



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 05:50 am GMT

PDB ID : 6G2I
EMDB ID : EMD-4344
Title : Filament of acetyl-CoA carboxylase and BRCT domains of BRCA1 (ACC-BRCT) at 5.9 Å resolution
Authors : Hunkeler, M.; Hagmann, A.; Stutfeld, E.; Chami, M.; Stahlberg, H.; Maier, T.
Deposited on : 2018-03-23
Resolution : 5.90 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

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

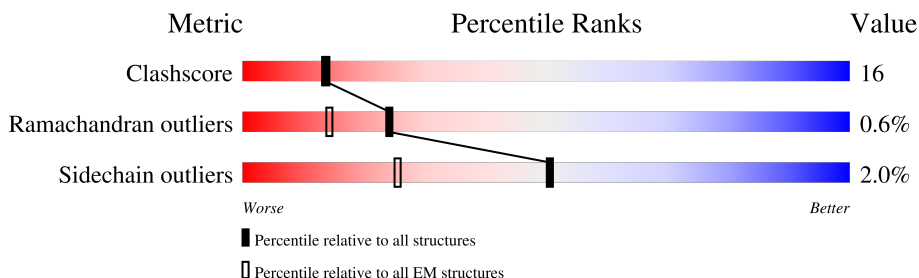
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2346	<div> <div>65%</div> <div>58%</div> <div>28%</div> <div>11%</div> </div>
1	B	2346	<div> <div>65%</div> <div>58%</div> <div>28%</div> <div>11%</div> </div>
1	C	2346	<div> <div>45%</div> <div>54%</div> <div>32%</div> <div>11%</div> </div>
1	D	2346	<div> <div>27%</div> <div>48%</div> <div>35%</div> <div>11%</div> </div>
1	E	2346	<div> <div>27%</div> <div>50%</div> <div>36%</div> <div>11%</div> </div>
1	F	2346	<div> <div>45%</div> <div>56%</div> <div>30%</div> <div>11%</div> </div>
1	G	2346	<div> <div>31%</div> <div>23%</div> <div>9%</div> <div>68%</div> </div>
1	J	2346	<div> <div>56%</div> <div>41%</div> <div>14%</div> <div>44%</div> </div>

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Mol	Chain	Length	Quality of chain
1	Q	2346	
1	R	2346	
2	H	240	
2	K	240	
2	M	240	
2	O	240	
2	S	240	
2	U	240	
2	W	240	
2	Y	240	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 288810 atoms, of which 143374 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	D	2080	Total	C	H	N	O	P	S	0	0
			32758	10493	16276	2855	3033	1	100		
1	E	2080	Total	C	H	N	O	P	S	0	0
			32758	10493	16276	2855	3033	1	100		
1	C	2080	Total	C	H	N	O	P	S	0	0
			32757	10493	16275	2855	3033	1	100		
1	F	2080	Total	C	H	N	O	P	S	0	0
			32757	10493	16275	2855	3033	1	100		
1	B	2080	Total	C	H	N	O	P	S	0	0
			32758	10493	16276	2855	3033	1	100		
1	A	2080	Total	C	H	N	O	P	S	0	0
			32758	10493	16276	2855	3033	1	100		
1	G	757	Total	C	H	N	O	S		0	0
			12055	3855	5997	1050	1124	29			
1	Q	757	Total	C	H	N	O	S		0	0
			12055	3855	5997	1050	1124	29			
1	J	1323	Total	C	H	N	O	P	S	0	0
			20703	6638	10279	1805	1909	1	71		
1	R	1323	Total	C	H	N	O	P	S	0	0
			20703	6638	10279	1805	1909	1	71		

- Molecule 2 is a protein called Breast cancer type 1 susceptibility protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	214	Total	C	H	N	O	S	0	0
			3347	1084	1648	289	312	14		
2	K	214	Total	C	H	N	O	S	0	0
			3340	1083	1644	286	313	14		
2	M	214	Total	C	H	N	O	S	0	0
			3347	1084	1648	289	312	14		
2	O	214	Total	C	H	N	O	S	0	0
			3340	1083	1644	286	313	14		
2	S	214	Total	C	H	N	O	S	0	0
			3347	1084	1648	289	312	14		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	U	214	Total	C	H	N	O	S	0	0
			3340	1083	1644	286	313	14		
2	Y	214	Total	C	H	N	O	S	0	0
			3347	1084	1648	289	312	14		
2	W	214	Total	C	H	N	O	S	0	0
			3340	1083	1644	286	313	14		

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1620	MET	-	initiating methionine	UNP P38398
H	1621	LYS	-	expression tag	UNP P38398
H	1622	HIS	-	expression tag	UNP P38398
H	1623	HIS	-	expression tag	UNP P38398
H	1624	HIS	-	expression tag	UNP P38398
H	1625	HIS	-	expression tag	UNP P38398
H	1626	HIS	-	expression tag	UNP P38398
H	1627	HIS	-	expression tag	UNP P38398
H	1628	PRO	-	expression tag	UNP P38398
H	1629	MET	-	expression tag	UNP P38398
H	1630	THR	-	expression tag	UNP P38398
H	1631	SER	-	expression tag	UNP P38398
H	1632	LEU	-	expression tag	UNP P38398
H	1633	TYR	-	expression tag	UNP P38398
H	1634	LYS	-	expression tag	UNP P38398
H	1635	LYS	-	expression tag	UNP P38398
H	1636	ALA	-	expression tag	UNP P38398
H	1637	GLY	-	expression tag	UNP P38398
H	1638	LEU	-	expression tag	UNP P38398
H	1639	GLU	-	expression tag	UNP P38398
H	1640	ASN	-	expression tag	UNP P38398
H	1641	LEU	-	expression tag	UNP P38398
H	1642	TYR	-	expression tag	UNP P38398
H	1643	PHE	-	expression tag	UNP P38398
H	1644	GLN	-	expression tag	UNP P38398
H	1645	GLY	-	expression tag	UNP P38398
K	1620	MET	-	initiating methionine	UNP P38398
K	1621	LYS	-	expression tag	UNP P38398
K	1622	HIS	-	expression tag	UNP P38398
K	1623	HIS	-	expression tag	UNP P38398
K	1624	HIS	-	expression tag	UNP P38398
K	1625	HIS	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1626	HIS	-	expression tag	UNP P38398
K	1627	HIS	-	expression tag	UNP P38398
K	1628	PRO	-	expression tag	UNP P38398
K	1629	MET	-	expression tag	UNP P38398
K	1630	THR	-	expression tag	UNP P38398
K	1631	SER	-	expression tag	UNP P38398
K	1632	LEU	-	expression tag	UNP P38398
K	1633	TYR	-	expression tag	UNP P38398
K	1634	LYS	-	expression tag	UNP P38398
K	1635	LYS	-	expression tag	UNP P38398
K	1636	ALA	-	expression tag	UNP P38398
K	1637	GLY	-	expression tag	UNP P38398
K	1638	LEU	-	expression tag	UNP P38398
K	1639	GLU	-	expression tag	UNP P38398
K	1640	ASN	-	expression tag	UNP P38398
K	1641	LEU	-	expression tag	UNP P38398
K	1642	TYR	-	expression tag	UNP P38398
K	1643	PHE	-	expression tag	UNP P38398
K	1644	GLN	-	expression tag	UNP P38398
K	1645	GLY	-	expression tag	UNP P38398
M	1620	MET	-	initiating methionine	UNP P38398
M	1621	LYS	-	expression tag	UNP P38398
M	1622	HIS	-	expression tag	UNP P38398
M	1623	HIS	-	expression tag	UNP P38398
M	1624	HIS	-	expression tag	UNP P38398
M	1625	HIS	-	expression tag	UNP P38398
M	1626	HIS	-	expression tag	UNP P38398
M	1627	HIS	-	expression tag	UNP P38398
M	1628	PRO	-	expression tag	UNP P38398
M	1629	MET	-	expression tag	UNP P38398
M	1630	THR	-	expression tag	UNP P38398
M	1631	SER	-	expression tag	UNP P38398
M	1632	LEU	-	expression tag	UNP P38398
M	1633	TYR	-	expression tag	UNP P38398
M	1634	LYS	-	expression tag	UNP P38398
M	1635	LYS	-	expression tag	UNP P38398
M	1636	ALA	-	expression tag	UNP P38398
M	1637	GLY	-	expression tag	UNP P38398
M	1638	LEU	-	expression tag	UNP P38398
M	1639	GLU	-	expression tag	UNP P38398
M	1640	ASN	-	expression tag	UNP P38398
M	1641	LEU	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
M	1642	TYR	-	expression tag	UNP P38398
M	1643	PHE	-	expression tag	UNP P38398
M	1644	GLN	-	expression tag	UNP P38398
M	1645	GLY	-	expression tag	UNP P38398
O	1620	MET	-	initiating methionine	UNP P38398
O	1621	LYS	-	expression tag	UNP P38398
O	1622	HIS	-	expression tag	UNP P38398
O	1623	HIS	-	expression tag	UNP P38398
O	1624	HIS	-	expression tag	UNP P38398
O	1625	HIS	-	expression tag	UNP P38398
O	1626	HIS	-	expression tag	UNP P38398
O	1627	HIS	-	expression tag	UNP P38398
O	1628	PRO	-	expression tag	UNP P38398
O	1629	MET	-	expression tag	UNP P38398
O	1630	THR	-	expression tag	UNP P38398
O	1631	SER	-	expression tag	UNP P38398
O	1632	LEU	-	expression tag	UNP P38398
O	1633	TYR	-	expression tag	UNP P38398
O	1634	LYS	-	expression tag	UNP P38398
O	1635	LYS	-	expression tag	UNP P38398
O	1636	ALA	-	expression tag	UNP P38398
O	1637	GLY	-	expression tag	UNP P38398
O	1638	LEU	-	expression tag	UNP P38398
O	1639	GLU	-	expression tag	UNP P38398
O	1640	ASN	-	expression tag	UNP P38398
O	1641	LEU	-	expression tag	UNP P38398
O	1642	TYR	-	expression tag	UNP P38398
O	1643	PHE	-	expression tag	UNP P38398
O	1644	GLN	-	expression tag	UNP P38398
O	1645	GLY	-	expression tag	UNP P38398
S	1620	MET	-	initiating methionine	UNP P38398
S	1621	LYS	-	expression tag	UNP P38398
S	1622	HIS	-	expression tag	UNP P38398
S	1623	HIS	-	expression tag	UNP P38398
S	1624	HIS	-	expression tag	UNP P38398
S	1625	HIS	-	expression tag	UNP P38398
S	1626	HIS	-	expression tag	UNP P38398
S	1627	HIS	-	expression tag	UNP P38398
S	1628	PRO	-	expression tag	UNP P38398
S	1629	MET	-	expression tag	UNP P38398
S	1630	THR	-	expression tag	UNP P38398
S	1631	SER	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
S	1632	LEU	-	expression tag	UNP P38398
S	1633	TYR	-	expression tag	UNP P38398
S	1634	LYS	-	expression tag	UNP P38398
S	1635	LYS	-	expression tag	UNP P38398
S	1636	ALA	-	expression tag	UNP P38398
S	1637	GLY	-	expression tag	UNP P38398
S	1638	LEU	-	expression tag	UNP P38398
S	1639	GLU	-	expression tag	UNP P38398
S	1640	ASN	-	expression tag	UNP P38398
S	1641	LEU	-	expression tag	UNP P38398
S	1642	TYR	-	expression tag	UNP P38398
S	1643	PHE	-	expression tag	UNP P38398
S	1644	GLN	-	expression tag	UNP P38398
S	1645	GLY	-	expression tag	UNP P38398
U	1620	MET	-	initiating methionine	UNP P38398
U	1621	LYS	-	expression tag	UNP P38398
U	1622	HIS	-	expression tag	UNP P38398
U	1623	HIS	-	expression tag	UNP P38398
U	1624	HIS	-	expression tag	UNP P38398
U	1625	HIS	-	expression tag	UNP P38398
U	1626	HIS	-	expression tag	UNP P38398
U	1627	HIS	-	expression tag	UNP P38398
U	1628	PRO	-	expression tag	UNP P38398
U	1629	MET	-	expression tag	UNP P38398
U	1630	THR	-	expression tag	UNP P38398
U	1631	SER	-	expression tag	UNP P38398
U	1632	LEU	-	expression tag	UNP P38398
U	1633	TYR	-	expression tag	UNP P38398
U	1634	LYS	-	expression tag	UNP P38398
U	1635	LYS	-	expression tag	UNP P38398
U	1636	ALA	-	expression tag	UNP P38398
U	1637	GLY	-	expression tag	UNP P38398
U	1638	LEU	-	expression tag	UNP P38398
U	1639	GLU	-	expression tag	UNP P38398
U	1640	ASN	-	expression tag	UNP P38398
U	1641	LEU	-	expression tag	UNP P38398
U	1642	TYR	-	expression tag	UNP P38398
U	1643	PHE	-	expression tag	UNP P38398
U	1644	GLN	-	expression tag	UNP P38398
U	1645	GLY	-	expression tag	UNP P38398
Y	1620	MET	-	initiating methionine	UNP P38398
Y	1621	LYS	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	1622	HIS	-	expression tag	UNP P38398
Y	1623	HIS	-	expression tag	UNP P38398
Y	1624	HIS	-	expression tag	UNP P38398
Y	1625	HIS	-	expression tag	UNP P38398
Y	1626	HIS	-	expression tag	UNP P38398
Y	1627	HIS	-	expression tag	UNP P38398
Y	1628	PRO	-	expression tag	UNP P38398
Y	1629	MET	-	expression tag	UNP P38398
Y	1630	THR	-	expression tag	UNP P38398
Y	1631	SER	-	expression tag	UNP P38398
Y	1632	LEU	-	expression tag	UNP P38398
Y	1633	TYR	-	expression tag	UNP P38398
Y	1634	LYS	-	expression tag	UNP P38398
Y	1635	LYS	-	expression tag	UNP P38398
Y	1636	ALA	-	expression tag	UNP P38398
Y	1637	GLY	-	expression tag	UNP P38398
Y	1638	LEU	-	expression tag	UNP P38398
Y	1639	GLU	-	expression tag	UNP P38398
Y	1640	ASN	-	expression tag	UNP P38398
Y	1641	LEU	-	expression tag	UNP P38398
Y	1642	TYR	-	expression tag	UNP P38398
Y	1643	PHE	-	expression tag	UNP P38398
Y	1644	GLN	-	expression tag	UNP P38398
Y	1645	GLY	-	expression tag	UNP P38398
W	1620	MET	-	initiating methionine	UNP P38398
W	1621	LYS	-	expression tag	UNP P38398
W	1622	HIS	-	expression tag	UNP P38398
W	1623	HIS	-	expression tag	UNP P38398
W	1624	HIS	-	expression tag	UNP P38398
W	1625	HIS	-	expression tag	UNP P38398
W	1626	HIS	-	expression tag	UNP P38398
W	1627	HIS	-	expression tag	UNP P38398
W	1628	PRO	-	expression tag	UNP P38398
W	1629	MET	-	expression tag	UNP P38398
W	1630	THR	-	expression tag	UNP P38398
W	1631	SER	-	expression tag	UNP P38398
W	1632	LEU	-	expression tag	UNP P38398
W	1633	TYR	-	expression tag	UNP P38398
W	1634	LYS	-	expression tag	UNP P38398
W	1635	LYS	-	expression tag	UNP P38398
W	1636	ALA	-	expression tag	UNP P38398
W	1637	GLY	-	expression tag	UNP P38398

