



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:47 PM UTC

PDB ID : 4LD7 / pdb\_00004ld7  
Title : Crystal structure of AnaPT from Neosartorya fischeri  
Authors : Zocher, G.; Stehle, T.  
Deposited on : 2013-06-24  
Resolution : 2.83 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

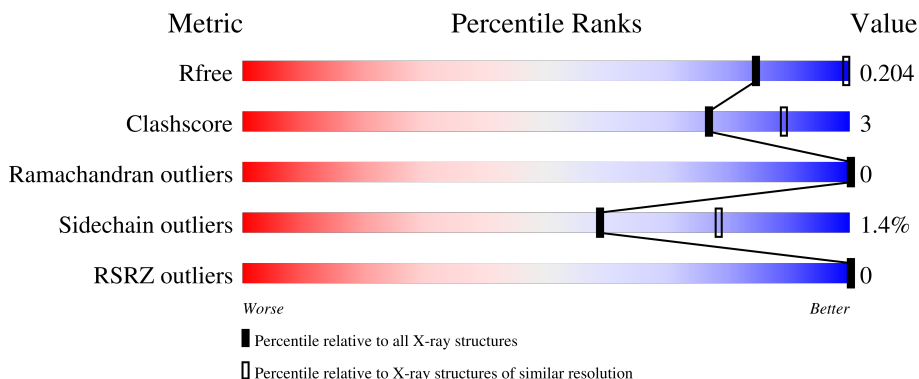
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.83 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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  $\geq 3$ , 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	A	445	83% 6% 11%
1	B	445	83% 6% 11%
1	C	445	83% 6% 11%
1	D	445	82% 7% 11%
1	E	445	84% 5% 11%

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Mol	Chain	Length	Quality of chain		
1	F	445		83%	6% 11%
1	G	445		82%	7% 11%
1	H	445		83%	6% 11%
1	I	445		83%	6% 11%
1	J	445		83%	6% 11%
1	K	445		82%	6% 12%
1	L	445		83%	6% 11%
1	M	445		84%	5% 11%
1	N	445		84%	. 11%
1	O	445		82%	6% 12%
1	P	445		83%	6% 11%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 48979 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 Dimethylallyl tryptophan synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	3057	1987	502	558	10	0	0	0
1	B	397	3056	1987	501	558	10	0	0	0
1	C	397	3058	1987	502	559	10	0	0	0
1	D	397	3054	1986	499	559	10	0	0	0
1	E	397	3050	1983	499	558	10	0	0	0
1	F	397	3056	1985	502	559	10	0	0	0
1	G	397	3058	1987	502	559	10	0	0	0
1	H	397	3058	1987	502	559	10	0	0	0
1	I	397	3056	1987	502	557	10	0	0	0
1	J	397	3058	1987	502	559	10	0	0	0
1	K	392	3022	1964	496	552	10	0	0	0
1	L	397	3058	1987	502	559	10	0	0	0
1	M	397	3050	1983	498	559	10	0	0	0
1	N	397	3058	1987	502	559	10	0	0	0
1	O	391	3012	1957	494	551	10	0	0	0
1	P	397	3058	1987	502	559	10	0	0	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	ARG	-	expression tag	UNP A1DN10
A	439	SER	-	expression tag	UNP A1DN10
A	440	HIS	-	expression tag	UNP A1DN10
A	441	HIS	-	expression tag	UNP A1DN10
A	442	HIS	-	expression tag	UNP A1DN10
A	443	HIS	-	expression tag	UNP A1DN10
A	444	HIS	-	expression tag	UNP A1DN10
A	445	HIS	-	expression tag	UNP A1DN10
B	438	ARG	-	expression tag	UNP A1DN10
B	439	SER	-	expression tag	UNP A1DN10
B	440	HIS	-	expression tag	UNP A1DN10
B	441	HIS	-	expression tag	UNP A1DN10
B	442	HIS	-	expression tag	UNP A1DN10
B	443	HIS	-	expression tag	UNP A1DN10
B	444	HIS	-	expression tag	UNP A1DN10
B	445	HIS	-	expression tag	UNP A1DN10
C	438	ARG	-	expression tag	UNP A1DN10
C	439	SER	-	expression tag	UNP A1DN10
C	440	HIS	-	expression tag	UNP A1DN10
C	441	HIS	-	expression tag	UNP A1DN10
C	442	HIS	-	expression tag	UNP A1DN10
C	443	HIS	-	expression tag	UNP A1DN10
C	444	HIS	-	expression tag	UNP A1DN10
C	445	HIS	-	expression tag	UNP A1DN10
D	438	ARG	-	expression tag	UNP A1DN10
D	439	SER	-	expression tag	UNP A1DN10
D	440	HIS	-	expression tag	UNP A1DN10
D	441	HIS	-	expression tag	UNP A1DN10
D	442	HIS	-	expression tag	UNP A1DN10
D	443	HIS	-	expression tag	UNP A1DN10
D	444	HIS	-	expression tag	UNP A1DN10
D	445	HIS	-	expression tag	UNP A1DN10
E	438	ARG	-	expression tag	UNP A1DN10
E	439	SER	-	expression tag	UNP A1DN10
E	440	HIS	-	expression tag	UNP A1DN10
E	441	HIS	-	expression tag	UNP A1DN10
E	442	HIS	-	expression tag	UNP A1DN10
E	443	HIS	-	expression tag	UNP A1DN10
E	444	HIS	-	expression tag	UNP A1DN10
E	445	HIS	-	expression tag	UNP A1DN10
F	438	ARG	-	expression tag	UNP A1DN10
F	439	SER	-	expression tag	UNP A1DN10

