



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 03:44 PM EST

PDB ID : 4V6H  
Title : Crystal structure of succinate-semialdehyde dehydrogenase from Burkholderia pseudomallei  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : unknown  
Resolution : 2.70 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

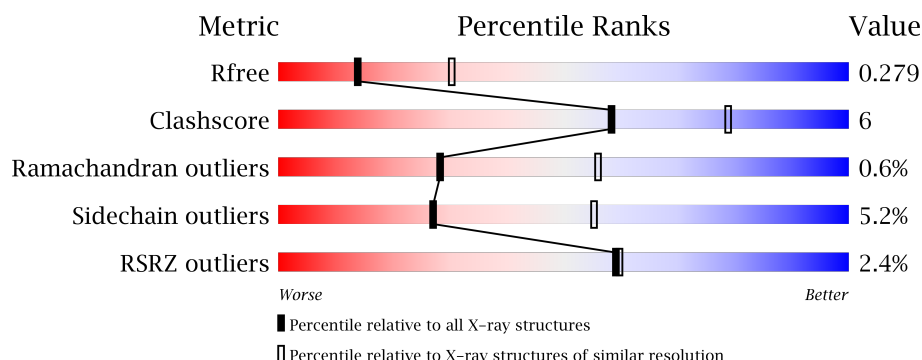
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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  $\geq 3$ , 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	1	484	<div> <div>11%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	2	484	<div> <div>%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	3	484	<div> <div>%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	4	484	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	5	484	<div> <div>%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	6	484	 89% 11%
1	A	484	 87% 11% .
1	B	484	 89% 10% .
1	C	484	 85% 13% .
1	D	484	 84% 15% .
1	E	484	 85% 13% .
1	F	484	 87% 11% .
1	G	484	 86% 12% .
1	H	484	 86% 13% .
1	I	484	 6% 80% 18% .
1	J	484	 83% 15% .
1	K	484	 % 88% 11% .
1	L	484	 86% 12% .
1	M	484	 83% 14% .
1	N	484	 87% 12% .
1	O	484	 87% 12% .
1	P	484	 87% 12% .
1	Q	484	 4% 83% 16% .
1	R	484	 3% 85% 13% .
1	S	484	 87% 12% .
1	T	484	 4% 82% 16% .
1	U	484	 12% 78% 20% .
1	V	484	 5% 82% 16% .
1	W	484	 88% 11%
1	X	484	 11% 78% 20% .

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Mol	Chain	Length	Quality of chain
1	Y	484	<div><div></div><div>3%</div><div>78%</div><div>20%</div><div></div></div>
1	Z	484	<div><div></div><div>11%</div><div>75%</div><div>24%</div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 114732 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 Succinate-semialdehyde dehydrogenase (NADP+).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	B	482	Total	C	N	O	S	0	0	0
			3553	2261	607	671	14			
1	C	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	D	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	E	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	F	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	G	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	H	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	I	482	Total	C	N	O	S	0	0	0
			3520	2242	597	667	14			
1	J	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	K	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	L	482	Total	C	N	O	S	0	0	0
			3543	2255	607	667	14			
1	M	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	N	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	O	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	P	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	R	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	S	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	T	482	Total	C	N	O	S	0	0	0
			3535	2248	606	667	14			
1	U	482	Total	C	N	O	S	0	0	0
			3521	2241	601	665	14			
1	V	482	Total	C	N	O	S	0	0	0
			3532	2248	603	667	14			
1	W	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	X	482	Total	C	N	O	S	0	0	0
			3515	2235	603	663	14			
1	Y	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	Z	482	Total	C	N	O	S	0	0	0
			3532	2248	603	667	14			
1	1	482	Total	C	N	O	S	0	0	0
			3510	2235	595	666	14			
1	2	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	3	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	4	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	5	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	6	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
A	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
A	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
A	4	SER	-	EXPRESSION TAG	UNP Q3JS51
B	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
B	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
B	3	GLY	-	EXPRESSION TAG	UNP Q3JS51

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	EXPRESSION TAG	UNP Q3JS51
C	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
C	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
C	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
C	4	SER	-	EXPRESSION TAG	UNP Q3JS51
D	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
D	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
D	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
D	4	SER	-	EXPRESSION TAG	UNP Q3JS51
E	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
E	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
E	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
E	4	SER	-	EXPRESSION TAG	UNP Q3JS51
F	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
F	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
F	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
F	4	SER	-	EXPRESSION TAG	UNP Q3JS51
G	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
G	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
G	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
G	4	SER	-	EXPRESSION TAG	UNP Q3JS51
H	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
H	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
H	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
H	4	SER	-	EXPRESSION TAG	UNP Q3JS51
I	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
I	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
I	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
I	4	SER	-	EXPRESSION TAG	UNP Q3JS51
J	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
J	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
J	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
J	4	SER	-	EXPRESSION TAG	UNP Q3JS51
K	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
K	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
K	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
K	4	SER	-	EXPRESSION TAG	UNP Q3JS51
L	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
L	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
L	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
L	4	SER	-	EXPRESSION TAG	UNP Q3JS51
M	1	GLY	-	EXPRESSION TAG	UNP Q3JS51

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Chain	Residue	Modelled	Actual	Comment	Reference
M	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
M	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
M	4	SER	-	EXPRESSION TAG	UNP Q3JS51
N	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
N	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
N	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
N	4	SER	-	EXPRESSION TAG	UNP Q3JS51
O	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
O	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
O	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
O	4	SER	-	EXPRESSION TAG	UNP Q3JS51
P	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
P	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
P	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
P	4	SER	-	EXPRESSION TAG	UNP Q3JS51
Q	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
Q	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
Q	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
Q	4	SER	-	EXPRESSION TAG	UNP Q3JS51
R	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
R	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
R	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
R	4	SER	-	EXPRESSION TAG	UNP Q3JS51
S	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
S	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
S	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
S	4	SER	-	EXPRESSION TAG	UNP Q3JS51
T	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
T	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
T	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
T	4	SER	-	EXPRESSION TAG	UNP Q3JS51
U	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
U	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
U	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
U	4	SER	-	EXPRESSION TAG	UNP Q3JS51
V	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
V	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
V	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
V	4	SER	-	EXPRESSION TAG	UNP Q3JS51
W	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
W	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
W	3	GLY	-	EXPRESSION TAG	UNP Q3JS51

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Chain	Residue	Modelled	Actual	Comment	Reference
W	4	SER	-	EXPRESSION TAG	UNP Q3JS51
X	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
X	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
X	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
X	4	SER	-	EXPRESSION TAG	UNP Q3JS51
Y	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
Y	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
Y	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
Y	4	SER	-	EXPRESSION TAG	UNP Q3JS51
Z	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
Z	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
Z	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
Z	4	SER	-	EXPRESSION TAG	UNP Q3JS51
1	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
1	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
1	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
1	4	SER	-	EXPRESSION TAG	UNP Q3JS51
2	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
2	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
2	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
2	4	SER	-	EXPRESSION TAG	UNP Q3JS51
3	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
3	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
3	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
3	4	SER	-	EXPRESSION TAG	UNP Q3JS51
4	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
4	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
4	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
4	4	SER	-	EXPRESSION TAG	UNP Q3JS51
5	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
5	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
5	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
5	4	SER	-	EXPRESSION TAG	UNP Q3JS51
6	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
6	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
6	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
6	4	SER	-	EXPRESSION TAG	UNP Q3JS51

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	46	Total O 46 46	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	59	Total O 59 59	0	0
2	C	56	Total O 56 56	0	0
2	D	60	Total O 60 60	0	0
2	E	72	Total O 72 72	0	0
2	F	75	Total O 75 75	0	0
2	G	66	Total O 66 66	0	0
2	H	58	Total O 58 58	0	0
2	I	24	Total O 24 24	0	0
2	J	35	Total O 35 35	0	0
2	K	55	Total O 55 55	0	0
2	L	57	Total O 57 57	0	0
2	M	40	Total O 40 40	0	0
2	N	46	Total O 46 46	0	0
2	O	39	Total O 39 39	0	0
2	P	74	Total O 74 74	0	0
2	Q	22	Total O 22 22	0	0
2	R	35	Total O 35 35	0	0
2	S	55	Total O 55 55	0	0
2	T	13	Total O 13 13	0	0
2	U	13	Total O 13 13	0	0
2	V	29	Total O 29 29	0	0

