



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 12:17 PM UTC

PDB ID : 8J4Z / pdb_00008j4z
EMDB ID : EMD-35980
Title : Human 3-methylcrotonyl-CoA carboxylase in BCCP-CTS state with substrate
Authors : Liu, D.S.; Su, J.Y.
Deposited on : 2023-04-21
Resolution : 2.73 Å(reported)

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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

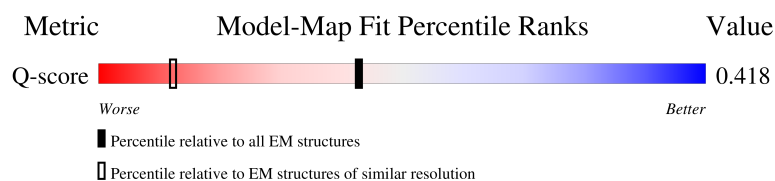
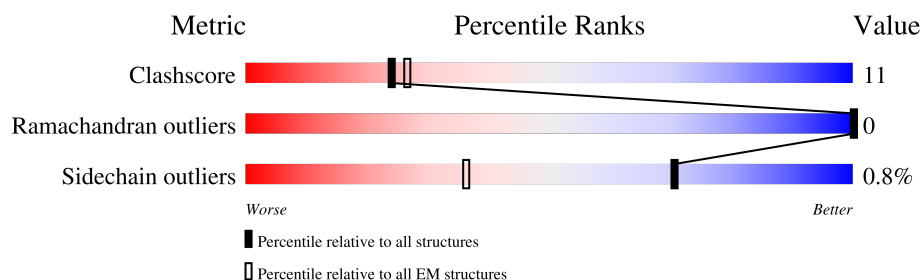
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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	10432 (2.23 - 3.23)

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	563	80% 16% .
1	C	563	80% 16% .
1	F	563	80% 16% .
1	H	563	80% 16% .

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Mol	Chain	Length	Quality of chain
1	J	563	
1	K	563	
2	B	725	
2	D	725	
2	E	725	
2	G	725	
2	I	725	
2	L	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
3	BTI	A	800	-	-	X	-
3	BTI	C	800	-	-	X	-
3	BTI	F	802	-	-	X	-
3	BTI	H	802	-	-	X	-
3	BTI	J	800	-	-	X	-
3	BTI	K	802	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 53664 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.

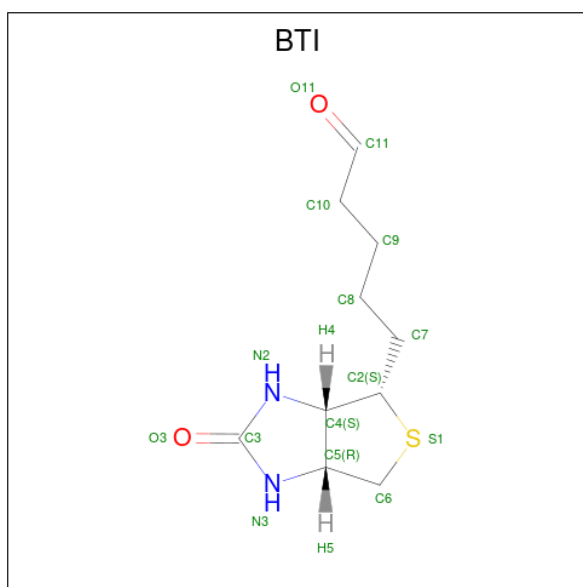
- Molecule 1 is a protein called Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	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	541	Total	C	N	O	S	0	0
			4154	2633	726	776	19		
1	F	541	Total	C	N	O	S	0	0
			4154	2633	726	776	19		
1	H	541	Total	C	N	O	S	0	0
			4154	2633	726	776	19		
1	K	541	Total	C	N	O	S	0	0
			4154	2633	726	776	19		

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

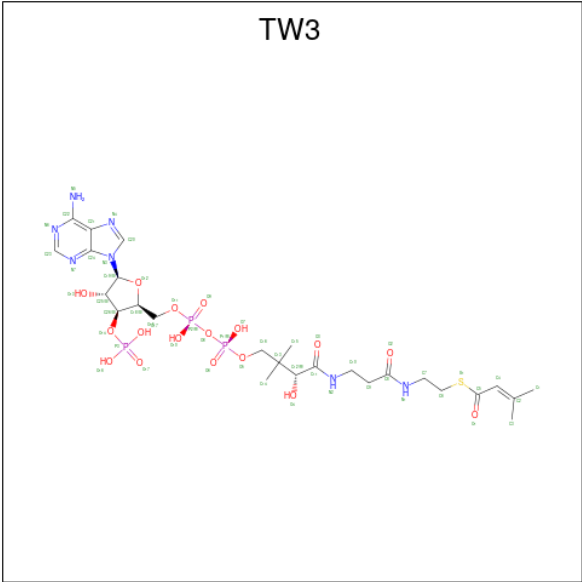
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	610	Total	C	N	O	S	0	0
			4721	2974	822	895	30		
2	B	610	Total	C	N	O	S	0	0
			4721	2974	822	895	30		
2	D	610	Total	C	N	O	S	0	0
			4721	2974	822	895	30		
2	G	610	Total	C	N	O	S	0	0
			4721	2974	822	895	30		
2	I	610	Total	C	N	O	S	0	0
			4721	2974	822	895	30		
2	L	610	Total	C	N	O	S	0	0
			4721	2974	822	895	30		

- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					AltConf
3	J	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	A	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	C	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	F	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	H	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	K	1	Total	C	N	O	S	0
			15	10	2	2	1	

- Molecule 4 is {S}-[2-[3-[(2 {R})-4-[[[(2 {S}),3 {S}),4 {S}),5 {S}]-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethyl] 3-methylbut-2-enethioate (CCD ID: TW3) (formula: C₂₆H₄₂N₇O₁₇P₃S).



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

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.

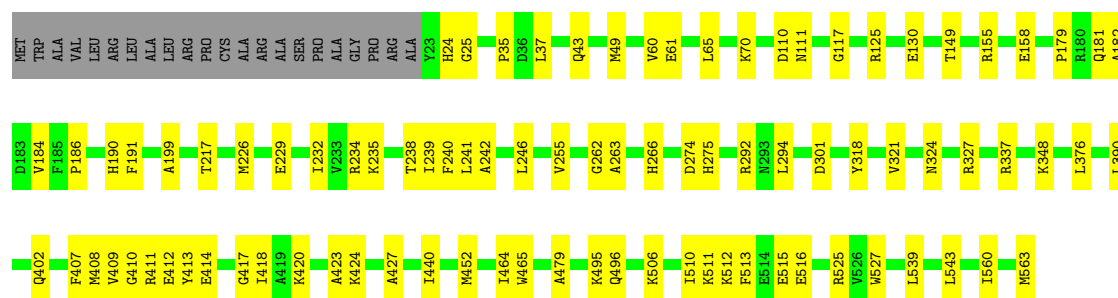
- Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

Chain J: 



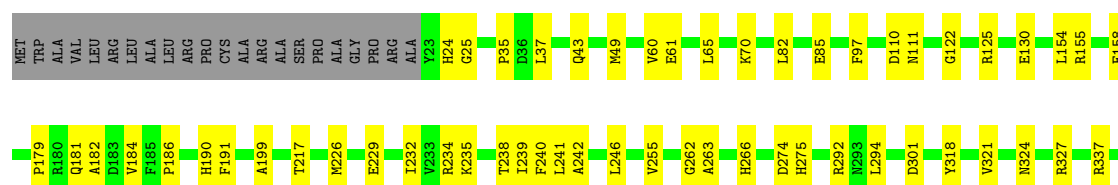
- Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

Chain A: 



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

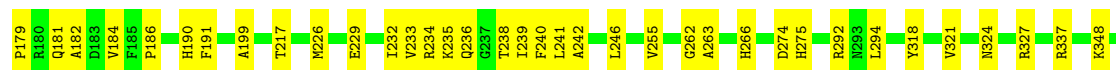
Chain C: 





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

Chain F: 80% 16%



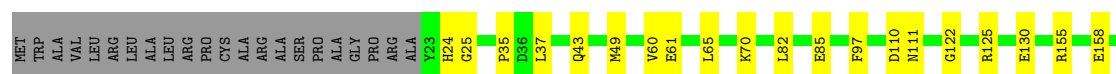
- Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

Chain H: 80% 16%



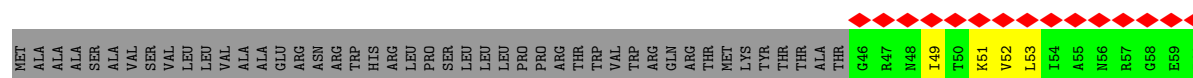
- Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

