



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 03:30 AM UTC

PDB ID : 8XKU / pdb_00008xku
EMDB ID : EMD-38425
Title : Cryo-EM structure of the Ycf2-FtsHi motor complex from Arabidopsis in ATP-bound state
Authors : Liang, K.; Zhan, X.; Xu, Q.; Wu, J.; Yan, Z.
Deposited on : 2023-12-24
Resolution : 3.20 Å(reported)

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

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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.dev132
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) : 2.49

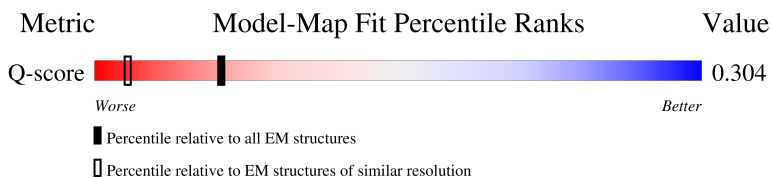
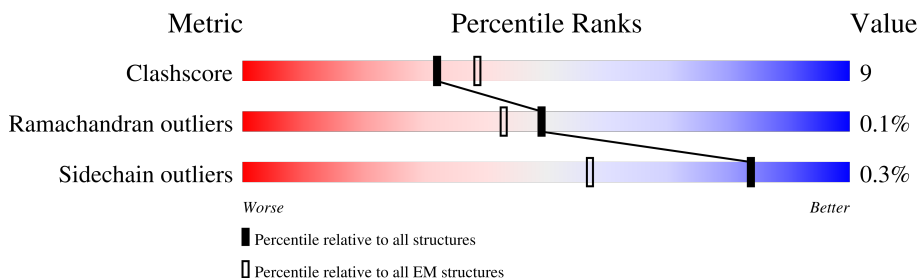
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	855	23% 66% 19% 15%
2	B	1008	13% 67% 17% 16%
3	C	1320	42% 56% 14% 30%
4	D	2294	10% 28% 7% 65%

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Mol	Chain	Length	Quality of chain
5	E	946	
6	F	876	
7	G	396	
8	H	348	
9	I	403	
9	J	403	
10	K	80	
11	L	18	
12	M	11	
13	N	37	
14	O	17	
15	P	19	
16	R	328	

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
18	ATP	A	902	-	-	X	-
18	ATP	B	1103	-	-	X	-
20	PX2	B	1104	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 45544 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 Probable inactive ATP-dependent zinc metalloprotease FTSHI 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	730	Total	C	N	O	S	0	0
			5841	3718	1000	1103	20		

- Molecule 2 is a protein called ATP-dependent zinc metalloprotease FTSH 12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	845	Total	C	N	O	S	0	0
			6879	4404	1195	1251	29		

- Molecule 3 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	921	Total	C	N	O	S	0	0
			7494	4775	1299	1386	34		

- Molecule 4 is a protein called Protein Ycf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	805	Total	C	N	O	S	0	0
			6659	4314	1145	1173	27		

- Molecule 5 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	498	Total	C	N	O	S	0	0
			3881	2451	690	729	11		

- Molecule 6 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	478	Total	C	N	O	S	0	0
			3744	2356	667	701	20		

- Molecule 7 is a protein called AtTam46.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	285	Total	C	N	O	S	0	0
			2375	1615	370	379	11		

- Molecule 8 is a protein called At4g28210.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	54	Total	C	N	O	S	0	0
			459	310	76	72	1		

- Molecule 9 is a protein called Malate dehydrogenase, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	317	Total	C	N	O	S	0	0
			2363	1503	396	457	7		
9	J	317	Total	C	N	O	S	0	0
			2363	1503	396	457	7		

- Molecule 10 is a protein called Aspartyl/glutamyl-tRNA (Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	67	Total	C	N	O	S	0	0
			555	359	98	97	1		

- Molecule 11 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	18	Total	C	N	O	S	0	0
			131	89	21	20	1		

- Molecule 12 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	11	Total	C	N	O	0	0
			84	59	13	12		

- Molecule 13 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	37	Total	C	N	O	S	0	0
			246	159	45	41	1		

- Molecule 14 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	17	Total	C	N	O	0	0
			132	89	25	18		

- Molecule 15 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	19	Total	C	N	O	0	0
			95	57	19	19		

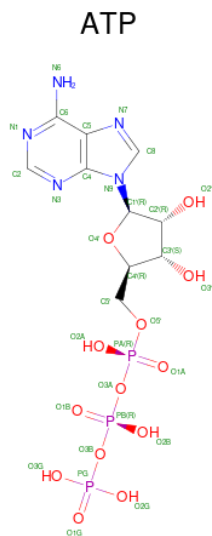
- Molecule 16 is a protein called Embryo defective 2737.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	267	Total	C	N	O	S	0	0
			2151	1371	367	397	16		

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mg	0
			1	1	
17	B	1	Total	Mg	0
			1	1	

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

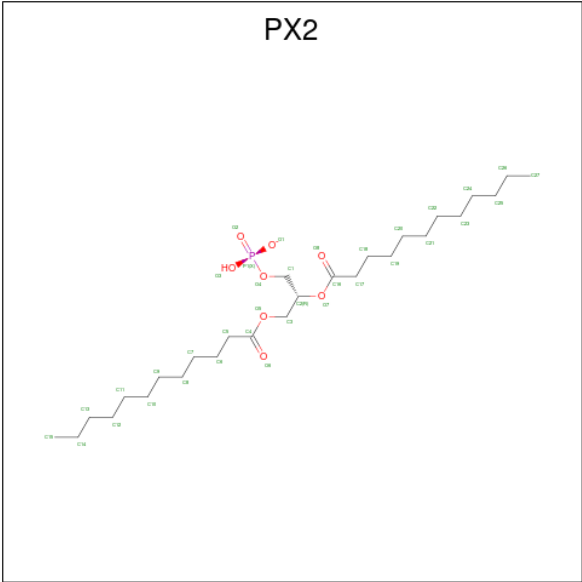


Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 31	C 10	N 5	O 13	P 3	0
18	B	1	Total 31	C 10	N 5	O 13	P 3	0

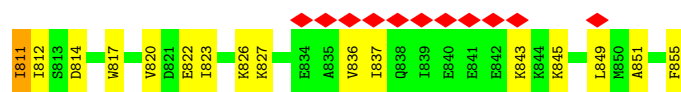
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total Zn 1 1	0
19	R	2	Total Zn 2 2	0

- Molecule 20 is 1,2-DILAUIOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).

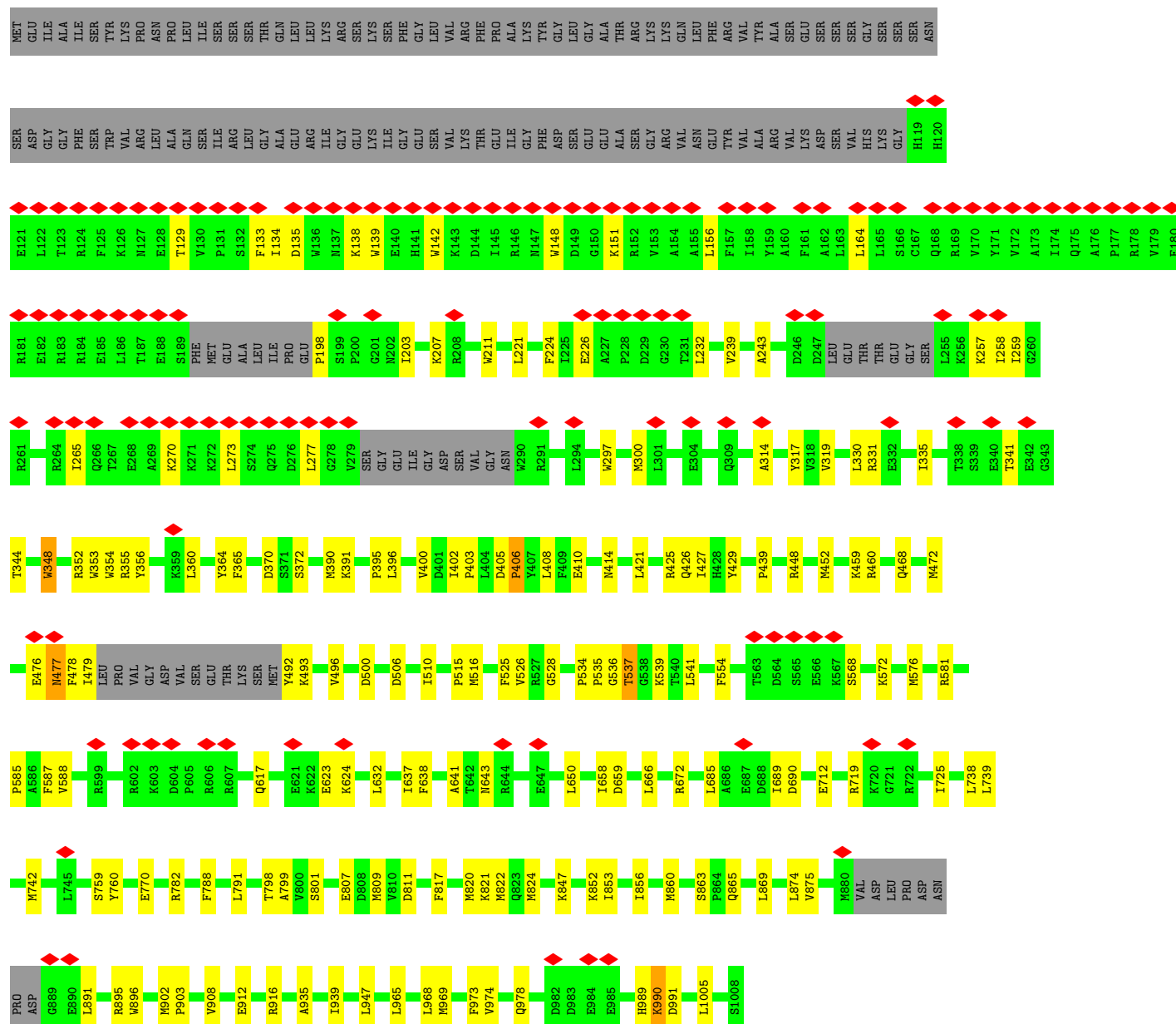


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	B	1	25	16	8	1	0



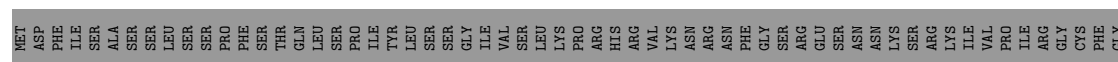
- Molecule 2: ATP-dependent zinc metalloprotease FTSH 12, chloroplastic

