



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:38 PM GMT

PDB ID : 3U9S
Title : Crystal structure of P. aeruginosa 3-methylcrotonyl-CoA carboxylase (MCC)
750 kD holoenzyme, CoA complex
Authors : Huang, C.S.; Tong, L.
Deposited on : 2011-10-19
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

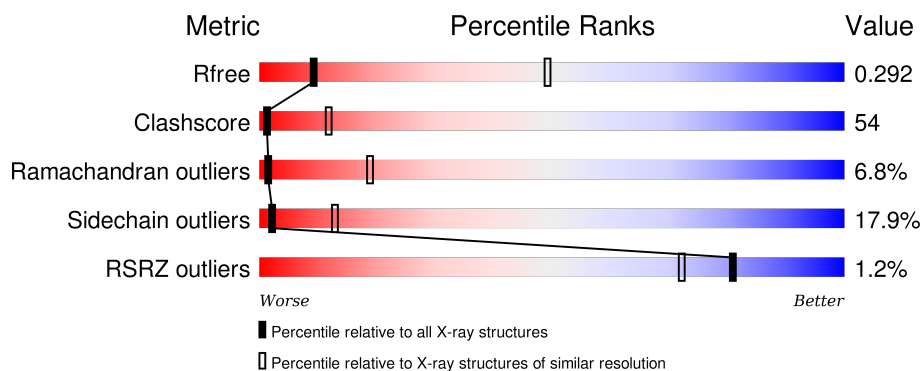
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	655	
1	C	655	
1	E	655	
1	G	655	
1	I	655	

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Mol	Chain	Length	Quality of chain
1	K	655	
2	B	555	
2	D	555	
2	F	555	
2	H	555	
2	J	555	
2	L	555	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BTI	A	801	-	-	-	X
3	BTI	I	801	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 49939 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Methylcrotonyl-CoA carboxylase, alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	0	0
			4778	2978	892	886	22			
1	C	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	E	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	G	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	I	498	Total	C	N	O	S	0	0	0
			3853	2399	731	707	16			
1	K	497	Total	C	N	O	S	0	0	0
			3844	2393	729	706	16			

- Molecule 2 is a protein called Methylcrotonyl-CoA carboxylase, beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	D	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	F	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	H	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	J	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	L	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	EXPRESSION TAG	UNP Q9I297

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	GLY	-	EXPRESSION TAG	UNP Q9I297
B	10	SER	-	EXPRESSION TAG	UNP Q9I297
B	11	SER	-	EXPRESSION TAG	UNP Q9I297
B	12	HIS	-	EXPRESSION TAG	UNP Q9I297
B	13	HIS	-	EXPRESSION TAG	UNP Q9I297
B	14	HIS	-	EXPRESSION TAG	UNP Q9I297
B	15	HIS	-	EXPRESSION TAG	UNP Q9I297
B	16	HIS	-	EXPRESSION TAG	UNP Q9I297
B	17	HIS	-	EXPRESSION TAG	UNP Q9I297
B	18	SER	-	EXPRESSION TAG	UNP Q9I297
B	19	SER	-	EXPRESSION TAG	UNP Q9I297
B	20	GLY	-	EXPRESSION TAG	UNP Q9I297
B	21	LEU	-	EXPRESSION TAG	UNP Q9I297
B	22	VAL	-	EXPRESSION TAG	UNP Q9I297
B	23	PRO	-	EXPRESSION TAG	UNP Q9I297
B	24	ARG	-	EXPRESSION TAG	UNP Q9I297
B	25	GLY	-	EXPRESSION TAG	UNP Q9I297
B	26	SER	-	EXPRESSION TAG	UNP Q9I297
B	27	HIS	-	EXPRESSION TAG	UNP Q9I297
D	8	MET	-	EXPRESSION TAG	UNP Q9I297
D	9	GLY	-	EXPRESSION TAG	UNP Q9I297
D	10	SER	-	EXPRESSION TAG	UNP Q9I297
D	11	SER	-	EXPRESSION TAG	UNP Q9I297
D	12	HIS	-	EXPRESSION TAG	UNP Q9I297
D	13	HIS	-	EXPRESSION TAG	UNP Q9I297
D	14	HIS	-	EXPRESSION TAG	UNP Q9I297
D	15	HIS	-	EXPRESSION TAG	UNP Q9I297
D	16	HIS	-	EXPRESSION TAG	UNP Q9I297
D	17	HIS	-	EXPRESSION TAG	UNP Q9I297
D	18	SER	-	EXPRESSION TAG	UNP Q9I297
D	19	SER	-	EXPRESSION TAG	UNP Q9I297
D	20	GLY	-	EXPRESSION TAG	UNP Q9I297
D	21	LEU	-	EXPRESSION TAG	UNP Q9I297
D	22	VAL	-	EXPRESSION TAG	UNP Q9I297
D	23	PRO	-	EXPRESSION TAG	UNP Q9I297
D	24	ARG	-	EXPRESSION TAG	UNP Q9I297
D	25	GLY	-	EXPRESSION TAG	UNP Q9I297
D	26	SER	-	EXPRESSION TAG	UNP Q9I297
D	27	HIS	-	EXPRESSION TAG	UNP Q9I297
F	8	MET	-	EXPRESSION TAG	UNP Q9I297
F	9	GLY	-	EXPRESSION TAG	UNP Q9I297
F	10	SER	-	EXPRESSION TAG	UNP Q9I297