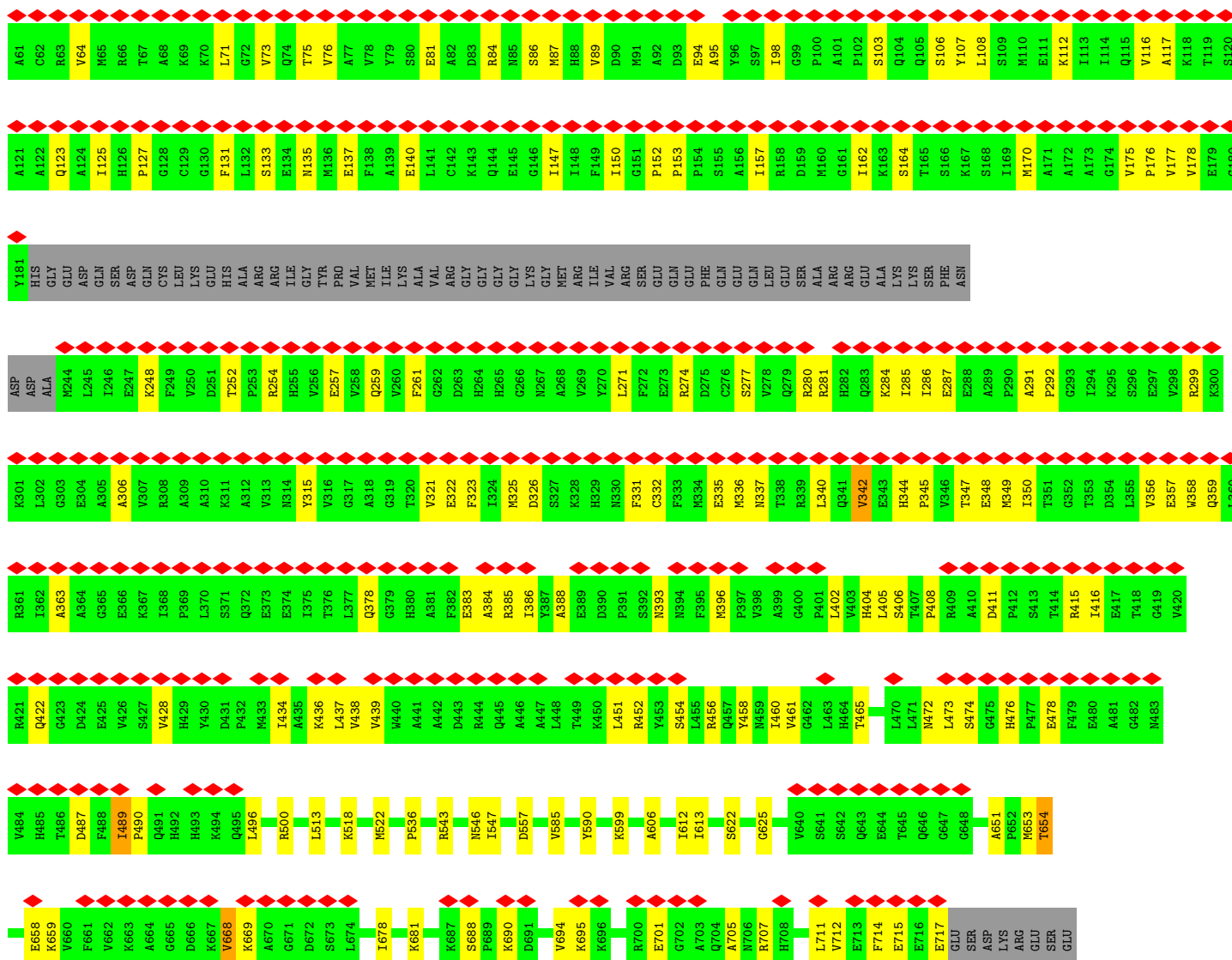
Chain K: 80% 16%



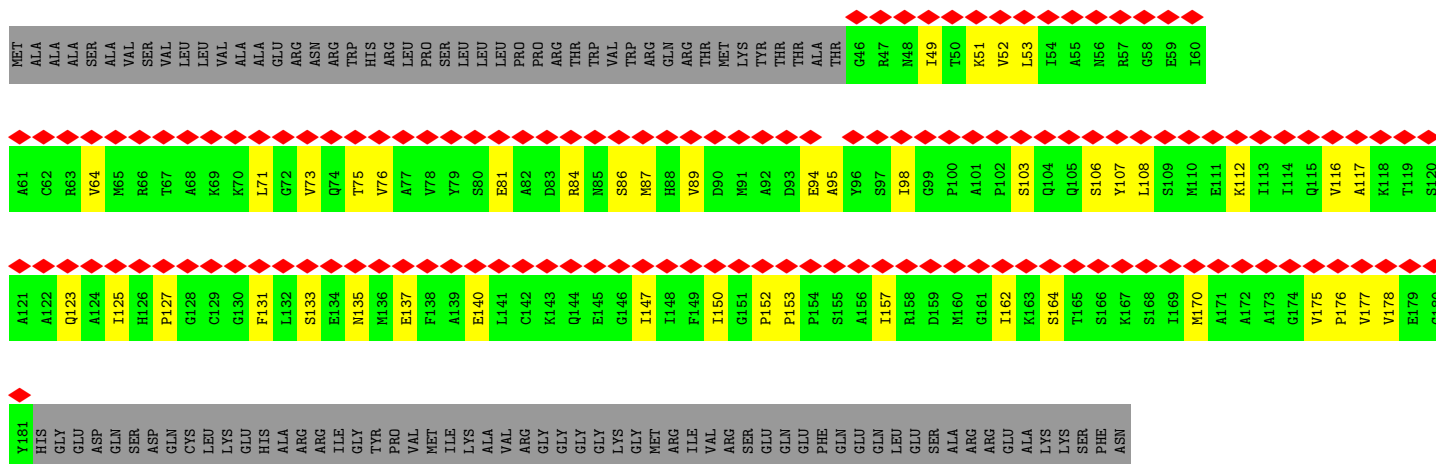
- Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial

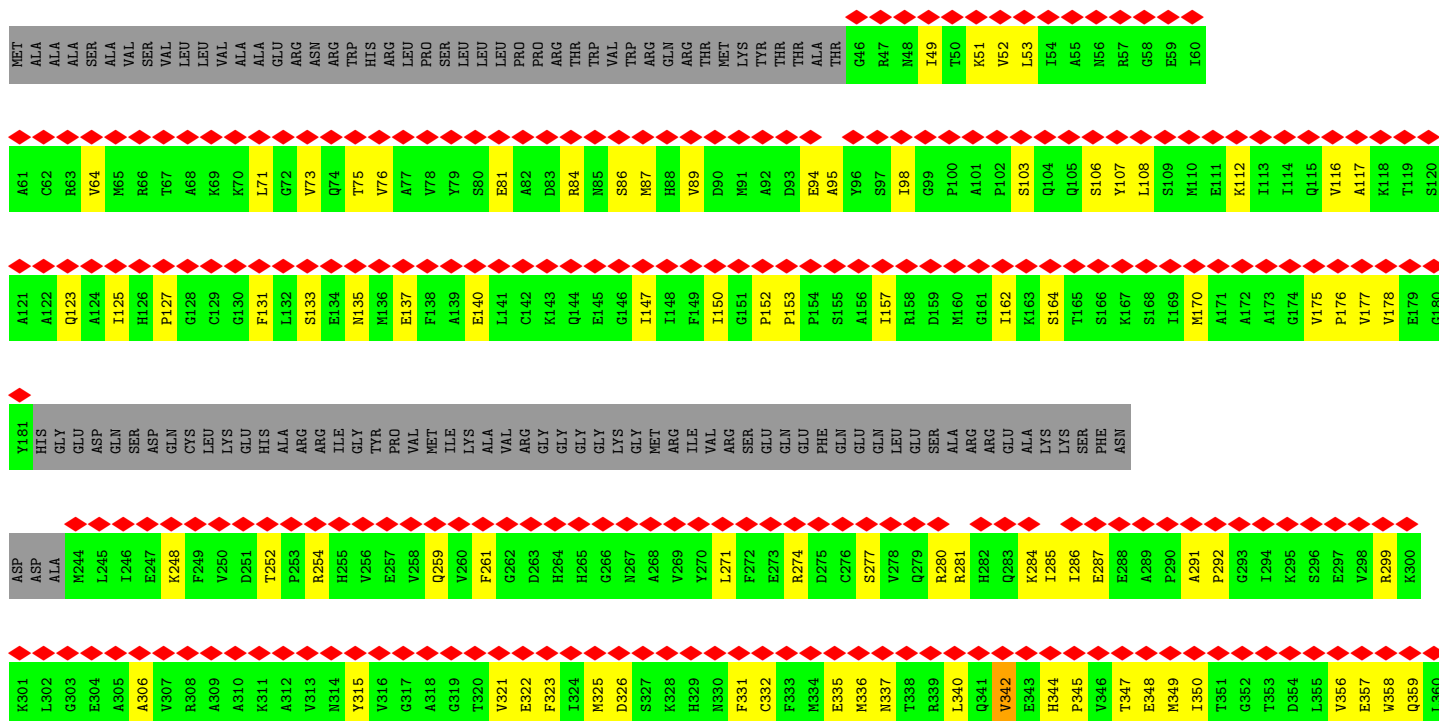
Chain E: 54% 61% 22% 16%

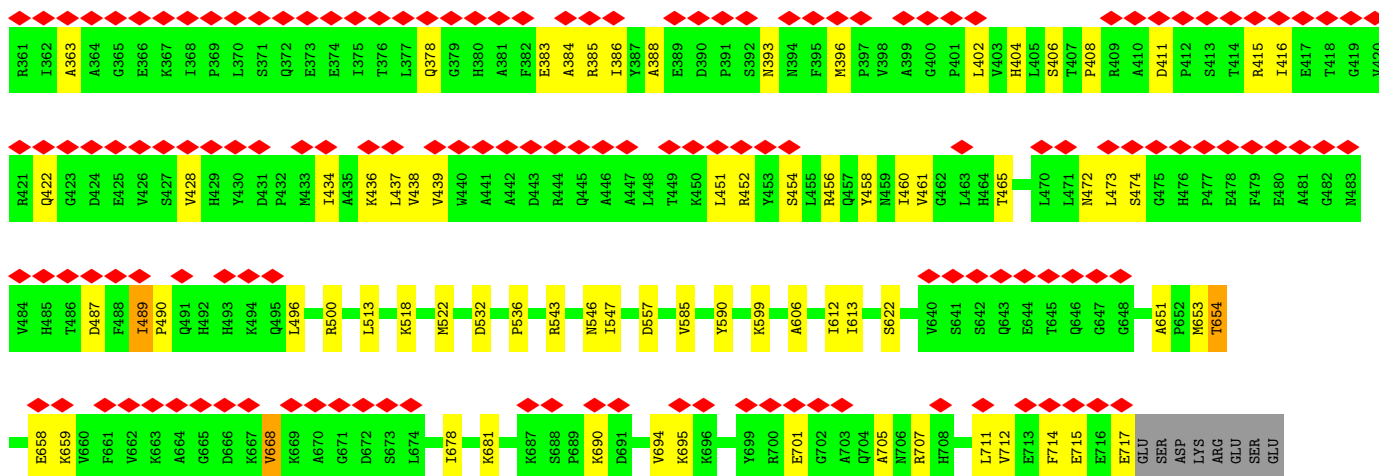




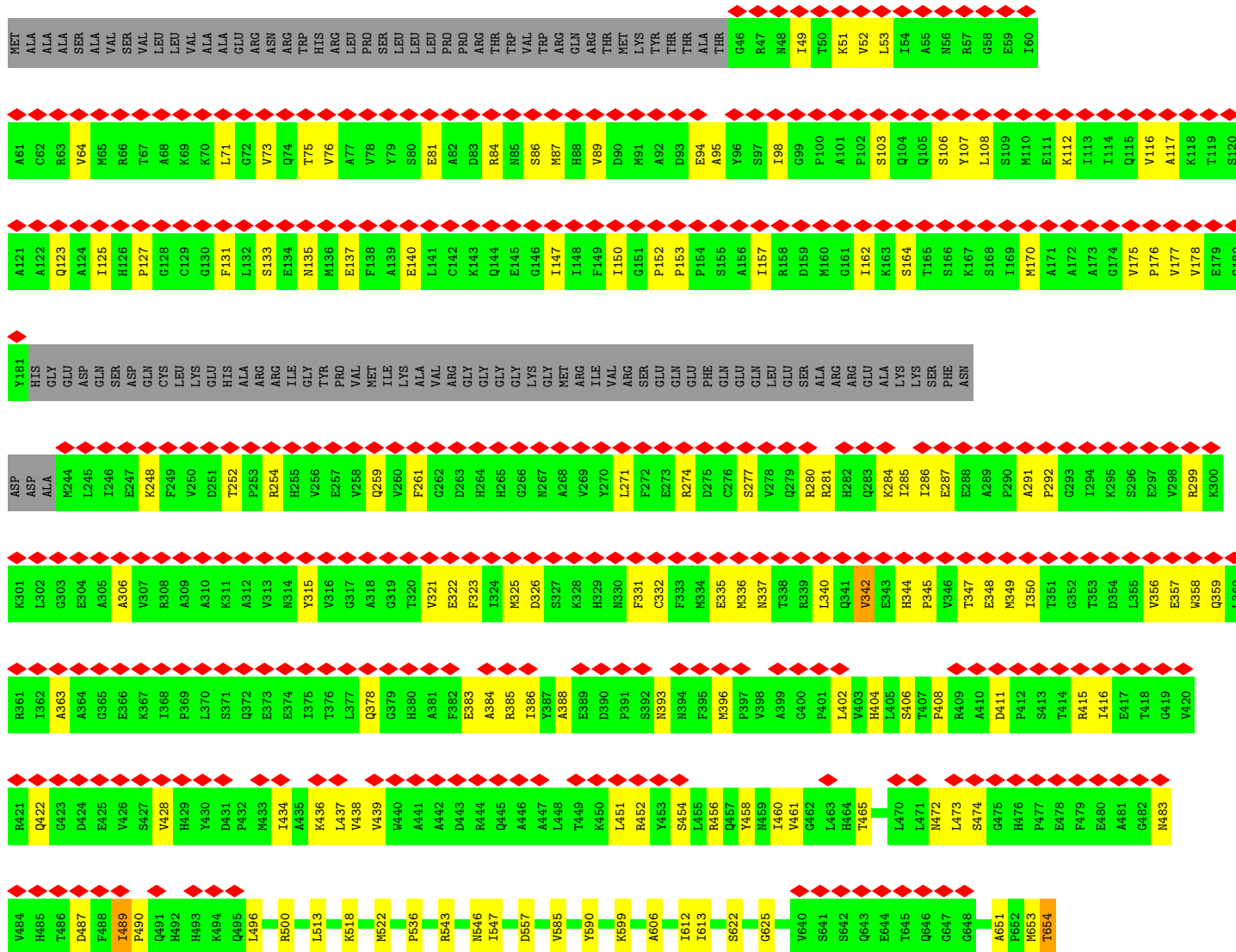
• Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial