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Chain	Residue	Modelled	Actual	Comment	Reference
F	440	HIS	-	expression tag	UNP A1DN10
F	441	HIS	-	expression tag	UNP A1DN10
F	442	HIS	-	expression tag	UNP A1DN10
F	443	HIS	-	expression tag	UNP A1DN10
F	444	HIS	-	expression tag	UNP A1DN10
F	445	HIS	-	expression tag	UNP A1DN10
G	438	ARG	-	expression tag	UNP A1DN10
G	439	SER	-	expression tag	UNP A1DN10
G	440	HIS	-	expression tag	UNP A1DN10
G	441	HIS	-	expression tag	UNP A1DN10
G	442	HIS	-	expression tag	UNP A1DN10
G	443	HIS	-	expression tag	UNP A1DN10
G	444	HIS	-	expression tag	UNP A1DN10
G	445	HIS	-	expression tag	UNP A1DN10
H	438	ARG	-	expression tag	UNP A1DN10
H	439	SER	-	expression tag	UNP A1DN10
H	440	HIS	-	expression tag	UNP A1DN10
H	441	HIS	-	expression tag	UNP A1DN10
H	442	HIS	-	expression tag	UNP A1DN10
H	443	HIS	-	expression tag	UNP A1DN10
H	444	HIS	-	expression tag	UNP A1DN10
H	445	HIS	-	expression tag	UNP A1DN10
I	438	ARG	-	expression tag	UNP A1DN10
I	439	SER	-	expression tag	UNP A1DN10
I	440	HIS	-	expression tag	UNP A1DN10
I	441	HIS	-	expression tag	UNP A1DN10
I	442	HIS	-	expression tag	UNP A1DN10
I	443	HIS	-	expression tag	UNP A1DN10
I	444	HIS	-	expression tag	UNP A1DN10
I	445	HIS	-	expression tag	UNP A1DN10
J	438	ARG	-	expression tag	UNP A1DN10
J	439	SER	-	expression tag	UNP A1DN10
J	440	HIS	-	expression tag	UNP A1DN10
J	441	HIS	-	expression tag	UNP A1DN10
J	442	HIS	-	expression tag	UNP A1DN10
J	443	HIS	-	expression tag	UNP A1DN10
J	444	HIS	-	expression tag	UNP A1DN10
J	445	HIS	-	expression tag	UNP A1DN10
K	438	ARG	-	expression tag	UNP A1DN10
K	439	SER	-	expression tag	UNP A1DN10
K	440	HIS	-	expression tag	UNP A1DN10
K	441	HIS	-	expression tag	UNP A1DN10

