



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:45 PM GMT

PDB ID : 1C2Y  
Title : CRYSTAL STRUCTURES OF A PENTAMERIC FUNGAL AND AN ICOSAHERAL PLANT LUMAZINE SYNTHASE REVEALS THE STRUCTURAL BASIS FOR DIFFERENCES IN ASSEMBLY  
Authors : Persson, K.; Schneider, G.; Jordan, D.B.; Viitanen, P.V.; Sandalova, T.  
Deposited on : 1999-07-27  
Resolution : 3.30 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

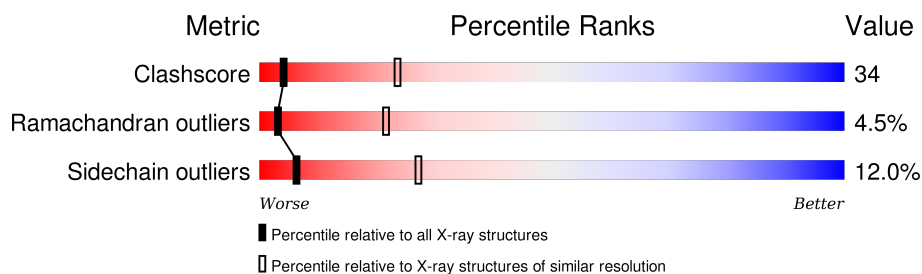
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	
1	B	156	
1	C	156	
1	D	156	
1	E	156	
1	F	156	
1	G	156	

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Mol	Chain	Length	Quality of chain
1	H	156	 40% 51% 6% ..
1	I	156	 49% 42% 7% ..
1	J	156	 40% 51% 7% ..
1	K	156	 44% 47% 6% ..
1	L	156	 47% 44% 8% ..
1	M	156	 41% 49% 8% ..
1	N	156	 44% 47% 7% ..
1	O	156	 44% 48% 6% ..
1	P	156	 48% 43% 7% ..
1	Q	156	 45% 46% 8% ..
1	R	156	 49% 42% 8% ..
1	S	156	 46% 45% 7% ..
1	T	156	 42% 49% 6% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMZ	E	205	-	-	X	-
2	LMZ	G	207	-	-	X	-
2	LMZ	I	209	-	-	X	-
2	LMZ	K	211	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23500 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 PROTEIN (LUMAZINE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	B	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	C	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	D	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	E	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	F	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	G	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	H	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	I	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	J	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	K	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	L	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	M	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	N	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	O	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	P	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	R	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	S	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	T	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			

There are 40 discrepancies between the modelled and reference sequences:

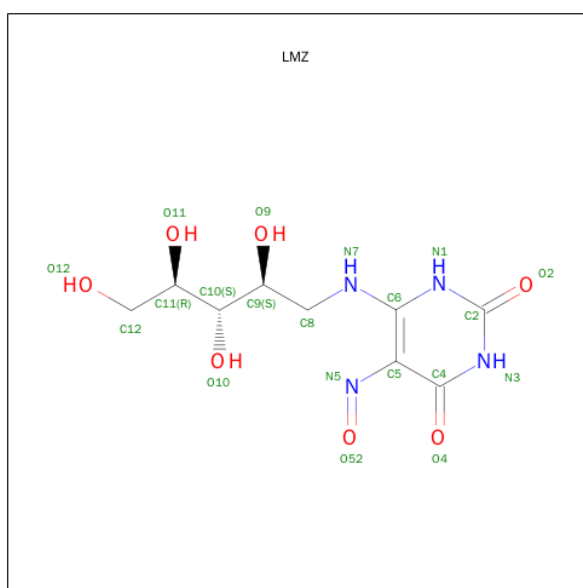
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	VAL	engineered	UNP Q9XH32
A	2	ASN	ARG	engineered	UNP Q9XH32
B	1	MET	VAL	engineered	UNP Q9XH32
B	2	ASN	ARG	engineered	UNP Q9XH32
C	1	MET	VAL	engineered	UNP Q9XH32
C	2	ASN	ARG	engineered	UNP Q9XH32
D	1	MET	VAL	engineered	UNP Q9XH32
D	2	ASN	ARG	engineered	UNP Q9XH32
E	1	MET	VAL	engineered	UNP Q9XH32
E	2	ASN	ARG	engineered	UNP Q9XH32
F	1	MET	VAL	engineered	UNP Q9XH32
F	2	ASN	ARG	engineered	UNP Q9XH32
G	1	MET	VAL	engineered	UNP Q9XH32
G	2	ASN	ARG	engineered	UNP Q9XH32
H	1	MET	VAL	engineered	UNP Q9XH32
H	2	ASN	ARG	engineered	UNP Q9XH32
I	1	MET	VAL	engineered	UNP Q9XH32
I	2	ASN	ARG	engineered	UNP Q9XH32
J	1	MET	VAL	engineered	UNP Q9XH32
J	2	ASN	ARG	engineered	UNP Q9XH32
K	1	MET	VAL	engineered	UNP Q9XH32
K	2	ASN	ARG	engineered	UNP Q9XH32
L	1	MET	VAL	engineered	UNP Q9XH32
L	2	ASN	ARG	engineered	UNP Q9XH32
M	1	MET	VAL	engineered	UNP Q9XH32
M	2	ASN	ARG	engineered	UNP Q9XH32
N	1	MET	VAL	engineered	UNP Q9XH32
N	2	ASN	ARG	engineered	UNP Q9XH32
O	1	MET	VAL	engineered	UNP Q9XH32
O	2	ASN	ARG	engineered	UNP Q9XH32
P	1	MET	VAL	engineered	UNP Q9XH32