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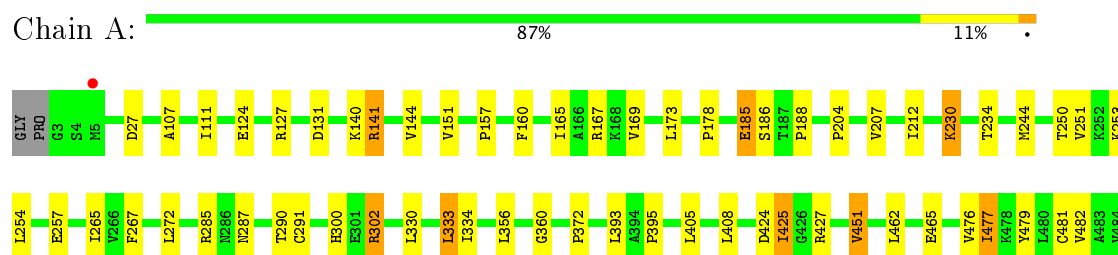
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	W	44	Total 44	O 44	0	0
2	X	8	Total 8	O 8	0	0
2	Y	36	Total 36	O 36	0	0
2	Z	20	Total 20	O 20	0	0
2	1	28	Total 28	O 28	0	0
2	2	37	Total 37	O 37	0	0
2	3	45	Total 45	O 45	0	0
2	4	46	Total 46	O 46	0	0
2	5	54	Total 54	O 54	0	0
2	6	57	Total 57	O 57	0	0

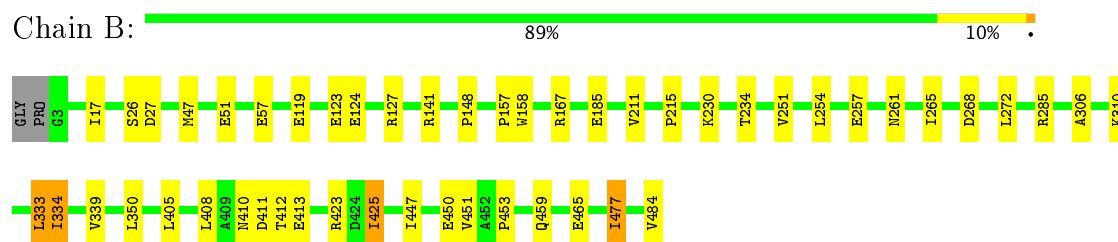
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

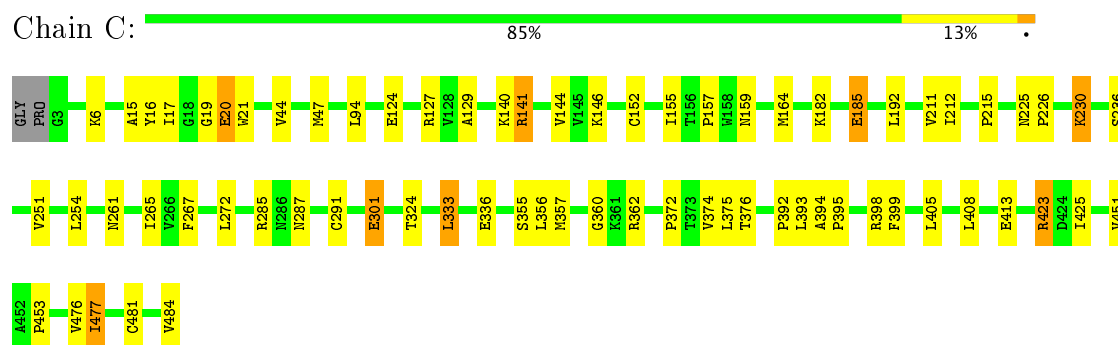
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



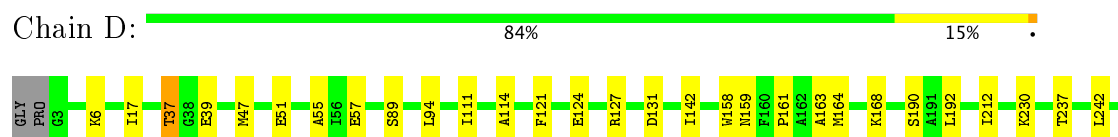
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

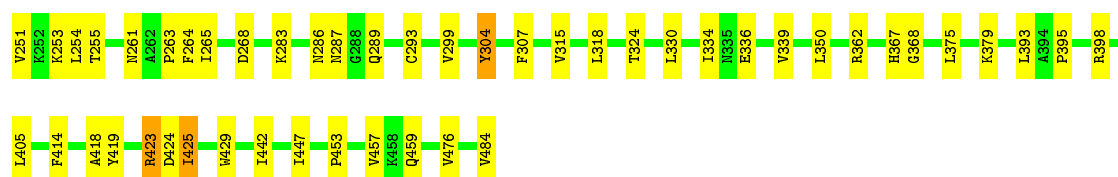


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



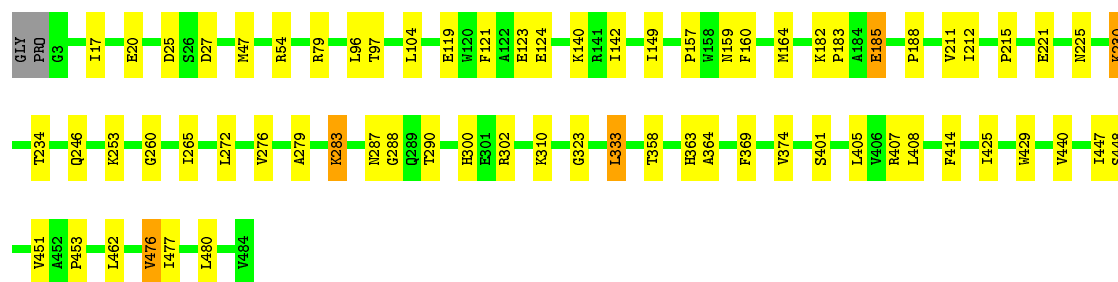
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)





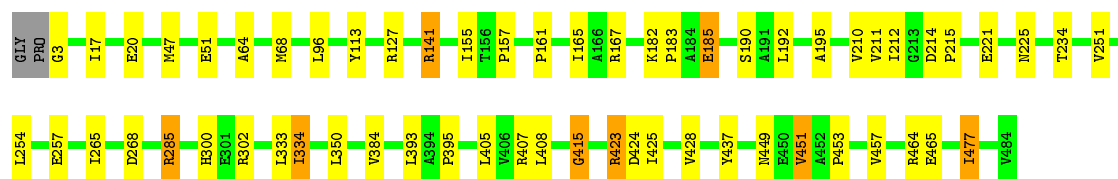
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain E: 85% 13%



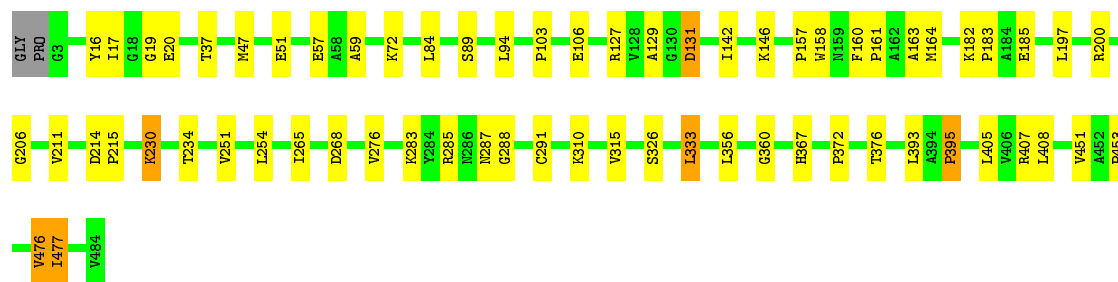
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain F: 87% 11%



