

Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 12:25 AM EDT

PDB ID	:	5IM4
Title	:	Crystal structure of designed two-component self-assembling icosahedral cage
		I52-32
Authors	:	Liu, Y.A.; Cascio, D.; Sawaya, M.R.; Bale, J.B.; Collazo, M.J.; Thomas, C.;
		Sheffler, W.; King, N.P.; Baker, D.; Yeates, T.O.
Deposited on	:	2016-03-05
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution $(//Entries - resolution - resolution)$		
	(#Entries)	(#Entries, resolution range(A))		
R _{free}	130704	1659 (3.60-3.40)		
Ramachandran outliers	138981	1005 (3.58-3.42)		
Sidechain outliers	138945	1006 (3.58-3.42)		
RSRZ outliers	127900	1559(3.60-3.40)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	А	162	4% 82%		17%
		102	3%	•	1770
1	В	162	82%	•	15%
1	С	162	82%	•	15%
1	D	169	4%		100/
	D	102	3%	•	19%
1	Е	162	80%	•	18%
1	K	162	2% 81%	•	17%



Mol	Chain	Length	Quality of chain	
1	т	169	5%	1.00/
1		102	<u> </u>	16%
1	М	162	82%	14%
1	N	100	4%	
<u>I</u>	IN	162	80% •	17%
1	Ο	162	7 8% •	20%
1	тт	1.60	2%	
	U	162	80% •	17%
1	V	162	81% •	16%
-		1.00	4%	
	W	162	79% ·	19%
1	Х	162	79% •	19%
			.%	
1	Y	162	81% ·	17%
1	е	162	80%	18%
			4%	
1	f	162	80% •	17%
1	g	162	78%	20%
	-		4%	
1	h	162	79% •	18%
1	i	162	81%	17%
			4%	
2	F	138	93%	• 5%
2	G	138	93%	• 5%
2	Н	138	91%	• 5%
2	Т	138	3% 	5%
	1	100	2%	• 570
2	J	138	92%	• 5%
2	Р	138	% •	. 5%
	1	100	3%	٥/ L •
2	Q	138	93%	• 5%
0	Ъ	128	3%	F0/
	10	190	<u>5%</u> 91%	• 5%
2	S	138	93%	• 5%
0	Т	190	%	
	1	138	92% 5%_	• 5%
2	Z	138	93%	• 5%



Mol	Chain	Length	Quality of chain	
2	a	138	% 92%	• 5%
2	b	138	% 93%	• 5%
2	с	138	% 92%	• 5%
2	d	138	^{2%} 92%	• 5%
2	j	138	% 92%	• 5%
2	k	138	3% 92%	• 5%
2	1	138	.% 92%	• 5%
2	m	138	93%	• 5%
2	n	138	% 92%	• 5%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 40538 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace								
1	Δ	195	Total	С	Ν	0	S	0	0	0								
1	A	199	1031	670	172	185	4	0	0	0								
1	Б	199	Total	С	Ν	0	S	0	0	0								
	E	100	1016	662	169	181	4	0	0	0								
1	C	127	Total	С	Ν	0	S	0	0	0								
		137	1051	680	177	190	4	0	0	0								
1	В	137	Total	С	Ν	0	S	0	0	0								
1	D	137	1051	682	179	186	4	0	0	0								
1	Л	139	Total	С	Ν	0	S	0	0	0								
1	D	132	1013	660	171	178	4	0	0	0								
1	K	135	Total	С	Ν	Ο	\mathbf{S}	0	0	0								
1	Γ	155	1032	670	174	184	4	0	0	0								
1	т	136	Total	С	Ν	0	S	0	0	0								
1		150	1045	677	175	189	4	0	0	0								
1	N	N	N	N	N	N	N	N	N	134	Total	С	Ν	0	S	0	0	0
	1	104	1023	664	172	183	4	0	0	0								
1	м	M 130	Total	С	Ν	0	S	0	0	0								
1	111	139	1072	693	181	194	4	0	0	0								
1	0	130	Total	С	Ν	0	S	0	0	0								
1		150	993	648	166	175	4		0	0	0							
1	II	134	Total	С	Ν	0	S	0	0	0								
1	U	134	1018	661	171	182	4	0	0	0								
1	V	136	Total	С	Ν	0	S	0	0	0								
1	v	150	1036	672	175	185	4	0	0	0								
1	v	139	Total	С	Ν	0	S	0	0	0								
1	Λ	132	1013	659	170	180	4	0	0	0								
1	W/	120	Total	С	Ν	0	S	0	0	0								
1	vv	132	1009	657	170	178	4	U	0	0								
1	v	125	Total	С	Ν	Ο	S	0	0	0								
	1	100	1017	659	170	184	4			U								
1	0	192	Total	С	Ν	Ο	S	0	0	0								
	е	100	1018	662	171	181	4	U	U	0								

• Molecule 1 is a protein called 6,7-dimethyl-8-ribityllumazine synthase.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1 (f	124	Total	С	Ν	0	S	0	0	0
1	1	134	1027	667	172	184	4	0		
1	h	199	Total	С	Ν	0	S	0	0	0
1 n	199	1008	657	168	179	4	0	0	0	
1		120	Total	С	Ν	0	S	0	0	0
1 g	190	995	648	168	175	4	0	0	U	
1 i	135	Total	С	Ν	0	S	0	0	0	
		1026	666	170	186	4			0	

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	11	MET	-	expression tag	UNP A0A0A3CUI3
А	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
А	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
А	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
А	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
А	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
А	165	LEU	-	expression tag	UNP A0A0A3CUI3
А	166	GLU	-	expression tag	UNP A0A0A3CUI3
A	167	HIS	-	expression tag	UNP A0A0A3CUI3
А	168	HIS	-	expression tag	UNP A0A0A3CUI3
А	169	HIS	-	expression tag	UNP A0A0A3CUI3
A	170	HIS	-	expression tag	UNP A0A0A3CUI3
А	171	HIS	-	expression tag	UNP A0A0A3CUI3
A	172	HIS	-	expression tag	UNP A0A0A3CUI3
Е	11	MET	-	expression tag	UNP A0A0A3CUI3
E	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
E	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
E	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
E	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
E	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
Е	165	LEU	-	expression tag	UNP A0A0A3CUI3
E	166	GLU	-	expression tag	UNP A0A0A3CUI3
Ε	167	HIS	-	expression tag	UNP A0A0A3CUI3
E	168	HIS	-	expression tag	UNP A0A0A3CUI3
E	169	HIS	-	expression tag	UNP A0A0A3CUI3
E	170	HIS	-	expression tag	UNP A0A0A3CUI3
E	171	HIS	-	expression tag	UNP A0A0A3CUI3
Е	172	HIS	-	expression tag	UNP A0A0A3CUI3
С	11	MET	-	expression tag	UNP A0A0A3CUI3
С	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
С	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3



