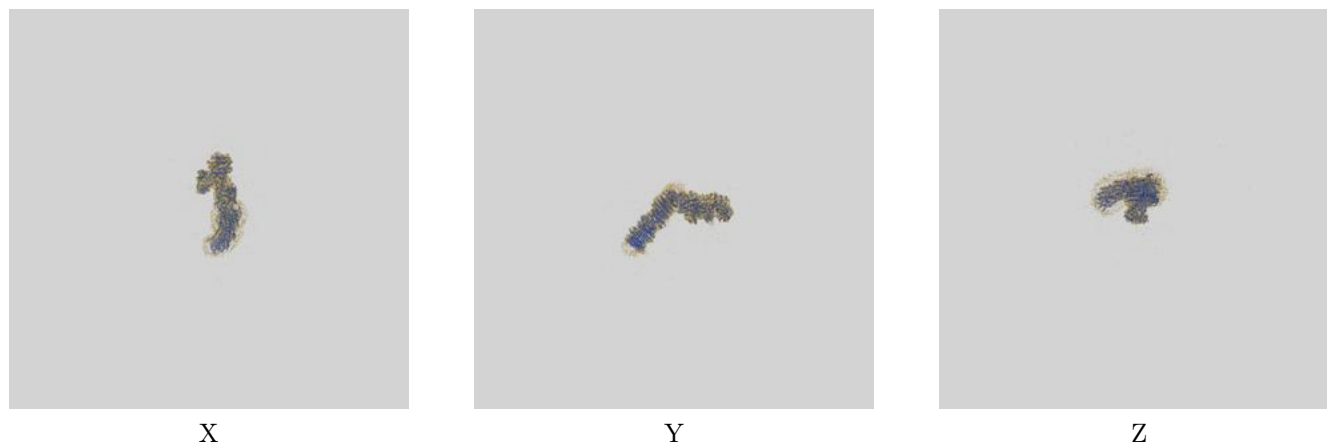
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.28	26.74	4.36
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

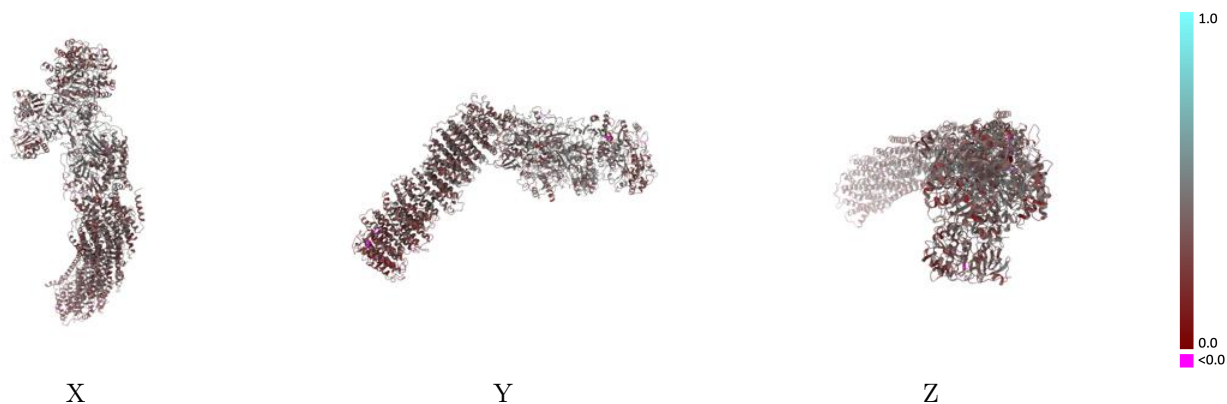
This section contains information regarding the fit between EMDB map EMD-11235 and PDB model 6ZJL. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



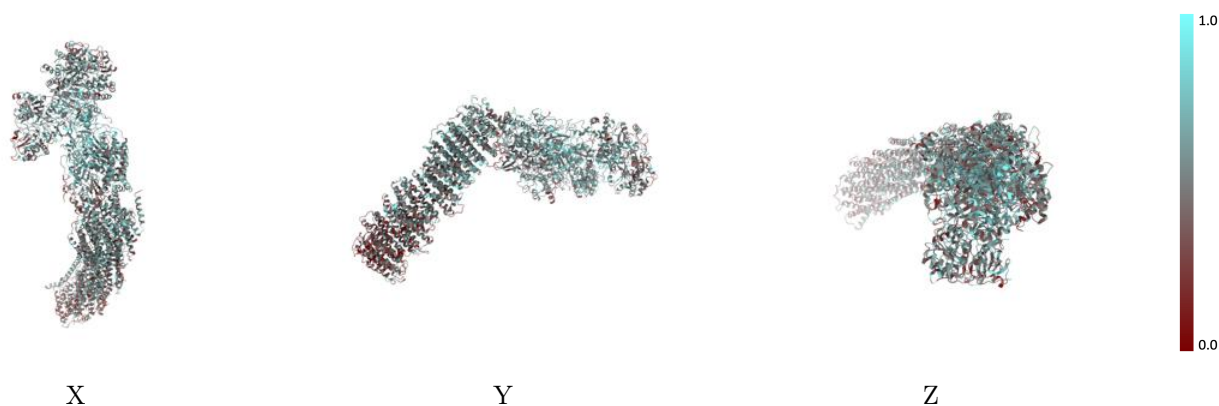
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



