



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 07:34 AM UTC

PDB ID : 4V6H / pdb_00004v6h
Title : Crystal structure of succinate-semialdehyde dehydrogenase from Burkholderia pseudomallei
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2009-07-24
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

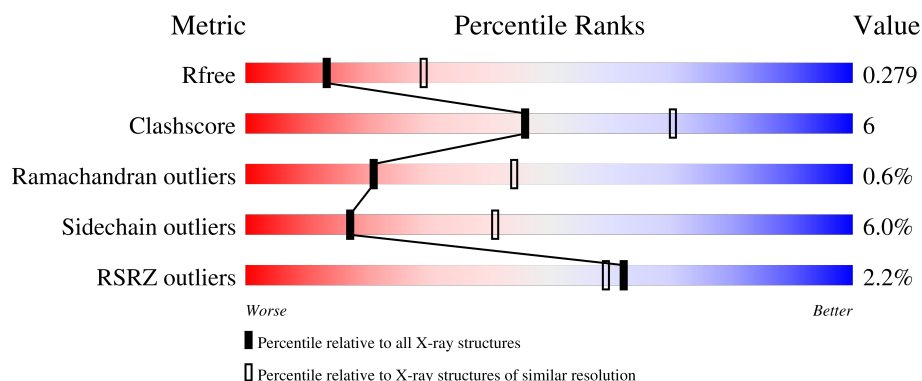
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	484	11% 77% 21% .
1	2	484	2% 77% 20% .
1	3	484	2% 81% 18% .
1	4	484	% 82% 16% .
1	5	484	% 83% 15% .

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Mol	Chain	Length	Quality of chain
1	6	484	 88% 12%
1	A	484	 86% 12% .
1	B	484	 89% 10% .
1	C	484	 85% 13% .
1	D	484	 82% 17%
1	E	484	 85% 13% .
1	F	484	 86% 12% .
1	G	484	 85% 13% .
1	H	484	 86% 13% .
1	I	484	 79% 20% .
1	J	484	 82% 15% .
1	K	484	 86% 12% .
1	L	484	 86% 13% .
1	M	484	 83% 15% .
1	N	484	 87% 12% .
1	O	484	 86% 13% .
1	P	484	 86% 13% .
1	Q	484	 81% 18% .
1	R	484	 84% 14% .
1	S	484	 86% 13% .
1	T	484	 81% 18% .
1	U	484	 77% 21% .
1	V	484	 81% 17% .
1	W	484	 88% 11% .
1	X	484	 77% 20% .

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Mol	Chain	Length	Quality of chain
1	Y	484	6% 77% 21%
1	Z	484	9% 73% 24%

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

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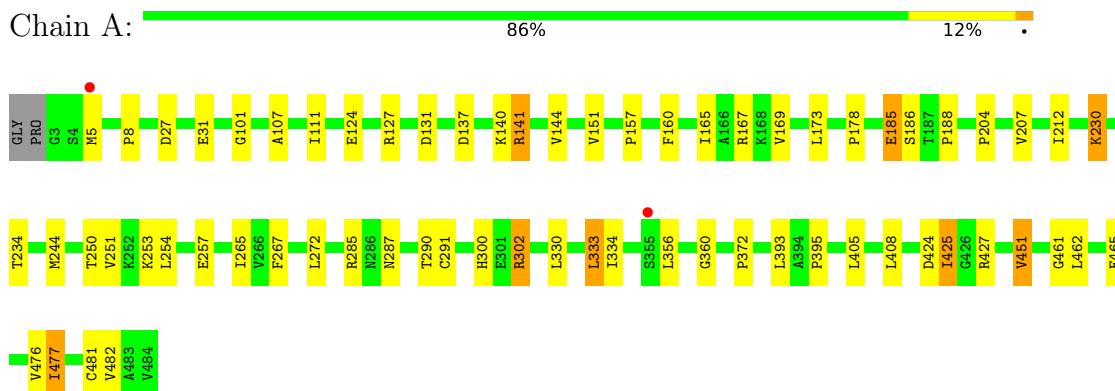
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	W	44	Total 44	O 44	0	0
2	X	8	Total 8	O 8	0	0
2	Y	36	Total 36	O 36	0	0
2	Z	20	Total 20	O 20	0	0
2	1	28	Total 28	O 28	0	0
2	2	37	Total 37	O 37	0	0
2	3	45	Total 45	O 45	0	0
2	4	46	Total 46	O 46	0	0
2	5	54	Total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

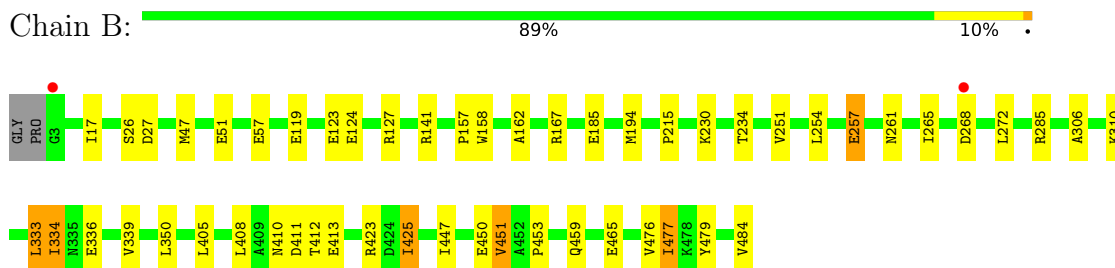
3 Residue-property plots

These plots are drawn for all protein, RNA, 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 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.

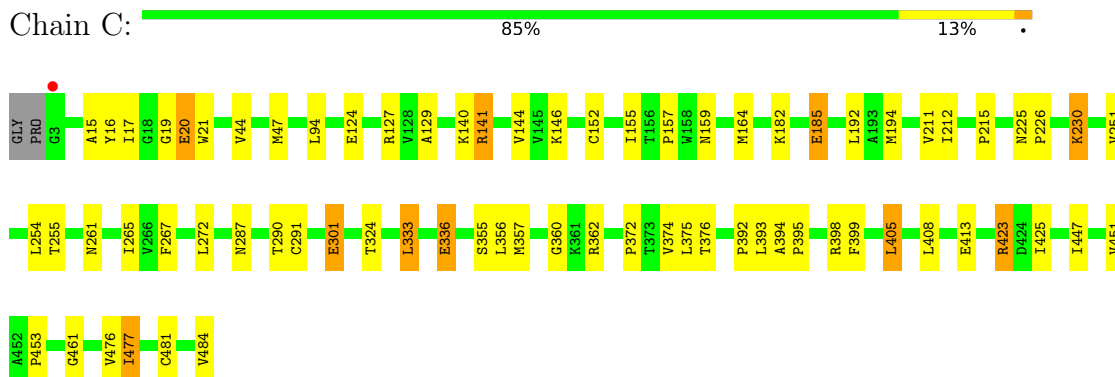
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



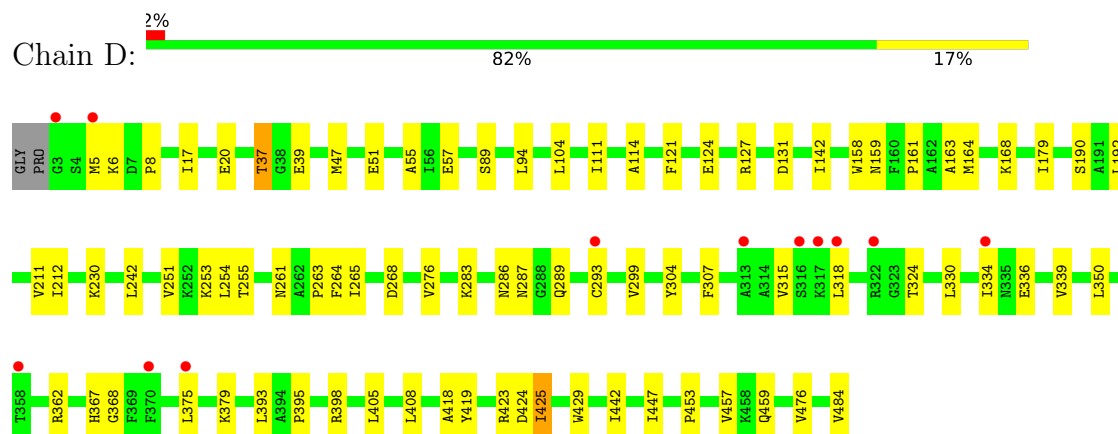
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