Chain	Residue	Modelled	Actual	Comment	Reference
С	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
C	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
C	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
C	165	LEU	_	expression tag	UNP A0A0A3CUI3
C	166	GLU	_	expression tag	UNP A0A0A3CUI3
С	167	HIS	_	expression tag	UNP A0A0A3CUI3
C	168	HIS	_	expression tag	UNP A0A0A3CUI3
С	169	HIS	-	expression tag	UNP A0A0A3CUI3
С	170	HIS	-	expression tag	UNP A0A0A3CUI3
С	171	HIS	-	expression tag	UNP A0A0A3CUI3
С	172	HIS	_	expression tag	UNP A0A0A3CUI3
В	11	MET	-	expression tag	UNP A0A0A3CUI3
В	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
В	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
В	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
В	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
В	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
В	165	LEU	_	expression tag	UNP A0A0A3CUI3
В	166	GLU	-	expression tag	UNP A0A0A3CUI3
В	167	HIS	_	expression tag	UNP A0A0A3CUI3
В	168	HIS	_	expression tag	UNP A0A0A3CUI3
В	169	HIS	_	expression tag	UNP A0A0A3CUI3
В	170	HIS	_	expression tag	UNP A0A0A3CUI3
В	171	HIS	_	expression tag	UNP A0A0A3CUI3
В	172	HIS	-	expression tag	UNP A0A0A3CUI3
D	11	MET	-	expression tag	UNP A0A0A3CUI3
D	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
D	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
D	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
D	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
D	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
D	165	LEU	-	expression tag	UNP A0A0A3CUI3
D	166	GLU	-	expression tag	UNP A0A0A3CUI3
D	167	HIS	-	expression tag	UNP A0A0A3CUI3
D	168	HIS	-	expression tag	UNP A0A0A3CUI3
D	169	HIS	-	expression tag	UNP A0A0A3CUI3
D	170	HIS	-	expression tag	UNP A0A0A3CUI3
D	171	HIS	-	expression tag	UNP A0A0A3CUI3
D	172	HIS	-	expression tag	UNP A0A0A3CUI3
Κ	11	MET	-	expression tag	UNP A0A0A3CUI3
K	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3

Continued on next page...

engineered mutation UNP A0A0A3CUI3



GLU

Κ

30

LYS

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
K	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
K	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
K	165	LEU	-	expression tag	UNP A0A0A3CUI3
K	166	GLU	_	expression tag	UNP A0A0A3CUI3
K	167	HIS	_	expression tag	UNP A0A0A3CUI3
K	168	HIS	-	expression tag	UNP A0A0A3CUI3
K	169	HIS	-	expression tag	UNP A0A0A3CUI3
K	170	HIS	-	expression tag	UNP A0A0A3CUI3
K	171	HIS	-	expression tag	UNP A0A0A3CUI3
K	172	HIS	-	expression tag	UNP A0A0A3CUI3
L	11	MET	-	expression tag	UNP A0A0A3CUI3
L	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
L	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
L	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
L	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
L	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
L	165	LEU	-	expression tag	UNP A0A0A3CUI3
L	166	GLU	-	expression tag	UNP A0A0A3CUI3
L	167	HIS	-	expression tag	UNP A0A0A3CUI3
L	168	HIS	-	expression tag	UNP A0A0A3CUI3
L	169	HIS	-	expression tag	UNP A0A0A3CUI3
L	170	HIS	-	expression tag	UNP A0A0A3CUI3
L	171	HIS	-	expression tag	UNP A0A0A3CUI3
L	172	HIS	-	expression tag	UNP A0A0A3CUI3
Ν	11	MET	-	expression tag	UNP A0A0A3CUI3
N	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
N	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
N	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
N	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
N	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
N	165	LEU	-	expression tag	UNP A0A0A3CUI3
N	166	GLU	-	expression tag	UNP A0A0A3CUI3
N	167	HIS	-	expression tag	UNP A0A0A3CUI3
N	168	HIS	-	expression tag	UNP A0A0A3CUI3
N	169	HIS	-	expression tag	UNP A0A0A3CUI3
N	170	HIS	-	expression tag	UNP A0A0A3CUI3
N	171	HIS	-	expression tag	UNP A0A0A3CUI3
N	172	HIS	-	expression tag	UNP A0A0A3CUI3
M	11	MET	-	expression tag	UNP A0A0A3CUI3
M	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
M	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3



5IM4

Chain		Modelled	Actual	Comment	Reference
М	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
M	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
М	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
M	165	LEU		expression tag	UNP A0A0A3CUI3
М	166	GLU	-	expression tag	UNP A0A0A3CUI3
М	167	HIS	_	expression tag	UNP A0A0A3CUI3
М	168	HIS	_	expression tag	UNP A0A0A3CUI3
М	169	HIS	_	expression tag	UNP A0A0A3CUI3
М	170	HIS	_	expression tag	UNP A0A0A3CUI3
М	171	HIS	-	expression tag	UNP A0A0A3CUI3
М	172	HIS	-	expression tag	UNP A0A0A3CUI3
0	11	MET	-	expression tag	UNP A0A0A3CUI3
0	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
0	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
0	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
0	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
0	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
0	165	LEU	-	expression tag	UNP A0A0A3CUI3
0	166	GLU	-	expression tag	UNP A0A0A3CUI3
0	167	HIS	-	expression tag	UNP A0A0A3CUI3
0	168	HIS	-	expression tag	UNP A0A0A3CUI3
0	169	HIS	-	expression tag	UNP A0A0A3CUI3
0	170	HIS	-	expression tag	UNP A0A0A3CUI3
0	171	HIS	_	expression tag	UNP A0A0A3CUI3
0	172	HIS	-	expression tag	UNP A0A0A3CUI3
U	11	MET	-	expression tag	UNP A0A0A3CUI3
U	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
U	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
U	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
U	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
U	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
U	165	LEU	-	expression tag	UNP A0A0A3CUI3
U	166	GLU	-	expression tag	UNP A0A0A3CUI3
U	167	HIS	-	expression tag	UNP A0A0A3CUI3
U	168	HIS	-	expression tag	UNP A0A0A3CUI3
U	169	HIS		expression tag	UNP A0A0A3CUI3
U	170	HIS	-	expression tag	UNP A0A0A3CUI3
U	171	HIS	-	expression tag	UNP A0A0A3CUI3
U	172	HIS	-	expression tag	UNP A0A0A3CUI3
V	11	MET	_	expression tag	UNP A0A0A3CUI3
V	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
V	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3



Chain	Residue	Modelled	Actual	Comment	Reference
V	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
V	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
V	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
V	165	LEU	-	expression tag	UNP A0A0A3CUI3
V	166	GLU	-	expression tag	UNP A0A0A3CUI3
V	167	HIS	-	expression tag	UNP A0A0A3CUI3
V	168	HIS	-	expression tag	UNP A0A0A3CUI3
V	169	HIS	-	expression tag	UNP A0A0A3CUI3
V	170	HIS	-	expression tag	UNP A0A0A3CUI3
V	171	HIS	-	expression tag	UNP A0A0A3CUI3
V	172	HIS	-	expression tag	UNP A0A0A3CUI3
Х	11	MET	-	expression tag	UNP A0A0A3CUI3
Х	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
Х	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
Х	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
Х	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
Х	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
Х	165	LEU	_	expression tag	UNP A0A0A3CUI3
Х	166	GLU	-	expression tag	UNP A0A0A3CUI3
Х	167	HIS	-	expression tag	UNP A0A0A3CUI3
Х	168	HIS	-	expression tag	UNP A0A0A3CUI3
Х	169	HIS	-	expression tag	UNP A0A0A3CUI3
Х	170	HIS	-	expression tag	UNP A0A0A3CUI3
Х	171	HIS	-	expression tag	UNP A0A0A3CUI3
Х	172	HIS	-	expression tag	UNP A0A0A3CUI3
W	11	MET	-	expression tag	UNP A0A0A3CUI3
W	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
W	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
W	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
W	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
W	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
W	165	LEU	-	expression tag	UNP A0A0A3CUI3
W	166	GLU	-	expression tag	UNP A0A0A3CUI3
W	167	HIS	-	expression tag	UNP A0A0A3CUI3
W	168	HIS	-	expression tag	UNP A0A0A3CUI3
W	169	HIS	-	expression tag	UNP A0A0A3CUI3
W	170	HIS	-	expression tag	UNP A0A0A3CUI3
W	171	HIS	-	expression tag	UNP A0A0A3CUI3
W	172	HIS	-	expression tag	UNP A0A0A3CUI3
Y	11	MET	-	expression tag	UNP A0A0A3CUI3
Y	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
Y	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3