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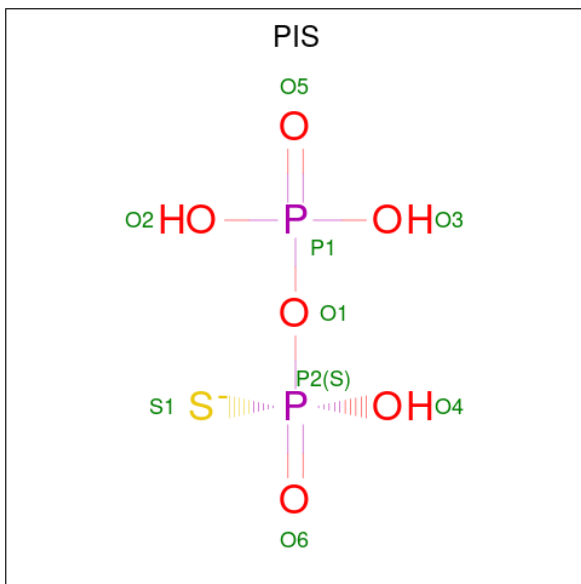
Chain	Residue	Modelled	Actual	Comment	Reference
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K	443	HIS	-	expression tag	UNP A1DN10
K	444	HIS	-	expression tag	UNP A1DN10
K	445	HIS	-	expression tag	UNP A1DN10
L	438	ARG	-	expression tag	UNP A1DN10
L	439	SER	-	expression tag	UNP A1DN10
L	440	HIS	-	expression tag	UNP A1DN10
L	441	HIS	-	expression tag	UNP A1DN10
L	442	HIS	-	expression tag	UNP A1DN10
L	443	HIS	-	expression tag	UNP A1DN10
L	444	HIS	-	expression tag	UNP A1DN10
L	445	HIS	-	expression tag	UNP A1DN10
M	438	ARG	-	expression tag	UNP A1DN10
M	439	SER	-	expression tag	UNP A1DN10
M	440	HIS	-	expression tag	UNP A1DN10
M	441	HIS	-	expression tag	UNP A1DN10
M	442	HIS	-	expression tag	UNP A1DN10
M	443	HIS	-	expression tag	UNP A1DN10
M	444	HIS	-	expression tag	UNP A1DN10
M	445	HIS	-	expression tag	UNP A1DN10
N	438	ARG	-	expression tag	UNP A1DN10
N	439	SER	-	expression tag	UNP A1DN10
N	440	HIS	-	expression tag	UNP A1DN10
N	441	HIS	-	expression tag	UNP A1DN10
N	442	HIS	-	expression tag	UNP A1DN10
N	443	HIS	-	expression tag	UNP A1DN10
N	444	HIS	-	expression tag	UNP A1DN10
N	445	HIS	-	expression tag	UNP A1DN10
O	438	ARG	-	expression tag	UNP A1DN10
O	439	SER	-	expression tag	UNP A1DN10
O	440	HIS	-	expression tag	UNP A1DN10
O	441	HIS	-	expression tag	UNP A1DN10
O	442	HIS	-	expression tag	UNP A1DN10
O	443	HIS	-	expression tag	UNP A1DN10
O	444	HIS	-	expression tag	UNP A1DN10
O	445	HIS	-	expression tag	UNP A1DN10
P	438	ARG	-	expression tag	UNP A1DN10
P	439	SER	-	expression tag	UNP A1DN10
P	440	HIS	-	expression tag	UNP A1DN10
P	441	HIS	-	expression tag	UNP A1DN10
P	442	HIS	-	expression tag	UNP A1DN10
P	443	HIS	-	expression tag	UNP A1DN10

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Chain	Residue	Modelled	Actual	Comment	Reference
P	444	HIS	-	expression tag	UNP A1DN10
P	445	HIS	-	expression tag	UNP A1DN10

- Molecule 2 is TRIHYDROGEN THIODIPHOSPHATE (CCD ID: PIS) (formula:  $H_3O_6P_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P	S		
2	A	1	Total 9	O 6	P 2	S 1	0	0
2	B	1	Total 9	O 6	P 2	S 1	0	0
2	C	1	Total 9	O 6	P 2	S 1	0	0
2	D	1	Total 9	O 6	P 2	S 1	0	0
2	E	1	Total 9	O 6	P 2	S 1	0	0
2	F	1	Total 9	O 6	P 2	S 1	0	0
2	G	1	Total 9	O 6	P 2	S 1	0	0
2	H	1	Total 9	O 6	P 2	S 1	0	0
2	I	1	Total 9	O 6	P 2	S 1	0	0
2	J	1	Total 9	O 6	P 2	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P	S		
2	K	1	9	6	2	1	0	0
2	L	1	9	6	2	1	0	0
2	M	1	9	6	2	1	0	0
2	N	1	9	6	2	1	0	0
2	O	1	9	6	2	1	0	0
2	P	1	9	6	2	1	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0
3	E	1	1	1	0	0
3	F	1	1	1	0	0
3	G	1	1	1	0	0
3	H	1	1	1	0	0
3	I	1	1	1	0	0
3	J	1	1	1	0	0
3	K	1	1	1	0	0
3	L	1	1	1	0	0
3	M	1	1	1	0	0