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Chain	Residue	Modelled	Actual	Comment	Reference
P	2	ASN	ARG	engineered	UNP Q9XH32
Q	1	MET	VAL	engineered	UNP Q9XH32
Q	2	ASN	ARG	engineered	UNP Q9XH32
R	1	MET	VAL	engineered	UNP Q9XH32
R	2	ASN	ARG	engineered	UNP Q9XH32
S	1	MET	VAL	engineered	UNP Q9XH32
S	2	ASN	ARG	engineered	UNP Q9XH32
T	1	MET	VAL	engineered	UNP Q9XH32
T	2	ASN	ARG	engineered	UNP Q9XH32

- Molecule 2 is 5-NITROSO-6-RIBITYL-AMINO-2,4(1H,3H)-PYRIMIDINEDIONE (three-letter code: LMZ) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>4</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	9	4	7		
2	B	1	Total	C	N	O	0	0
			20	9	4	7		
2	C	1	Total	C	N	O	0	0
			20	9	4	7		
2	D	1	Total	C	N	O	0	0
			20	9	4	7		
2	E	1	Total	C	N	O	0	0
			20	9	4	7		
2	F	1	Total	C	N	O	0	0
			20	9	4	7		

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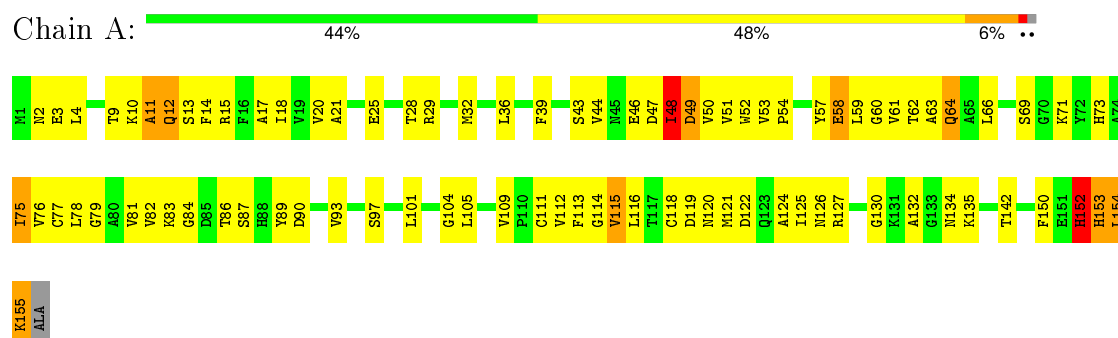
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			20	9	4	7		
2	H	1	Total	C	N	O	0	0
			20	9	4	7		
2	I	1	Total	C	N	O	0	0
			20	9	4	7		
2	J	1	Total	C	N	O	0	0
			20	9	4	7		
2	K	1	Total	C	N	O	0	0
			20	9	4	7		
2	L	1	Total	C	N	O	0	0
			20	9	4	7		
2	M	1	Total	C	N	O	0	0
			20	9	4	7		
2	N	1	Total	C	N	O	0	0
			20	9	4	7		
2	O	1	Total	C	N	O	0	0
			20	9	4	7		
2	P	1	Total	C	N	O	0	0
			20	9	4	7		
2	Q	1	Total	C	N	O	0	0
			20	9	4	7		
2	R	1	Total	C	N	O	0	0
			20	9	4	7		
2	S	1	Total	C	N	O	0	0
			20	9	4	7		
2	T	1	Total	C	N	O	0	0
			20	9	4	7		

### 3 Residue-property plots

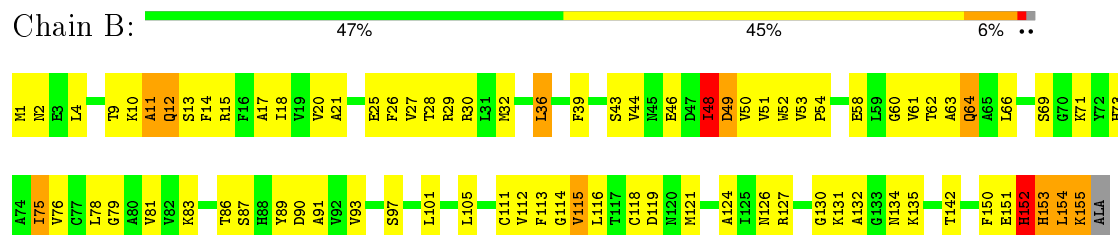
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

