W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 06:05 pm GMT

|		
PDB ID	:	6G2D
EMDB ID	:	EMD-4342
Title	:	Citrate-induced acetyl-CoA carboxylase (ACC-Cit) filament at 5.4 A resolution
Authors	:	Hunkeler, M.; Hagmann, A.; Stuttfeld, E.; Chami, M.; Stahlberg, H.; Maier, T.
Deposited on	:	2018-03-23
Resolution	:	5.40 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
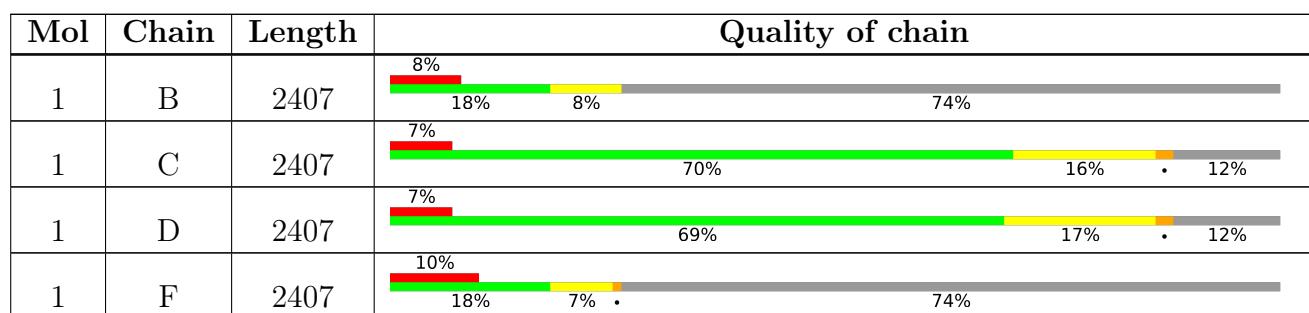
The reported resolution of this entry is 5.40 Å.

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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0.6%
Sidechain outliers		3.1%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

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

Mol	Chain	Length	Quality of chain
1	B	2407	8% — 18% 8% 74%
1	C	2407	7% — 70% 16% • 12%
1	D	2407	7% — 69% 17% • 12%
1	F	2407	10% — 18% 7% • 74%

2   Entry composition   ⓘ

There is only 1 type of molecule in this entry. The entry contains 88169 atoms, of which 43991 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 Acetyl-CoA carboxylase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	625	Total	C	H	N	O	S	0	0
			10226	3267	5114	888	922	35		
1	C	2121	Total	C	H	N	O	S	0	0
			33781	10771	16841	2945	3124	100		
1	D	2121	Total	C	H	N	O	S	0	0
			33782	10771	16842	2945	3124	100		
1	F	634	Total	C	H	N	O	S	0	0
			10380	3310	5194	905	936	35		

There are 244 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-60	MET	-	initiating methionine	UNP Q13085
B	-59	ALA	-	expression tag	UNP Q13085
B	-58	HIS	-	expression tag	UNP Q13085
B	-57	HIS	-	expression tag	UNP Q13085
B	-56	HIS	-	expression tag	UNP Q13085
B	-55	HIS	-	expression tag	UNP Q13085
B	-54	HIS	-	expression tag	UNP Q13085
B	-53	HIS	-	expression tag	UNP Q13085
B	-52	HIS	-	expression tag	UNP Q13085
B	-51	HIS	-	expression tag	UNP Q13085
B	-50	HIS	-	expression tag	UNP Q13085
B	-49	HIS	-	expression tag	UNP Q13085
B	-48	GLY	-	expression tag	UNP Q13085
B	-47	SER	-	expression tag	UNP Q13085
B	-46	THR	-	expression tag	UNP Q13085
B	-45	SER	-	expression tag	UNP Q13085
B	-44	GLY	-	expression tag	UNP Q13085
B	-43	SER	-	expression tag	UNP Q13085
B	-42	GLY	-	expression tag	UNP Q13085
B	-41	GLU	-	expression tag	UNP Q13085
B	-40	GLN	-	expression tag	UNP Q13085
B	-39	LYS	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	LEU	-	expression tag	UNP Q13085
B	-37	ILE	-	expression tag	UNP Q13085
B	-36	SER	-	expression tag	UNP Q13085
B	-35	GLU	-	expression tag	UNP Q13085
B	-34	GLU	-	expression tag	UNP Q13085
B	-33	ASP	-	expression tag	UNP Q13085
B	-32	LEU	-	expression tag	UNP Q13085
B	-31	GLY	-	expression tag	UNP Q13085
B	-30	SER	-	expression tag	UNP Q13085
B	-29	THR	-	expression tag	UNP Q13085
B	-28	SER	-	expression tag	UNP Q13085
B	-27	GLY	-	expression tag	UNP Q13085
B	-26	SER	-	expression tag	UNP Q13085
B	-25	GLY	-	expression tag	UNP Q13085
B	-24	ASP	-	expression tag	UNP Q13085
B	-23	TYR	-	expression tag	UNP Q13085
B	-22	LYS	-	expression tag	UNP Q13085
B	-21	ASP	-	expression tag	UNP Q13085
B	-20	ASP	-	expression tag	UNP Q13085
B	-19	ASP	-	expression tag	UNP Q13085
B	-18	ASP	-	expression tag	UNP Q13085
B	-17	LYS	-	expression tag	UNP Q13085
B	-16	LEU	-	expression tag	UNP Q13085
B	-15	THR	-	expression tag	UNP Q13085
B	-14	SER	-	expression tag	UNP Q13085
B	-13	LEU	-	expression tag	UNP Q13085
B	-12	TYR	-	expression tag	UNP Q13085
B	-11	LYS	-	expression tag	UNP Q13085
B	-10	LYS	-	expression tag	UNP Q13085
B	-9	ALA	-	expression tag	UNP Q13085
B	-8	GLY	-	expression tag	UNP Q13085
B	-7	LEU	-	expression tag	UNP Q13085
B	-6	GLU	-	expression tag	UNP Q13085
B	-5	ASN	-	expression tag	UNP Q13085
B	-4	LEU	-	expression tag	UNP Q13085
B	-3	TYR	-	expression tag	UNP Q13085
B	-2	PHE	-	expression tag	UNP Q13085
B	-1	GLN	-	expression tag	UNP Q13085
B	0	GLY	-	expression tag	UNP Q13085
C	-60	MET	-	initiating methionine	UNP Q13085
C	-59	ALA	-	expression tag	UNP Q13085
C	-58	HIS	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-57	HIS	-	expression tag	UNP Q13085
C	-56	HIS	-	expression tag	UNP Q13085
C	-55	HIS	-	expression tag	UNP Q13085
C	-54	HIS	-	expression tag	UNP Q13085
C	-53	HIS	-	expression tag	UNP Q13085
C	-52	HIS	-	expression tag	UNP Q13085
C	-51	HIS	-	expression tag	UNP Q13085
C	-50	HIS	-	expression tag	UNP Q13085
C	-49	HIS	-	expression tag	UNP Q13085
C	-48	GLY	-	expression tag	UNP Q13085
C	-47	SER	-	expression tag	UNP Q13085
C	-46	THR	-	expression tag	UNP Q13085
C	-45	SER	-	expression tag	UNP Q13085
C	-44	GLY	-	expression tag	UNP Q13085
C	-43	SER	-	expression tag	UNP Q13085
C	-42	GLY	-	expression tag	UNP Q13085
C	-41	GLU	-	expression tag	UNP Q13085
C	-40	GLN	-	expression tag	UNP Q13085
C	-39	LYS	-	expression tag	UNP Q13085
C	-38	LEU	-	expression tag	UNP Q13085
C	-37	ILE	-	expression tag	UNP Q13085
C	-36	SER	-	expression tag	UNP Q13085
C	-35	GLU	-	expression tag	UNP Q13085
C	-34	GLU	-	expression tag	UNP Q13085
C	-33	ASP	-	expression tag	UNP Q13085
C	-32	LEU	-	expression tag	UNP Q13085
C	-31	GLY	-	expression tag	UNP Q13085
C	-30	SER	-	expression tag	UNP Q13085
C	-29	THR	-	expression tag	UNP Q13085
C	-28	SER	-	expression tag	UNP Q13085
C	-27	GLY	-	expression tag	UNP Q13085
C	-26	SER	-	expression tag	UNP Q13085
C	-25	GLY	-	expression tag	UNP Q13085