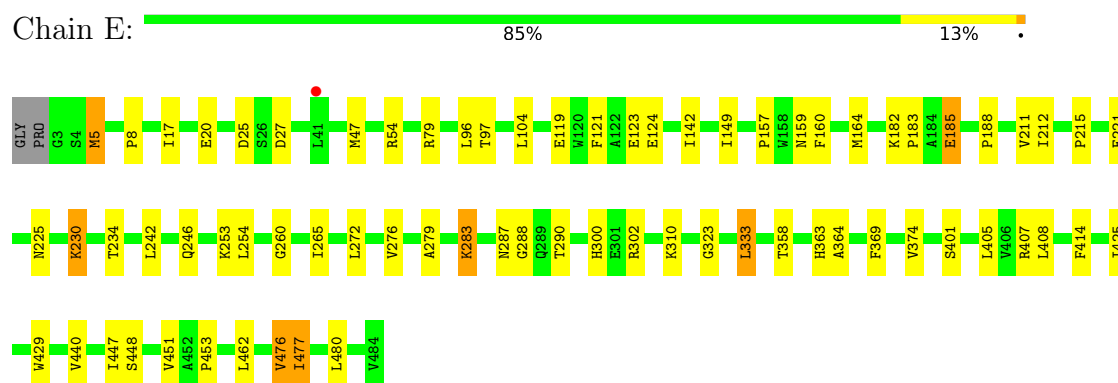
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



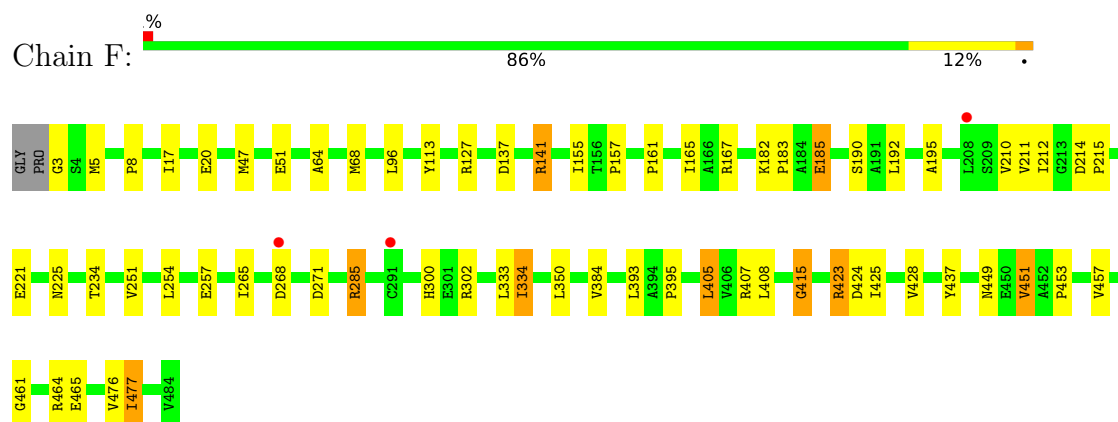
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



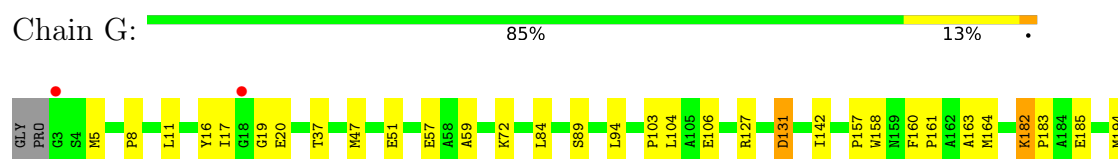
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

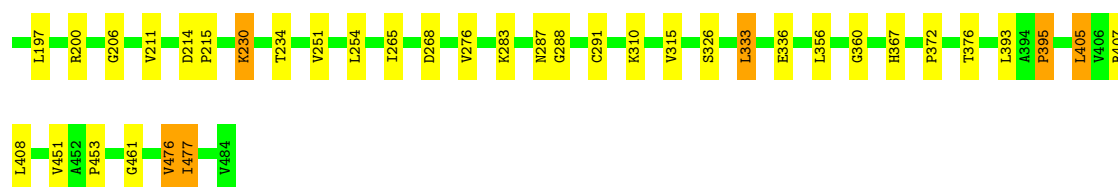


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

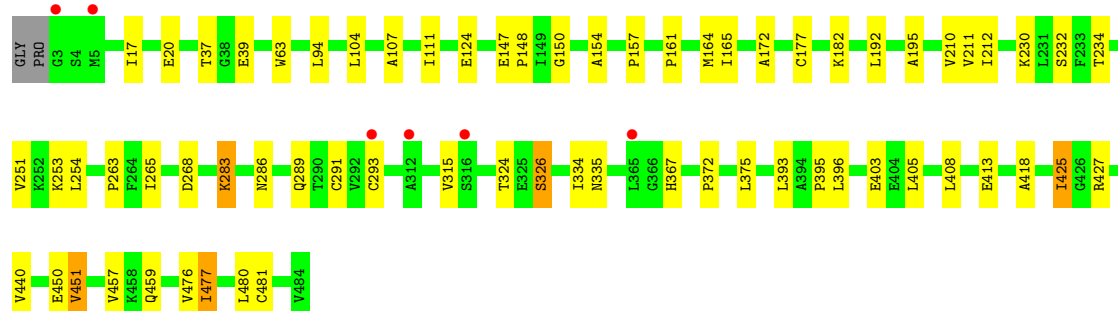
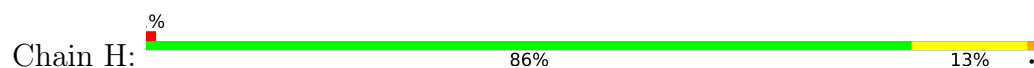


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

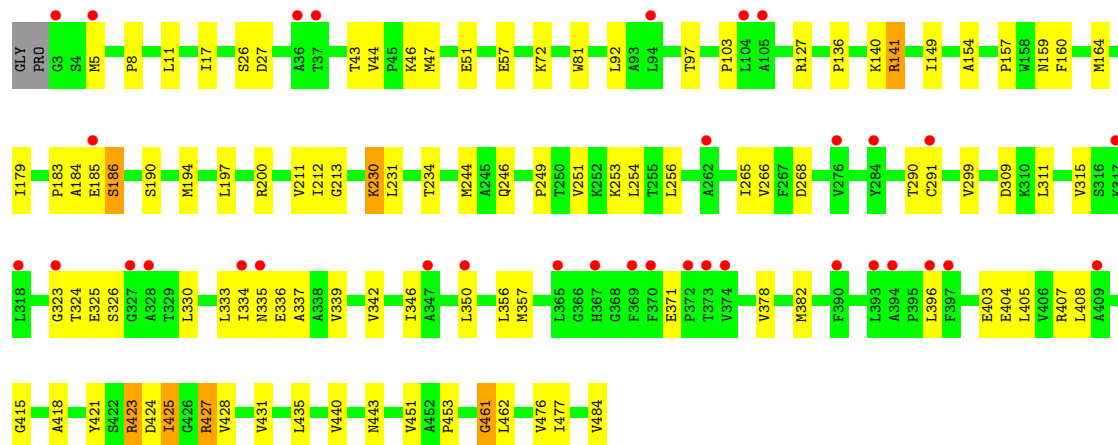
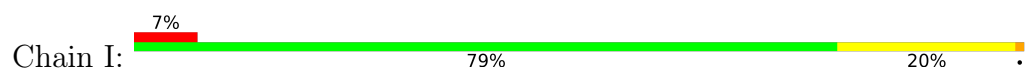