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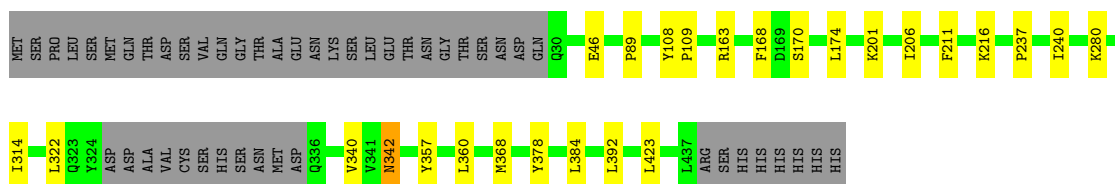
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	N	1	Total 1	Na 1	0	0
3	O	1	Total 1	Na 1	0	0
3	P	1	Total 1	Na 1	0	0

### 3 Residue-property plots [i](#)


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.

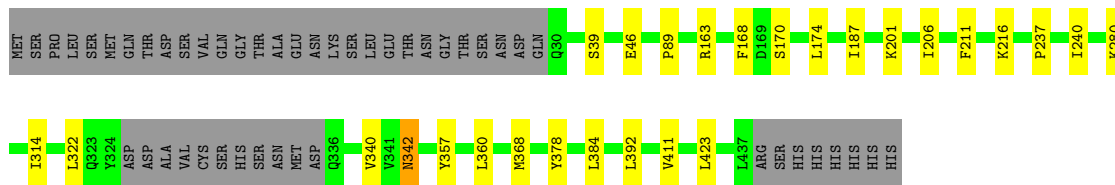
- Molecule 1: Dimethylallyl tryptophan synthase

Chain A:  83% 6% 11%




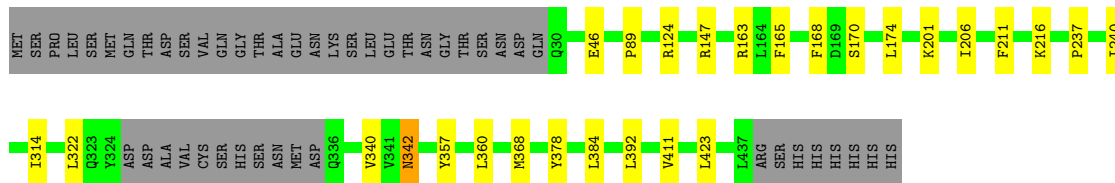
- Molecule 1: Dimethylallyl tryptophan synthase

Chain B:  83% 6% 11%




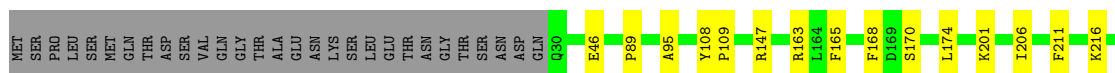
- Molecule 1: Dimethylallyl tryptophan synthase

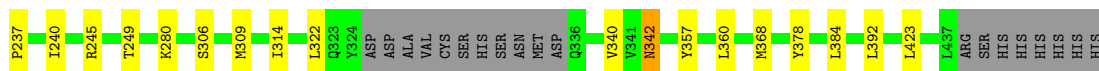
Chain C:  83% 6% 11%



- Molecule 1: Dimethylallyl tryptophan synthase

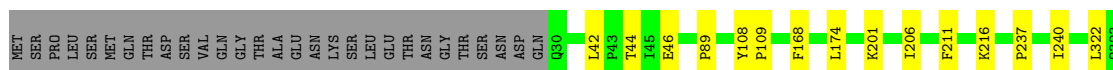
Chain D:  82% 7% 11%





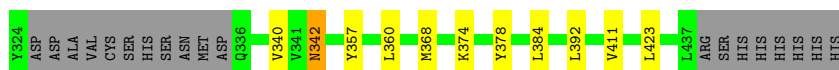
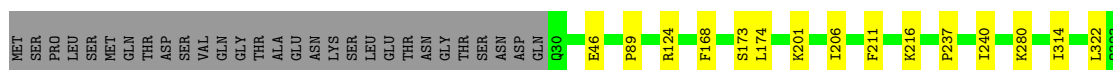
- Molecule 1: Dimethylallyl tryptophan synthase

Chain E: 84% 5% 11%



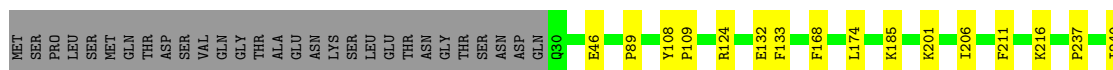
- Molecule 1: Dimethylallyl tryptophan synthase