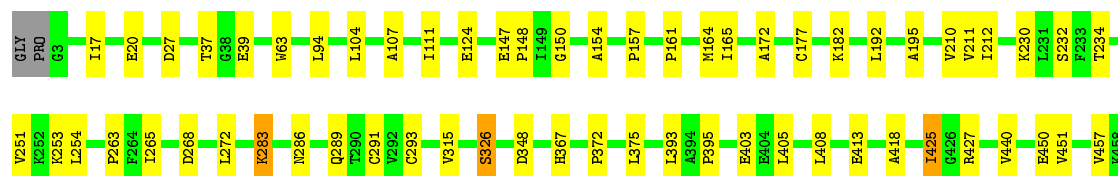
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain G: 86% 12%



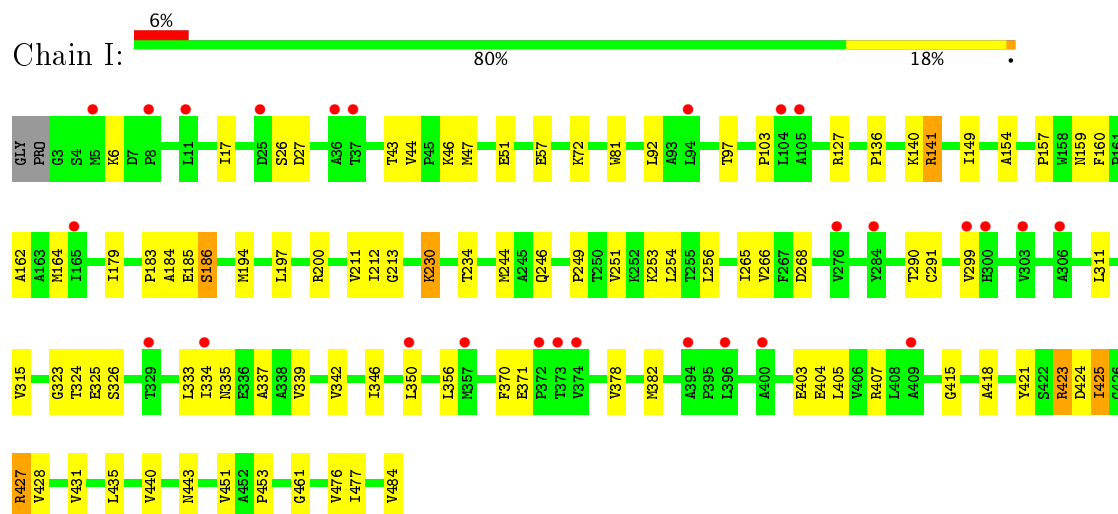
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain H: 86% 13%

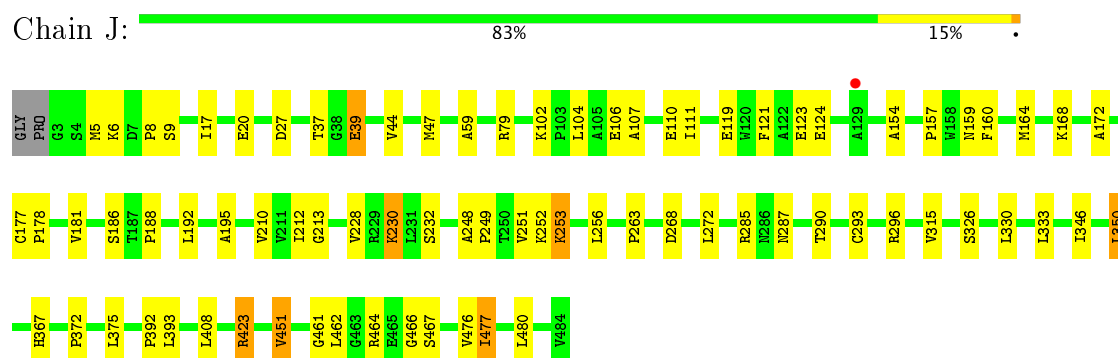




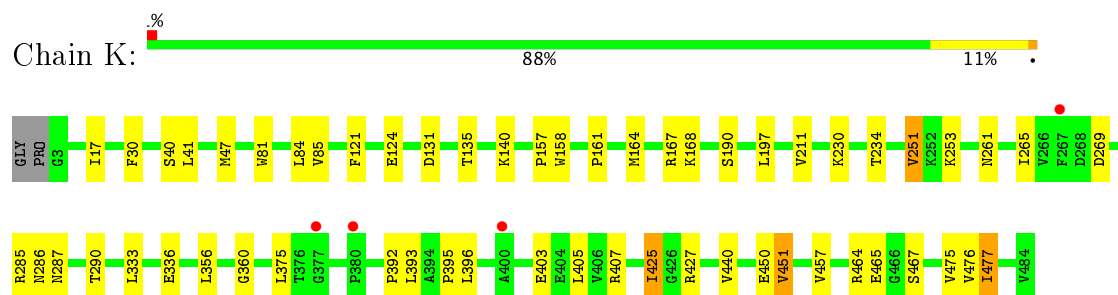
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



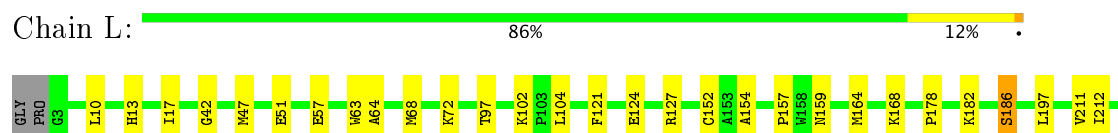
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

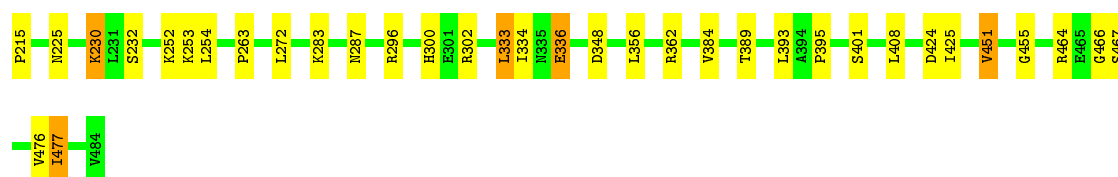


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



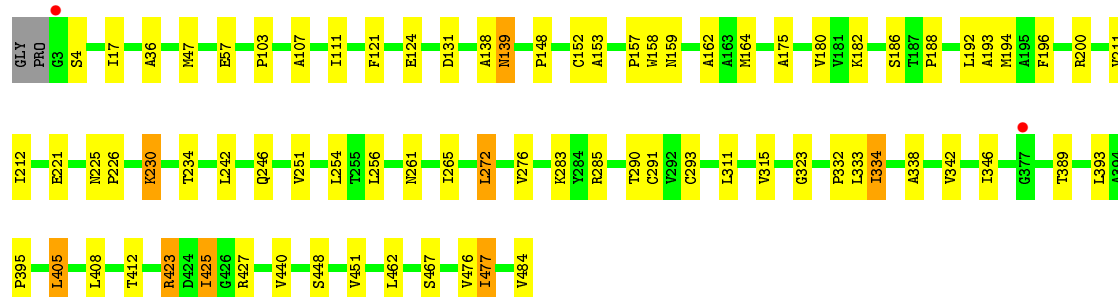
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)





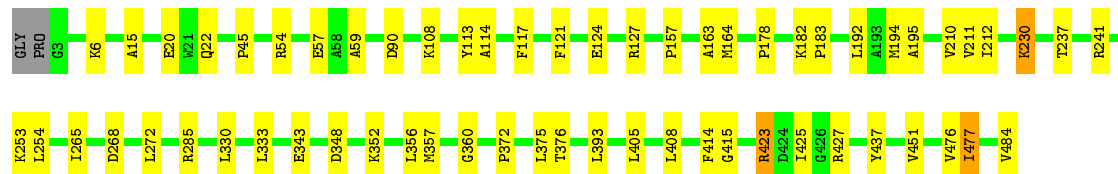
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain M: 83% 14%



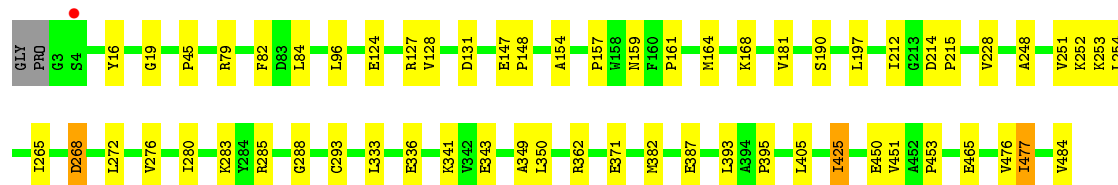
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain N: 87% 12%