C	-24	ASP	-	expression tag	UNP Q13085
C	-23	TYR	-	expression tag	UNP Q13085
C	-22	LYS	-	expression tag	UNP Q13085
C	-21	ASP	-	expression tag	UNP Q13085
C	-20	ASP	-	expression tag	UNP Q13085
C	-19	ASP	-	expression tag	UNP Q13085
C	-18	ASP	-	expression tag	UNP Q13085
C	-17	LYS	-	expression tag	UNP Q13085
C	-16	LEU	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	THR	-	expression tag	UNP Q13085
C	-14	SER	-	expression tag	UNP Q13085
C	-13	LEU	-	expression tag	UNP Q13085
C	-12	TYR	-	expression tag	UNP Q13085
C	-11	LYS	-	expression tag	UNP Q13085
C	-10	LYS	-	expression tag	UNP Q13085
C	-9	ALA	-	expression tag	UNP Q13085
C	-8	GLY	-	expression tag	UNP Q13085
C	-7	LEU	-	expression tag	UNP Q13085
C	-6	GLU	-	expression tag	UNP Q13085
C	-5	ASN	-	expression tag	UNP Q13085
C	-4	LEU	-	expression tag	UNP Q13085
C	-3	TYR	-	expression tag	UNP Q13085
C	-2	PHE	-	expression tag	UNP Q13085
C	-1	GLN	-	expression tag	UNP Q13085
C	0	GLY	-	expression tag	UNP Q13085
D	-60	MET	-	initiating methionine	UNP Q13085
D	-59	ALA	-	expression tag	UNP Q13085
D	-58	HIS	-	expression tag	UNP Q13085
D	-57	HIS	-	expression tag	UNP Q13085
D	-56	HIS	-	expression tag	UNP Q13085
D	-55	HIS	-	expression tag	UNP Q13085
D	-54	HIS	-	expression tag	UNP Q13085
D	-53	HIS	-	expression tag	UNP Q13085
D	-52	HIS	-	expression tag	UNP Q13085
D	-51	HIS	-	expression tag	UNP Q13085
D	-50	HIS	-	expression tag	UNP Q13085
D	-49	HIS	-	expression tag	UNP Q13085
D	-48	GLY	-	expression tag	UNP Q13085
D	-47	SER	-	expression tag	UNP Q13085
D	-46	THR	-	expression tag	UNP Q13085
D	-45	SER	-	expression tag	UNP Q13085
D	-44	GLY	-	expression tag	UNP Q13085
D	-43	SER	-	expression tag	UNP Q13085
D	-42	GLY	-	expression tag	UNP Q13085
D	-41	GLU	-	expression tag	UNP Q13085
D	-40	GLN	-	expression tag	UNP Q13085
D	-39	LYS	-	expression tag	UNP Q13085
D	-38	LEU	-	expression tag	UNP Q13085
D	-37	ILE	-	expression tag	UNP Q13085
D	-36	SER	-	expression tag	UNP Q13085
D	-35	GLU	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-34	GLU	-	expression tag	UNP Q13085
D	-33	ASP	-	expression tag	UNP Q13085
D	-32	LEU	-	expression tag	UNP Q13085
D	-31	GLY	-	expression tag	UNP Q13085
D	-30	SER	-	expression tag	UNP Q13085
D	-29	THR	-	expression tag	UNP Q13085
D	-28	SER	-	expression tag	UNP Q13085
D	-27	GLY	-	expression tag	UNP Q13085
D	-26	SER	-	expression tag	UNP Q13085
D	-25	GLY	-	expression tag	UNP Q13085
D	-24	ASP	-	expression tag	UNP Q13085
D	-23	TYR	-	expression tag	UNP Q13085
D	-22	LYS	-	expression tag	UNP Q13085
D	-21	ASP	-	expression tag	UNP Q13085
D	-20	ASP	-	expression tag	UNP Q13085
D	-19	ASP	-	expression tag	UNP Q13085
D	-18	ASP	-	expression tag	UNP Q13085
D	-17	LYS	-	expression tag	UNP Q13085
D	-16	LEU	-	expression tag	UNP Q13085
D	-15	THR	-	expression tag	UNP Q13085
D	-14	SER	-	expression tag	UNP Q13085
D	-13	LEU	-	expression tag	UNP Q13085
D	-12	TYR	-	expression tag	UNP Q13085
D	-11	LYS	-	expression tag	UNP Q13085
D	-10	LYS	-	expression tag	UNP Q13085
D	-9	ALA	-	expression tag	UNP Q13085
D	-8	GLY	-	expression tag	UNP Q13085
D	-7	LEU	-	expression tag	UNP Q13085
D	-6	GLU	-	expression tag	UNP Q13085
D	-5	ASN	-	expression tag	UNP Q13085
D	-4	LEU	-	expression tag	UNP Q13085
D	-3	TYR	-	expression tag	UNP Q13085
D	-2	PHE	-	expression tag	UNP Q13085
D	-1	GLN	-	expression tag	UNP Q13085
D	0	GLY	-	expression tag	UNP Q13085
F	-60	MET	-	initiating methionine	UNP Q13085
F	-59	ALA	-	expression tag	UNP Q13085
F	-58	HIS	-	expression tag	UNP Q13085
F	-57	HIS	-	expression tag	UNP Q13085
F	-56	HIS	-	expression tag	UNP Q13085
F	-55	HIS	-	expression tag	UNP Q13085
F	-54	HIS	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-53	HIS	-	expression tag	UNP Q13085
F	-52	HIS	-	expression tag	UNP Q13085
F	-51	HIS	-	expression tag	UNP Q13085
F	-50	HIS	-	expression tag	UNP Q13085
F	-49	HIS	-	expression tag	UNP Q13085
F	-48	GLY	-	expression tag	UNP Q13085
F	-47	SER	-	expression tag	UNP Q13085
F	-46	THR	-	expression tag	UNP Q13085
F	-45	SER	-	expression tag	UNP Q13085
F	-44	GLY	-	expression tag	UNP Q13085
F	-43	SER	-	expression tag	UNP Q13085
F	-42	GLY	-	expression tag	UNP Q13085
F	-41	GLU	-	expression tag	UNP Q13085
F	-40	GLN	-	expression tag	UNP Q13085
F	-39	LYS	-	expression tag	UNP Q13085
F	-38	LEU	-	expression tag	UNP Q13085
F	-37	ILE	-	expression tag	UNP Q13085
F	-36	SER	-	expression tag	UNP Q13085
F	-35	GLU	-	expression tag	UNP Q13085
F	-34	GLU	-	expression tag	UNP Q13085
F	-33	ASP	-	expression tag	UNP Q13085
F	-32	LEU	-	expression tag	UNP Q13085
F	-31	GLY	-	expression tag	UNP Q13085
F	-30	SER	-	expression tag	UNP Q13085
F	-29	THR	-	expression tag	UNP Q13085
F	-28	SER	-	expression tag	UNP Q13085
F	-27	GLY	-	expression tag	UNP Q13085
F	-26	SER	-	expression tag	UNP Q13085
F	-25	GLY	-	expression tag	UNP Q13085
F	-24	ASP	-	expression tag	UNP Q13085
F	-23	TYR	-	expression tag	UNP Q13085
F	-22	LYS	-	expression tag	UNP Q13085
F	-21	ASP	-	expression tag	UNP Q13085
F	-20	ASP	-	expression tag	UNP Q13085
F	-19	ASP	-	expression tag	UNP Q13085
F	-18	ASP	-	expression tag	UNP Q13085
F	-17	LYS	-	expression tag	UNP Q13085
F	-16	LEU	-	expression tag	UNP Q13085
F	-15	THR	-	expression tag	UNP Q13085
F	-14	SER	-	expression tag	UNP Q13085
F	-13	LEU	-	expression tag	UNP Q13085
F	-12	TYR	-	expression tag	UNP Q13085