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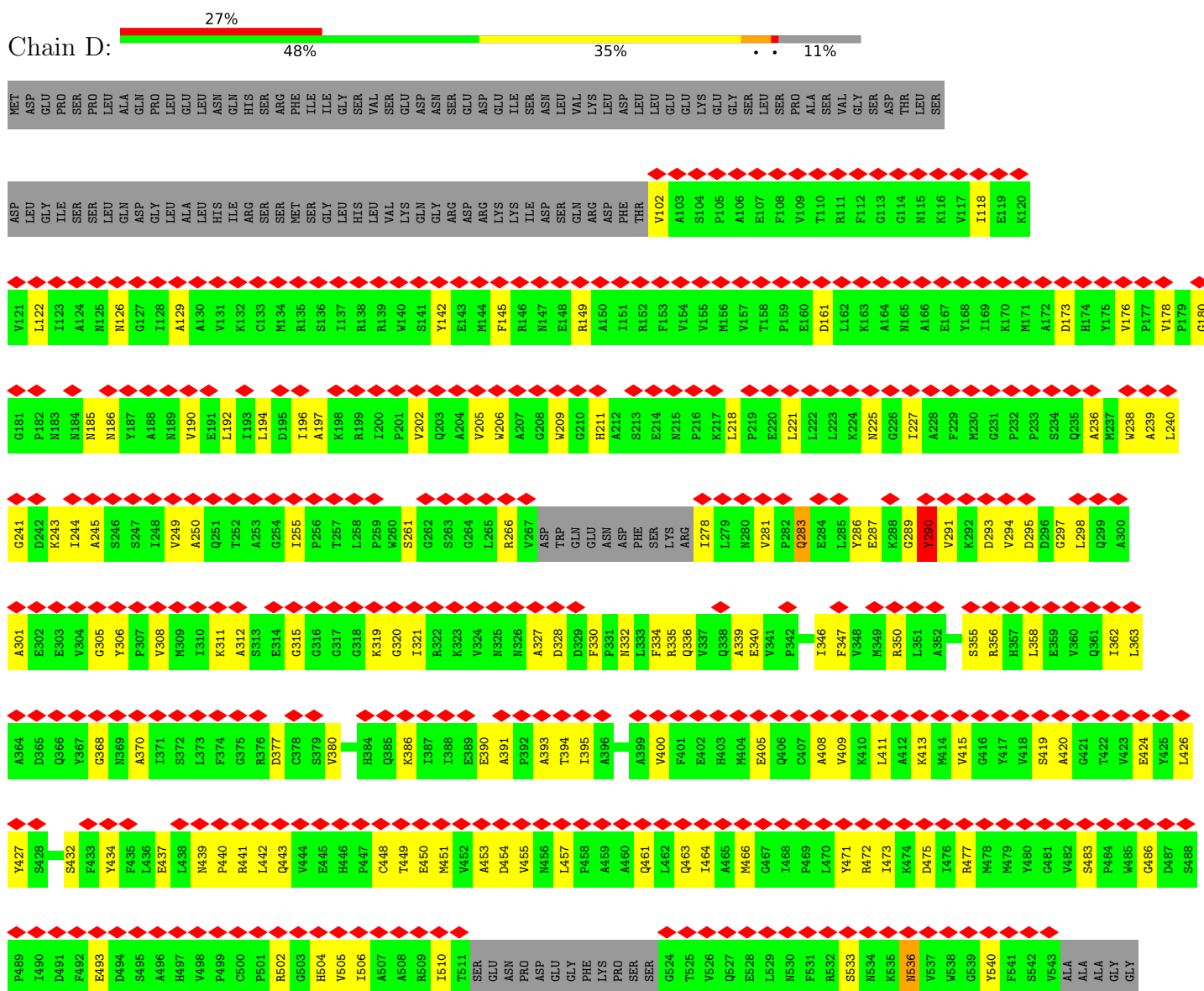
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Chain	Residue	Modelled	Actual	Comment	Reference
W	1638	LEU	-	expression tag	UNP P38398
W	1639	GLU	-	expression tag	UNP P38398
W	1640	ASN	-	expression tag	UNP P38398
W	1641	LEU	-	expression tag	UNP P38398
W	1642	TYR	-	expression tag	UNP P38398
W	1643	PHE	-	expression tag	UNP P38398
W	1644	GLN	-	expression tag	UNP P38398
W	1645	GLY	-	expression tag	UNP P38398

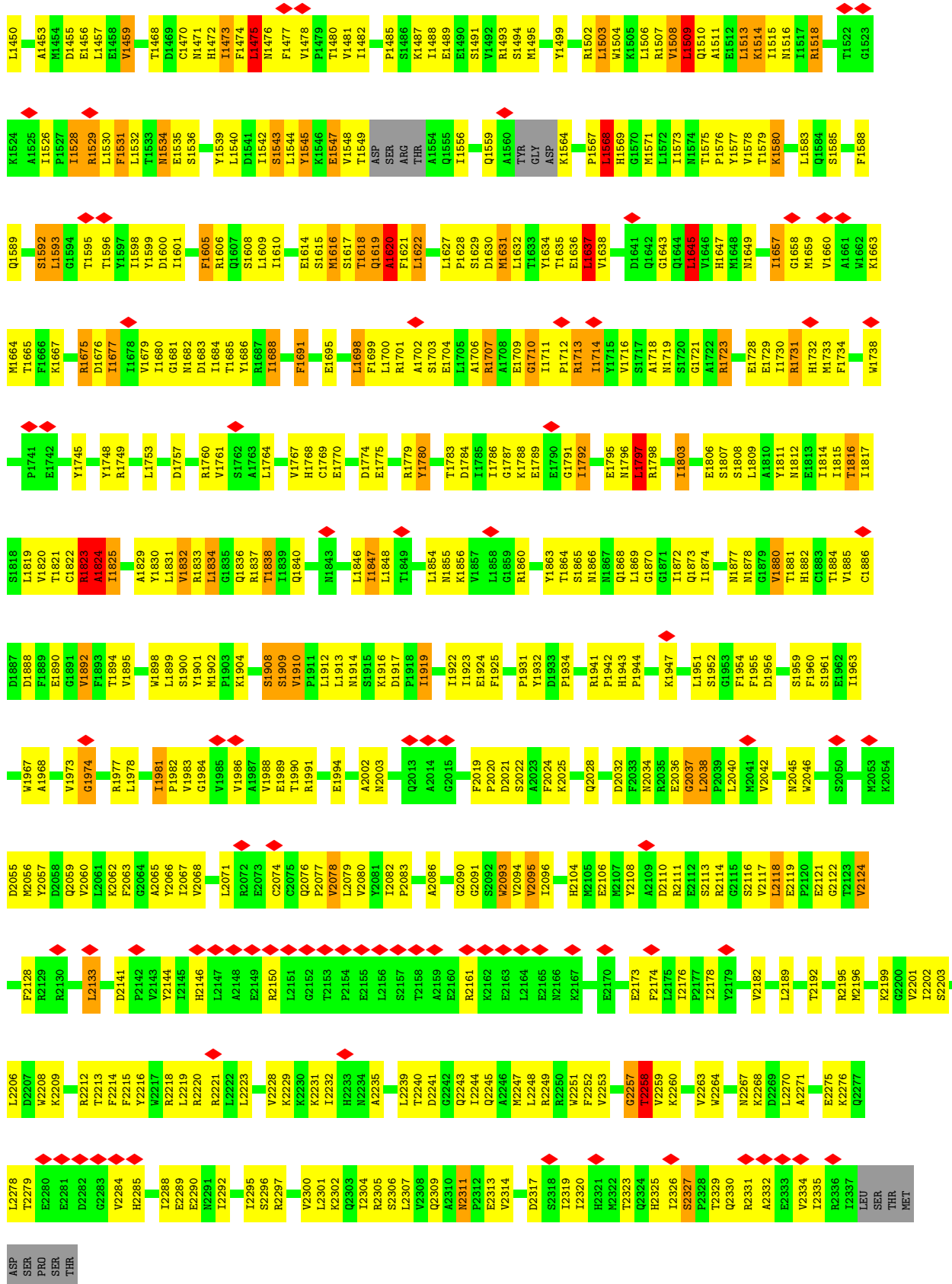
3 Residue-property plots

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





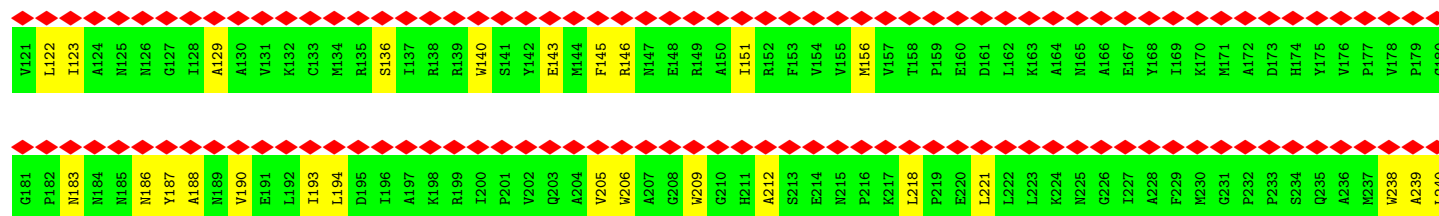


• Molecule 1: Acetyl-CoA carboxylase 1

Chain E:  27% 50% 36% 11%

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

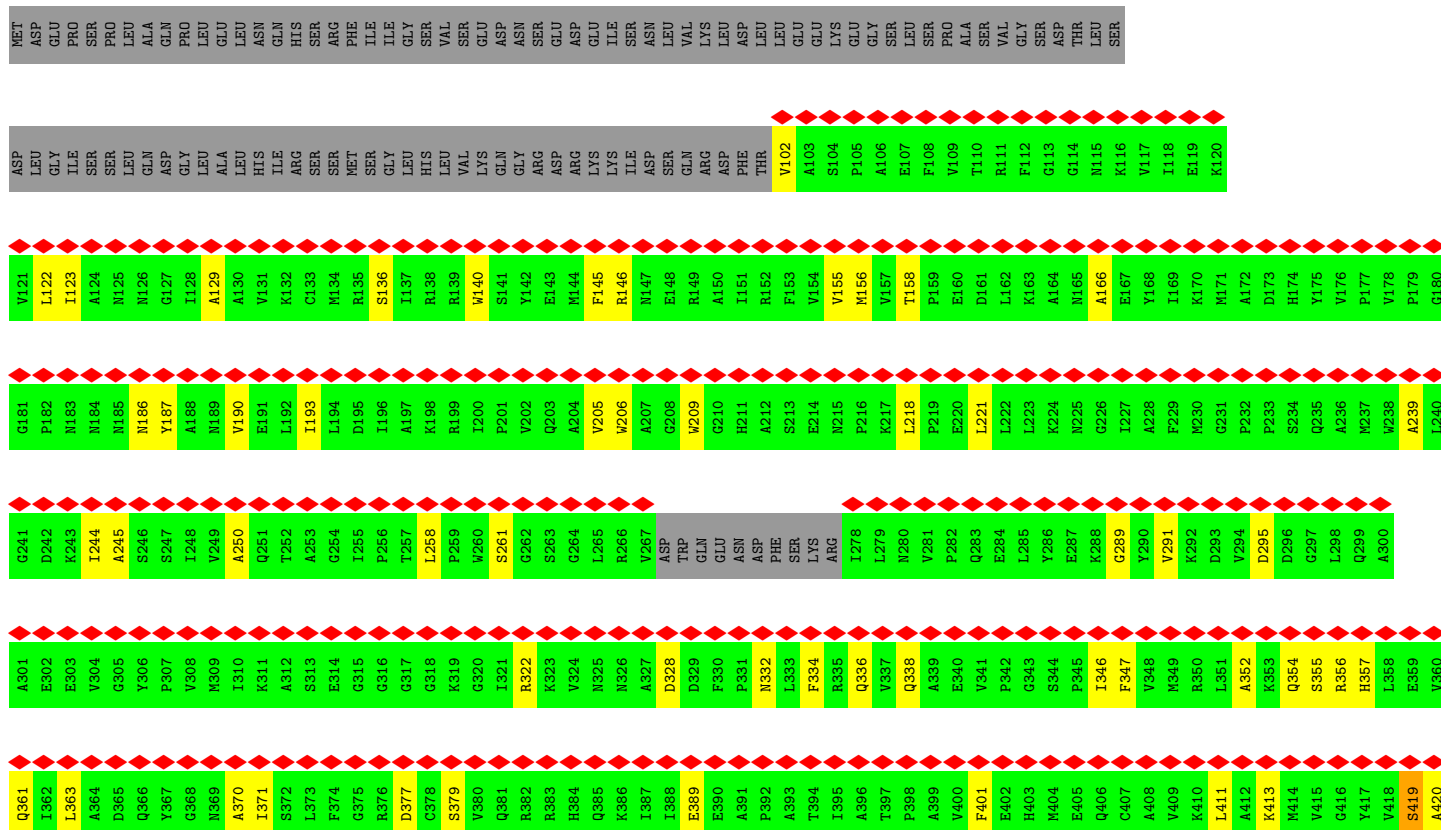
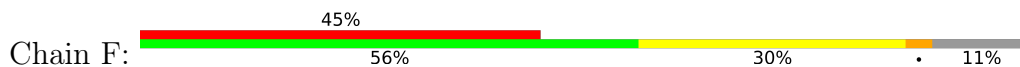




G241	A301	Q361	G421	G481	F541	E601	L661	S721	E781	D901	M963
D242	E302	I362	T422	V482	S542	S602	P662	S722	I782	I902	N964
K243	E303	L363	V423	S483	V543	F603	A663	Y723	E783	M903	T965
I244	V304	A364	E424	P484	ALA	Q604	H664	T724	W784	T904	Q966
A245	G305	A485	Y425	G486	ALA	M605	T665	Y725	M785	S905	S967
S246	G306	Q366	L426	G487	GLY	N606	L666	Y726	K786	V906	I968
S247	P307	Y367	Y427	D487	GLY	R607	L667	M727	M787	S907	V969
I248	V308	G368	S428	S488	LEU	I608	N668	K728	V788	G908	Q970
V249	M309	N369	Q429	P489	HIS	D609	T669	E729	M789	R909	G971
A250	I310	A370	D430	I490	GLU	T610	V670	E730	T790	R910	Q972
Q251	K311	I371	G431	D491	PHE	G611	D671	V731	L791	P911	Q973
T252	A312	S372	S432	E492	ASP	G612	V672	D732	T792	P912	R974
G253	S133	L373	F433	E493	SER	L613	E673	R733	A793	M913	Y975
A254	E314	F374	Y434	D494	Q556	D614	L674	Y734	W794	R914	R976
I255	G315	G375	F435	S495	F557	R615	L675	R735	E795	E915	S977
P256	G316	R376	L436	A496	G558	L616	Y676	T736	S796	K916	G978
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L258	G318	C378	L438	V498	C560	ALA	G678	I738	C798	I918	R980
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W260	G320	V380	P440	C500	S562	LYS	K680	N740	H800	K920	H982
S261	I321	Q381	R441	F501	M563	VAL	Y681	K741	W801	E921	M983
G262	R322	R382	L442	R502	G564	GLN	V682	T742	A802	M922	A984
S263	K323	R383	Q443	G503	E565	ALA	L683	C743	R803	K923	V986
G264	V324	H384	V444	H504	N566	R625	K684	V744	R804	Q924	Y987
L265	N325	Q385	E445	V505	R567	P626	V685	F745	P805	Y925	M988
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V267	A327	I387	P447	A507	E569	T628	R687	K747	A807	S927	L990
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TRP	D329	E389	T449	R509	I571	L630	S689	ASP	L809	P929	R992
GLU	F330	E390	E450	R510	S572	G631	P690	PRD	L810	T930	Q993
ASN	P331	A391	M451	I511	N573	V632	M691	S752	D810	S931	Y994
ASP	N332	P392	V452	SER	M574	V633	S692	W753	P811	G932	L995
PHE	L333	A393	A453	GLU	V575	C634	Y693	W754	G812	L933	C994
SER	F334	T394	D454	ASN	V576	G635	V694	R755	C813	C994	Q995
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ARG	Q336	A396	M456	ASP	L578	L637	V696	S757	L815		
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L279	Q338	T397	L457	GLY	E580	V639	M697	S758	K817	Q940	Q940
N280	V339	P398	P458	PHE	L581	G639	N698	A759	W818	I941	I941
V281	A339	A399	A459	LYS	S582	A640	G699	G760	Q819	D942	D942
P282	E340	V400	A460	PRD	S583	D641	S700	K761	L820	N943	N943
Q283	V341	F401	Q461	SER	I583	V642	C701	K762	D821	I944	I944
E284	P942	E402	L462	G524	R584	S643	V702	L762	ASN	E945	E945
L285	G343	H403	Q463	T525	G585	L644	E703	Q764	PRD	L946	L946
Y286	M404	M404	I464	V526	D586	R645	W704	Y765	SER	Y1006	Y1006
Y287	P345	E405	A465	Q527	F587	N646	D705	I766	LYS	S947	S947
K288	P346	Q406	M466	E528	R588	S647	V706	V767	VAL	H948	H948
G289	I346	C407	G467	L529	T589	V648	W707	E768	GLN	A949	A949
Y290	F347	A408	I468	N530	T590	S649	ARG	D769	GLN	R950	R950
V291	V949	V409	P469	V591	V591	N650	L650	G770	LEU	T951	T951
K292	M349	M349	M349	F531	E592	F651	SER	G771	ARG	L952	L952
D293	R350	L411	L470	R532	Y593	L652	ASP	H772	SER	N953	N953
V294	L351	L411	Y471	S533	Y594	H653	GLY	H773	GLY	R954	R954
D295	A352	A412	R472	N534	L594	S654	L714	V773	ALA	K955	K955
D296	K353	K413	I473	K535	I595	S654	L714	F774	LEU	P956	P956
G297	Q354	M414	K474	N536	K596	L655	L715	A775	GLU	E957	E957
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Q299	R356	G416	I476	N538	L598	R657	S717	Q777	ALA	E959	E959
A300	H357	Y417	R477	G539	E599	G658	Y718	C778	LYS	Y960	Y960
	L358	V418	M478	Y540	T600	Q659	D719	Y779	GLN	F961	F961
	E359	S419	M479			V660	G720	A780		N962	N962