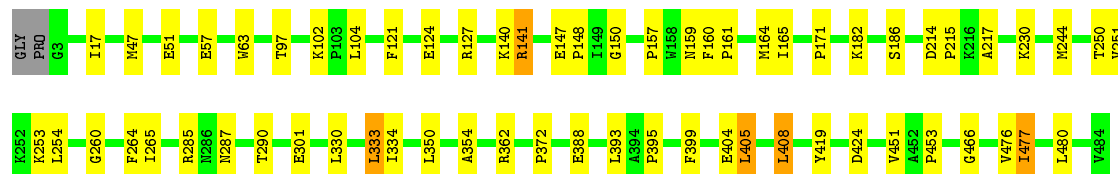
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain O: 87% 12%

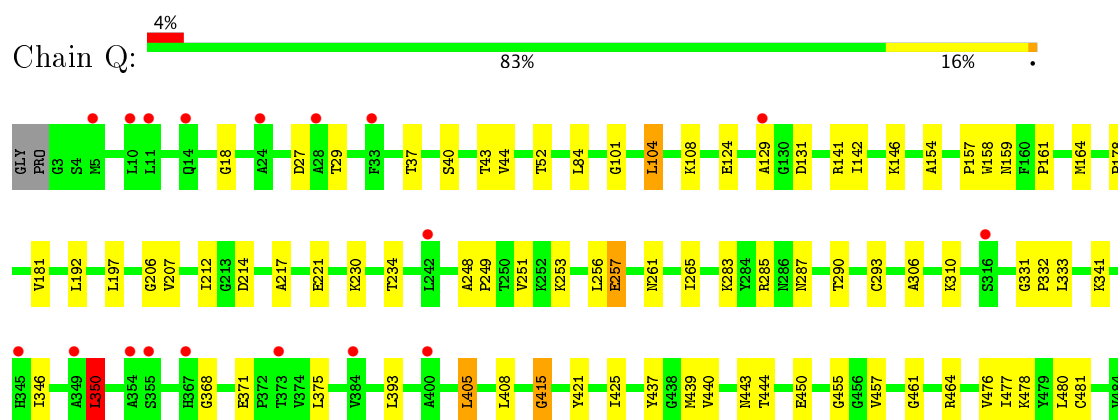


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

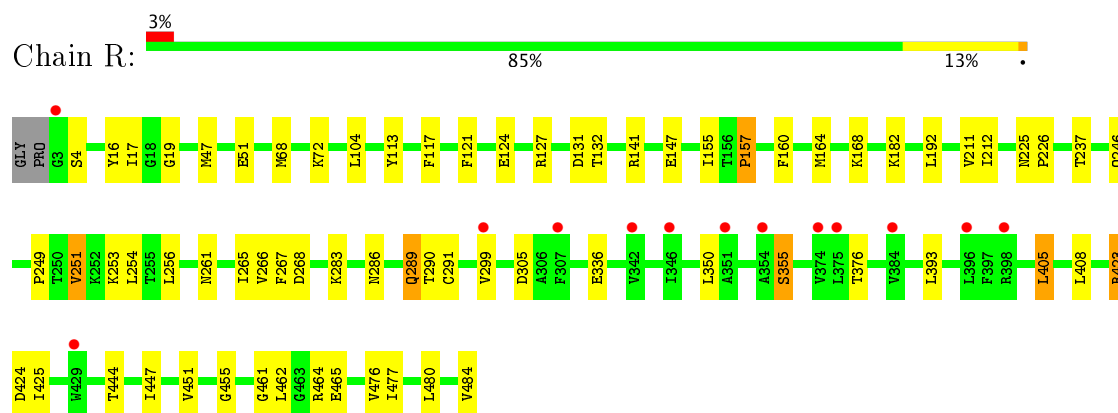
Chain P: 87% 12%



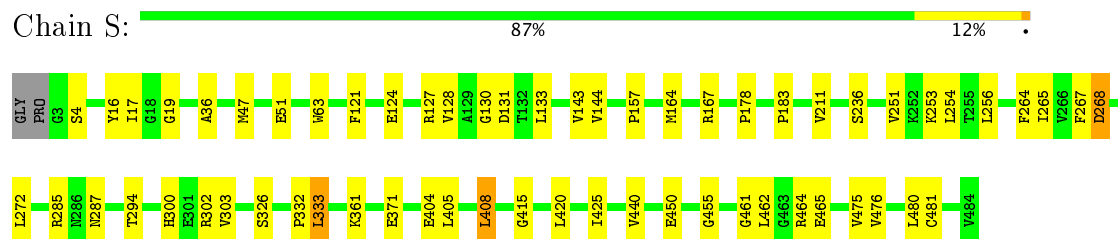
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



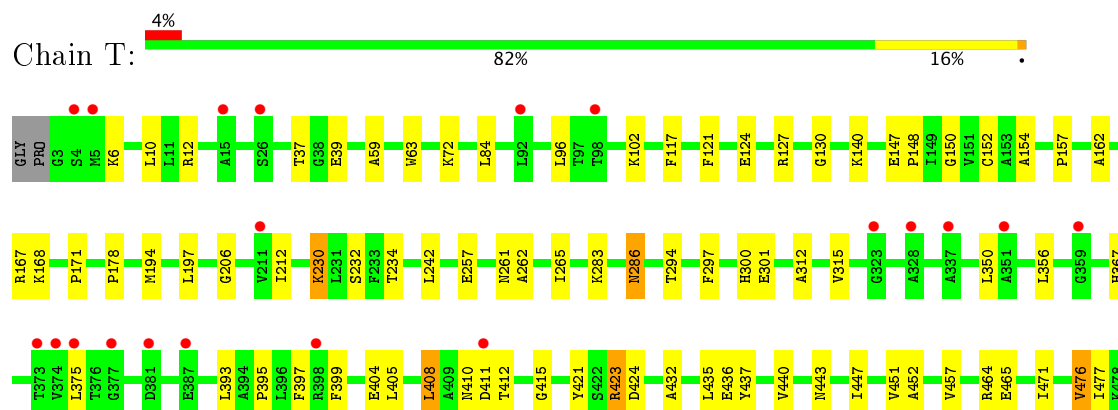
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