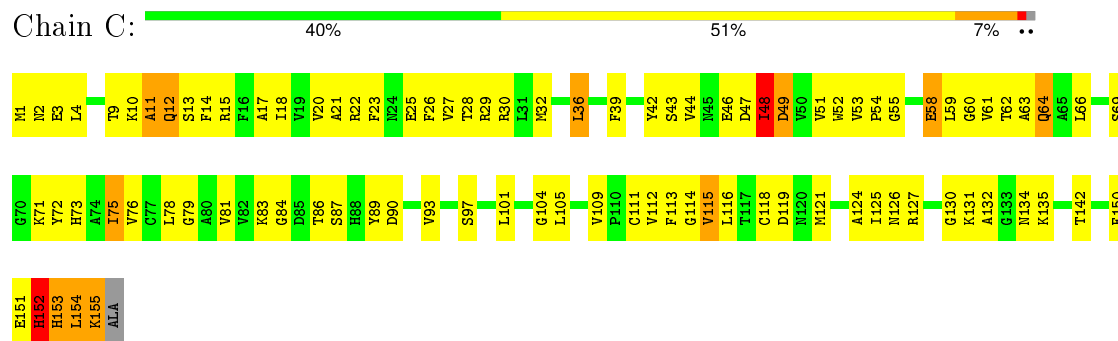
#### • Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



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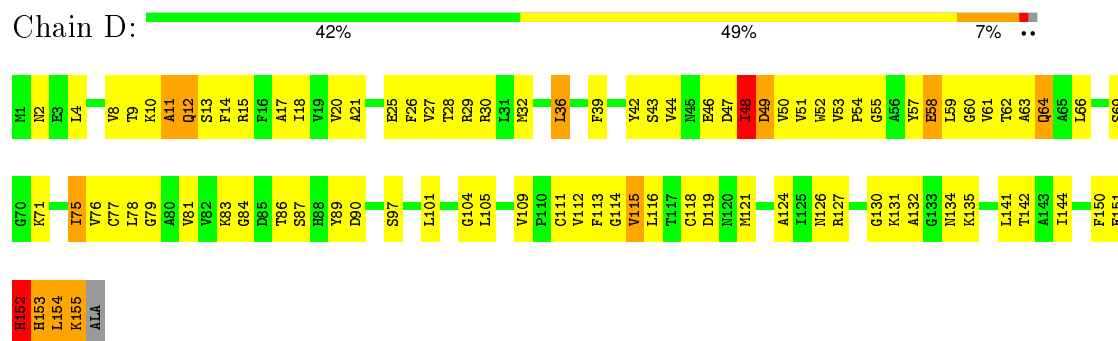


#### • Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

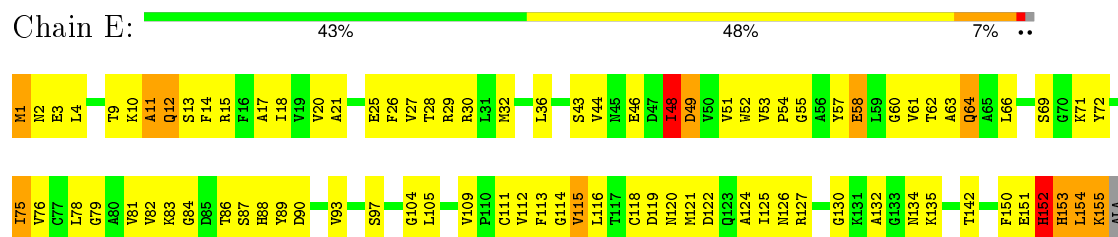


#### • Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

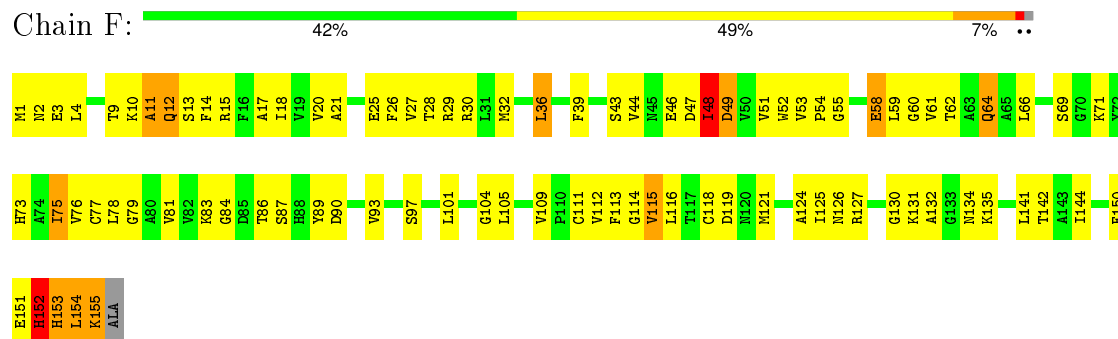




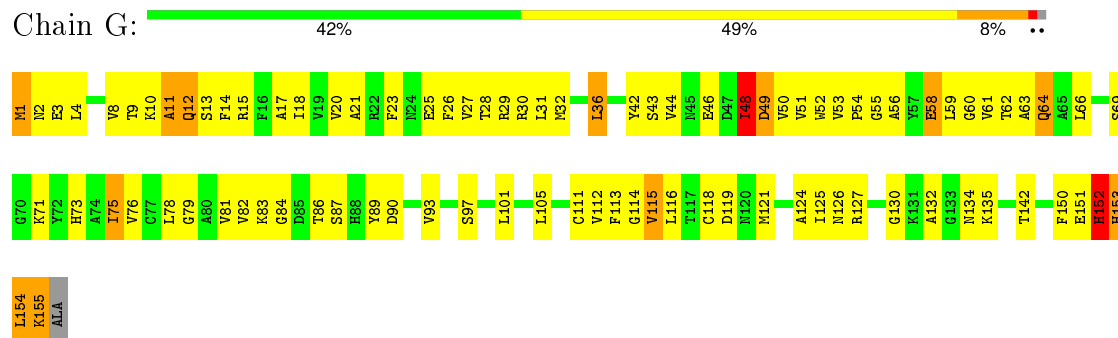
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

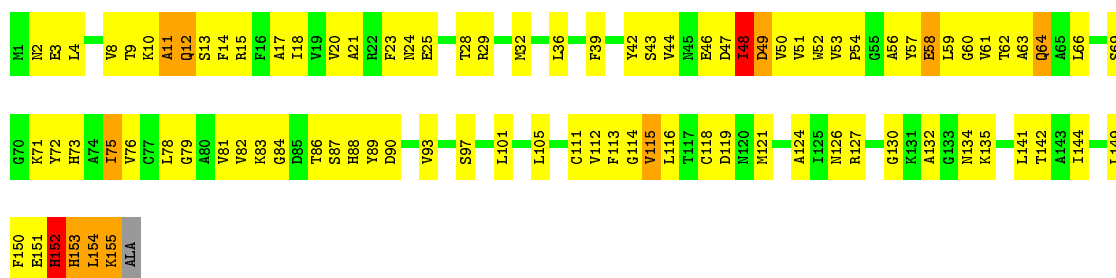


• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



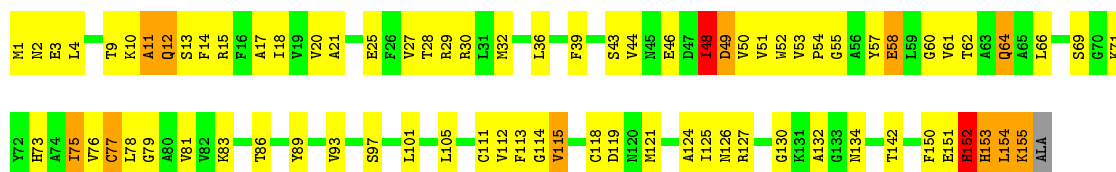
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)





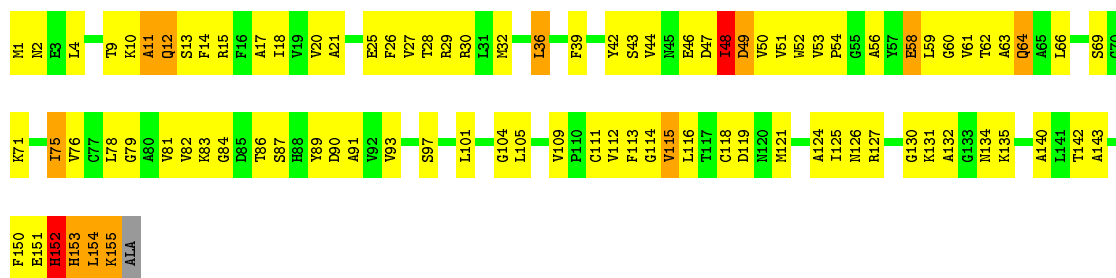
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain I: 49% 42% 7% ..