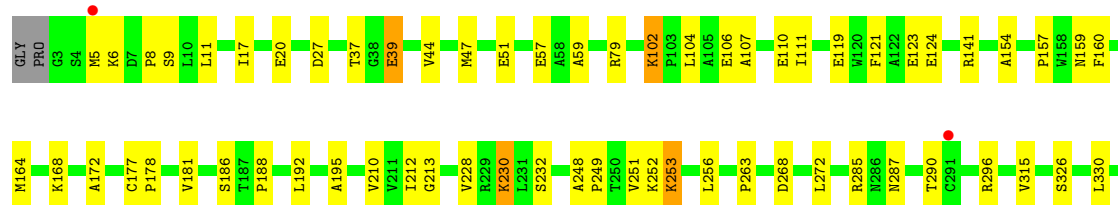
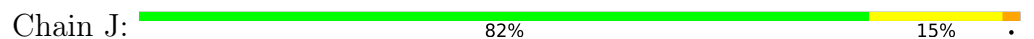
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

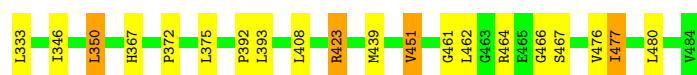


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

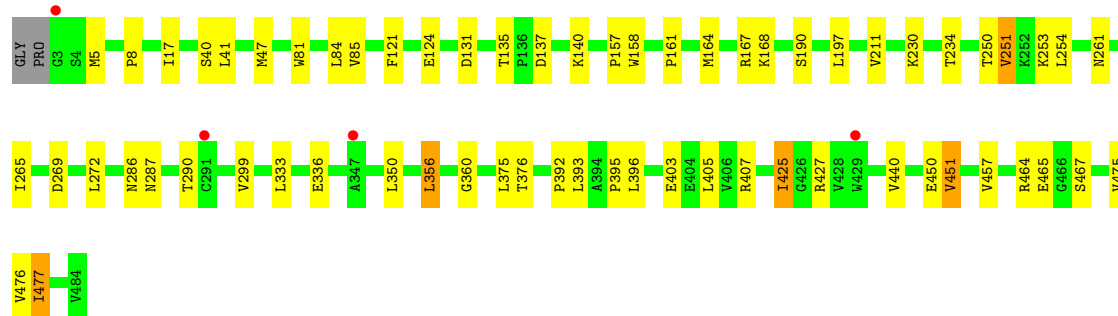
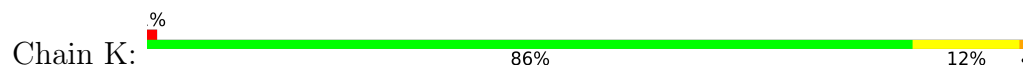


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

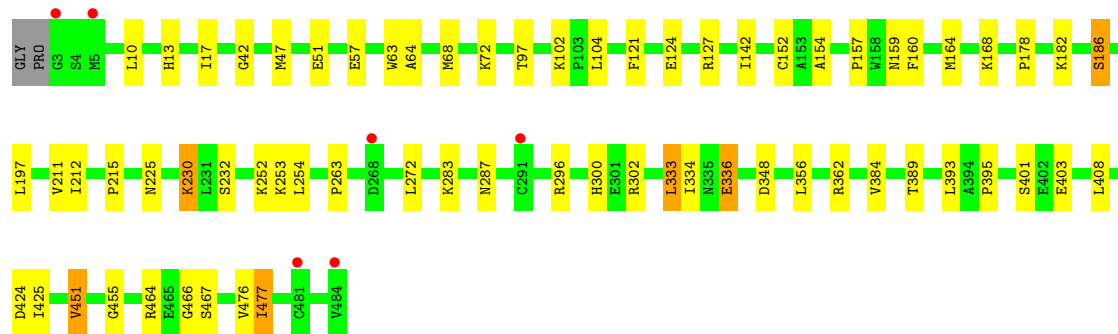
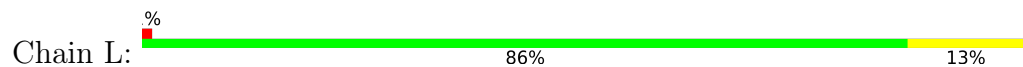




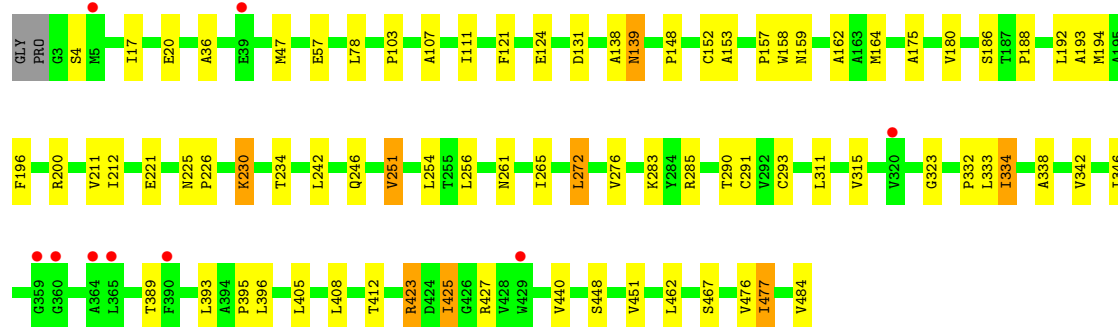
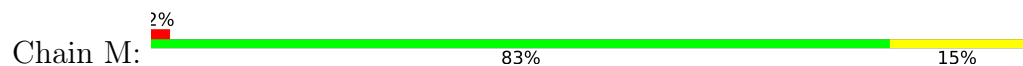
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



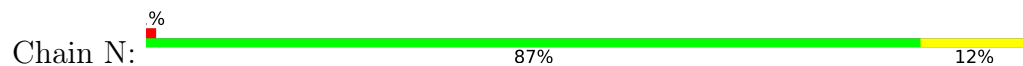
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



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

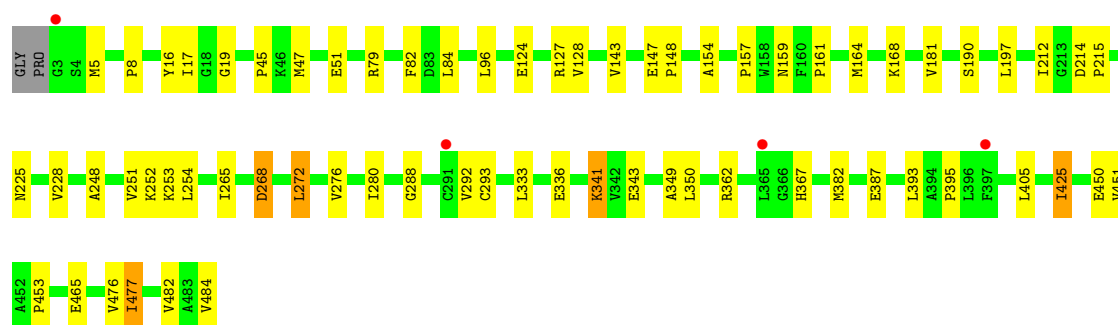
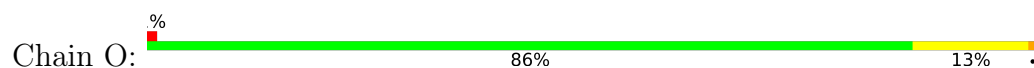


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

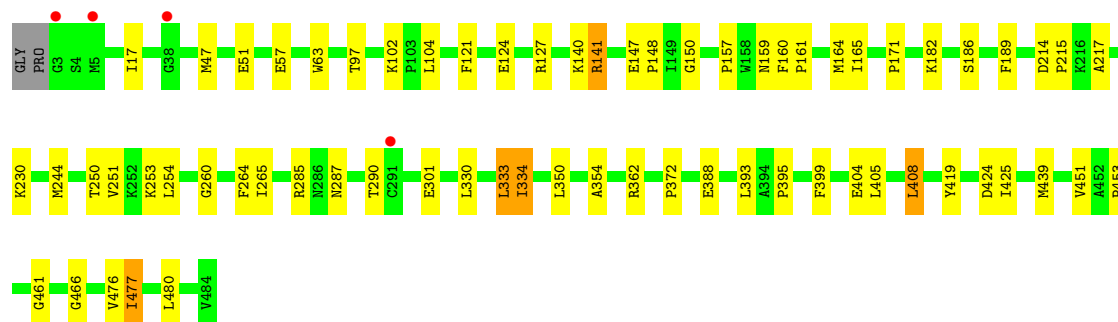
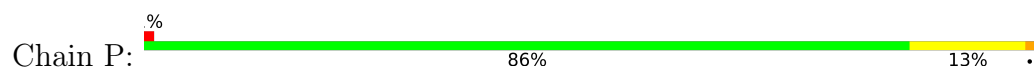




