



## wwPDB EM Validation Summary Report ⓘ

Jun 25, 2024 – 10:31 AM JST

PDB ID : 8JXM  
EMDB ID : EMD-36705  
Title : Human 3-methylcrotonyl-CoA carboxylase in BCCP-H2 state with MCoA  
Authors : Liu, D.S.; Su, J.Y.; Tian, X.Y.  
Deposited on : 2023-06-30  
Resolution : 3.49 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](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:

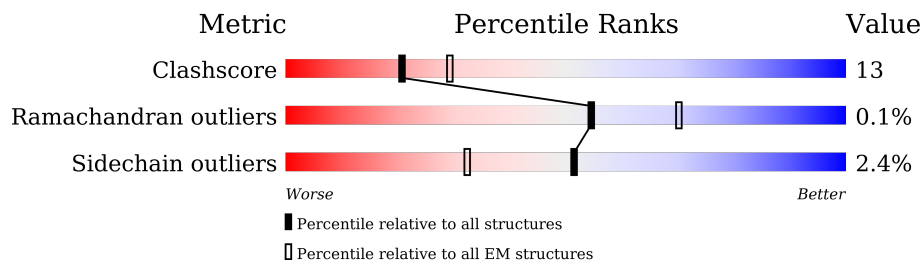
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 3.49 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	A	563	76% 19% .
1	C	563	73% 19% 8%
1	E	563	77% 17% 7%
1	H	563	72% 19% . 8%
1	J	563	75% 17% 7%
1	K	563	78% 18% .
2	B	725	52% 48% 26% 25%
2	F	725	61% 68% 15% 16%

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Mol	Chain	Length	Quality of chain
2	G	725	
2	I	725	
2	L	725	
2	M	725	

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
4	BTI	C	601	-	-	X	-
4	BTI	H	601	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 51993 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 Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial.

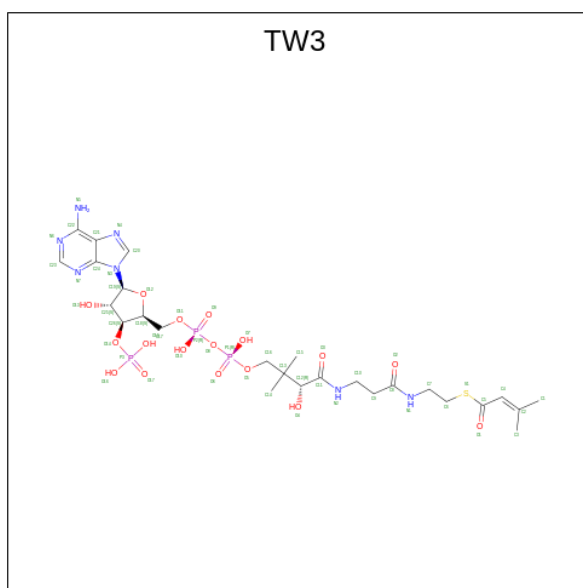
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	K	541	Total	C	N	O	S	0	0
			4154	2633	726	776	19		
1	A	541	Total	C	N	O	S	0	0
			4154	2633	726	776	19		
1	C	520	Total	C	N	O	S	0	0
			4006	2538	704	745	19		
1	H	520	Total	C	N	O	S	0	0
			4006	2538	704	745	19		
1	E	524	Total	C	N	O	S	0	0
			4038	2562	708	749	19		
1	J	522	Total	C	N	O	S	0	0
			4025	2553	706	747	19		

- Molecule 2 is a protein called Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	541	Total	C	N	O	S	0	0
			4192	2646	730	790	26		
2	B	541	Total	C	N	O	S	0	0
			4192	2646	730	790	26		
2	F	607	Total	C	N	O	S	0	0
			4703	2961	821	892	29		
2	G	607	Total	C	N	O	S	0	0
			4703	2961	821	892	29		
2	I	607	Total	C	N	O	S	0	0
			4703	2961	821	892	29		
2	M	607	Total	C	N	O	S	0	0
			4703	2961	821	892	29		

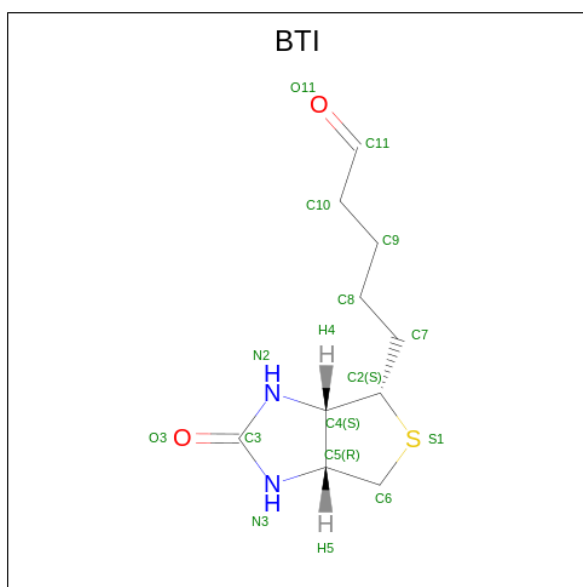
- Molecule 3 is {S}-[2-[3-[(2 {R})-4-[[[(2 {S}),3 {S}),4 {S}),5 {S}]-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonoxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethyl] 3-methylbut-2-enethioate (three-letter code: TW3) (formula: C<sub>26</sub>H<sub>42</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by

depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
3	K	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	A	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	C	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	H	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	E	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	J	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>S).

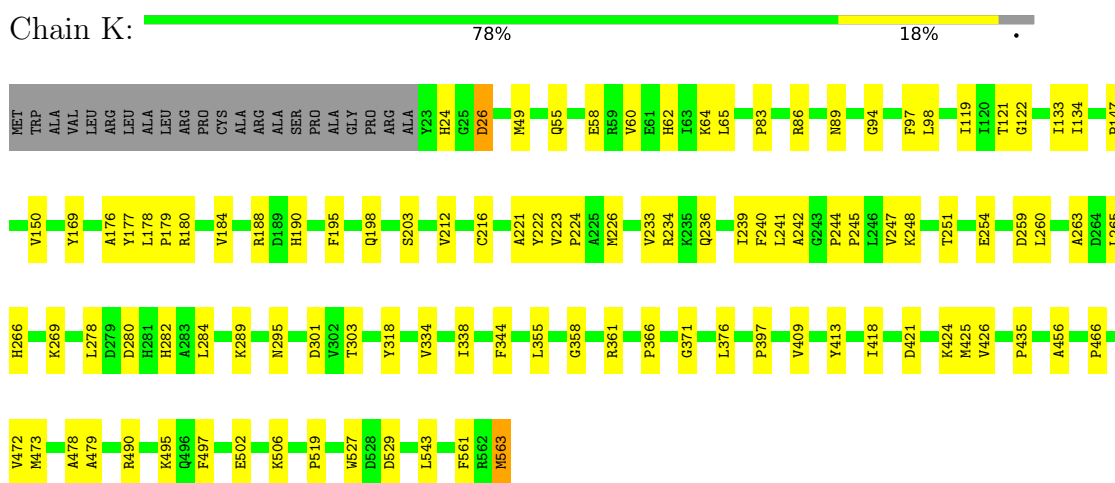


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
4	C	1	Total 15	10	2	2	1	0
4	F	1	Total 15	10	2	2	1	0
4	G	1	Total 15	10	2	2	1	0
4	H	1	Total 15	10	2	2	1	0
4	I	1	Total 15	10	2	2	1	0
4	M	1	Total 15	10	2	2	1	0

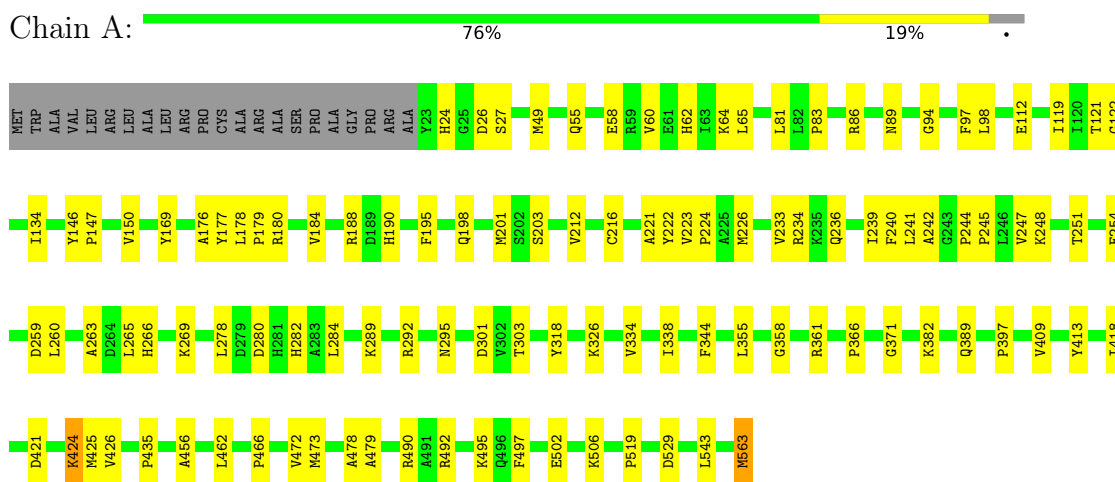
### 3 Residue-property plots

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: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

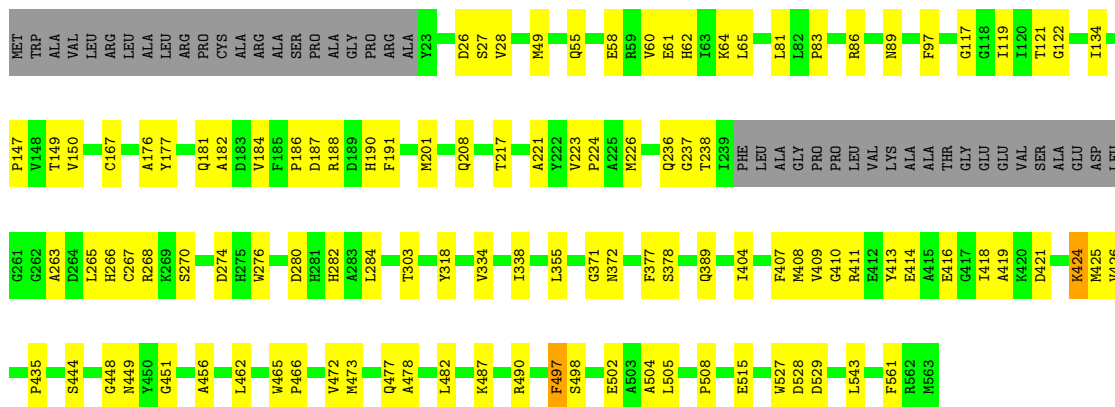


- Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

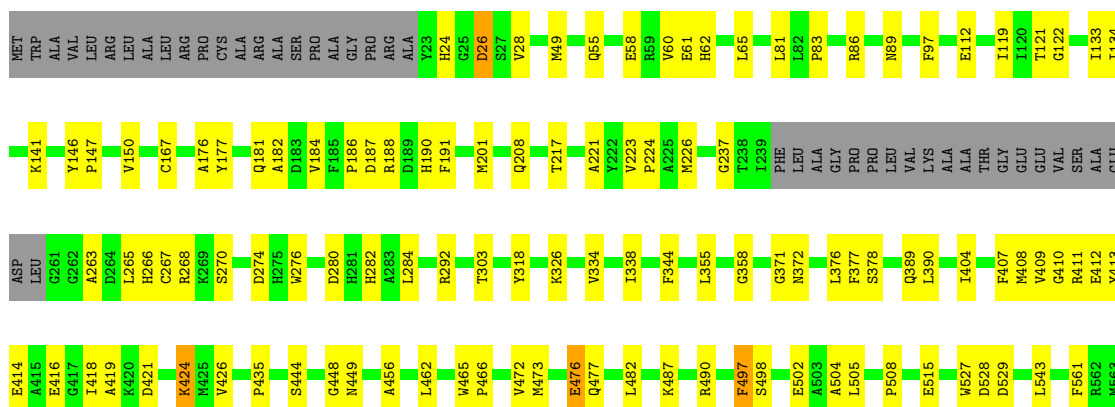


- Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

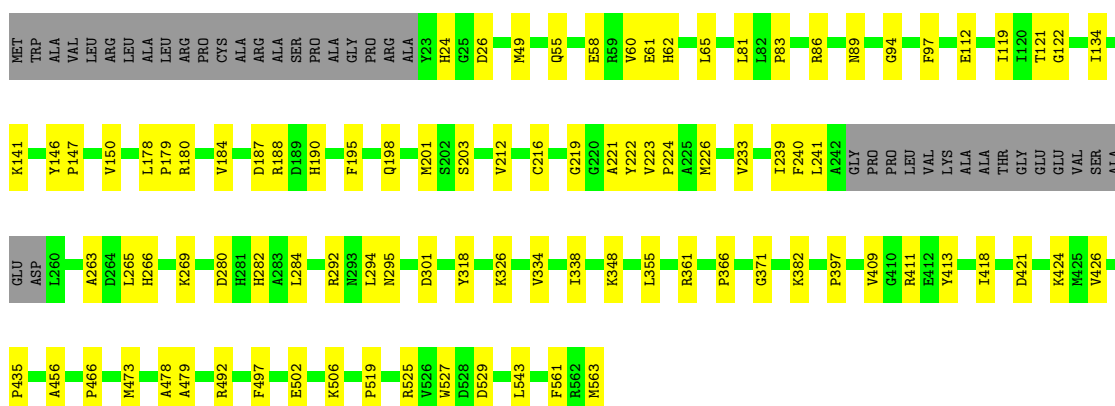
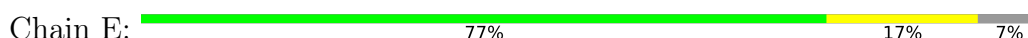




• Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial



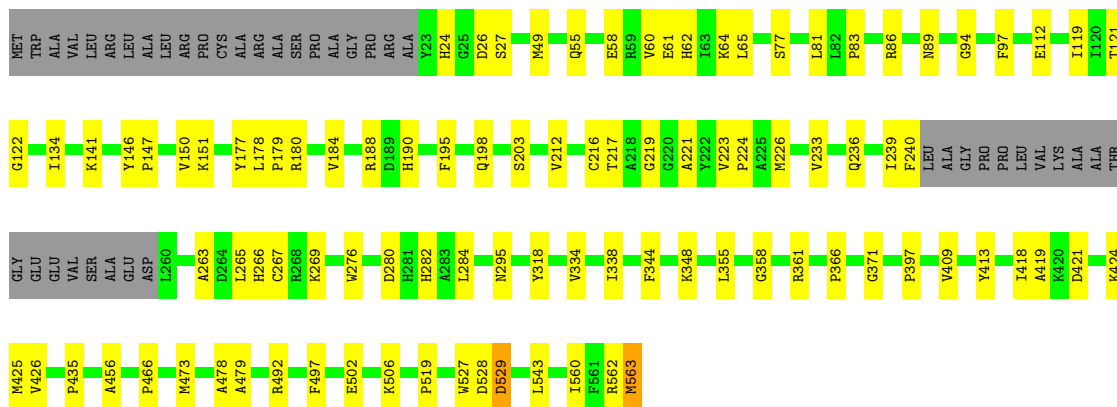
• Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial



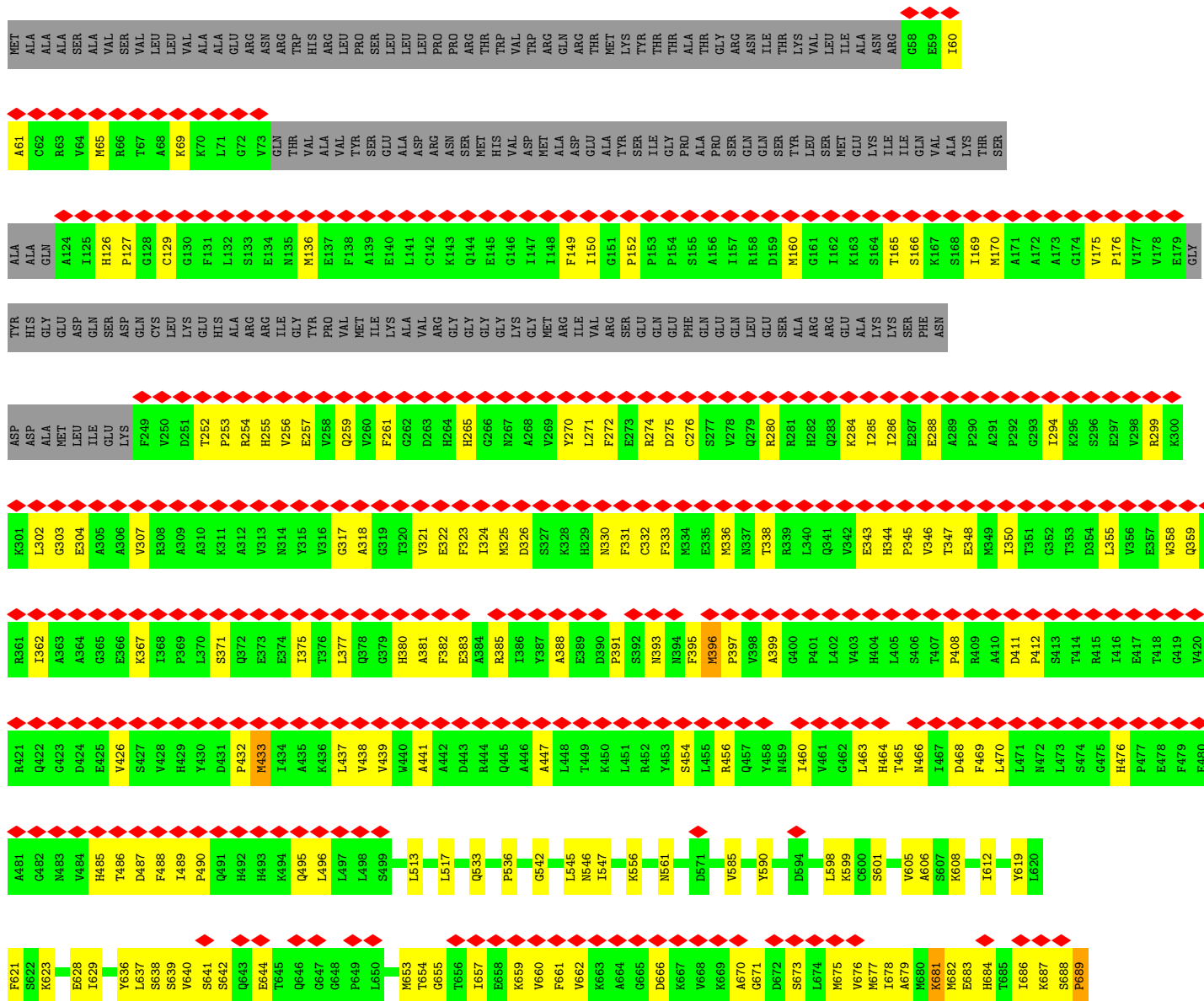
• Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial







● Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial





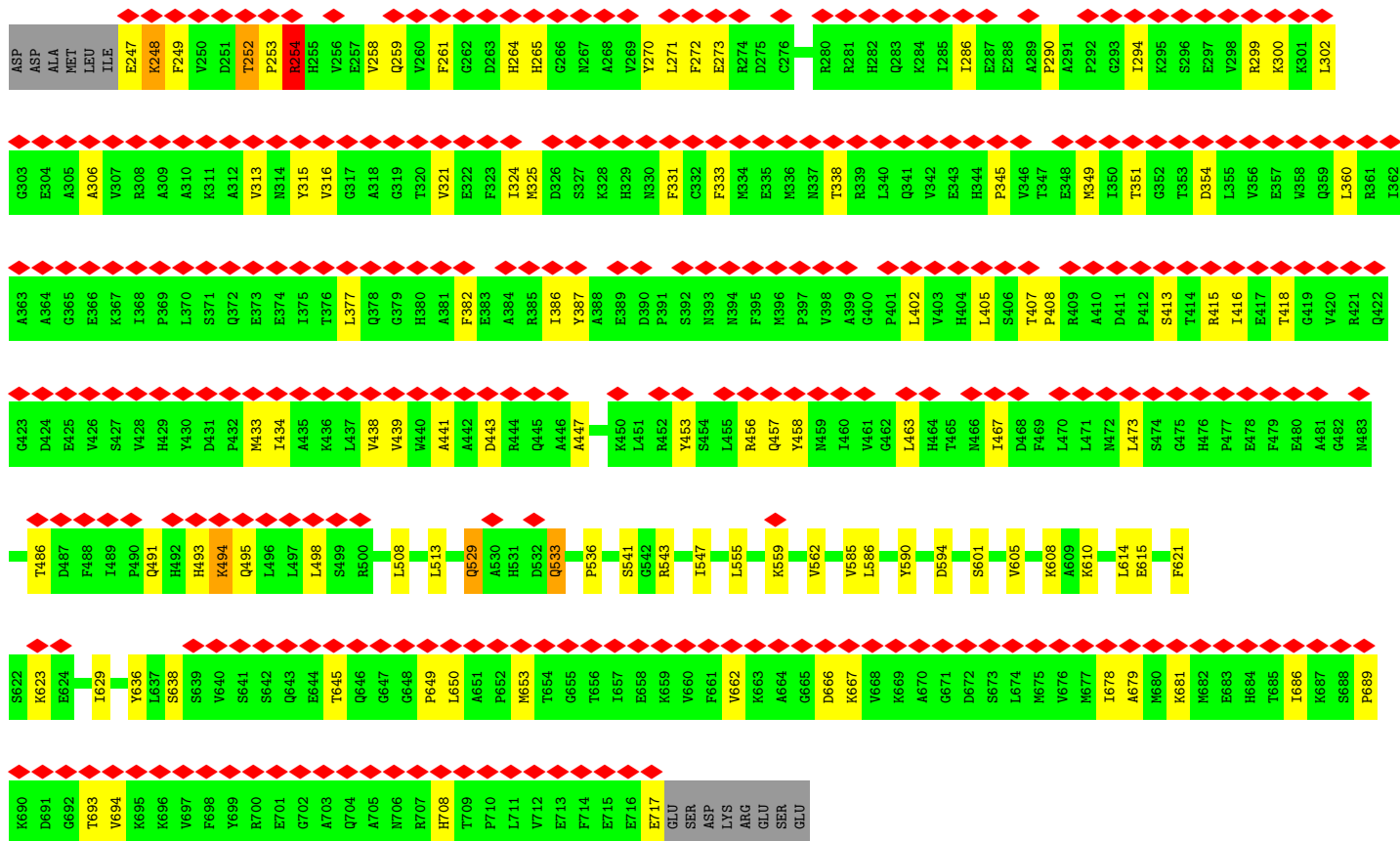


Q123	GLY
A124	GLU
I125	ASP
H126	GLN
P127	SER
G128	ASP
C129	GLN
G130	CYS
F131	LYS
L132	GLU
S133	HIS
E134	ALA
M135	ARG
M136	ARG
E137	ILE
F138	LEU
A139	PRO
E140	GLY
C142	TRP
K143	VAL
E144	ARG
E145	GLY
G146	GLY
I147	GLY
I148	LYS
F149	MET
I150	ARG
G151	ILE
P152	VAL
P153	ARG
P154	SER
S155	GLU
A156	GLN
I157	GLU
R158	GLN
D159	LEU
M160	LEU
G161	SER
I162	ALA
K163	ALA
S164	ARG
T165	GLU
S166	ALA
K167	LYS
S168	LYS
I169	SER
M170	PHE
A171	ASN
A172	ASP
A173	ASP
G174	ASP
V175	ASP
P176	ASP
V177	ASP
E178	ASP
E179	ASP
G180	ASP
Y181	ASP
Y182	ASP
H182	ASP
ALA	ALA
MET	MET
LEU	LEU
ILE	ILE
E247	E247
K248	K248
F249	F249
V250	V250
D251	D251
T252	T252
P253	P253
R254	R254
H255	H255
V256	V256
E257	E257
V258	V258
Q259	Q259
V260	V260
F261	F261
G262	G262
D263	D263
H264	H264
H265	H265
G266	G266
H267	H267
A268	A268
V269	V269
Y270	Y270
L271	L271
F272	F272
E273	E273
R274	R274
D275	D275
C276	C276
S277	S277
V278	V278
Q279	Q279
R280	R280
R281	R281
H282	H282
Q283	Q283
K284	K284
I285	I285
L286	L286
A288	A288
P290	P290
A291	A291
P292	P292
G293	G293
L294	L294
K295	K295
S296	S296
E297	E297
V298	V298
R299	R299
K300	K300
K301	K301
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G303	G303
E304	E304
A305	A305
A306	A306
V307	V307
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A309	A309
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F312	F312
V313	V313
H314	H314
Y315	Y315
V316	V316
G317	G317
A318	A318
G319	G319
T320	T320
Y321	Y321
E322	E322
F323	F323
I324	I324
M325	M325
D326	D326
S327	S327
K328	K328
H329	H329
M330	M330
F331	F331
C332	C332
F333	F333
M334	M334
E335	E335
M336	M336
H337	H337
T338	T338
R339	R339
L340	L340
Q341	Q341
V342	V342
E343	E343
H344	H344
F345	F345
V346	V346
T347	T347
E348	E348
M349	M349
I350	I350
T351	T351
G352	G352
T353	T353
D354	D354
S355	S355
V356	V356
E357	E357
W358	W358
R359	R359
K360	K360
L361	L361
L362	L362
A363	A363
A364	A364
G365	G365
E366	E366
K367	K367
I368	I368
P369	P369
L370	L370
F371	F371
S372	S372
V373	V373
E374	E374
I375	I375
T376	T376
L377	L377
Q378	Q378
G379	G379
H380	H380
A381	A381
F382	F382
E383	E383
A384	A384
R385	R385
I386	I386
S387	S387
A388	A388
E389	E389
S392	S392
R393	R393
F395	F395
M396	M396
P397	P397
V398	V398
A399	A399
G400	G400
P401	P401
L402	L402
V403	V403
H404	H404
L405	L405
S406	S406
T407	T407
P408	P408
R409	R409
A410	A410
D411	D411
P412	P412
S413	S413
T414	T414
R415	R415
L416	L416
F417	F417
T418	T418
G419	G419
V420	V420
R421	R421
Q422	Q422
G423	G423
D424	D424
E425	E425
V426	V426
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H429	H429
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M433	M433
I434	I434
A435	A435
K436	K436
L437	L437
V438	V438
V439	V439
W440	W440
A441	A441
A442	A442
D443	D443
R444	R444
Q445	Q445
A446	A446
A447	A447
L448	L448
K449	K449
L450	L450
L451	L451
R452	R452
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Q457	Q457
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M472	M472
L473	L473
S474	S474
G475	G475
H476	H476
P477	P477
E478	E478
F479	F479
S640	S640
S641	S641
S642	S642
Q643	Q643
P490	P490
Q491	Q491
H492	H492
H493	H493
K494	K494
Q495	Q495
L496	L496
L497	L497
L498	L498
S499	S499
R500	R500
L508	L508
L513	L513
P536	P536
S541	S541
G542	G542
R543	R543
I547	I547
L555	L555
V562	V562
V585	V585
Y590	Y590
D594	D594
S601	S601
V605	V605
K608	K608
A609	A609
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E615	E615
F621	F621
S622	S622
K623	K623
I629	I629
K635	K635
V636	V636
L637	L637
S638	S638
S639	S639
V640	V640
S641	S641
S642	S642
Q643	Q643
E644	E644
T645	T645
Q646	Q646
G647	G647
G648	G648
P649	P649
L650	L650
A651	A651
P652	P652
M653	M653
T654	T654
G655	G655
T656	T656
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K659	K659
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G665	G665
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A670	A670
G671	G671
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G702	G702
A703	A703
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A705	A705
W706	W706
R707	R707
H708	H708
T709	T709
L710	L710
L711	L711
W712	W712
E713	E713
F714	F714
E716	E716
E717	E717
GLU	GLU
SER	SER
ASP	ASP
LYS	LYS
ARG	ARG
PRO	PRO
LEU	LEU
SER	SER
GLU	GLU

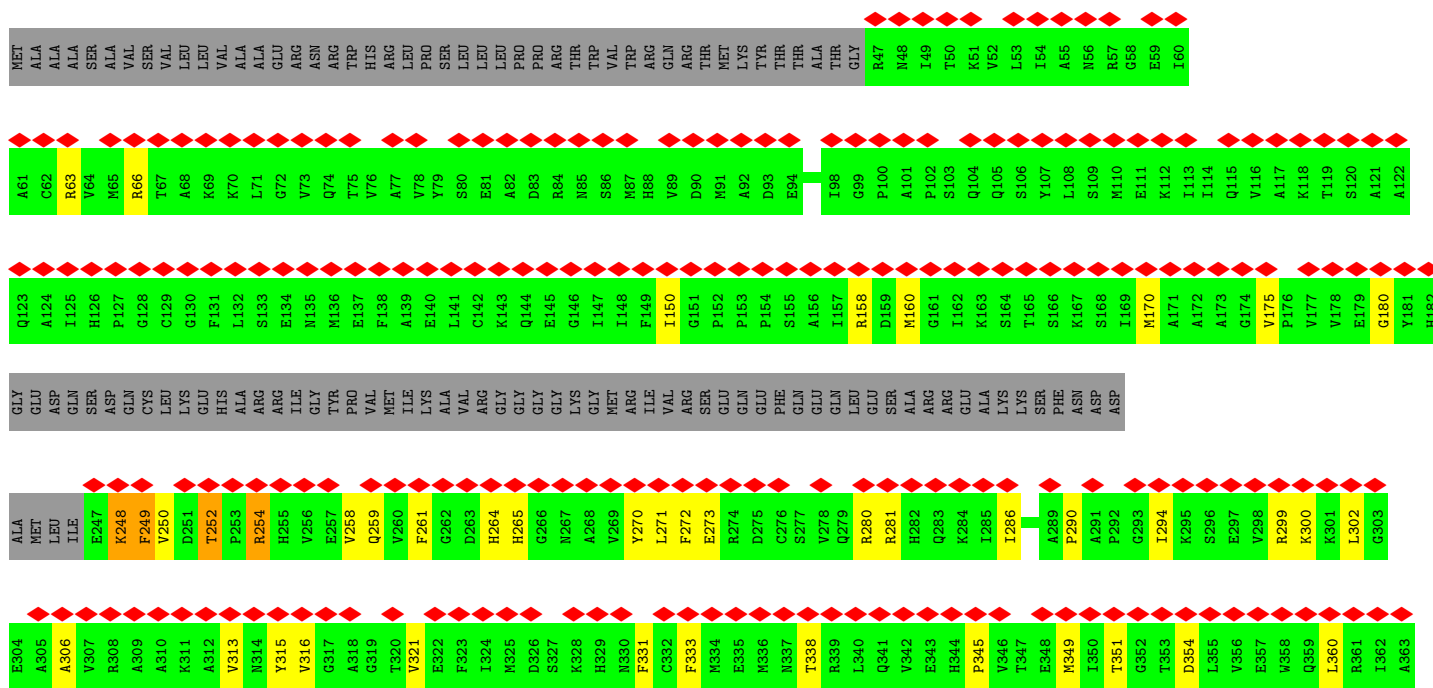
• Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial



MET	R47
ALA	M48
ALA	I49
ALA	I54
SER	A55
VAL	N56
VAL	R57
VAL	G58
VAL	E59
VAL	I60
GLU	
ASP	A61
GLN	C62
GLN	R63
ASP	V64
GLN	M65
ASP	R66
GLN	T67
CYS	A68
LEU	K69
LEU	G70
ALA	L71
ALA	G72
ARG	V73
ASN	Q74
TRP	T75
HIS	V76
LEU	A77
LEU	F78
PRO	Y79
LEU	S80
LEU	E81
PRO	A82
ARG	D83
GLY	R84
GLY	N85
LYS	S86
LYS	M87
ARG	H88
ARG	V89
ILE	D90
VAL	M91
ARG	A92
GLU	D93
GLU	E94
PHE	A95
GLN	Y96
GLU	S97
GLN	I98
GLU	G99
ALA	P100
ARG	A101
ARG	V102
GLU	L103
ALA	I104
LYS	A105
LYS	Q106
SER	Y107
PHE	L108
ASN	E109
	M110
	E111
	K112
	I113
	I114
	Q115
	V116
	A117
	K118
	T119
	S120
A121	A121
Q123	Q123
A124	A124
I125	I125
H126	H126
P127	P127
G128	G128
C129	C129
G130	G130
F131	F131
L132	L132
E134	E134
S133	S133
N135	N135
M136	M136
E137	E137
F138	F138
A139	A139
E140	E140
L141	L141
C142	C142
K143	K143
Q144	Q144
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I147	I147
I148	I148
F149	F149
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G151	G151
P152	P152
P153	P153
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S155	S155
A156	A156
I157	I157
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D159	D159
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S164	S164
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K167	K167
S168	S168
I169	I169
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A172	A172
A173	A173
G174	G174
V175	V175
P176	P176
V177	V177
V178	V178
E179	E179
G180	G180
Y181	Y181
H182	H182
GLY	GLY
GLU	GLU
GLN	GLN
ASP	ASP
GLN	GLN
ASP	ASP
GLN	GLN
CYS	CYS
LEU	LEU
LYS	LYS
HIS	HIS
ALA	ALA
ALA	ALA
ARG	ARG
ARG	ARG
ILE	ILE
GLY	GLY
TRP	TRP
PRO	PRO
VAL	VAL
MET	MET
ILE	ILE
LYS	LYS
LYS	LYS
GLY	GLY
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GLY	GLY
MET	MET
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ILE	ILE
VAL	VAL
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SER	SER
GLU	GLU
GLN	GLN
GLU	GLU
PHE	PHE
GLN	GLN
GLU	GLU
GLN	GLN
LEU	LEU
SER	SER
ALA	ALA
ARG	ARG
ARG	ARG
GLU	GLU
LYS	LYS
LYS	



• Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44531	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.782	Depositor
Minimum map value	-0.224	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.09	Depositor
Map size ( $\text{\AA}$ )	349.2, 349.2, 349.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.97, 0.97, 0.97	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: BTI, TW3

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	0.36	1/4239 (0.0%)	0.51	0/5731
1	C	0.41	1/4087 (0.0%)	0.56	0/5521
1	E	0.36	1/4120 (0.0%)	0.51	0/5566
1	H	0.41	1/4087 (0.0%)	0.56	0/5521
1	J	0.36	1/4107 (0.0%)	0.51	0/5548
1	K	0.36	1/4239 (0.0%)	0.51	0/5731
2	B	0.27	0/4273	0.46	0/5771
2	F	0.55	0/4793	0.73	2/6476 (0.0%)
2	G	0.54	0/4793	0.73	2/6476 (0.0%)
2	I	0.55	0/4793	0.73	2/6476 (0.0%)
2	L	0.27	1/4273 (0.0%)	0.46	0/5771
2	M	0.55	0/4793	0.73	2/6476 (0.0%)
All	All	0.43	7/52597 (0.0%)	0.60	8/71064 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	PRO	N-CD	5.26	1.55	1.47
1	K	435	PRO	N-CD	5.25	1.55	1.47
1	H	435	PRO	N-CD	5.22	1.55	1.47
1	C	435	PRO	N-CD	5.21	1.55	1.47
1	E	435	PRO	N-CD	5.21	1.55	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	158	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	I	158	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	M	158	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	G	158	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	I	66	ARG	NE-CZ-NH1	5.52	123.06	120.30



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	4154	0	4130	147	0
1	C	4006	0	3982	133	0
1	E	4038	0	4018	122	0
1	H	4006	0	3982	138	0
1	J	4025	0	4002	124	0
1	K	4154	0	4130	134	0
2	B	4192	0	4199	223	0
2	F	4703	0	4703	88	0
2	G	4703	0	4703	90	0
2	I	4703	0	4703	95	0
2	L	4192	0	4199	223	0
2	M	4703	0	4703	91	0
3	A	54	0	0	2	0
3	C	54	0	0	6	0
3	E	54	0	0	4	0
3	H	54	0	0	7	0
3	J	54	0	0	5	0
3	K	54	0	0	2	0
4	C	15	0	16	7	0
4	F	15	0	15	3	0
4	G	15	0	15	3	0
4	H	15	0	16	9	0
4	I	15	0	15	3	0
4	M	15	0	15	3	0
All	All	51993	0	51546	1383	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 13.