Chain B: 13% 67% 17% 16%

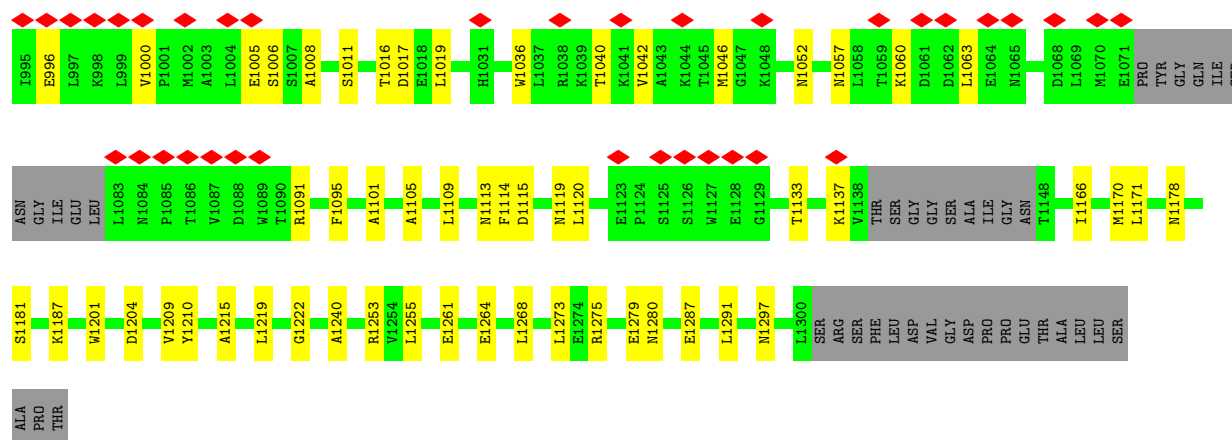


- Molecule 3: Probable inactive ATP-dependent zinc metalloprotease FTSHI 5, chloroplastic

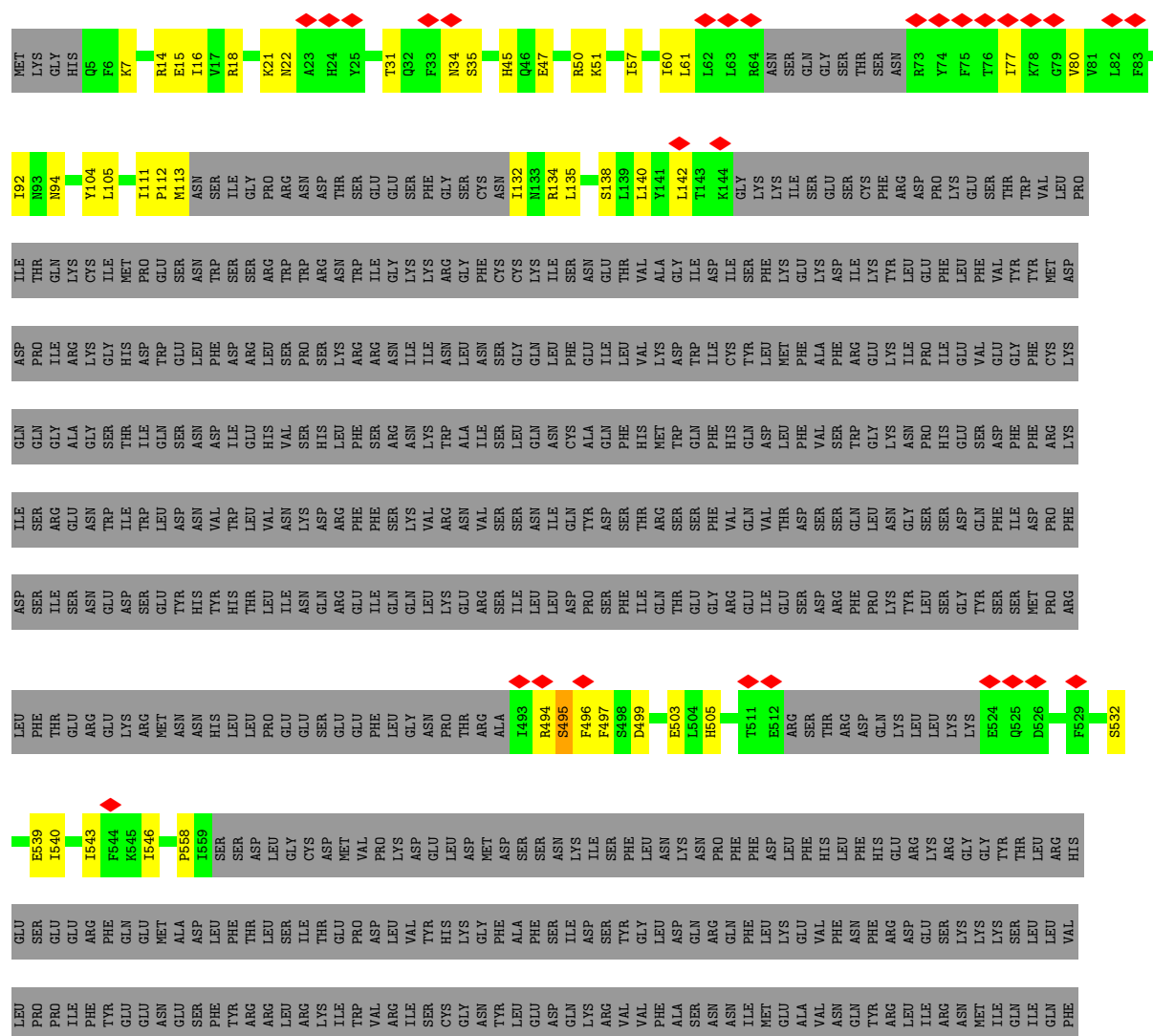
Chain C: 42% 56% 14% 30%



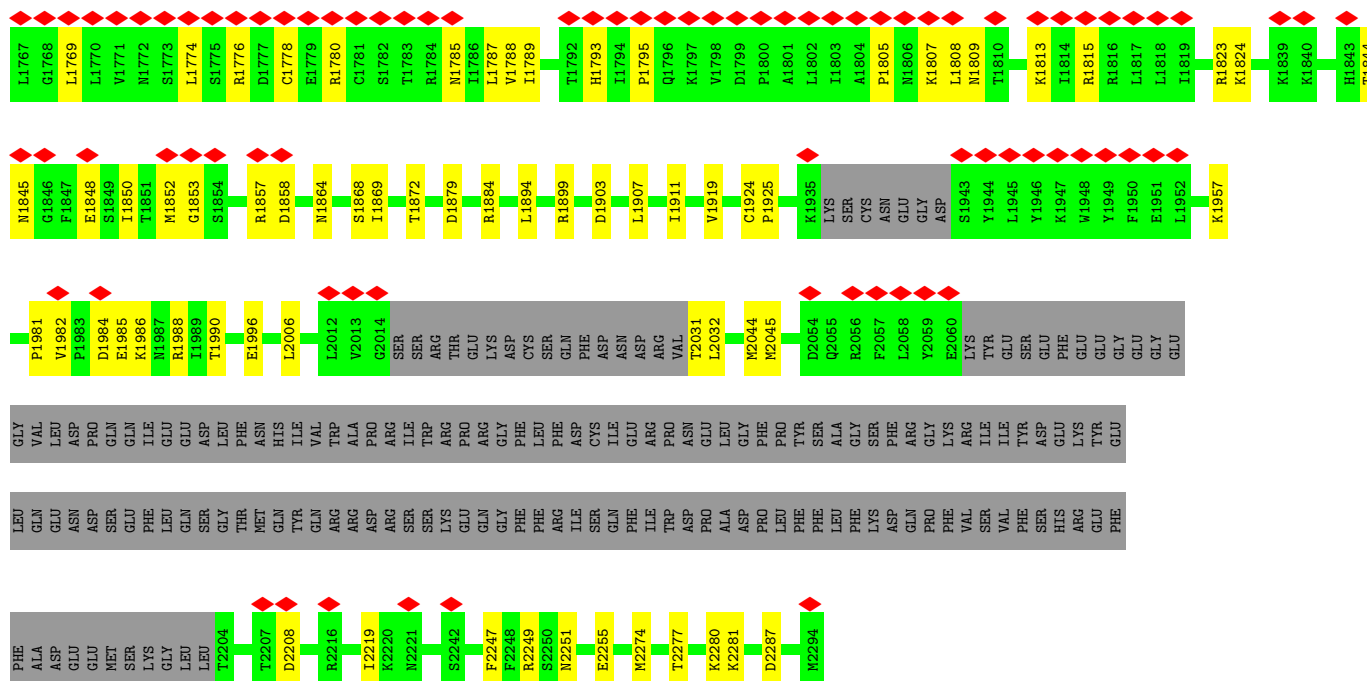
H933	K934	Q935	I936	D937	E938	A939	L940	R941	R942	P943	G944	R945	M946	D947	R948	V949	F950	H951	L952	Q953	S954	P955	T956	E957	M958	T959	R960	Q961	L962	I963	L964	H965	A966	A967	A968	E969	E970	T971	M972	D973	R974	E975	L976	V977	D978	L979	V980	D981	V982	R983	K984	E987	T990	L991	L992	R993	P994				
G813	A814	R815	A816	P817	R818	G819	V820	L821	I822	V823	G824	E825	R826	G827	T828	G829	K830	T831	S832	L833	A834	L835	A836	I837	R838	A839	K840	L783	A841	R842	V843	P844	V845	V846	N847	V848	E849	A850	Q851	L912	V913	E914	L915	D916	G917	F918	E919	K920	Q921	D922	G923	V924	V925	L926	M927	A928	T929	T930	R931	N932	T872
ARG	ARG	ILE	LYS	GLN	LYS	ARG	LYS	ALA	GLY	ILE	D764	P765	I766	K767	T768	A769	F770	D771	R772	M773	K774	R775	V776	K777	M778	P779	P780	I781	P782	L783	K784	F785	F786	A787	S788	I789	E790	V848	S791	M792	R793	E794	E795	I796	N797	P798	V799	V800	A801	F802	L803	Q804	N805	P806	K807	A808	F809	Q810	E811	M812	
GLU	ASP	PHE	GLN	TRP	PHE	LEU	TRP	PHE	ALA	ILE	ARG	SER	SER	TYR	GLY	PHE	VAL	HIS	VAL	VAL	M773	K774	R775	V776	K777	M778	P779	P780	I781	P782	L783	K784	F785	F786	A787	S788	I789	E790	V848	S791	M792	R793	E794	E795	I796	N797	P798	V799	V800	A801	F802	L803	Q804	N805	P806	K807	A808	F809	Q810	E811	M812
ASN	ILE	ASN	ASP	ASP	ILE	MET	MET	ALA	VAL	VAL	PHE	PRO	VAL	ILE	GLU	PHE	ILE	PRO	TYR	GLN	ARG	ARG	ARG	LEU	LEU	ARG	MET	ALA	TRP	PRO	GLU	ILE	GLY	THR	VAL	GLY	ARG	ASP	PRO	ASN	LEU	GLN	TRP	GLN	TRP	PHE	ASN	LYS	THR	ARG	ASN	ASN	ALA	LYS	ASP	THR	VAL	LEU	LYS	ILE	ARG
F568	M575	L576	A577	C578	G579	I580	P581	T582	S583	V584	H585	L586	M587	M588	S510	I589	P590	M591	S592	E593	L594	S595	L596	Q597	Q598	Q599	F600	L601	L602	V603	T604	R605	V606	V607	S608	R609	V610	F611	N612	A613	L614	R615	K616	T617	GLN	VAL	VAL	ASN	ALA	LYS	ASP	THR	VAL	LEU	LYS	ILE	ARG				
Q491	V492	L493	R496	D497	R498	V499	V500	W504	Y505	N506	E507	D508	K509	S510	R511	W512	E513	P516	M517	A518	V519	P520	L527	A531	R532	I533	H534	H535	D536	M540	V541	G546	D547	D548	K467	A468	D469	L470	K471	Q472	K473	L474	L475	K556	E557	M560	L561	F562	E563	K564	F565	I485	A486	Q489	E490						
E426	A427	V428	K429	G430	F431	P432	F433	A434	F435	V436	K437	W438	F440	G441	E442	K443	E444	V445	V446	V447	P448	K449	A450	I451	Q452	R456	H457	K460	K461	W462	E464	A465	A466	K467	A468	D469	L470	K471	Q472	K473	L474	L475	K556	E557	M560	L561	F562	E563	K564	F565	I485	A486	Q489	E490							
LEU	PRO	ASN	VAL	LEU	GLU	LEU	GLU	VAL	ASP	PHE	ASP	R378	D379	S380	V381	D382	F383	S384	L385	R386	I387	K388	R389	R390	L391	E392	E393	S394	Q398	R399	D400	L401	R404	I405	R406	R408	M409	K410	K411	F412	G413	E414	E415	E287	K416	L417	F418	V419	Q420	K421	T422	P423	E424	G425							
G303	V304	R305	E306	L307	I308	F309	I310	E311	R312	E313	C314	V315	E316	L317	V318	K319	S320	F321	N322	R323	E324	L325	Q327	N326	Q327	K328	S329	F330	E331	SER	VAL	PRO	GLU	SER	SER	ILE	THR	LYS	THR	LEU	SER	ARG	SER	GLU	ILE	LYS	GLN	GLU	GLU	MET	ILE										
V242	D243	E244	A245	L246	S247	L248	K249	K250	Q251	S252	E253	K254	L255	L256	R257	K258	G259	A260	R261	E262	K263	M264	E265	K266	L267	E268	E269	S270	S271	D272	I273	M274	E275	S276	E277	V278	N279	K280	I281	W282	E283	R284	I285	D286	E287	I288	D289	D290	I291	I292	K294	K295	E296	T297	L300	D239	K240	F302			
ILE	ALA	GLY	LEU	SER	PRO	ILE	ARG	SER	PHE	GLN	ALA	ALA	VAL	VAL	PRO	PHE	VAL	ASP	VAL	ILE	TRP	LYS	LYS	LYS	GLU	VAL	ARG	GLU	GLY	TVR	ASN	SER	VAL	VAL	LYS	THR	ARG	GLU	SER	SER	VAL	ILE	GLN	PHE	S168	D169	Y170	T171	R172	A173	L174	L175	E176	T177	R178	S179	V180				
PHE	SER	GLY	SER	PHE	LEU	ARG	SER	SER	GLN	ASP	TVR	GLY	SER	GLU	ALA	ALA	VAL	SER	GLU	SER	ARG	LEU	CYS	GLY	GLY	ASN	GLU	VAL	VAL	ASN	SER	ALA	LYS	THR	ARG	GLU	SER	SER	VAL	ILE	GLN	PHE	PHE	VAL	THR	PRO	LEU	VAL	TVR	ALA	LEU	PHE	CYS								