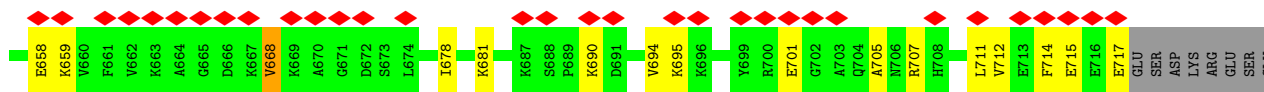




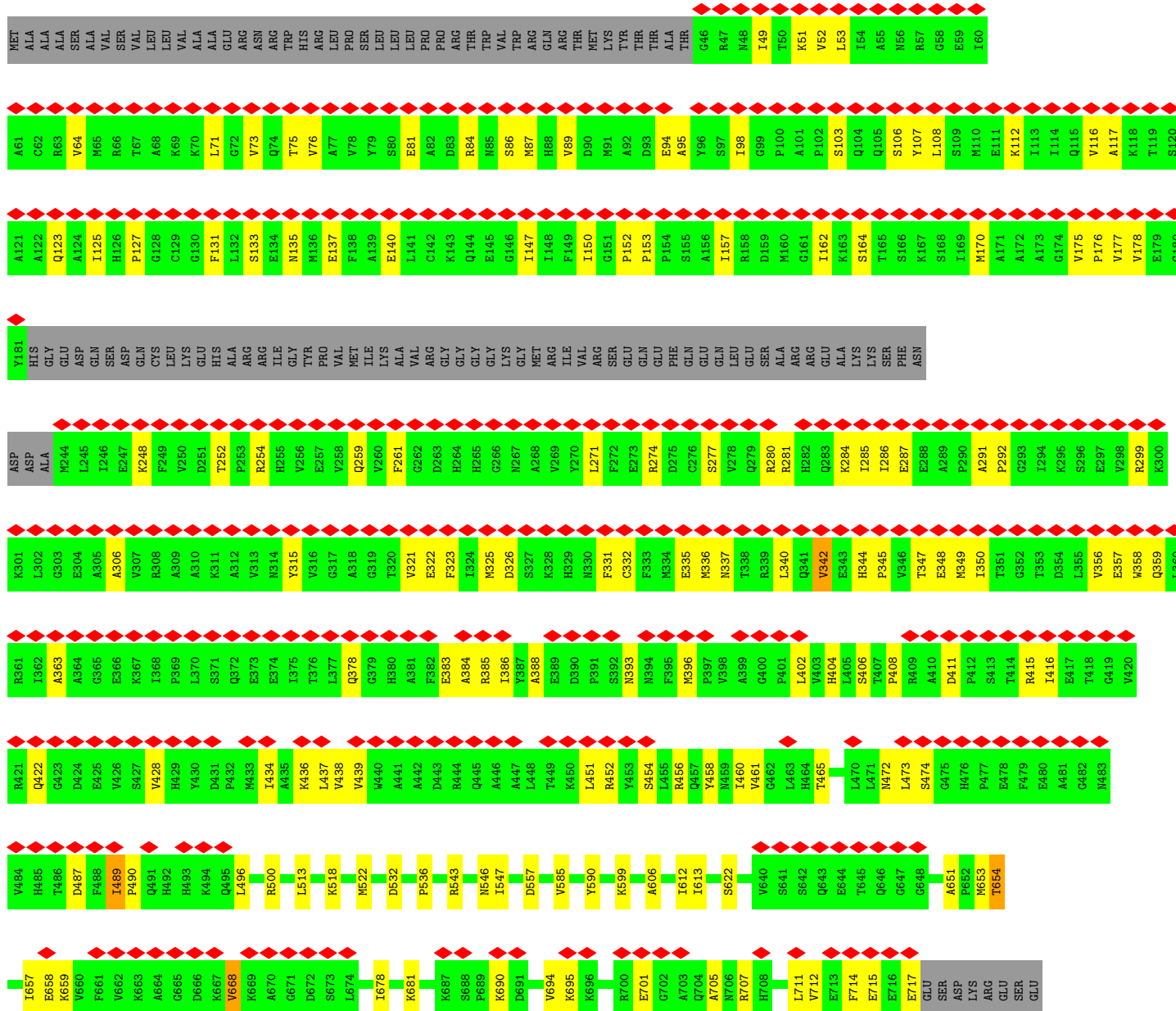


• Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial

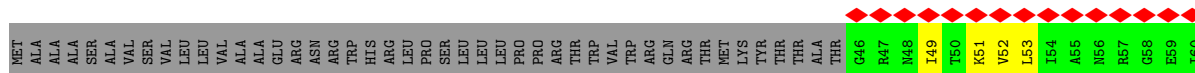




• Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial



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



A61	A121	A131	K301	R361	R421	V484	A651	ARG
C62	A122	HIS	L302	I362	Q422	H485	P652	GLU
R63	Q123	GLU	G303	A363	G423	T486	M653	SER
V64	A124	ASP	E304	A364	D424	D487	T654	GLU
M65	I125	GLN	A305	G365	E425	F488	E658	
R66	H126	SER	A306	E366	V426	I489	K659	
T67	P127	ASP	V307	K367	S427	P490	V660	
A68	G128	GLN	R308	I368	V428	Q491	F661	
K69	C129	CYS	A309	P369	H429	H492	V662	
K70	G130	LEU	A310	L370	Y430	H493	K663	
L71	F131	LYS	K311	S371	D431	K494	A664	
G72	L132	GLU	A312	Q372	P432	Q495	G665	
V73	S133	HIS	V313	E373	M433	L496	D666	
Q74	E134	ALA	N314	E374	I434	R500	K667	
T75	N135	ARG	Y315	I375	A435	L513	V668	
V76	M136	ILE	V316	T376	K436	A670	K669	
A77	M137	TYR	G317	L377	L437	K518	A671	
V78	E138	PRO	A318	Q378	V438	M522	D672	
Y79	F138	VAL	G319	G379	V439	D532	S673	
Y79	A139	MET	T320	H380	A441	P536	L674	
S80	E140	ILE	T321	A381	A442	R543		
E81	L141	LYS	V321	E382	D443	R546		
A82	C142	ALA	E322	F382	R444	N546		
D83	K143	VAL	F323	E383	Q445	I547		
R84	Q144	GLY	I324	A384	A446	D557		
M85	G145	GLY	M325	R385	A447	L557		
S86	E146	LYS	D326	I386	L448	V585		
M87	G146	GLY	S327	A387	T449	K590		
H88	I147	MET	K328	E388	K450	K599		
V89	F149	ARG	H329	D390	L451	K695		
D90	I150	ILE	N330	P391	R452	K696		
M91	G151	ARG	F331	S392	Y453			
A92	P152	SER	C332	N393	S454			
D93	P153	GLU	F333	K394	L455			
E94	P154	GLU	M334	F395	R456			
A95	S155	PHE	E335	M396	Q457			
Y96	A156	GLN	M336	P397	Y458			
S97	I157	GLU	N337	V398	P459			
I98	R158	LEU	T338	A399	T460			
G99	D159	GLU	R339	G400	V461			
P100	M160	SER	L340	P401	L463			
A101	G161	ALA	Q341	L402	H464			
P102	A162	ARG	V342	Y403	T465			
P102	I162	ARG	E343	L405	L470			
S103	K163	ALA	H344	S406	L471			
Q104	S164	LYS	P345	T407	M472			
Q105	T165	LYS	V346	R409	L473			
S106	S166	SER	T347	A410	S474			
Y107	K167	PHE	E348	D411	G475			
L108	S168	ASP	M349	P412	H476			
S109	I169	LYS	I350	S413	P477			
M110	M170	ASN	T351	T414	E478			
E111	A171		G352	R415	F479			
K112	A172		T353	T416	E480			
I113	A173		D354	E417	A481			
I114	G174		L355	T418	G482			
Q115	V175		V356	G419	M483			
V116	P176		E357					
A117	V177		M358					
K118	V178		Q359					
T119	E179		L360					
S120	G180							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	273383	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)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.915	Depositor
Minimum map value	-0.316	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.092	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	0.19	0/4239	0.33	0/5731
1	C	0.16	0/4239	0.31	0/5731
1	F	0.16	0/4239	0.31	0/5731
1	H	0.17	0/4239	0.30	0/5731
1	J	0.17	0/4239	0.30	0/5731
1	K	0.17	0/4239	0.30	0/5731
2	B	0.17	0/4810	0.34	0/6498
2	D	0.16	0/4810	0.34	0/6498
2	E	0.17	0/4810	0.34	0/6498
2	G	0.16	0/4810	0.34	0/6498
2	I	0.17	0/4810	0.34	0/6498
2	L	0.17	0/4810	0.34	0/6498
All	All	0.17	0/54294	0.32	0/73374

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4154	0	4130	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4154	0	4130	113	0
1	F	4154	0	4130	108	0
1	H	4154	0	4130	103	0
1	J	4154	0	4130	105	0
1	K	4154	0	4130	109	0
2	B	4721	0	4732	115	0
2	D	4721	0	4732	117	0
2	E	4721	0	4732	123	0
2	G	4721	0	4732	120	0
2	I	4721	0	4732	119	0
2	L	4721	0	4732	118	0
3	A	15	0	16	14	0
3	C	15	0	16	15	0
3	F	15	0	16	17	0
3	H	15	0	16	16	0
3	J	15	0	16	16	0
3	K	15	0	16	13	0
4	A	54	0	0	11	0
4	C	54	0	0	11	0
4	F	54	0	0	11	0
4	H	54	0	0	11	0
4	J	54	0	0	11	0
4	K	54	0	0	11	0
All	All	53664	0	53268	1155	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 11.