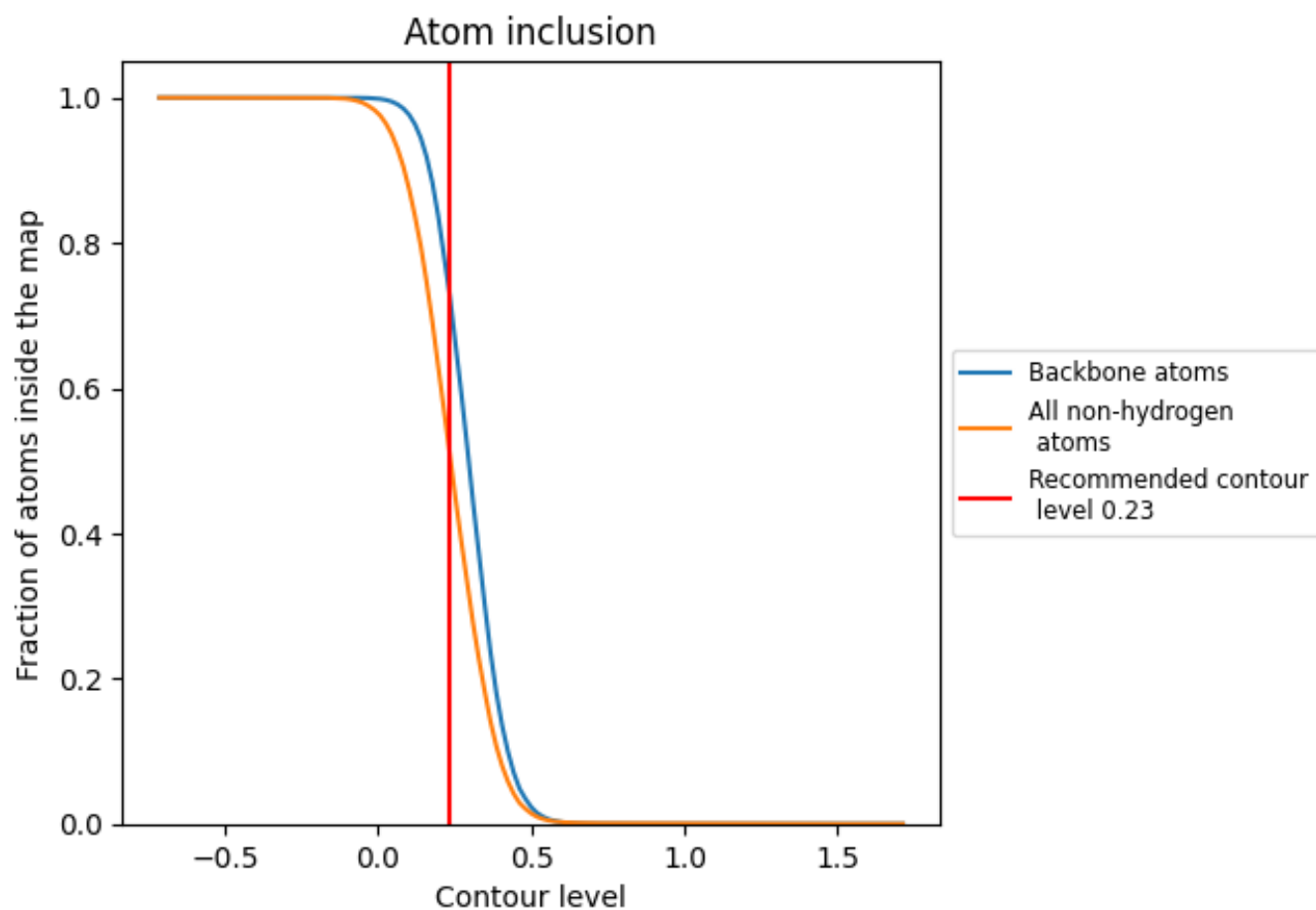
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.23).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 52% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5201	 0.3730
1	 0.5279	 0.3690
2	 0.5344	 0.3800
3	 0.5511	 0.3880
4	 0.5921	 0.4160
5	 0.5688	 0.4060
6	 0.5843	 0.4100
7	 0.5240	 0.3910
9	 0.6557	 0.4300
A	 0.4564	 0.3670
H	 0.5259	 0.3700
J	 0.5248	 0.3820
K	 0.5407	 0.3720
L	 0.3694	 0.2950
M	 0.4823	 0.3490
N	 0.5349	 0.3820