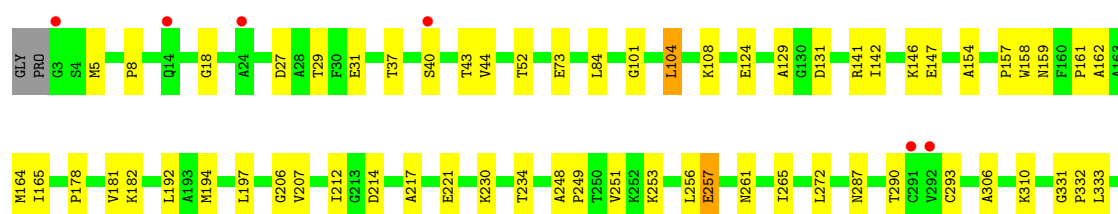
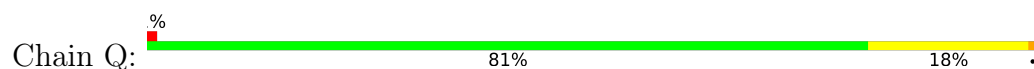
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

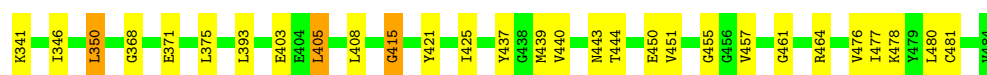


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

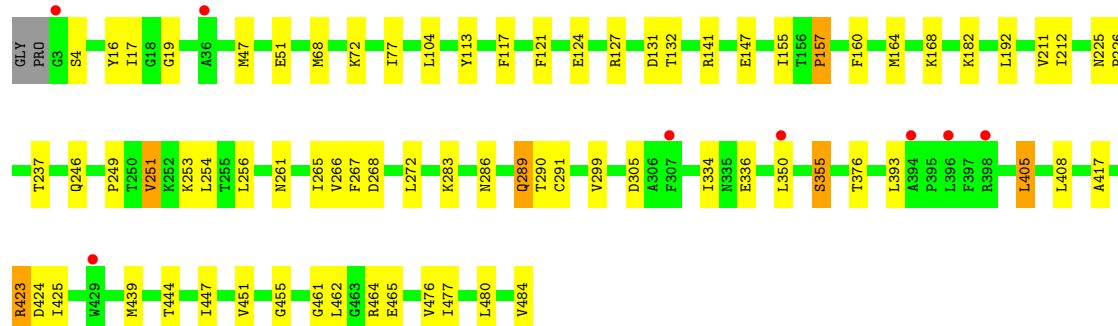
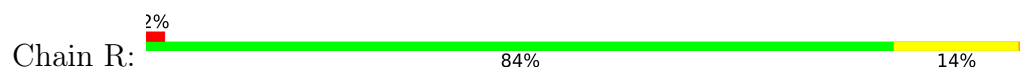


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

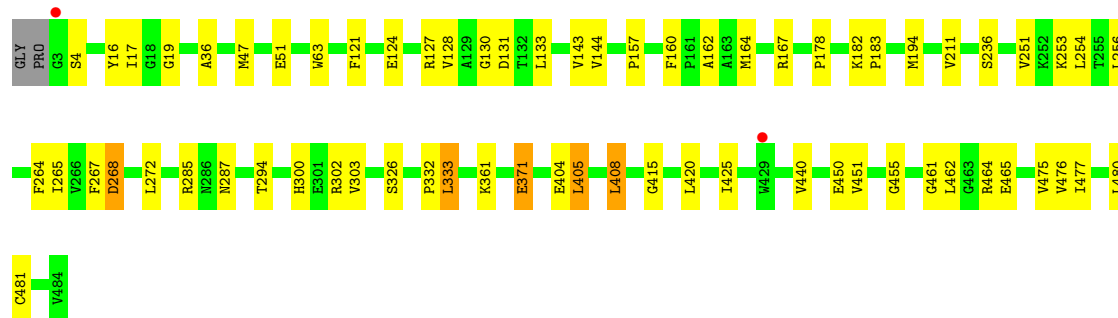
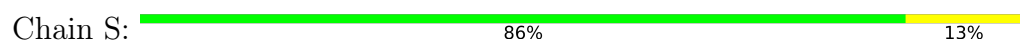




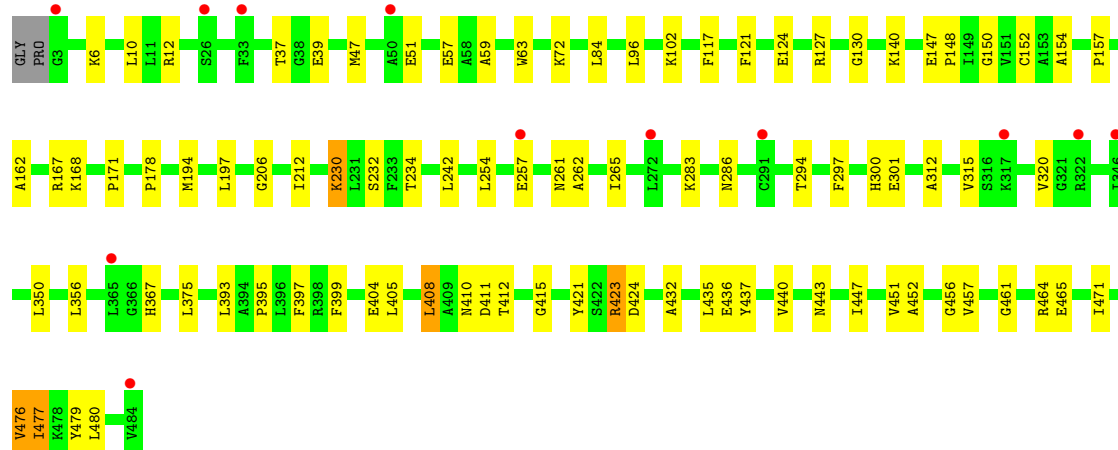
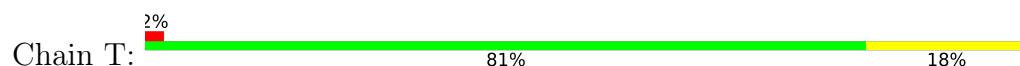
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP⁺)



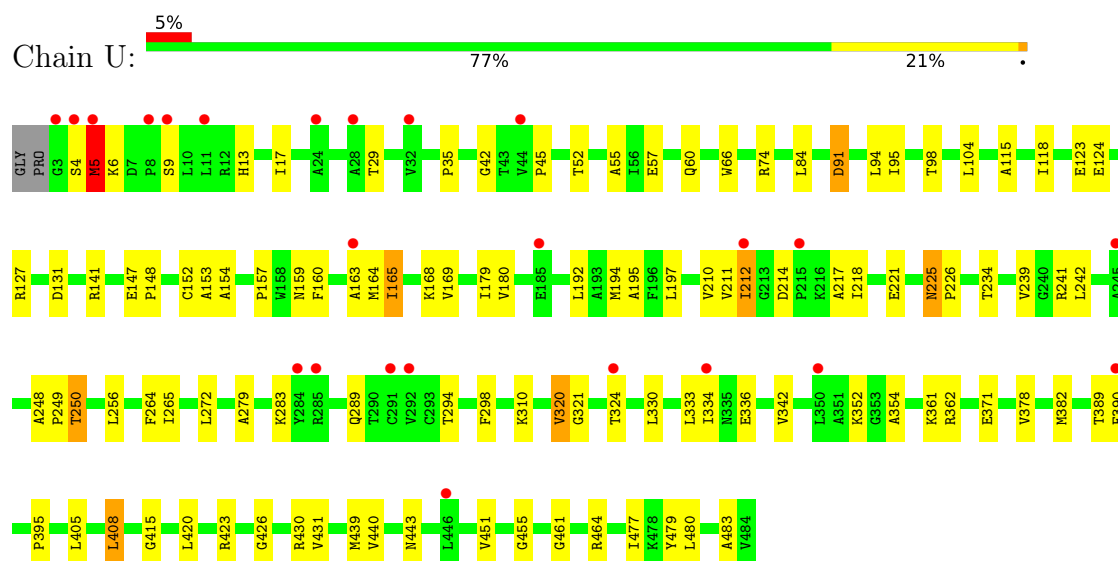
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP⁺)