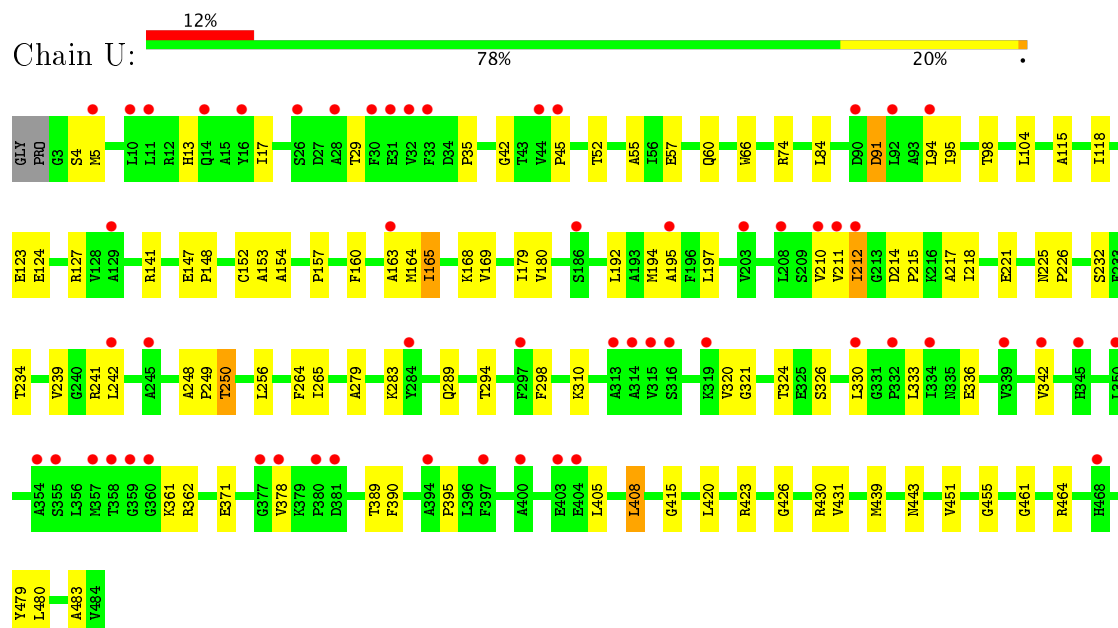


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

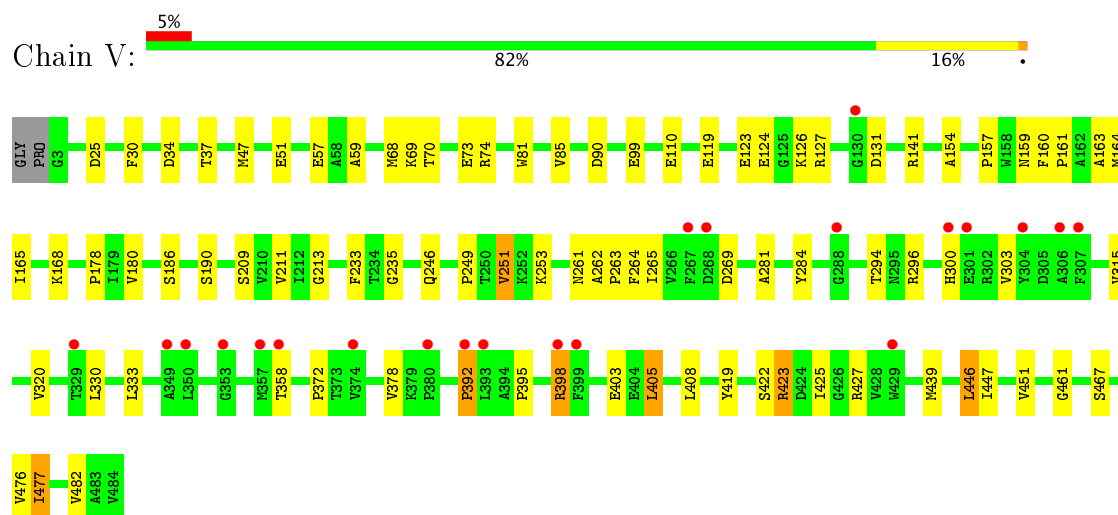




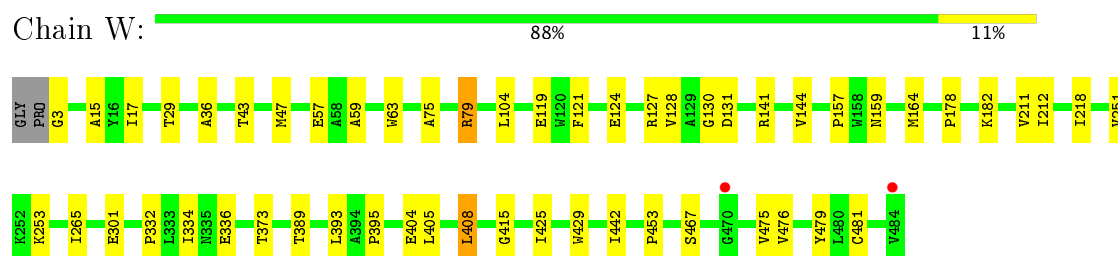
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



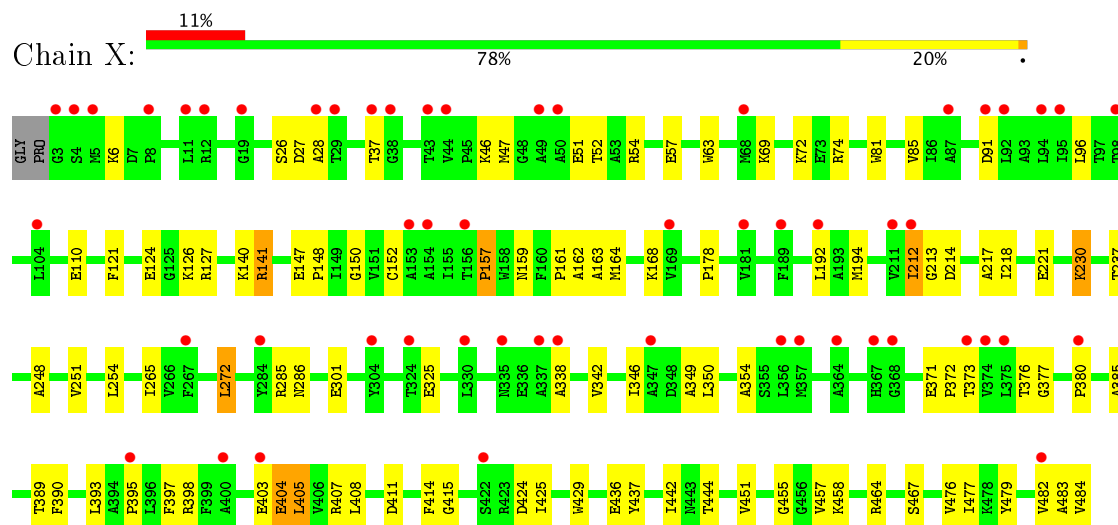
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



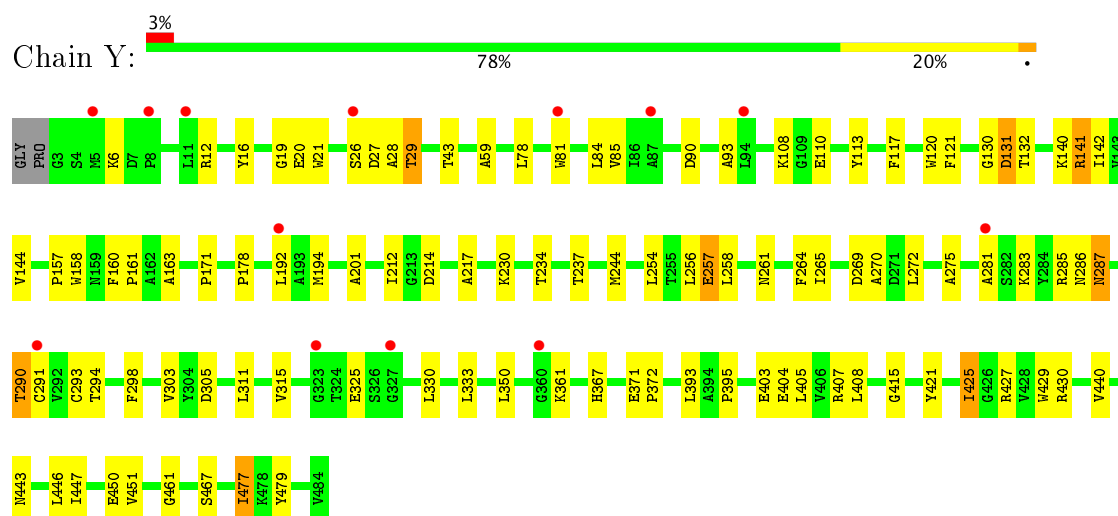
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



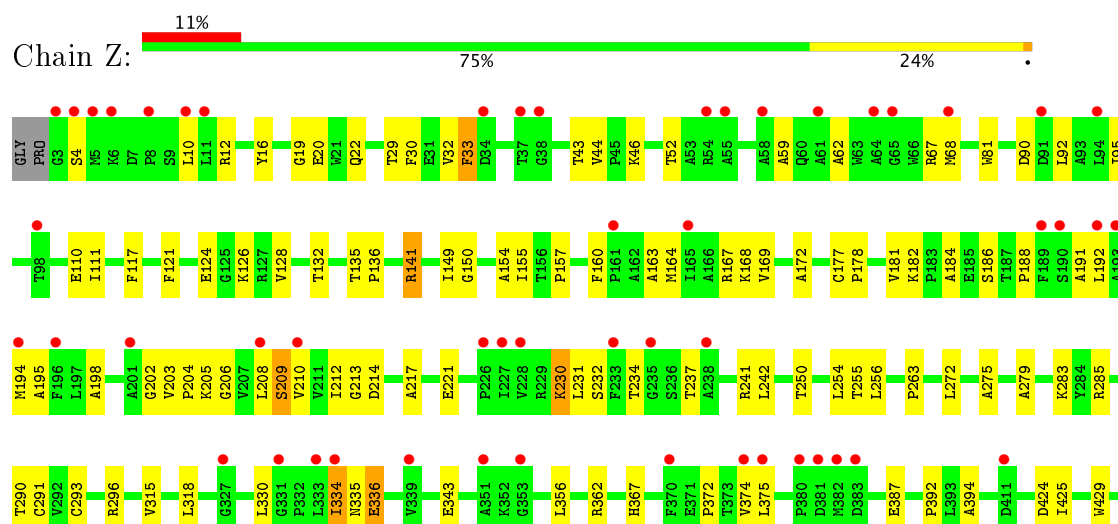
● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