Chain F: 83% 6% 11%



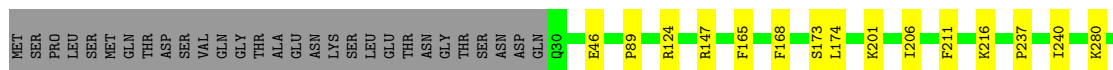
- Molecule 1: Dimethylallyl tryptophan synthase

Chain G: 82% 7% 11%



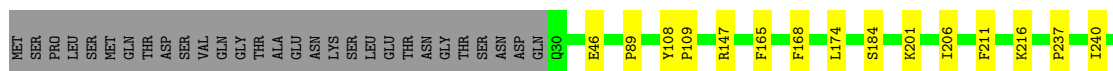
- Molecule 1: Dimethylallyl tryptophan synthase

Chain H: 83% 6% 11%



- Molecule 1: Dimethylallyl tryptophan synthase

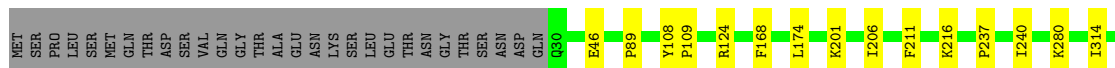
Chain I: 83% 6% 11%





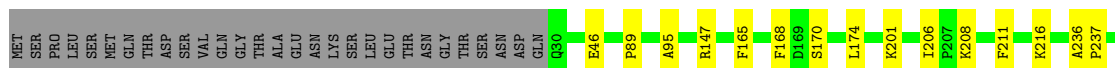
- Molecule 1: Dimethylallyl tryptophan synthase

Chain J: 83% 6% 11%



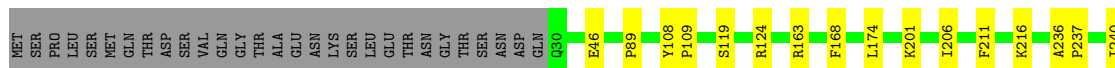
- Molecule 1: Dimethylallyl tryptophan synthase

Chain K: 82% 6% 12%



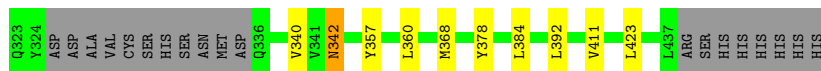
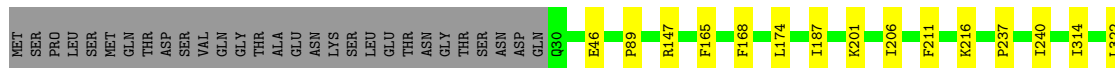
- Molecule 1: Dimethylallyl tryptophan synthase

Chain L: 83% 6% 11%



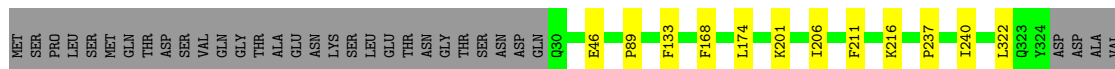
- Molecule 1: Dimethylallyl tryptophan synthase

Chain M: 84% 5% 11%



- Molecule 1: Dimethylallyl tryptophan synthase

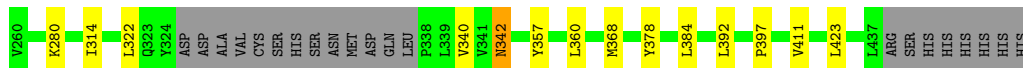
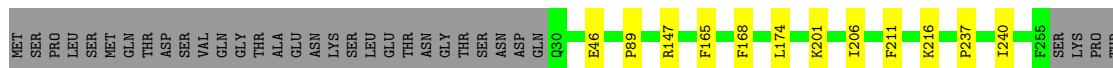
Chain N: 84% 0% 11%





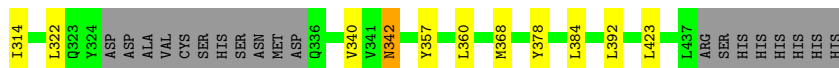
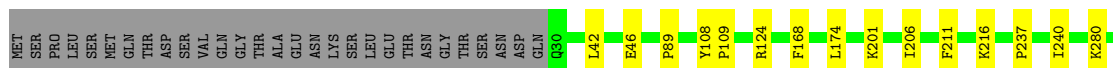
- Molecule 1: Dimethylallyl tryptophan synthase