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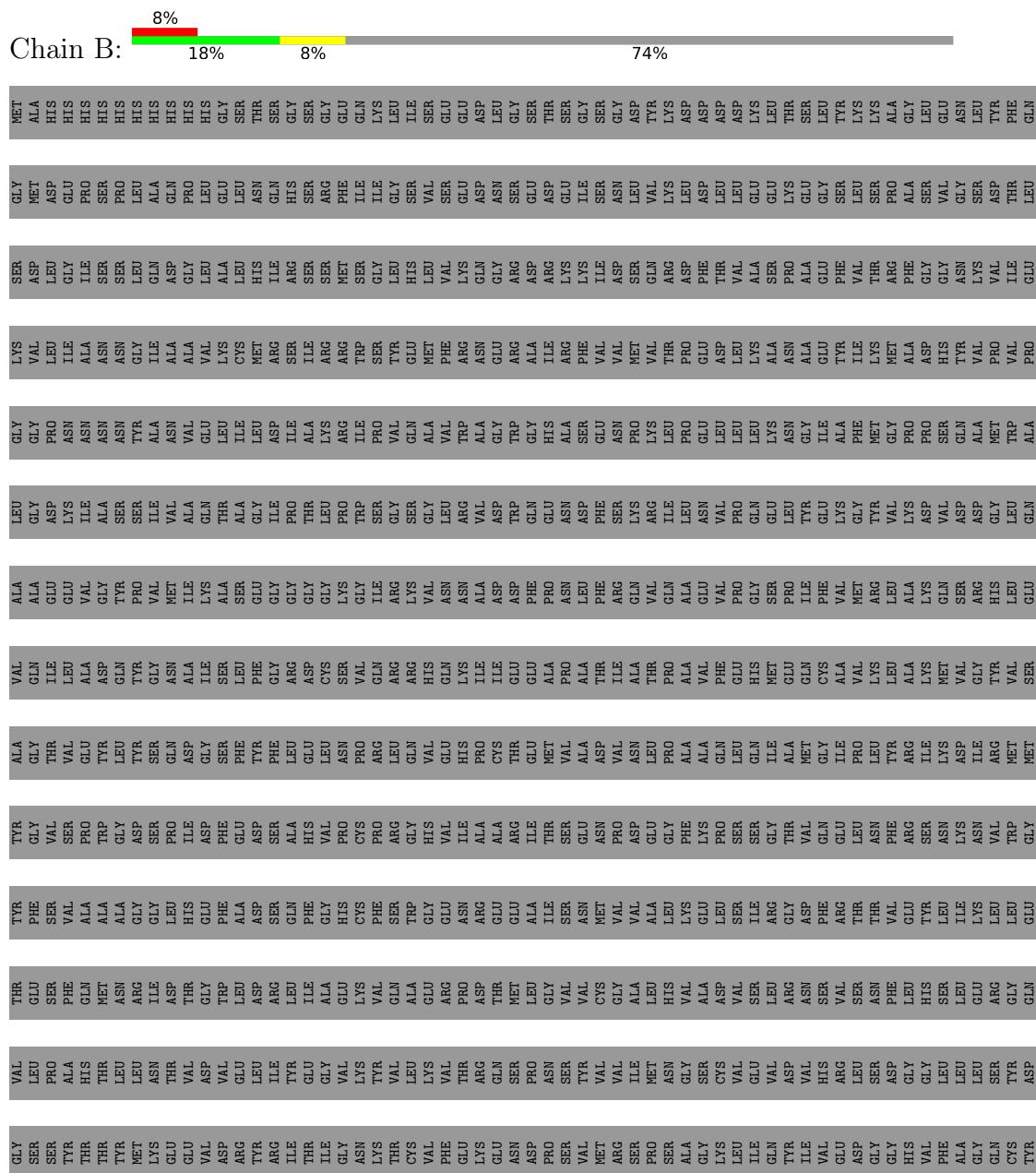
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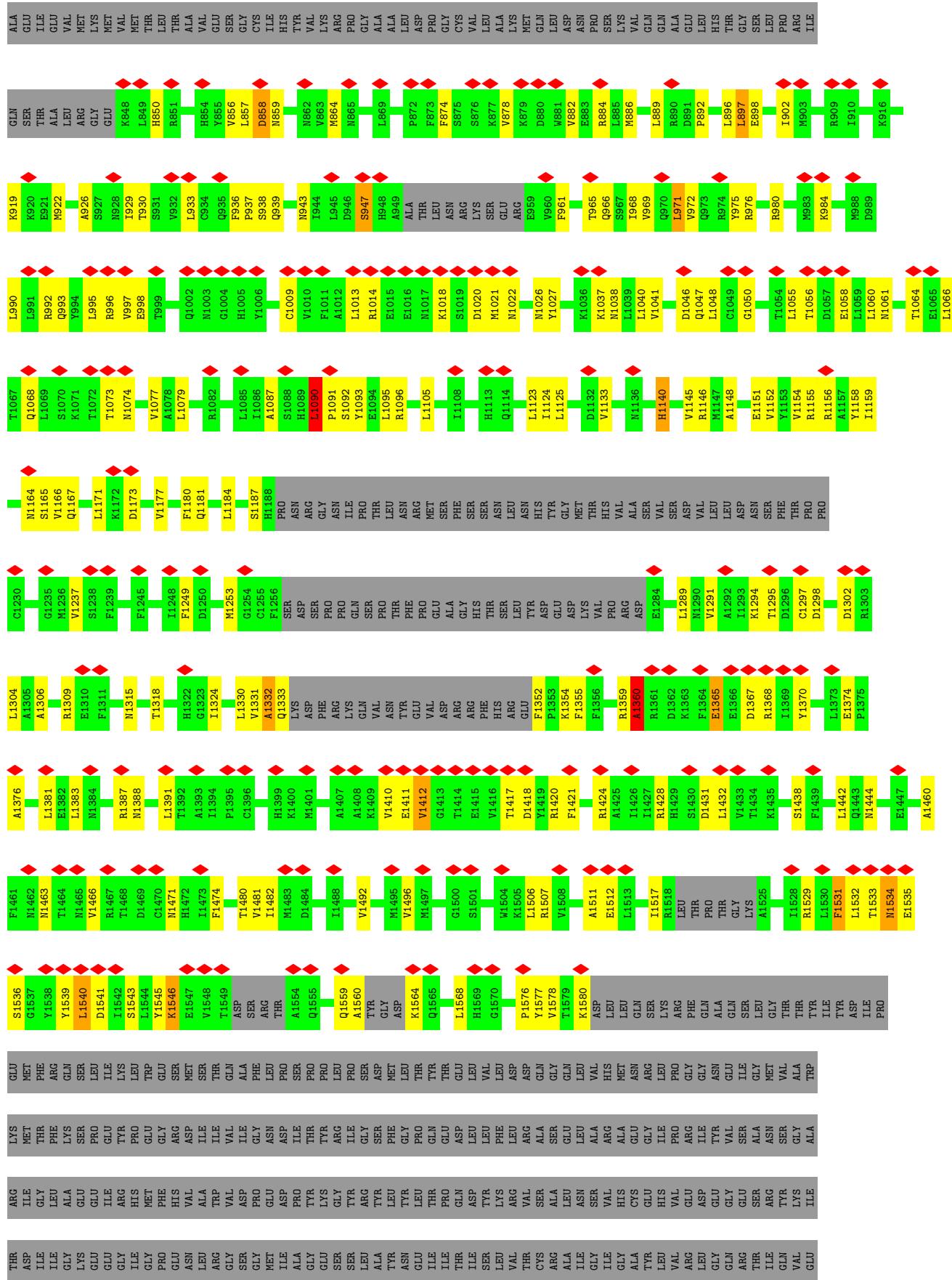
Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	LYS	-	expression tag	UNP Q13085
F	-10	LYS	-	expression tag	UNP Q13085
F	-9	ALA	-	expression tag	UNP Q13085
F	-8	GLY	-	expression tag	UNP Q13085
F	-7	LEU	-	expression tag	UNP Q13085
F	-6	GLU	-	expression tag	UNP Q13085
F	-5	ASN	-	expression tag	UNP Q13085
F	-4	LEU	-	expression tag	UNP Q13085
F	-3	TYR	-	expression tag	UNP Q13085
F	-2	PHE	-	expression tag	UNP Q13085
F	-1	GLN	-	expression tag	UNP Q13085
F	0	GLY	-	expression tag	UNP Q13085
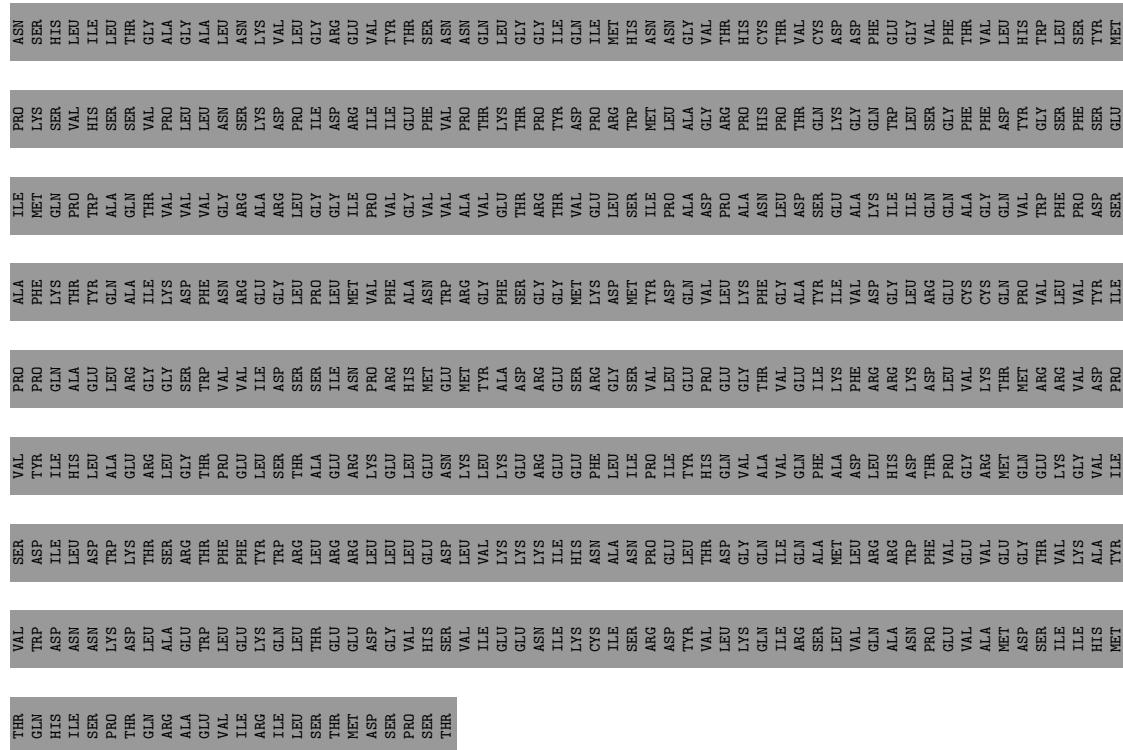
3 Residue-property plots ⓘ