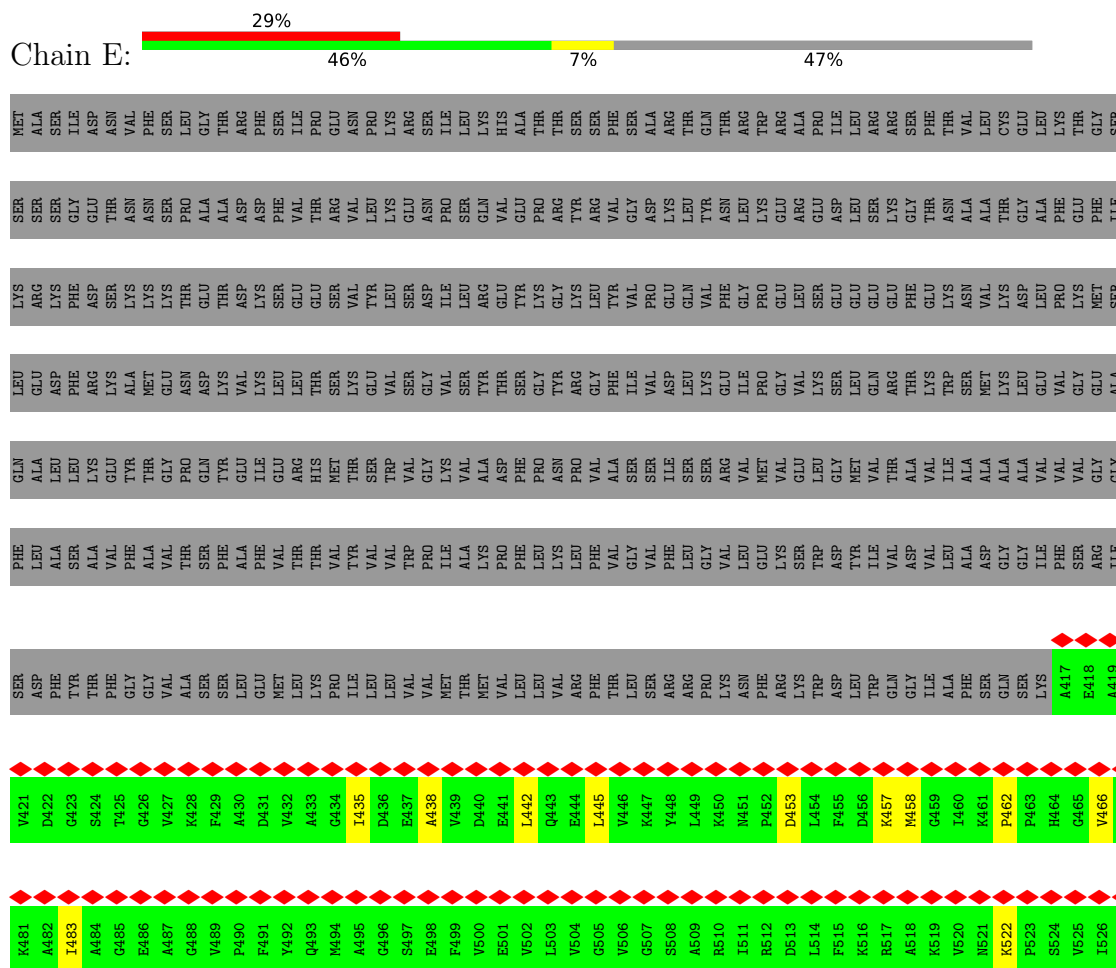
• Molecule 4: Protein Ycf2





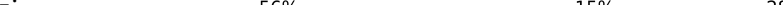


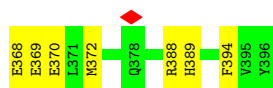
- Molecule 5: Probable inactive ATP-dependent zinc metalloprotease FTSHI 1, chloroplastic

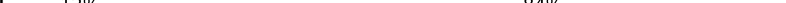


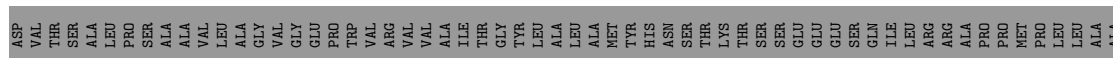
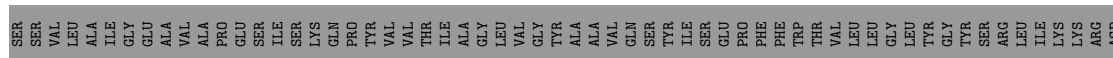
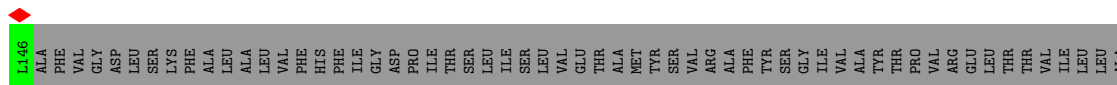
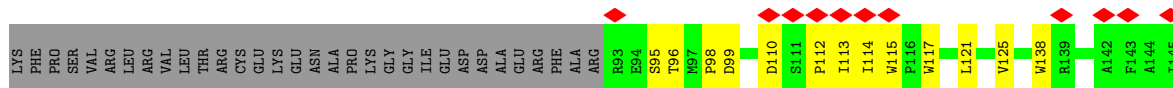




Chain G: 



Chain H:  12% 84%



ALA
LEU
ALA
ALA
ILE
GLY
VAL
ARG
LEU
ALA
ALA
LYS
TRP
GLY
TYR
ARG
HIS
LEU
THR
TRP
MET
MET
ILE
VAL

- Molecule 9: Malate dehydrogenase, chloroplastic

Chain I:



MET
ALA
THR
THR
THR
SER
ALA
SER
LEU
PHE
SER
THR
VAL
SER
SER
SER
TYR
PHE
HIS
LYS
ALA
SER
SER
ILE
PRO
HIS
SER
ARG
LEU
GLN
SER
VAL
LYS
PHE
ASN
SER
VAL
PRO
SER
PHE
THR
GLY
LEU
LYS
SER
THR
SER
LEU
ILE
SER
GLY
SER
ASP
SER
SER
SER
LEU
ALA
LYS
THR
LEU

ARG
GLY
SER
VAL
LYS
THR
ALA
GLN
THR
SER
ASP
LYS
LYS
PRO
TYR
GLY
PHE
LYS
ILE
ASN
ALA
S82
Y83
K84
I94
L101
I102
K103
M104
S105
V108
S109
T110
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H112
T131
R136
P141
L144
A145
D146
K149
N152
V153
V154
V155
I156
P157
R162
K163