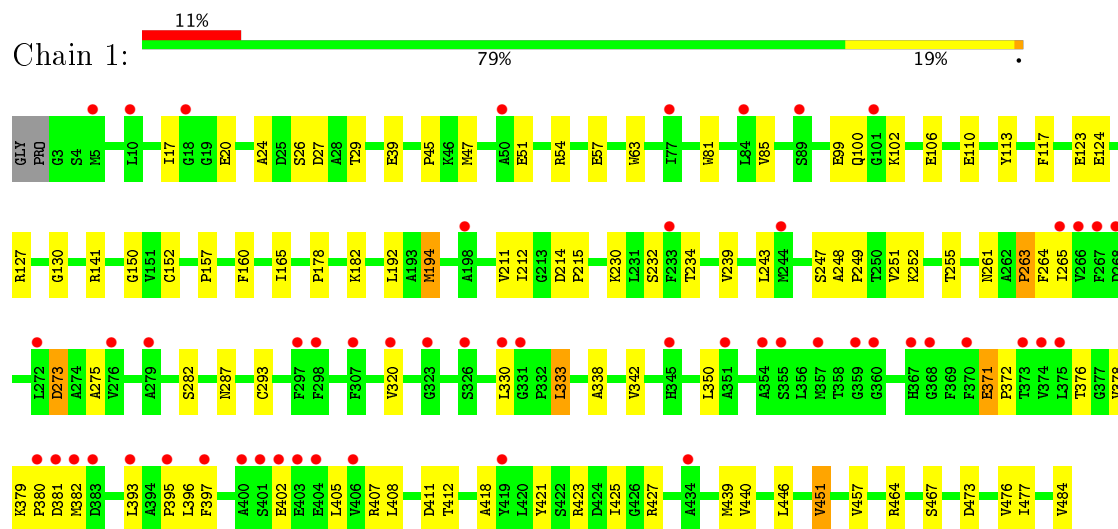


● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

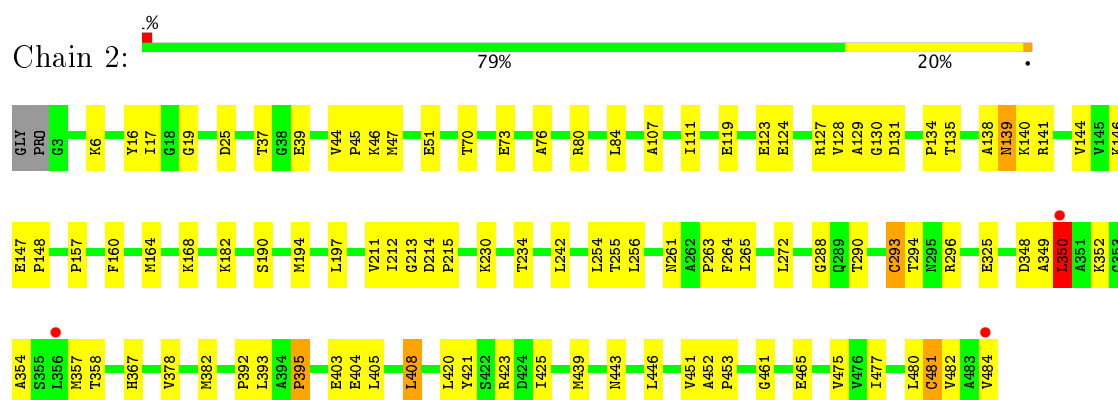




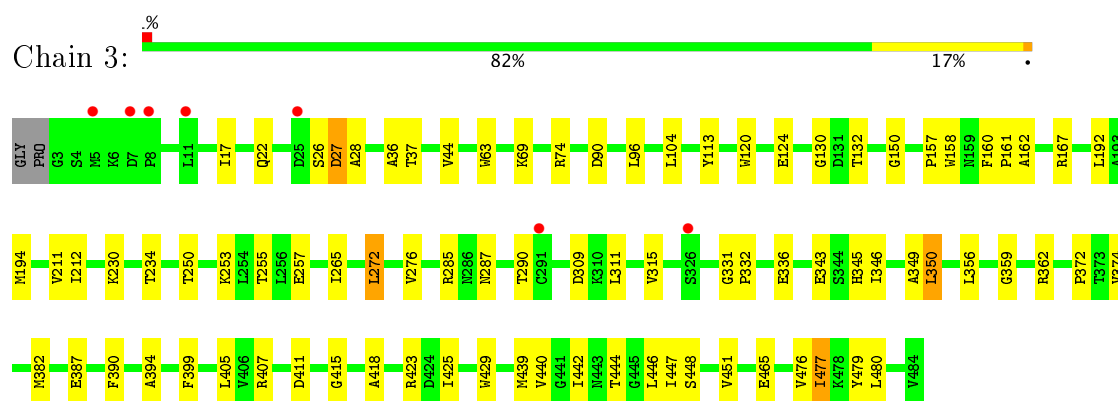
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



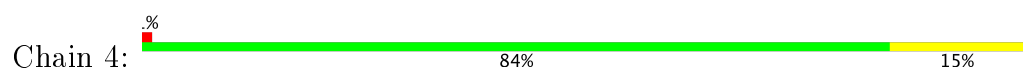
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

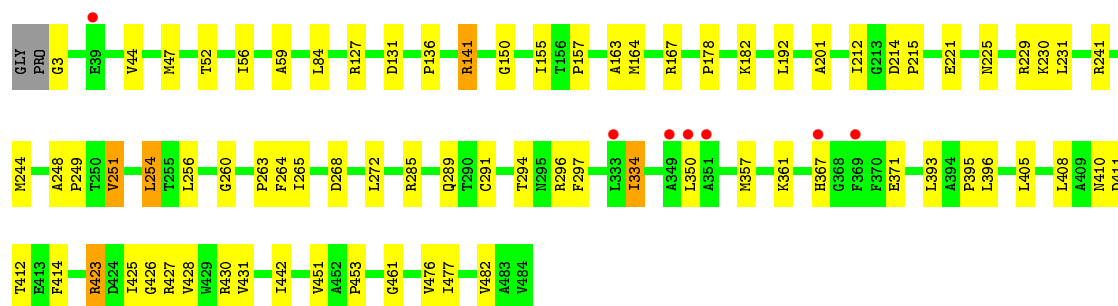


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

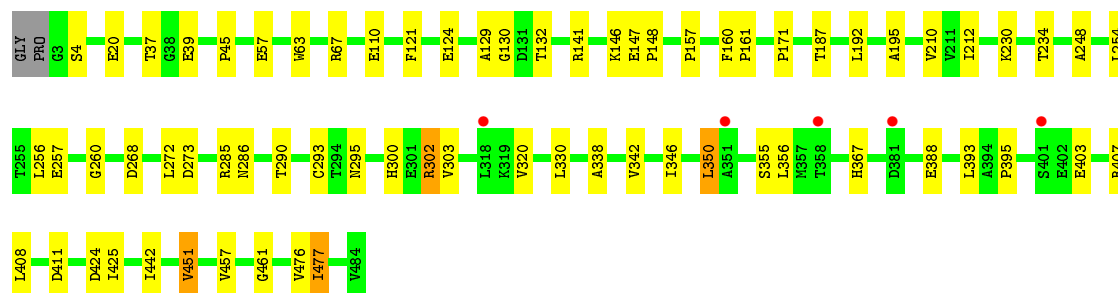
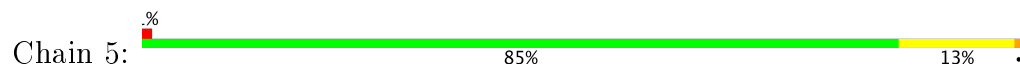