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: Acetyl-CoA carboxylase 1
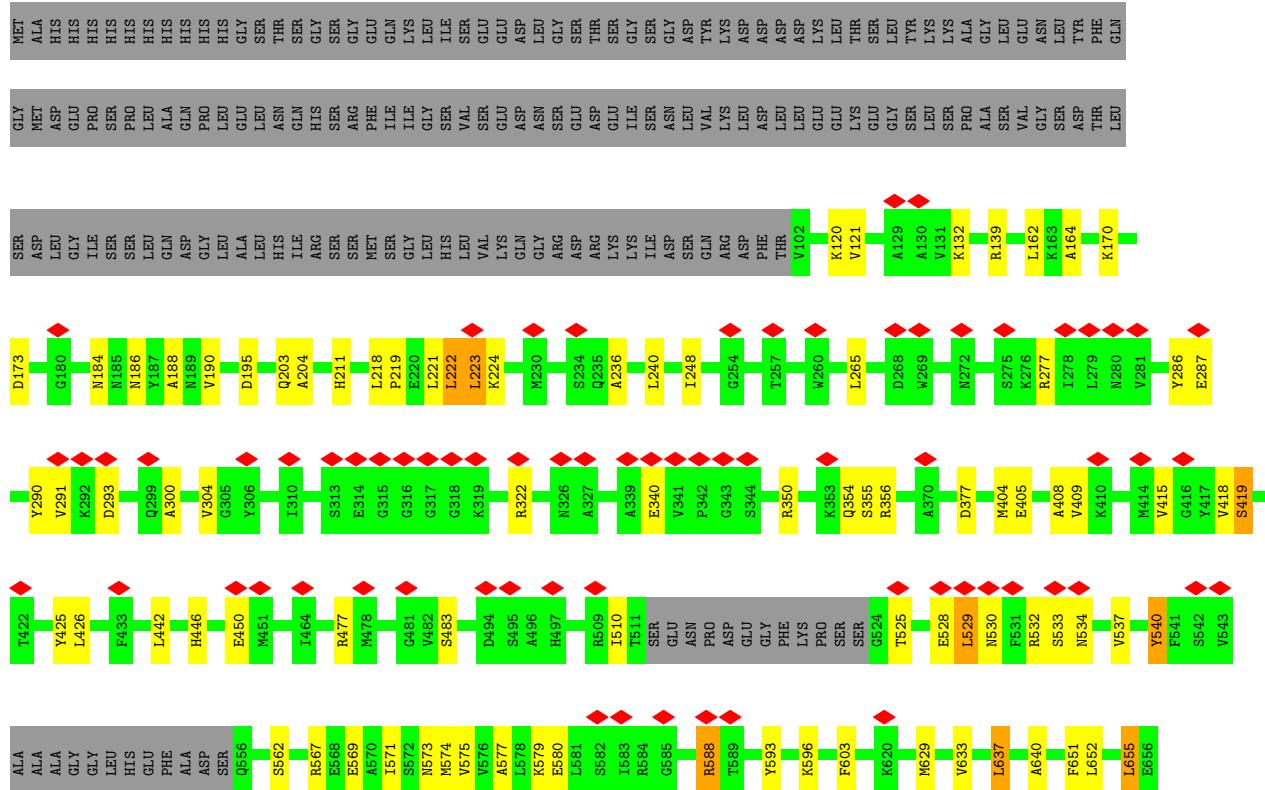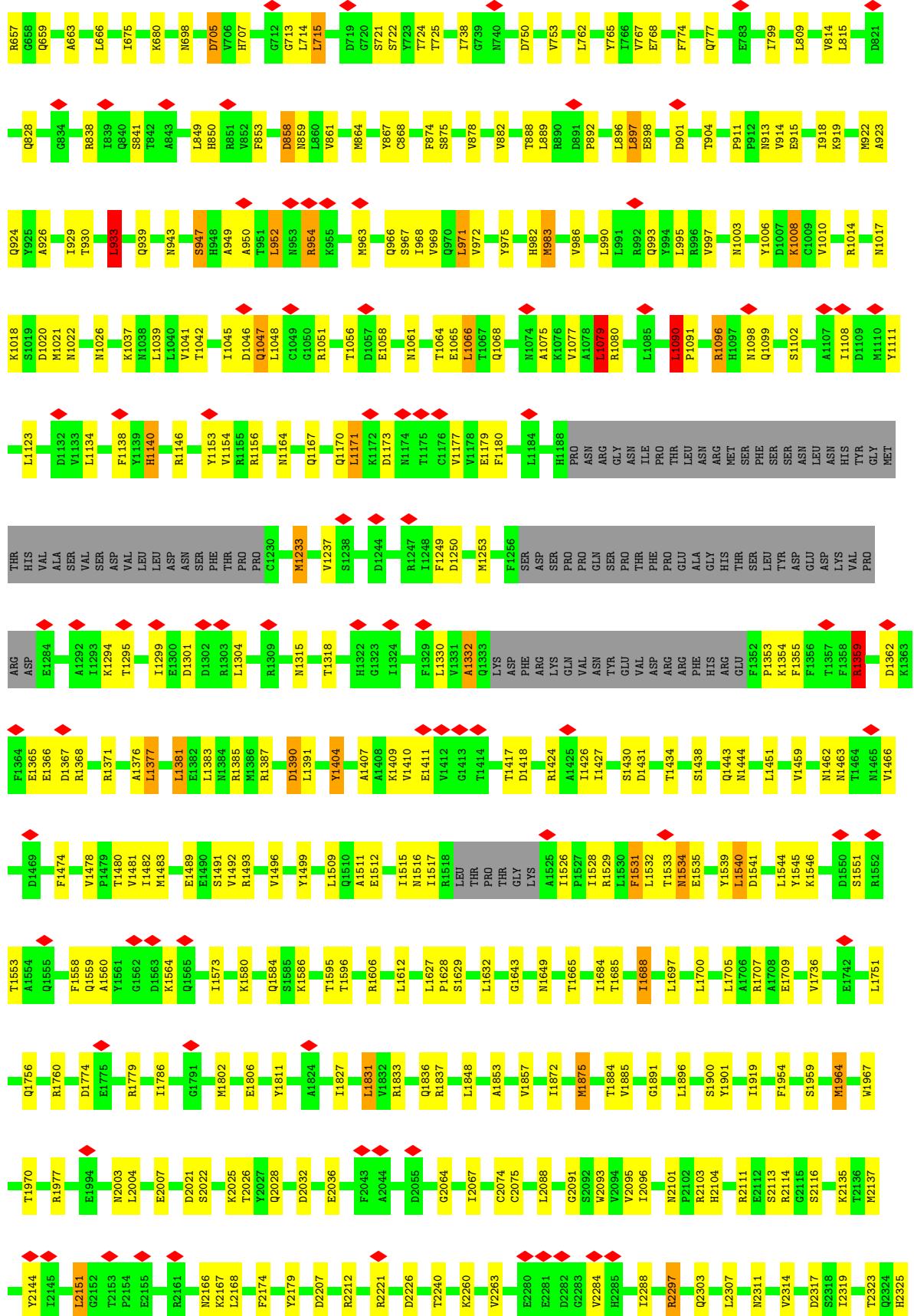
• Molecule 1: Acetyl-CoA carboxylase 1
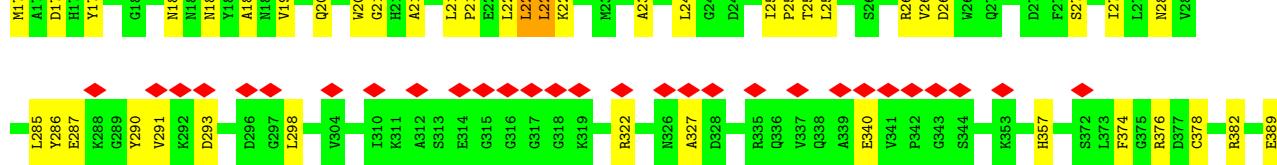
Chain C:

7%
70%
16%
12%

• Molecule 1: Acetyl-CoA carboxylase 1

• Molecule 1: Acetyl-CoA carboxylase 1

Chain F:

10%

18%   7% •   74%
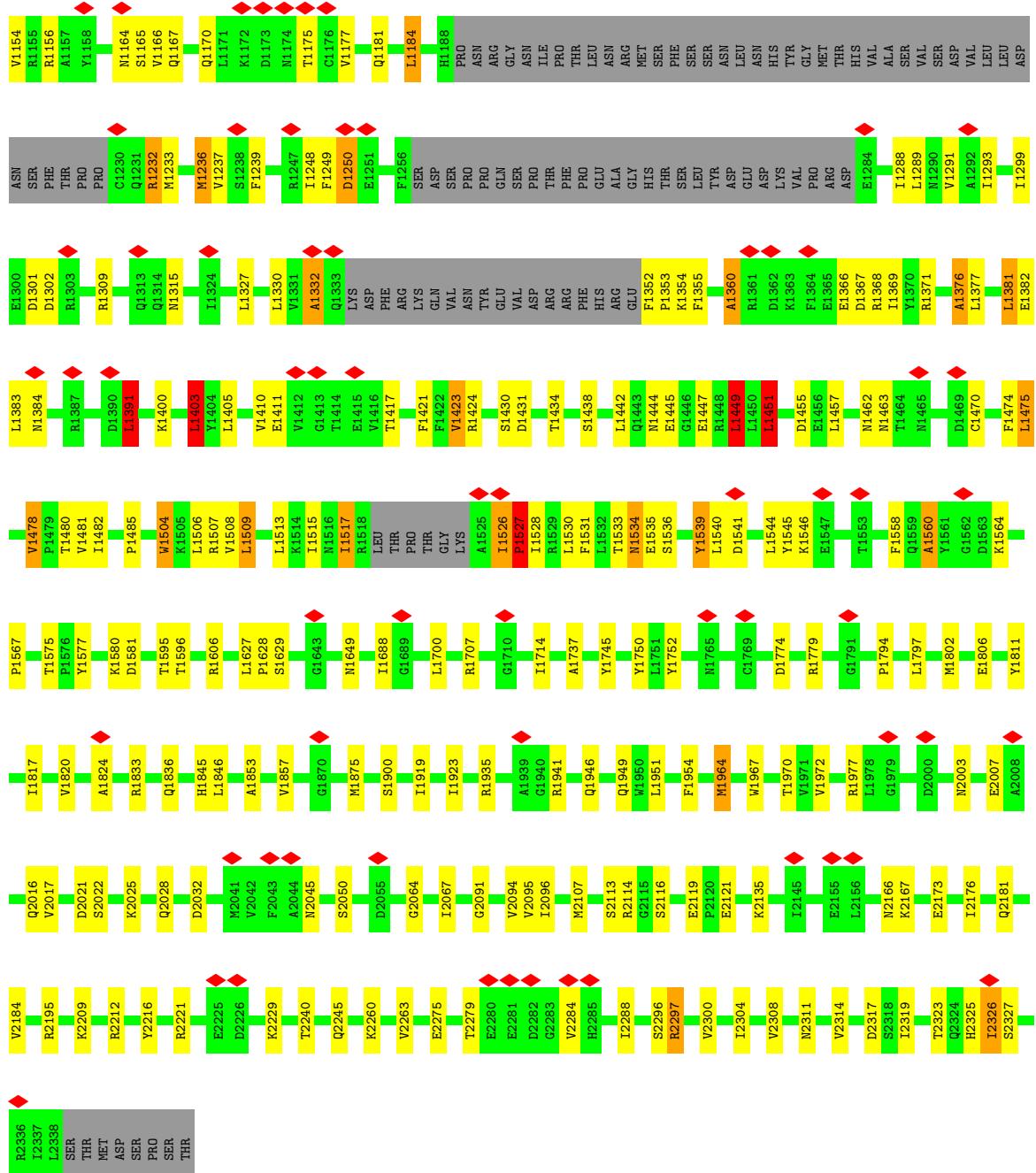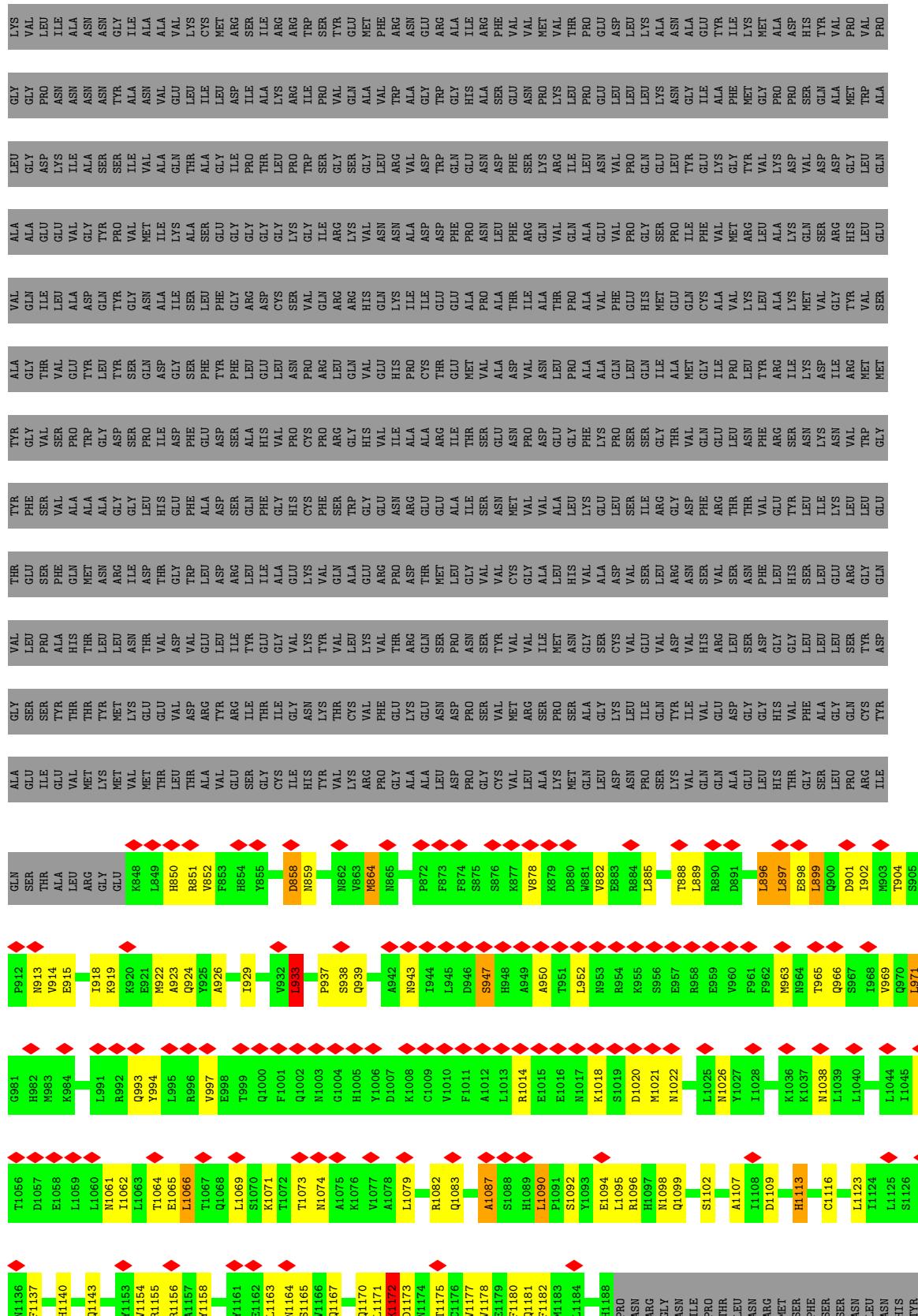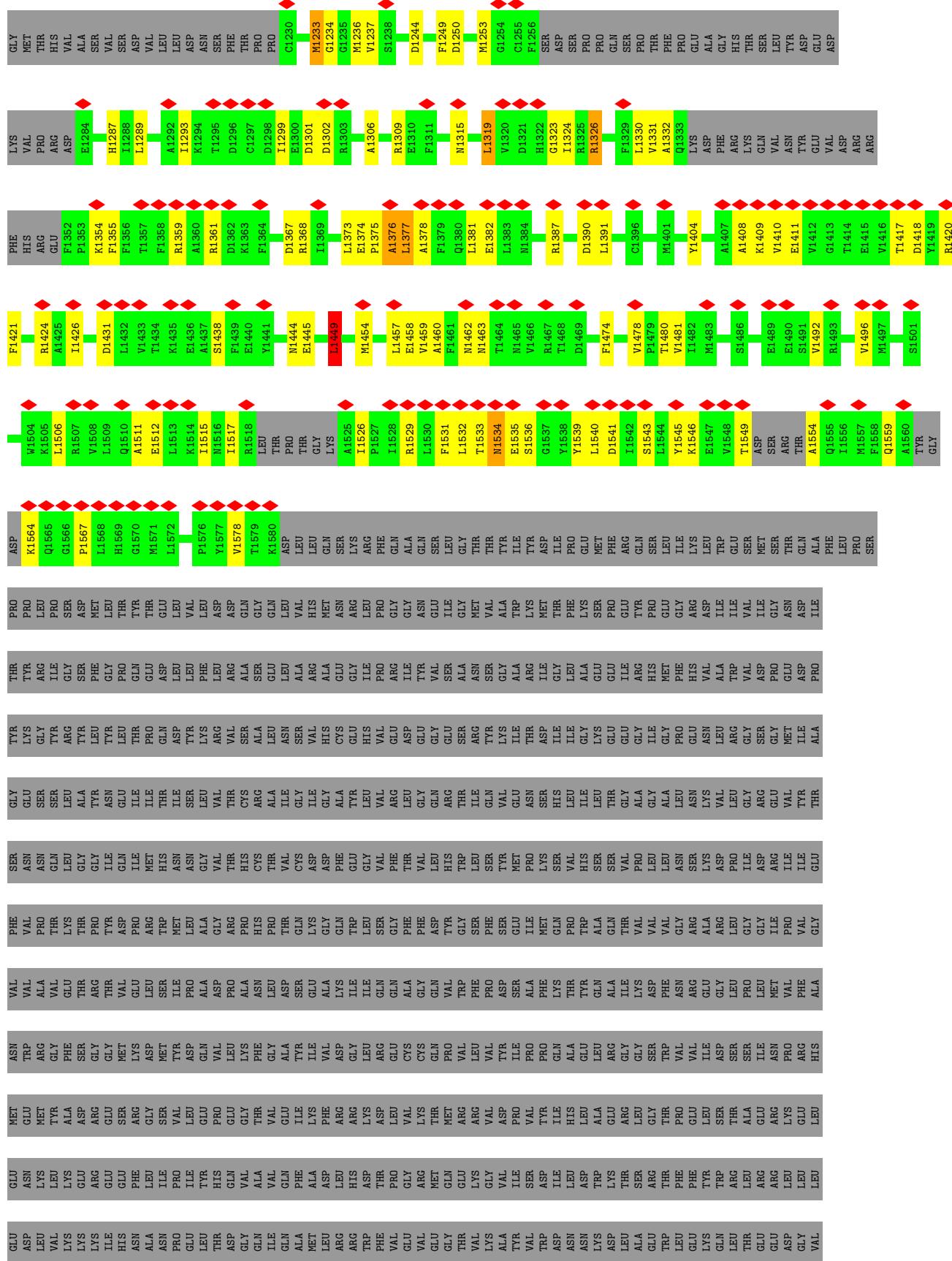
HIS SER VAL ILE GLU GLU ASN ILE LYS CYS ILE SER ARG ASP TYR VAL LEU LYS GLN ILE ARG SER LEU VAL GLN ALA ASN PRO GLU VAL ALA MET ASP SER ILE ILE HIS MET THR GLN HIS ILE SER PRO THR GLN ARG ALA GLU VAL ILE ARG ILE LEU SER THR MET ASP SER PRO

SER THR

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131062	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 $(e^-/Å^2)$	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0172	Depositor
Map size (Å)	476.09998, 476.09998, 476.09998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5　Model quality ⓘ

5.1　Standard geometry ⓘ

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	B	0.42	0/5209	0.95	13/7030 (0.2%)
1	C	0.40	1/17302 (0.0%)	0.88	34/23432 (0.1%)
1	D	0.42	2/17302 (0.0%)	0.94	59/23432 (0.3%)
1	F	0.42	0/5284	0.96	12/7131 (0.2%)
All	All	0.41	3/45097 (0.0%)	0.92	118/61025 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	8
1	C	0	16
1	D	0	16
1	F	0	10
All	All	0	50

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1526	ILE	C-N	7.03	1.47	1.34
1	D	1527	PRO	CB-CG	-5.58	1.22	1.50
1	C	1138	PHE	CA-C	5.14	1.66	1.52

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	971	LEU	CA-CB-CG	13.49	146.33	115.30
1	D	1526	ILE	C-N-CD	-13.29	91.36	120.60
1	D	585	GLY	N-CA-C	12.22	143.64	113.10
1	D	222	LEU	CA-CB-CG	10.98	140.56	115.30
1	D	1527	PRO	C-N-CA	10.94	149.04	121.70

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1171	LEU	Peptide
1	B	1173	ASP	Peptide
1	B	1249	PHE	Peptide
1	B	1315	ASN	Peptide
1	B	1332	ALA	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	B	5112	5114	5134	108	0
1	C	16940	16841	16897	255	0
1	D	16940	16842	16897	282	0
1	F	5186	5194	5214	113	0
All	All	44178	43991	44142	728	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 8.