P164
G165
M166
T167
R168
D169
D170
M173
A176
M177
I178
V179
A185
M189
F194
I195
H196
I197
I198
L247
P253
V254
L255
L264
P265
L266
V286
N290
V295
K299
A302
G303
S304
A305
T306
L307
S308
M309
F335
L340
A347
L357

L365
P397
A398
ALA
ALA
ALA
ALA
ASN

- Molecule 9: Malate dehydrogenase, chloroplastic

Chain J:



MET
ALA
THR
THR
SER
SER
ALA
SER
LEU
PHE
SER
THR
VAL
SER
SER
TYR
PHE
SER
LYS
ALA
SER
SER
ILE
PRO
HIS
SER
ARG
LEU
GLN
SER
VAL
LYS
PHE
ASN
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SER
VAL
PRO
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PHE
THR
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GLY
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ASP
SER
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SER
LEU
ALA
LYS
THR
LEU

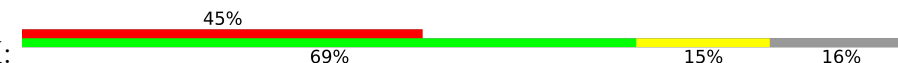
ARG
GLY
SER
VAL
LYS
THR
ALA
GLN
THR
SER
ASP
LYS
LYS
PRO
TYR
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ILE
ASN
ALA
S82
Y83
K84
L100
L101
I102
K103
V108
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V135
F138
D146
G147
L148
K149
V153
V154
V155
I156
P157
R162
K163
P164
G165
M166
T167

R168
D169
M173
M177
I178
V179
A185
V186
M189
C190
F194
T205
I208
K222
T229
L230
I248
G257
T262
K271
V286
N290
T293
V296
K299
A300
G301
A302
G303
S304
A305
M309
A310
Y311
A312
D327
F335
A347

L357
Y371
K374
E377
A378
L379
A394
A398
ALA
ALA
ALA
ALA
ASN

- Molecule 10: Aspartyl/glutamyl-tRNA (Asn/Gln) amidotransferase subunit B

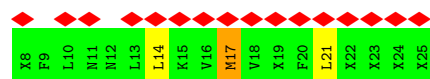
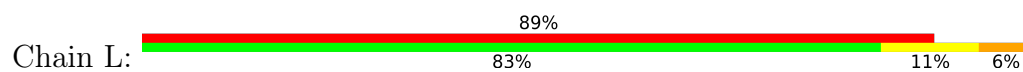
Chain K:



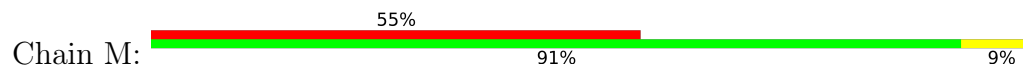
MET
GLY
ASN
LYS
ALA
THR
THR
VAL
LYS
GLU
GLU
ARG
GLU
E14
I15
H16
L17
V20
D24
F27
W30
L31
D34
R37
V38
H39
G40
F41
K42
P43
K44
N45
N46
T47
R48
P52
S55
Y56
F59
L62
S65
L66
D67
V68
D69
L70
D71
D72
P73

D74
L75
A76
H77
L78
F79
K80

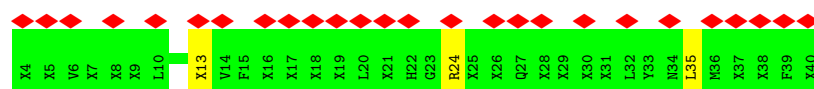
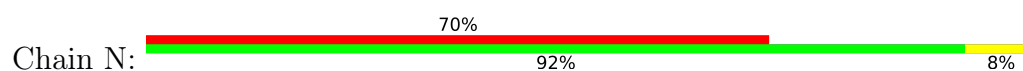
- Molecule 11: UNK



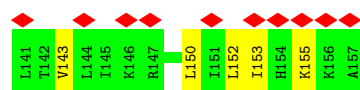
• Molecule 12: UNK



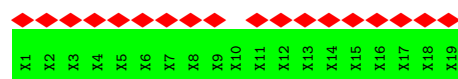
• Molecule 13: UNK



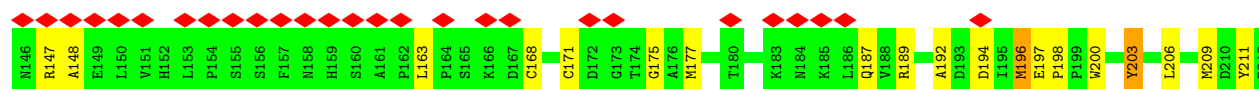
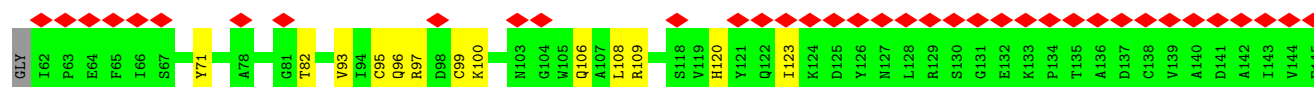
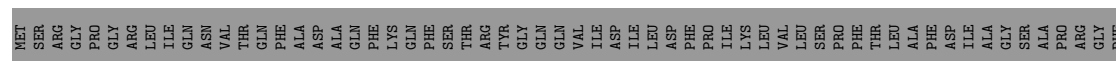
• Molecule 14: UNK

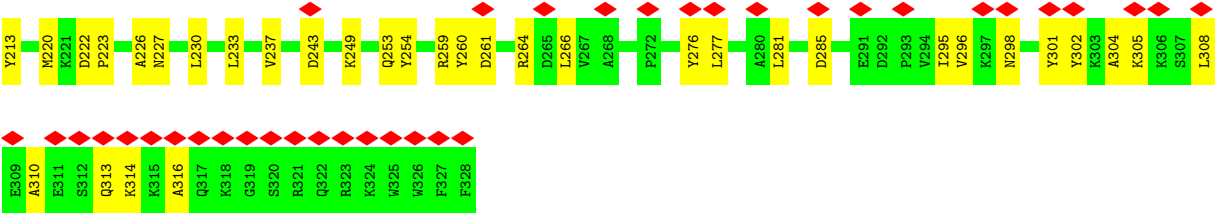


• Molecule 15: UNK



• Molecule 16: Embryo defective 2737





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	738896	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: MG, PX2, ZN, ATP

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	0.17	0/5952	0.47	0/8038
2	B	0.23	1/7022 (0.0%)	0.55	5/9460 (0.1%)
3	C	0.16	0/7627	0.46	0/10262
4	D	0.18	0/6804	0.49	1/9177 (0.0%)
5	E	0.14	0/3953	0.38	0/5357
6	F	0.16	0/3798	0.44	1/5115 (0.0%)
7	G	0.23	0/2470	0.58	2/3375 (0.1%)
8	H	0.17	0/477	0.41	0/651
9	I	0.15	0/2399	0.41	0/3261
9	J	0.15	0/2399	0.42	2/3261 (0.1%)
10	K	0.21	0/570	0.47	0/772
11	L	0.28	0/101	0.95	1/133 (0.8%)
12	M	0.23	0/74	0.72	0/99
13	N	0.15	0/142	0.52	0/179
14	O	0.22	0/132	0.59	0/175
16	R	0.19	0/2206	0.49	0/2986
All	All	0.18	1/46126 (0.0%)	0.48	12/62301 (0.0%)

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	A	0	1
2	B	0	3
4	D	0	2
5	E	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	406	PRO	CG-CD	-9.93	1.17	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	406	PRO	CA-N-CD	-12.98	93.82	112.00
2	B	406	PRO	N-CD-CG	-11.01	86.69	103.20
11	L	17	MET	CB-CG-SD	7.94	136.51	112.70
2	B	406	PRO	CA-CB-CG	-6.63	91.91	104.50
7	G	293	MET	CA-CB-CG	6.01	126.13	114.10

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	811	ILE	Peptide
2	B	476	GLU	Peptide
2	B	477	ASN	Peptide
2	B	990	LYS	Peptide
4	D	495	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5841	0	5858	153	0
2	B	6879	0	6912	176	0
3	C	7494	0	7625	129	0
4	D	6659	0	6763	139	0
5	E	3881	0	3926	44	0
6	F	3744	0	3823	74	0
7	G	2375	0	2353	52	0
8	H	459	0	455	10	0
9	I	2363	0	2437	29	0
9	J	2363	0	2437	35	0
10	K	555	0	561	12	0
11	L	131	0	123	4	0
12	M	84	0	97	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	246	0	175	5	0
14	O	132	0	161	5	0
15	P	95	0	21	0	0
16	R	2151	0	2123	55	0
17	A	1	0	0	0	0
17	B	1	0	0	0	0
18	A	31	0	12	33	0
18	B	31	0	12	19	0
19	B	1	0	0	0	0
19	R	2	0	0	0	0
20	B	25	0	23	32	0
All	All	45544	0	45897	790	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 790 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:TRP:CZ2	20:B:1104:PX2:H33	1.28	1.65
2:B:354:TRP:CE2	20:B:1104:PX2:H33	1.11	1.59
2:B:354:TRP:CH2	20:B:1104:PX2:C16	1.89	1.53
2:B:354:TRP:CZ2	20:B:1104:PX2:C18	1.94	1.48
2:B:354:TRP:CE2	20:B:1104:PX2:C18	1.98	1.46