Chain O: 82% 6% 12%



- Molecule 1: Dimethylallyl tryptophan synthase

Chain P: 83% 6% 11%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.55Å 242.59Å 145.32Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	39.95 – 2.83 39.95 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.95-2.83) 99.8 (39.95-2.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0044	Depositor
R, $R_{free}$	0.203 , 0.202 0.201 , 0.204	Depositor DCC
$R_{free}$ test set	3202 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 19.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.449 for h,-k,-l	Xtriage
Reported twinning fraction	0.544 for H, K, L 0.456 for -h,-k,l	Depositor
Outliers	0 of 160059 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	48979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

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

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	0.41	0/3136	0.75	0/4276
1	B	0.41	0/3135	0.76	0/4275
1	C	0.41	0/3137	0.76	0/4277
1	D	0.41	0/3133	0.76	0/4273
1	E	0.41	0/3129	0.76	0/4267
1	F	0.41	0/3135	0.76	0/4275
1	G	0.41	0/3137	0.76	0/4277
1	H	0.41	0/3137	0.76	0/4277
1	I	0.41	0/3135	0.76	0/4275
1	J	0.41	0/3137	0.76	0/4277
1	K	0.41	0/3099	0.76	0/4223
1	L	0.41	0/3137	0.76	0/4277
1	M	0.41	0/3129	0.76	0/4268
1	N	0.41	0/3137	0.76	0/4277
1	O	0.41	0/3089	0.76	0/4210
1	P	0.41	0/3137	0.76	0/4277
All	All	0.41	0/50079	0.76	0/68281

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3057	0	2943	18	0
1	B	3056	0	2947	19	0
1	C	3058	0	2946	19	0
1	D	3054	0	2942	26	0
1	E	3050	0	2930	16	0
1	F	3056	0	2942	17	0
1	G	3058	0	2946	28	0
1	H	3058	0	2946	17	0
1	I	3056	0	2940	18	0
1	J	3058	0	2946	18	0
1	K	3022	0	2904	22	0
1	L	3058	0	2946	19	0
1	M	3050	0	2928	20	0
1	N	3058	0	2946	14	0
1	O	3012	0	2890	17	0
1	P	3058	0	2946	17	0
2	A	9	0	0	1	0
2	B	9	0	0	1	0
2	C	9	0	0	1	0
2	D	9	0	0	1	0
2	E	9	0	0	0	0
2	F	9	0	0	2	0
2	G	9	0	0	3	0
2	H	9	0	0	2	0
2	I	9	0	0	0	0
2	J	9	0	0	2	0
2	K	9	0	0	1	0
2	L	9	0	0	1	0
2	M	9	0	0	0	0
2	N	9	0	0	0	0
2	O	9	0	0	1	0
2	P	9	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
All	All	48979	0	46988	281	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 3.

The worst 5 of 281 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:F:374:LYS:CB	1:L:119:SER:HB3	2.16	0.75
1:D:245:ARG:O	1:D:249:THR:HG23	1.87	0.75
1:G:185:LYS:HB3	1:M:187:ILE:HG21	1.70	0.74
1:D:95:ALA:CB	1:K:95:ALA:HB2	2.18	0.72
1:D:95:ALA:HB2	1:K:95:ALA:HB2	1.71	0.72

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	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	B	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	C	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	D	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	E	393/445 (88%)	387 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	393/445 (88%)	386 (98%)	7 (2%)	0	100	100
1	G	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	H	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	I	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	J	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	K	386/445 (87%)	380 (98%)	6 (2%)	0	100	100
1	L	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	M	393/445 (88%)	386 (98%)	7 (2%)	0	100	100
1	N	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	O	385/445 (86%)	379 (98%)	6 (2%)	0	100	100
1	P	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
All	All	6273/7120 (88%)	6175 (98%)	98 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	307/382 (80%)	303 (99%)	4 (1%)	61	79
1	B	308/382 (81%)	303 (98%)	5 (2%)	55	76
1	C	308/382 (81%)	304 (99%)	4 (1%)	61	79
1	D	308/382 (81%)	304 (99%)	4 (1%)	61	79
1	E	306/382 (80%)	302 (99%)	4 (1%)	61	79
1	F	308/382 (81%)	303 (98%)	5 (2%)	55	76
1	G	308/382 (81%)	304 (99%)	4 (1%)	61	79
1	H	308/382 (81%)	303 (98%)	5 (2%)	55	76
1	I	306/382 (80%)	302 (99%)	4 (1%)	61	79
1	J	308/382 (81%)	304 (99%)	4 (1%)	61	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	303/382 (79%)	299 (99%)	4 (1%)	61	79
1	L	308/382 (81%)	304 (99%)	4 (1%)	61	79
1	M	306/382 (80%)	302 (99%)	4 (1%)	61	79
1	N	308/382 (81%)	304 (99%)	4 (1%)	61	79
1	O	302/382 (79%)	298 (99%)	4 (1%)	61	79
1	P	308/382 (81%)	304 (99%)	4 (1%)	61	79
All	All	4910/6112 (80%)	4843 (99%)	67 (1%)	59	78