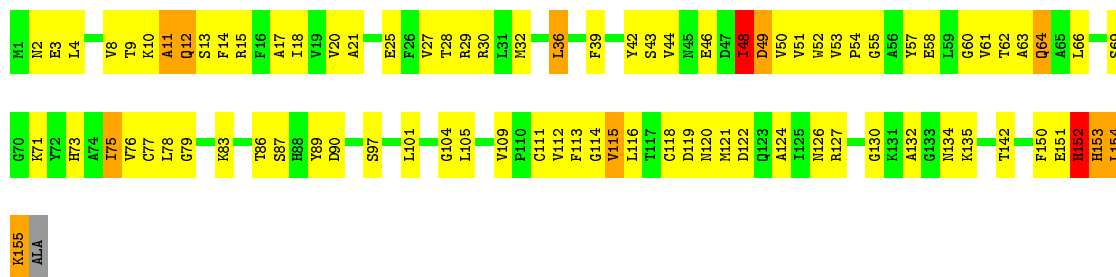
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain J: 40% 51% 7% ..



• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain K: 44% 47% 6% ..



• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

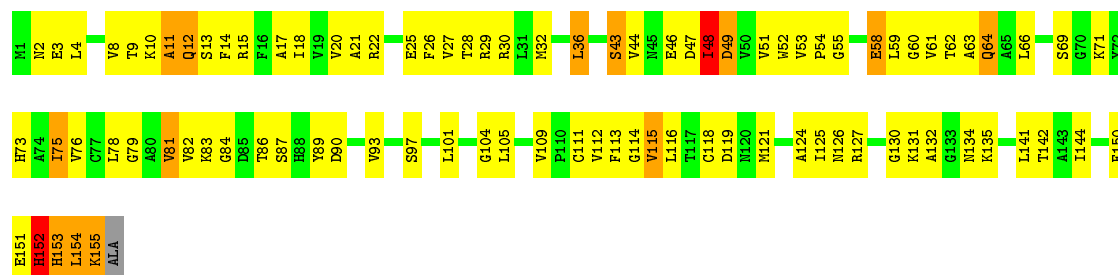
Chain L: 47% 44% 8% ..





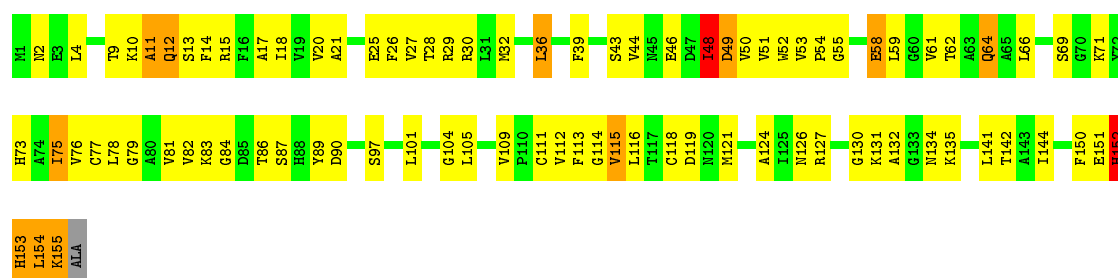
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain M: 41% 49% 8% ..



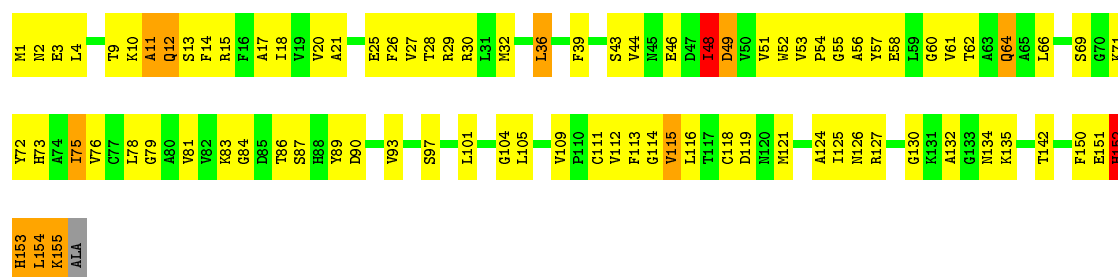
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain N: 44% 47% 7% ..



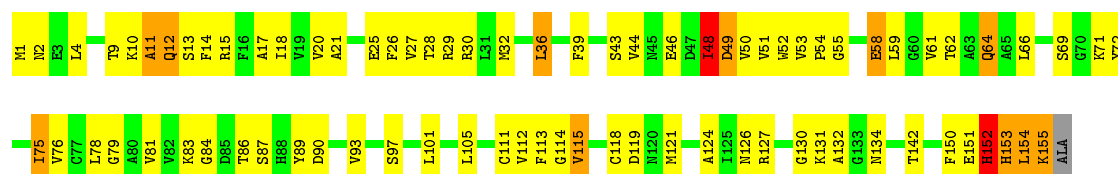
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain O: 44% 48% 6% ..