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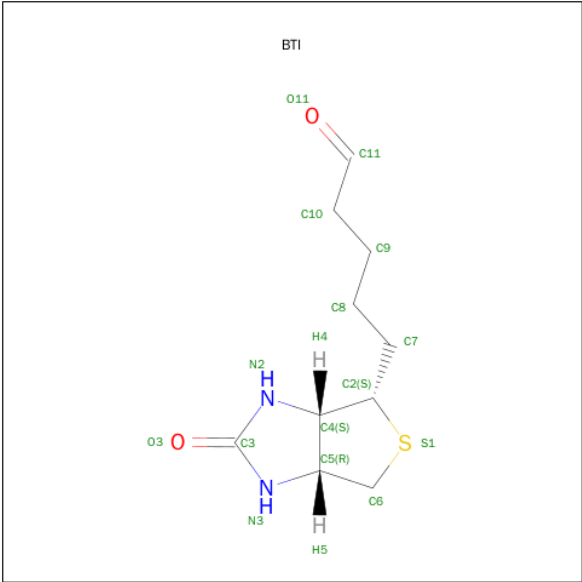
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F	12	HIS	-	EXPRESSION TAG	UNP Q9I297
F	13	HIS	-	EXPRESSION TAG	UNP Q9I297
F	14	HIS	-	EXPRESSION TAG	UNP Q9I297
F	15	HIS	-	EXPRESSION TAG	UNP Q9I297
F	16	HIS	-	EXPRESSION TAG	UNP Q9I297
F	17	HIS	-	EXPRESSION TAG	UNP Q9I297
F	18	SER	-	EXPRESSION TAG	UNP Q9I297
F	19	SER	-	EXPRESSION TAG	UNP Q9I297
F	20	GLY	-	EXPRESSION TAG	UNP Q9I297
F	21	LEU	-	EXPRESSION TAG	UNP Q9I297
F	22	VAL	-	EXPRESSION TAG	UNP Q9I297
F	23	PRO	-	EXPRESSION TAG	UNP Q9I297
F	24	ARG	-	EXPRESSION TAG	UNP Q9I297
F	25	GLY	-	EXPRESSION TAG	UNP Q9I297
F	26	SER	-	EXPRESSION TAG	UNP Q9I297
F	27	HIS	-	EXPRESSION TAG	UNP Q9I297
H	8	MET	-	EXPRESSION TAG	UNP Q9I297
H	9	GLY	-	EXPRESSION TAG	UNP Q9I297
H	10	SER	-	EXPRESSION TAG	UNP Q9I297
H	11	SER	-	EXPRESSION TAG	UNP Q9I297
H	12	HIS	-	EXPRESSION TAG	UNP Q9I297
H	13	HIS	-	EXPRESSION TAG	UNP Q9I297
H	14	HIS	-	EXPRESSION TAG	UNP Q9I297
H	15	HIS	-	EXPRESSION TAG	UNP Q9I297
H	16	HIS	-	EXPRESSION TAG	UNP Q9I297
H	17	HIS	-	EXPRESSION TAG	UNP Q9I297
H	18	SER	-	EXPRESSION TAG	UNP Q9I297
H	19	SER	-	EXPRESSION TAG	UNP Q9I297
H	20	GLY	-	EXPRESSION TAG	UNP Q9I297
H	21	LEU	-	EXPRESSION TAG	UNP Q9I297
H	22	VAL	-	EXPRESSION TAG	UNP Q9I297
H	23	PRO	-	EXPRESSION TAG	UNP Q9I297
H	24	ARG	-	EXPRESSION TAG	UNP Q9I297
H	25	GLY	-	EXPRESSION TAG	UNP Q9I297
H	26	SER	-	EXPRESSION TAG	UNP Q9I297
H	27	HIS	-	EXPRESSION TAG	UNP Q9I297
J	8	MET	-	EXPRESSION TAG	UNP Q9I297
J	9	GLY	-	EXPRESSION TAG	UNP Q9I297
J	10	SER	-	EXPRESSION TAG	UNP Q9I297
J	11	SER	-	EXPRESSION TAG	UNP Q9I297
J	12	HIS	-	EXPRESSION TAG	UNP Q9I297

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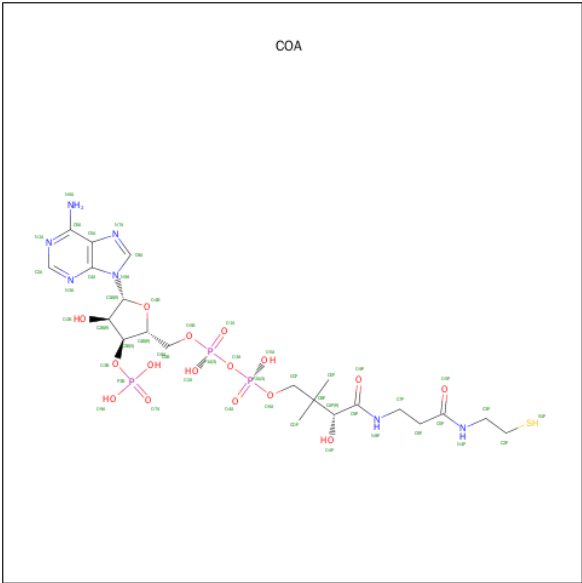
Chain	Residue	Modelled	Actual	Comment	Reference
J	13	HIS	-	EXPRESSION TAG	UNP Q9I297
J	14	HIS	-	EXPRESSION TAG	UNP Q9I297
J	15	HIS	-	EXPRESSION TAG	UNP Q9I297
J	16	HIS	-	EXPRESSION TAG	UNP Q9I297
J	17	HIS	-	EXPRESSION TAG	UNP Q9I297
J	18	SER	-	EXPRESSION TAG	UNP Q9I297
J	19	SER	-	EXPRESSION TAG	UNP Q9I297
J	20	GLY	-	EXPRESSION TAG	UNP Q9I297
J	21	LEU	-	EXPRESSION TAG	UNP Q9I297
J	22	VAL	-	EXPRESSION TAG	UNP Q9I297
J	23	PRO	-	EXPRESSION TAG	UNP Q9I297
J	24	ARG	-	EXPRESSION TAG	UNP Q9I297
J	25	GLY	-	EXPRESSION TAG	UNP Q9I297
J	26	SER	-	EXPRESSION TAG	UNP Q9I297
J	27	HIS	-	EXPRESSION TAG	UNP Q9I297
L	8	MET	-	EXPRESSION TAG	UNP Q9I297
L	9	GLY	-	EXPRESSION TAG	UNP Q9I297
L	10	SER	-	EXPRESSION TAG	UNP Q9I297
L	11	SER	-	EXPRESSION TAG	UNP Q9I297
L	12	HIS	-	EXPRESSION TAG	UNP Q9I297
L	13	HIS	-	EXPRESSION TAG	UNP Q9I297
L	14	HIS	-	EXPRESSION TAG	UNP Q9I297
L	15	HIS	-	EXPRESSION TAG	UNP Q9I297
L	16	HIS	-	EXPRESSION TAG	UNP Q9I297
L	17	HIS	-	EXPRESSION TAG	UNP Q9I297
L	18	SER	-	EXPRESSION TAG	UNP Q9I297
L	19	SER	-	EXPRESSION TAG	UNP Q9I297
L	20	GLY	-	EXPRESSION TAG	UNP Q9I297
L	21	LEU	-	EXPRESSION TAG	UNP Q9I297
L	22	VAL	-	EXPRESSION TAG	UNP Q9I297
L	23	PRO	-	EXPRESSION TAG	UNP Q9I297
L	24	ARG	-	EXPRESSION TAG	UNP Q9I297
L	25	GLY	-	EXPRESSION TAG	UNP Q9I297
L	26	SER	-	EXPRESSION TAG	UNP Q9I297
L	27	HIS	-	EXPRESSION TAG	UNP Q9I297