The worst 5 of 1155 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)
3:F:802:BTI:C11	2:G:681:LYS:NZ	1.80	1.45
3:H:802:BTI:H11	2:I:681:LYS:NZ	1.14	1.45
3:J:800:BTI:C11	2:E:681:LYS:NZ	1.80	1.45
3:K:802:BTI:C11	2:L:681:LYS:NZ	1.80	1.45
3:C:800:BTI:C11	2:D:681:LYS:NZ	1.80	1.43

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	539/563 (96%)	521 (97%)	18 (3%)	0	100	100
1	C	539/563 (96%)	521 (97%)	18 (3%)	0	100	100
1	F	539/563 (96%)	521 (97%)	18 (3%)	0	100	100
1	H	539/563 (96%)	521 (97%)	18 (3%)	0	100	100
1	J	539/563 (96%)	521 (97%)	18 (3%)	0	100	100
1	K	539/563 (96%)	521 (97%)	18 (3%)	0	100	100
2	B	606/725 (84%)	589 (97%)	17 (3%)	0	100	100
2	D	606/725 (84%)	589 (97%)	17 (3%)	0	100	100
2	E	606/725 (84%)	589 (97%)	17 (3%)	0	100	100
2	G	606/725 (84%)	589 (97%)	17 (3%)	0	100	100
2	I	606/725 (84%)	589 (97%)	17 (3%)	0	100	100
2	L	606/725 (84%)	589 (97%)	17 (3%)	0	100	100
All	All	6870/7728 (89%)	6660 (97%)	210 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	430/445 (97%)	430 (100%)	0	100	100
1	C	430/445 (97%)	430 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	430/445 (97%)	430 (100%)	0	100	100
1	H	430/445 (97%)	430 (100%)	0	100	100
1	J	430/445 (97%)	430 (100%)	0	100	100
1	K	430/445 (97%)	429 (100%)	1 (0%)	87	94
2	B	513/609 (84%)	506 (99%)	7 (1%)	59	74
2	D	513/609 (84%)	506 (99%)	7 (1%)	59	74
2	E	513/609 (84%)	506 (99%)	7 (1%)	59	74
2	G	513/609 (84%)	506 (99%)	7 (1%)	59	74
2	I	513/609 (84%)	506 (99%)	7 (1%)	59	74
2	L	513/609 (84%)	506 (99%)	7 (1%)	59	74
All	All	5658/6324 (90%)	5615 (99%)	43 (1%)	70	83

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	87	MET
1	K	408	MET
2	I	140	GLU
2	I	489	ILE
2	L	140	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	123	GLN
1	H	489	GLN
2	G	255	HIS
2	G	704	GLN
2	I	255	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	TW3	H	801	-	53,56,56	0.46	0	77,83,83	1.24	5 (6%)
4	TW3	A	801	-	53,56,56	0.46	0	77,83,83	1.24	5 (6%)
4	TW3	F	801	-	53,56,56	0.46	0	77,83,83	1.24	5 (6%)
3	BTI	J	800	-	15,16,16	0.43	0	20,21,21	1.13	2 (10%)
4	TW3	J	801	-	53,56,56	0.46	0	77,83,83	1.24	5 (6%)
3	BTI	A	800	-	15,16,16	0.43	0	20,21,21	1.13	2 (10%)
4	TW3	K	801	-	53,56,56	0.45	0	77,83,83	1.24	5 (6%)
4	TW3	C	801	-	53,56,56	0.45	0	77,83,83	1.24	5 (6%)
3	BTI	F	802	-	15,16,16	0.43	0	20,21,21	1.13	2 (10%)
3	BTI	H	802	-	15,16,16	0.44	0	20,21,21	1.13	2 (10%)
3	BTI	C	800	-	15,16,16	0.43	0	20,21,21	1.13	2 (10%)
3	BTI	K	802	-	15,16,16	0.44	0	20,21,21	1.13	2 (10%)

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
4	TW3	H	801	-	-	14/54/71/71	0/3/3/3
4	TW3	A	801	-	-	14/54/71/71	0/3/3/3
4	TW3	F	801	-	-	14/54/71/71	0/3/3/3
3	BTI	J	800	-	-	0/6/27/27	0/2/2/2
4	TW3	J	801	-	-	14/54/71/71	0/3/3/3
3	BTI	A	800	-	-	0/6/27/27	0/2/2/2
4	TW3	K	801	-	-	14/54/71/71	0/3/3/3
4	TW3	C	801	-	-	14/54/71/71	0/3/3/3
3	BTI	F	802	-	-	0/6/27/27	0/2/2/2
3	BTI	H	802	-	-	0/6/27/27	0/2/2/2
3	BTI	C	800	-	-	0/6/27/27	0/2/2/2
3	BTI	K	802	-	-	0/6/27/27	0/2/2/2

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	801	TW3	C4-C5-S1	7.81	121.25	111.32
4	H	801	TW3	C4-C5-S1	7.80	121.24	111.32
4	C	801	TW3	C4-C5-S1	7.80	121.23	111.32
4	K	801	TW3	C4-C5-S1	7.80	121.23	111.32
4	J	801	TW3	C4-C5-S1	7.79	121.22	111.32

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	801	TW3	N2-C11-C12-C13
4	J	801	TW3	N2-C11-C12-O4
4	J	801	TW3	O3-C11-C12-C13
4	J	801	TW3	O3-C11-C12-O4
4	J	801	TW3	C18-C17-O11-P2

There are no ring outliers.

12 monomers are involved in 157 short contacts:

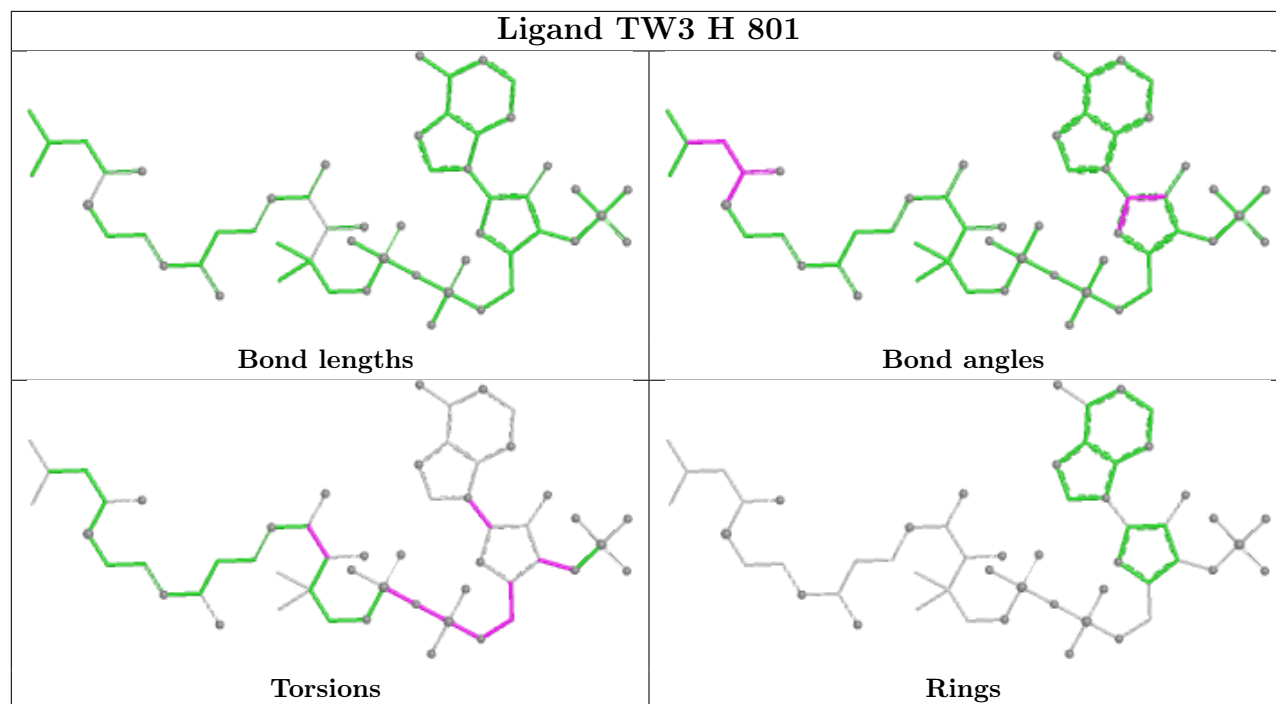
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	801	TW3	11	0
4	A	801	TW3	11	0
4	F	801	TW3	11	0

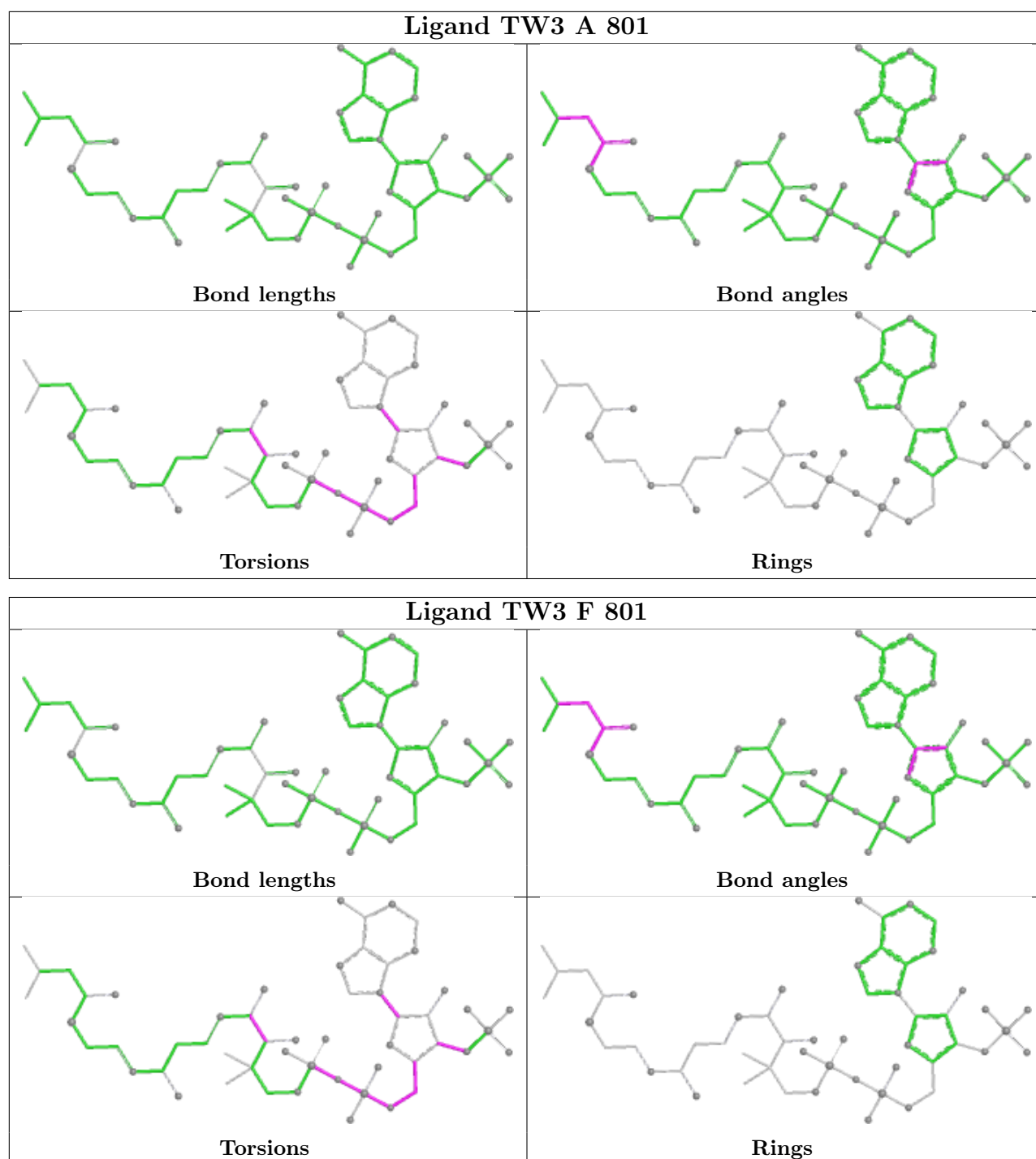
Continued on next page...