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

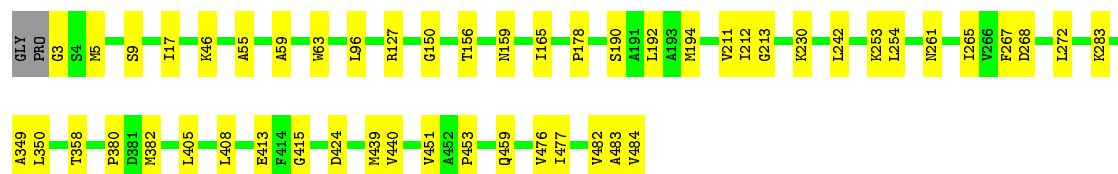
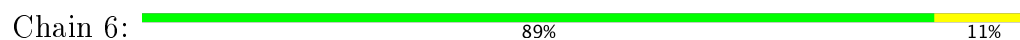




- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.66Å 164.87Å 278.90Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	49.47 – 2.70 49.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.47-2.70) 98.3 (49.47-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.236 , 0.282 0.235 , 0.279	Depositor DCC
$R_{free}$ test set	22724 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	114732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.06 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8625e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.48	0/3584	0.56	0/4884
1	2	0.41	0/3619	0.56	1/4925 (0.0%)
1	3	0.42	0/3619	0.56	0/4925
1	4	0.41	0/3619	0.55	0/4925
1	5	0.41	0/3619	0.56	0/4925
1	6	0.41	0/3619	0.56	0/4925
1	A	0.39	0/3623	0.55	0/4930
1	B	0.40	0/3627	0.55	0/4935
1	C	0.41	0/3623	0.56	0/4930
1	D	0.41	0/3623	0.56	0/4930
1	E	0.40	0/3623	0.56	0/4930
1	F	0.41	0/3623	0.55	0/4930
1	G	0.41	0/3623	0.56	0/4930
1	H	0.41	0/3623	0.56	0/4930
1	I	0.44	0/3594	0.54	0/4896
1	J	0.41	0/3623	0.55	0/4930
1	K	0.41	0/3619	0.53	0/4925
1	L	0.40	0/3617	0.56	0/4922
1	M	0.41	0/3619	0.54	0/4925
1	N	0.39	0/3619	0.53	0/4925
1	O	0.41	0/3619	0.54	0/4925
1	P	0.39	0/3619	0.55	0/4925
1	Q	0.43	0/3619	0.54	1/4925 (0.0%)
1	R	0.41	0/3619	0.54	0/4925
1	S	0.39	0/3619	0.54	0/4925
1	T	0.43	0/3609	0.53	0/4913
1	U	0.47	0/3594	0.54	0/4894
1	V	0.44	0/3606	0.55	0/4910
1	W	0.42	0/3619	0.54	0/4925
1	X	0.47	0/3588	0.55	0/4885
1	Y	0.43	0/3619	0.57	0/4925
1	Z	0.46	0/3606	0.56	0/4910
All	All	0.42	0/115694	0.55	2/157464 (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	6	0	1
1	U	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	350	LEU	CA-CB-CG	7.05	131.51	115.30
1	Q	350	LEU	CA-CB-CG	5.35	127.60	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	6	267	PHE	Peptide
1	U	4	SER	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	1	3510	0	3426	54	0
1	2	3545	0	3503	61	0
1	3	3545	0	3503	52	0
1	4	3545	0	3503	44	0
1	5	3545	0	3503	40	0
1	6	3545	0	3503	21	0
1	A	3549	0	3507	37	0
1	B	3553	0	3511	34	0
1	C	3549	0	3507	41	0
1	D	3549	0	3507	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3549	0	3507	44	0
1	F	3549	0	3507	47	0
1	G	3549	0	3507	36	0
1	H	3549	0	3507	38	0
1	I	3520	0	3450	49	0
1	J	3549	0	3507	50	0
1	K	3545	0	3503	34	0
1	L	3543	0	3496	34	0
1	M	3545	0	3503	46	0
1	N	3545	0	3503	26	0
1	O	3545	0	3503	28	0
1	P	3545	0	3503	38	0
1	Q	3545	0	3503	46	0
1	R	3545	0	3503	33	0
1	S	3545	0	3503	38	0
1	T	3535	0	3474	51	0
1	U	3521	0	3463	50	0
1	V	3532	0	3472	47	0
1	W	3545	0	3503	37	0
1	X	3515	0	3438	62	0
1	Y	3545	0	3503	66	0
1	Z	3532	0	3472	77	0
2	1	28	0	0	0	0
2	2	37	0	0	2	0
2	3	45	0	0	1	0
2	4	46	0	0	2	0
2	5	54	0	0	1	0
2	6	57	0	0	1	0
2	A	46	0	0	0	0
2	B	59	0	0	1	0
2	C	56	0	0	1	0
2	D	60	0	0	3	0
2	E	72	0	0	2	0
2	F	75	0	0	4	0
2	G	66	0	0	1	0
2	H	58	0	0	1	0
2	I	24	0	0	1	0
2	J	35	0	0	2	0
2	K	55	0	0	2	0
2	L	57	0	0	2	0
2	M	40	0	0	1	0
2	N	46	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	39	0	0	0	0
2	P	74	0	0	1	0
2	Q	22	0	0	0	0
2	R	35	0	0	0	0
2	S	55	0	0	1	0
2	T	13	0	0	0	0
2	U	13	0	0	1	0
2	V	29	0	0	1	0
2	W	44	0	0	1	0
2	X	8	0	0	0	0
2	Y	36	0	0	2	0
2	Z	20	0	0	5	0
All	All	114732	0	111803	1241	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 6.

The worst 5 of 1241 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:D:242:LEU:HD22	1:1:26:SER:HA	1.18	1.18
1:4:476:VAL:HG21	1:5:457:VAL:HG12	1.36	1.04
1:Z:192:LEU:HD11	1:Z:212:ILE:HD11	1.39	1.02
1:X:237:THR:HG1	1:X:414:PHE:HE1	1.09	0.97
1:H:265:ILE:HG21	1:H:405:LEU:HD21	1.51	0.91

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	1	480/484 (99%)	441 (92%)	33 (7%)	6 (1%)	14	35
1	2	480/484 (99%)	443 (92%)	31 (6%)	6 (1%)	14	35
1	3	480/484 (99%)	451 (94%)	27 (6%)	2 (0%)	38	66
1	4	480/484 (99%)	459 (96%)	18 (4%)	3 (1%)	28	56
1	5	480/484 (99%)	459 (96%)	18 (4%)	3 (1%)	28	56
1	6	480/484 (99%)	463 (96%)	13 (3%)	4 (1%)	22	49
1	A	480/484 (99%)	457 (95%)	21 (4%)	2 (0%)	38	66
1	B	480/484 (99%)	464 (97%)	13 (3%)	3 (1%)	28	56
1	C	480/484 (99%)	465 (97%)	14 (3%)	1 (0%)	51	79
1	D	480/484 (99%)	450 (94%)	27 (6%)	3 (1%)	28	56
1	E	480/484 (99%)	456 (95%)	24 (5%)	0	100	100
1	F	480/484 (99%)	463 (96%)	15 (3%)	2 (0%)	38	66
1	G	480/484 (99%)	462 (96%)	16 (3%)	2 (0%)	38	66
1	H	480/484 (99%)	454 (95%)	24 (5%)	2 (0%)	38	66
1	I	480/484 (99%)	445 (93%)	32 (7%)	3 (1%)	28	56
1	J	480/484 (99%)	451 (94%)	27 (6%)	2 (0%)	38	66
1	K	480/484 (99%)	459 (96%)	19 (4%)	2 (0%)	38	66
1	L	480/484 (99%)	460 (96%)	19 (4%)	1 (0%)	51	79
1	M	480/484 (99%)	458 (95%)	19 (4%)	3 (1%)	28	56
1	N	480/484 (99%)	463 (96%)	16 (3%)	1 (0%)	51	79
1	O	480/484 (99%)	460 (96%)	19 (4%)	1 (0%)	51	79
1	P	480/484 (99%)	458 (95%)	22 (5%)	0	100	100
1	Q	480/484 (99%)	456 (95%)	21 (4%)	3 (1%)	28	56
1	R	480/484 (99%)	458 (95%)	17 (4%)	5 (1%)	18	43
1	S	480/484 (99%)	462 (96%)	17 (4%)	1 (0%)	51	79
1	T	480/484 (99%)	447 (93%)	29 (6%)	4 (1%)	22	49
1	U	480/484 (99%)	438 (91%)	41 (8%)	1 (0%)	51	79
1	V	480/484 (99%)	443 (92%)	33 (7%)	4 (1%)	22	49
1	W	480/484 (99%)	456 (95%)	21 (4%)	3 (1%)	28	56
1	X	480/484 (99%)	429 (89%)	48 (10%)	3 (1%)	28	56
1	Y	480/484 (99%)	427 (89%)	45 (9%)	8 (2%)	11	27
1	Z	480/484 (99%)	430 (90%)	45 (9%)	5 (1%)	18	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	15360/15488 (99%)	14487 (94%)	784 (5%)	89 (1%)	28	56