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D1418	Y1419	R1420	F1421	V1422	G1423	R1424	I1427	R1428	H1429	S1430	ASP	LEU	VAL	THR	LYS	E1436	A1437	S1438	F1439	E1440	Y1441	N1444	E1447	R1448	L1449	L1450	L1451	E1452	N1462	L1463	T1464	N1465	V1466	R1467	T1468	D1469	C1470	N1471	H1472	I1473	F1474	L1475	N1476	T1480	V1481	I1482	M1483	D1484	V1492	R1493	M1494	M1495	V1496				
VAL	ASP	ARG	PHE	HIS	ARG	GLU	F1352	K1353	F1354	F1355	F1358	R1359	A1360	R1361	D1362	K1363	F1364	E1365	E1366	D1367	R1368	I1369	H1372	L1373	L1377	A1378	F1379	Q1380	L1381	M1384	R1385	M1386	R1387	M1388	F1389	D1390	L1391	I1394	H1399	K1400	M1401	H1402	L1403	Y1404	E1411	V1412	G1413	T1414	E1415	V1416	T1417						
PRO	ARG	ASP	E1284	H1287	L1288	L1289	V1291	A1292	I1293	K1294	T1295	D1296	C1297	D1298	I1299	D1301	D1302	R1303	L1304	A1305	M1307	F1308	R1309	E1310	F1311	T1312	Q1313	Q1314	M1315	T1318	L1319	V1320	D1321	H1322	R1325	R1326	L1327	T1328	F1329	L1330	V1331	A1332	Q1333	LYS	ASP	PHE	ARG	LYS	GLN	VAL	ASN	TYR	GLU				
SER	VAL	ASP	SER	VAL	LEU	LEU	ASP	ASN	ASN	PHE	THR	PRO	C1230	Q1231	R1232	M1236	S1238	F1239	R1240	E1243	D1244	F1245	V1246	R1247	I1248	F1249	G1253	M1254	C1255	F1256	SER	ASP	PRO	P1261	Q1262	S1263	P1264	T1265	P1267	E1268	A1269	G1270	HIS	THR	SER	LEU	ASN	TYR	GLY	ASP	GLU	LYS	VAL				
RI156	A1157	Y1158	LI159	LI160	LI161	LI162	LI163	LI164	LI165	LI166	LI167	LI168	LI169	LI170	LI171	LI172	LI173	LI174	LI175	LI176	LI177	LI178	LI179	LI180	LI181	LI182	LI183	LI184	LI185	LI186	LI187	LI188	PRO	ASN	ARG	GLY	ASN	THR	LEU	ASN	ARG	MET	SER	PHE	SER	SER	ASN	LEU	ASN	TYR	GLY	MET	GLN	THR	HIS	VAL	ALA
I1086	A1087	S1088	H1089	L1090	P1091	S1092	Y1093	E1094	L1095	Q1096	Q1099	V1100	E1101	S1102	L1103	L1104	L1105	S1106	A1107	I1108	D1109	M1110	Y1111	G1112	H1113	Q1114	F1115	C1116	I1117	E1118	N1119	L1120	Q1121	K1122	L1123	I1124	L1125	S1126	S1129	I1130	F1131	D1132	F1138	Y1139	H1140	S1141	N1142	Q1143	V1144	V1145	R1146	M1147	A1148	V1152	Y1153		

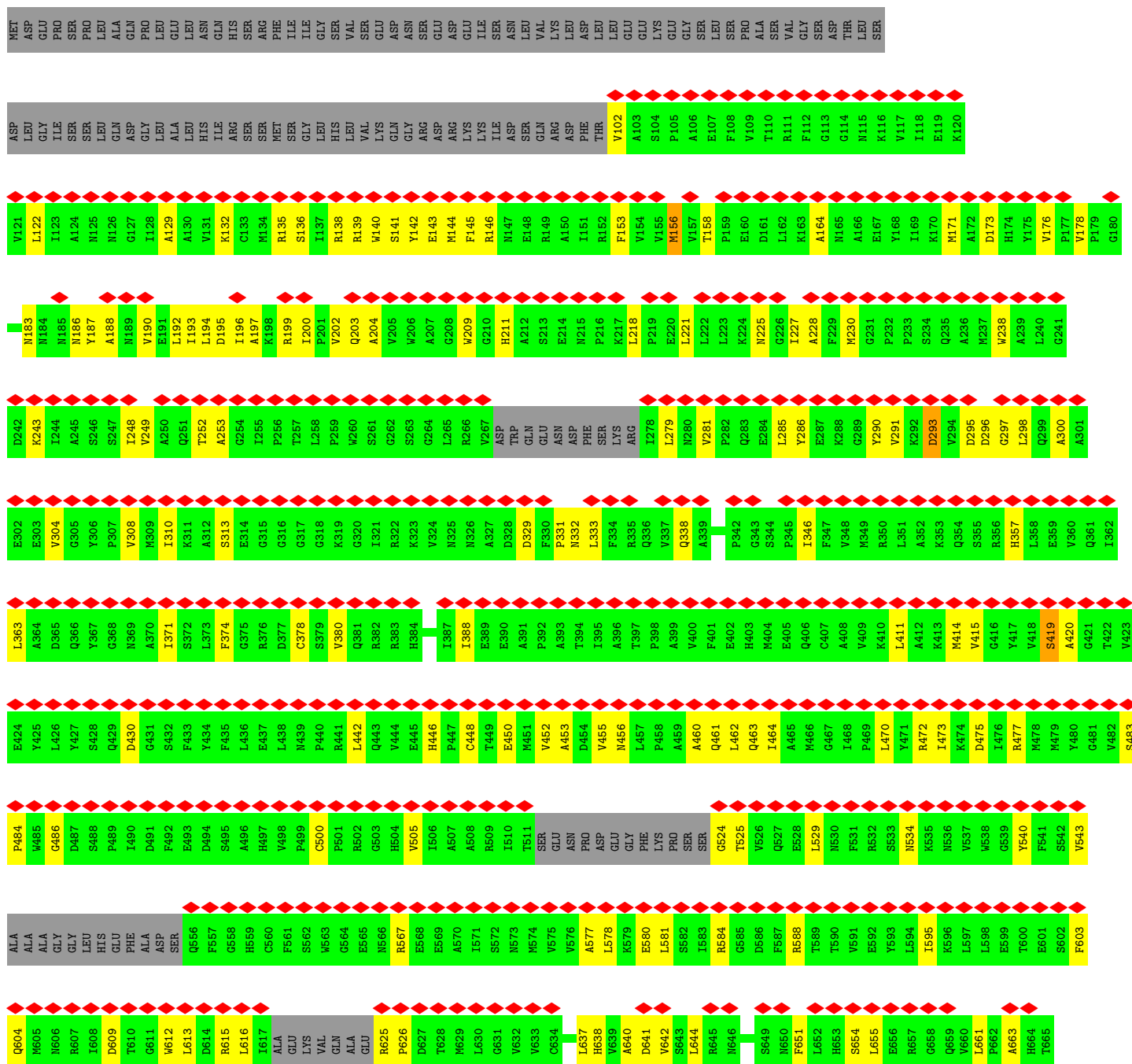
- Molecule 1: Acetyl-CoA carboxylase 1



G421	G481	F541	E501	L661	S721	E781	SER	D901	F962	M1022	V1084	V1144
T422	V482	S542	S602	P662	S722	I782	THR	I902	M963	T1023	L1085	V1145
V423	S483	V543	F603	A663	T723	E783	ALA	I903	N964	T1024	I1086	R1146
E424	P484	ALA	Q604	H664	T724	V784	LEU	T904	T965	L1025	A1087	M1147
Y425	W485	ALA	M605	T665	T725	M785	ARG	S905	Q966	M1026	S1088	A1148
L426	W486	GLY	N606	L666	T726	K786	GLY	V906	S967	I1027	H1089	A1149
Y427	D487	GLY	R607	L667	M727	M787	GLU	S907	I968	I1028	L1090	V1152
S428	S488	LEU	I608	N668	K728	V788	L849	G908	V969	F1029	P1091	V1153
Q429	P489	HIS	D609	T669	E729	M789	H850	R909	Q970	S1030	S1092	V1154
D430	I490	PIE	T610	V670	E730	T790	R851	I910	L971	H1031	Y1093	E1155
G431	D491	ALA	G611	D671	V731	L791	W852	P911	V972	A1032	E1094	E1156
S432	F492	ASP	W612	V672	D732	T792	F853	P912	Q973	Q1033	L1095	A1157
F433	E493	SER	L613	E673	R733	A793	H854	N913	R974	T1034	R1096	Y1158
Y434	D494	Q556	D614	L674	R734	V794	Y855	E915	R975	V1035	R1097	I1159
F435	S495	F557	R615	I675	R735	E795	V856	E916	R976	K1036	Q1098	A1160
L436	A496	G558	L616	V676	I736	S796	L857	S917	G977	K1037	E1100	E1162
E437	H497	H559	I617	E677	T737	G797	D858	I918	S978	M1038	S1102	L1163
L438	V498	C560	ALA	G678	I738	C798	R859	I919	R980	L1040	E1094	F1104
N439	P499	F561	GLU	V679	G739	I799	L860	K920	G981	L1041	L1105	S1165
P440	C500	S562	LYS	K680	K740	H800	V861	E921	H882	V1042	S1106	Q1167
R441	P501	W563	VAL	Y681	T741	Y801	R862	N922	M883	M1043	A1107	H1168
L442	R502	G564	GLN	V682	T742	V802	V863	A923	K984	I1044	D1108	Q1170
Q443	G503	E565	ALA	L683	C743	K603	M864	Q924	R985	I1045	D1109	K1172
V444	H504	P567	GLU	K684	V744	R604	N865	Y925	V986	D1046	M1110	D1173
E445	V505	R567	P626	V685	T745	P605	G866	A926	V987	Q1047	G1111	T1174
H446	I506	E568	D627	T686	E746	G806	C868	S927	M988	L1048	H1112	T1175
P447	A507	E569	T628	R687	K747	A607	L869	N928	D989	G1050	Q1114	G1176
C448	R508	I571	M629	Q688	E748	A608	P870	I929	L991	R1051	F1115	E1179
T449	R509	S572	L630	V689	ASP	L809	D871	T930	R992	D1052	I1117	F1180
E450	I510	N573	G631	P690	PRO	D810	F872	S931	Q993	P1053	E1118	M1183
M451	T511	M574	V632	N691	S752	P611	F873	Y932	Y994	T1054	M1119	L1184
V452	SER	V575	C634	S692	V753	G812	S874	L933	L995	L1055	L1120	P1185
A453	ASN	V576	G635	Y693	M754	C813	S875	C934	R996	T1056	Q1121	T1186
D454	P80	A577	A636	V694	R755	V814	S876	Q935	V997	D1057	K1122	S1187
V455	ASP	L578	L637	V695	S756	L815	K877	S938	E998	E1058	L1123	H1188
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P458	PHE	L581	A640	N698	A759	M618	D880	I941	F1001	M1061	S1126	ARG
A459	LYS	S582	D641	G699	G760	Q619	V881	I942	Q1002	I1062	E1127	GLY
A460	SER	I583	V642	S700	K761	L820	E882	A942	N1003	L1063	T1128	ILE
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L462	T525	G585	L644	V702	E703	PRO	R884	I944	L1005	E1065	I1130	THR
Q463	V526	D586	R645	E703	Q764	SER	L885	L945	Y1006	L1066	F1131	LEU
I464	I464	F587	N646	V704	Y765	LYS	M886	D946	D1007	T1067	D1132	ASN
A465	Q527	R588	S647	D705	I766	VAL	K887	S947	K1008	Q1068	E1133	LEU
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G467	L529	N530	S649	V707	E768	ALA	R890	A949	V1010	S1070	F1137	MET
I468	F531	V591	N650	ARG	D769	LEU	R890	I951	F1011	A1012	F1138	PHE
P469	R532	E592	F651	SER	G770	SER	D891	L952	A1013	K1071	Y1139	SER
L470	S533	Y593	L652	ASP	G771	GLY	P892	N953	L1013	T1072	H1140	SER
Y471	N534	L594	H553	GLY	H772	GLY	S893	R954	R1014	T1073	S1141	ASN
R472	K535	I595	S654	L714	V773	L714	L894	K955	E1015	K1076	N1142	LEU
I473	N536	K596	L555	L715	F774	L715	P895	R956	E1016	V1077	A1078	
K474	V537	L597	E556	L716	A775	L716	L896	S957	L897	L1079	L1079	
D475	W538	L598	R657	S717	G776	S717	L897	R958	K1018	R1080	Q1083	
I476	G539	E599	G658	Y718	Q777	Y718	E898	E959	S1019			
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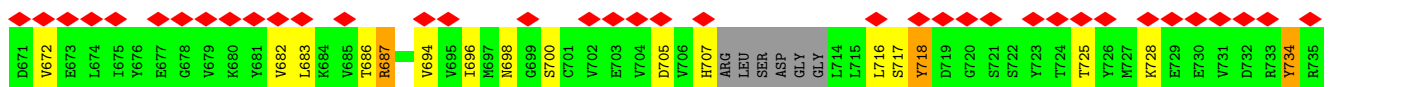
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V2124	K2054	G1980	Y1801	L1831	P1755	V1660	ASP	V1496	V1412	ARG	LEU	TYR
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L2133	L2061	V1983	K1904	G1835	L1760	M1664	ASP	S1501	V1416	ASN	GLU	HIS
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V2140	V2068	V1993	S1915	H1845	S1766	L1579	ASP	L1506	F1422	PHE	ASP	VAL
D2141	R2072	E1994	I1919	H1846	H1767	K1580	ASP	R1507	V1423	HIS	LEU	LEU
I2145	C2073	S1996	I1923	I1847	D1774	D1581	ASP	L1508	R1424	ARG	ASP	ASP
A2148	C2074	I1997	F1925	L1848	E1773	K1586	ASP	Q1510	F1352	LEU	ASP	ASN
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F2177	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO
L2178	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO
R2180	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO
Q2181	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO
V2182	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO
A2187	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO
D2188	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO
L2189	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO
R2195	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO
K2199	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO
I2205	Q2085	E2007	M1837	E1861	D1784	N1682	ASP	I1515	C1287	PRO	PRO	PRO