The worst 5 of 728 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:C:1511:ALA:HB3	1:C:1532:LEU:HD12	1.36	1.07
1:C:721:SER:OG	1:D:173:ASP:O	1.92	0.86
1:C:1533:THR:OG1	1:C:1541:ASP:O	1.94	0.84
1:D:357:HIS:ND1	1:D:378:CYS:SG	2.50	0.83
1:C:1387:ARG:O	1:C:1409:LYS:NZ	2.12	0.81

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	B	609/2407 (25%)	522 (86%)	81 (13%)	6 (1%)	15	54
1	C	2107/2407 (88%)	1908 (91%)	191 (9%)	8 (0%)	34	72
1	D	2107/2407 (88%)	1901 (90%)	193 (9%)	13 (1%)	25	65
1	F	620/2407 (26%)	521 (84%)	91 (15%)	8 (1%)	12	48
All	All	5443/9628 (56%)	4852 (89%)	556 (10%)	35 (1%)	29	65

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1087	ALA
1	B	1304	LEU
1	B	1365	GLU
1	C	1304	LEU
1	D	1527	PRO

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	B	571/2108 (27%)	552 (97%)	19 (3%)	38	61
1	C	1855/2108 (88%)	1806 (97%)	49 (3%)	46	67
1	D	1855/2108 (88%)	1800 (97%)	55 (3%)	41	63
1	F	579/2108 (28%)	552 (95%)	27 (5%)	26	52
All	All	4860/8432 (58%)	4710 (97%)	150 (3%)	43	62

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2003	ASN
1	F	1438	SER
1	D	2240	THR
1	F	947	SER
1	C	1463	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1534	ASN
1	F	1534	ASN
1	D	2003	ASN
1	F	1170	GLN
1	C	698	ASN

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 monosaccharides in this entry.

5.6　Ligand geometry ⓘ

There are no ligands in this entry.

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.
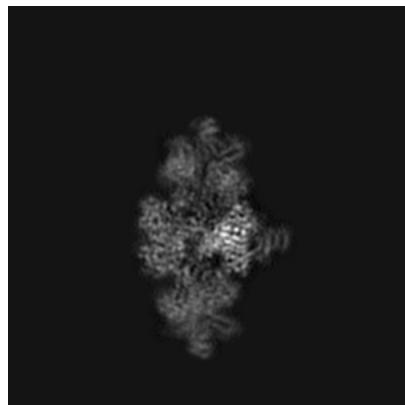
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-4342. These allow visual inspection of the internal detail of the map and identification of artifacts.
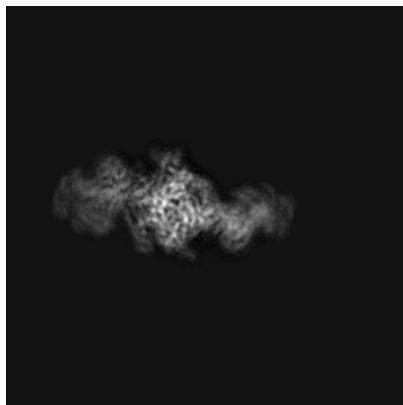
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ
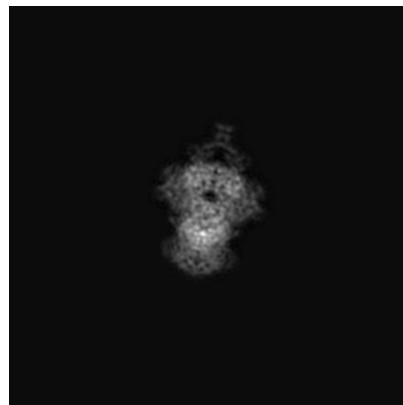
6.1.1 Primary map

| X | Y | Z |
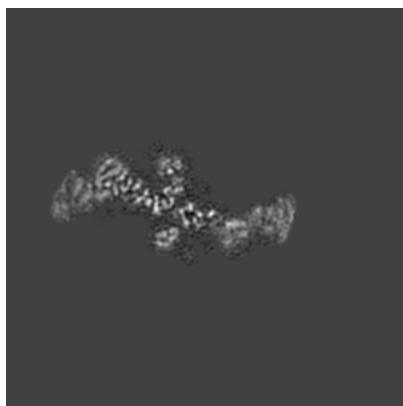
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 225 | Y Index: 225 | Z Index: 225 |
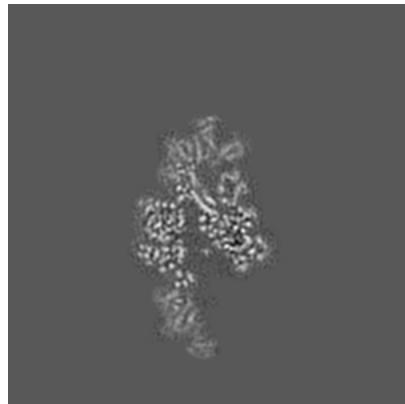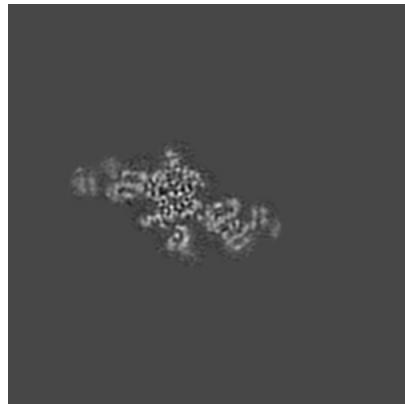
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices (i)
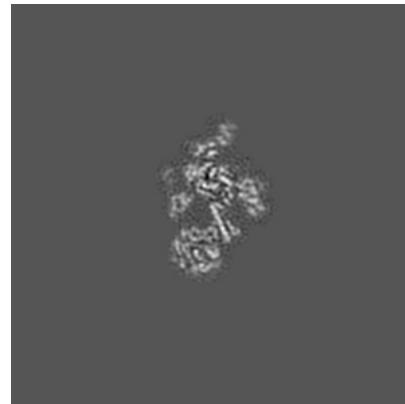
6.3.1   Primary map

| X Index: 217 | Y Index: 247 | Z Index: 177 |
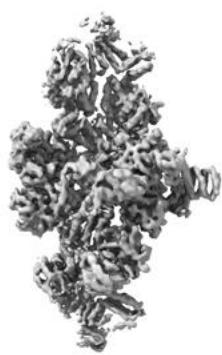
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal surface views (i)

6.4.1   Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0172. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.
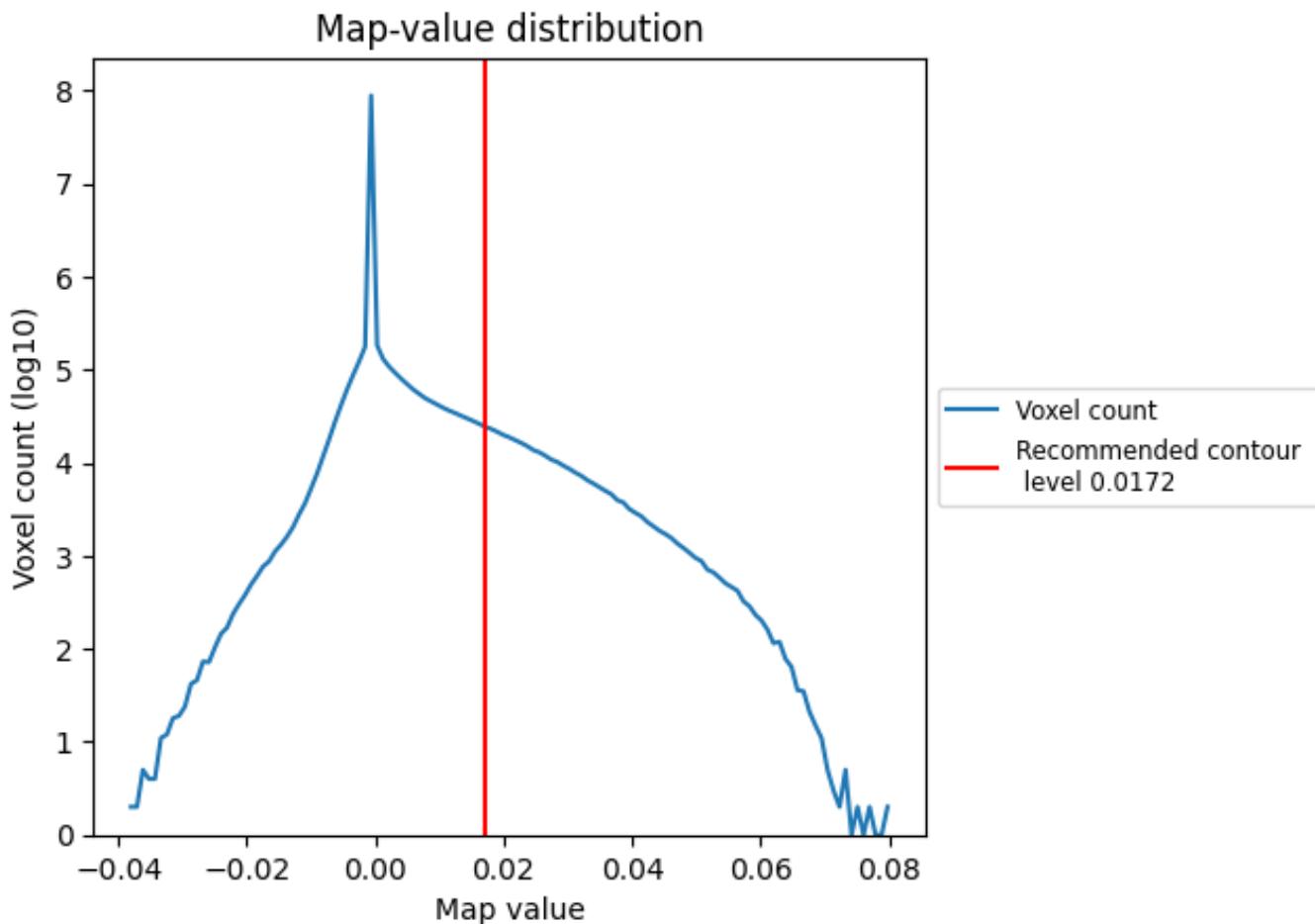
6.5 Mask visualisation ⓘ