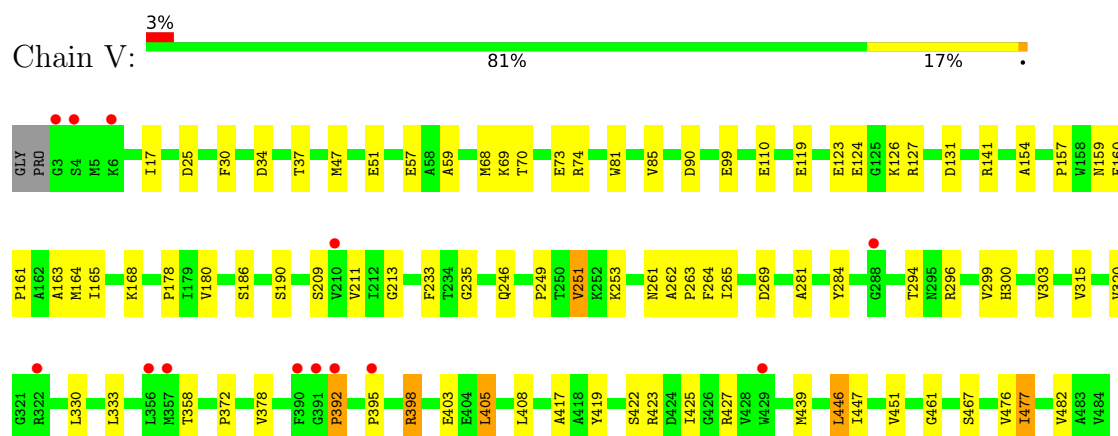
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP⁺)



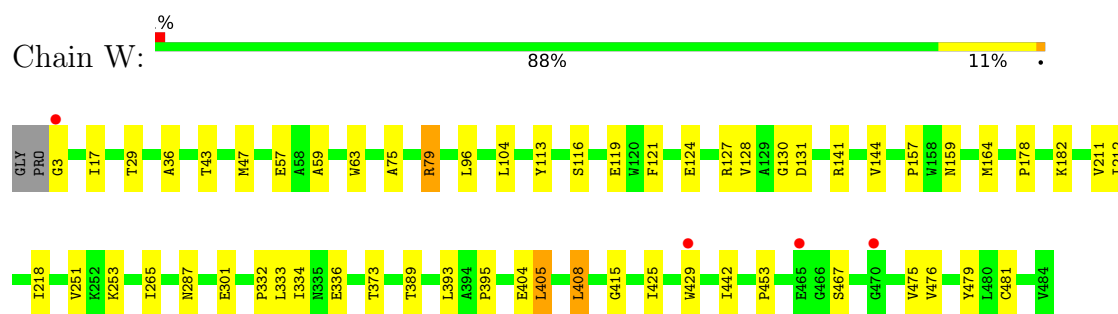
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



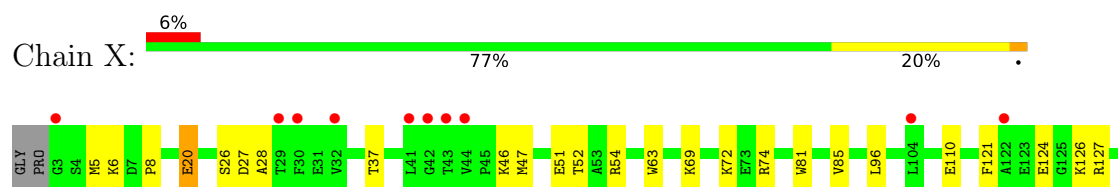
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