The worst 5 of 1383 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:A:278:LEU:HD11	2:B:641:SER:CB	1.30	1.61
1:K:278:LEU:HD11	2:L:641:SER:CB	1.30	1.56
2:F:681:LYS:NZ	4:F:801:BTI:C11	1.71	1.54
2:M:681:LYS:NZ	4:M:801:BTI:C11	1.71	1.53
2:G:681:LYS:NZ	4:G:801:BTI:C11	1.71	1.52

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	539/563 (96%)	521 (97%)	18 (3%)	0	100	100
1	C	516/563 (92%)	502 (97%)	14 (3%)	0	100	100
1	E	520/563 (92%)	502 (96%)	17 (3%)	1 (0%)	47	81
1	H	516/563 (92%)	503 (98%)	12 (2%)	1 (0%)	47	81
1	J	518/563 (92%)	500 (96%)	17 (3%)	1 (0%)	47	81
1	K	539/563 (96%)	520 (96%)	17 (3%)	2 (0%)	34	72
2	B	535/725 (74%)	524 (98%)	11 (2%)	0	100	100
2	F	603/725 (83%)	585 (97%)	18 (3%)	0	100	100
2	G	603/725 (83%)	579 (96%)	24 (4%)	0	100	100
2	I	603/725 (83%)	584 (97%)	18 (3%)	1 (0%)	47	81
2	L	535/725 (74%)	524 (98%)	11 (2%)	0	100	100
2	M	603/725 (83%)	585 (97%)	18 (3%)	0	100	100
All	All	6630/7728 (86%)	6429 (97%)	195 (3%)	6 (0%)	54	84

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	26	ASP

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Mol	Chain	Res	Type
1	K	529	ASP
1	H	26	ASP
1	E	529	ASP
1	J	529	ASP

### 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	430/445 (97%)	418 (97%)	12 (3%)	43	72
1	C	415/445 (93%)	405 (98%)	10 (2%)	49	76
1	E	418/445 (94%)	409 (98%)	9 (2%)	52	78
1	H	415/445 (93%)	405 (98%)	10 (2%)	49	76
1	J	417/445 (94%)	404 (97%)	13 (3%)	40	70
1	K	430/445 (97%)	420 (98%)	10 (2%)	50	77
2	B	456/609 (75%)	452 (99%)	4 (1%)	78	90
2	F	511/609 (84%)	495 (97%)	16 (3%)	40	70
2	G	511/609 (84%)	497 (97%)	14 (3%)	44	73
2	I	511/609 (84%)	494 (97%)	17 (3%)	38	68
2	L	456/609 (75%)	452 (99%)	4 (1%)	78	90
2	M	511/609 (84%)	497 (97%)	14 (3%)	44	73
All	All	5481/6324 (87%)	5348 (98%)	133 (2%)	51	76

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	240	PHE
1	E	563	MET
1	J	560	ILE
2	F	458	TYR
2	F	443	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	477	GLN
2	M	259	GLN
1	H	518	ASN
2	I	429	HIS
2	M	457	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](#)

12 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	$\# Z  > 2$
3	TW3	A	601	-	47,56,56	0.55	0	60,83,83	1.39	5 (8%)
4	BTI	M	801	-	16,16,16	0.54	0	21,21,21	0.89	1 (4%)
4	BTI	G	801	-	16,16,16	0.54	0	21,21,21	0.90	1 (4%)
4	BTI	F	801	-	16,16,16	0.55	0	21,21,21	0.90	1 (4%)
4	BTI	C	601	-	16,16,16	1.27	1 (6%)	21,21,21	2.18	6 (28%)
3	TW3	C	602	-	47,56,56	0.55	0	60,83,83	1.41	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BTI	H	601	-	16,16,16	1.27	1 (6%)	21,21,21	2.03	7 (33%)
3	TW3	J	601	-	47,56,56	0.55	0	60,83,83	1.40	5 (8%)
4	BTI	I	801	-	16,16,16	0.53	0	21,21,21	0.91	1 (4%)
3	TW3	E	601	-	47,56,56	0.55	0	60,83,83	1.41	5 (8%)
3	TW3	K	601	-	47,56,56	0.55	0	60,83,83	1.39	5 (8%)
3	TW3	H	602	-	47,56,56	0.55	0	60,83,83	1.40	5 (8%)

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
3	TW3	A	601	-	-	13/50/71/71	0/3/3/3
4	BTI	M	801	-	-	2/5/27/27	0/2/2/2
4	BTI	G	801	-	-	2/5/27/27	0/2/2/2
4	BTI	F	801	-	-	2/5/27/27	0/2/2/2
4	BTI	C	601	-	-	4/5/27/27	0/2/2/2
3	TW3	C	602	-	-	13/50/71/71	0/3/3/3
4	BTI	H	601	-	-	4/5/27/27	0/2/2/2
3	TW3	J	601	-	-	13/50/71/71	0/3/3/3
4	BTI	I	801	-	-	2/5/27/27	0/2/2/2
3	TW3	E	601	-	-	13/50/71/71	0/3/3/3
3	TW3	K	601	-	-	13/50/71/71	0/3/3/3
3	TW3	H	602	-	-	13/50/71/71	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	BTI	C2-S1	-3.56	1.76	1.82
4	H	601	BTI	C2-S1	-3.39	1.77	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	TW3	C4-C5-S1	7.96	121.18	111.24
3	C	602	TW3	C4-C5-S1	7.96	121.17	111.24
3	J	601	TW3	C4-C5-S1	7.92	121.13	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	602	TW3	C4-C5-S1	7.92	121.12	111.24
3	A	601	TW3	C4-C5-S1	7.88	121.07	111.24

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

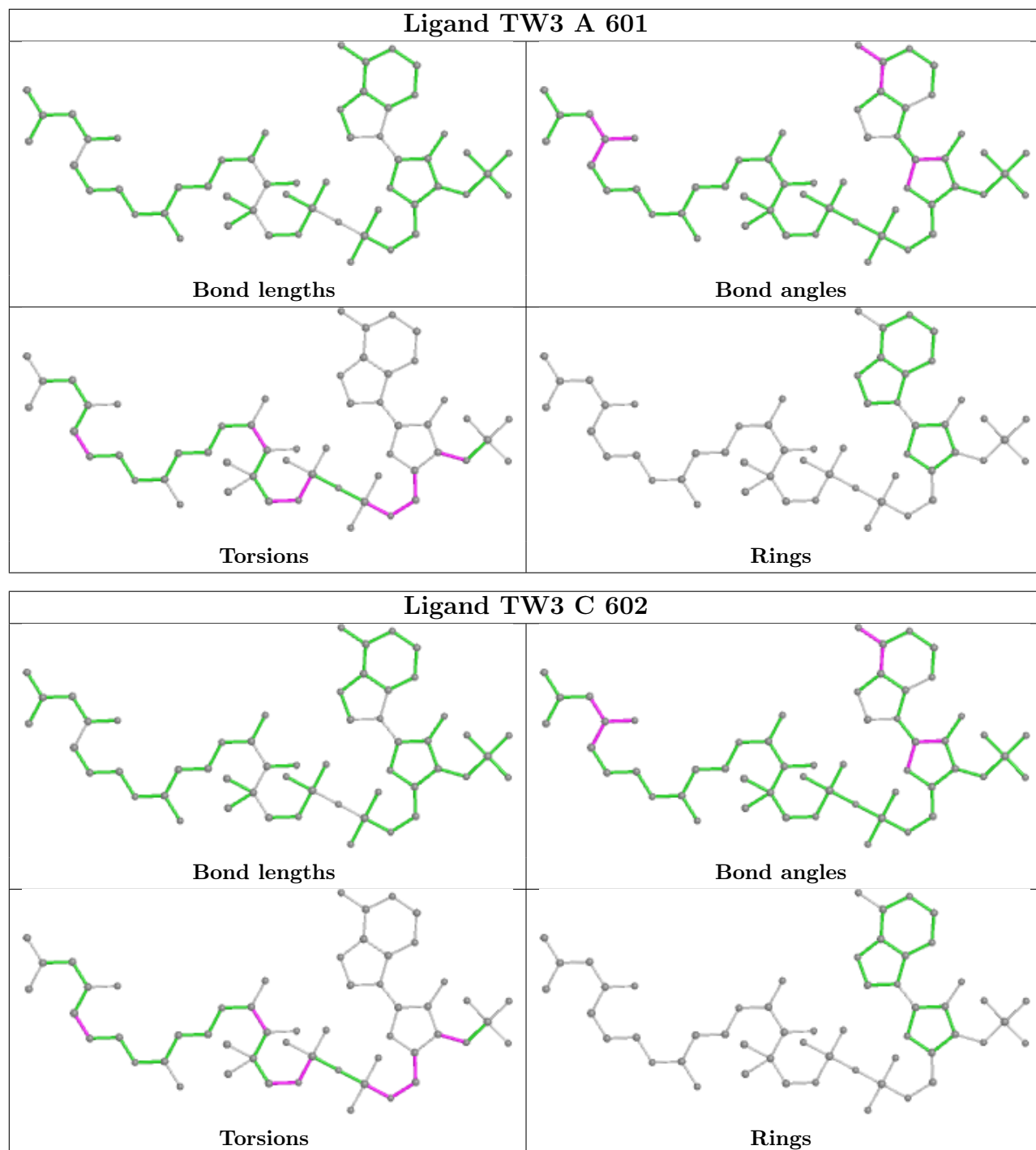
Mol	Chain	Res	Type	Atoms
3	K	601	TW3	N2-C11-C12-C13
3	K	601	TW3	N2-C11-C12-O4
3	K	601	TW3	O3-C11-C12-C13
3	K	601	TW3	O3-C11-C12-O4
3	K	601	TW3	C18-C17-O11-P2

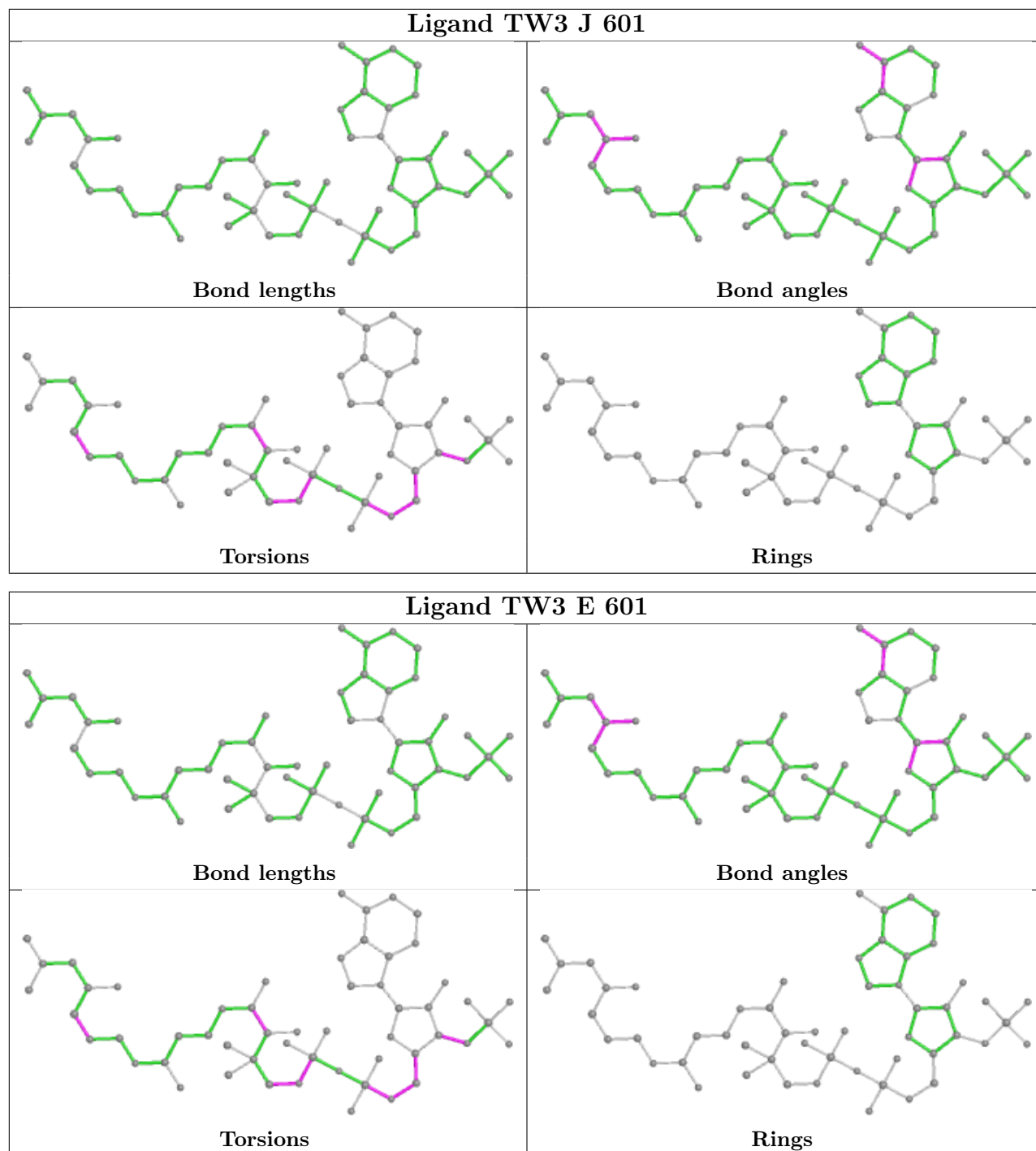
There are no ring outliers.