- Molecule 1: Acetyl-CoA carboxylase 1





L2239	L2240	D2241	Q2243	Q2244	Q2245	A2246	M2247	L2248	R2249	R2250	W2251	Q2252	Q2253	E2254	Q2255	E2256	Q2257	T2258	Q2259	K2260	A2261	Q2262	Q2263	Q2264	Q2265	L2270	K2276	T2279	E2280	E2281	E2282	G2283	V2284	I2288	E2289	E2290	N2291	L2292	K2293	C2294	L2295	S2296	R2297	D2298	V2299	V2300	L2301	K2302	Q2303	L2304	R2305	S2306	L2307							
P2177	I2178	Y2179	H2180	Q2181	W2182	A2183	V2184	Q2185	T2186	A2187	D2188	L2189	H2190	D2191	T2192	T2193	Q2194	R2195	M2196	Q2197	E2198	K2199	Q2200	V2201	V2202	S2203	D2204	I2205	L2206	D2207	W2208	K2209	R2212	T2213	F2214	F2215	T2216	R2217	L2218	L2219	R2220	R2221	L2222	L2223	L2224	L2227	W2228	K2229	K2230	K2231	L2232	H2233	N2234	A2235	W2236	P2237	E2238			
V2117	L2118	E2119	P2120	E2121	Q2122	T2123	V2124	E2125	L2126	K2127	F2128	R2129	R2130	K2131	D2132	L2133	V2134	K2135	T2136	M2137	R2138	R2139	V2140	D2141	P2142	V2143	Y2144	I2145	L2146	L2147	A2148	E2149	R2150	L2151	G2152	T2153	P2154	E2155	L2156	S2157	T2158	A2159	E2160	R2161	K2162	E2163	L2164	E2165	N2166	K2167	L2168	A2169	D2170	R2171	E2172	E2173	F2174	L2175	I2176	
Y2057	D2058	Q2059	V2060	L2061	K2062	F2063	G2064	A2065	T2066	I2067	V2068	D2069	G2070	L2071	R2072	E2073	C2074	C2075	Q2076	P2077	V2078	L2079	V2080	Y2081	L2082	P2083	Q2084	Q2085	A2086	E2087	L2088	R2089	G2090	G2091	S2092	W2093	V2094	V2095	I2096	D2097	S2098	S2099	L2100	N2101	P2102	R2103	H2104	M2105	E2106	M2107	Y2108	A2109	D2110	R2111	E2112	S2113	R2114	G2115	S2116	
I1997	P1998	A1999	D2000	P2001	A2002	N2003	L2004	D2005	S2006	E2007	A2008	K2009	T2010	I2011	Q2012	Q2013	A2014	G2015	Q2016	V2017	W2018	F2019	P2020	D2021	S2022	A2023	F2024	K2025	T2026	Y2027	Q2028	A2029	T2030	K2031	D2032	F2033	N2034	R2035	E2036	G2037	L2038	P2039	G1980	I1981	P1982	V1983	G1984	N1985	V1986	V1987	V1988	E1989	T1990	S2050	G2051	G2052	M2053	K2054	D2055	M2056
M1937	L1938	A1939	G1940	R1941	P1942	H1943	P1944	T1945	Q1946	K1947	G1948	Q1949	W1950	L1951	S1952	G1953	F1954	F1955	D1956	Y1957	G1958	S1959	F1960	S1961	E1962	I1963	M1964	Q1965	P1966	V1967	A1968	Q1969	T1970	V1971	V1972	V1973	G1974	R1975	A1976	R1977	L1978	G1979	G1980	I1981	P1982	V1983	G1984	N1985	V1986	V1987	V1988	E1989	T1990	R1991	T1992	V1993	E1994	L1995	S1996	
M1877	M1878	G1879	V1880	T1881	H1882	C1883	T1884	V1885	C1886	D1887	D1888	F1889	E1890	G1891	V1892	F1893	T1894	V1895	L1896	H1897	M1898	L1899	S1900	Y1901	M1902	P1903	K1904	S1905	V1906	H1907	S1908	S1909	V1910	P1911	L1912	L1913	N1914	S1915	K1916	D1917	P1918	G1919	I1919	D1920	E1861	I1922	I1923	E1924	F1925	V1926	P1927	T1928	K1929	T1930	P1931	Y1932	D1933	P1934	R1935	W1936
I1817	S1818	L1819	V1820	T1821	C1822	R1823	A1824	I1825	G1826	I1827	G1828	A1829	Y1830	L1831	V1832	R1833	L1834	G1835	Q1836	R1837	T1838	I1839	Q1840	V1841	E1842	M1843	S1844	H1845	L1846	I1847	L1848	T1849	G1850	A1851	G1852	A1853	L1854	N1855	K1856	V1857	L1858	G1859	R1860	E1861	V1862	Y1863	T1864	S1865	N1866	M1867	Q1868	L1869	G1870	G1871	I1872	Q1873	L1874	M1875	H1876	
D1757	Y1758	K1759	R1760	V1761	S1762	A1763	L1764	M1765	S1766	V1767	H1768	C1769	E1770	H1771	V1772	E1773	D1774	E1775	G1776	E1777	S1778	R1779	Y1780	K1781	I1782	T1783	D1784	I1785	I1786	G1787	K1788	E1789	E1790	G1791	I1792	G1793	P1794	E1795	M1796	L1797	R1798	G1799	S1800	G1801	M1802	I1803	A1804	G1805	E1806	S1807	S1808	L1809	A1810	Y1811	M1812	I1813	I1814	I1815	T1816	
L1697	L1698	F1699	L1700	R1701	A1702	S1703	E1704	L1705	A1706	R1707	A1708	E1709	G1710	I1711	P1712	R1713	I1714	Y1715	V1716	S1717	A1718	M1719	G1720	G1721	A1722	R1723	I1724	G1725	L1726	A1727	E1728	E1729	I1730	R1731	H1732	M1733	F1734	H1735	V1736	A1737	W1738	V1739	D1740	P1741	E1742	D1743	P1744	Y1745	K1746	G1747	Y1748	R1749	Y1750	F1691	G1692	P1693	Q1694	E1695	D1696	
L1637	V1638	L1639	D1640	D1641	Q1642	L1643	Q1644	L1645	V1646	H1647	M1648	R1649	L1650	L1651	P1652	G1653	G1654	M1655	E1656	I1657	G1658	M1659	V1660	A1661	W1662	L1663	M1664	T1665	F1666	K1667	S1668	P1669	E1670	Y1671	P1672	E1673	G1674	H1675	D1676	S1677	I1678	V1679	I1680	G1681	M1682	D1683	L1684	T1685	Y1686	R1687	L1688	G1689	S1690	F1691	G1692	P1693	Q1694	E1695	D1696	
Y1577	V1578	T1579	K1580	D1581	L1582	L1583	Q1584	S1585	K1586	R1587	F1588	Q1589	A1590	Q1591	S1592	L1593	G1594	T1595	T1596	Y1597	I1598	Y1599	D1600	I1601	P1602	E1603	M1604	F1605	R1606	Q1607	S1608	L1609	I1610	K1611	L1612	W1613	E1614	S1615	M1616	S1617	L1618	Q1619	A1620	F1621	L1622	P1623	S1624	P1625	P1626	L1627	P1628	S1629	D1630	M1631	L1632	T1633	Y1634	L1635	E1636	
A1511	E1512	L1513	K1514	I1515	N1516	T1517	R1518	L1519	T1520	P1521	T1522	G1523	K1524	A1525	P1526	I1527	R1528	R1529	L1530	F1531	L1532	T1533	N1534	E1535	I1538	Y1539	L1540	D1541	I1542	S1543	L1544	Y1545	K1546	E1547	V1548	T1549	ASP	SER	ARG	THR	A1554	Q1555	T1556	M1557	F1558	Q1559	A1560	TYR	GLY	ASP	K1564	G1570	M1571	L1572	T1576	P1576				



G1523	A1452	T1392	H1325	P1264	D1132	K1071	E998	N925	V856	S796	I736
K1524	A1453	A1393	R1326	T1265	V1133	T1072	T999	I929	L857	G797	T737
I1525	M1454	I1394	L1330	F1266	N1136	T1073	S931	T930	V863	C798	I738
P1527	D1455	P1395	V1331	P1267	F1137	A1075	M964	V932	M965	I799	G739
I1528	A1456	A1396	A1332	E1268	F1138	A1076	N966	N933	N967	H800	N740
R1529	L1457	A1397	Q1333	A1269	Y1139	V1077	G1004	L933	G866	Y801	K741
L1530	A1458	N1398	LYS	G1270	H1140	A1078	Y1006	C934	Y867	V802	T742
F1531	V1459	H1399	ASP	HIS	S1141	L1079	V1010	I941	G863	K803	C743
A1460	A1460	K1400	PHE	THR	R1146	R1080	L1013	A942	L869	R804	V744
F1461	GLN	ARG	VAL	VAL	M1147	A1081	R1014	N943	P870	R805	F745
N1462	LYS	LYS	ALA	TTR	M1148	Q1083	L1015	I944	P872	G806	E746
L1463	VAL	ASP	SER	GLU	A1149	V1084	E1016	L945	F873	A807	K747
T1464	ASN	GLN	VAL	VAL	Y1153	L1085	H1017	D946	C863	A808	E748
N1465	TYR	ASP	ASP	ASP	V1154	I1087	K1018	S947	S876	ASN	
V1466	LYS	LYS	VAL	VAL	R1155	A1087	S1019	A950	K877	ASP	
R1467	GLU	VAL	VAL	VAL	R1156	S1088	D1020	T951	V878	PRO	
T1468	ASP	PRO	LEU	LEU	A1157	H1089	M1021	T952	K879	S752	
D1469	ARG	ARG	ARG	ARG	Y1158	P1091	V1024	N953	D880	V753	
C1470	ASN	THR	ASP	ASP	I1159	S1092	H1026	S956	V882	M754	
N1471	PHE	THR	ASP	ASP	A1160	Y1093	Y1027	E957	V883	R755	
H1472	ARG	GLU	ASP	ASP	Y1161	E1094	I1028	E958	R884	M756	
I1473	ARG	GLU	ASP	ASP	E1162	L1095	L1029	E959	T888	P757	
F1474	GLN	GLU	ASP	ASP	L1163	L1096	S1030	V960	L889	M758	
L1475	VAL	GLU	ASP	ASP	N1164	H1097	H1031	F961	S893	A759	
N1476	ASP	GLU	ASP	ASP	H1168	Q1099	V1034	F962	L894	C760	
F1477	PHE	THR	ASP	ASP	R1169	Y1100	T1035	T965	L897	K761	
V1478	GLN	THR	ASP	ASP	Q1170	S1102	K1036	T966	I763	L762	
T1479	GLU	THR	ASP	ASP	L1171	T1103	K1037	S967	E898	I763	
F1480	ASP	THR	ASP	ASP	K1172	F1104	M1038	Q900	Q764	Q764	
L1481	ASP	THR	ASP	ASP	C1176	L1105	L1039	D901	Y765	Y765	
N1482	ASP	THR	ASP	ASP	V1177	S1106	I1045	I902	I766	I766	
M1483	ASP	THR	ASP	ASP	V1178	A1107	D1046	M903	V767	V767	
D1484	ASP	THR	ASP	ASP	E1179	I1108	Q1047	T904	E768	E768	
K1487	ASP	THR	ASP	ASP	F1180	D1109	T1054	S905	D769	D769	
S1491	ASP	THR	ASP	ASP	L1184	M1110	T1055	I910	G770	G770	
M1495	ASP	THR	ASP	ASP	P1185	Y1111	T1056	P911	G771	G771	
R1498	ASP	THR	ASP	ASP	T1186	H1112	D1057	P912	H772	H772	
S1501	ASP	THR	ASP	ASP	S1187	H1113	T1058	N913	V773	V773	
L1502	ASP	THR	ASP	ASP	H1188	Q1114	E1059	V914	F774	F774	
L1503	ASP	THR	ASP	ASP	PRO	Q1115	L1061	E915	A775	A775	
W1504	ASP	THR	ASP	ASP	ARG	C1116	T1062	K916	G776	G776	
K1505	ASP	THR	ASP	ASP	ASN	T1117	L1063	S917	C777	C777	
L1506	ASP	THR	ASP	ASP	T1188	M1119	T1064	K918	Q778	Q778	
R1507	ASP	THR	ASP	ASP	S1189	Q1120	E1065	K919	C779	C779	
L1508	ASP	THR	ASP	ASP	H1188	Q1121	L1066	K920	Y779	Y779	
Q1510	ASP	THR	ASP	ASP	PRO	K1122	L1067	E921	A780	A780	
Q1511	ASP	THR	ASP	ASP	ARG	L1123	E1068	M922	E781	E781	
E1512	ASP	THR	ASP	ASP	GLY	I1124	Q1068	Q924	I782	I782	
I1515	ASP	THR	ASP	ASP	ILE	L1125	L1069	A926	V784	V784	
N1516	ASP	THR	ASP	ASP	THR	S1126	S1070	S927	M785	M785	
I1517	ASP	THR	ASP	ASP	ASN	S1129			H850	H850	
R1518	ASP	THR	ASP	ASP	MET	I1130			R851	R851	
L1521	ASP	THR	ASP	ASP	SER	F1131			V852	V852	
L1522	ASP	THR	ASP	ASP					F853	F853	
L1523	ASP	THR	ASP	ASP					H854	H854	
L1524	ASP	THR	ASP	ASP					Y855	Y855	
L1525	ASP	THR	ASP	ASP							
L1526	ASP	THR	ASP	ASP							
L1527	ASP	THR	ASP	ASP							
L1528	ASP	THR	ASP	ASP							
L1529	ASP	THR	ASP	ASP							
L1530	ASP	THR	ASP	ASP							
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L1532	ASP	THR	ASP	ASP							
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L1534	ASP	THR	ASP	ASP							
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L1586	ASP	THR	ASP	ASP							
L1587	ASP	THR	ASP	ASP							
L1588	ASP	THR	ASP	ASP							
L1589	ASP	THR	ASP	ASP							
L1590	ASP	THR	ASP	ASP							
L1591	ASP	THR	ASP	ASP							
L1592	ASP	THR	ASP	ASP							



Chain G:

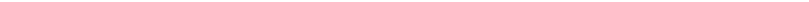
[illegible]