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

7   Map analysis ⓘ
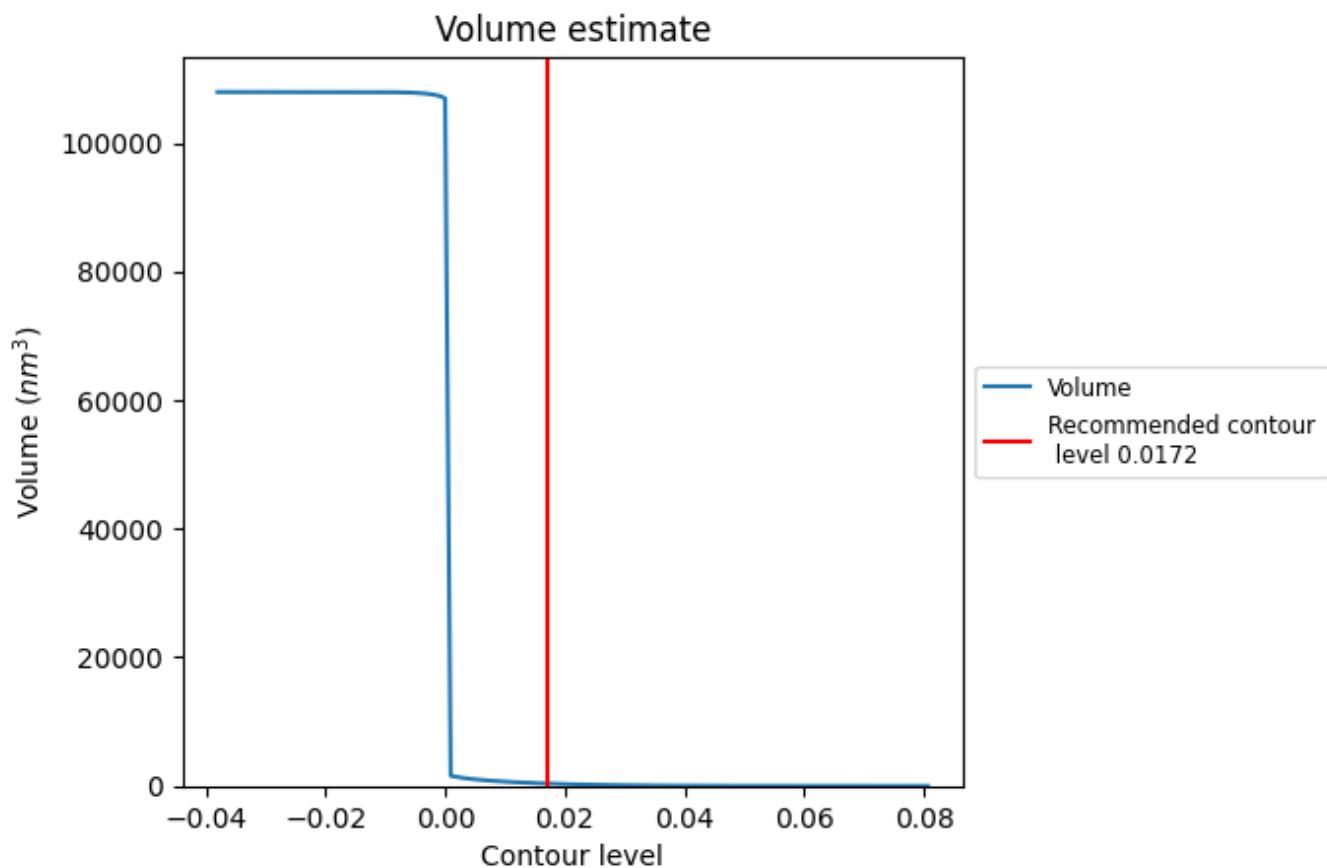
This section contains the results of statistical analysis of the map.

7.1   Map-value distribution ⓘ

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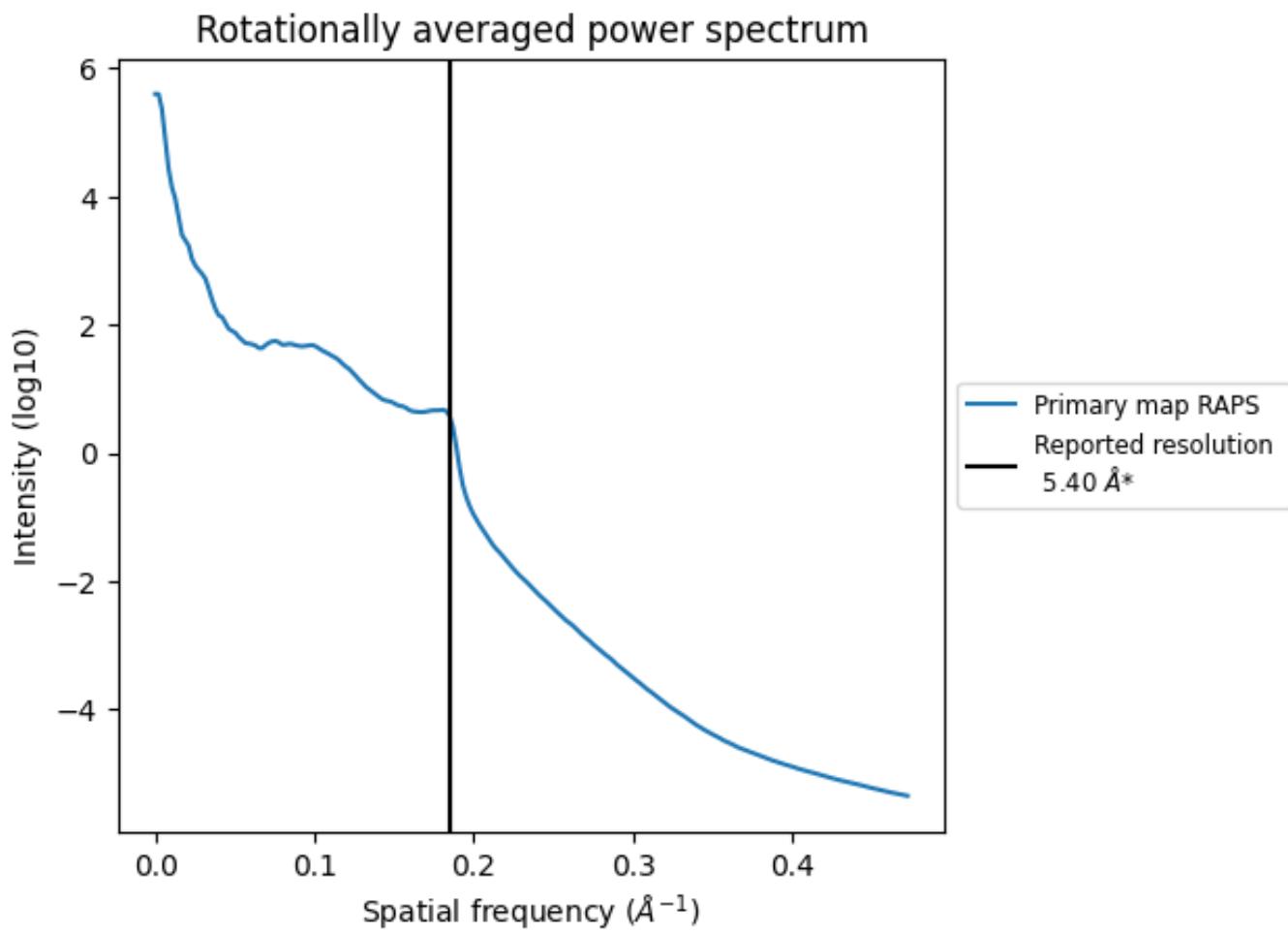
7.2   Volume estimate (i)