12 monomers are involved in 54 short contacts:

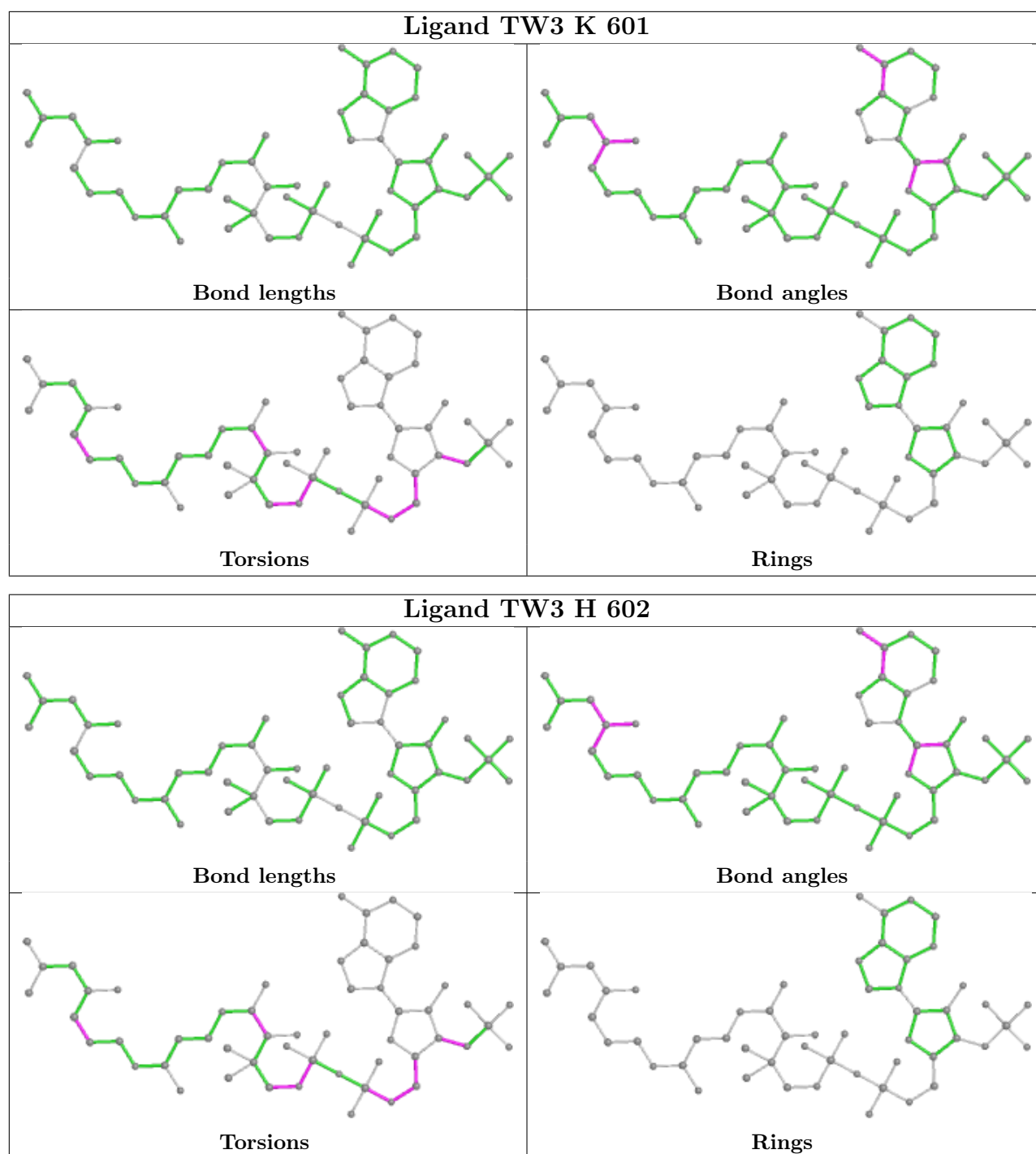
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	TW3	2	0
4	M	801	BTI	3	0
4	G	801	BTI	3	0
4	F	801	BTI	3	0
4	C	601	BTI	7	0
3	C	602	TW3	6	0
4	H	601	BTI	9	0
3	J	601	TW3	5	0
4	I	801	BTI	3	0
3	E	601	TW3	4	0
3	K	601	TW3	2	0
3	H	602	TW3	7	0

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.

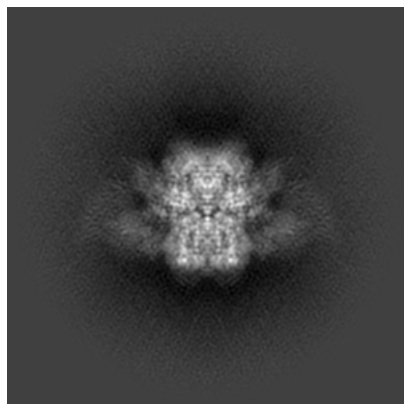
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36705. These allow visual inspection of the internal detail of the map and identification of artifacts.

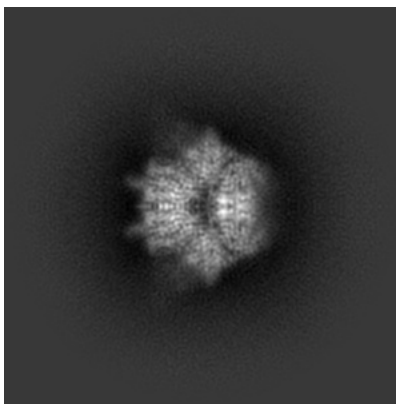
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

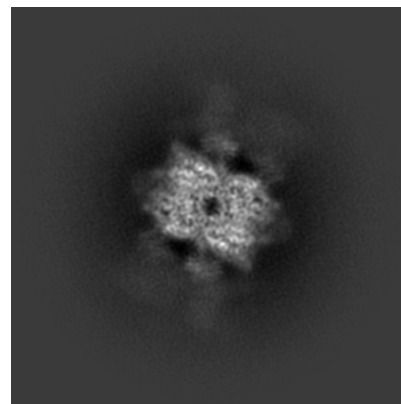
#### 6.1.1 Primary map



X

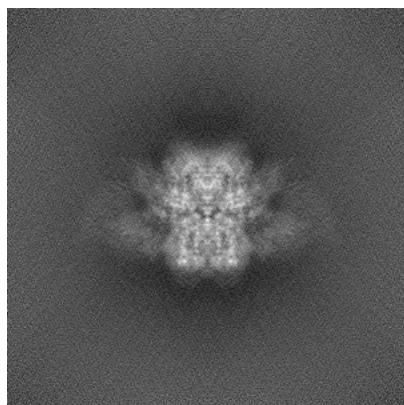


Y

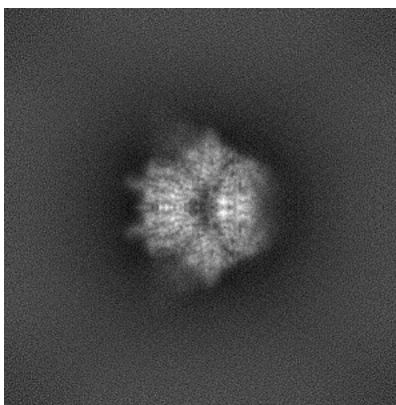


Z

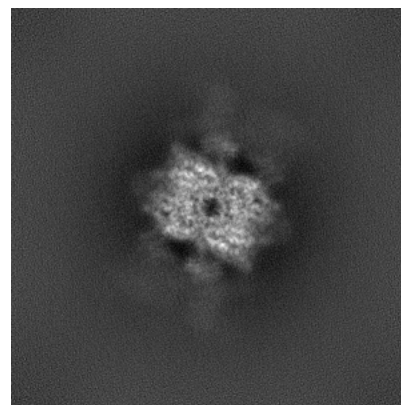
#### 6.1.2 Raw map



X



Y

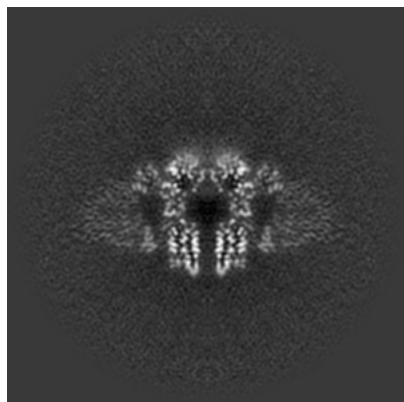


Z

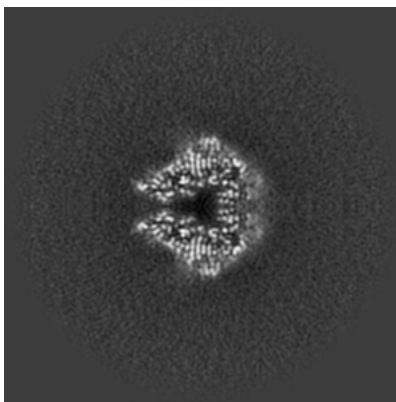
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

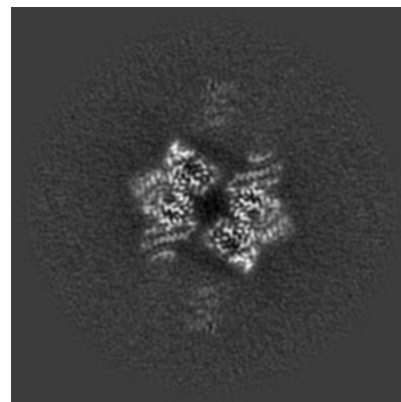
### 6.2.1 Primary map



X Index: 180

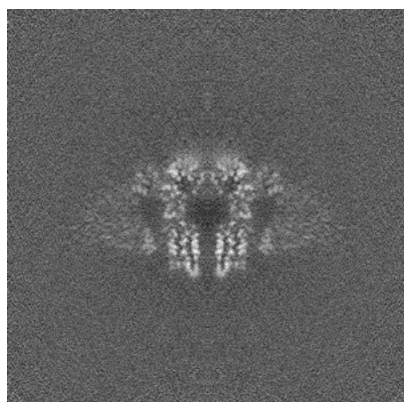


Y Index: 180

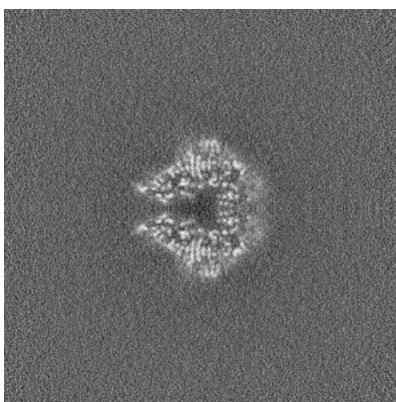


Z Index: 180

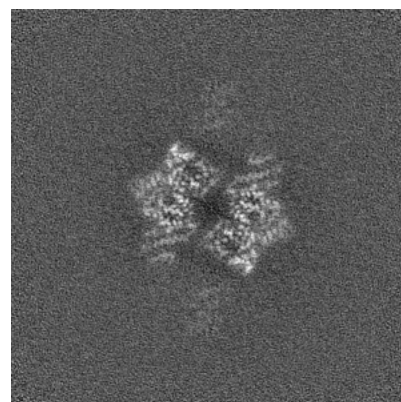
### 6.2.2 Raw map



X Index: 180



Y Index: 180

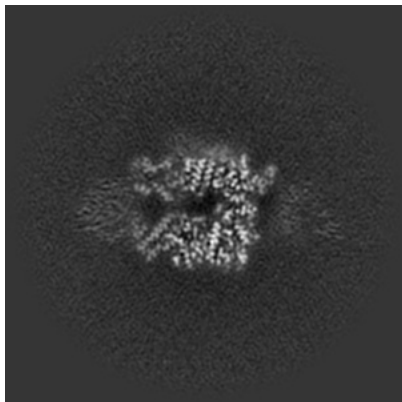


Z Index: 180

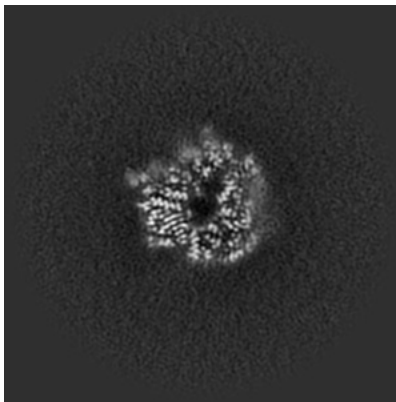
The images above show central slices of the map in three orthogonal directions.