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	724/855 (85%)	691 (95%)	31 (4%)	2 (0%)	36 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	833/1008 (83%)	798 (96%)	33 (4%)	2 (0%)	43	73
3	C	911/1320 (69%)	890 (98%)	21 (2%)	0	100	100
4	D	775/2294 (34%)	719 (93%)	56 (7%)	0	100	100
5	E	494/946 (52%)	478 (97%)	15 (3%)	1 (0%)	43	73
6	F	476/876 (54%)	460 (97%)	16 (3%)	0	100	100
7	G	283/396 (72%)	272 (96%)	11 (4%)	0	100	100
8	H	52/348 (15%)	51 (98%)	1 (2%)	0	100	100
9	I	315/403 (78%)	310 (98%)	5 (2%)	0	100	100
9	J	315/403 (78%)	309 (98%)	6 (2%)	0	100	100
10	K	65/80 (81%)	59 (91%)	6 (9%)	0	100	100
11	L	12/18 (67%)	11 (92%)	1 (8%)	0	100	100
12	M	8/11 (73%)	5 (62%)	3 (38%)	0	100	100
13	N	17/37 (46%)	13 (76%)	4 (24%)	0	100	100
14	O	15/17 (88%)	11 (73%)	4 (27%)	0	100	100
16	R	265/328 (81%)	252 (95%)	13 (5%)	0	100	100
All	All	5560/9340 (60%)	5329 (96%)	226 (4%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	478	PHE
5	E	821	VAL
1	A	208	PRO
2	B	477	ASN
1	A	812	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	628/744 (84%)	626 (100%)	2 (0%)	86	88
2	B	734/872 (84%)	730 (100%)	4 (0%)	81	85
3	C	817/1177 (69%)	816 (100%)	1 (0%)	88	91
4	D	753/2151 (35%)	752 (100%)	1 (0%)	88	91
5	E	422/817 (52%)	422 (100%)	0	100	100
6	F	399/757 (53%)	397 (100%)	2 (0%)	81	85
7	G	246/347 (71%)	245 (100%)	1 (0%)	84	86
8	H	46/287 (16%)	46 (100%)	0	100	100
9	I	261/332 (79%)	261 (100%)	0	100	100
9	J	261/332 (79%)	260 (100%)	1 (0%)	84	86
10	K	62/73 (85%)	62 (100%)	0	100	100
11	L	12/12 (100%)	12 (100%)	0	100	100
12	M	9/9 (100%)	9 (100%)	0	100	100
13	N	16/16 (100%)	16 (100%)	0	100	100
14	O	14/15 (93%)	13 (93%)	1 (7%)	13	44
16	R	236/286 (82%)	234 (99%)	2 (1%)	73	82
All	All	4916/8227 (60%)	4901 (100%)	15 (0%)	84	88

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	1666	TYR
16	R	196	MET
6	F	577	ILE
16	R	203	TYR
9	J	120	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	1555	HIS
5	E	555	GLN
16	R	278	GLN
16	R	96	GLN
4	D	1558	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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
18	ATP	B	1103	17	32,33,33	1.21	3 (9%)	48,52,52	1.87	10 (20%)
20	PX2	B	1104	-	24,24,35	2.02	7 (29%)	27,29,40	2.68	13 (48%)
18	ATP	A	902	17	32,33,33	1.21	3 (9%)	48,52,52	1.86	10 (20%)

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
18	ATP	B	1103	17	-	3/22/38/38	0/3/3/3
20	PX2	B	1104	-	-	9/26/26/37	-
18	ATP	A	902	17	-	3/22/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1104	PX2	O5-C4	4.58	1.46	1.33
20	B	1104	PX2	O7-C2	-4.50	1.36	1.46
20	B	1104	PX2	O8-C16	-4.08	1.10	1.22
18	B	1103	ATP	C5-C4	3.69	1.45	1.39
18	A	902	ATP	C5-C4	3.60	1.45	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	902	ATP	C5-C4-N3	-6.01	118.45	126.72
18	B	1103	ATP	C5-C4-N3	-5.99	118.47	126.72
18	A	902	ATP	N3-C4-N9	4.94	135.57	127.17
18	B	1103	ATP	N3-C4-N9	4.94	135.57	127.17
20	B	1104	PX2	O5-C4-C5	4.73	126.24	111.83

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	902	ATP	C5'-O5'-PA-O1A
18	A	902	ATP	C5'-O5'-PA-O3A
18	B	1103	ATP	C5'-O5'-PA-O1A
18	B	1103	ATP	C5'-O5'-PA-O3A
20	B	1104	PX2	C1-O4-P1-O1

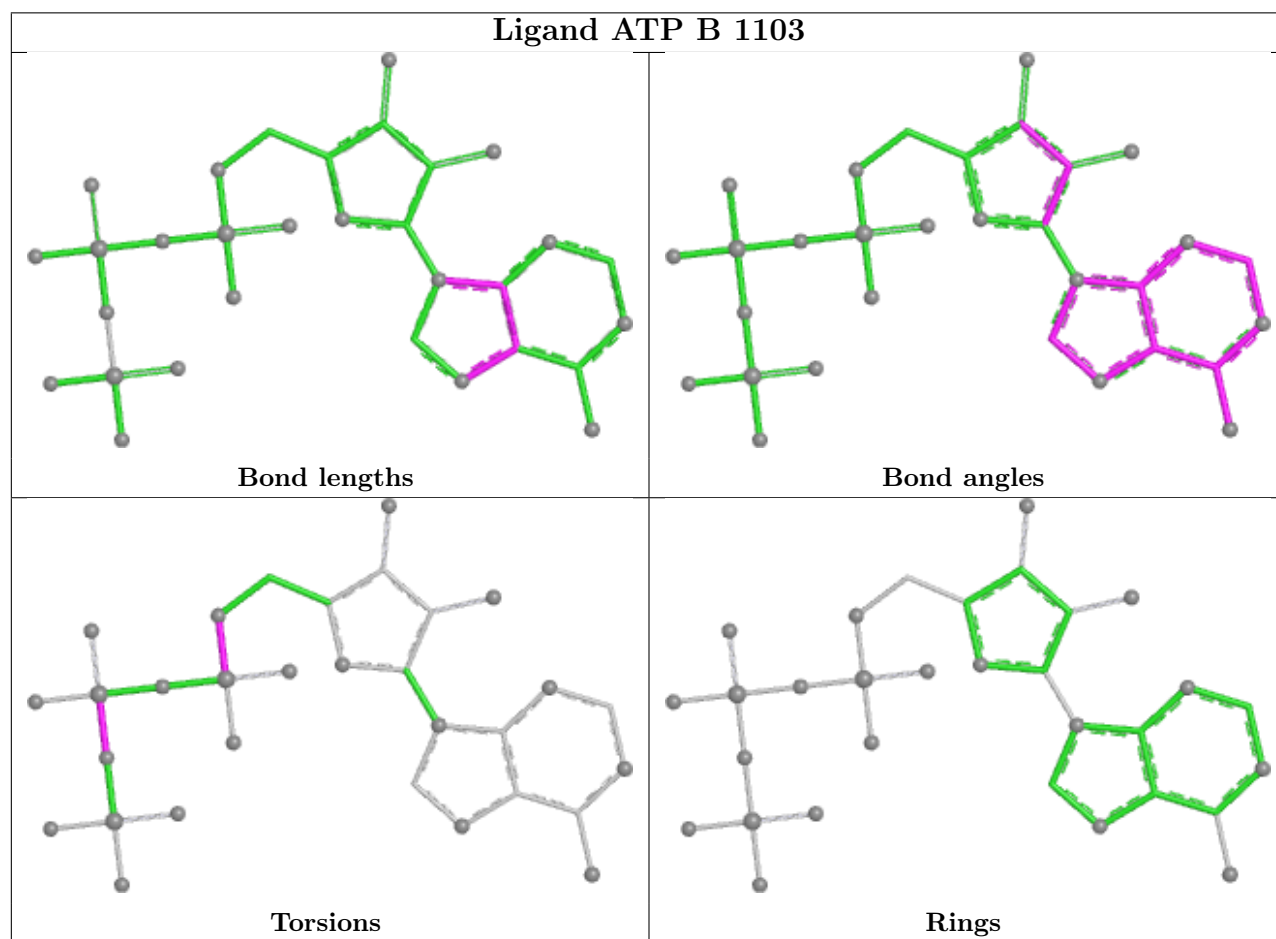
There are no ring outliers.

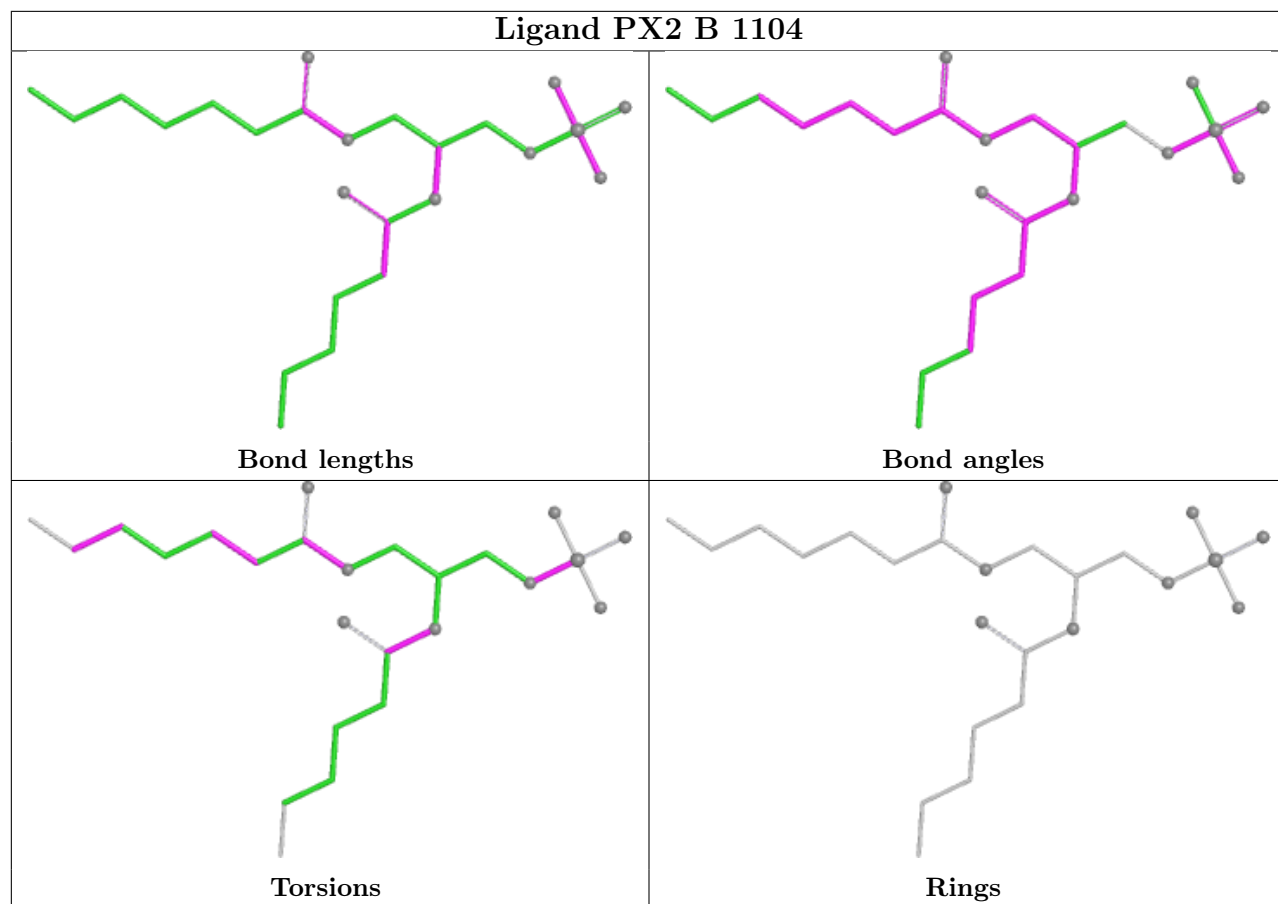
3 monomers are involved in 84 short contacts:

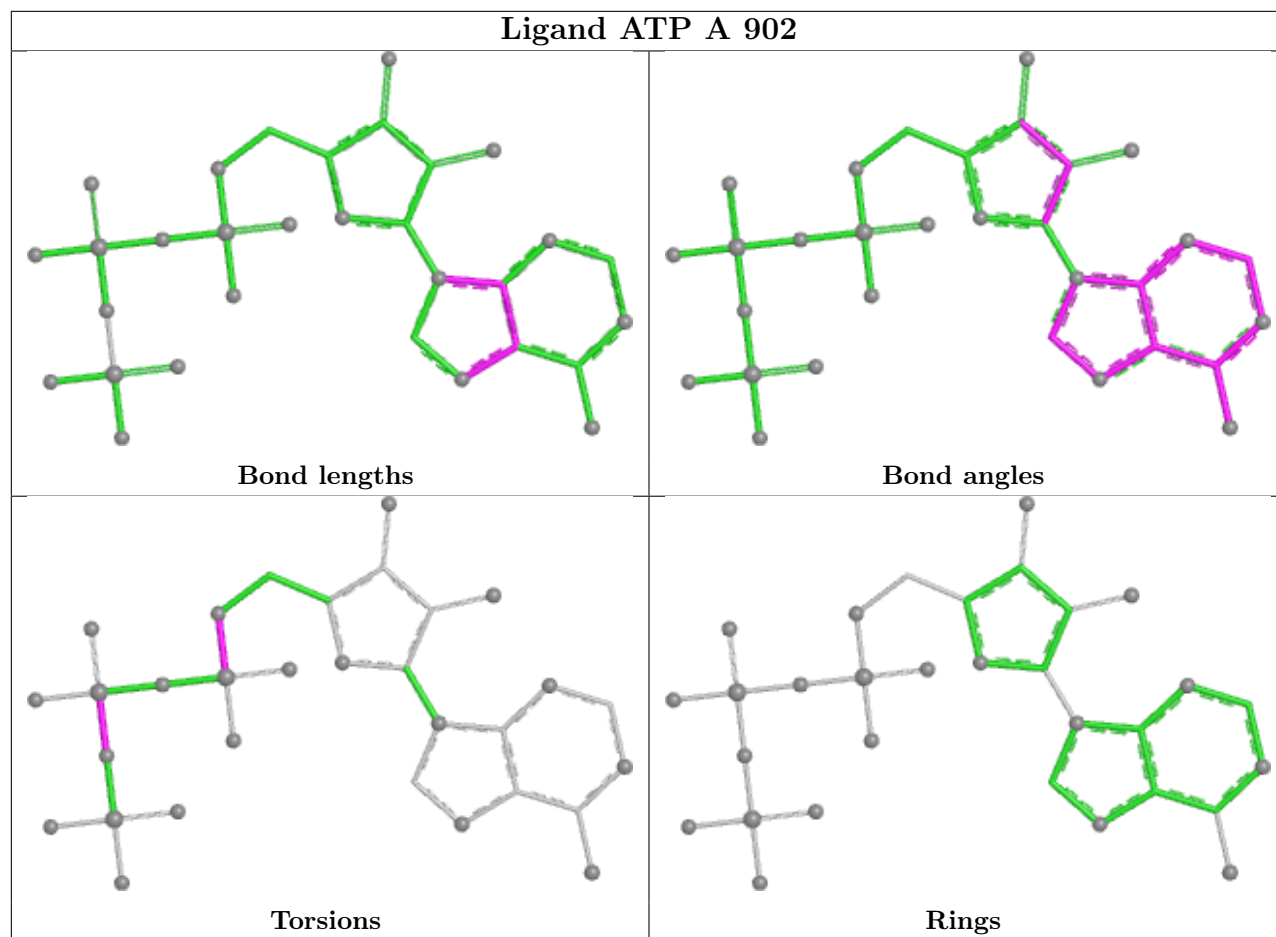
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	1103	ATP	19	0
20	B	1104	PX2	32	0
18	A	902	ATP	33	0

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.

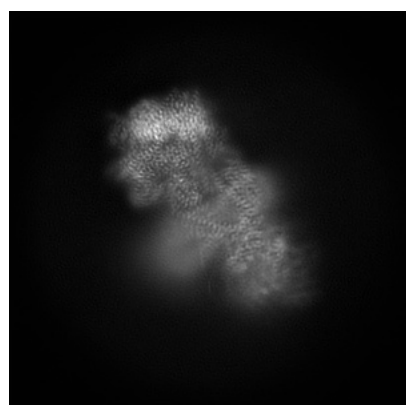
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38425. These allow visual inspection of the internal detail of the map and identification of artifacts.

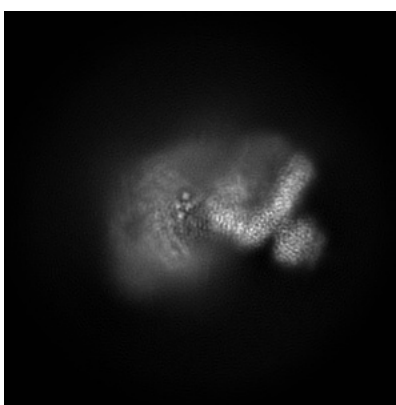
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

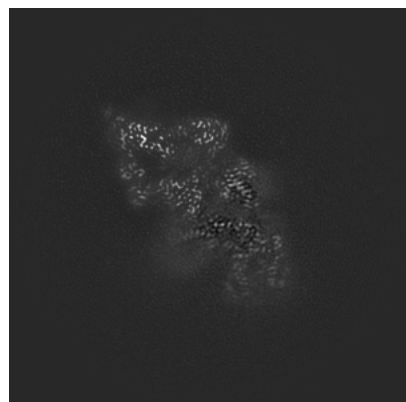


Z

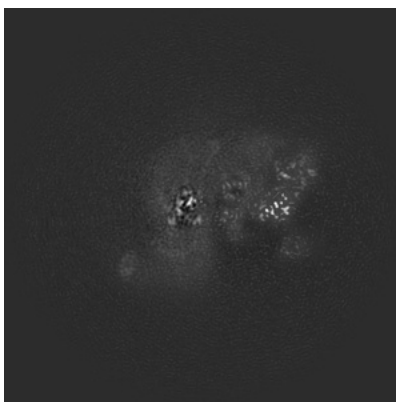
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

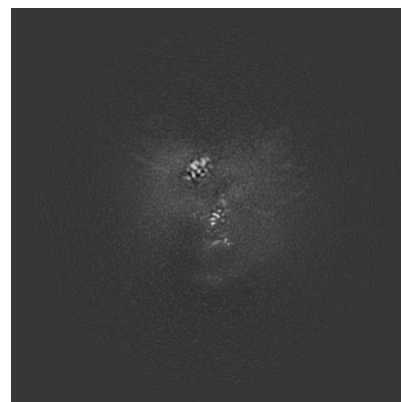
6.2.1 Primary map



X Index: 180



Y Index: 180

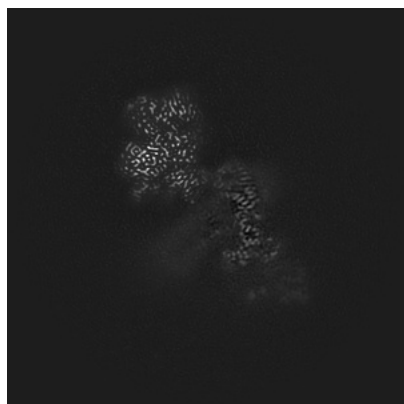


Z Index: 180

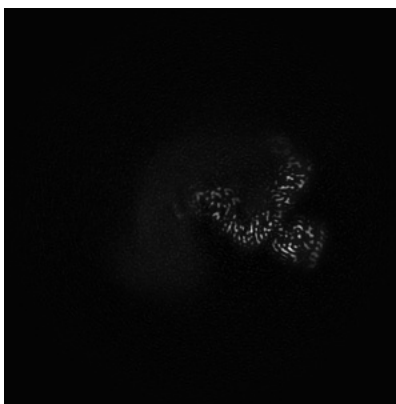
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

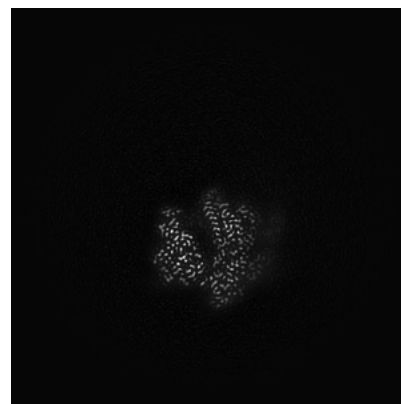
6.3.1 Primary map



X Index: 163



Y Index: 156

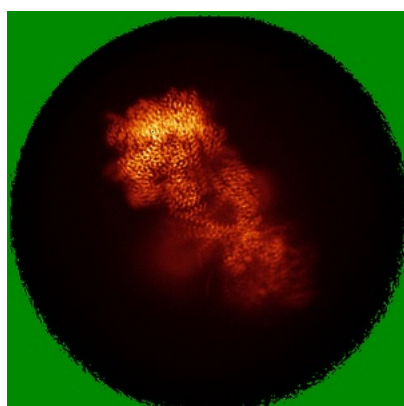


Z Index: 254

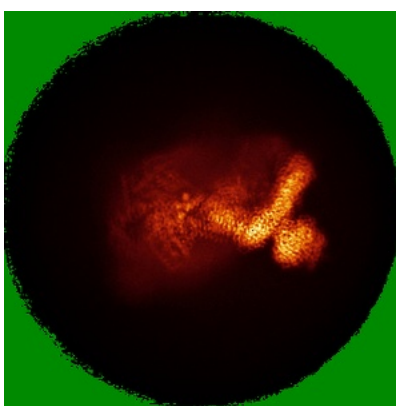
The images above show the largest variance slices of the map in three orthogonal directions.