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	I	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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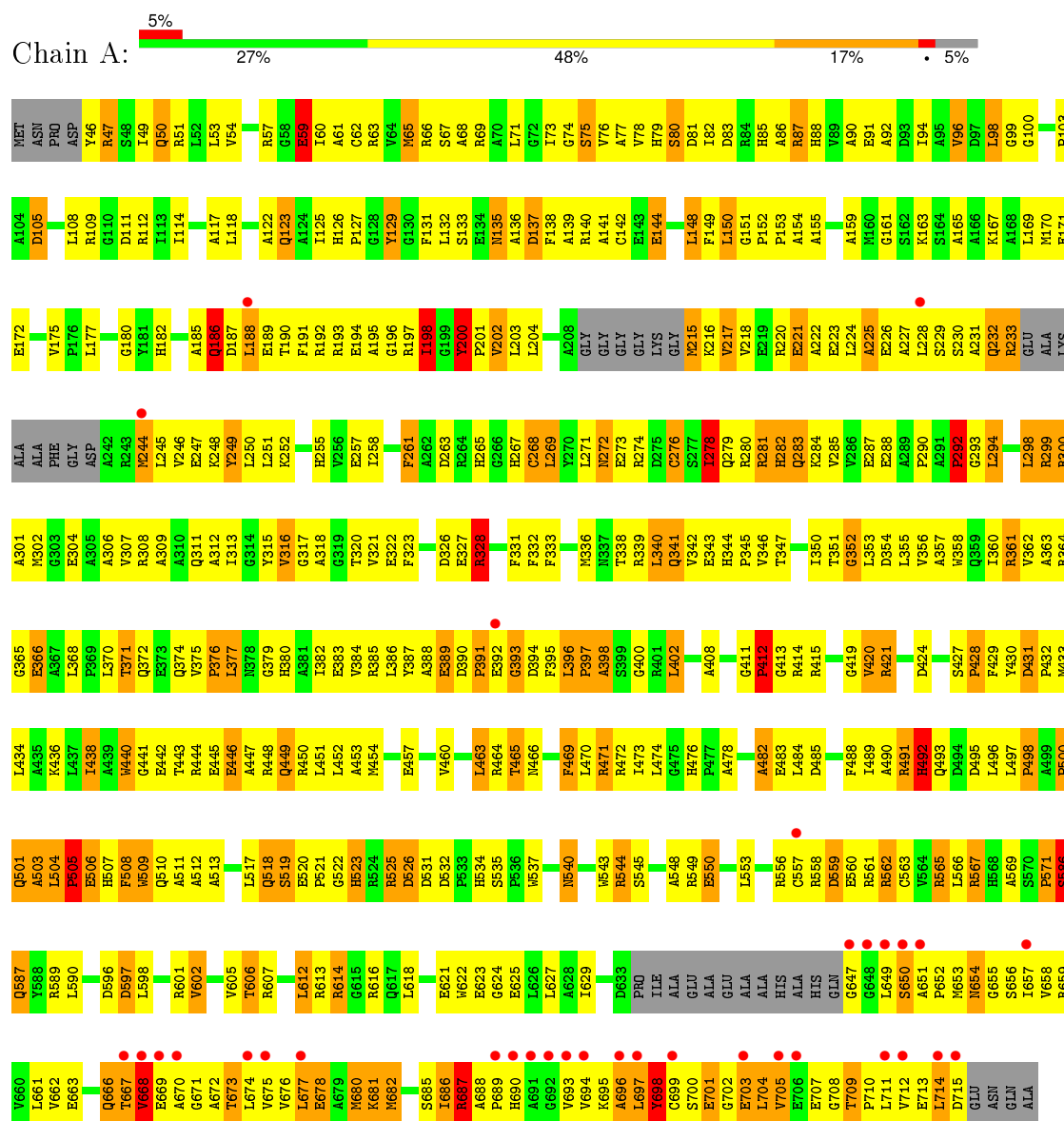
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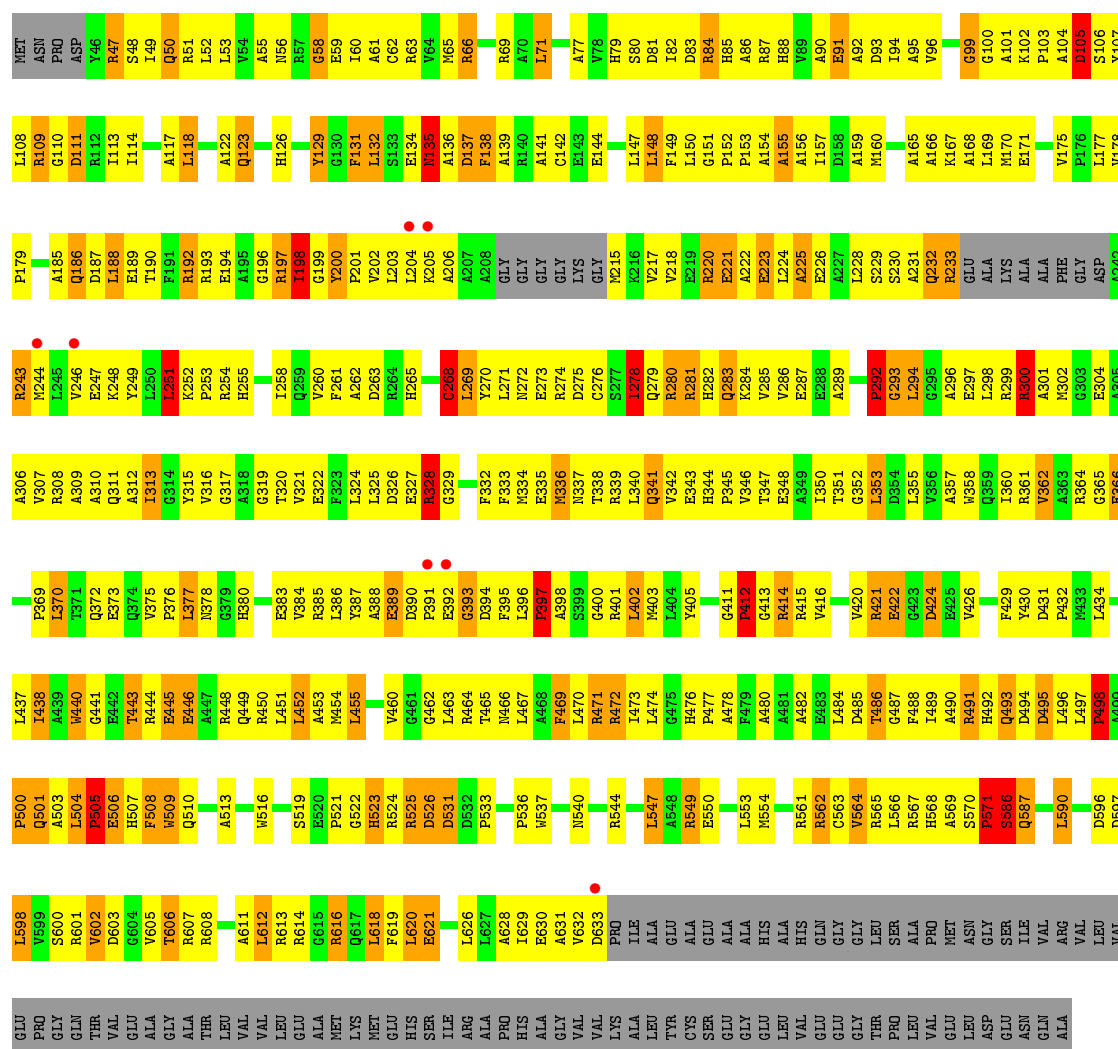
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

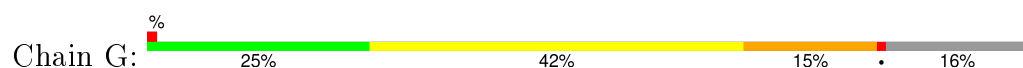
- Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit