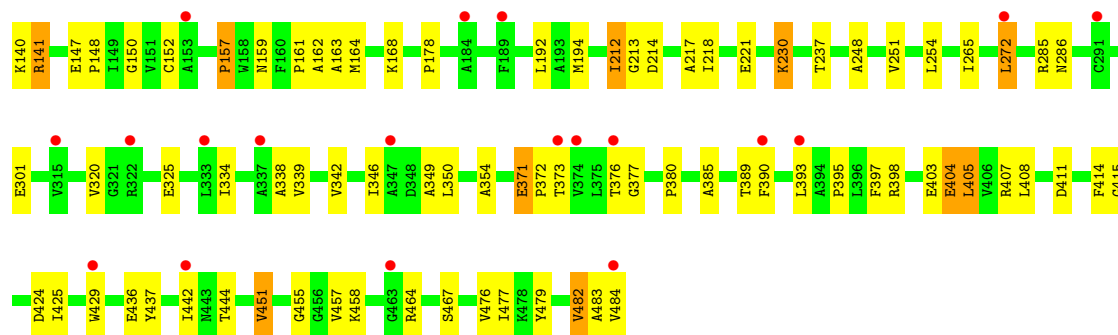


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

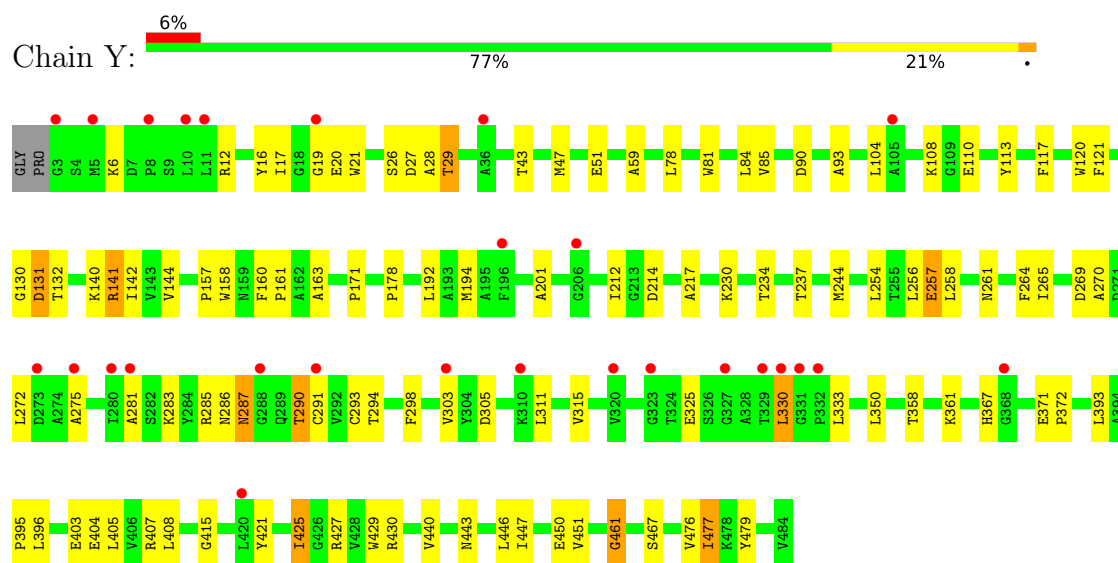


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

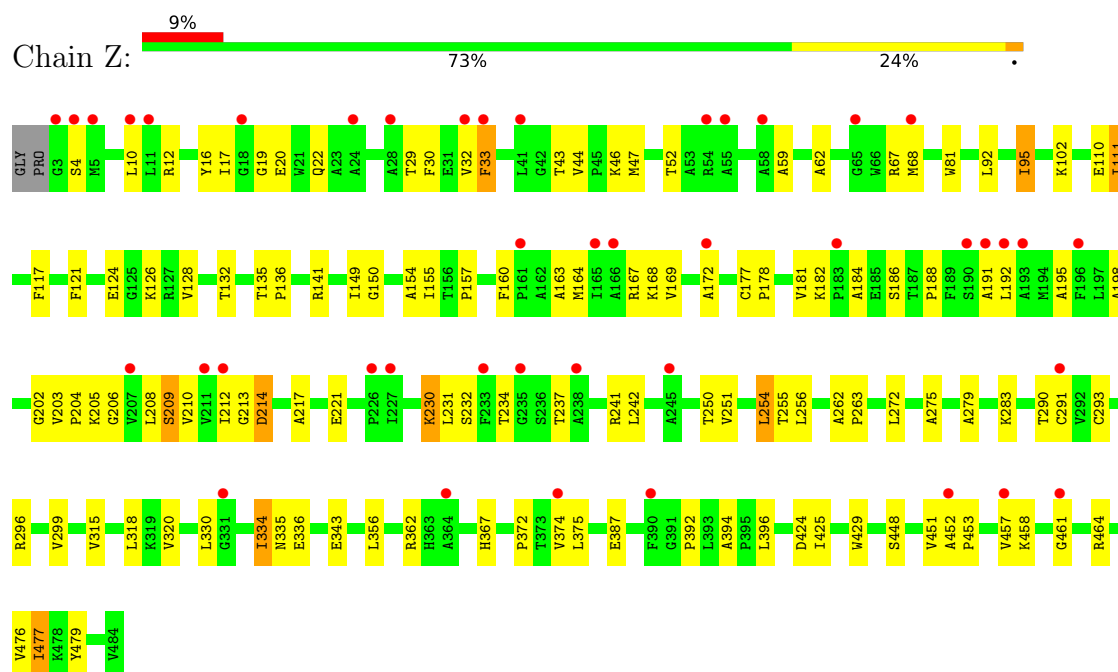




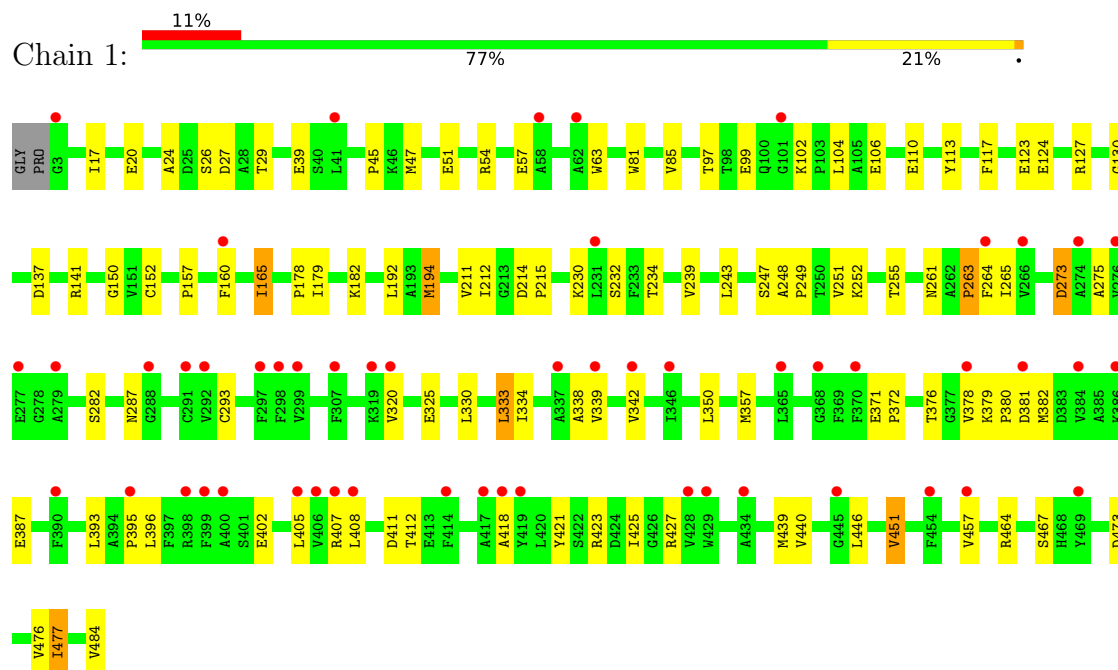
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



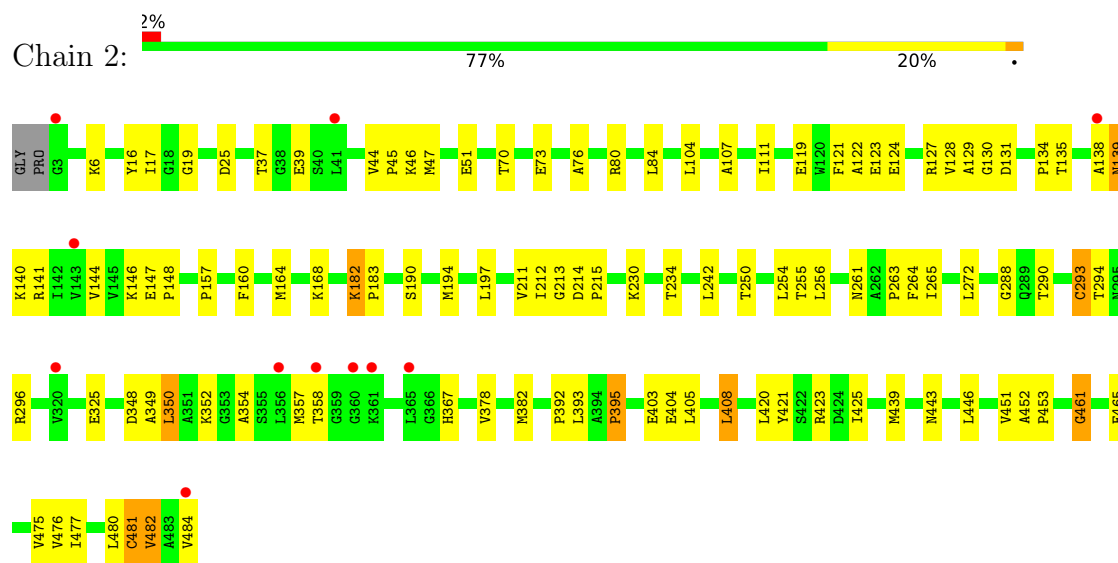
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



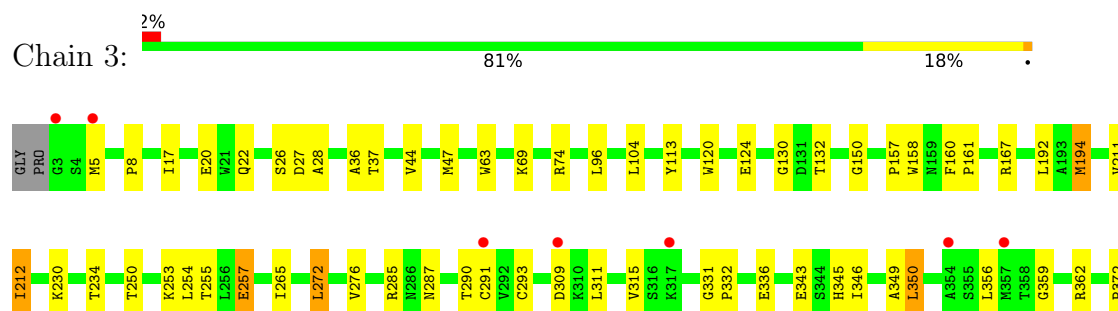
● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

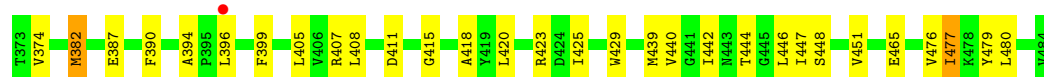


● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

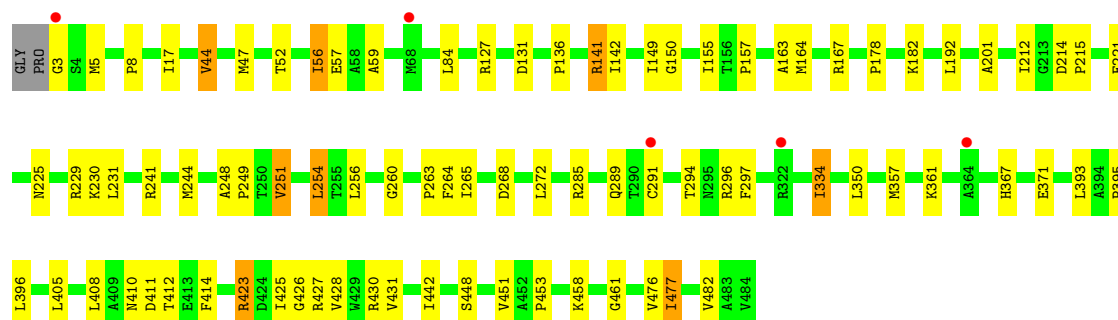
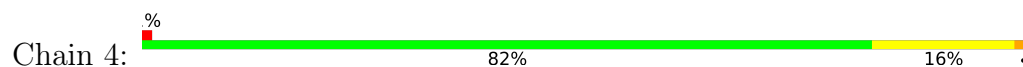


● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

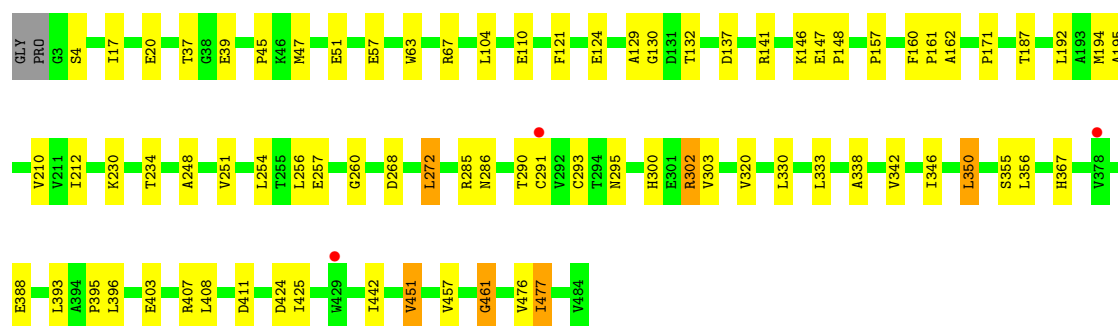
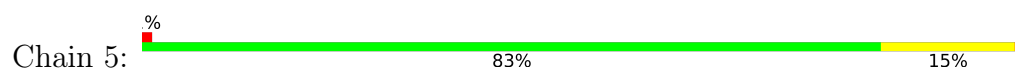




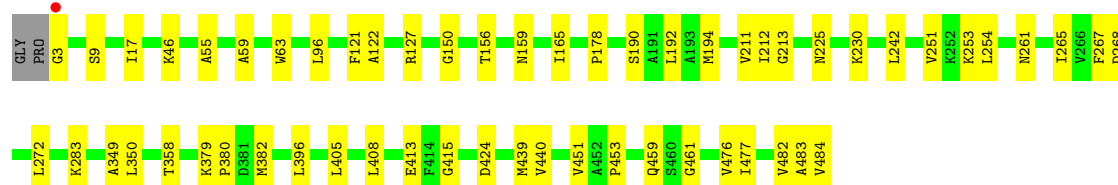
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



- 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, α , β , γ	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) 98.5 (49.47-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	22748 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.62	0/3584	0.90	1/4884 (0.0%)
1	2	0.53	0/3619	0.87	1/4925 (0.0%)
1	3	0.54	0/3619	0.90	0/4925
1	4	0.53	0/3619	0.90	4/4925 (0.1%)
1	5	0.53	0/3619	0.87	1/4925 (0.0%)
1	6	0.54	0/3619	0.89	5/4925 (0.1%)
1	A	0.52	0/3623	0.86	2/4930 (0.0%)
1	B	0.52	0/3627	0.85	0/4935
1	C	0.53	0/3623	0.88	1/4930 (0.0%)
1	D	0.54	0/3623	0.85	1/4930 (0.0%)
1	E	0.53	0/3623	0.84	0/4930
1	F	0.53	0/3623	0.86	1/4930 (0.0%)
1	G	0.52	0/3623	0.87	1/4930 (0.0%)
1	H	0.53	0/3623	0.87	1/4930 (0.0%)
1	I	0.55	0/3594	0.87	1/4896 (0.0%)
1	J	0.52	0/3623	0.86	2/4930 (0.0%)
1	K	0.52	0/3619	0.86	0/4925
1	L	0.54	0/3617	0.87	0/4922
1	M	0.53	0/3619	0.87	0/4925
1	N	0.51	0/3619	0.84	0/4925
1	O	0.53	0/3619	0.89	3/4925 (0.1%)
1	P	0.51	0/3619	0.86	2/4925 (0.0%)
1	Q	0.55	0/3619	0.88	1/4925 (0.0%)
1	R	0.54	0/3619	0.88	1/4925 (0.0%)
1	S	0.52	0/3619	0.87	2/4925 (0.0%)
1	T	0.55	0/3609	0.86	2/4913 (0.0%)
1	U	0.60	0/3594	0.90	5/4894 (0.1%)
1	V	0.56	0/3606	0.89	0/4910
1	W	0.54	0/3619	0.86	0/4925
1	X	0.62	0/3588	0.91	3/4885 (0.1%)
1	Y	0.55	0/3619	0.85	1/4925 (0.0%)
1	Z	0.59	0/3606	0.92	6/4910 (0.1%)
All	All	0.54	0/115694	0.87	48/157464 (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.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	461	GLY	N-CA-C	10.40	122.03	111.21
1	6	461	GLY	N-CA-C	7.56	119.19	111.56
1	Z	461	GLY	N-CA-C	7.32	118.82	111.21
1	C	461	GLY	N-CA-C	7.01	119.90	110.43
1	T	461	GLY	N-CA-C	6.64	119.40	110.43

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	56	0
1	2	3545	0	3503	65	0
1	3	3545	0	3503	56	0
1	4	3545	0	3503	45	0
1	5	3545	0	3503	44	0
1	6	3545	0	3503	22	0
1	A	3549	0	3507	40	0
1	B	3553	0	3511	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3549	0	3507	43	0
1	D	3549	0	3507	51	0
1	E	3549	0	3507	47	0
1	F	3549	0	3507	50	0
1	G	3549	0	3507	40	0
1	H	3549	0	3507	38	0
1	I	3520	0	3450	55	0
1	J	3549	0	3507	52	0
1	K	3545	0	3503	38	0
1	L	3543	0	3496	36	0
1	M	3545	0	3503	46	0
1	N	3545	0	3503	26	0
1	O	3545	0	3503	31	0
1	P	3545	0	3503	42	0
1	Q	3545	0	3503	49	0
1	R	3545	0	3503	35	0
1	S	3545	0	3503	38	0
1	T	3535	0	3474	52	0
1	U	3521	0	3463	54	0
1	V	3532	0	3472	49	0
1	W	3545	0	3503	35	0
1	X	3515	0	3438	63	0
1	Y	3545	0	3503	69	0
1	Z	3532	0	3472	80	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	40	0	0	1	0
2	N	46	0	0	0	0
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	1315	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 1315 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:S:17:ILE:HD11	1:S:47:MET:HE1	1.27	1.13
1:L:17:ILE:HD11	1:L:47:MET:HE1	1.34	1.07
1:D:47:MET:HE3	1:D:51:GLU:HB3	1.38	1.04
1:4:476:VAL:HG21	1:5:457:VAL:HG12	1.36	1.04