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

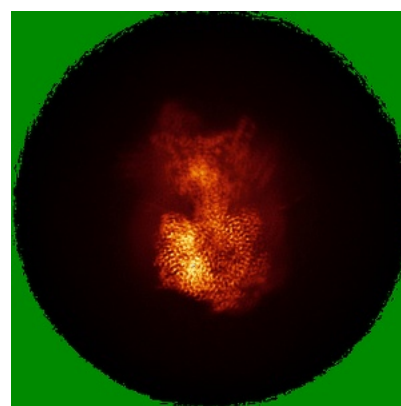
6.4.1 Primary map



X



Y

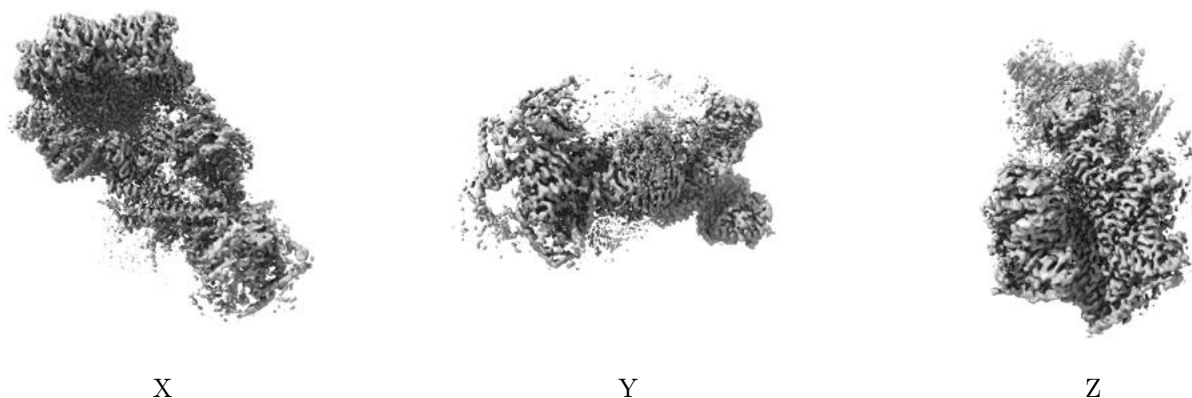


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

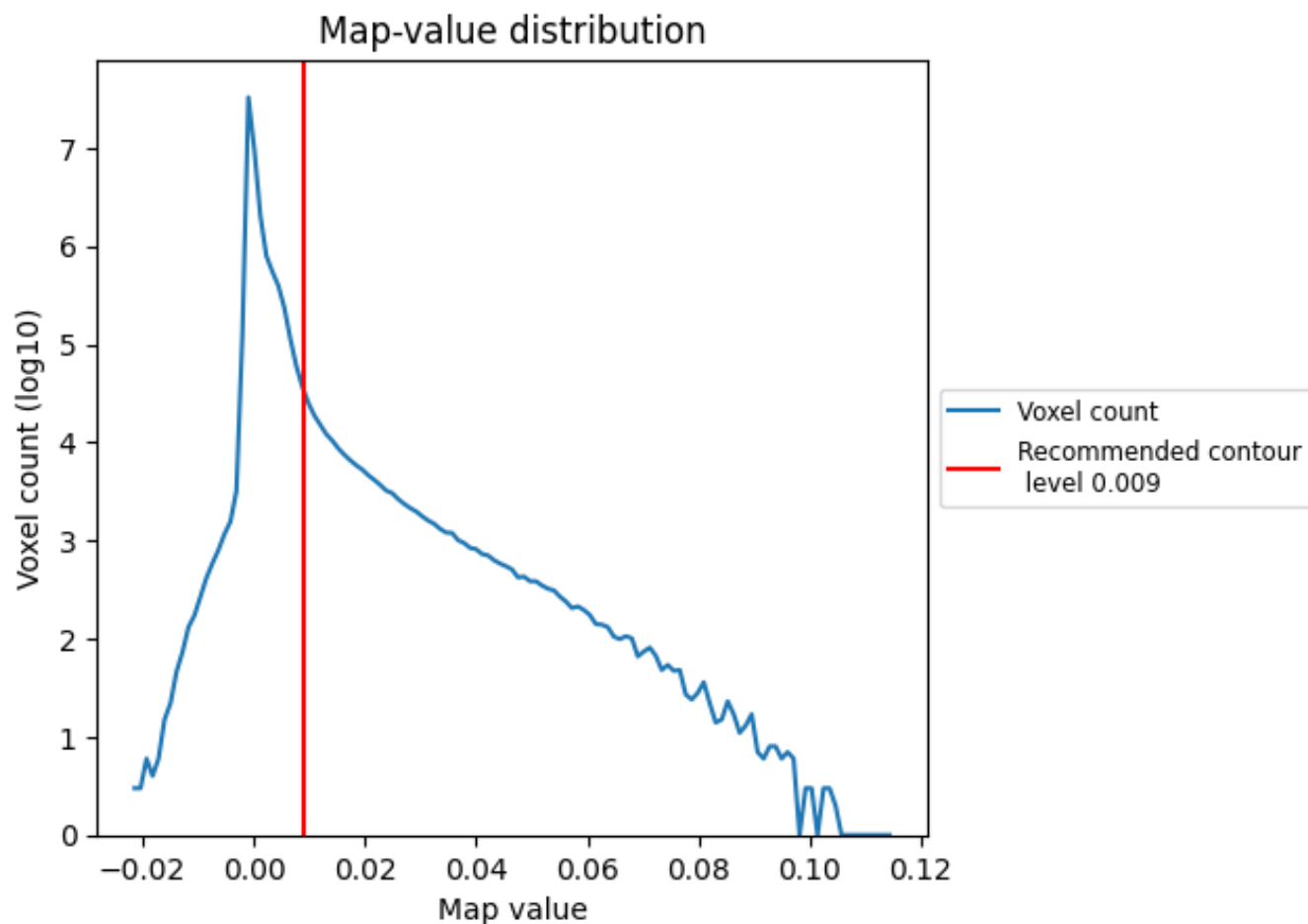
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

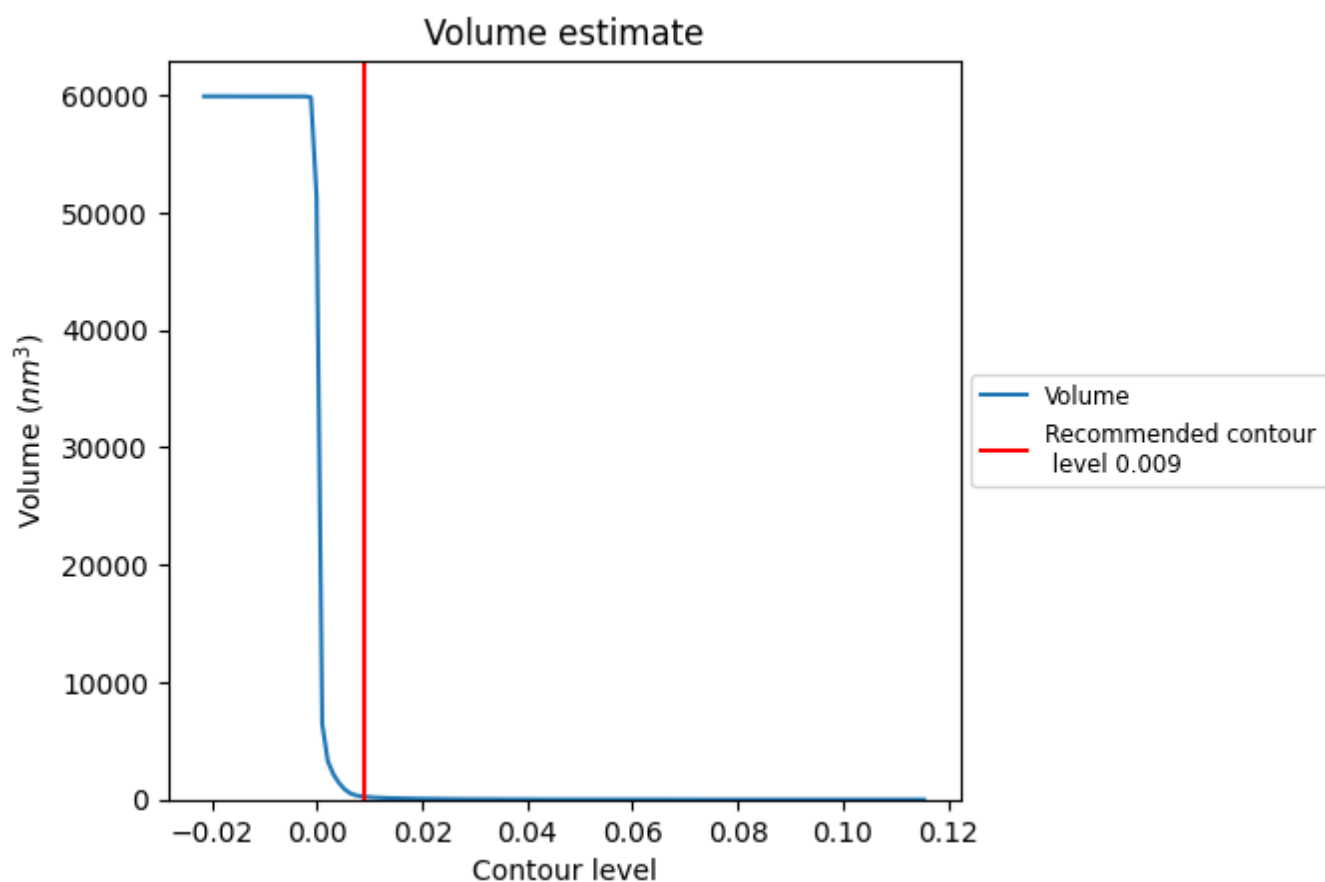
This section contains the results of statistical analysis of the map.

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.