Chain	Residue	Modelled	Actual	Comment	Reference
Y	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
Y	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
Y	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
Y	165	LEU	-	expression tag	UNP A0A0A3CUI3
Y	166	GLU	-	expression tag	UNP A0A0A3CUI3
Y	167	HIS	_	expression tag	UNP A0A0A3CUI3
Y	168	HIS	_	expression tag	UNP A0A0A3CUI3
Y	169	HIS	-	expression tag	UNP A0A0A3CUI3
Y	170	HIS	-	expression tag	UNP A0A0A3CUI3
Y	171	HIS	-	expression tag	UNP A0A0A3CUI3
Y	172	HIS	_	expression tag	UNP A0A0A3CUI3
е	11	MET	-	expression tag	UNP A0A0A3CUI3
е	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
е	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
е	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
е	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
е	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
е	165	LEU	-	expression tag	UNP A0A0A3CUI3
е	166	GLU	-	expression tag	UNP A0A0A3CUI3
е	167	HIS	-	expression tag	UNP A0A0A3CUI3
е	168	HIS	-	expression tag	UNP A0A0A3CUI3
е	169	HIS	-	expression tag	UNP A0A0A3CUI3
e	170	HIS	-	expression tag	UNP A0A0A3CUI3
e	171	HIS	-	expression tag	UNP A0A0A3CUI3
е	172	HIS	-	expression tag	UNP A0A0A3CUI3
f	11	MET	-	expression tag	UNP A0A0A3CUI3
f	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
f	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
f	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
f	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
f	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
f	165	LEU	-	expression tag	UNP A0A0A3CUI3
f	166	GLU	-	expression tag	UNP A0A0A3CUI3
f	167	HIS	-	expression tag	UNP A0A0A3CUI3
f	168	HIS	-	expression tag	UNP A0A0A3CUI3
f	169	HIS	-	expression tag	UNP A0A0A3CUI3
f	170	HIS	-	expression tag	UNP A0A0A3CUI3
f	171	HIS	-	expression tag	UNP A0A0A3CUI3
f	172	HIS	-	expression tag	UNP A0A0A3CUI3
h	11	MET	-	expression tag	UNP A0A0A3CUI3
h	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
h	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3



Chain	Residue	Modelled	Actual	Comment	Reference
h	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
h	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
h	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
h	165	LEU	-	expression tag	UNP A0A0A3CUI3
h	166	GLU	_	expression tag	UNP A0A0A3CUI3
h	167	HIS	-	expression tag	UNP A0A0A3CUI3
h	168	HIS	-	expression tag	UNP A0A0A3CUI3
h	169	HIS	-	expression tag	UNP A0A0A3CUI3
h	170	HIS	-	expression tag	UNP A0A0A3CUI3
h	171	HIS	-	expression tag	UNP A0A0A3CUI3
h	172	HIS	-	expression tag	UNP A0A0A3CUI3
g	11	MET	-	expression tag	UNP A0A0A3CUI3
g	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
g	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
g	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
g	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
g	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
g	165	LEU	-	expression tag	UNP A0A0A3CUI3
g	166	GLU	-	expression tag	UNP A0A0A3CUI3
g	167	HIS	-	expression tag	UNP A0A0A3CUI3
g	168	HIS	-	expression tag	UNP A0A0A3CUI3
g	169	HIS	-	expression tag	UNP A0A0A3CUI3
g	170	HIS	-	expression tag	UNP A0A0A3CUI3
g	171	HIS	-	expression tag	UNP A0A0A3CUI3
g	172	HIS	-	expression tag	UNP A0A0A3CUI3
i	11	MET	-	expression tag	UNP A0A0A3CUI3
i	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
i	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
i	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
i	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
i	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
i	165	LEU	-	expression tag	UNP A0A0A3CUI3
i	166	GLU	-	expression tag	UNP A0A0A3CUI3
i	167	HIS	-	expression tag	UNP A0A0A3CUI3
i	168	HIS	-	expression tag	UNP A0A0A3CUI3
i	169	HIS	-	expression tag	UNP A0A0A3CUI3
i	170	HIS	-	expression tag	UNP A0A0A3CUI3
i	171	HIS	-	expression tag	UNP A0A0A3CUI3
i	172	HIS	-	expression tag	UNP A0A0A3CUI3

• Molecule 2 is a protein called Phosphotransferase system, mannose/fructose-specific component IIA.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	Б	121	Total	С	Ν	Ο	S	0	0	0
	Г	101	1000	649	160	185	6	0	0	0
9	ц	121	Total	С	Ν	0	S	0	0	0
	11	131	1004	651	160	187	6	0	0	0
2	G	131	Total	С	Ν	0	S	0	0	0
	u	101	996	646	159	185	6	0	0	0
2	Т	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	1	101	1000	649	160	185	6	0	0	0
2	I	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	0	101	1004	651	160	187	6	0	0	0
2	Р	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	1	101	1004	651	160	187	6	0	0	0
2	0	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	<u>بر</u>	101	1004	651	160	187	6	Ŭ		
2	S	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
		101	1000	649	160	185	6	Ŭ		
2	В	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	10	101	1008	653	160	189	6	0	0	0
2	Т	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	-	101	1004	651	160	187	6	0	0	0
2	h	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	0	101	1000	649	160	185	6	0	0	0
2	d	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	u	101	1004	651	160	187	6	0	0	0
2	C	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	Ŭ	101	1000	649	160	185	6	0	0	0
2	Z	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	2	101	1004	651	160	187	6	Ŭ		0
2	а	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	a	101	1004	651	160	187	6	0	0	0
2	i	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	J	101	1004	651	160	187	6	0	0	0
2	k	131	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	К	101	1008	653	160	189	6	0	0	0
2	m	131	Total	\mathbf{C}	Ν	0	S	0	0	0
		101	1000	649	160	185	6			0
2	1	131	Total	С	Ν	Ο	\mathbf{S}	0	0	Ο
	1	101	996	647	160	183	6			0
2	n	131	Total	C	N	0	\mathbf{S}	0	0	0
	11	101	1000	649	160	185	6			0