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

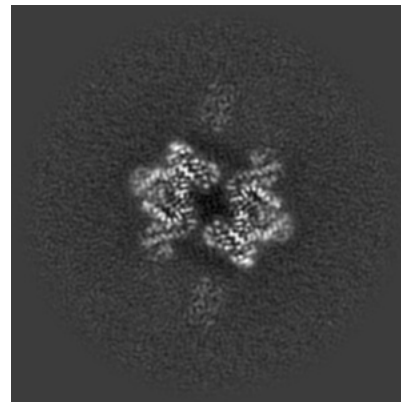
### 6.3.1 Primary map



X Index: 171

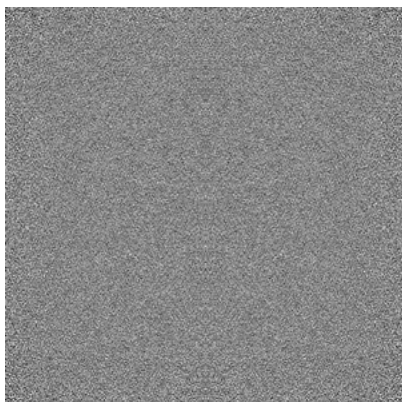


Y Index: 170

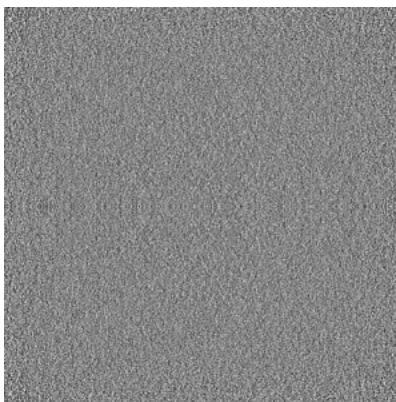


Z Index: 182

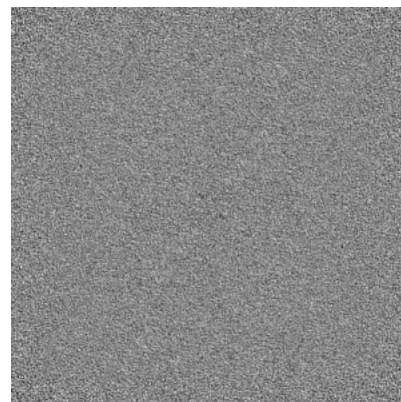
### 6.3.2 Raw map



X Index: 0



Y Index: 0

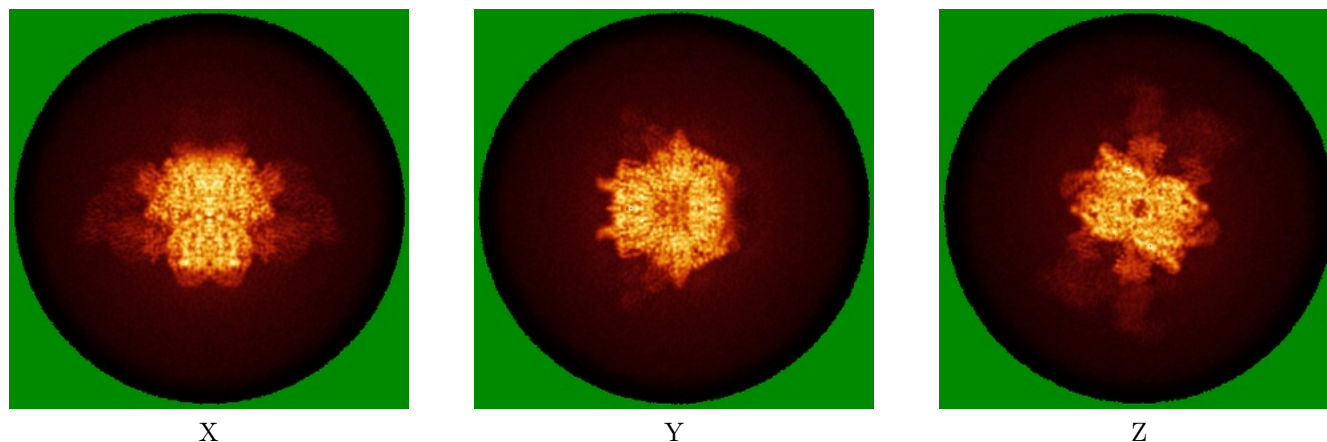


Z Index: 0

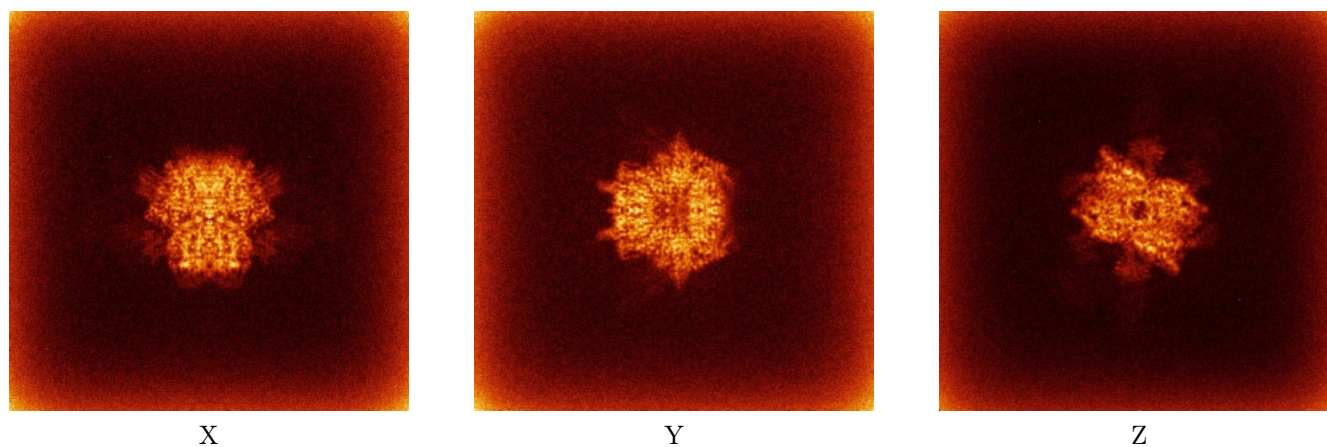
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



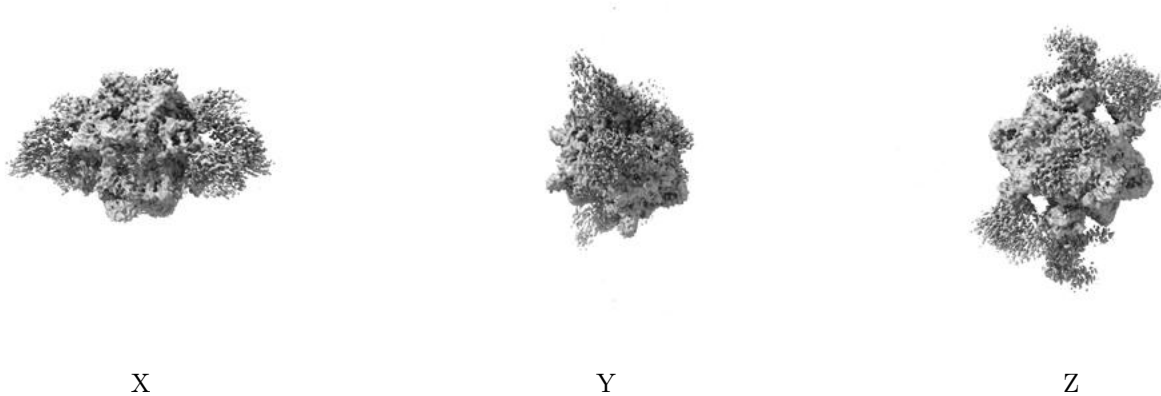
### 6.4.2 Raw map



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.

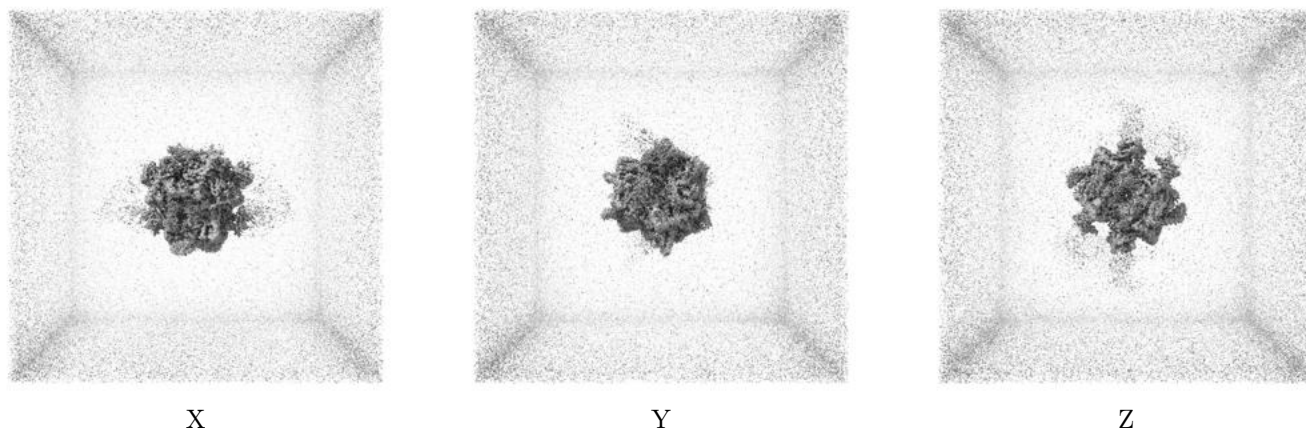
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