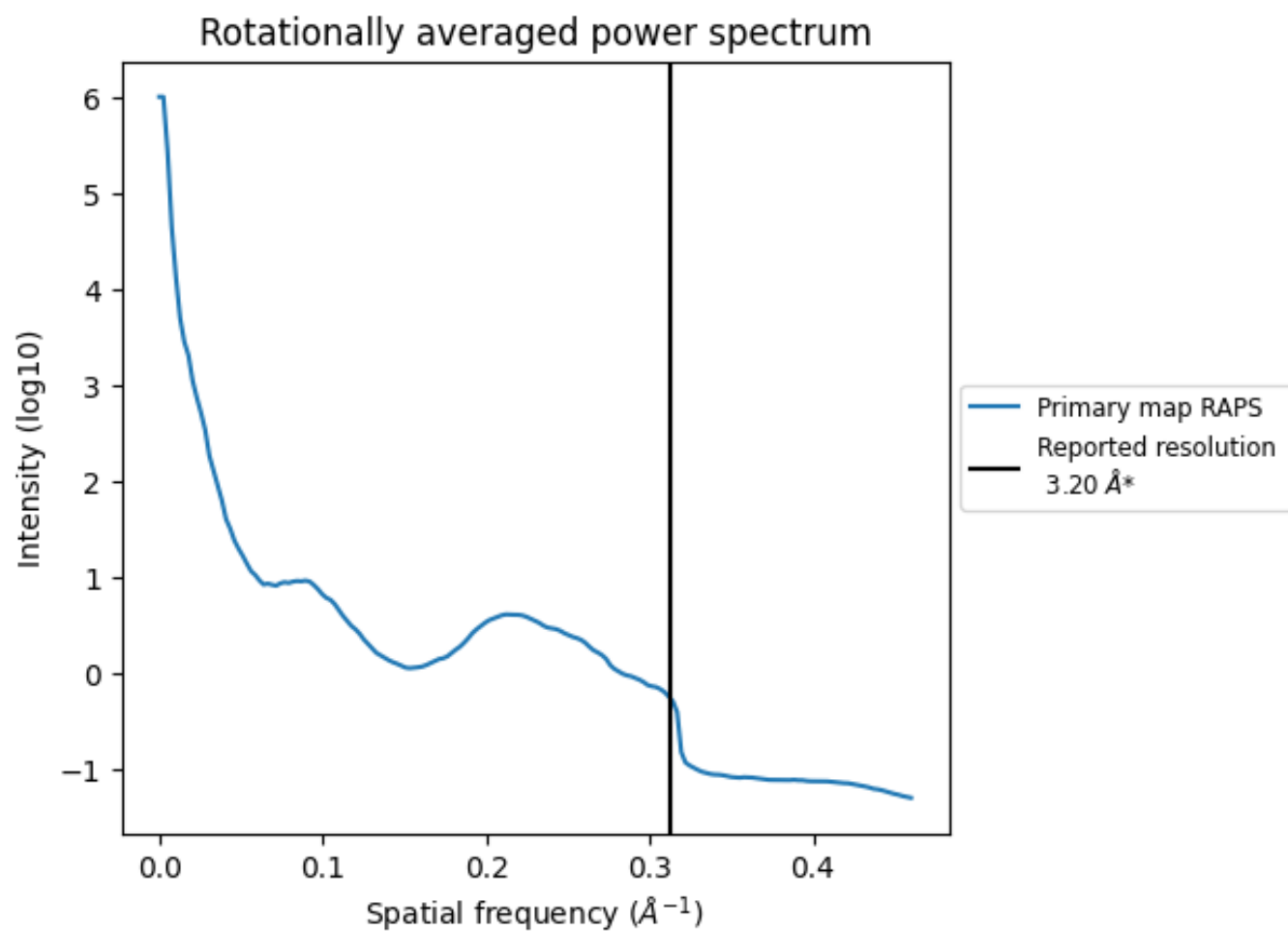
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm³; this corresponds to an approximate mass of 225 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

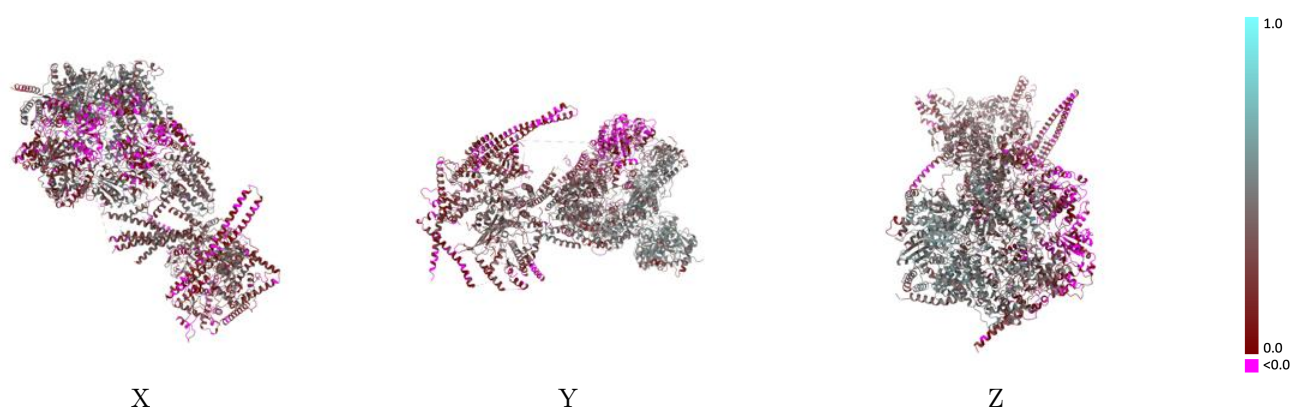
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-38425 and PDB model 8XKU. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)

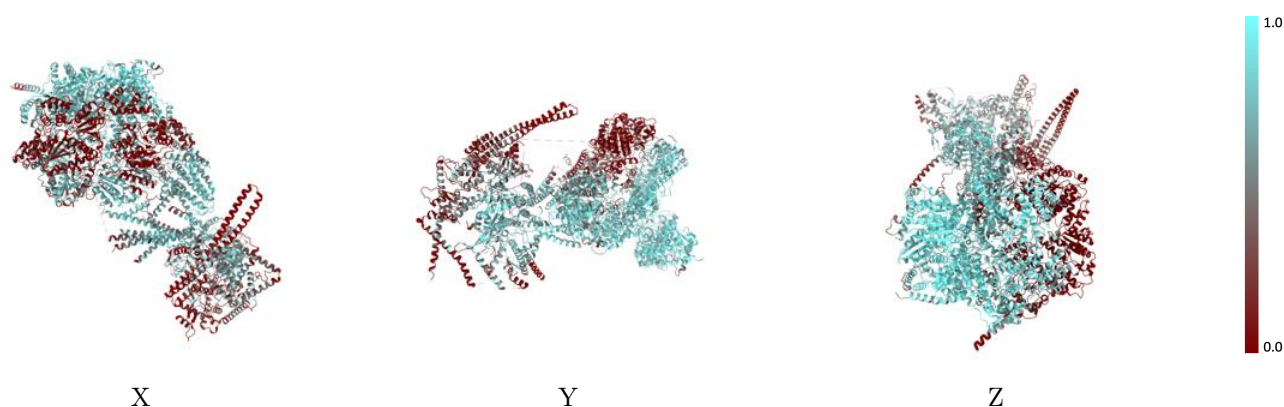
This section was not generated.

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



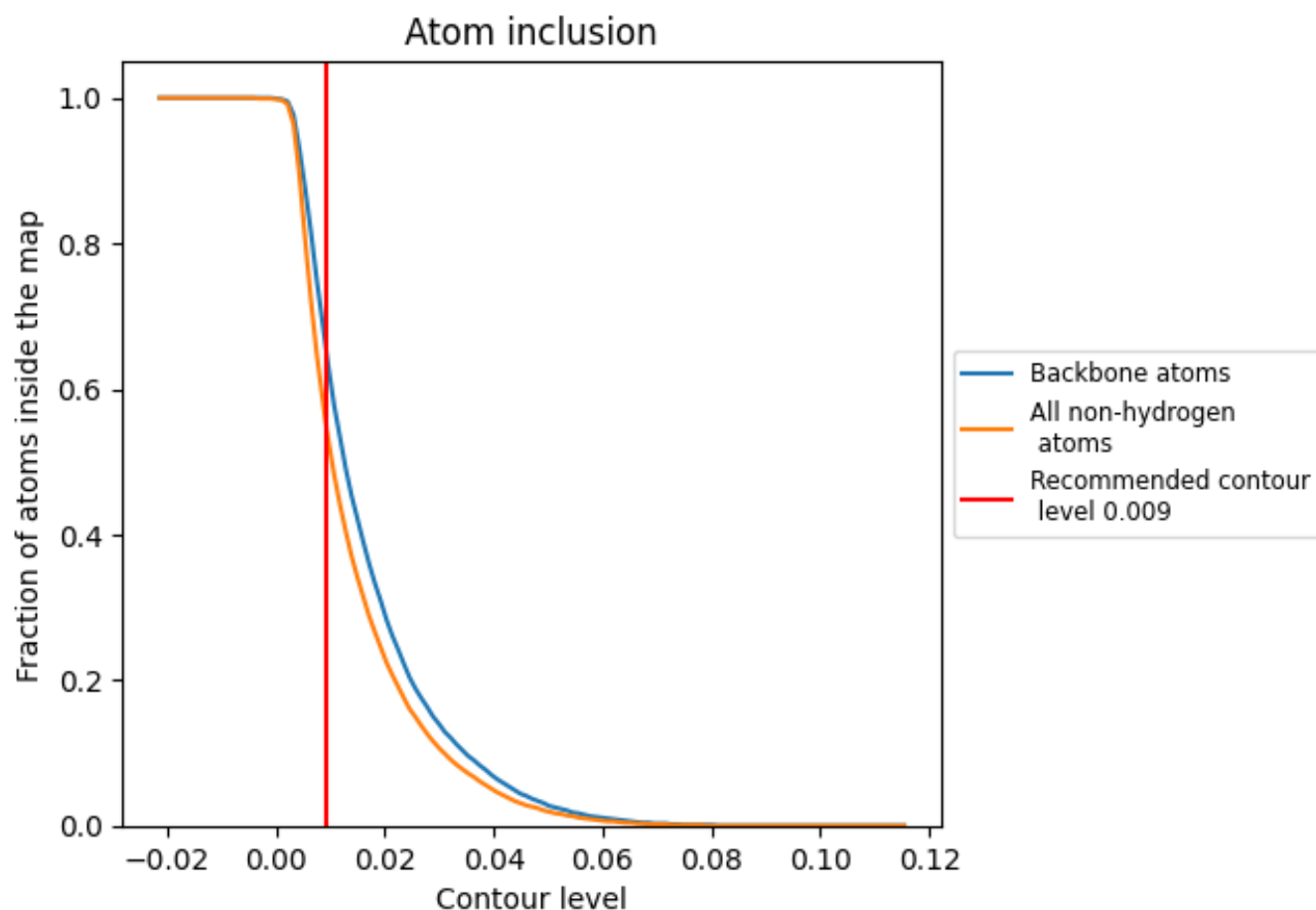
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5580	 0.3040
A	 0.6090	 0.3260
B	 0.7080	 0.3600
C	 0.3380	 0.2030
D	 0.5830	 0.3230
E	 0.4010	 0.2060
F	 0.3870	 0.2610
G	 0.7150	 0.3440
H	 0.6660	 0.3500
I	 0.8660	 0.4610
J	 0.8700	 0.4660
K	 0.3460	 0.2390
L	 0.1680	 0.1950
M	 0.3610	 0.2750
N	 0.2880	 0.2530
O	 0.3540	 0.3120
P	 0.1160	 0.1110
R	 0.4750	 0.2460