Q374	T443	A513	D597	LEU
V375	R444	E514	L596	VAL
P376	E445	A515	V599	GLU
L377	E446	W516	S600	PRO
N378	A447	S519	V601	GLN
G379	R448	E520	V602	GLY
H380	Q449	F521	D603	THR
A381	R450	G522	G604	VAL
L382	L451	G521	V605	GLU
E383	L452	H523	R606	ALA
V384	A453	R524	R607	GLY
R385	M454	B525	R608	ALA
L386	L455	D526	A611	THR
Y387	T458	D531	L612	LEU
A388	S459	D532	R613	VAL
E389	V460	F533	R614	VAL
D390	P391	H534	G615	LEU
P391	T463	S535	R616	GLU
E392	R464	P536	R617	ALA
G393	T465	R539	Q617	MET
L394	M466	N540	F619	LYS
F395	L467	D541	R621	MET
L396	L470	R544	R622	HIS
P397	F469	S545	R623	SER
A398	L471	A546	L626	ILE
S399	L474	L547	L627	ARG
G400	L475	L548	R628	ALA
R401	L476	R549	L629	PRO
L404	P479	A550	E630	HIS
Y405	A482	S551	D633	ALA
R406	E483	L552	PRO	GLY
E407	L484	M554	ILE	VAL
G411	D485	L555	ALA	LYS
P412	T486	R556	ALA	LEU
G413	Q487	C557	GLU	TYR
R414	F488	D558	ALA	CYS
S418	F489	R560	ALA	SER
R421	R491	R561	ALA	GLU
E422	H492	R562	HIS	GLY
V426	Q493	V564	ALA	LEU
F429	L497	R565	HIS	VAL
Y430	A499	L566	GLN	GLU
D431	P500	R567	GLY	GLU
P432	Q501	H568	LEU	THR
M433	A503	A569	SER	PRO
L434	L504	S570	ALA	LEU
A435	P505	P571	VAL	VAL
K436	E506	R587	PRO	GLU
L437	E507	Y588	ASN	LEU
T438	F508	R589	GLY	ASP
A439	F509	L590	SER	GLU
W440	Q510	D591	ILE	ASN
G441	G511	G592	ARG	ALA
E442	A512	D596	VAL	GLN

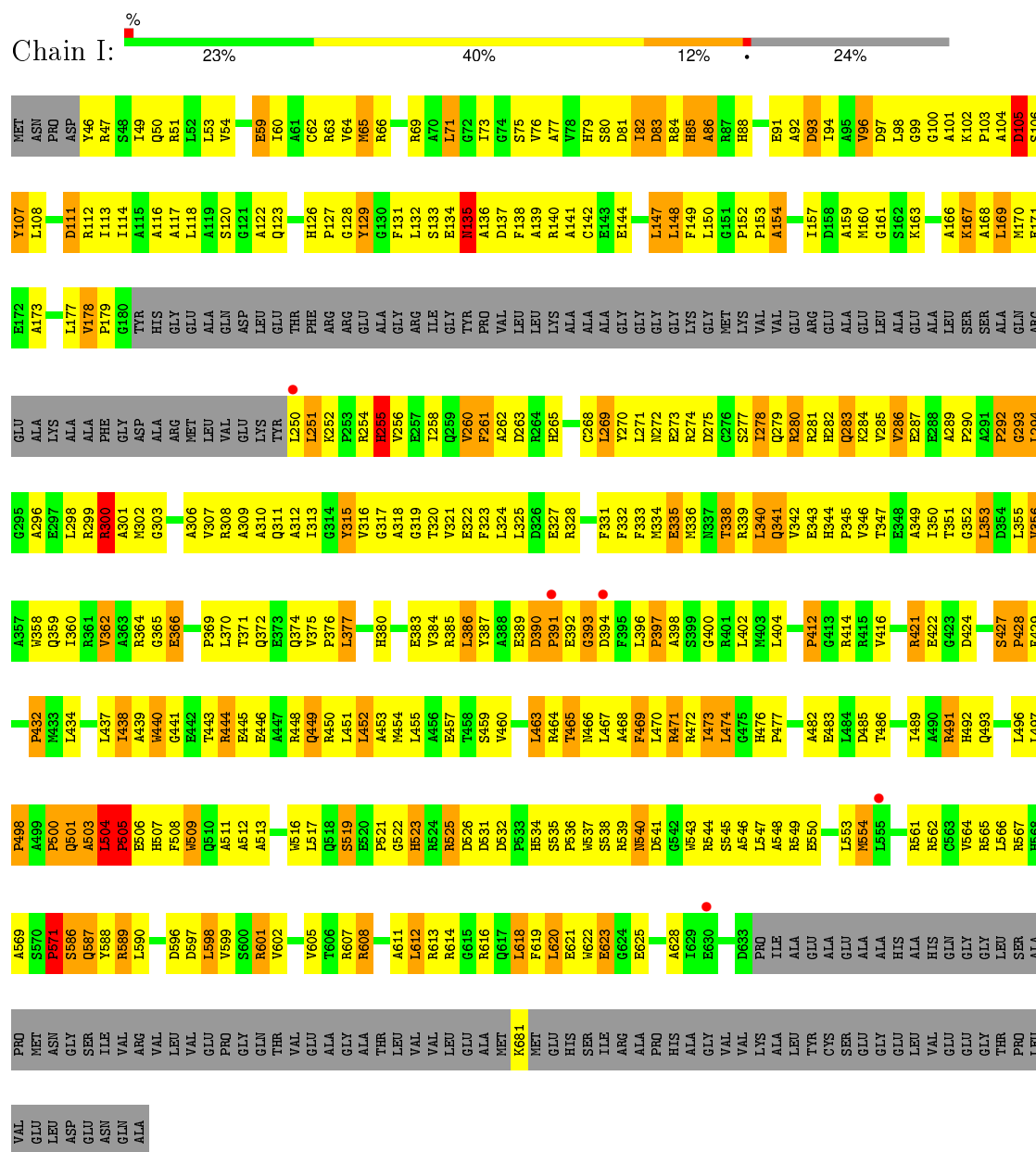
• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