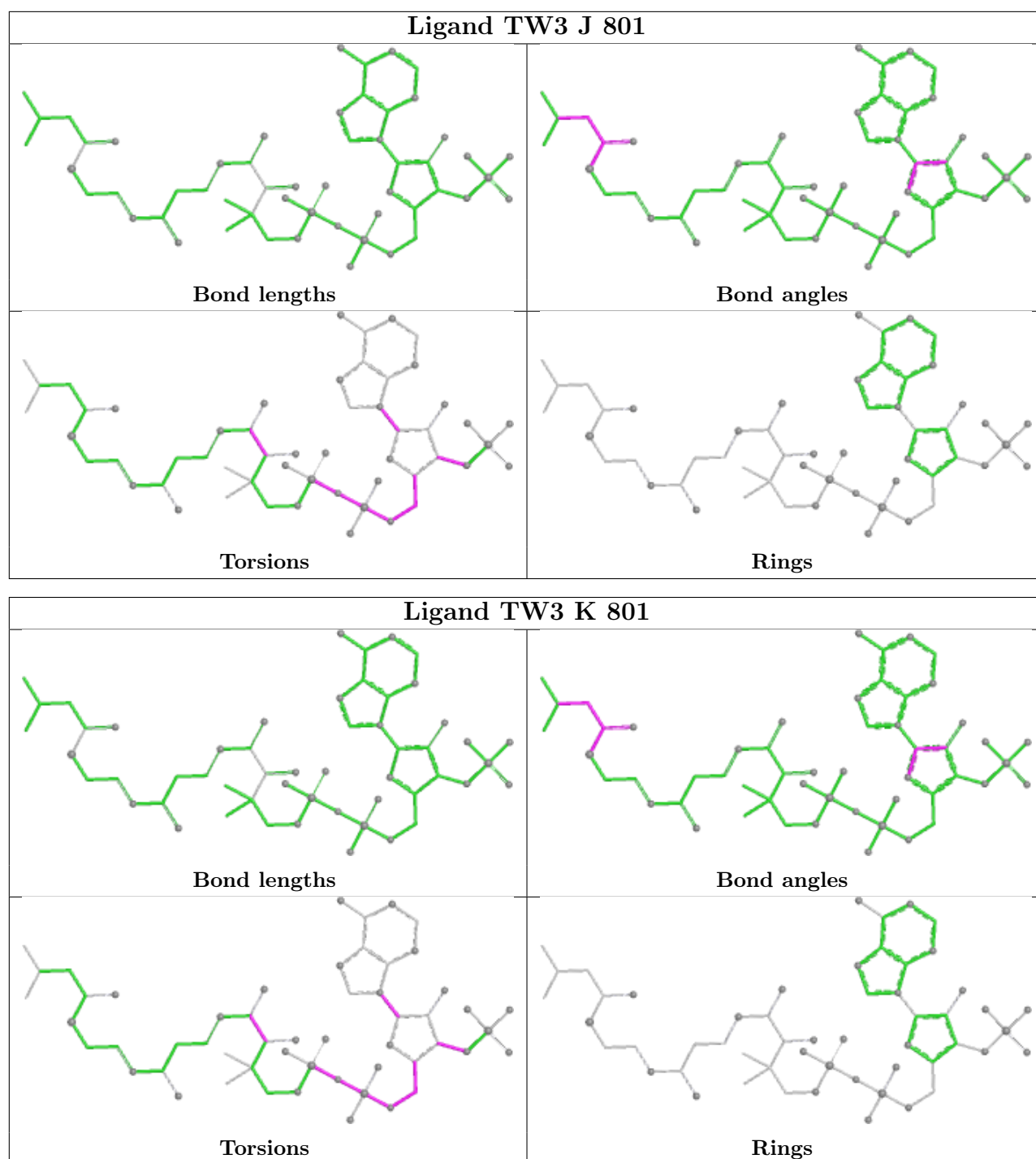
Continued from previous page...

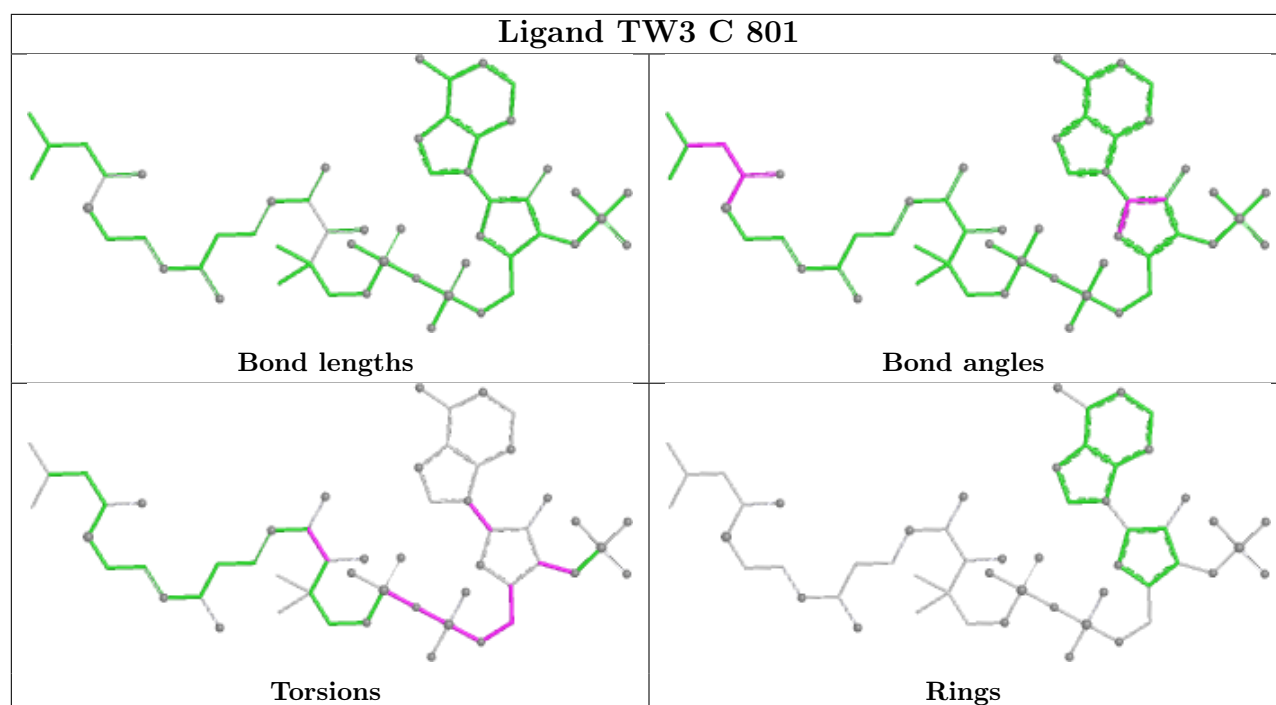
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	800	BTI	16	0
4	J	801	TW3	11	0
3	A	800	BTI	14	0
4	K	801	TW3	11	0
4	C	801	TW3	11	0
3	F	802	BTI	17	0
3	H	802	BTI	16	0
3	C	800	BTI	15	0
3	K	802	BTI	13	0

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.

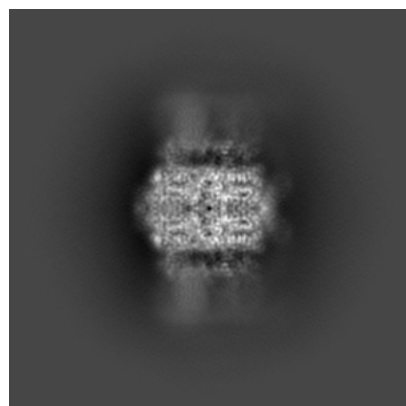
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35980. These allow visual inspection of the internal detail of the map and identification of artifacts.

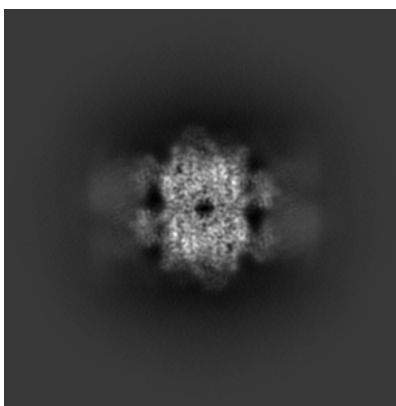
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

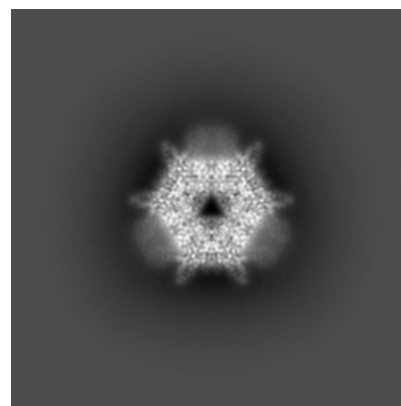
6.1.1 Primary map



X

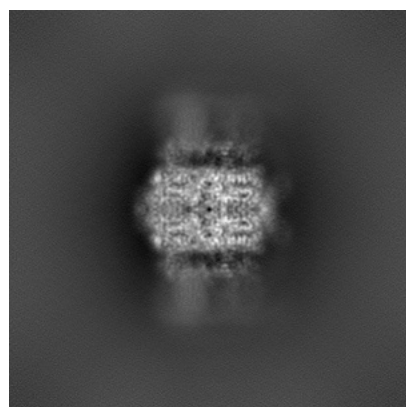


Y

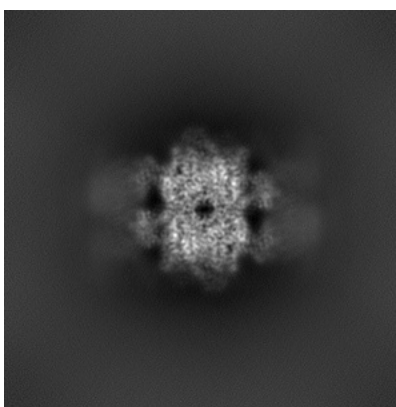


Z

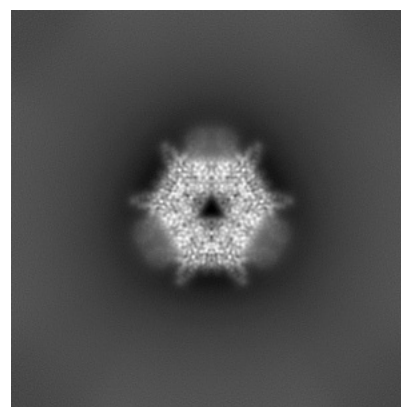
6.1.2 Raw map



X



Y

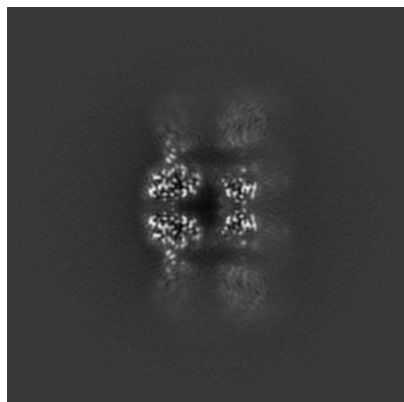


Z

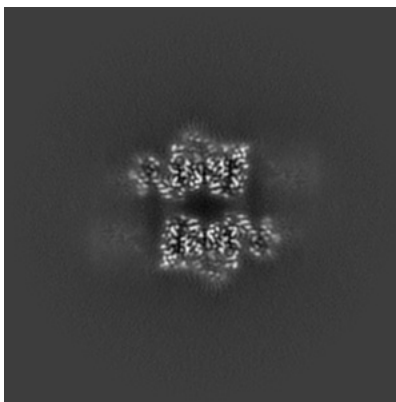
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