MET
ASP
SER
PRO
SER
THR

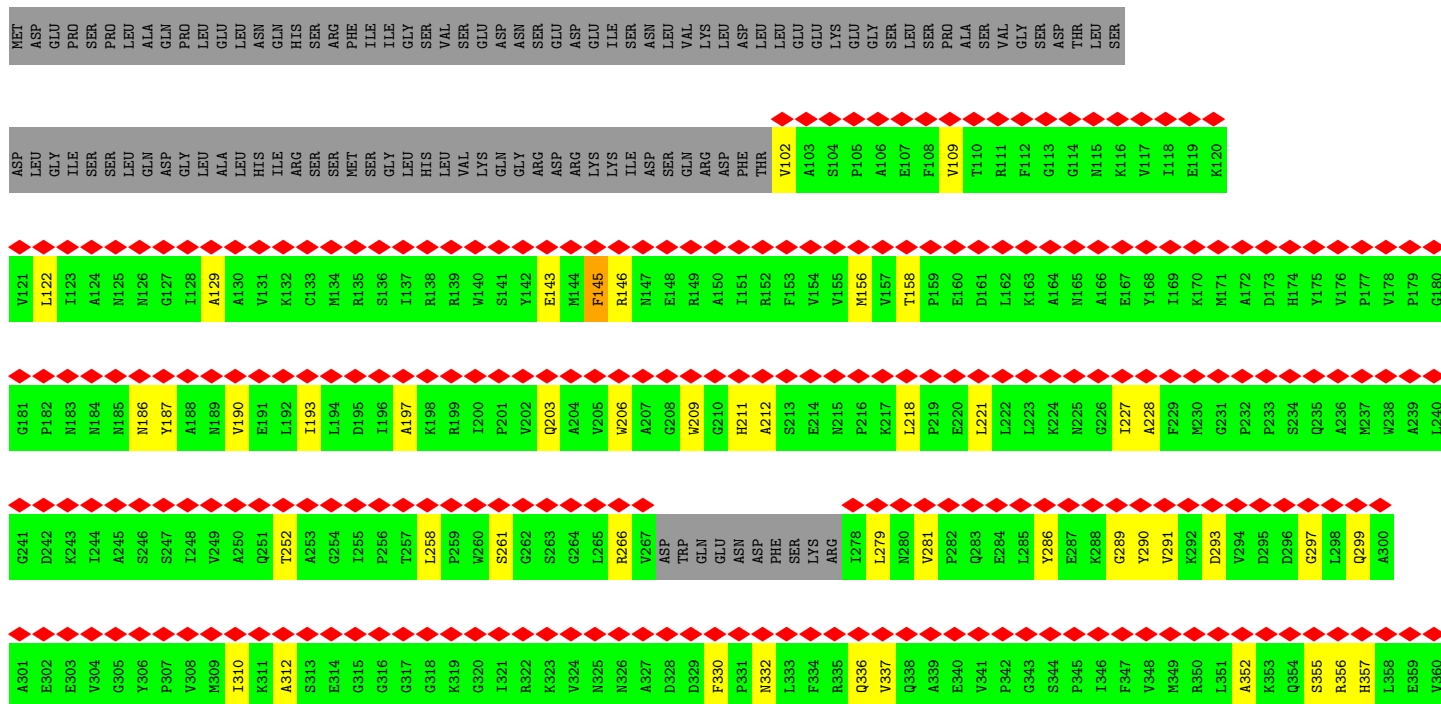
Chain J:  56% 41% 14% 44%

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

D901	SER	G181	G241	A301	Q361	G421	G481	F541	E601	L661	S721	E761	S88	D901	D901
I902	THR	L122	D242	E302	I362	T422	V482	S542	S602	P662	S722	I782	THR	D902	D902
M903	ALA	I123	K243	E303	L363	V423	S483	S543	F603	A663	Y723	E783	ALA	D903	D903
T904	ARG	A124	I244	V304	A364	E424	P484	ALA	Q604	H664	T724	V784	ARG	D904	D904
S905	GLY	N125	A245	G305	D365	Y425	V485	ALA	M605	T665	T725	M785	GLY	D905	D905
N906	GLU	N126	S246	Y306	Q366	L426	G486	GLY	N606	L666	T726	K786	GLU	D906	D906
S907		G127	S247	P307	Y367	Y427	D487	GLY	R607	L667	M727	M787		D907	D907
G908		I128	I248	V308	G368	S428	S488	LEU	T608	N668	K728	V788		D908	D908
R909		A129	V249	M309	N369	Q429	P489	HIS	D609	T669	K729	M789		D909	D909
I910		A130	A250	I310	N369	Q430	P490	PHE	T610	V670	E730	M790		D910	D910
P911		V131	Q251	K311	I371	G431	D491	ALA	G611	D671	V731	L791		D911	D911
P912		K132	T252	L192	S372	S432	F492	ASP	V612	V672	D732	T792		D912	D912
M913		C133	I193	A253	L373	F433	E493	SER	L613	E673	R733	A793		D913	D913
Y914		M134	G254	E314	F374	Y434	D494	Q556	D614	L674	Y734	V794		D914	D914
E915		R135	G254	E315	G375	F435	S495	F557	R615	L675	R735	E795		D915	D915
K916		R136	I255	G315	G375	F436	S496	Q558	L616	V676	T736	S796		D916	D916
S917		S137	P256	G316	R376	L436	A496	H559	L617	E677	T737	G797		D917	D917
I918		I138	T257	G317	D377	E437	H497	C560	ALA	V677	I738	C798		D918	D918
K919		R138	L258	G318	C378	L438	V498	F561	GLU	G678	T739	G799		D919	D919
K920		R139	P259	K319	S379	M439	P499	S562	LYS	V679	Y740	H800		D920	D920
E921		I200	W260	G320	V380	P440	C500	W563	VAL	K680	K741	H801		D921	D921
M922		S141	S261	I321	Q381	R441	F502	G564	GLN	V681	T742	V802		D922	D922
A923		Y142	S262	R322	R382	L442	R502	E565	ALA	L682	C743	K803		D923	D923
Q924		E143	S263	K323	R383	Q443	G503	N566	GLU	L683	C744	R804		D924	D924
Y925		M144	G264	V324	H384	V444	H504	R567	P626	K684	F745	P805		D925	D925
A926		F145	G264	A204	Q385	E445	V505	E568	D627	V685	E746	G806		D926	D926
S927		R146	L265	N325	K386	H446	I506	E569	T628	T686	K747	A807		D927	D927
N928		R146	R266	N326	I387	P447	A507	A570	H629	R687	E748	K808		D928	D928
I929		M147	V267	A327	I388	C448	A508	I571	L630	Q688	S749	L809		D929	D929
T930		E148	ASP	D328	E389	T449	R509	S572	G631	S689	ASP	D810		D930	D930
S931		E149	TRP	D329	E390	T449	R510	N573	V632	P690	PRO	P811		D931	D931
V932		A150	GLU	F330	E391	E450	I510	N574	V633	M691	S752	C812		D932	D932
L933		I151	ASN	P331	A391	M451	T511	S574	C634	K692	C753	C813		D933	D933
C934		R152	GLU	N332	P392	V452	GLY	V575	G635	V693	W754	V814		D934	D934
Q935		F153	PHE	L333	A393	A453	ASN	V576	A636	V694	R755	L815		D935	D935
S936		E214	LYS	F334	T394	D454	PRO	A577	L637	V695	S756	A816		D936	D936
N937		N215	ARG	R335	I395	V455	ASP	L578	T637	T696	R757	R817		D937	D937
P938		N216	I278	Q336	A396	N456	GLY	K579	H638	M697	S758	L818		D938	D938
Y939		K217	L279	V337	T397	L457	PHE	E580	V639	N698	A759	Q819		D939	D939
Q940		T158	N280	Q338	P398	P458	LYS	L581	A640	V699	K760	L820		D940	D940
I941		P159	V281	A339	A399	A459	PRO	S582	D641	S699	K761	D821		D941	D941
A942		E160	E220	E340	V400	A460	SER	I583	V642	T700	L762	ASN		D942	D942
N943		D161	Q283	V341	F401	Q461	G524	R584	S643	C701	R763	PRO		D943	D943
I944		L162	E284	P342	E402	L462	T525	G585	L644	V702	W764	SER		D944	D944
L945		K163	L285	G343	H403	Q463	V526	D586	R645	E703	Y765	LYS		D945	D945
D946		A164	Y286	S344	M404	T464	Q527	F587	N646	W704	T766	VAL		D946	D946
S947		N165	E287	P345	E405	A465	E528	R588	S647	T705	I767	GLN		D947	D947
K948		N166	K288	I346	Q406	M466	L529	T589	V648	V706	E768	ALA		D948	D948
A949		E167	G289	F347	C407	G467	N530	T590	S649	H707	D769	LEU		D949	D949
R950		Y168	Y290	V348	A408	T468	F531	V591	N650	ARG	G770	LEU		D950	D950
T951		I169	V291	M349	V409	P469	R532	E592	F651	THR	G771	ASP		D951	D951
L952		K170	K292	R350	K410	L470	S533	E593	L652	SER	H771	GLY		D952	D952
N953		M171	D293	L351	L411	Y471	N534	L594	H653	GLY	V773	GLY		D953	D953
K954		A172	Y294	A352	A412	R472	K535	I595	S654	L714	F774	L715		D954	D954
R955		D173	D295	K353	K413	T473	N536	K596	L655	L716	A775	L716		D955	D955
Y956		H174	D296	Q354	M414	K474	V537	L597	E656	S717	G776	L717		D956	D956
S957		Y175	G297	S355	V415	D475	M538	L598	R657	T718	A777	L718		D957	D957
P958		V176	L298	R356	G416	T476	M539	E599	T658	Y719	G777	L719		D958	D958
V959		P177	Q299	H357	Y417	R477	G539	T600	Q659	D720	V778	GLN		D959	D959
G960		V178	A300	L358	Y418	M478	V540		V660		A780			D960	D960
		P179		E359	S419	M479									
		G180		V360	A420	Y480									



- Molecule 1: Acetyl-CoA carboxylase 1



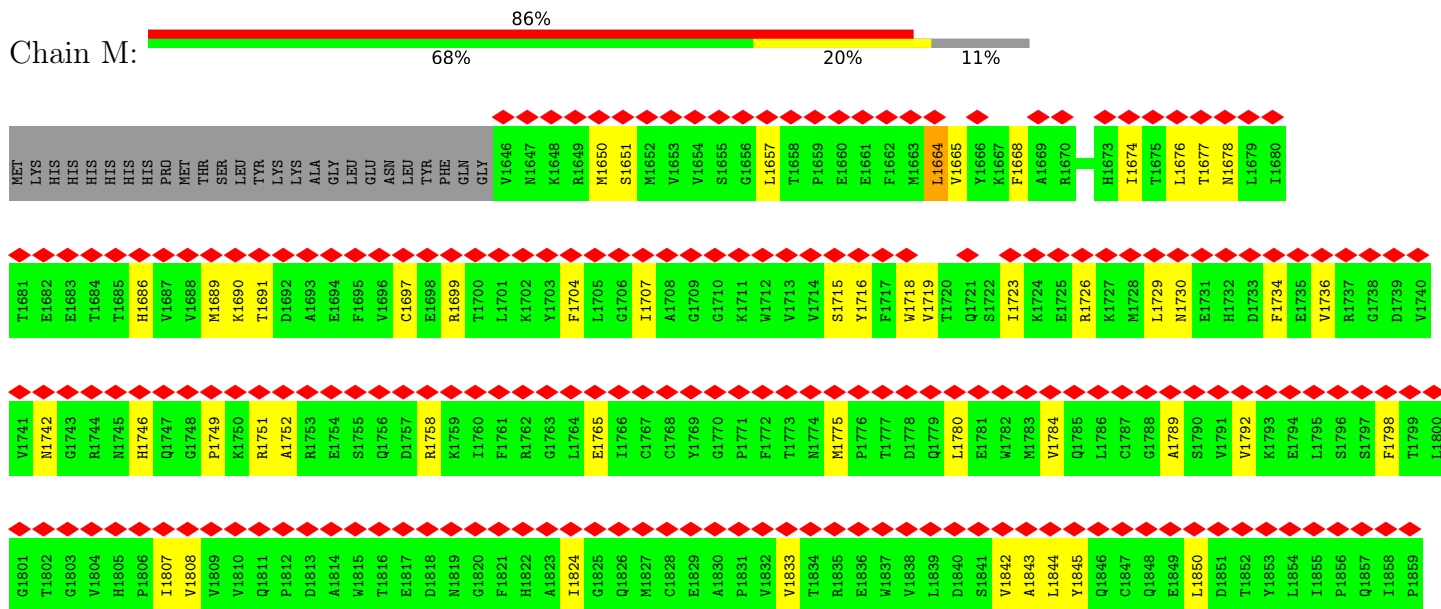
A1081	R1082	Q1083	V1084	L1085	I1086	A1087	S1088	H1089	L1090	P1091	S1092	E1094	L1095	R1096	H1097	N1098	Q1099	V1100	E1101	S1102	I1103	F1104	L1105	S1106	A1107	I1108	L1109	M1110	Y1111	G1112	H1113	Q1114	F1115	C1116	I1117	E1118	N1119	Y1120	Q1121	K1122	L1123	I1124	L1125	E1126	T1127	Q1128	S1129	F1130	D1131	V1132	L1133	P1134	N1135	F1136	Y1137	Y1138	Y1139				
M1021	N1022	T1023	V1024	L1025	N1026	Y1027	I1028	F1029	S1030	H1031	A1032	Q1033	V1034	T1035	K1036	N1037	L1038	L1039	L1040	V1041	T1042	M1043	L1044	I1045	D1046	Q1047	L1048	C1049	G1050	R1051	D1052	P1053	T1054	L1055	T1056	D1057	E1058	L1059	L1060	N1061	I1062	L1063	T1064	E1065	L1066	T1067	Q1068	L1069	S1070	F1131	D1132	T1072	T1073	N1074	A1075	K1076	Y1077	A1078	L1079	R1080	
F961	F962	M963	N964	T965	Q966	S967	I968	V969	Q970	L971	V972	Q973	R974	Y975	R976	S977	Q978	R980	G981	H982	M983	K984	A985	V986	V987	M988	D989	L990	L991	R992	Q993	Y994	L995	R996	V997	E998	T999	Q1000	F1001	Q1002	N1003	G1004	H1005	Y1006	D1007	S947	K1008	C1009	V1010	F1011	A1012	L1013	R1014	E1015	E1016	N1017	S1019	D1020			
D901	I902	M903	T904	S905	V906	S907	G908	R909	I910	P911	P912	N913	V914	E915	K916	S917	I918	K919	K920	E921	M922	A923	Q924	Y925	A926	S927	N928	I929	T930	S931	V932	L933	C934	Q935	F936	P937	S938	Q939	Q940	I941	A942	N943	I944	L945	D946	D1007	H948	A949	A950	T951	L952	N953	R954	K955	S956	E957	R958	E959	V960		
SER	THR	ALA	LEU	ARG	GLY	GLU	K848	L849	R851	V852	F853	H854	Y855	V856	L857	D858	H859	L860	V861	N862	V863	M864	R865	G866	Y867	C868	L869	P870	D871	P872	F873	F874	S875	S876	K877	V878	K879	D880	W881	E883	R884	L885	M886	K887	T888	L889	R890	D891	P892	S893	L894	P895	L896	L897	E898	L899	Q900				
E781	I782	E783	V784	M785	K786	M787	V788	M789	T790	L791	T792	A793	V794	E795	S796	G797	C798	I799	H800	Y801	V802	K803	R804	P805	G806	A807	A808	L809	D810	P811	G812	C813	V814	L815	A816	K817	M818	Q819	L820	D821	ASN	P80	L762	I763	Q764	V765	I766	V767	E768	D769	G770	H771	G772	V773	F774	A775	G776	Q777	C778	Y779	A780
L661	P662	A663	H664	T665	L666	L667	N668	T669	D670	G671	V672	E673	L674	I675	V676	E677	G678	V679	K680	Y681	V682	L683	K684	V685	T686	R687	Q688	S689	P690	N691	S692	Y693	V694	V695	I696	M697	N698	G699	S700	C701	V702	E703	V704	D705	V706	H707	ARG	LEU	SER	ASP	GLY	L714	L715	L716	S717	Y718	D719	G720			
E601	S602	F603	Q604	M605	N606	R607	I608	G609	T610	G611	V612	L613	D614	R615	L616	I617	ALA	GLU	LYS	VAL	GLN	ALA	GLU	R625	P626	D627	T628	M629	L630	G631	V632	V633	C634	G635	A636	L637	H638	V639	A640	D641	S642	L644	R645	N646	S647	V648	S649	N650	F651	L652	H653	S654	L655	E656	R657	G658	Q659	V660			
F541	S542	V543	ALA	ALA	GLY	GLY	LEU	HIS	PHE	ALA	ASP	SER	Q556	F557	G558	H559	C560	F561	S562	W563	G564	E565	N566	R567	E568	E569	A570	I571	S572	N573	M574	V575	V576	A577	L578	K579	E580	L581	S582	I583	R584	G585	D586	F587	R588	T589	T590	V591	R592	Y593	L594	I595	K596	L597	L598	E599	T600				
G481	V482	S483	P484	W485	G486	D487	S488	P489	I490	D491	F492	E493	D494	S495	A496	H497	V498	P499	C500	P501	R502	G503	H504	V505	I506	A507	A508	R509	I510	T511	SER	GLU	ASN	ASP	GLY	PHE	LYS	PRO	SER	G524	T525	V526	Q527	E528	L529	N530	F531	R532	S533	N534	K535	N536	V537	W538	G539	Y540					
Q361	I362	L363	A364	D365	Q366	Y367	G368	N369	A370	I371	S372	L373	F374	G375	R376	D377	C378	S379	V380	Q381	R382	R383	H384	Q385	K386	I387	I388	E389	A391	P392	A393	T394	I395	A396	T397	P398	A399	V400	F401	E402	H403	M404	E405	Q406	C407	A408	V409	K410	L411	A412	K413	M414	V415	G416	Y417	V418	S419	A420			
G421	T422	V423	E424	Y425	L426	Y427	S428	Q429	D430	G431	S432	F433	Y434	F435	L436	E437	L438	N439	P440	R441	L442	Q443	V444	E445	H446	P447	C448	T449	E450	M451	V452	A453	D454	V455	N456	L457	P458	A459	A460	Q461	L462	Q463	I464	A465	M466	G467	I468	P469	L470	Y471	R472	I473	K474	D475	I476	R477	M478	Y480			