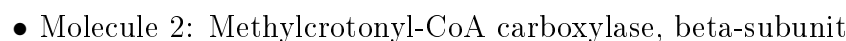


RET	R109	E172	GLU	L298	R361	A439	E506	S586	ARG
ASN	G110	A173	ALA	R299	V362	W440	H507	Q587	VAL
PRO	D111	G174	LYS	R300	A363	G441	F508	R588	LEU
ASP	R112	V175	ALA	A301	R364	A445	M509	L590	VAL
	I113	P176	ALA	R302	G365	R444	A513	D596	PRO
	I114	L177	PHE	G303	E366	E445	B514	D597	GLY
	A115	V178	GLY	E304	A367	E446	A515	D598	GLN
	A116	P179	ASP	A305	L368	A447	H516	L598	THR
	A117		A242	A306	T371	Q449	A517	R599	GLU
	L118	H182	R243	V307	Q372	Q449	L517	E506	VAL
	G121	G183	R244	R308	E373	Q449	Q518	R601	GLU
	A122	E184	L245	A309	Q374	L451	S519	V602	ALA
	Q123	A185	V246	A310	V375	L452	E520	D603	GLY
	I125	Q186	E247	Q311	P376	L453	P521	G604	ALA
	H126	D187	K248	A312	L377	M454	G522	V605	THR
	E128	L188	L250	R313	N378	L455	H523	R606	LEU
	R66	A195	L251	G314	G379	S459	R524	R607	VAL
	S67	A196	K252	G315	H380	V460	D526	A611	LEU
	E621	R197	P253	G316	E383	L463	D531	L612	GLU
	A68	I198	R254	G317	V384	R464	D532	R613	ALA
	R69	G199	E257	A318	R385	T465	F533	R614	ALA
	A70	Y200	D261	G319	R386	N466	H534	P533	MET
	L71	P201	D263	T320	L386	Y387	S535	P536	LYS
	F131	A195	L268	G321	Y387	A388	R539	L537	MET
	L132	A196	Q259	E322	A389	F469	N540	W622	GLU
	R133	R197	V260	E323	E392	L470	D541	L626	ALA
	E134	R197	R260	E324	G393	G475	A542	L629	PRO
	E134	R197	R260	E325	R394	H476	R543	E630	HIS
	E134	R197	R260	E326	F395	P477	R544	A631	ALA
	E134	R197	R260	E327	L396	A478	S545	V632	GLY
	E134	R197	R260	E328	P397	F479	L547	D633	VAL
	E134	R197	R260	E329	A398	S399	A548	PRO	LYS
	E134	R197	R260	E330	C400	L404	R549	ILE	ALA
	E134	R197	R260	E331	L404	E483	E550	ALA	LEU
	E134	R197	R260	E332	L404	D485	D552	GLU	TYR
	E134	R197	R260	E333	L404	T486	S551	ALA	CYS
	E134	R197	R260	E334	L404	G487	L553	SER	GLY
	E134	R197	R260	E335	L404	F488	M554	ALA	GLU
	E134	R197	R260	E336	L404	I489	L555	GLY	GLU
	E134	R197	R260	E337	L404	A490	C557	LEU	ALA
	E134	R197	R260	E338	L404	R491	R558	HIS	VAL
	E134	R197	R260	E339	L404	H492	D559	GLN	GLU
	E134	R197	R260	E340	L404	Q493	E560	GLY	GLY
	E134	R197	R260	E341	L404	D494	R561	GLY	THR
	E134	R197	R260	E342	L404	D495	R562	LEU	PRO
	E134	R197	R260	E343	L404	L496	C563	SER	PRO
	E134	R197	R260	E344	L404	L497	V564	ALA	LEU
	E134	R197	R260	E345	L404	P498	R565	VAL	VAL
	E134	R197	R260	E346	L404	A499	L566	GLU	GLU
	E134	R197	R260	E347	L404	P500	R567	MET	ASP
	E134	R197	R260	E348	L404	Q501	H568	GLY	GLY
	E134	R197	R260	E349	L404	A503	A569	SER	GLU
	E134	R197	R260	E350	L404	L504	S570	ASN	ASN
	E134	R197	R260	E351	L404	P505	P571	ILE	VAL

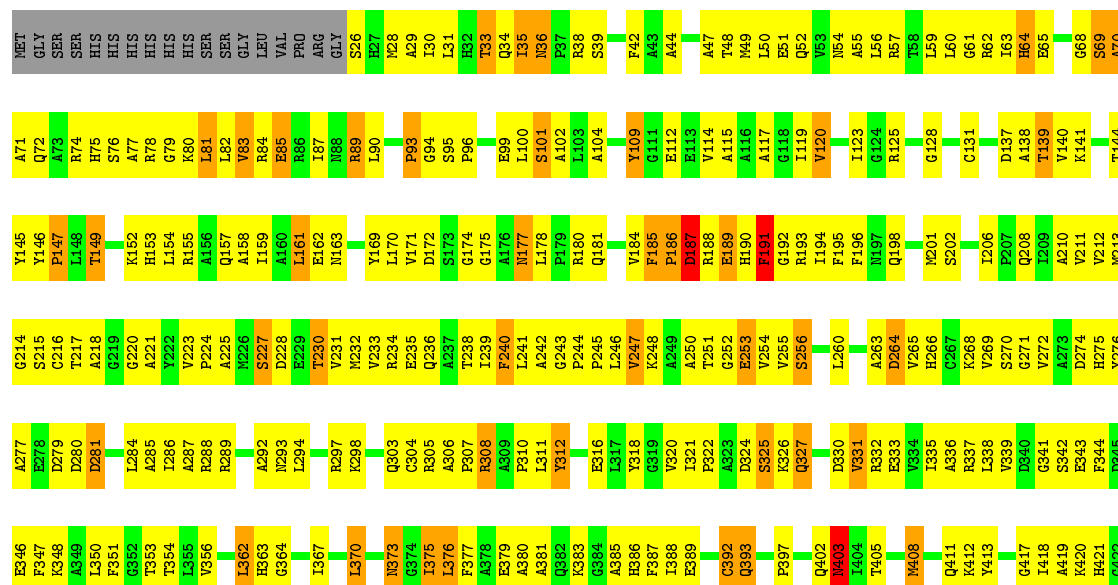
ALA

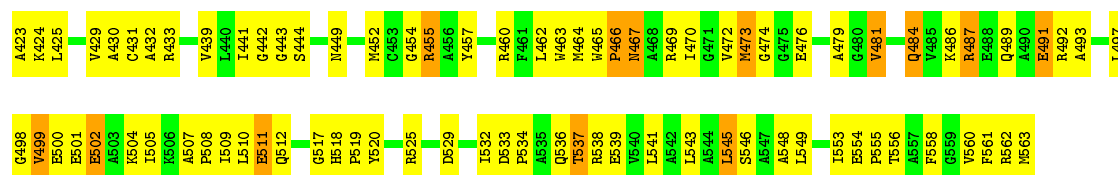
- Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit