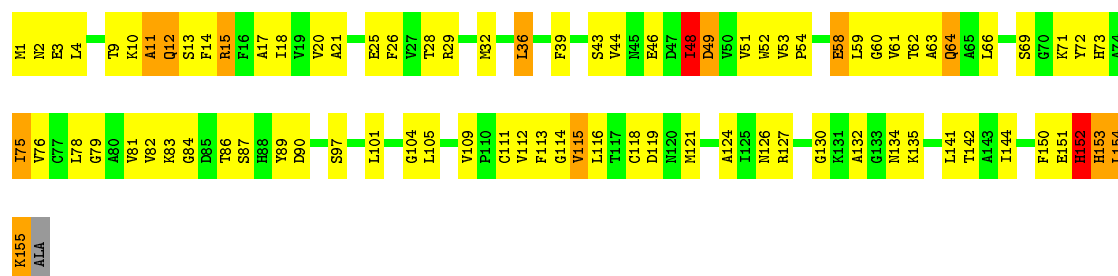
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain P: 48% 43% 7% ..



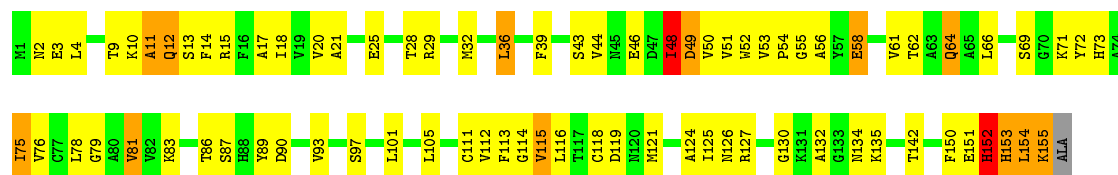
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain Q:  45% 46% 8% ..



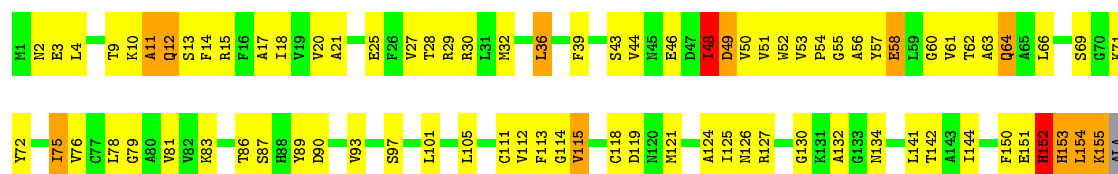
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain R:  49% 42% 8% ..



• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain S:  46% 45% 7% ..



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.24Å 218.24Å 218.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-3.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	11.10	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.310 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.73	0/1174	0.76	0/1586
1	B	0.75	0/1174	0.76	0/1586
1	C	0.74	0/1174	0.76	0/1586
1	D	0.73	0/1174	0.77	0/1586
1	E	0.74	0/1174	0.76	0/1586
1	F	0.72	0/1174	0.76	0/1586
1	G	0.72	0/1174	0.76	0/1586
1	H	0.72	0/1174	0.76	0/1586
1	I	0.72	0/1174	0.77	0/1586
1	J	0.73	0/1174	0.76	0/1586
1	K	0.70	0/1174	0.76	0/1586
1	L	0.71	0/1174	0.76	0/1586
1	M	0.72	0/1174	0.76	0/1586
1	N	0.72	0/1174	0.77	0/1586
1	O	0.74	0/1174	0.75	0/1586
1	P	0.73	0/1174	0.76	0/1586
1	Q	0.74	0/1174	0.76	0/1586
1	R	0.73	0/1174	0.76	0/1586
1	S	0.74	0/1174	0.75	0/1586
1	T	0.73	0/1174	0.76	0/1586
All	All	0.73	0/23480	0.76	0/31720

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	1155	0	1145	87	0
1	B	1155	0	1145	84	0
1	C	1155	0	1145	98	0
1	D	1155	0	1145	96	0
1	E	1155	0	1145	90	0
1	F	1155	0	1145	95	0
1	G	1155	0	1145	92	0
1	H	1155	0	1145	99	0
1	I	1155	0	1145	87	0
1	J	1155	0	1145	95	0
1	K	1155	0	1145	84	0
1	L	1155	0	1145	89	0
1	M	1155	0	1145	99	0
1	N	1155	0	1145	88	0
1	O	1155	0	1145	90	0
1	P	1155	0	1145	88	0
1	Q	1155	0	1145	90	0
1	R	1155	0	1145	83	0
1	S	1155	0	1145	85	0
1	T	1155	0	1145	88	0
2	A	20	0	14	5	0
2	B	20	0	14	4	0
2	C	20	0	14	4	0
2	D	20	0	14	4	0
2	E	20	0	14	7	0
2	F	20	0	14	4	0
2	G	20	0	14	7	0
2	H	20	0	14	4	0
2	I	20	0	14	7	0
2	J	20	0	14	5	0
2	K	20	0	14	7	0
2	L	20	0	14	5	0
2	M	20	0	14	5	0
2	N	20	0	14	3	0
2	O	20	0	14	5	0
2	P	20	0	14	5	0
2	Q	20	0	14	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	20	0	14	4	0
2	S	20	0	14	4	0
2	T	20	0	14	3	0
All	All	23500	0	23180	1573	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 34.