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%)	9	25
1	2	480/484 (99%)	443 (92%)	31 (6%)	6 (1%)	9	25
1	3	480/484 (99%)	451 (94%)	27 (6%)	2 (0%)	30	54
1	4	480/484 (99%)	459 (96%)	18 (4%)	3 (1%)	21	44
1	5	480/484 (99%)	459 (96%)	18 (4%)	3 (1%)	21	44
1	6	480/484 (99%)	463 (96%)	13 (3%)	4 (1%)	16	37
1	A	480/484 (99%)	457 (95%)	21 (4%)	2 (0%)	30	54
1	B	480/484 (99%)	464 (97%)	13 (3%)	3 (1%)	21	44
1	C	480/484 (99%)	465 (97%)	14 (3%)	1 (0%)	43	68
1	D	480/484 (99%)	450 (94%)	27 (6%)	3 (1%)	21	44
1	E	480/484 (99%)	456 (95%)	24 (5%)	0	100	100
1	F	480/484 (99%)	463 (96%)	15 (3%)	2 (0%)	30	54
1	G	480/484 (99%)	462 (96%)	16 (3%)	2 (0%)	30	54
1	H	480/484 (99%)	454 (95%)	24 (5%)	2 (0%)	30	54
1	I	480/484 (99%)	445 (93%)	32 (7%)	3 (1%)	21	44
1	J	480/484 (99%)	451 (94%)	27 (6%)	2 (0%)	30	54
1	K	480/484 (99%)	459 (96%)	19 (4%)	2 (0%)	30	54
1	L	480/484 (99%)	460 (96%)	19 (4%)	1 (0%)	43	68
1	M	480/484 (99%)	458 (95%)	19 (4%)	3 (1%)	21	44
1	N	480/484 (99%)	463 (96%)	16 (3%)	1 (0%)	43	68
1	O	480/484 (99%)	460 (96%)	19 (4%)	1 (0%)	43	68
1	P	480/484 (99%)	458 (95%)	22 (5%)	0	100	100
1	Q	480/484 (99%)	456 (95%)	21 (4%)	3 (1%)	21	44
1	R	480/484 (99%)	458 (95%)	17 (4%)	5 (1%)	12	32
1	S	480/484 (99%)	462 (96%)	17 (4%)	1 (0%)	43	68
1	T	480/484 (99%)	447 (93%)	29 (6%)	4 (1%)	16	37
1	U	480/484 (99%)	438 (91%)	41 (8%)	1 (0%)	43	68
1	V	480/484 (99%)	443 (92%)	33 (7%)	4 (1%)	16	37
1	W	480/484 (99%)	456 (95%)	21 (4%)	3 (1%)	21	44
1	X	480/484 (99%)	429 (89%)	48 (10%)	3 (1%)	21	44
1	Y	480/484 (99%)	427 (89%)	45 (9%)	8 (2%)	7	19
1	Z	480/484 (99%)	430 (90%)	45 (9%)	5 (1%)	12	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	15360/15488 (99%)	14487 (94%)	784 (5%)	89 (1%)	21	44

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%)	314 (92%)	27 (8%)	11	28
1	2	349/363 (96%)	327 (94%)	22 (6%)	16	39
1	3	349/363 (96%)	325 (93%)	24 (7%)	14	34
1	4	349/363 (96%)	329 (94%)	20 (6%)	18	43
1	5	349/363 (96%)	327 (94%)	22 (6%)	16	39
1	6	349/363 (96%)	330 (95%)	19 (5%)	20	45
1	A	350/363 (96%)	334 (95%)	16 (5%)	24	51
1	B	351/363 (97%)	334 (95%)	17 (5%)	23	50
1	C	350/363 (96%)	324 (93%)	26 (7%)	13	32
1	D	350/363 (96%)	331 (95%)	19 (5%)	20	45
1	E	350/363 (96%)	330 (94%)	20 (6%)	18	43
1	F	350/363 (96%)	335 (96%)	15 (4%)	26	54
1	G	350/363 (96%)	329 (94%)	21 (6%)	17	41
1	H	350/363 (96%)	330 (94%)	20 (6%)	18	43
1	I	344/363 (95%)	315 (92%)	29 (8%)	10	26
1	J	350/363 (96%)	330 (94%)	20 (6%)	18	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	349/363 (96%)	332 (95%)	17 (5%)	22	49
1	L	348/363 (96%)	326 (94%)	22 (6%)	16	39
1	M	349/363 (96%)	325 (93%)	24 (7%)	14	34
1	N	349/363 (96%)	329 (94%)	20 (6%)	18	43
1	O	349/363 (96%)	331 (95%)	18 (5%)	21	47
1	P	349/363 (96%)	333 (95%)	16 (5%)	24	51
1	Q	349/363 (96%)	325 (93%)	24 (7%)	14	34
1	R	349/363 (96%)	322 (92%)	27 (8%)	12	30
1	S	349/363 (96%)	332 (95%)	17 (5%)	22	49
1	T	346/363 (95%)	331 (96%)	15 (4%)	26	54
1	U	344/363 (95%)	321 (93%)	23 (7%)	15	36
1	V	346/363 (95%)	322 (93%)	24 (7%)	14	34
1	W	349/363 (96%)	334 (96%)	15 (4%)	26	54
1	X	340/363 (94%)	317 (93%)	23 (7%)	14	35
1	Y	349/363 (96%)	327 (94%)	22 (6%)	16	39
1	Z	346/363 (95%)	324 (94%)	22 (6%)	16	38
All	All	11141/11616 (96%)	10475 (94%)	666 (6%)	17	41

5 of 666 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	425	ILE
1	2	408	LEU
1	X	339	VAL
1	W	408	LEU
1	Z	254	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	367	HIS
1	X	286	ASN
1	4	289	GLN
1	R	468	HIS
1	U	88	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 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 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, 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	1	482/484 (99%)	1.05	53 (10%) 10 9	36, 52, 63, 68	1 (0%)
1	2	482/484 (99%)	0.40	11 (2%) 61 58	28, 42, 57, 62	1 (0%)
1	3	482/484 (99%)	0.41	8 (1%) 69 67	27, 43, 56, 64	1 (0%)
1	4	482/484 (99%)	0.25	5 (1%) 79 78	33, 44, 57, 64	1 (0%)
1	5	482/484 (99%)	0.26	3 (0%) 85 85	31, 44, 58, 63	1 (0%)
1	6	482/484 (99%)	0.06	1 (0%) 91 90	26, 37, 51, 55	1 (0%)
1	A	482/484 (99%)	0.11	2 (0%) 88 87	29, 41, 52, 64	1 (0%)
1	B	482/484 (99%)	0.05	2 (0%) 88 87	26, 38, 49, 59	1 (0%)
1	C	482/484 (99%)	0.08	1 (0%) 91 90	25, 38, 51, 62	1 (0%)
1	D	482/484 (99%)	0.26	12 (2%) 58 55	25, 40, 54, 63	1 (0%)
1	E	482/484 (99%)	0.05	1 (0%) 91 90	24, 37, 47, 59	1 (0%)
1	F	482/484 (99%)	0.03	3 (0%) 85 85	25, 36, 47, 58	1 (0%)
1	G	482/484 (99%)	0.08	2 (0%) 88 87	26, 38, 51, 61	1 (0%)
1	H	482/484 (99%)	0.13	6 (1%) 76 75	25, 39, 53, 62	1 (0%)
1	I	482/484 (99%)	0.74	34 (7%) 22 19	33, 49, 62, 67	1 (0%)
1	J	482/484 (99%)	0.21	2 (0%) 88 87	29, 43, 54, 63	1 (0%)
1	K	482/484 (99%)	0.12	4 (0%) 82 81	28, 41, 57, 60	1 (0%)
1	L	482/484 (99%)	0.05	6 (1%) 76 75	28, 39, 47, 54	1 (0%)
1	M	482/484 (99%)	0.26	9 (1%) 66 63	32, 43, 55, 63	1 (0%)
1	N	482/484 (99%)	0.11	5 (1%) 79 78	29, 41, 51, 62	1 (0%)
1	O	482/484 (99%)	0.16	4 (0%) 82 81	28, 42, 56, 61	1 (0%)
1	P	482/484 (99%)	-0.02	4 (0%) 82 81	28, 36, 46, 54	1 (0%)
1	Q	482/484 (99%)	0.45	6 (1%) 76 75	38, 50, 61, 67	1 (0%)
1	R	482/484 (99%)	0.24	8 (1%) 69 67	31, 43, 57, 60	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	S	482/484 (99%)	0.04	2 (0%) 88 87	32, 40, 49, 58	1 (0%)
1	T	482/484 (99%)	0.56	12 (2%) 58 55	39, 51, 62, 68	1 (0%)
1	U	482/484 (99%)	0.88	24 (4%) 34 30	43, 53, 64, 69	1 (0%)
1	V	482/484 (99%)	0.56	13 (2%) 56 53	38, 47, 60, 64	1 (0%)
1	W	482/484 (99%)	0.27	4 (0%) 82 81	35, 44, 52, 59	1 (0%)
1	X	482/484 (99%)	0.97	29 (6%) 27 24	43, 54, 63, 69	1 (0%)
1	Y	482/484 (99%)	0.74	27 (5%) 30 26	30, 48, 59, 67	1 (0%)
1	Z	482/484 (99%)	1.06	43 (8%) 15 13	40, 52, 62, 71	1 (0%)
All	All	15424/15488 (99%)	0.33	346 (2%) 62 59	24, 43, 59, 71	32 (0%)

The worst 5 of 346 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	3	GLY	5.5
1	L	3	GLY	4.8
1	2	3	GLY	4.5
1	V	3	GLY	4.4
1	U	32	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.