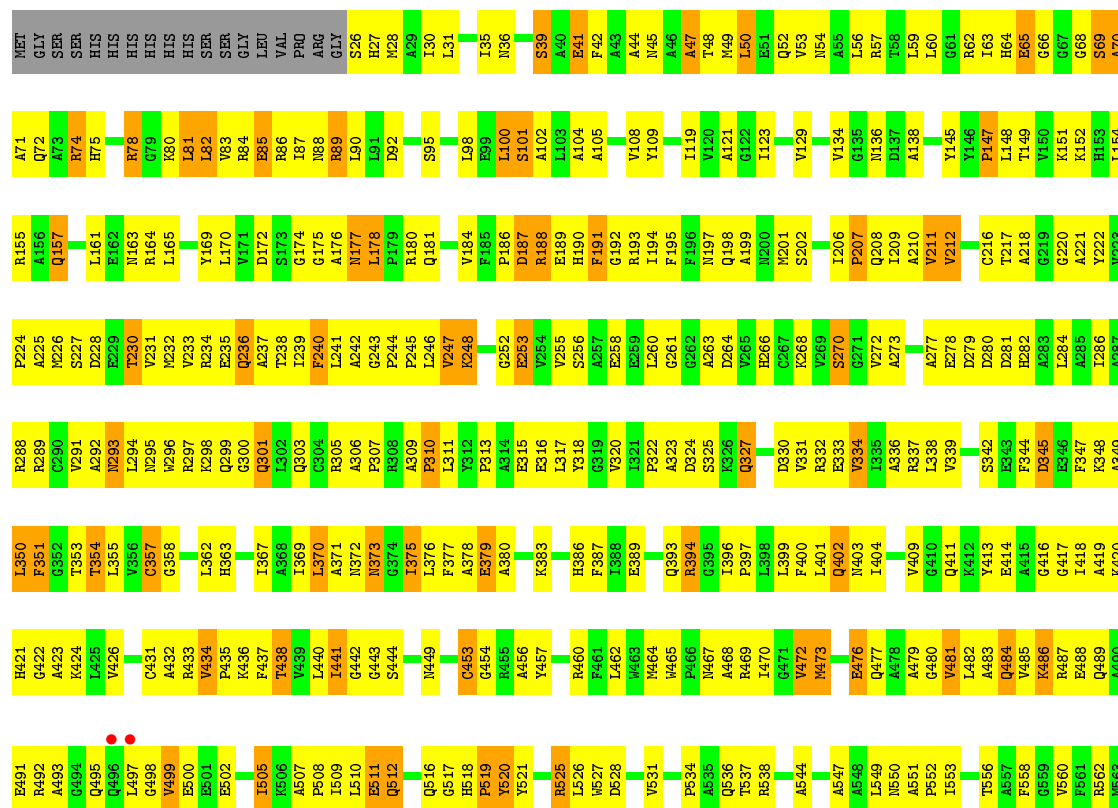
Chain B: 35% 51% 10% . .





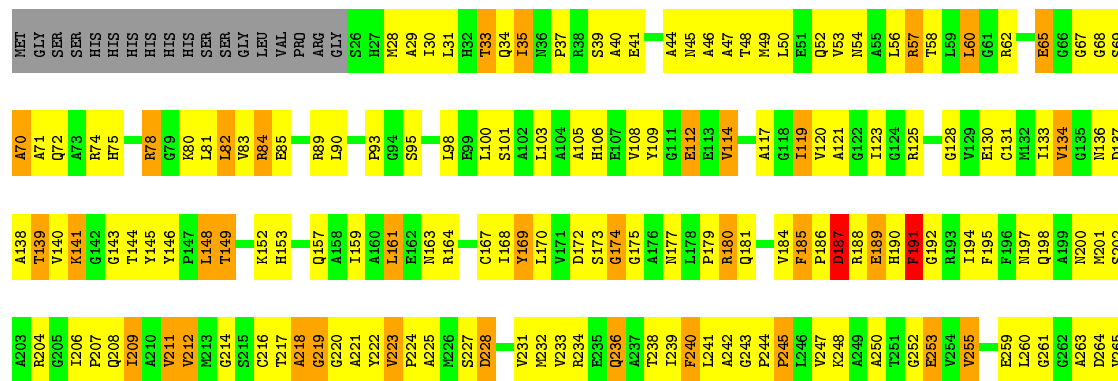
• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