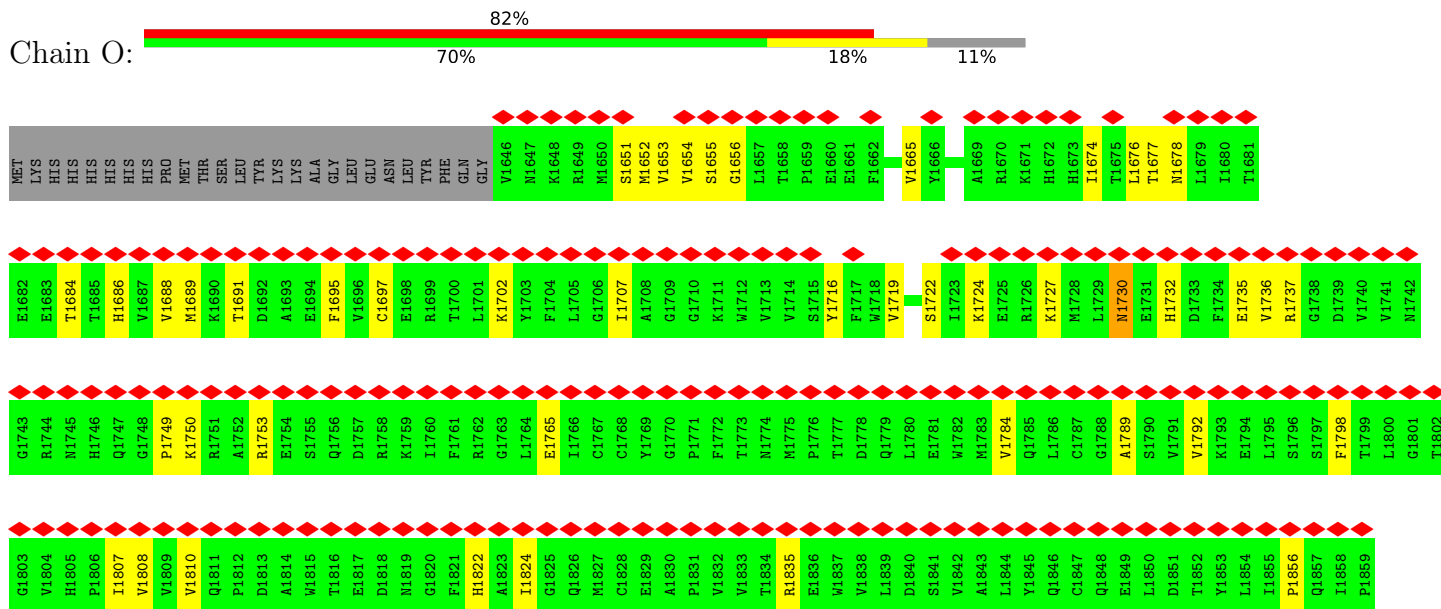
● Molecule 2: Breast cancer type 1 susceptibility protein

Chain M:



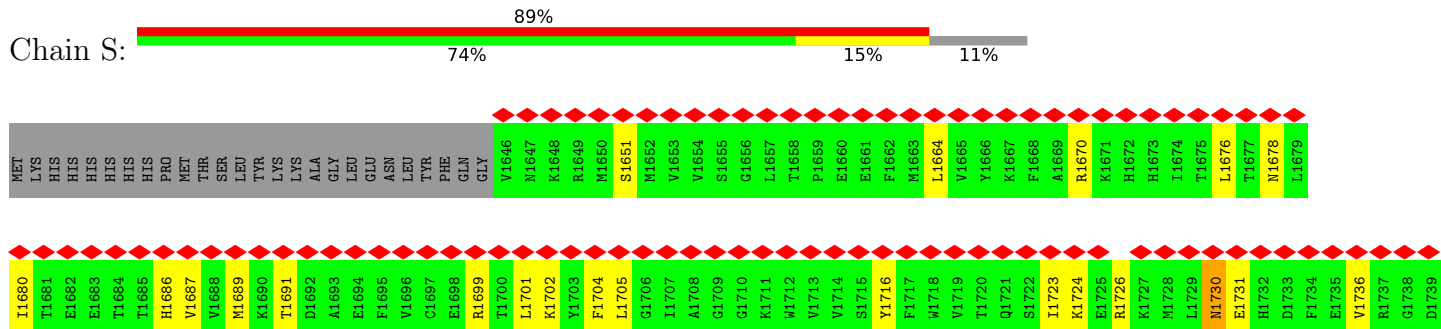
● Molecule 2: Breast cancer type 1 susceptibility protein

Chain O:



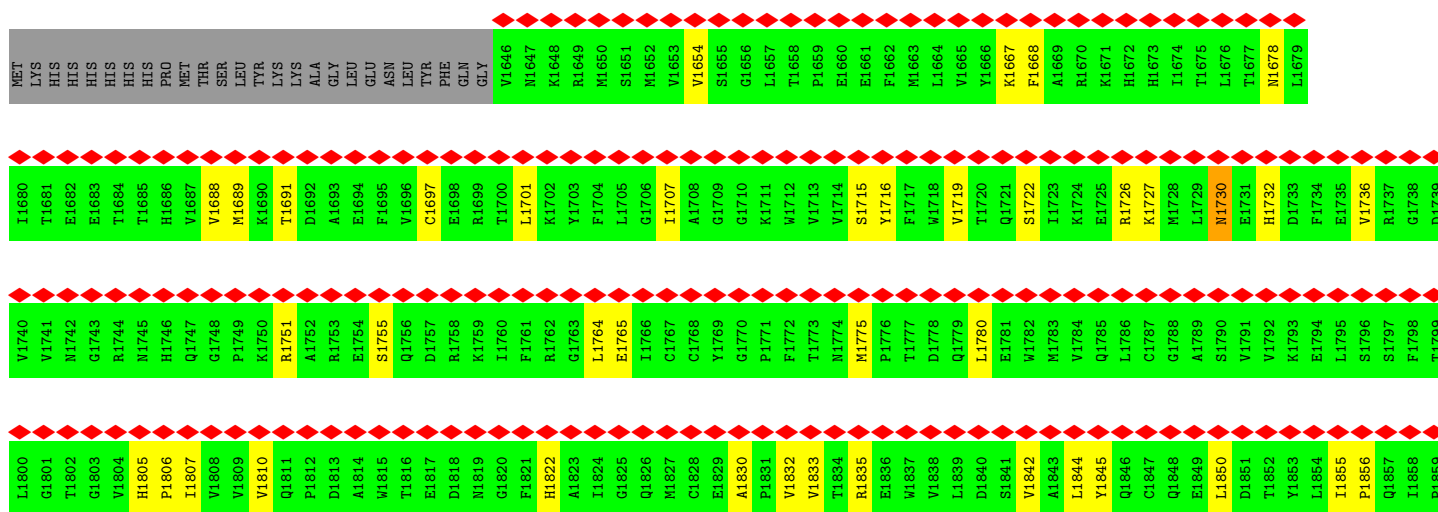
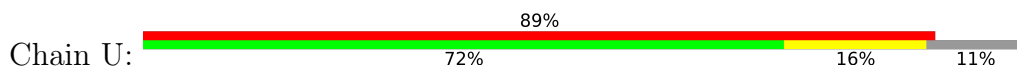
● Molecule 2: Breast cancer type 1 susceptibility protein

Chain S:

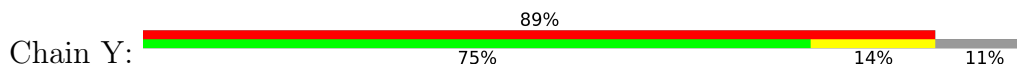




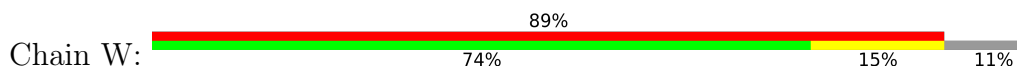
• Molecule 2: Breast cancer type 1 susceptibility protein



• Molecule 2: Breast cancer type 1 susceptibility protein



• Molecule 2: Breast cancer type 1 susceptibility protein



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	48483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	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	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	397.80798, 397.80798, 397.80798	wwPDB
Map dimensions	376, 376, 376	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

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

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	0.51	3/16819 (0.0%)	1.02	65/22785 (0.3%)
1	B	0.52	4/16819 (0.0%)	1.06	76/22785 (0.3%)
1	C	0.60	3/16819 (0.0%)	1.05	63/22785 (0.3%)
1	D	0.67	8/16819 (0.0%)	1.20	144/22785 (0.6%)
1	E	0.66	4/16819 (0.0%)	1.11	72/22785 (0.3%)
1	F	0.59	3/16819 (0.0%)	1.04	56/22785 (0.2%)
1	G	0.43	0/6199	0.87	7/8406 (0.1%)
1	J	0.41	0/10619	0.91	26/14376 (0.2%)
1	Q	0.43	0/6199	0.88	10/8406 (0.1%)
1	R	0.41	0/10619	0.92	32/14376 (0.2%)
2	H	0.44	0/1740	0.87	1/2364 (0.0%)
2	K	0.40	0/1737	0.79	0/2360
2	M	0.40	0/1740	0.81	0/2364
2	O	0.43	0/1737	0.84	1/2360 (0.0%)
2	S	0.36	0/1740	0.81	4/2364 (0.2%)
2	U	0.36	0/1737	0.75	0/2360
2	W	0.37	0/1737	0.77	2/2360 (0.1%)
2	Y	0.37	0/1740	0.78	0/2364
All	All	0.54	25/148458 (0.0%)	1.02	559/201170 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	B	0	13
1	C	0	12
1	D	1	18
1	E	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	12
1	J	0	11
1	R	0	11
All	All	1	101

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	2018	TRP	CB-CG	-7.39	1.36	1.50
1	B	1539	TYR	CB-CG	-7.33	1.40	1.51
1	C	2018	TRP	CB-CG	-7.25	1.37	1.50
1	E	1116	CYS	CB-SG	-7.02	1.70	1.82
1	D	1780	TYR	CD2-CE2	-6.97	1.28	1.39

The worst 5 of 559 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1503	LEU	CA-CB-CG	10.94	140.47	115.30
1	E	1449	LEU	CA-CB-CG	10.48	139.40	115.30
1	A	991	LEU	CA-CB-CG	10.27	138.93	115.30
1	E	290	TYR	CB-CG-CD2	10.07	127.04	121.00
1	B	290	TYR	CB-CG-CD2	9.91	126.95	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	1838	THR	CB

5 of 101 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1052	ASP	Peptide
1	D	1087	ALA	Peptide
1	D	1110	MET	Peptide
1	D	924	GLN	Peptide
1	D	957	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16482	16276	16330	551	0
1	B	16482	16276	16330	552	0
1	C	16482	16275	16329	647	0
1	D	16482	16276	16329	769	0
1	E	16482	16276	16330	704	0
1	F	16482	16275	16330	615	0
1	G	6058	5997	6015	151	0
1	J	10424	10279	10314	212	0
1	Q	6058	5997	6015	159	0
1	R	10424	10279	10314	217	0
2	H	1699	1648	1655	30	0
2	K	1696	1644	1651	35	0
2	M	1699	1648	1655	36	0
2	O	1696	1644	1651	30	0
2	S	1699	1648	1655	20	0
2	U	1696	1644	1651	29	0
2	W	1696	1644	1651	23	0
2	Y	1699	1648	1655	20	0
All	All	145436	143374	143860	4549	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 16.

The worst 5 of 4549 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:B:2264:TRP:HA	1:B:2270:LEU:HD21	1.42	1.00
1:A:197:ALA:HB1	1:A:227:ILE:HD13	1.42	0.98
1:B:197:ALA:HB1	1:B:227:ILE:HD13	1.44	0.97
1:F:1123:LEU:HD12	1:F:1152:VAL:HG21	1.48	0.95
1:C:1123:LEU:HD12	1:C:1152:VAL:HG21	1.48	0.93

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	2047/2346 (87%)	1889 (92%)	147 (7%)	11 (0%)	25	65
1	B	2047/2346 (87%)	1888 (92%)	146 (7%)	13 (1%)	22	61
1	C	2047/2346 (87%)	1884 (92%)	150 (7%)	13 (1%)	22	61
1	D	2047/2346 (87%)	1879 (92%)	154 (8%)	14 (1%)	19	57
1	E	2047/2346 (87%)	1895 (93%)	138 (7%)	14 (1%)	19	57
1	F	2047/2346 (87%)	1884 (92%)	150 (7%)	13 (1%)	22	61
1	G	755/2346 (32%)	727 (96%)	25 (3%)	3 (0%)	30	68
1	J	1290/2346 (55%)	1157 (90%)	125 (10%)	8 (1%)	22	61
1	Q	755/2346 (32%)	727 (96%)	24 (3%)	4 (0%)	25	65
1	R	1290/2346 (55%)	1158 (90%)	124 (10%)	8 (1%)	22	61
2	H	212/240 (88%)	207 (98%)	5 (2%)	0	100	100
2	K	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
2	M	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
2	O	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
2	S	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
2	U	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
2	W	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
2	Y	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
All	All	18068/25380 (71%)	16732 (93%)	1235 (7%)	101 (1%)	24	61

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	211	HIS
1	D	419	SER
1	D	868	CYS
1	D	1688	ILE

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Mol	Chain	Res	Type
1	E	211	HIS

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	1784/2056 (87%)	1748 (98%)	36 (2%)	50	68
1	B	1784/2056 (87%)	1755 (98%)	29 (2%)	58	73
1	C	1784/2056 (87%)	1745 (98%)	39 (2%)	47	65
1	D	1784/2056 (87%)	1739 (98%)	45 (2%)	42	61
1	E	1784/2056 (87%)	1734 (97%)	50 (3%)	38	57
1	F	1784/2056 (87%)	1750 (98%)	34 (2%)	52	69
1	G	660/2056 (32%)	655 (99%)	5 (1%)	79	85
1	J	1124/2056 (55%)	1093 (97%)	31 (3%)	38	57
1	Q	660/2056 (32%)	654 (99%)	6 (1%)	75	83
1	R	1124/2056 (55%)	1089 (97%)	35 (3%)	35	54
2	H	186/214 (87%)	185 (100%)	1 (0%)	86	89
2	K	186/214 (87%)	185 (100%)	1 (0%)	86	89
2	M	186/214 (87%)	184 (99%)	2 (1%)	70	80
2	O	186/214 (87%)	185 (100%)	1 (0%)	86	89
2	S	186/214 (87%)	184 (99%)	2 (1%)	70	80
2	U	186/214 (87%)	185 (100%)	1 (0%)	86	89
2	W	186/214 (87%)	185 (100%)	1 (0%)	86	89
2	Y	186/214 (87%)	184 (99%)	2 (1%)	70	80
All	All	15760/22272 (71%)	15439 (98%)	321 (2%)	50	68