There are 240 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	MET	-	expression tag	UNP Q8RD55
F	0	GLY	-	expression tag	UNP Q8RD55
F	45	LYS	VAL	engineered mutation	UNP Q8RD55
F	47	ALA	ARG	engineered mutation	UNP Q8RD55
F	51	MET	GLU	engineered mutation	UNP Q8RD55
F	52	ARG	LYS	engineered mutation	UNP Q8RD55
F	55	ILE	LYS	engineered mutation	UNP Q8RD55
F	56	ALA	GLU	engineered mutation	UNP Q8RD55
F	59	ALA	GLN	engineered mutation	UNP Q8RD55
F	81	GLU	SER	engineered mutation	UNP Q8RD55
F	85	THR	GLU	engineered mutation	UNP Q8RD55
F	86	PHE	TYR	engineered mutation	UNP Q8RD55
Н	-1	MET	-	expression tag	UNP Q8RD55
Н	0	GLY	-	expression tag	UNP Q8RD55
Н	45	LYS	VAL	engineered mutation	UNP Q8RD55
Н	47	ALA	ARG	engineered mutation	UNP Q8RD55
Н	51	MET	GLU	engineered mutation	UNP Q8RD55
Н	52	ARG	LYS	engineered mutation	UNP Q8RD55
Н	55	ILE	LYS	engineered mutation	UNP Q8RD55
Н	56	ALA	GLU	engineered mutation	UNP Q8RD55
Н	59	ALA	GLN	engineered mutation	UNP Q8RD55
Н	81	GLU	SER	engineered mutation	UNP Q8RD55
Н	85	THR	GLU	engineered mutation	UNP Q8RD55
Н	86	PHE	TYR	engineered mutation	UNP Q8RD55
G	-1	MET	-	expression tag	UNP Q8RD55
G	0	GLY	-	expression tag	UNP Q8RD55
G	45	LYS	VAL	engineered mutation	UNP Q8RD55
G	47	ALA	ARG	engineered mutation	UNP Q8RD55
G	51	MET	GLU	engineered mutation	UNP Q8RD55
G	52	ARG	LYS	engineered mutation	UNP Q8RD55
G	55	ILE	LYS	engineered mutation	UNP Q8RD55
G	56	ALA	GLU	engineered mutation	UNP Q8RD55
G	59	ALA	GLN	engineered mutation	UNP Q8RD55
G	81	GLU	SER	engineered mutation	UNP Q8RD55
G	85	THR	GLU	engineered mutation	UNP Q8RD55
G	86	PHE	TYR	engineered mutation	UNP Q8RD55
I	-1	MET	-	expression tag	UNP Q8RD55
I	0	GLY	-	expression tag	UNP Q8RD55
I	45	LYS	VAL	engineered mutation	UNP Q8RD55
	47	ALA	ARG	engineered mutation	UNP Q8RD55
1	51	MET	GLU	engineered mutation	UNP Q8RD55
	52	ARG	LYS	engineered mutation	UNP Q8RD55
I	55	ILE	LYS	engineered mutation	UNP Q8RD55
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Chain	Residue	Modelled	Actual	Comment	Reference
Ι	56	ALA	GLU	engineered mutation	UNP Q8RD55
Ι	59	ALA	GLN	engineered mutation	UNP Q8RD55
Ι	81	GLU	SER	engineered mutation	UNP Q8RD55
Ι	85	THR	GLU	engineered mutation	UNP Q8RD55
Ι	86	PHE	TYR	engineered mutation	UNP Q8RD55
J	-1	MET	-	expression tag	UNP Q8RD55
J	0	GLY	-	expression tag	UNP Q8RD55
J	45	LYS	VAL	engineered mutation	UNP Q8RD55
J	47	ALA	ARG	engineered mutation	UNP Q8RD55
J	51	MET	GLU	engineered mutation	UNP Q8RD55
J	52	ARG	LYS	engineered mutation	UNP Q8RD55
J	55	ILE	LYS	engineered mutation	UNP Q8RD55
J	56	ALA	GLU	engineered mutation	UNP Q8RD55
J	59	ALA	GLN	engineered mutation	UNP Q8RD55
J	81	GLU	SER	engineered mutation	UNP Q8RD55
J	85	THR	GLU	engineered mutation	UNP Q8RD55
J	86	PHE	TYR	engineered mutation	UNP Q8RD55
P	-1	MET	-	expression tag	UNP Q8RD55
P	0	GLY	-	expression tag	UNP Q8RD55
P	45	LYS	VAL	engineered mutation	UNP Q8RD55
P	47	ALA	ARG	engineered mutation	UNP Q8RD55
P	51	MET	GLU	engineered mutation	UNP Q8RD55
P	52	ARG	LYS	engineered mutation	UNP Q8RD55
P	55	ILE	LYS	engineered mutation	UNP Q8RD55
P	56	ALA	GLU	engineered mutation	UNP Q8RD55
P	59	ALA	GLN	engineered mutation	UNP Q8RD55
P	81	GLU	SER	engineered mutation	UNP Q8RD55
P	85	THR	GLU	engineered mutation	UNP Q8RD55
Р	86	PHE	TYR	engineered mutation	UNP Q8RD55
Q	-1	MET	-	expression tag	UNP Q8RD55
Q	0	GLY	-	expression tag	UNP Q8RD55
Q	45	LYS	VAL	engineered mutation	UNP Q8RD55
Q	47	ALA	ARG	engineered mutation	UNP Q8RD55
Q	51	MET	GLU	engineered mutation	UNP Q8RD55
Q	52	ARG	LYS	engineered mutation	UNP Q8RD55
Q	55	ILE	LYS	engineered mutation	UNP Q8RD55
Q	56	ALA	GLU	engineered mutation	UNP Q8RD55
Q	59	ALA	GLN	engineered mutation	UNP Q8RD55
Q	81	GLU	SER	engineered mutation	UNP Q8RD55
Q	85	'THR	GLU	engineered mutation	UNP Q8RD55
Q	86	PHE	TYR	engineered mutation	UNP Q8RD55
S	-1	MET	-	expression tag	UNP Q8RD55



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GLY	-	expression tag	UNP Q8RD55
LYS	VAL	engineered mutation	UNP Q8RD55
ALA	ARG	engineered mutation	UNP Q8RD55
MET	GLU	engineered mutation	UNP Q8RD55
ARG	LYS	engineered mutation	UNP Q8RD55
ILE	LYS	engineered mutation	UNP Q8RD55
ALA	GLU	engineered mutation	UNP Q8RD55
ALA	GLN	engineered mutation	UNP Q8RD55
GLU	SER	engineered mutation	UNP Q8RD55
THR	GLU	engineered mutation	UNP Q8RD55
PHE	TYR	engineered mutation	UNP Q8RD55
MET	-	expression tag	UNP Q8RD55
GLY	-	expression tag	UNP Q8RD55
LYS	VAL	engineered mutation	UNP Q8RD55
ALA	ARG	engineered mutation	UNP Q8RD55
MET	GLU	engineered mutation	UNP Q8RD55
ARG	LYS	engineered mutation	UNP Q8RD55
ILE	LYS	engineered mutation	UNP Q8RD55
ALA	GLU	engineered mutation	UNP Q8RD55
ALA	GLN	engineered mutation	UNP Q8RD55
GLU	SER	engineered mutation	UNP Q8RD55
THR	GLU	engineered mutation	UNP Q8RD55
PHE	TYR	engineered mutation	UNP Q8RD55
MET	-	expression tag	UNP Q8RD55
GLY	-	expression tag	UNP Q8RD55
LYS	VAL	engineered mutation	UNP Q8RD55
ALA	ARG	engineered mutation	UNP Q8RD55
MET	GLU	engineered mutation	UNP Q8RD55
ARG	LYS	engineered mutation	UNP Q8RD55
ILE	LYS	engineered mutation	UNP Q8RD55
ALA	GLU	engineered mutation	UNP Q8RD55