Volume estimate

The volume at the recommended contour level is 370 nm³; this corresponds to an approximate mass of 334 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 0.185 Å^{-1}
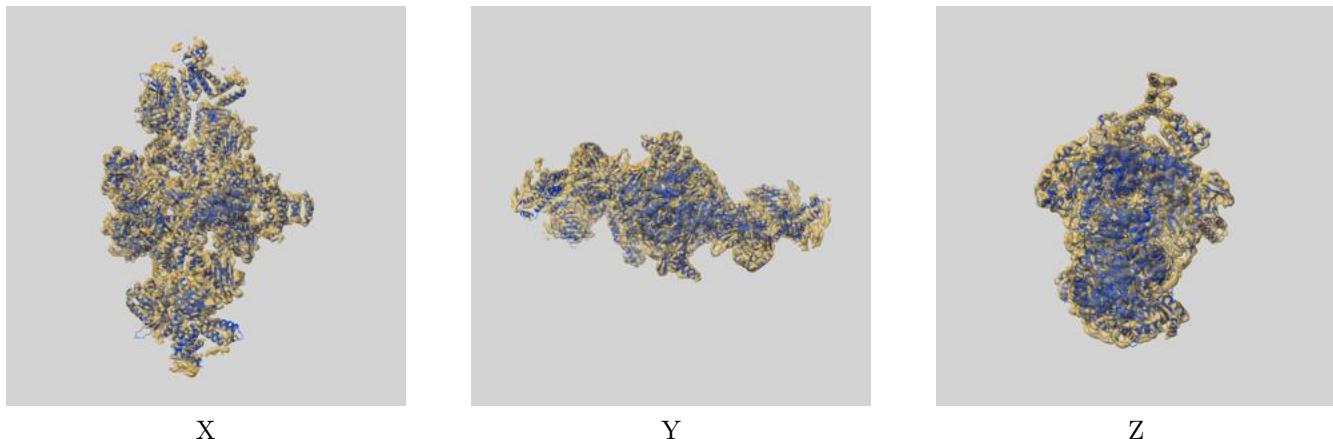
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit (i)
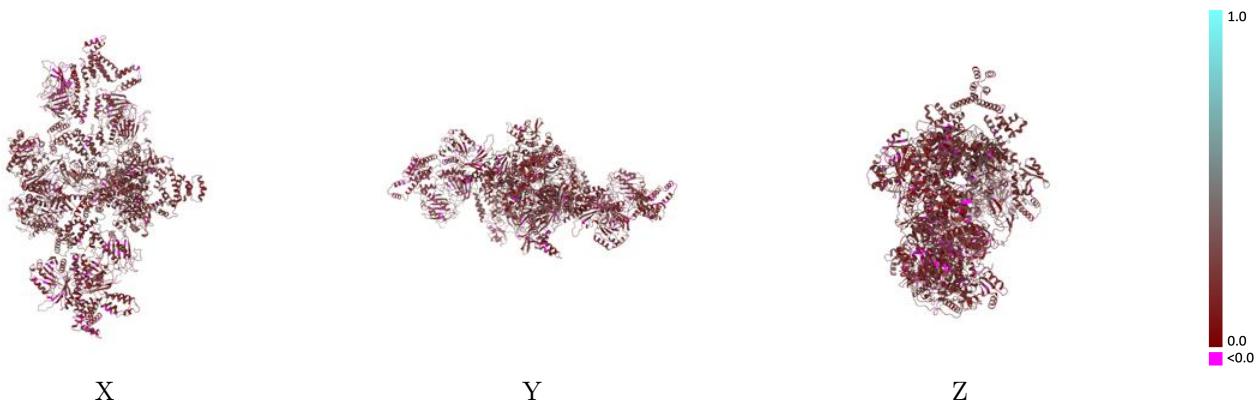
This section contains information regarding the fit between EMDB map EMD-4342 and PDB model 6G2D. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay (i)
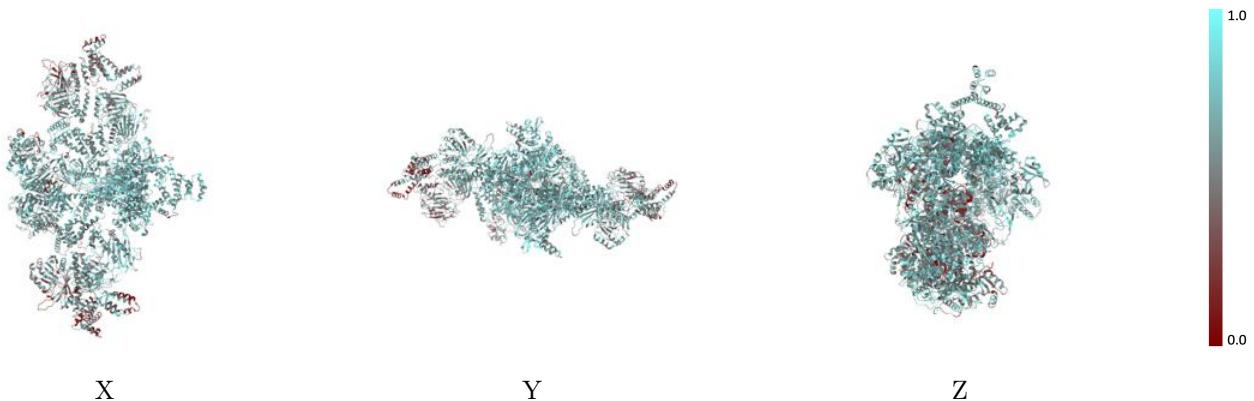
X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.0172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model (i)

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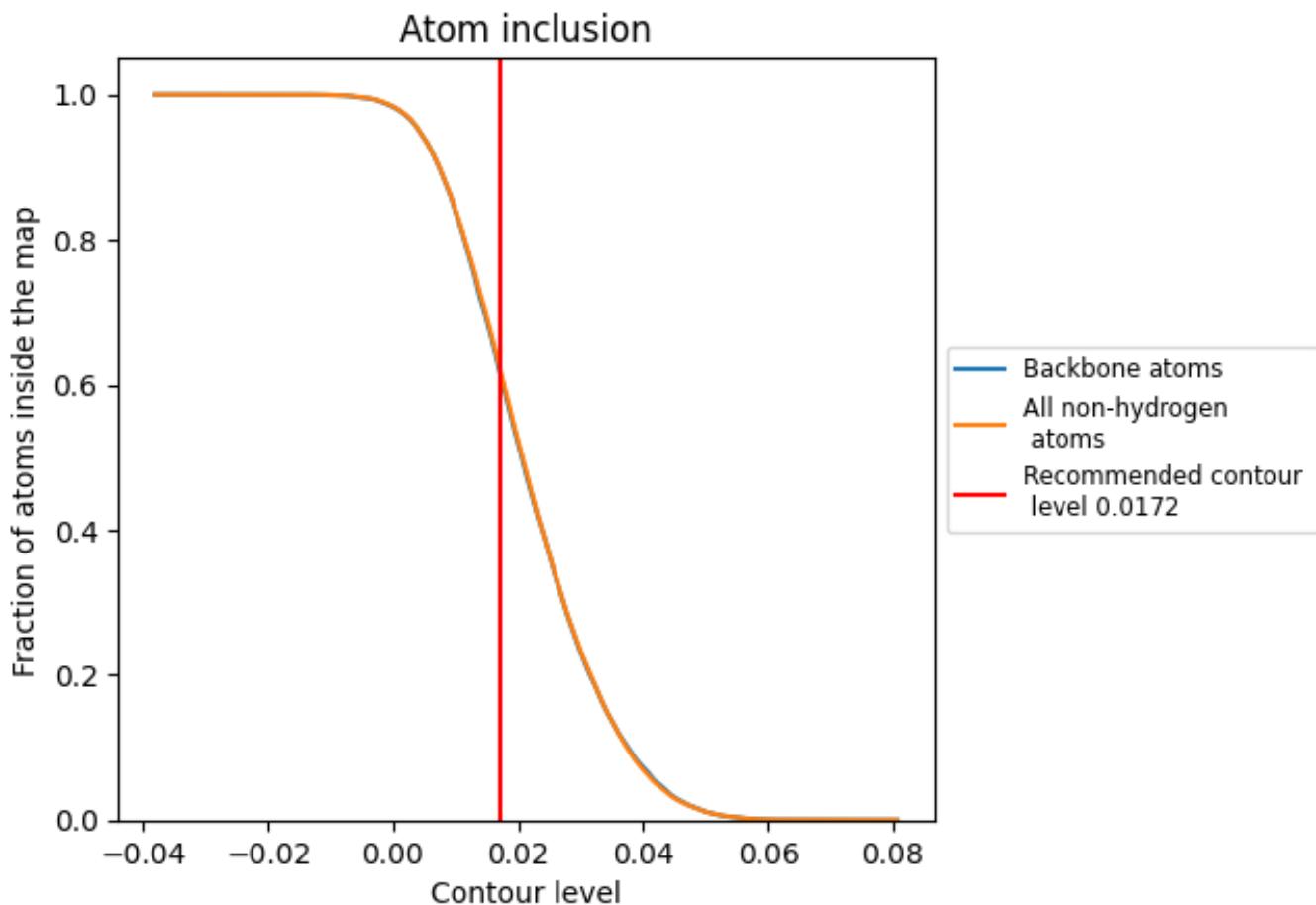
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model (i)

X   Y   Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0172).

9.4　Atom inclusion ⓘ

At the recommended contour level, 61% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6199	0.2160
B	0.5194	0.1810
C	0.6712	0.2260
D	0.6747	0.2280
F	0.4604	0.1760

1.0

0.0
<0.0