5 of 321 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2245	GLN

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Mol	Chain	Res	Type
1	R	916	LYS
1	Q	1667	LYS
1	J	1080	ARG
1	R	1388	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 233 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1619	GLN
2	O	1730	ASN
1	B	1181	GLN
2	M	1730	ASN
1	J	1444	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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$
1	SEP	F	1263	1	8,9,10	1.54	1 (12%)	8,12,14	0.92	0
1	SEP	J	1263	1	8,9,10	1.56	1 (12%)	8,12,14	1.42	2 (25%)
1	SEP	D	1263	1	8,9,10	1.51	1 (12%)	8,12,14	1.22	2 (25%)
1	SEP	R	1263	1	8,9,10	1.57	1 (12%)	8,12,14	1.32	2 (25%)
1	SEP	B	1263	1	8,9,10	1.53	1 (12%)	8,12,14	0.89	0
1	SEP	E	1263	1	8,9,10	1.52	1 (12%)	8,12,14	1.32	2 (25%)
1	SEP	A	1263	1	8,9,10	1.54	1 (12%)	8,12,14	1.74	2 (25%)
1	SEP	C	1263	1	8,9,10	1.55	1 (12%)	8,12,14	1.83	2 (25%)

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
1	SEP	F	1263	1	-	1/5/8/10	-
1	SEP	J	1263	1	-	1/5/8/10	-
1	SEP	D	1263	1	-	1/5/8/10	-
1	SEP	R	1263	1	-	1/5/8/10	-
1	SEP	B	1263	1	-	1/5/8/10	-
1	SEP	E	1263	1	-	1/5/8/10	-
1	SEP	A	1263	1	-	1/5/8/10	-
1	SEP	C	1263	1	-	1/5/8/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1263	SEP	P-O1P	3.47	1.61	1.50
1	R	1263	SEP	P-O1P	3.41	1.61	1.50
1	J	1263	SEP	P-O1P	3.40	1.61	1.50
1	B	1263	SEP	P-O1P	3.39	1.61	1.50
1	F	1263	SEP	P-O1P	3.36	1.61	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1263	SEP	OG-CB-CA	3.54	111.59	108.14
1	C	1263	SEP	P-OG-CB	-3.26	109.33	118.30
1	C	1263	SEP	OG-CB-CA	2.92	110.99	108.14
1	J	1263	SEP	OG-CB-CA	2.72	110.79	108.14
1	A	1263	SEP	P-OG-CB	-2.64	111.02	118.30

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	1263	SEP	N-CA-CB-OG
1	E	1263	SEP	N-CA-CB-OG
1	C	1263	SEP	N-CA-CB-OG
1	F	1263	SEP	N-CA-CB-OG
1	B	1263	SEP	N-CA-CB-OG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	1263	SEP	2	0
1	D	1263	SEP	1	0
1	E	1263	SEP	1	0
1	C	1263	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

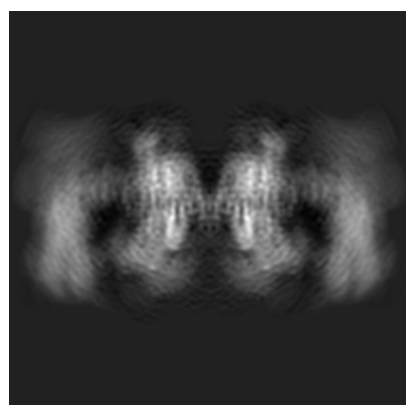
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4344. These allow visual inspection of the internal detail of the map and identification of artifacts.

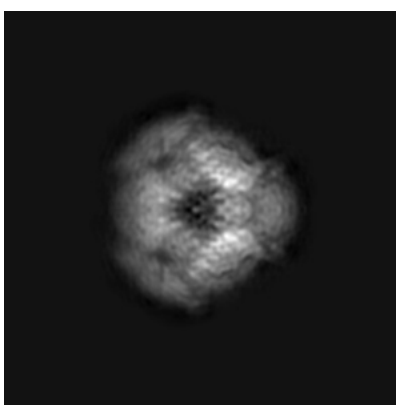
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

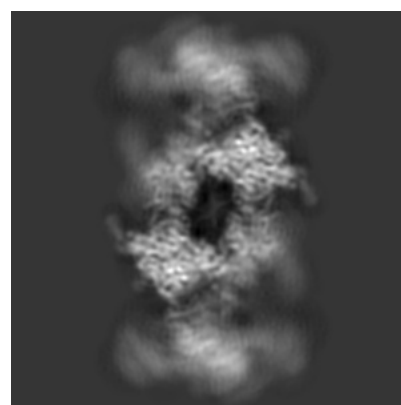
6.1.1 Primary map



X



Y

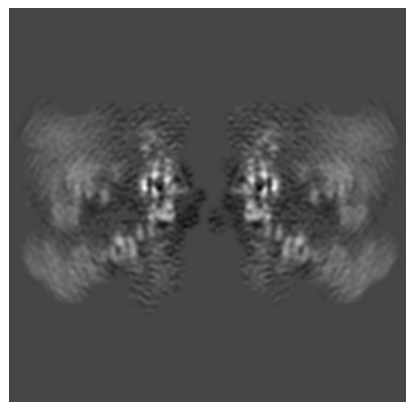


Z

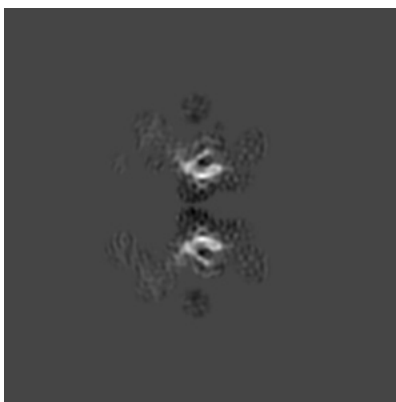
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

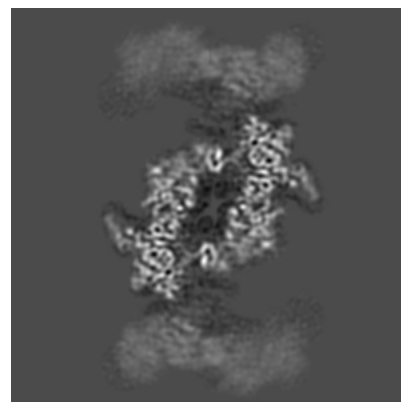
6.2.1 Primary map



X Index: 188



Y Index: 188

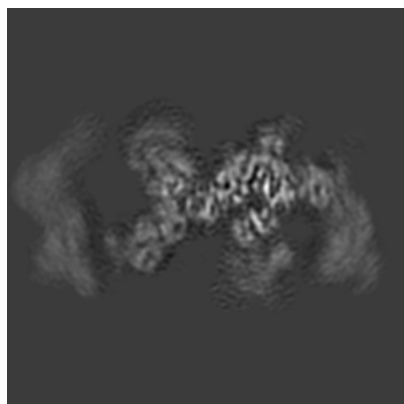


Z Index: 188

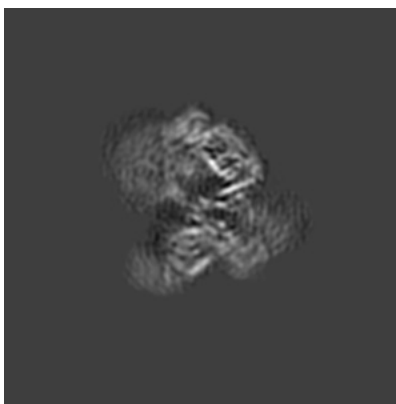
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

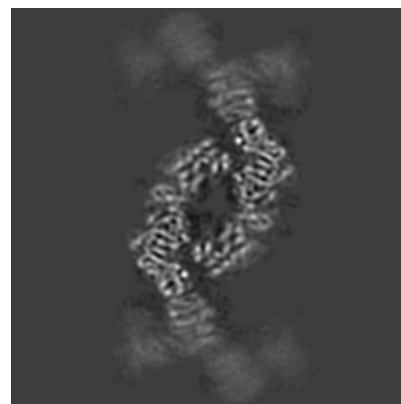
6.3.1 Primary map



X Index: 219



Y Index: 223

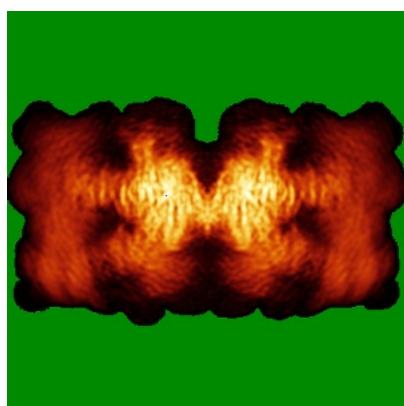


Z Index: 201

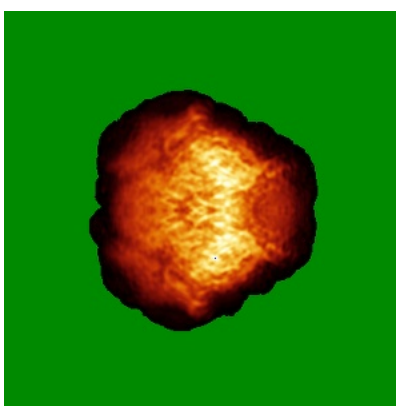
The images above show the largest variance slices of the map in three orthogonal directions.

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

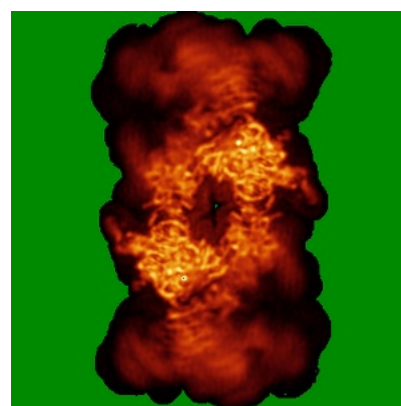
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

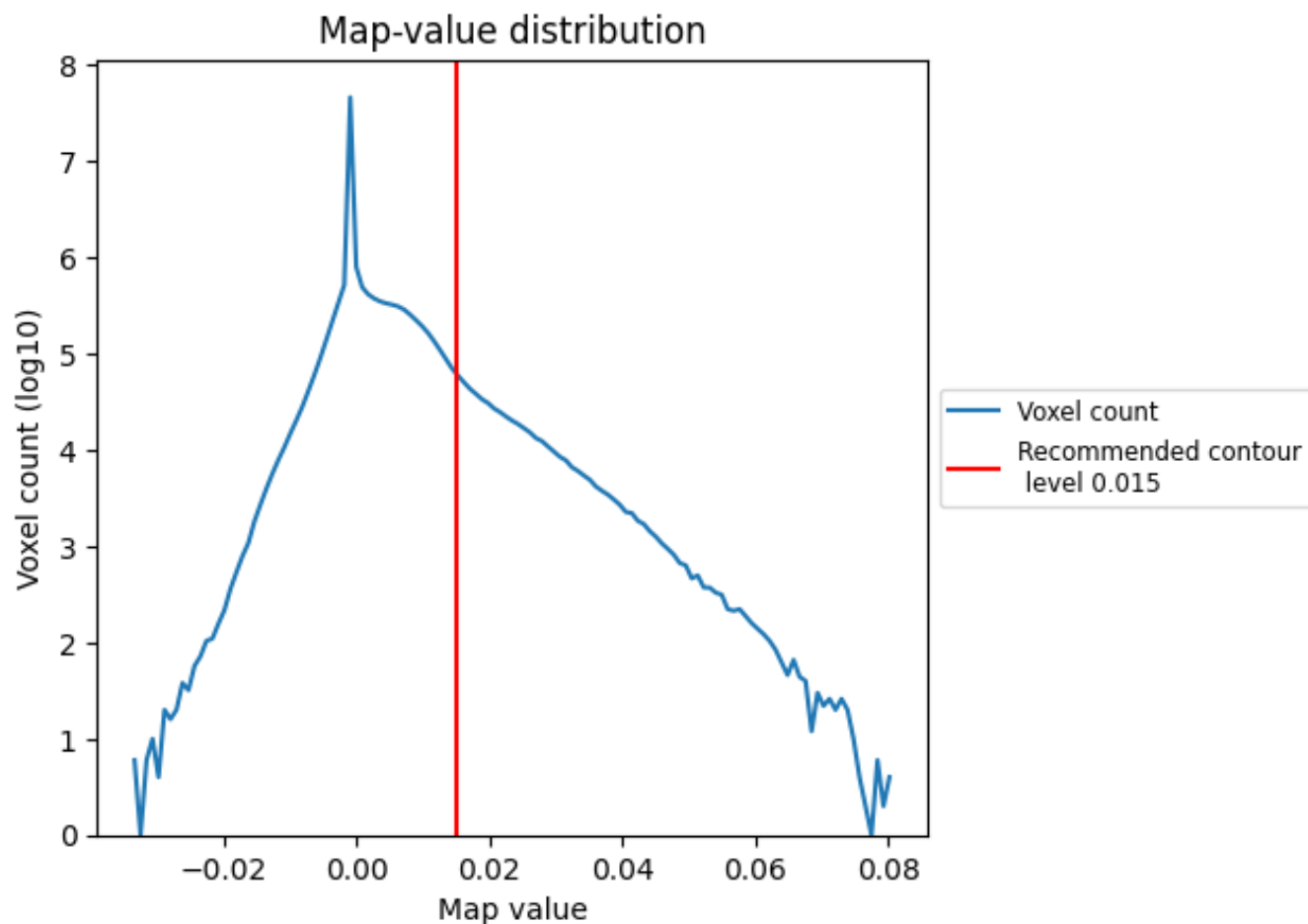
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

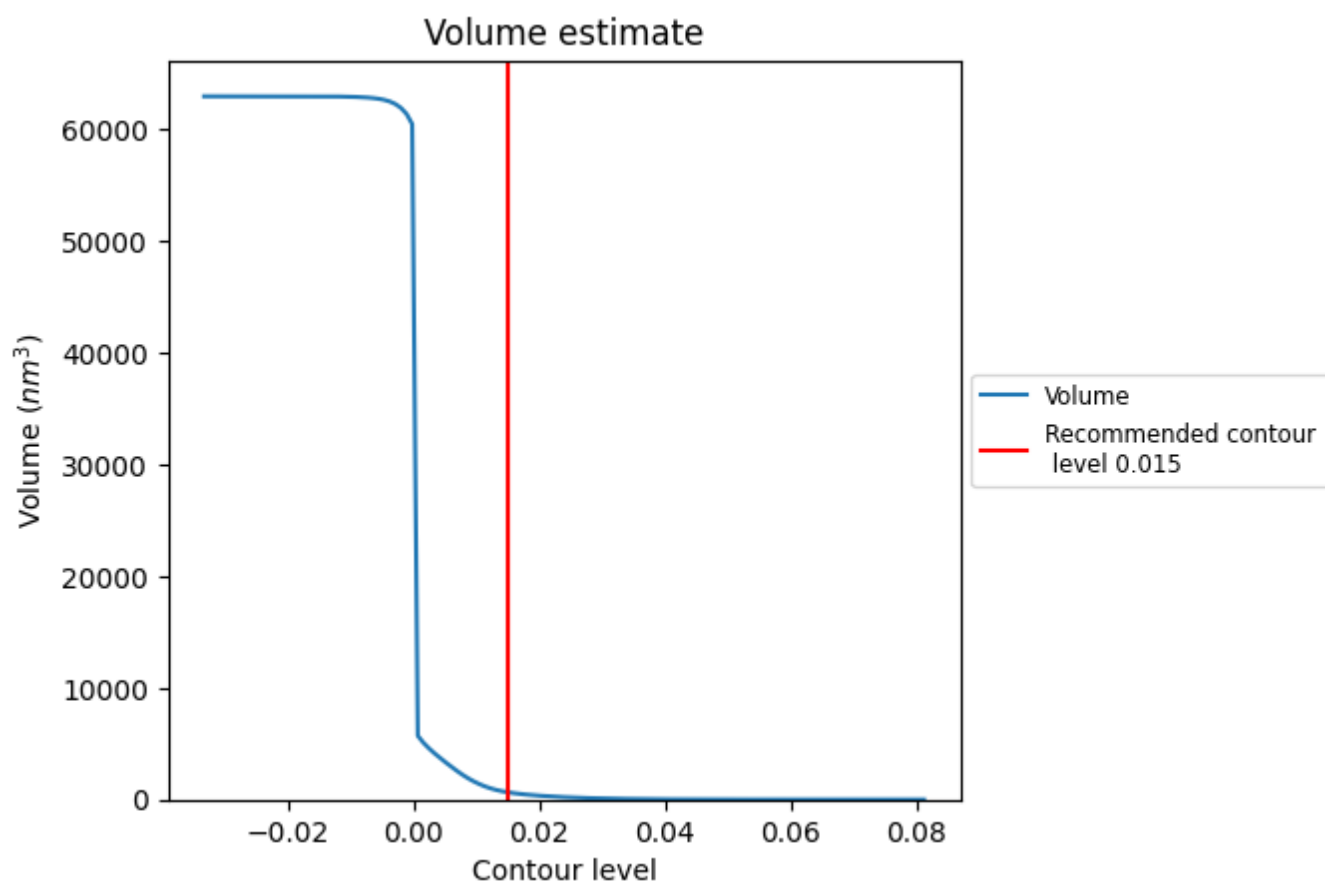
This section contains the results of statistical analysis of the map.