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Residue Modelled Actual

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UNP Q8RD55

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Chain	Residue	Modelled	Actual	Comment	Reference
b	56	ALA	GLU	engineered mutation	UNP Q8RD55
b	59	ALA	GLN	engineered mutation	UNP Q8RD55
b	81	GLU	SER	engineered mutation	UNP Q8RD55
b	85	THR	GLU	engineered mutation	UNP Q8RD55
b	86	PHE	TYR	engineered mutation	UNP Q8RD55
d	-1	MET	-	expression tag	UNP Q8RD55
d	0	GLY	-	expression tag	UNP Q8RD55
d	45	LYS	VAL	engineered mutation	UNP Q8RD55
d	47	ALA	ARG	engineered mutation	UNP Q8RD55
d	51	MET	GLU	engineered mutation	UNP Q8RD55
d	52	ARG	LYS	engineered mutation	UNP Q8RD55
d	55	ILE	LYS	engineered mutation	UNP Q8RD55
d	56	ALA	GLU	engineered mutation	UNP Q8RD55
d	59	ALA	GLN	engineered mutation	UNP Q8RD55
d	81	GLU	SER	engineered mutation	UNP Q8RD55
d	85	THR	GLU	engineered mutation	UNP Q8RD55
d	86	PHE	TYR	engineered mutation	UNP Q8RD55
с	-1	MET	-	expression tag	UNP Q8RD55
с	0	GLY	-	expression tag	UNP Q8RD55
с	45	LYS	VAL	engineered mutation	UNP Q8RD55
с	47	ALA	ARG	engineered mutation	UNP Q8RD55
с	51	MET	GLU	engineered mutation	UNP Q8RD55
с	52	ARG	LYS	engineered mutation	UNP Q8RD55
с	55	ILE	LYS	engineered mutation	UNP Q8RD55
с	56	ALA	GLU	engineered mutation	UNP Q8RD55
с	59	ALA	GLN	engineered mutation	UNP Q8RD55
с	81	GLU	SER	engineered mutation	UNP Q8RD55
с	85	THR	GLU	engineered mutation	UNP Q8RD55
с	86	PHE	TYR	engineered mutation	UNP Q8RD55
Ζ	-1	MET	-	expression tag	UNP Q8RD55
Z	0	GLY	-	expression tag	UNP Q8RD55
Z	45	LYS	VAL	engineered mutation	UNP Q8RD55
Z	47	ALA	ARG	engineered mutation	UNP Q8RD55
Z	51	MET	GLU	engineered mutation	UNP Q8RD55
Z	52	ARG	LYS	engineered mutation	UNP Q8RD55
Ζ	55	ILE	LYS	engineered mutation	UNP Q8RD55
Ζ	56	ALA	GLU	engineered mutation	UNP Q8RD55
Z	59	ALA	GLN	engineered mutation	UNP Q8RD55
Ζ	81	GLU	SER	engineered mutation	UNP Q8RD55
Ζ	85	THR	GLU	engineered mutation	UNP Q8RD55
Z	86	PHE	TYR	engineered mutation	UNP Q8RD55
a	-1	MET	_	expression tag	UNP Q8RD55



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Chain	Residue	Modelled	Actual	Comment	Reference
a	0	GLY	-	expression tag	UNP Q8RD55
a	45	LYS	VAL	engineered mutation	UNP Q8RD55
a	47	ALA	ARG	engineered mutation	UNP Q8RD55
a	51	MET	GLU	engineered mutation	UNP Q8RD55
a	52	ARG	LYS	engineered mutation	UNP Q8RD55
a	55	ILE	LYS	engineered mutation	UNP Q8RD55
a	56	ALA	GLU	engineered mutation	UNP Q8RD55
a	59	ALA	GLN	engineered mutation	UNP Q8RD55
a	81	GLU	SER	engineered mutation	UNP Q8RD55
a	85	THR	GLU	engineered mutation	UNP Q8RD55
a	86	PHE	TYR	engineered mutation	UNP Q8RD55
j	-1	MET	-	expression tag	UNP Q8RD55
j	0	GLY	-	expression tag	UNP Q8RD55
j	45	LYS	VAL	engineered mutation	UNP Q8RD55
j	47	ALA	ARG	engineered mutation	UNP Q8RD55
j	51	MET	GLU	engineered mutation	UNP Q8RD55
j	52	ARG	LYS	engineered mutation	UNP Q8RD55
j	55	ILE	LYS	engineered mutation	UNP Q8RD55
j	56	ALA	GLU	engineered mutation	UNP Q8RD55
j	59	ALA	GLN	engineered mutation	UNP Q8RD55
j	81	GLU	SER	engineered mutation	UNP Q8RD55
j	85	THR	GLU	engineered mutation	UNP Q8RD55
j	86	PHE	TYR	engineered mutation	UNP Q8RD55
k	-1	MET	-	expression tag	UNP Q8RD55
k	0	GLY	-	expression tag	UNP Q8RD55
k	45	LYS	VAL	engineered mutation	UNP Q8RD55
k	47	ALA	ARG	engineered mutation	UNP Q8RD55
k	51	MET	GLU	engineered mutation	UNP Q8RD55
k	52	ARG	LYS	engineered mutation	UNP Q8RD55
k	55	ILE	LYS	engineered mutation	UNP Q8RD55
k	56	ALA	GLU	engineered mutation	UNP Q8RD55
k	59	ALA	GLN	engineered mutation	UNP Q8RD55
k	81	GLU	SER	engineered mutation	UNP Q8RD55
k	85	THR	GLU	engineered mutation	UNP Q8RD55
k	86	PHE	TYR	engineered mutation	UNP Q8RD55
m	-1	MET	-	expression tag	UNP Q8RD55
m	0	GLY	-	expression tag	UNP Q8RD55
m	45	LYS	VAL	engineered mutation	UNP Q8RD55
m	47	ALA	ARG	engineered mutation	UNP Q8RD55
m	51	MET	GLU	engineered mutation	UNP Q8RD55
m	52	ARG	LYS	engineered mutation	UNP Q8RD55
m	55	ILE	LYS	engineered mutation	UNP Q8RD55



Chain	Residue	Modelled	Actual	Comment	Reference
m	56	ALA	GLU	engineered mutation	UNP Q8RD55
m	59	ALA	GLN	engineered mutation	UNP Q8RD55
m	81	GLU	SER	engineered mutation	UNP Q8RD55
m	85	THR	GLU	engineered mutation	UNP Q8RD55
m	86	PHE	TYR	engineered mutation	UNP Q8RD55
1	-1	MET	-	expression tag	UNP Q8RD55
1	0	GLY	-	expression tag	UNP Q8RD55
1	45	LYS	VAL	engineered mutation	UNP Q8RD55
1	47	ALA	ARG	engineered mutation	UNP Q8RD55
1	51	MET	GLU	engineered mutation	UNP Q8RD55
1	52	ARG	LYS	engineered mutation	UNP Q8RD55
1	55	ILE	LYS	engineered mutation	UNP Q8RD55
1	56	ALA	GLU	engineered mutation	UNP Q8RD55
1	59	ALA	GLN	engineered mutation	UNP Q8RD55
1	81	GLU	SER	engineered mutation	UNP Q8RD55
1	85	THR	GLU	engineered mutation	UNP Q8RD55
1	86	PHE	TYR	engineered mutation	UNP Q8RD55
n	-1	MET	-	expression tag	UNP Q8RD55
n	0	GLY	-	expression tag	UNP Q8RD55
n	45	LYS	VAL	engineered mutation	UNP Q8RD55
n	47	ALA	ARG	engineered mutation	UNP Q8RD55
n	51	MET	GLU	engineered mutation	UNP Q8RD55
n	52	ARG	LYS	engineered mutation	UNP Q8RD55
n	55	ILE	LYS	engineered mutation	UNP Q8RD55
n	56	ALA	GLU	engineered mutation	UNP Q8RD55
n	59	ALA	GLN	engineered mutation	UNP Q8RD55
n	81	GLU	SER	engineered mutation	UNP Q8RD55
n	85	THR	GLU	engineered mutation	UNP Q8RD55
n	86	PHE	TYR	engineered mutation	UNP Q8RD55



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.