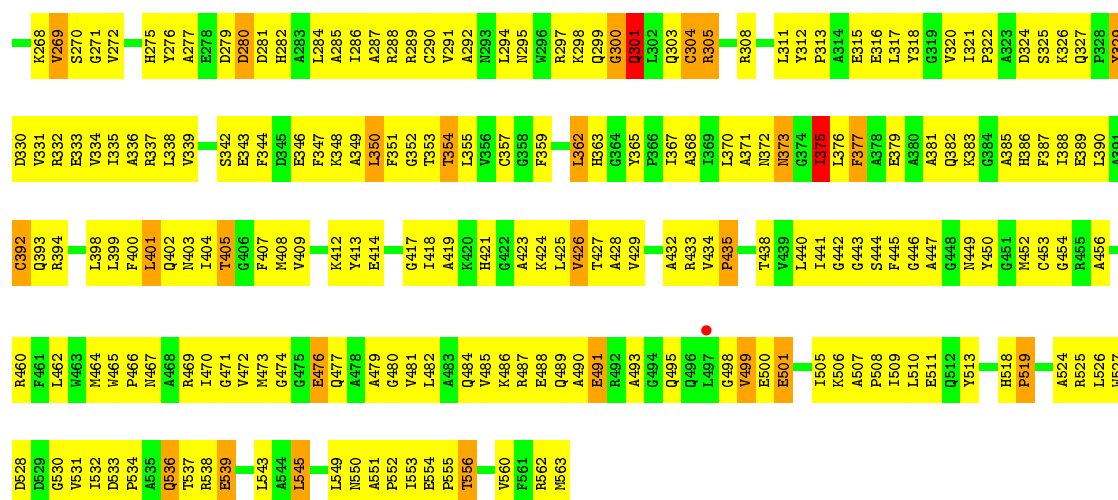
Chain D: 35% 50% 12%

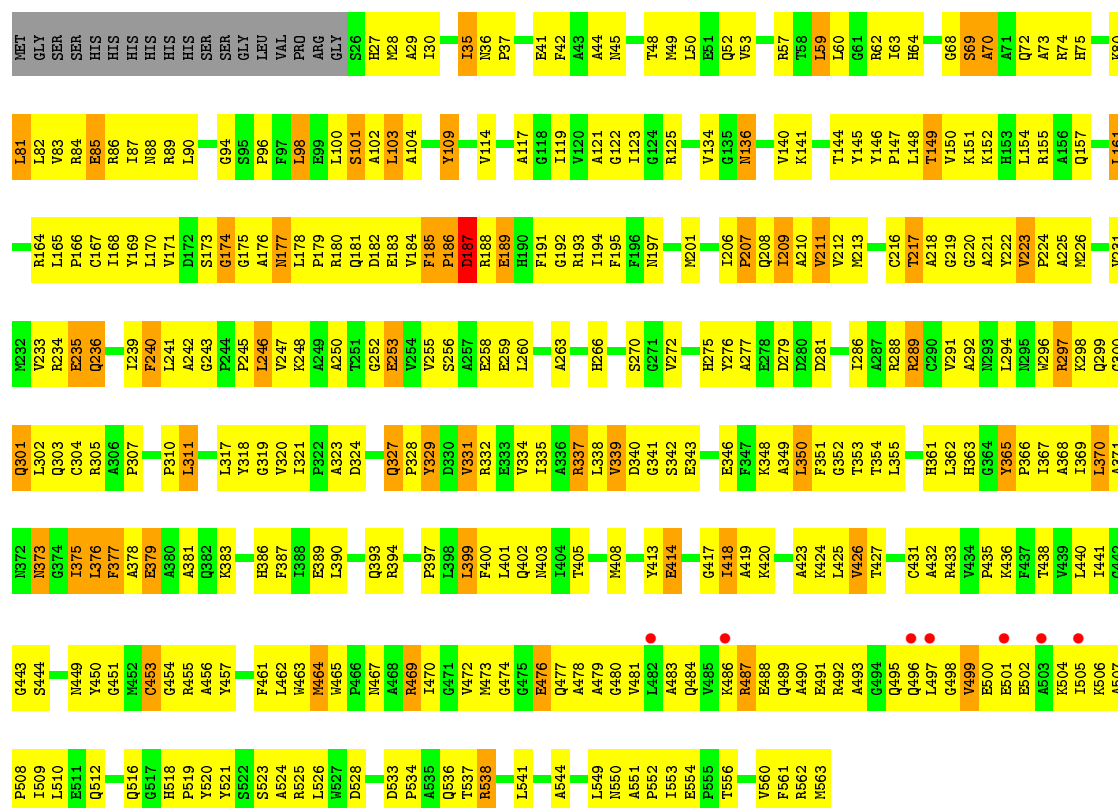


• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

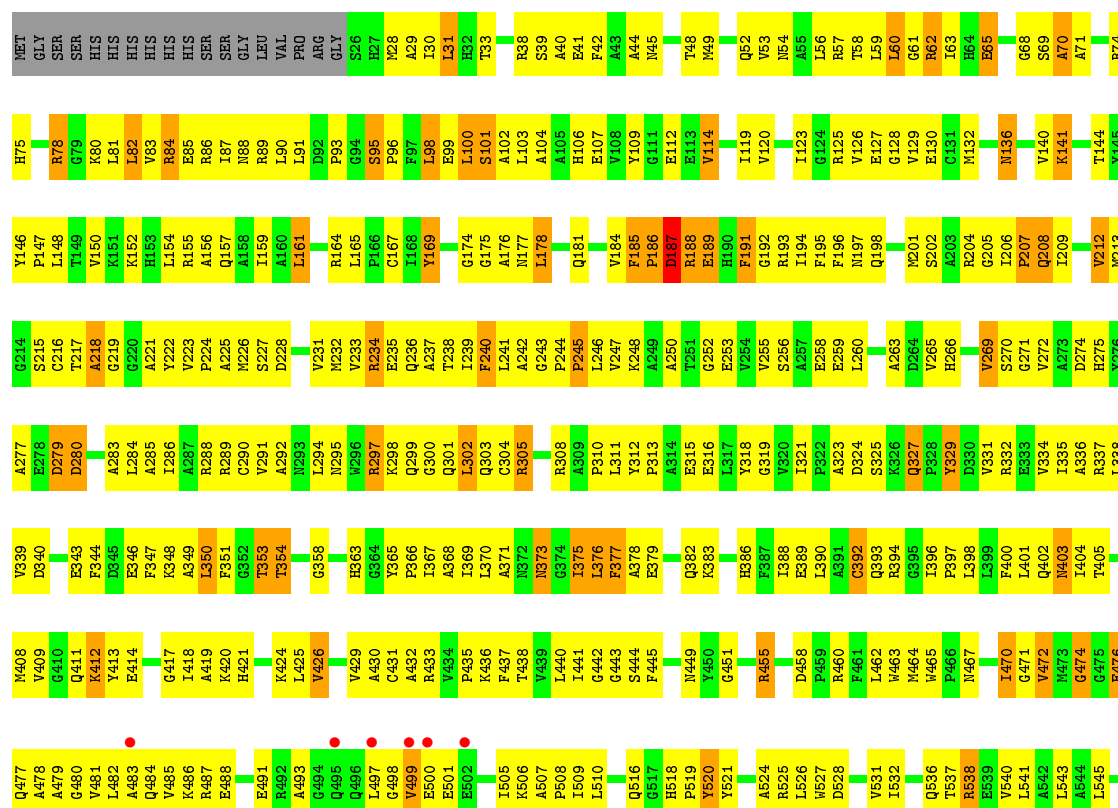
Chain F: 30% 55% 11%







• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit



L549	H550	A551	P552	I553	E554	P555	T556	A557	F558	G559	V560	R561	K562	H563
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.51Å 255.34Å 152.67Å 90.00° 95.74° 90.00°	Depositor
Resolution (Å)	48.90 – 3.50 48.90 – 3.28	Depositor EDS
% Data completeness (in resolution range)	83.0 (48.90-3.50) 76.9 (48.90-3.28)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 3.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.292 0.234 , 0.292	Depositor DCC
R_{free} test set	5256 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.971	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 134143 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	49939	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.68	0/4866	0.87	4/6581 (0.1%)
1	C	0.63	0/4362	0.86	3/5897 (0.1%)
1	E	0.65	1/4362 (0.0%)	0.85	3/5897 (0.1%)
1	G	0.65	0/4362	0.87	0/5897
1	I	0.66	0/3929	0.84	1/5315 (0.0%)
1	K	0.68	0/3921	0.85	2/5307 (0.0%)
2	B	0.67	0/4135	0.86	1/5605 (0.0%)
2	D	0.67	0/4135	0.86	3/5605 (0.1%)
2	F	0.64	0/4135	0.87	3/5605 (0.1%)
2	H	0.67	3/4135 (0.1%)	0.83	1/5605 (0.0%)
2	J	0.68	0/4135	0.87	2/5605 (0.0%)
2	L	0.67	0/4135	0.87	0/5605
All	All	0.66	4/50612 (0.0%)	0.86	23/68524 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	G	0	2
1	I	0	1
2	B	0	1
2	H	0	1
2	J	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	131	CYS	CB-SG	-7.11	1.70	1.82
1	E	563	CYS	CB-SG	5.92	1.92	1.82
2	H	189	GLU	CB-CG	5.11	1.61	1.52
2	H	189	GLU	CG-CD	5.11	1.59	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	399	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	E	506	GLU	N-CA-C	-6.63	93.10	111.00
1	C	506	GLU	N-CA-C	-6.45	93.60	111.00
1	E	566	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	298	LEU	CA-CB-CG	-5.94	101.63	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	698	TYR	Sidechain
2	B	109	TYR	Sidechain
1	E	129	TYR	Sidechain
1	G	129	TYR	Sidechain
1	G	588	TYR	Sidechain

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	4778	0	4730	583	0
1	C	4280	0	4227	535	0
1	E	4280	0	4227	519	0
1	G	4280	0	4227	516	0
1	I	3853	0	3795	477	0
1	K	3844	0	3786	485	0
2	B	4051	0	4023	401	0
2	D	4051	0	4023	425	0
2	F	4051	0	4023	437	0
2	H	4051	0	4023	422	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	4051	0	4023	425	0
2	L	4051	0	4023	419	0
3	A	15	0	15	3	0
3	I	15	0	15	4	0
4	B	48	0	32	4	0
4	D	48	0	32	3	0
4	F	48	0	32	3	0
4	H	48	0	32	6	0
4	J	48	0	32	4	0
4	L	48	0	32	2	0
All	All	49939	0	49352	5408	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 54.