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	392	LEU
1	O	342	ASN
1	P	392	LEU
1	F	392	LEU
1	F	384	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	408	GLN
1	M	82	HIS
1	K	82	HIS
1	L	82	HIS
1	M	408	GLN

### 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](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

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
2	PIS	C	501	-	5,8,8	1.30	0	8,13,13	1.65	1 (12%)
2	PIS	E	501	-	5,8,8	3.17	2 (40%)	8,13,13	1.47	1 (12%)
2	PIS	P	501	-	5,8,8	3.21	2 (40%)	8,13,13	1.64	1 (12%)
2	PIS	I	501	-	5,8,8	3.19	2 (40%)	8,13,13	1.59	1 (12%)
2	PIS	J	501	-	5,8,8	1.40	1 (20%)	8,13,13	1.76	1 (12%)
2	PIS	O	501	-	5,8,8	1.38	1 (20%)	8,13,13	1.72	1 (12%)
2	PIS	F	501	-	5,8,8	3.20	2 (40%)	8,13,13	1.74	2 (25%)
2	PIS	N	501	-	5,8,8	1.43	1 (20%)	8,13,13	1.65	1 (12%)
2	PIS	K	501	-	5,8,8	1.38	1 (20%)	8,13,13	1.54	1 (12%)
2	PIS	A	501	-	5,8,8	3.21	2 (40%)	8,13,13	1.59	1 (12%)
2	PIS	G	501	-	5,8,8	1.30	1 (20%)	8,13,13	1.73	1 (12%)
2	PIS	B	501	-	5,8,8	1.25	0	8,13,13	1.79	2 (25%)
2	PIS	L	501	-	5,8,8	3.20	2 (40%)	8,13,13	1.59	1 (12%)
2	PIS	M	501	-	5,8,8	3.27	2 (40%)	8,13,13	1.65	1 (12%)
2	PIS	D	501	-	5,8,8	3.22	2 (40%)	8,13,13	1.73	1 (12%)
2	PIS	H	501	-	5,8,8	3.17	2 (40%)	8,13,13	1.66	1 (12%)

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
2	PIS	C	501	-	-	3/4/6/6	-
2	PIS	E	501	-	-	0/4/6/6	-
2	PIS	P	501	-	-	0/4/6/6	-
2	PIS	I	501	-	-	0/4/6/6	-
2	PIS	J	501	-	-	0/4/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PIS	O	501	-	-	1/4/6/6	-
2	PIS	F	501	-	-	0/4/6/6	-
2	PIS	N	501	-	-	0/4/6/6	-
2	PIS	K	501	-	-	0/4/6/6	-
2	PIS	A	501	-	-	0/4/6/6	-
2	PIS	G	501	-	-	0/4/6/6	-
2	PIS	B	501	-	-	1/4/6/6	-
2	PIS	L	501	-	-	0/4/6/6	-
2	PIS	M	501	-	-	0/4/6/6	-
2	PIS	D	501	-	-	1/4/6/6	-
2	PIS	H	501	-	-	0/4/6/6	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	501	PIS	P2-O6	6.86	1.61	1.46
2	P	501	PIS	P2-O6	6.74	1.61	1.46
2	D	501	PIS	P2-O6	6.72	1.61	1.46
2	L	501	PIS	P2-O6	6.71	1.61	1.46
2	A	501	PIS	P2-O6	6.71	1.61	1.46

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PIS	O4-P2-O6	4.09	118.78	109.86
2	D	501	PIS	O4-P2-O6	4.08	118.75	109.86
2	J	501	PIS	O4-P2-O6	4.06	118.72	109.86
2	G	501	PIS	O4-P2-O6	4.05	118.69	109.86
2	F	501	PIS	O4-P2-O6	4.00	118.59	109.86

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PIS	P1-O1-P2-O4
2	C	501	PIS	P2-O1-P1-O2
2	D	501	PIS	P1-O1-P2-O4
2	O	501	PIS	P1-O1-P2-O4
2	C	501	PIS	P2-O1-P1-O5