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	ASP
1	D	261	ASN
1	D	268	ASP
1	G	268	ASP
1	H	268	ASP

### 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	1	341/363 (94%)	320 (94%)	21 (6%)	21	46
1	2	349/363 (96%)	331 (95%)	18 (5%)	27	55
1	3	349/363 (96%)	333 (95%)	16 (5%)	31	61
1	4	349/363 (96%)	333 (95%)	16 (5%)	31	61
1	5	349/363 (96%)	332 (95%)	17 (5%)	29	58
1	6	349/363 (96%)	331 (95%)	18 (5%)	27	55
1	A	350/363 (96%)	334 (95%)	16 (5%)	31	61
1	B	351/363 (97%)	337 (96%)	14 (4%)	36	67
1	C	350/363 (96%)	325 (93%)	25 (7%)	17	39
1	D	350/363 (96%)	333 (95%)	17 (5%)	29	58
1	E	350/363 (96%)	332 (95%)	18 (5%)	28	56
1	F	350/363 (96%)	337 (96%)	13 (4%)	39	70
1	G	350/363 (96%)	332 (95%)	18 (5%)	28	56
1	H	350/363 (96%)	331 (95%)	19 (5%)	26	54
1	I	344/363 (95%)	319 (93%)	25 (7%)	16	38
1	J	350/363 (96%)	332 (95%)	18 (5%)	28	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	349/363 (96%)	336 (96%)	13 (4%)	39	70
1	L	348/363 (96%)	328 (94%)	20 (6%)	24	51
1	M	349/363 (96%)	327 (94%)	22 (6%)	21	46
1	N	349/363 (96%)	330 (95%)	19 (5%)	26	54
1	O	349/363 (96%)	332 (95%)	17 (5%)	29	58
1	P	349/363 (96%)	334 (96%)	15 (4%)	33	64
1	Q	349/363 (96%)	330 (95%)	19 (5%)	26	54
1	R	349/363 (96%)	324 (93%)	25 (7%)	17	39
1	S	349/363 (96%)	337 (97%)	12 (3%)	42	73
1	T	346/363 (95%)	334 (96%)	12 (4%)	41	72
1	U	344/363 (95%)	324 (94%)	20 (6%)	23	50
1	V	346/363 (95%)	322 (93%)	24 (7%)	18	41
1	W	349/363 (96%)	338 (97%)	11 (3%)	44	75
1	X	340/363 (94%)	321 (94%)	19 (6%)	25	51
1	Y	349/363 (96%)	332 (95%)	17 (5%)	29	58
1	Z	346/363 (95%)	326 (94%)	20 (6%)	23	50
All	All	11141/11616 (96%)	10567 (95%)	574 (5%)	27	55

5 of 574 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	159	ASN
1	R	350	LEU
1	4	285	ARG
1	O	350	LEU
1	Q	44	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	286	ASN
1	Z	13	HIS
1	1	443	ASN
1	Q	468	HIS
1	1	286	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	482/484 (99%)	0.71	54 (11%) 6 4	36, 52, 63, 68	1 (0%)
1	2	482/484 (99%)	-0.04	3 (0%) 89 90	28, 42, 57, 62	1 (0%)
1	3	482/484 (99%)	0.11	7 (1%) 74 75	27, 43, 56, 64	1 (0%)
1	4	482/484 (99%)	-0.00	7 (1%) 74 75	33, 44, 57, 64	1 (0%)
1	5	482/484 (99%)	0.02	5 (1%) 82 82	31, 44, 58, 63	1 (0%)
1	6	482/484 (99%)	-0.18	0 100 100	26, 37, 51, 55	1 (0%)
1	A	482/484 (99%)	-0.14	1 (0%) 94 96	29, 41, 52, 64	1 (0%)
1	B	482/484 (99%)	-0.19	0 100 100	26, 38, 49, 59	1 (0%)
1	C	482/484 (99%)	-0.17	0 100 100	25, 38, 51, 62	1 (0%)
1	D	482/484 (99%)	-0.03	0 100 100	25, 40, 54, 63	1 (0%)
1	E	482/484 (99%)	-0.14	0 100 100	24, 37, 47, 59	1 (0%)
1	F	482/484 (99%)	-0.14	0 100 100	25, 36, 47, 58	1 (0%)
1	G	482/484 (99%)	-0.18	0 100 100	26, 38, 51, 61	1 (0%)
1	H	482/484 (99%)	-0.11	0 100 100	25, 39, 53, 62	1 (0%)
1	I	482/484 (99%)	0.36	27 (5%) 25 23	33, 49, 62, 67	1 (0%)
1	J	482/484 (99%)	-0.09	1 (0%) 94 96	29, 43, 54, 63	1 (0%)
1	K	482/484 (99%)	-0.08	4 (0%) 86 86	28, 41, 57, 60	1 (0%)
1	L	482/484 (99%)	-0.25	0 100 100	28, 39, 47, 54	1 (0%)
1	M	482/484 (99%)	-0.02	2 (0%) 92 93	32, 43, 55, 63	1 (0%)
1	N	482/484 (99%)	-0.13	0 100 100	29, 41, 51, 62	1 (0%)
1	O	482/484 (99%)	-0.05	1 (0%) 94 96	28, 42, 56, 61	1 (0%)
1	P	482/484 (99%)	-0.22	0 100 100	28, 36, 46, 54	1 (0%)
1	Q	482/484 (99%)	0.21	18 (3%) 42 41	38, 50, 61, 67	1 (0%)
1	R	482/484 (99%)	0.06	13 (2%) 55 55	31, 43, 57, 60	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	S	482/484 (99%)	-0.20	0 <span>100</span> <span>100</span>	32, 40, 49, 58	1 (0%)
1	T	482/484 (99%)	0.32	20 (4%) <span>38</span> <span>36</span>	39, 51, 62, 68	1 (0%)
1	U	482/484 (99%)	0.74	57 (11%) <span>5</span> <span>4</span>	43, 53, 64, 69	1 (0%)
1	V	482/484 (99%)	0.20	22 (4%) <span>33</span> <span>31</span>	38, 47, 60, 64	1 (0%)
1	W	482/484 (99%)	-0.07	2 (0%) <span>92</span> <span>93</span>	35, 44, 52, 59	1 (0%)
1	X	482/484 (99%)	0.77	55 (11%) <span>6</span> <span>4</span>	43, 54, 63, 69	1 (0%)
1	Y	482/484 (99%)	0.31	13 (2%) <span>55</span> <span>55</span>	30, 48, 59, 67	1 (0%)
1	Z	482/484 (99%)	0.68	52 (10%) <span>6</span> <span>5</span>	40, 52, 62, 71	1 (0%)
All	All	15424/15488 (99%)	0.07	364 (2%) <span>59</span> <span>60</span>	24, 43, 59, 71	32 (0%)

The worst 5 of 364 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	484	VAL	5.6
1	Z	8	PRO	5.4
1	Y	8	PRO	5.1
1	U	32	VAL	5.0
1	X	211	VAL	5.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.