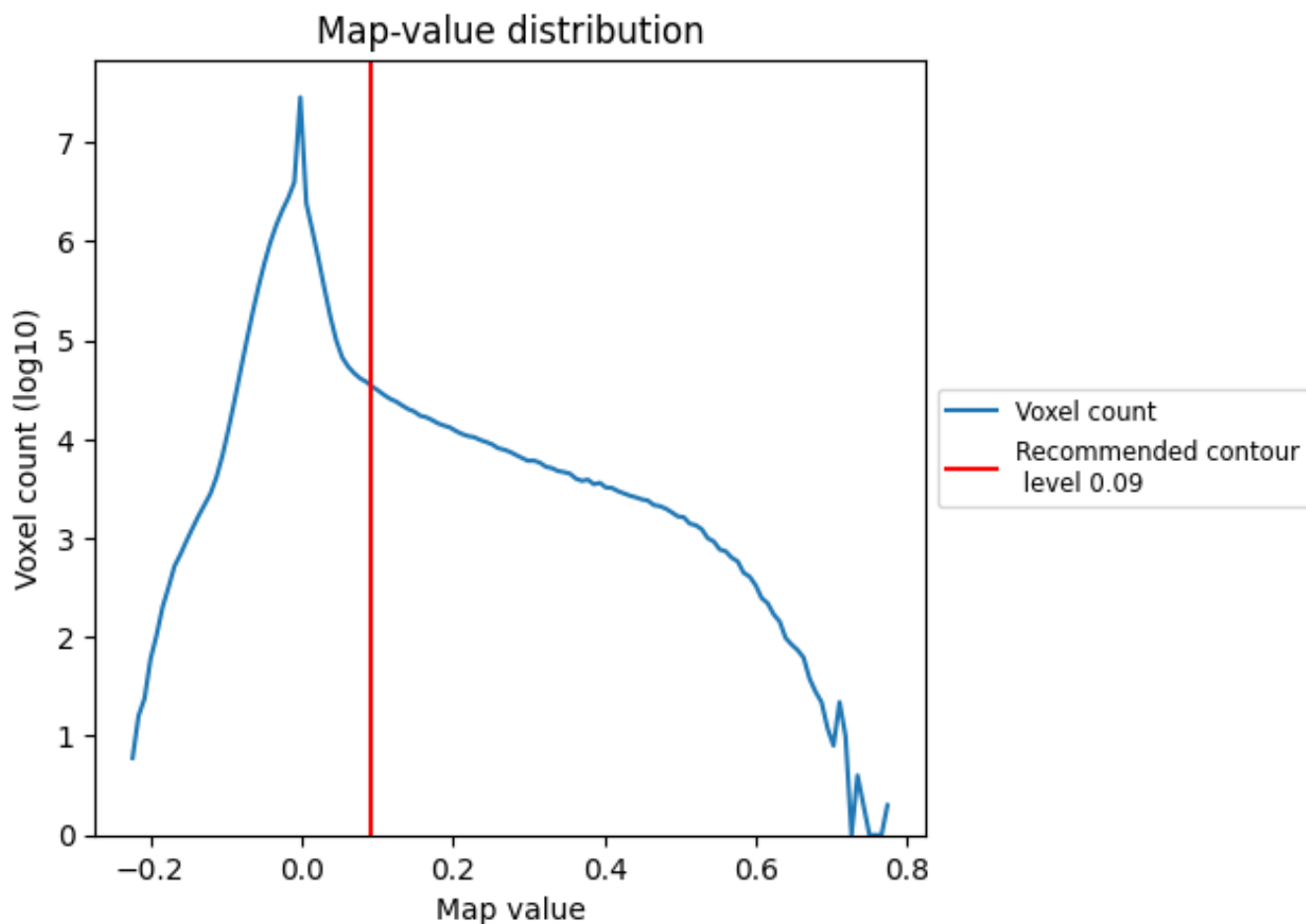
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

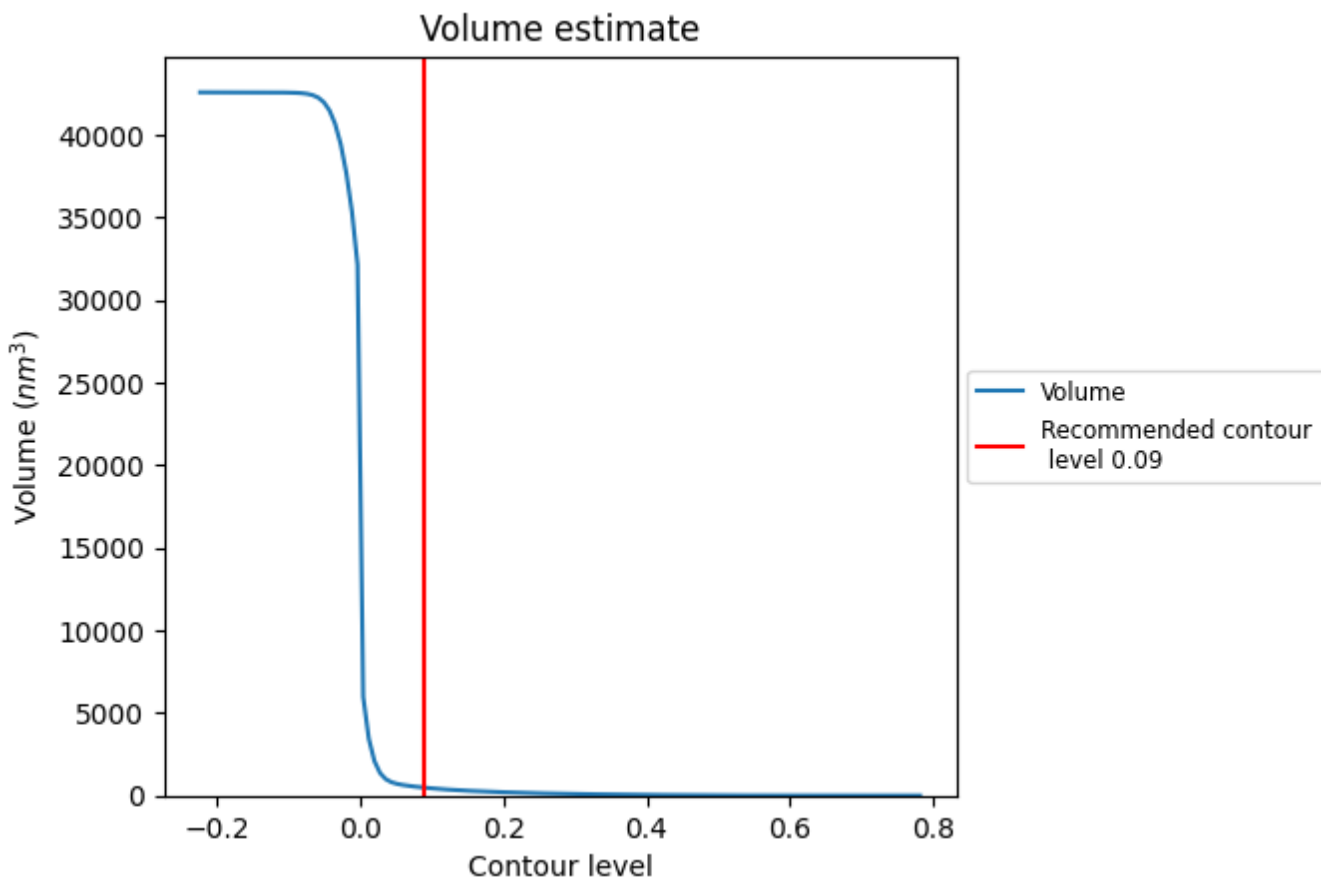
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

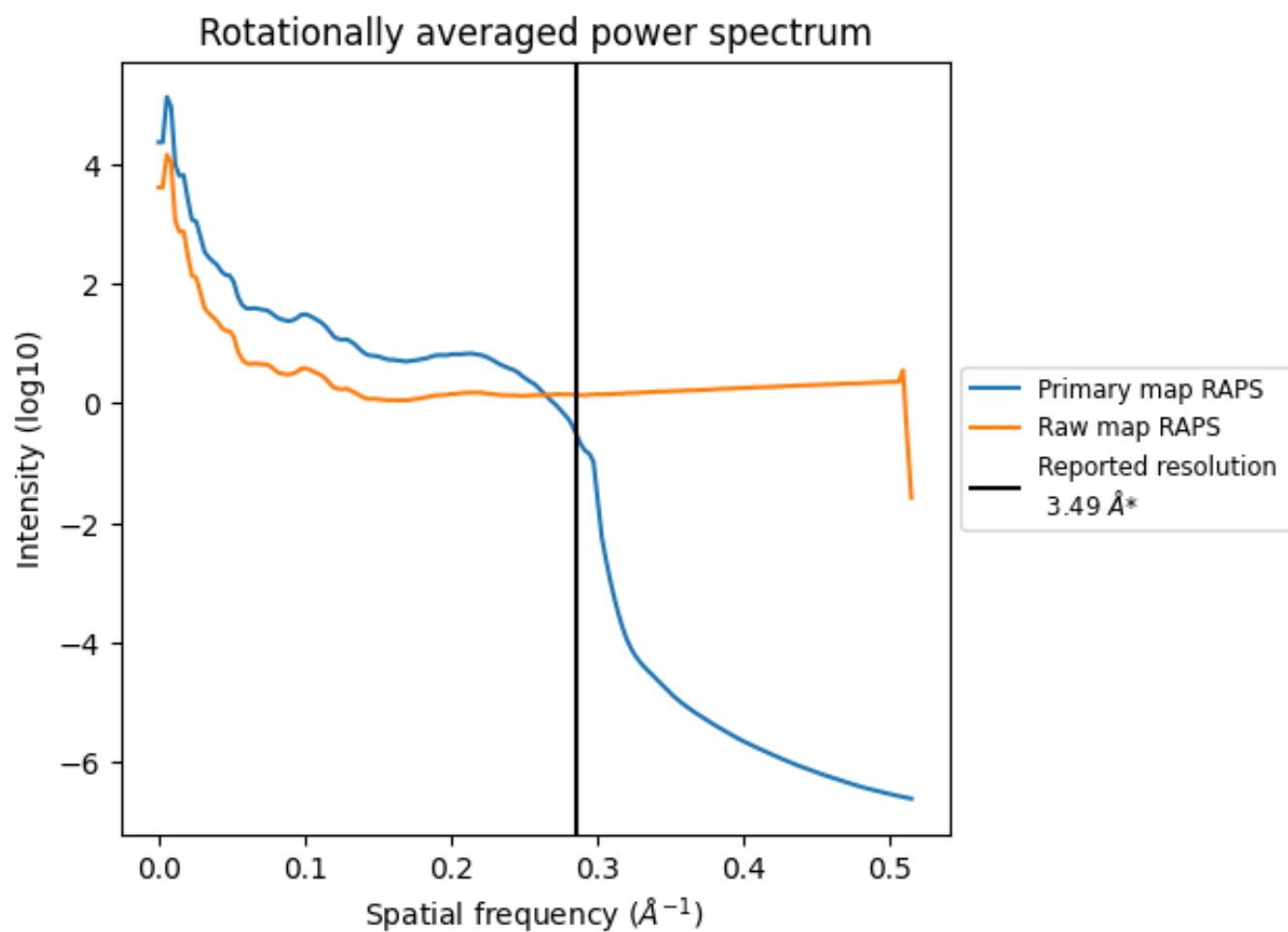


The volume at the recommended contour level is 477 nm<sup>3</sup>; this corresponds to an approximate mass of 431 kDa.