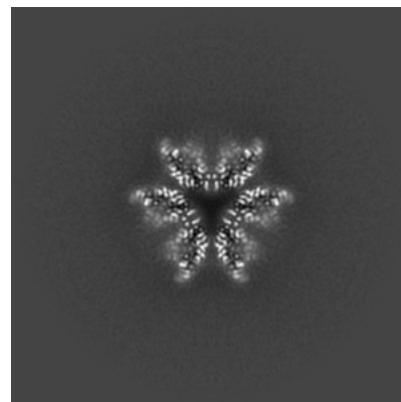
6.2.1 Primary map



X Index: 180

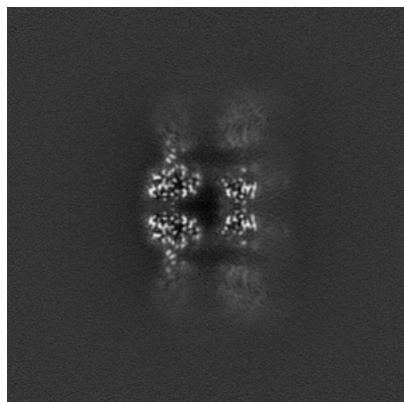


Y Index: 180

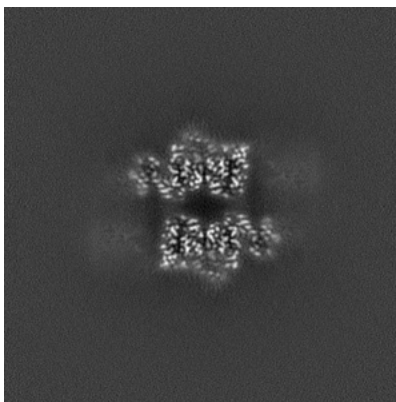


Z Index: 180

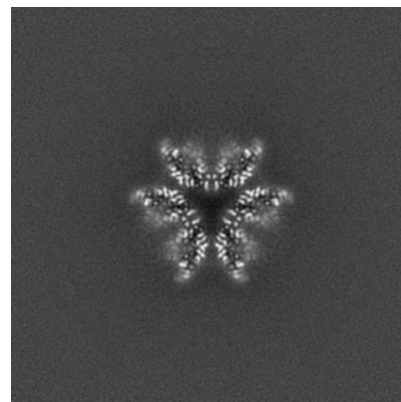
6.2.2 Raw map



X Index: 180



Y Index: 180

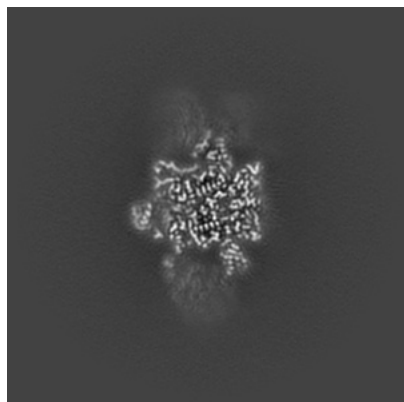


Z Index: 180

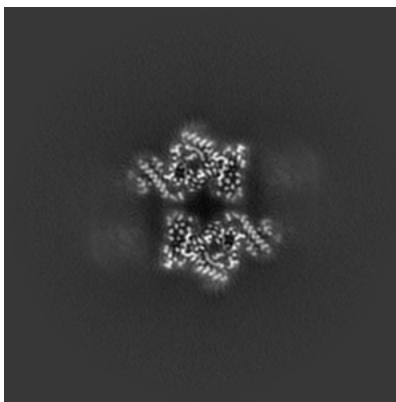
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

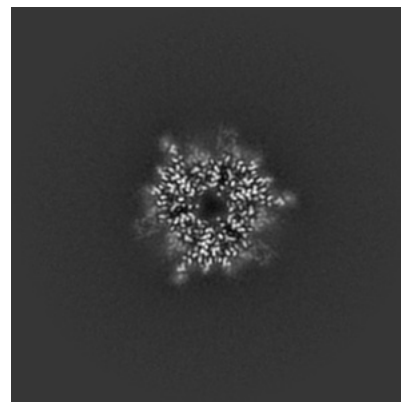
6.3.1 Primary map



X Index: 152

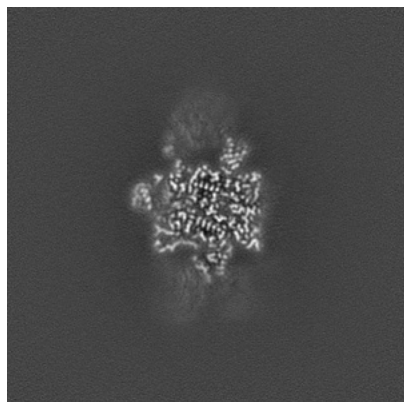


Y Index: 183

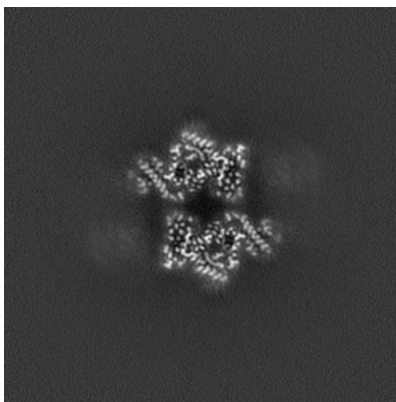


Z Index: 170

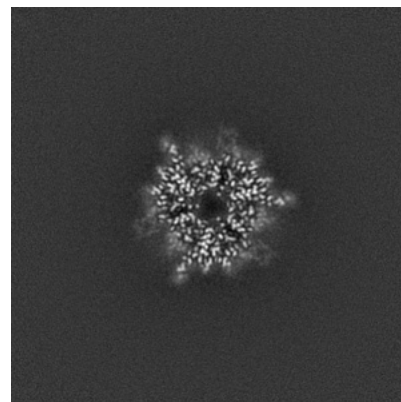
6.3.2 Raw map



X Index: 208



Y Index: 183

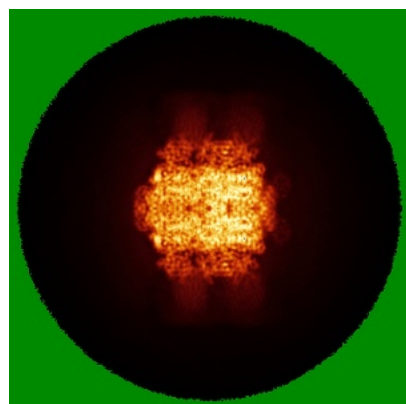


Z Index: 170

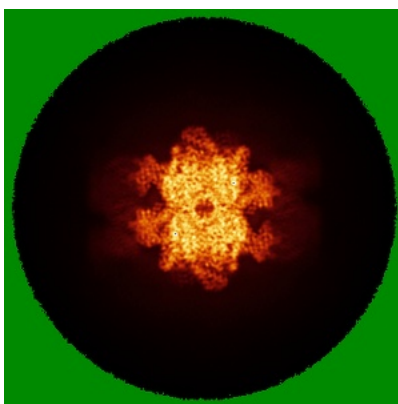
The images above show the largest variance slices of the map in three orthogonal directions.

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

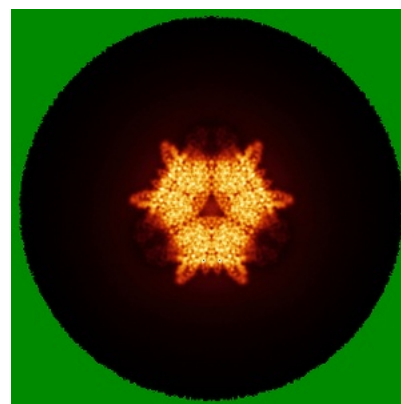
6.4.1 Primary map



X

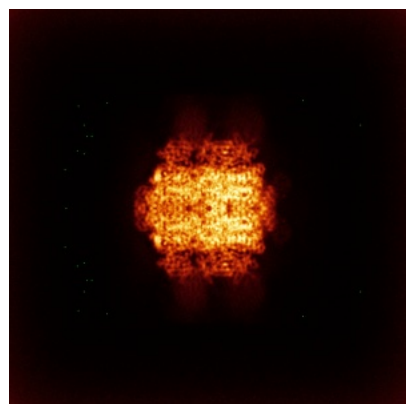


Y

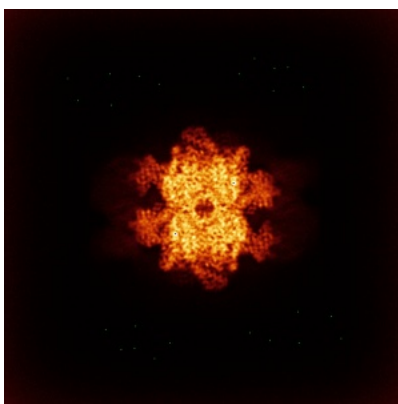


Z

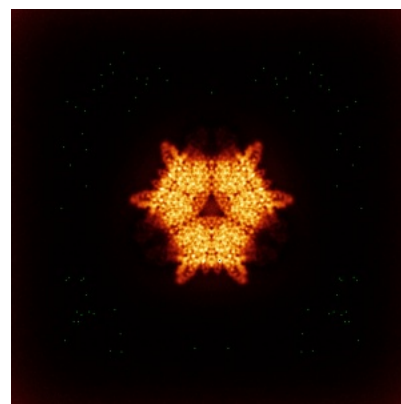
6.4.2 Raw map



X



Y

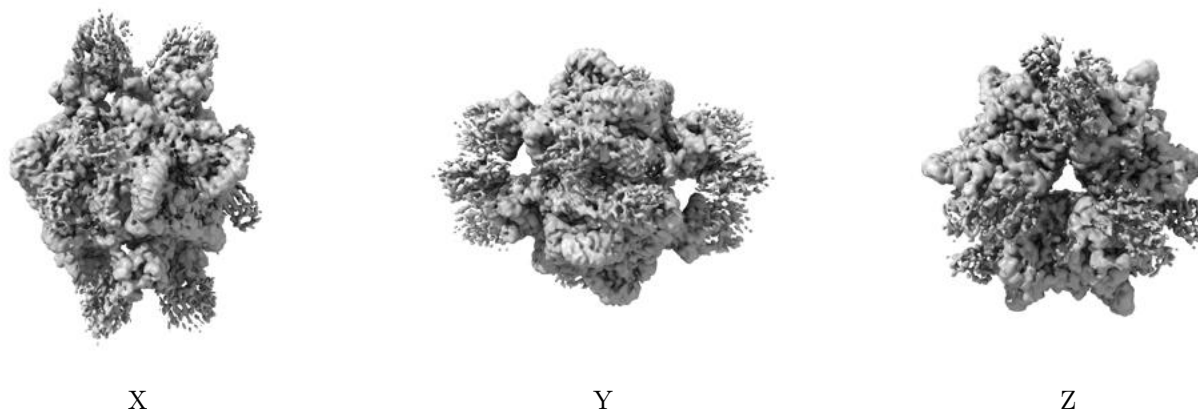


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.092. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