The worst 5 of 5408 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:504:LEU:HB3	1:C:505:PRO:HD2	1.23	1.17
1:G:200:TYR:CE1	1:G:221:GLU:HA	1.82	1.15
1:G:278:ILE:H	1:G:278:ILE:HD12	1.10	1.14
1:K:101:ALA:HB1	1:K:429:PHE:CE1	1.83	1.14
2:F:231:VAL:HG22	2:F:275:HIS:HB2	1.18	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	613/655 (94%)	427 (70%)	114 (19%)	72 (12%)	0 7
1	C	546/655 (83%)	382 (70%)	113 (21%)	51 (9%)	1 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	546/655 (83%)	384 (70%)	109 (20%)	53 (10%)	1	10
1	G	546/655 (83%)	381 (70%)	113 (21%)	52 (10%)	1	10
1	I	493/655 (75%)	353 (72%)	101 (20%)	39 (8%)	1	14
1	K	493/655 (75%)	364 (74%)	88 (18%)	41 (8%)	1	13
2	B	535/555 (96%)	448 (84%)	63 (12%)	24 (4%)	3	30
2	D	535/555 (96%)	456 (85%)	62 (12%)	17 (3%)	5	40
2	F	535/555 (96%)	439 (82%)	73 (14%)	23 (4%)	3	31
2	H	535/555 (96%)	450 (84%)	60 (11%)	25 (5%)	3	29
2	J	535/555 (96%)	452 (84%)	65 (12%)	18 (3%)	5	39
2	L	535/555 (96%)	438 (82%)	76 (14%)	21 (4%)	4	34
All	All	6447/7260 (89%)	4974 (77%)	1037 (16%)	436 (7%)	1	19

5 of 436 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	225	ALA
1	A	230	SER
1	A	294	LEU
1	A	366	GLU

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 X-ray entries followed by that with respect to entries of similar resolution.

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	477/496 (96%)	384 (80%)	93 (20%)	2	10
1	C	423/496 (85%)	336 (79%)	87 (21%)	1	8
1	E	423/496 (85%)	330 (78%)	93 (22%)	1	7
1	G	423/496 (85%)	329 (78%)	94 (22%)	1	6
1	I	382/496 (77%)	305 (80%)	77 (20%)	1	9
1	K	381/496 (77%)	300 (79%)	81 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	401/418 (96%)	341 (85%)	60 (15%)	3	21
2	D	401/418 (96%)	340 (85%)	61 (15%)	3	21
2	F	401/418 (96%)	339 (84%)	62 (16%)	3	20
2	H	401/418 (96%)	338 (84%)	63 (16%)	3	19
2	J	401/418 (96%)	354 (88%)	47 (12%)	7	32
2	L	401/418 (96%)	341 (85%)	60 (15%)	3	21
All	All	4915/5484 (90%)	4037 (82%)	878 (18%)	2	13

5 of 878 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	57	ARG
1	G	250	LEU
1	K	606	THR
2	F	119	ILE
2	F	435	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	236	GLN
1	G	372	GLN
2	L	157	GLN
2	F	293	ASN
2	F	467	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 carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	BTI	A	801	1	14,16,16	1.89	1 (7%)	13,21,21	3.27	5 (38%)
4	COA	B	591	-	40,50,50	0.84	1 (2%)	50,75,75	1.74	4 (8%)
4	COA	D	591	-	40,50,50	0.84	1 (2%)	50,75,75	1.78	5 (10%)
4	COA	F	591	-	40,50,50	0.85	1 (2%)	50,75,75	1.86	5 (10%)
4	COA	H	591	-	40,50,50	0.85	1 (2%)	50,75,75	1.78	6 (12%)
3	BTI	I	801	1	14,16,16	1.88	1 (7%)	13,21,21	3.26	6 (46%)
4	COA	J	591	-	40,50,50	0.85	1 (2%)	50,75,75	1.79	4 (8%)
4	COA	L	591	-	40,50,50	0.84	0	50,75,75	1.92	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BTI	A	801	1	-	0/5/27/27	0/2/2/2
4	COA	B	591	-	-	0/44/64/64	0/3/3/3
4	COA	D	591	-	-	0/44/64/64	0/3/3/3
4	COA	F	591	-	-	0/44/64/64	0/3/3/3
4	COA	H	591	-	-	0/44/64/64	0/3/3/3
3	BTI	I	801	1	-	0/5/27/27	0/2/2/2
4	COA	J	591	-	-	0/44/64/64	0/3/3/3
4	COA	L	591	-	-	0/44/64/64	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	591	COA	O4B-C1B	2.00	1.43	1.41
4	B	591	COA	O4B-C1B	2.08	1.43	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	591	COA	O4B-C1B	2.13	1.43	1.41
4	J	591	COA	O4B-C1B	2.17	1.43	1.41
4	F	591	COA	O4B-C1B	2.17	1.43	1.41

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	591	COA	N3A-C2A-N1A	-9.84	121.36	128.89
4	J	591	COA	N3A-C2A-N1A	-9.55	121.58	128.89
4	L	591	COA	N3A-C2A-N1A	-9.49	121.62	128.89
4	B	591	COA	N3A-C2A-N1A	-9.41	121.69	128.89
4	F	591	COA	N3A-C2A-N1A	-9.30	121.77	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	BTI	3	0
4	B	591	COA	4	0
4	D	591	COA	3	0
4	F	591	COA	3	0
4	H	591	COA	6	0
3	I	801	BTI	4	0
4	J	591	COA	4	0
4	L	591	COA	2	0

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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	621/655 (94%)	0.14	34 (5%) 29 22	71, 115, 170, 200	0
1	C	552/655 (84%)	-0.01	7 (1%) 79 70	69, 113, 154, 187	0
1	E	552/655 (84%)	-0.02	4 (0%) 89 82	71, 113, 154, 189	0
1	G	552/655 (84%)	-0.02	4 (0%) 89 82	76, 112, 155, 187	0
1	I	498/655 (76%)	0.01	5 (1%) 84 76	73, 113, 146, 193	0
1	K	497/655 (75%)	0.07	10 (2%) 68 59	65, 115, 146, 187	0
2	B	537/555 (96%)	-0.36	0 100 100	60, 87, 140, 169	0
2	D	537/555 (96%)	-0.30	2 (0%) 93 90	58, 89, 143, 171	0
2	F	537/555 (96%)	-0.33	1 (0%) 95 93	58, 88, 142, 167	0
2	H	537/555 (96%)	-0.32	0 100 100	59, 88, 138, 169	0
2	J	537/555 (96%)	-0.18	7 (1%) 79 70	55, 88, 142, 168	0
2	L	537/555 (96%)	-0.26	6 (1%) 82 73	57, 88, 139, 167	0
All	All	6494/7260 (89%)	-0.13	80 (1%) 81 72	55, 103, 153, 200	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	647	GLY	6.3
1	A	648	GLY	5.0
1	A	715	ASP	4.5
1	C	391	PRO	4.4
2	L	497	LEU	4.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BTI	A	801	15/15	0.84	0.50	4.58	140,152,154,155	0
3	BTI	I	801	15/15	0.84	0.43	3.21	142,152,155,158	0
4	COA	L	591	48/48	0.91	0.29	0.83	98,125,132,135	0
4	COA	F	591	48/48	0.89	0.28	0.49	97,124,134,135	0
4	COA	B	591	48/48	0.89	0.24	-0.07	103,129,139,142	0
4	COA	D	591	48/48	0.88	0.28	-0.18	102,129,142,145	0
4	COA	H	591	48/48	0.93	0.22	-0.30	102,128,137,139	0
4	COA	J	591	48/48	0.91	0.21	-0.64	101,127,136,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.