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

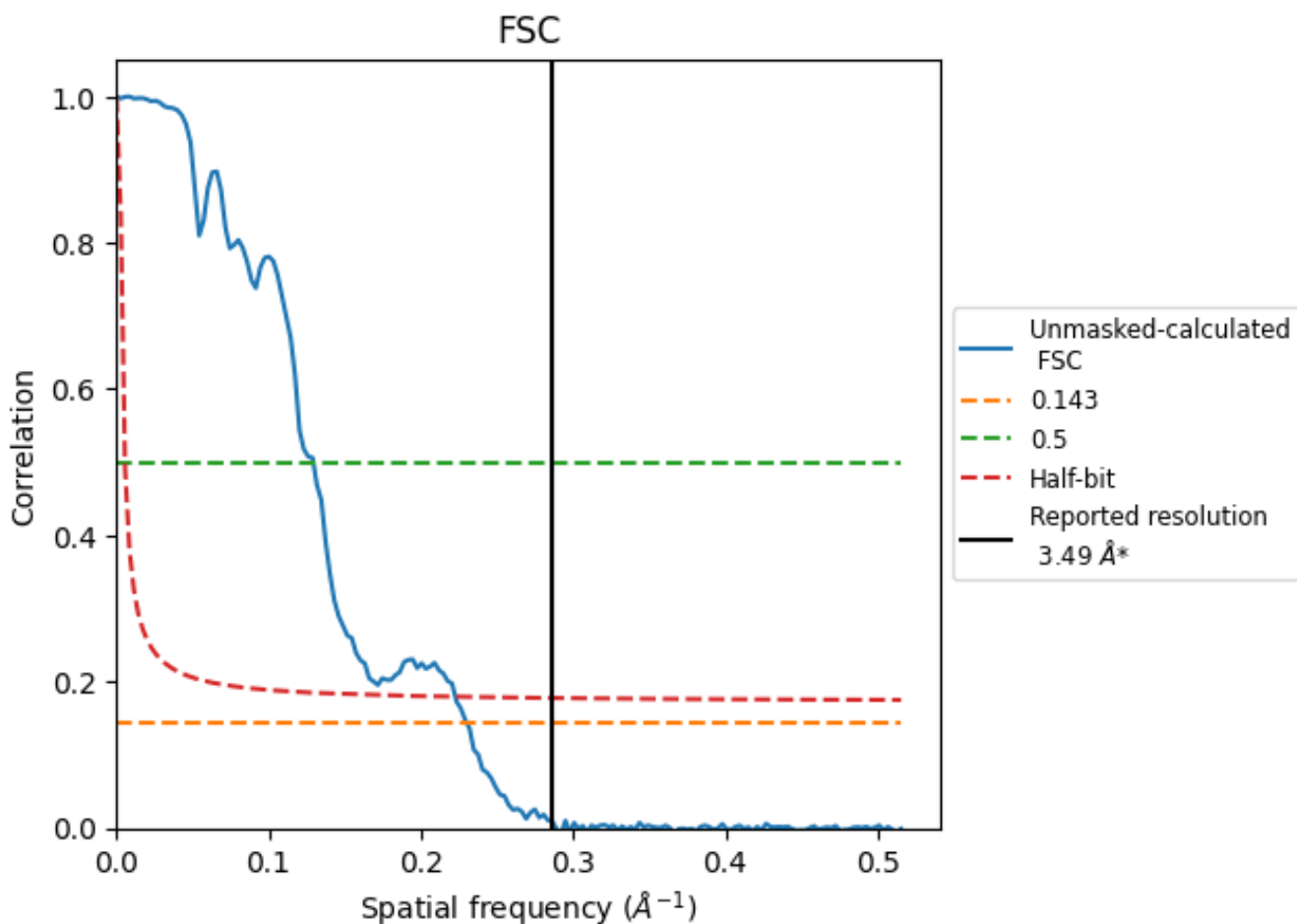


\*Reported resolution corresponds to spatial frequency of 0.287 Å<sup>-1</sup>

## 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 0.287 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

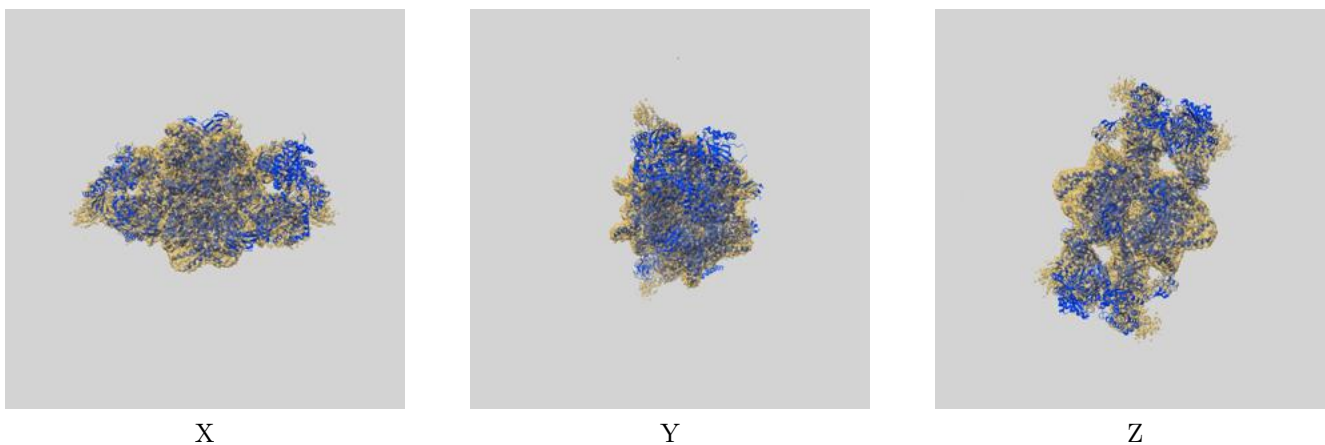
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.34	7.73	4.49

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.49 by more than 10 %

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

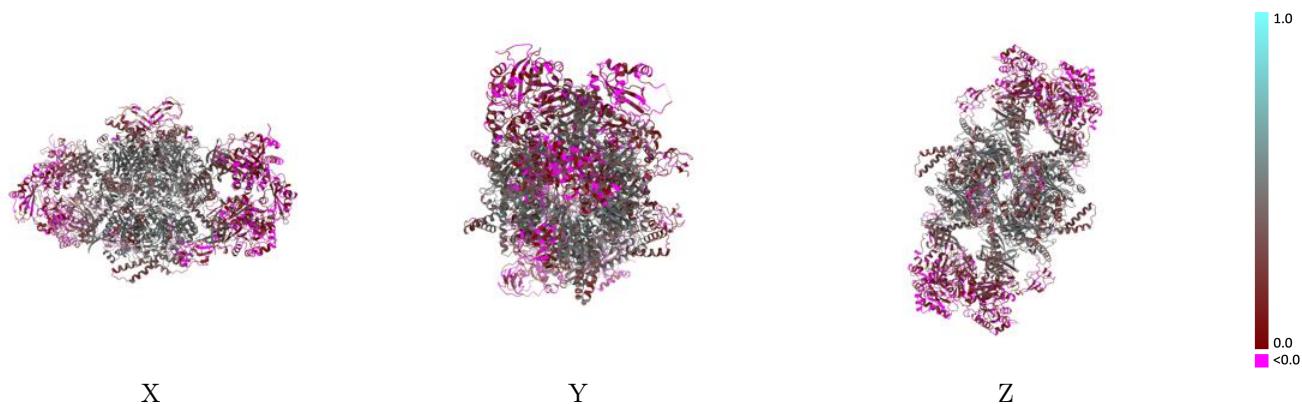
This section contains information regarding the fit between EMDB map EMD-36705 and PDB model 8JXM. Per-residue inclusion information can be found in section 3 on page 7.

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



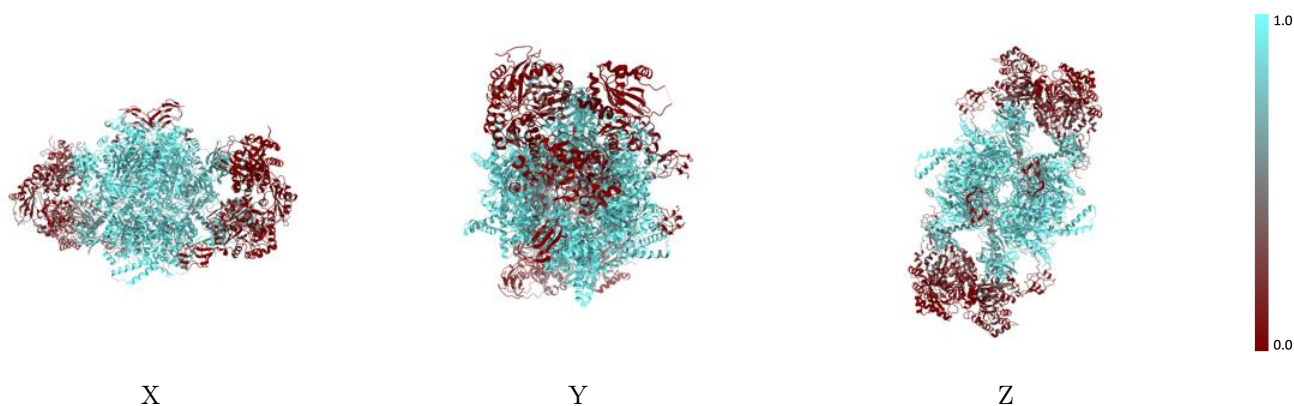
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



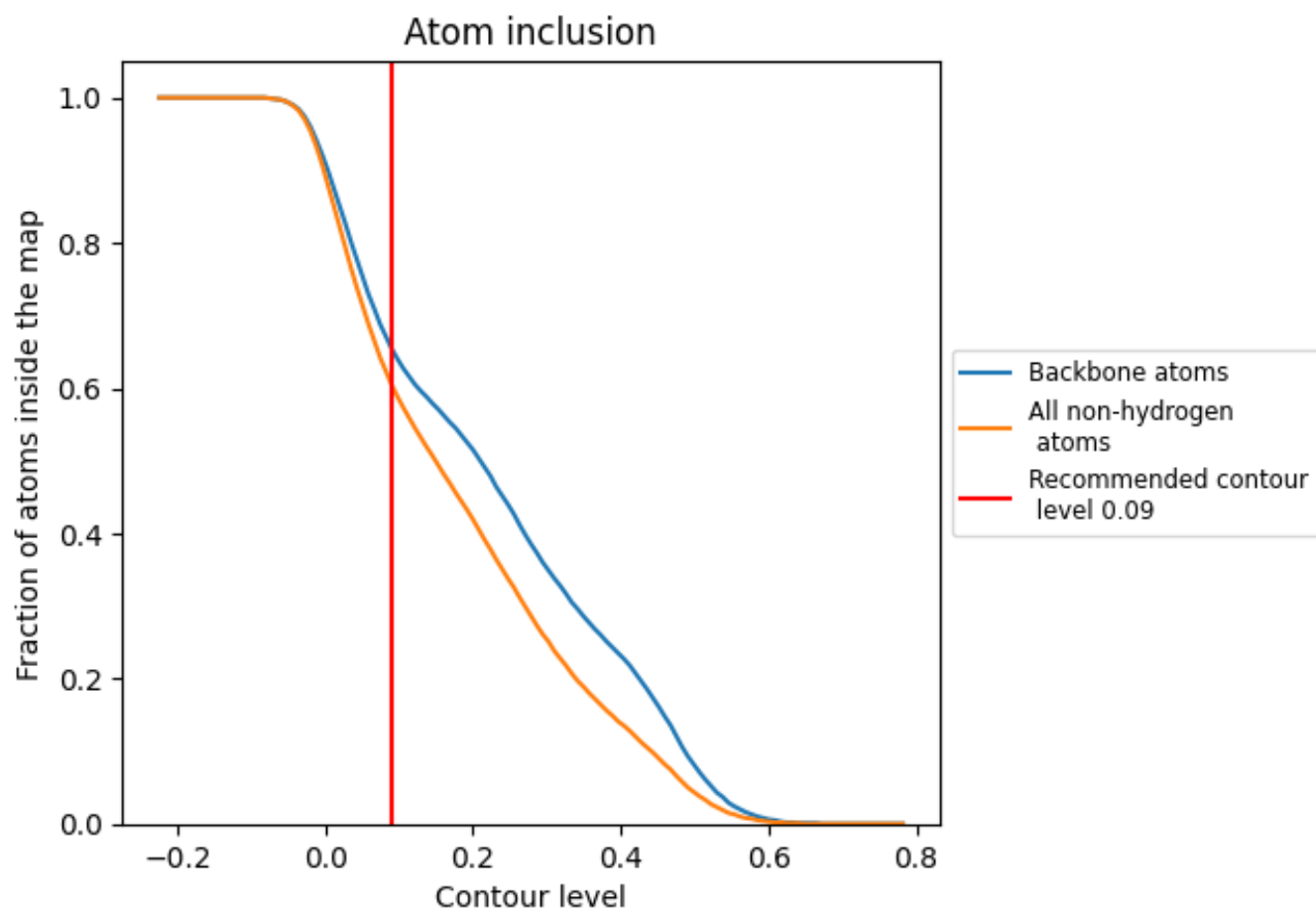
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 61% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6060	 0.2890
A	 0.9580	 0.4320
B	 0.2930	 0.1610
C	 0.9510	 0.4320
E	 0.9610	 0.4420
F	 0.2640	 0.1550
G	 0.3110	 0.1530
H	 0.9530	 0.4310
I	 0.2620	 0.1540
J	 0.9610	 0.4430
K	 0.9580	 0.4330
L	 0.2920	 0.1600
M	 0.3100	 0.1510