The worst 5 of 1573 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:N:12:GLN:HA	1:N:44:VAL:HA	1.46	0.97
1:K:12:GLN:HA	1:K:44:VAL:HA	1.47	0.97
1:E:12:GLN:HA	1:E:44:VAL:HA	1.48	0.96
1:H:12:GLN:HA	1:H:44:VAL:HA	1.48	0.96
1:F:86:THR:HG21	1:J:118:CYS:HA	1.48	0.95

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	153/156 (98%)	120 (78%)	26 (17%)	7 (5%)	3	21
1	B	153/156 (98%)	120 (78%)	26 (17%)	7 (5%)	3	21
1	C	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	3	21
1	D	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	3	21
1	E	153/156 (98%)	117 (76%)	29 (19%)	7 (5%)	3	21
1	F	153/156 (98%)	119 (78%)	27 (18%)	7 (5%)	3	21
1	G	153/156 (98%)	119 (78%)	27 (18%)	7 (5%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	153/156 (98%)	120 (78%)	26 (17%)	7 (5%)	3	21
1	I	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	3	21
1	J	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	3	21
1	K	153/156 (98%)	119 (78%)	27 (18%)	7 (5%)	3	21
1	L	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	3	21
1	M	153/156 (98%)	119 (78%)	27 (18%)	7 (5%)	3	21
1	N	153/156 (98%)	118 (77%)	29 (19%)	6 (4%)	4	25
1	O	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	3	21
1	P	153/156 (98%)	121 (79%)	26 (17%)	6 (4%)	4	25
1	Q	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	3	21
1	R	153/156 (98%)	119 (78%)	28 (18%)	6 (4%)	4	25
1	S	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	3	21
1	T	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	3	21
All	All	3060/3120 (98%)	2373 (78%)	550 (18%)	137 (4%)	3	21

5 of 137 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	48	ILE
1	B	12	GLN
1	B	48	ILE
1	C	12	GLN

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/120 (100%)	106 (88%)	14 (12%)	7	28
1	B	120/120 (100%)	106 (88%)	14 (12%)	7	28
1	C	120/120 (100%)	106 (88%)	14 (12%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	120/120 (100%)	105 (88%)	15 (12%)	6	24
1	E	120/120 (100%)	106 (88%)	14 (12%)	7	28
1	F	120/120 (100%)	105 (88%)	15 (12%)	6	24
1	G	120/120 (100%)	105 (88%)	15 (12%)	6	24
1	H	120/120 (100%)	107 (89%)	13 (11%)	8	32
1	I	120/120 (100%)	106 (88%)	14 (12%)	7	28
1	J	120/120 (100%)	106 (88%)	14 (12%)	7	28
1	K	120/120 (100%)	106 (88%)	14 (12%)	7	28
1	L	120/120 (100%)	105 (88%)	15 (12%)	6	24
1	M	120/120 (100%)	106 (88%)	14 (12%)	7	28
1	N	120/120 (100%)	105 (88%)	15 (12%)	6	24
1	O	120/120 (100%)	105 (88%)	15 (12%)	6	24
1	P	120/120 (100%)	105 (88%)	15 (12%)	6	24
1	Q	120/120 (100%)	104 (87%)	16 (13%)	5	21
1	R	120/120 (100%)	106 (88%)	14 (12%)	7	28
1	S	120/120 (100%)	106 (88%)	14 (12%)	7	28
1	T	120/120 (100%)	105 (88%)	15 (12%)	6	24
All	All	2400/2400 (100%)	2111 (88%)	289 (12%)	6	27

5 of 289 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	36	LEU
1	L	49	ASP
1	S	64	GLN
1	J	58	GLU
1	K	48	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	88	HIS
1	K	153	HIS
1	S	12	GLN
1	I	153	HIS