- Chain A: 82% 17% GLU GLU GLN GLN GLU GLU GLU GLY GLY TLE TLE 3LU 3LU CYS • Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase Chain E: 80% 18% THR MET HIS PHE GLU TYR GLU GLU GLN GLU GLV GLY GLY CLEU CLEU CLEU • Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase Chain C: 82% 15% ALA GLU ALA ALA ALA GLY GLY GLY GLY GLY SER MET MET HIS PHE GLU GLU TYR ILE • Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase Chain B: 82% 15% • Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase Chain D: 78% 19% HIS PHE GLU TYR GLU GLN GLN GLN GLU AALA AALA AALA AALA AALA CLEU LEU LLEU CLVS
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase













• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA











• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA





4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	258.82Å 258.82Å 641.73Å	Deneriten
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{B}_{\mathrm{ascolution}}(\hat{\boldsymbol{\lambda}})$	110.72 - 3.50	Depositor
Resolution (A)	213.91 - 3.50	EDS
% Data completeness	99.0 (110.72-3.50)	Depositor
(in resolution range)	$99.1 \ (213.91 - 3.50)$	EDS
R _{merge}	0.13	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.51 (at 3.49 \text{\AA})$	Xtriage
Refinement program	PHENIX	Depositor
D D	0.227 , 0.233	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.227 , 0.234	DCC
R_{free} test set	20042 reflections (10.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	104.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 60.7	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
	0.000 for -1/3 *h+1/3 *k+1/3 *l,-k,8/3 *h+4/	
	$3^{*}k+1/3^{*}l$	
	0.000 for -2/3 + 1/3 +	
	$1/3^{+}l,-4/3^{+}h+4/3^{+}k+1/3^{+}l$	
	$0.000 \text{ IOI} -\Pi, 1/3 \Pi - 1/3 K - 1/3 \Pi - 4/3 \Pi - 0/3 K$	
Estimated twinning fraction	$^{+1/3}_{0.000 \text{ for -h} 2/3*h+1/3*k+1/3*l}4/3*h+8/3$	Xtriage
	*k-1/3*l	Attrage
	$0.000 \text{ for } 1/3^{*}h+2/3^{*}k-1/3^{*}l,-k,-8/3^{*}h-4/3^{*}$	
	k-1/3*l	
	0.000 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-	
	1/3*l, $4/3$ *h- $4/3$ *k- $1/3$ *l	
	0.000 for -h-k,k,-l	
F_o, F_c correlation	0.92	EDS
Total number of atoms	40538	wwPDB-VP
Average B, all atoms $(Å^2)$	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.

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.



 $^{^1 \}mathrm{Intensities}$ estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bond	lengths	Bond angles		
WIOI	Ullaill	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.41	0/1049	0.49	0/1417	
1	В	0.36	0/1069	0.50	0/1442	
1	С	0.40	0/1069	0.52	0/1444	
1	D	0.39	0/1030	0.51	0/1389	
1	Е	0.42	0/1033	0.50	0/1394	
1	Κ	0.36	0/1049	0.49	0/1416	
1	L	0.44	0/1062	0.51	0/1433	
1	М	0.40	0/1090	0.51	0/1469	
1	Ν	0.39	0/1040	0.50	0/1405	
1	0	0.41	0/1010	0.49	0/1362	
1	U	0.35	0/1035	0.55	0/1398	
1	V	0.42	0/1053	0.50	0/1421	
1	W	0.38	0/1026	0.51	0/1385	
1	Х	0.41	0/1030	0.50	0/1390	
1	Y	0.38	0/1032	0.51	0/1393	
1	е	0.42	0/1035	0.51	0/1397	
1	f	0.41	0/1044	0.51	0/1409	
1	g	0.41	0/1012	0.51	0/1365	
1	h	0.40	0/1025	0.51	0/1384	
1	i	0.41	0/1043	0.52	0/1410	
2	F	0.55	0/1009	0.54	0/1356	
2	G	0.57	0/1005	0.56	0/1352	
2	Н	0.54	0/1013	0.55	0/1361	
2	Ι	0.51	0/1009	0.55	0/1356	
2	J	0.54	0/1013	0.54	0/1361	
2	Р	0.58	0/1013	0.56	0/1361	
2	Q	0.57	0/1013	0.54	0/1361	
2	R	0.54	0/1017	0.55	0/1366	
2	S	0.58	0/1009	0.55	0/1356	
2	Т	0.55	0/1013	0.55	0/1361	
2	Ζ	0.49	0/1013	0.56	0/1361	
2	a	0.57	0/1013	0.55	0/1361	
2	b	0.59	0/1009	0.56	0/1356	
2	с	0.54	0/1009	0.56	0/1356	



Mal	Chain	Bond lengths		Bond angles	
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
2	d	0.55	0/1013	0.56	0/1361
2	j	0.55	0/1013	0.56	0/1361
2	k	0.56	0/1017	0.56	0/1366
2	l	0.54	0/1005	0.56	0/1351
2	m	0.59	0/1009	0.56	0/1356
2	n	0.51	0/1009	0.57	0/1356
All	All	0.48	0/41060	0.53	0/55299

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 (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	Perce	ntiles
1	А	129/162~(80%)	127 (98%)	2(2%)	0	100	100
1	В	131/162~(81%)	129 (98%)	2(2%)	0	100	100
1	С	131/162~(81%)	128 (98%)	3~(2%)	0	100	100
1	D	126/162~(78%)	124 (98%)	2(2%)	0	100	100
1	Ε	127/162~(78%)	125~(98%)	2(2%)	0	100	100
1	Κ	129/162~(80%)	127~(98%)	2(2%)	0	100	100
1	L	130/162~(80%)	127 (98%)	3 (2%)	0	100	100
1	М	133/162~(82%)	131 (98%)	2(2%)	0	100	100



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Contentaca	JION	precious	pagem