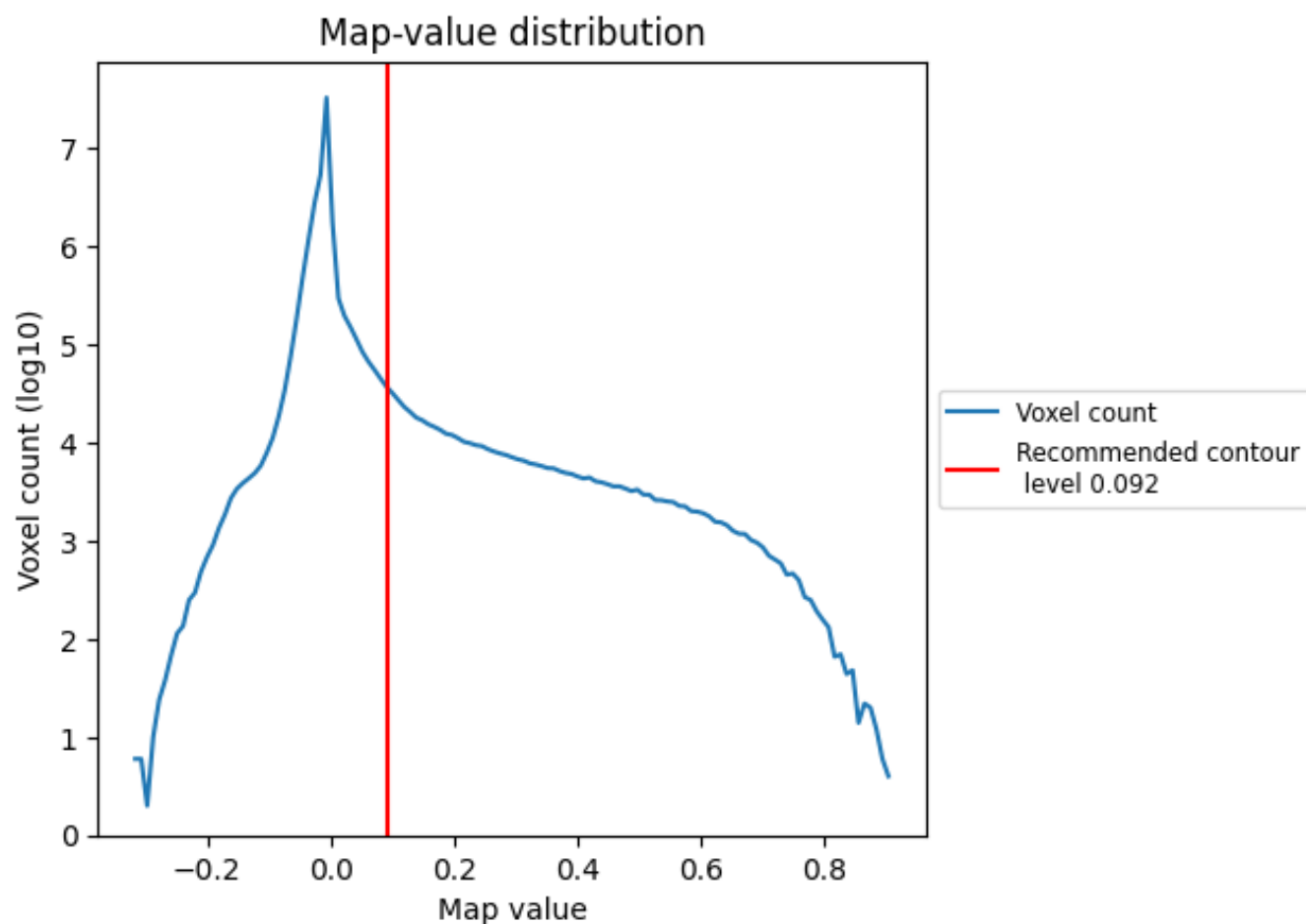
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

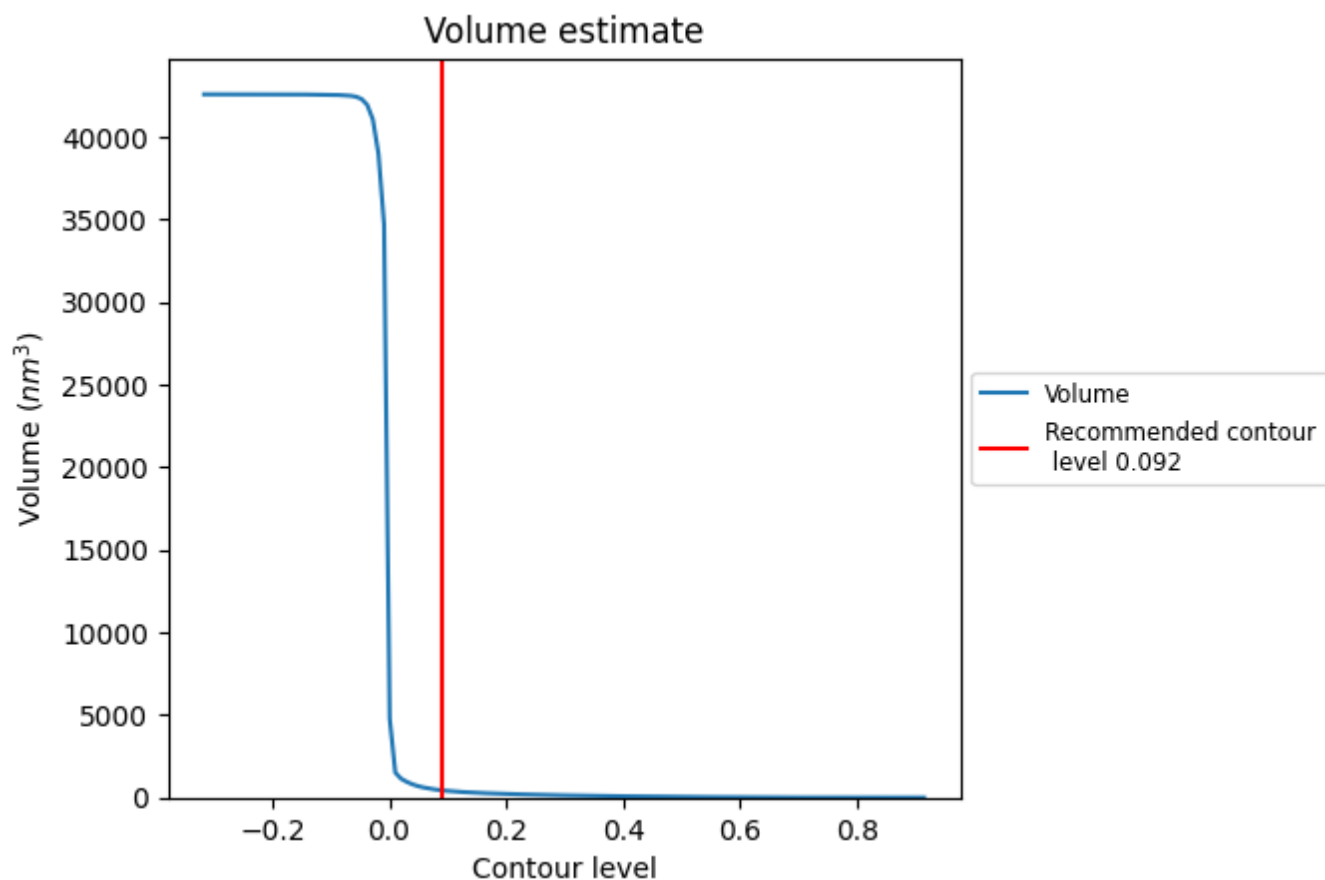
This section contains the results of statistical analysis of the map.

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.

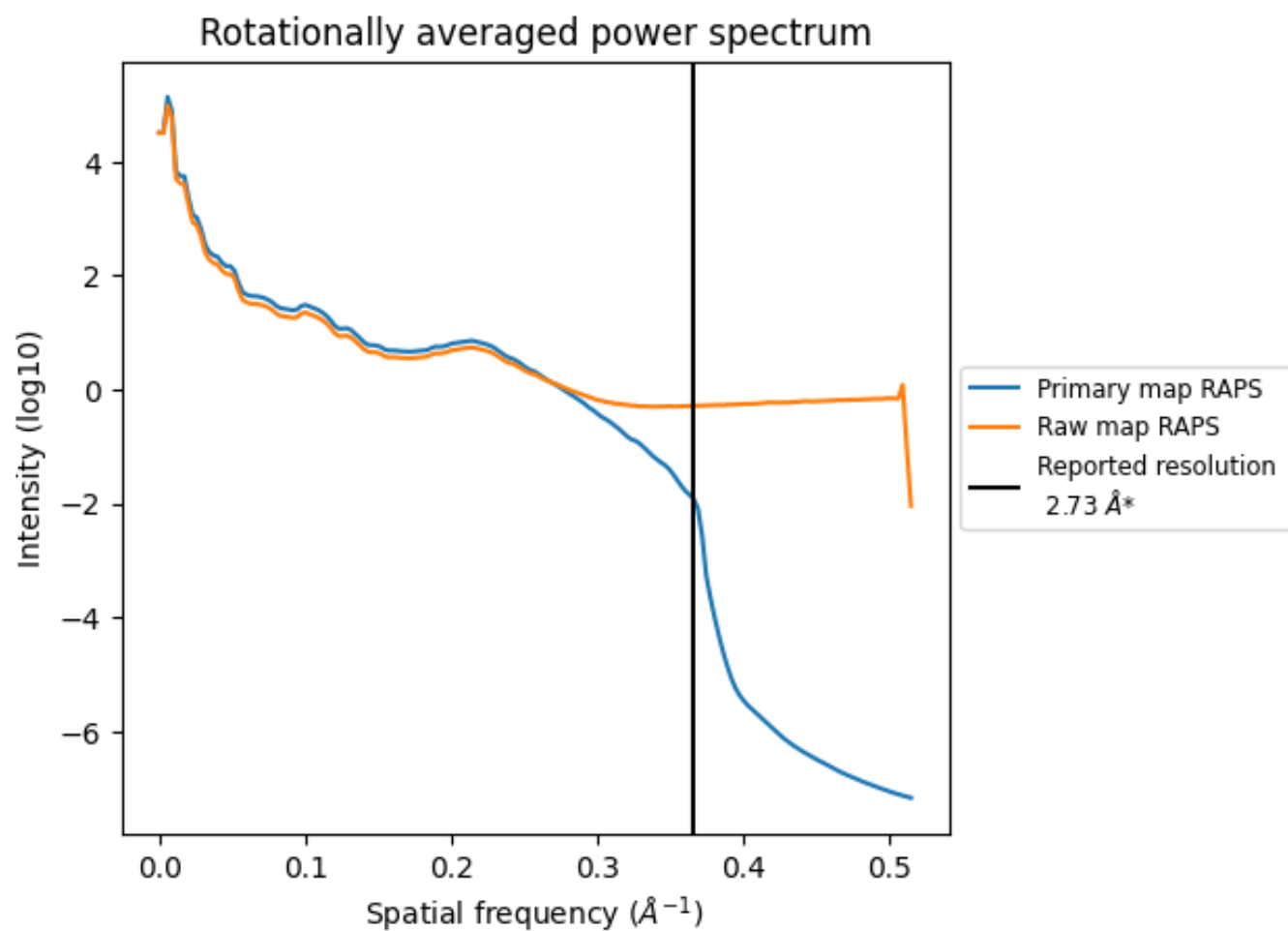
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 432 nm³; this corresponds to an approximate mass of 390 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 ⓘ