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Mol	Chain	Res	Type
1	J	153	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	LMZ	A	201	-	15,20,20	2.52	7 (46%)	18,27,27	3.88	8 (44%)
2	LMZ	B	202	-	15,20,20	2.65	6 (40%)	18,27,27	4.08	9 (50%)
2	LMZ	C	203	-	15,20,20	2.93	7 (46%)	18,27,27	4.06	8 (44%)
2	LMZ	D	204	-	15,20,20	2.88	8 (53%)	18,27,27	4.16	8 (44%)
2	LMZ	E	205	-	15,20,20	2.89	8 (53%)	18,27,27	3.94	9 (50%)
2	LMZ	F	206	-	15,20,20	2.78	6 (40%)	18,27,27	4.02	7 (38%)
2	LMZ	G	207	-	15,20,20	2.87	7 (46%)	18,27,27	4.21	8 (44%)
2	LMZ	H	208	-	15,20,20	2.64	9 (60%)	18,27,27	3.99	8 (44%)
2	LMZ	I	209	-	15,20,20	3.09	9 (60%)	18,27,27	3.90	8 (44%)
2	LMZ	J	210	-	15,20,20	3.02	8 (53%)	18,27,27	4.10	8 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LMZ	K	211	-	15,20,20	3.05	10 (66%)	18,27,27	4.22	9 (50%)
2	LMZ	L	212	-	15,20,20	2.60	6 (40%)	18,27,27	3.90	9 (50%)
2	LMZ	M	213	-	15,20,20	3.22	7 (46%)	18,27,27	4.06	8 (44%)
2	LMZ	N	214	-	15,20,20	3.01	8 (53%)	18,27,27	4.06	8 (44%)
2	LMZ	O	215	-	15,20,20	2.82	6 (40%)	18,27,27	4.08	9 (50%)
2	LMZ	P	216	-	15,20,20	2.57	7 (46%)	18,27,27	3.93	8 (44%)
2	LMZ	Q	217	-	15,20,20	2.76	6 (40%)	18,27,27	4.06	9 (50%)
2	LMZ	R	218	-	15,20,20	2.75	8 (53%)	18,27,27	3.85	8 (44%)
2	LMZ	S	219	-	15,20,20	2.64	8 (53%)	18,27,27	3.99	8 (44%)
2	LMZ	T	220	-	15,20,20	2.97	7 (46%)	18,27,27	4.23	8 (44%)

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	LMZ	A	201	-	-	0/17/17/17	0/1/1/1
2	LMZ	B	202	-	-	0/17/17/17	0/1/1/1
2	LMZ	C	203	-	-	0/17/17/17	0/1/1/1
2	LMZ	D	204	-	-	0/17/17/17	0/1/1/1
2	LMZ	E	205	-	-	0/17/17/17	0/1/1/1
2	LMZ	F	206	-	-	0/17/17/17	0/1/1/1
2	LMZ	G	207	-	-	0/17/17/17	0/1/1/1
2	LMZ	H	208	-	-	0/17/17/17	0/1/1/1
2	LMZ	I	209	-	-	0/17/17/17	0/1/1/1
2	LMZ	J	210	-	-	0/17/17/17	0/1/1/1
2	LMZ	K	211	-	-	0/17/17/17	0/1/1/1
2	LMZ	L	212	-	-	0/17/17/17	0/1/1/1
2	LMZ	M	213	-	-	0/17/17/17	0/1/1/1
2	LMZ	N	214	-	-	0/17/17/17	0/1/1/1
2	LMZ	O	215	-	-	0/17/17/17	0/1/1/1
2	LMZ	P	216	-	-	0/17/17/17	0/1/1/1
2	LMZ	Q	217	-	-	0/17/17/17	0/1/1/1
2	LMZ	R	218	-	-	0/17/17/17	0/1/1/1
2	LMZ	S	219	-	-	0/17/17/17	0/1/1/1
2	LMZ	T	220	-	-	0/17/17/17	0/1/1/1

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	211	LMZ	O9-C9	-2.08	1.38	1.43
2	H	208	LMZ	O10-C10	-2.08	1.38	1.43
2	I	209	LMZ	C12-C11	2.00	1.57	1.52
2	H	208	LMZ	C5-N5	2.01	1.42	1.35
2	J	210	LMZ	C5-N5	2.01	1.42	1.35

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	207	LMZ	O11-C11-C10	-6.42	92.88	109.02
2	H	208	LMZ	O11-C11-C10	-6.26	93.28	109.02
2	K	211	LMZ	O11-C11-C10	-6.12	93.62	109.02
2	F	206	LMZ	O11-C11-C10	-5.98	93.97	109.02
2	D	204	LMZ	O11-C11-C10	-5.94	94.07	109.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	LMZ	5	0
2	B	202	LMZ	4	0
2	C	203	LMZ	4	0
2	D	204	LMZ	4	0
2	E	205	LMZ	7	0
2	F	206	LMZ	4	0
2	G	207	LMZ	7	0
2	H	208	LMZ	4	0
2	I	209	LMZ	7	0
2	J	210	LMZ	5	0
2	K	211	LMZ	7	0
2	L	212	LMZ	5	0
2	M	213	LMZ	5	0
2	N	214	LMZ	3	0
2	O	215	LMZ	5	0
2	P	216	LMZ	5	0
2	Q	217	LMZ	4	0
2	R	218	LMZ	4	0
2	S	219	LMZ	4	0
2	T	220	LMZ	3	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.