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	Ν	128/162~(79%)	126 (98%)	2(2%)	0	100	100
1	Ο	124/162~(76%)	121 (98%)	3~(2%)	0	100	100
1	U	128/162~(79%)	125~(98%)	3~(2%)	0	100	100
1	V	130/162~(80%)	127 (98%)	3 (2%)	0	100	100
1	W	126/162~(78%)	124 (98%)	2 (2%)	0	100	100
1	Х	126/162~(78%)	124 (98%)	2 (2%)	0	100	100
1	Y	129/162~(80%)	126 (98%)	3 (2%)	0	100	100
1	е	127/162~(78%)	125 (98%)	2 (2%)	0	100	100
1	f	128/162~(79%)	126 (98%)	2 (2%)	0	100	100
1	g	124/162~(76%)	122 (98%)	2 (2%)	0	100	100
1	h	127/162~(78%)	124 (98%)	3 (2%)	0	100	100
1	i	129/162~(80%)	125 (97%)	4 (3%)	0	100	100
2	F	129/138~(94%)	128 (99%)	1 (1%)	0	100	100
2	G	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	Н	129/138~(94%)	128 (99%)	1 (1%)	0	100	100
2	Ι	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	J	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	Р	129/138~(94%)	128 (99%)	1 (1%)	0	100	100
2	Q	129/138~(94%)	128 (99%)	1 (1%)	0	100	100
2	R	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	S	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	Т	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	Ζ	129/138~(94%)	127 (98%)	2 (2%)	0	100	100
2	a	129/138~(94%)	128 (99%)	1 (1%)	0	100	100
2	b	129/138~(94%)	128 (99%)	1 (1%)	0	100	100
2	с	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	d	129/138~(94%)	127 (98%)	2 (2%)	0	100	100
2	j	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	k	129/138~(94%)	128 (99%)	1 (1%)	0	100	100
2	l	129/138~(94%)	128 (99%)	1 (1%)	0	100	100
2	m	129/138~(94%)	128 (99%)	1 (1%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles			
2	n	129/138~(94%)	128 (99%)	1 (1%)	0	100	100			
All	All	5142/6000~(86%)	5071 (99%)	71 (1%)	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 side chain 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	Perce	ntiles
1	А	107/133~(80%)	105 (98%)	2(2%)	57	80
1	В	109/133~(82%)	105~(96%)	4 (4%)	34	65
1	С	109/133~(82%)	105 (96%)	4 (4%)	34	65
1	D	106/133~(80%)	101 (95%)	5(5%)	26	60
1	Ε	106/133~(80%)	103 (97%)	3~(3%)	43	72
1	Κ	107/133~(80%)	103 (96%)	4 (4%)	34	65
1	L	109/133~(82%)	105 (96%)	4 (4%)	34	65
1	М	112/133~(84%)	106 (95%)	6~(5%)	22	55
1	Ν	106/133~(80%)	102 (96%)	4 (4%)	33	65
1	Ο	103/133~(77%)	100 (97%)	3~(3%)	42	71
1	U	105/133~(79%)	101 (96%)	4 (4%)	33	65
1	V	107/133~(80%)	102 (95%)	5 (5%)	26	60
1	W	105/133~(79%)	101 (96%)	4 (4%)	33	65
1	Х	106/133~(80%)	102 (96%)	4 (4%)	33	65
1	Y	105/133~(79%)	102 (97%)	3~(3%)	42	71
1	е	106/133~(80%)	103~(97%)	3~(3%)	43	72
1	f	107/133~(80%)	103 (96%)	4 (4%)	34	65
1	g	103/133~(77%)	100 (97%)	3~(3%)	42	71
1	h	$10\overline{4/133}~(78\%)$	99~(95%)	5 (5%)	25	60
1	i	106/133~(80%)	102 (96%)	4 (4%)	33	65



Mol	Chain	Analysed	Rotameric	Outliers	Perce	\mathbf{n} tiles
2	F	112/120~(93%)	109~(97%)	3~(3%)	44	73
2	G	111/120~(92%)	108~(97%)	3~(3%)	44	73
2	Н	113/120~(94%)	107~(95%)	6~(5%)	22	55
2	Ι	112/120~(93%)	107~(96%)	5 (4%)	27	61
2	J	113/120~(94%)	109~(96%)	4 (4%)	36	67
2	Р	113/120~(94%)	109~(96%)	4 (4%)	36	67
2	Q	113/120~(94%)	110~(97%)	3~(3%)	44	73
2	R	114/120~(95%)	109~(96%)	5 (4%)	28	62
2	S	112/120~(93%)	109~(97%)	3(3%)	44	73
2	Т	113/120 (94%)	109 (96%)	4 (4%)	36	67
2	Ζ	113/120 (94%)	110 (97%)	3(3%)	44	73
2	a	113/120~(94%)	109~(96%)	4 (4%)	36	67
2	b	112/120~(93%)	109~(97%)	3~(3%)	44	73
2	с	112/120~(93%)	108 (96%)	4 (4%)	35	66
2	d	113/120 (94%)	109 (96%)	4 (4%)	36	67
2	j	113/120~(94%)	109~(96%)	4 (4%)	36	67
2	k	114/120~(95%)	110~(96%)	4 (4%)	36	67
2	1	111/120~(92%)	107~(96%)	4 (4%)	35	66
2	m	112/120~(93%)	109 (97%)	3(3%)	44	73
2	n	112/120~(93%)	108 (96%)	4 (4%)	35	66
All	All	4379/5060~(86%)	4224 (96%)	155~(4%)	36	67

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	43	LEU
1	А	148	HIS
1	Е	43	LEU
1	Е	78	LEU
1	Е	148	HIS
1	С	43	LEU
1	С	51	GLU
1	С	78	LEU
1	С	148	HIS
1	В	43	LEU



Mol	Chain	Res	Type
1	В	51	GLU
1	В	78	LEU
1	В	148	HIS
1	D	43	LEU
1	D	51	GLU
1	D	77	ARG
1	D	78	LEU
1	D	148	HIS
2	F	70	LEU
2	F	95	ASN
2	F	106	ILE
2	Н	70	LEU
2	Н	81	GLU
2	Н	87	ASP
2	Н	95	ASN
2	Н	106	ILE
2	Н	131	LYS
2	G	70	LEU
2	G	95	ASN
2	G	106	ILE
2	Ι	70	LEU
2	Ι	87	ASP
2	Ι	95	ASN
2	Ι	106	ILE
2	Ι	130	GLU
2	J	70	LEU
2	J	87	ASP
2	J	95	ASN
2	J	106	ILE
1	K	43	LEU
1	K	51	GLU
1	K	78	LEU
1	K	148	HIS
1	L	12	LYS
1	L	43	LEU
1	L	78	LEU
1	L	148	HIS
1	N	43	LEU
1	N	78	LEU
1	N	148	HIS
1	N	165	LEU
1	М	43	LEU



Mol	Chain	Res	Type
1	М	51	GLU
1	М	77	ARG
1	М	78	LEU
1	М	148	HIS
1	М	167	HIS
1	0	43	LEU
1	0	78	LEU
1	0	148	HIS
2	Р	70	LEU
2	Р	87	ASP
2	Р	95	ASN
2	Р	106	ILE
2	Q	70	LEU
2	Q	95	ASN
2	Q	106	ILE
2	S	70	LEU
2	S	95	ASN
2	S	106	ILE
2	R	70	LEU
2	R	81	GLU
2	R	87	ASP
2	R	95	ASN
2	R	106	ILE
2	Т	70	LEU
2	Т	87	ASP
2	Т	95	ASN
2	Т	106	ILE
1	U	43	LEU
1	U	77	ARG
1	U	78	LEU
1	U	148	HIS
1	V	43	LEU
1	V	51	GLU
1	V	77	ARG
1	V	78	LEU
1	V	148	HIS
1	Х	43	LEU
1	Х	77	ARG
1	X	78	LEU
1	X	148	HIS
1	W	43	LEU
1	W	51	GLU



Mol	Chain	Res	Type
1	W	78	LEU
1	W	148	HIS
1	Y	43	LEU
1	Y	78	LEU
1	Y	148	HIS
2	b	70	LEU
2	b	95	ASN
2	b	106	ILE
2	d	70	LEU
2	d	95	ASN
2	d	106	ILE
2	d	131	LYS
2	с	70	LEU
2	с	95	ASN
2	с	106	ILE
2	с	131	LYS
2	Ζ	70	LEU
2	Ζ	95	ASN
2	Ζ	106	ILE
2	a	70	LEU
2	a	87	ASP
2	a	95	ASN
2	a	106	ILE
1	е	43	LEU
1	е	78	LEU
1	е	148	HIS
1	f	43	LEU
1	f	51	GLU
1	f	78	LEU
1	f	148	HIS
1	h	43	LEU
1	h	51	GLU
1	h	78	LEU
1	h	148	HIS
1	h	165	LEU
1	g	43	LEU
1	g	78	LEU
1	g	148	HIS
1	i	43	LEU
1	i	51	GLU
1	i	78	LEU
1	i	148	HIS