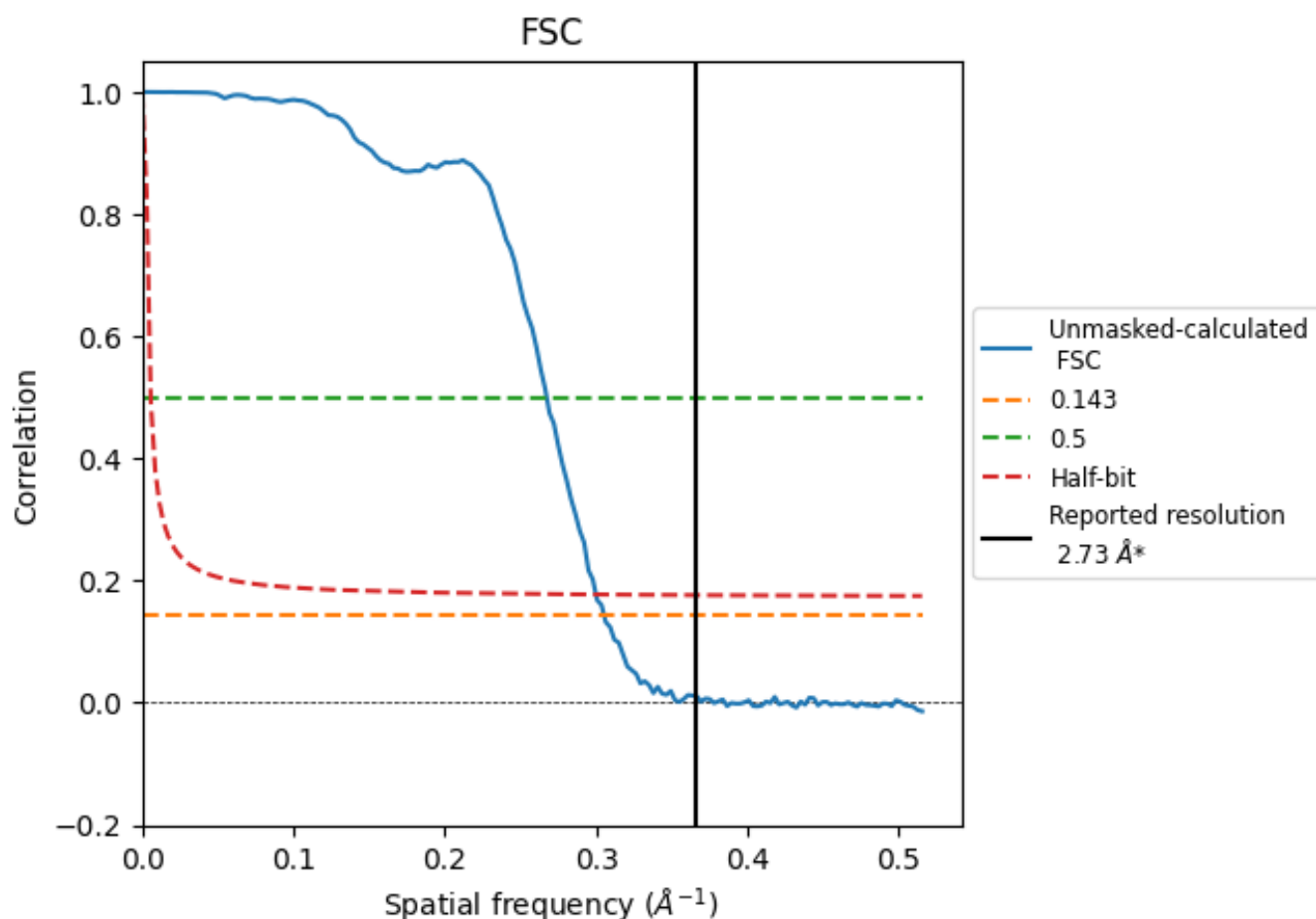


*Reported resolution corresponds to spatial frequency of $0.366 \text{ \AA}^{-1}$

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 0.366 Å⁻¹

8.2 Resolution estimates [i](#)

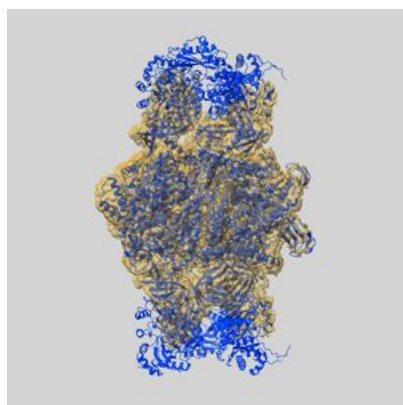
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	3.74	3.33

*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 3.28 differs from the reported value 2.73 by more than 10 %

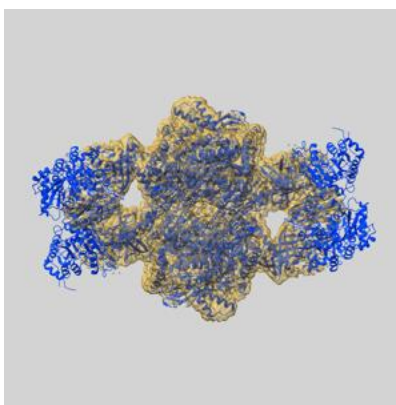
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35980 and PDB model 8J4Z. Per-residue inclusion information can be found in section 3 on page 7.

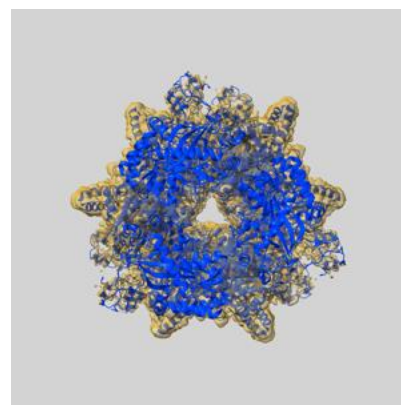
9.1 Map-model overlay [i](#)



X



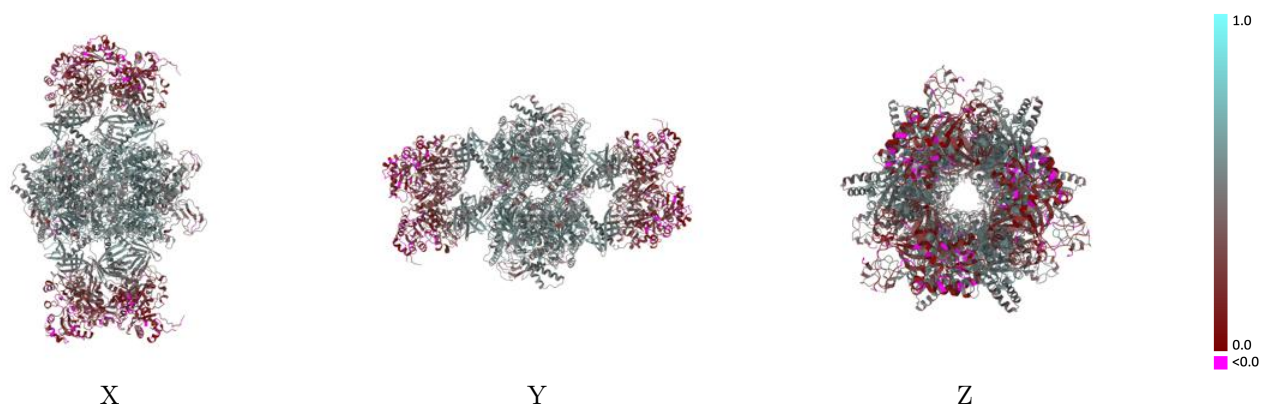
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.092 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](#)

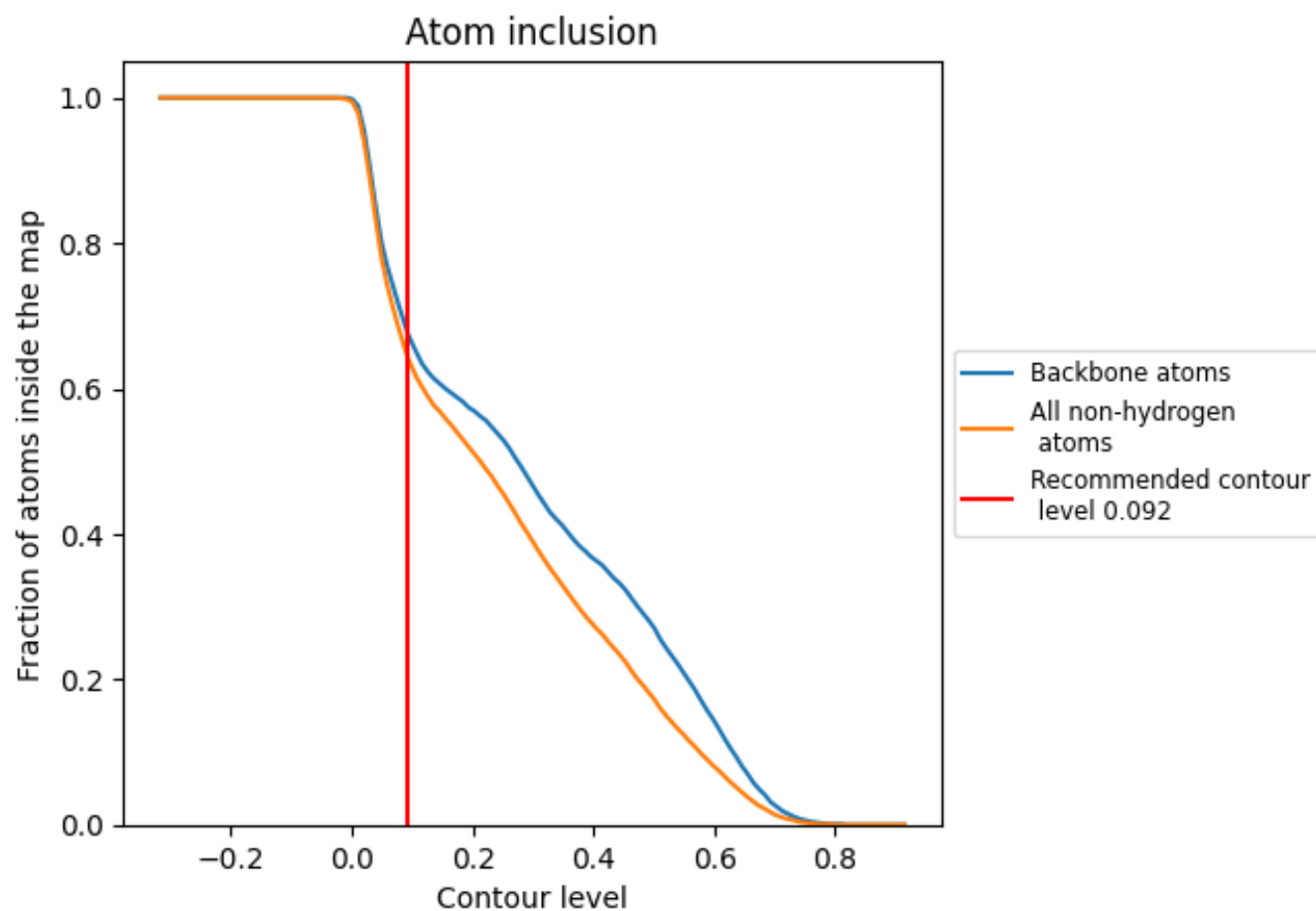


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 64% 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 (0.092) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6440	0.4180
A	0.9850	0.5500
B	0.3410	0.3030
C	0.9850	0.5510
D	0.3400	0.3010
E	0.3420	0.3010
F	0.9850	0.5510
G	0.3410	0.2980
H	0.9850	0.5520
I	0.3410	0.2980
J	0.9840	0.5510
K	0.9850	0.5500
L	0.3400	0.2990