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.

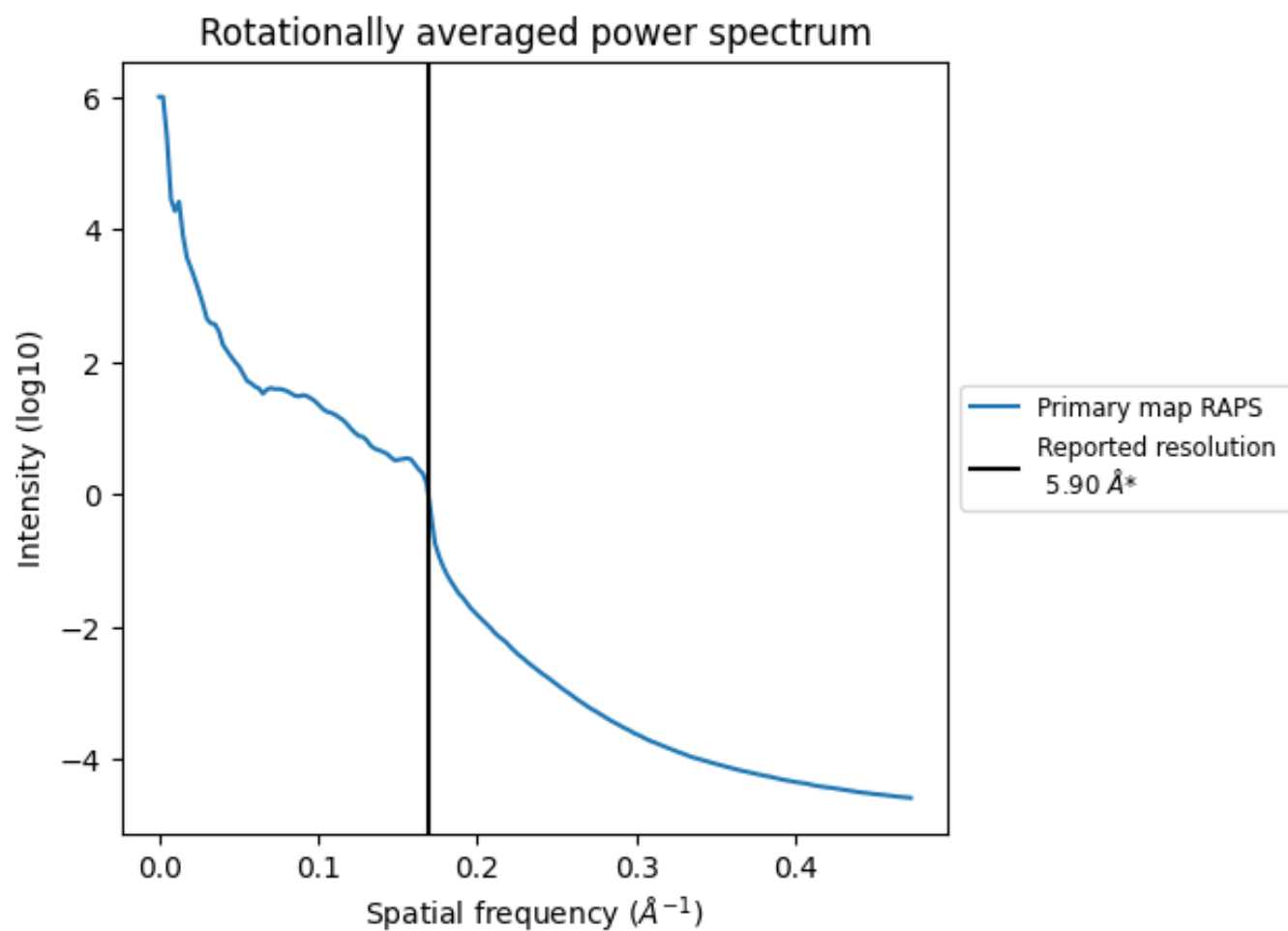
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 649 nm³; this corresponds to an approximate mass of 587 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 0.169 Å⁻¹

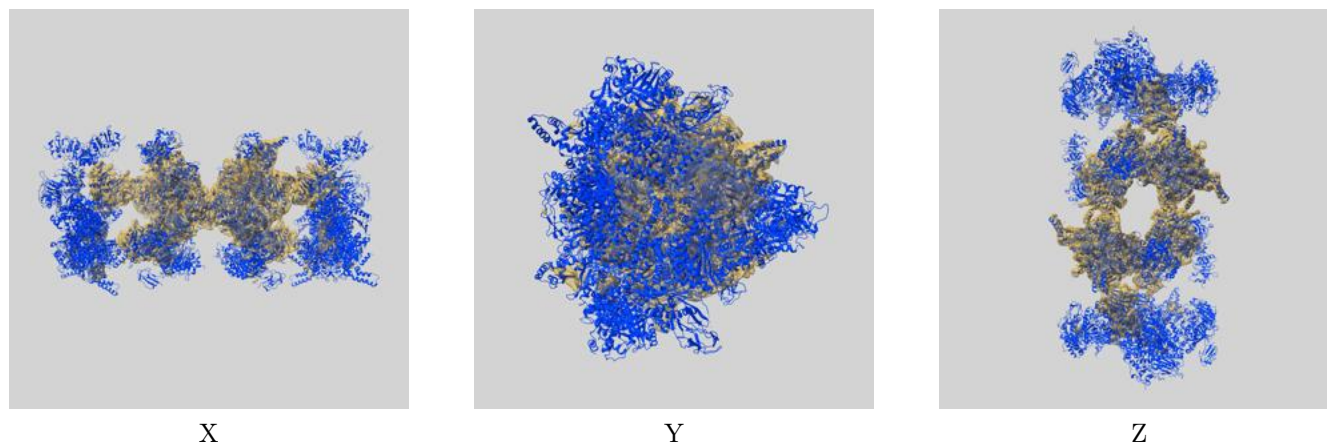
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

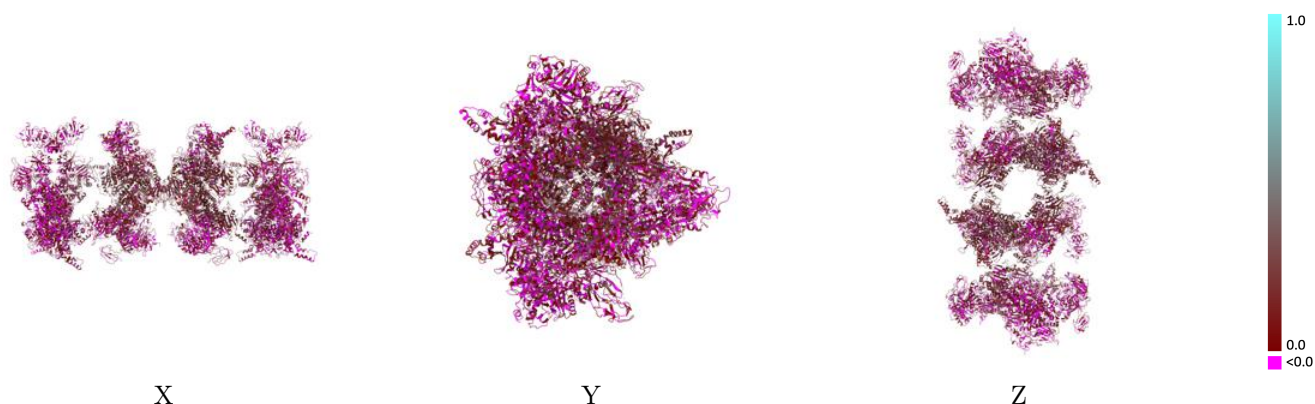
This section contains information regarding the fit between EMDB map EMD-4344 and PDB model 6G2I. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



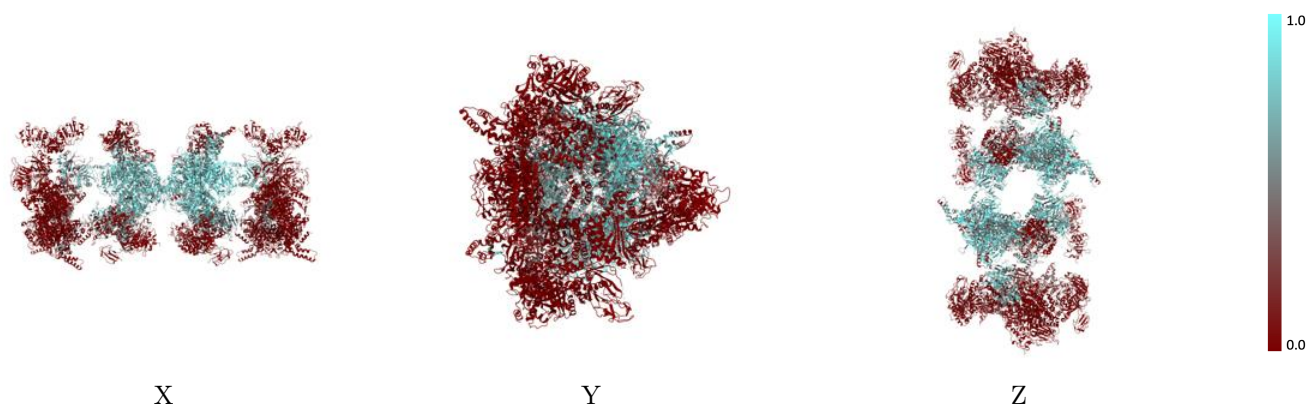
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



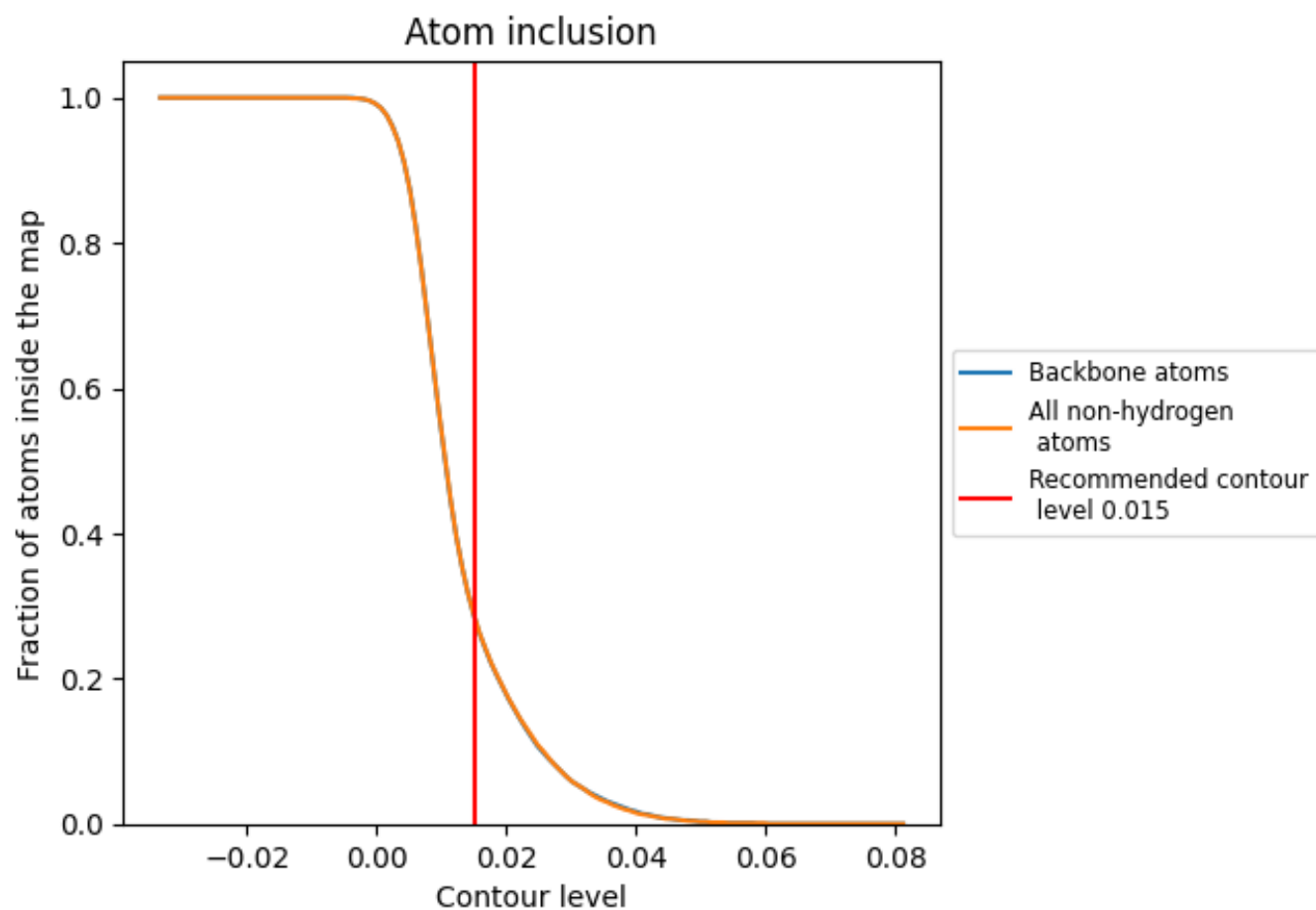
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 29% of all backbone atoms, 29% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2880	 0.1080
A	 0.2280	 0.0990
B	 0.2300	 0.1000
C	 0.4240	 0.1330
D	 0.5950	 0.1610
E	 0.5900	 0.1610
F	 0.4230	 0.1330
G	 0.0360	 0.0800
H	 0.0710	 0.0540
J	 0.0060	 0.0540
K	 0.0520	 0.0450
M	 0.0470	 0.0510
O	 0.0730	 0.0580
Q	 0.0350	 0.0770
R	 0.0060	 0.0540
S	 0.0020	 0.0510
U	 0.0020	 0.0510
W	 0.0000	 0.0370
Y	 0.0010	 0.0380