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PIS	1	0
2	P	501	PIS	2	0
2	J	501	PIS	2	0
2	O	501	PIS	1	0
2	F	501	PIS	2	0
2	K	501	PIS	1	0
2	A	501	PIS	1	0
2	G	501	PIS	3	0
2	B	501	PIS	1	0
2	L	501	PIS	1	0
2	D	501	PIS	1	0
2	H	501	PIS	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, 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	A	397/445 (89%)	-1.52	0 100 100	28, 43, 66, 77	0
1	B	397/445 (89%)	-1.49	0 100 100	29, 48, 73, 86	0
1	C	397/445 (89%)	-1.47	0 100 100	28, 46, 70, 84	0
1	D	397/445 (89%)	-1.49	0 100 100	31, 46, 72, 88	0
1	E	397/445 (89%)	-1.47	0 100 100	31, 50, 69, 83	0
1	F	397/445 (89%)	-1.36	0 100 100	32, 54, 89, 100	0
1	G	397/445 (89%)	-1.47	0 100 100	30, 50, 72, 85	0
1	H	397/445 (89%)	-1.47	0 100 100	31, 49, 78, 97	0
1	I	397/445 (89%)	-1.07	0 100 100	50, 78, 110, 121	0
1	J	397/445 (89%)	-1.42	0 100 100	37, 55, 81, 92	0
1	K	392/445 (88%)	-1.13	0 100 100	53, 76, 106, 116	0
1	L	397/445 (89%)	-0.87	0 100 100	59, 92, 133, 148	0
1	M	397/445 (89%)	-1.07	0 100 100	58, 80, 110, 119	0
1	N	397/445 (89%)	-1.32	0 100 100	47, 62, 76, 88	0
1	O	391/445 (87%)	-1.12	0 100 100	57, 78, 103, 113	0
1	P	397/445 (89%)	-1.10	0 100 100	57, 75, 98, 119	0
All	All	6341/7120 (89%)	-1.30	0 100 100	28, 62, 103, 148	0

There are no RSRZ outliers to report.

### 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](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	I	502	1/1	0.94	0.06	121,121,121,121	0
3	NA	O	502	1/1	0.97	0.05	59,59,59,59	0
3	NA	L	502	1/1	0.98	0.04	89,89,89,89	0
3	NA	K	502	1/1	0.98	0.03	70,70,70,70	0
2	PIS	L	501	9/9	0.99	0.02	49,51,54,55	0
2	PIS	N	501	9/9	0.99	0.03	38,40,41,41	0
2	PIS	P	501	9/9	0.99	0.03	42,47,49,50	0
3	NA	A	502	1/1	0.99	0.03	51,51,51,51	0
3	NA	D	502	1/1	0.99	0.02	43,43,43,43	0
3	NA	F	502	1/1	0.99	0.06	92,92,92,92	0
3	NA	H	502	1/1	0.99	0.05	60,60,60,60	0
2	PIS	E	501	9/9	0.99	0.03	33,34,37,42	0
3	NA	J	502	1/1	0.99	0.08	104,104,104,104	0
2	PIS	F	501	9/9	0.99	0.03	37,38,40,42	0
2	PIS	I	501	9/9	0.99	0.02	44,46,48,48	0
3	NA	M	502	1/1	0.99	0.02	49,49,49,49	0
3	NA	N	502	1/1	0.99	0.03	60,60,60,60	0
2	PIS	K	501	9/9	0.99	0.03	45,49,52,56	0
3	NA	P	502	1/1	0.99	0.03	58,58,58,58	0
2	PIS	C	501	9/9	1.00	0.02	32,33,36,39	0
3	NA	E	502	1/1	1.00	0.02	51,51,51,51	0
2	PIS	J	501	9/9	1.00	0.02	30,31,32,35	0
3	NA	G	502	1/1	1.00	0.02	39,39,39,39	0
2	PIS	D	501	9/9	1.00	0.03	30,31,34,37	0
2	PIS	A	501	9/9	1.00	0.02	32,34,35,36	0
2	PIS	M	501	9/9	1.00	0.02	45,47,48,50	0
2	PIS	B	501	9/9	1.00	0.02	29,31,32,34	0
2	PIS	O	501	9/9	1.00	0.02	47,50,52,55	0
2	PIS	G	501	9/9	1.00	0.02	32,35,37,37	0
2	PIS	H	501	9/9	1.00	0.03	34,35,36,38	0
3	NA	B	502	1/1	1.00	0.04	60,60,60,60	0
3	NA	C	502	1/1	1.00	0.04	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.