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Mol	Chain	Res	Type
2	j	70	LEU
2	j	87	ASP
2	j	95	ASN
2	j	106	ILE
2	k	70	LEU
2	k	87	ASP
2	k	95	ASN
2	k	106	ILE
2	m	70	LEU
2	m	95	ASN
2	m	106	ILE
2	1	70	LEU
2	1	87	ASP
2	1	95	ASN
2	1	106	ILE
2	n	70	LEU
2	n	87	ASP
2	n	95	ASN
2	n	106	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	108	HIS
1	Е	108	HIS
1	С	108	HIS
1	В	108	HIS
1	D	108	HIS
2	F	33	HIS
2	F	95	ASN
2	Н	33	HIS
2	Н	95	ASN
2	G	33	HIS
2	G	95	ASN
2	Ι	33	HIS
2	Ι	95	ASN
2	J	33	HIS
2	J	95	ASN
1	K	108	HIS
1	L	108	HIS
1	Ν	108	HIS
1	М	108	HIS



Mol	Chain	Res	Type
1	М	167	HIS
1	0	108	HIS
2	Р	33	HIS
2	Р	95	ASN
2	Q	95	ASN
2	S	33	HIS
2	S	95	ASN
2	R	33	HIS
2	R	95	ASN
2	Т	33	HIS
2	Т	95	ASN
1	U	108	HIS
1	V	108	HIS
1	Х	108	HIS
1	W	108	HIS
1	Y	108	HIS
2	b	33	HIS
2	b	95	ASN
2	d	33	HIS
2	d	95	ASN
2	с	33	HIS
2	с	95	ASN
2	Z	33	HIS
2	Z	95	ASN
2	a	33	HIS
2	a	95	ASN
1	e	108	HIS
1	f	108	HIS
1	h	108	HIS
1	g	108	HIS
1	i	108	HIS
2	j	95	ASN
2	k	33	HIS
2	k	95	ASN
2	m	33	HIS
2	m	95	ASN
2	1	33	HIS
2	1	95	ASN
2	n	33	HIS
2	n	95	ASN

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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 monosaccharides 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 (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^{th} 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		>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	135/162~(83%)	0.73	6~(4%)	34	30	66, 93, 176, 231	0
1	В	137/162~(84%)	0.69	5 (3%)	42	38	55, 91, 168, 243	0
1	С	137/162~(84%)	0.68	5 (3%)	42	38	47, 73, 170, 239	0
1	D	132/162~(81%)	0.83	7 (5%)	26	24	47, 77, 158, 225	0
1	Ε	133/162~(82%)	0.69	5 (3%)	40	36	56, 86, 159, 236	0
1	K	135/162~(83%)	0.69	3 (2%)	62	56	55, 90, 167, 250	0
1	L	136/162~(83%)	0.77	8 (5%)	22	20	59, 89, 171, 245	0
1	М	139/162~(85%)	0.83	6 (4%)	35	31	58, 96, 192, 231	0
1	Ν	134/162~(82%)	0.72	7 (5%)	27	24	69, 98, 174, 256	0
1	Ο	130/162~(80%)	0.73	4 (3%)	49	43	64, 94, 154, 219	0
1	U	134/162~(82%)	0.69	3~(2%)	62	56	48, 77, 169, 229	0
1	V	136/162~(83%)	0.70	4 (2%)	51	45	44, 79, 178, 246	0
1	W	132/162~(81%)	0.75	7 (5%)	26	24	52, 82, 170, 226	0
1	Х	132/162~(81%)	0.69	8 (6%)	21	19	61, 94, 168, 210	0
1	Y	135/162~(83%)	0.66	2(1%)	73	68	58, 90, 179, 244	0
1	е	133/162~(82%)	0.81	9~(6%)	17	16	58, 91, 165, 222	0
1	f	134/162~(82%)	0.75	6 (4%)	33	29	64, 96, 173, 221	0
1	g	130/162~(80%)	0.70	6 (4%)	32	28	68, 96, 170, 203	0
1	h	133/162~(82%)	0.71	6 (4%)	33	29	60, 93, 161, 242	0
1	i	135/162~(83%)	0.77	10 (7%)	14	14	59,87,167,245	0
2	F	131/138~(94%)	0.57	5 (3%)	40	36	78, 107, 158, 174	0
2	G	131/138~(94%)	0.59	2(1%)	73	68	66, 92, 146, 184	0
2	Н	131/138~(94%)	0.49	0 100) 1	00	55, 88, 149, 172	0
2	Ι	131/138~(94%)	0.54	4 (3%)	49	43	64, 97, 145, 176	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
2	J	131/138 (94%)	0.57	3 (2%) 60 54	73, 101, 146, 177	0
2	Р	131/138 (94%)	0.53	2 (1%) 73 68	69, 101, 146, 168	0
2	Q	131/138 (94%)	0.55	4 (3%) 49 43	72, 96, 140, 166	0
2	R	131/138 (94%)	0.47	4 (3%) 49 43	75, 102, 150, 170	0
2	S	131/138~(94%)	0.56	7 (5%) 26 24	80, 109, 156, 174	0
2	Т	131/138~(94%)	0.53	1 (0%) 86 81	65, 93, 146, 167	0
2	Z	131/138~(94%)	0.64	7 (5%) 26 24	72, 101, 152, 193	0
2	a	131/138 (94%)	0.52	2 (1%) 73 68	65, 92, 149, 166	0
2	b	131/138 (94%)	0.44	2 (1%) 73 68	62, 91, 142, 165	0
2	с	131/138 (94%)	0.54	2 (1%) 73 68	66, 93, 146, 181	0
2	d	131/138~(94%)	0.51	3 (2%) 60 54	78, 107, 157, 178	0
2	j	131/138~(94%)	0.55	2 (1%) 73 68	73, 99, 148, 163	0
2	k	131/138~(94%)	0.52	4 (3%) 49 43	76, 103, 154, 183	0
2	1	131/138~(94%)	0.53	2 (1%) 73 68	80, 108, 151, 190	0
2	m	131/138 (94%)	0.52	2 (1%) 73 68	66, 98, 151, 162	0
2	n	131/138~(94%)	0.50	1 (0%) 86 81	66, 88, 132, 147	0
All	All	5302/6000 (88%)	0.63	176 (3%) 46 41	44, 95, 160, 256	0

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All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	h	129	LEU	5.1
1	М	103	CYS	4.9
1	Ν	134	ALA	4.6
1	Ν	129	LEU	4.3
1	Κ	103	CYS	4.2
1	D	129	LEU	4.2
1	М	134	ALA	4.2
1	В	103	CYS	4.2
1	i	129	LEU	4.1
1	i	134	ALA	3.8
1	h	103	CYS	3.7
1	g	103	CYS	3.6
1	f	129	LEU	3.4
1	Х	103	CYS	3.4
2	J	111	THR	3.4



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Continued	from	previous	page
	9	1	1 0

Mol	Chain	Res	Type	RSRZ
1	С	103	CYS	3.4
1	Х	123	PHE	3.2
2	S	111	THR	3.2
1	0	123	PHE	3.2
1	А	123	PHE	3.1
1	е	126	LEU	3.1
1	е	90	VAL	3.1
1	С	129	LEU	3.1
2	Ι	122	GLY	3.1
1	U	103	CYS	3.1
1	е	129	LEU	3.0
1	С	111	MET	3.0
1	W	103	CYS	3.0
1	V	103	CYS	3.0
1	g	90	VAL	3.0
1	L	62	PHE	2.9
1	е	103	CYS	2.9
1	Ν	123	PHE	2.9
1	Ν	103	CYS	2.9
1	Y	103	CYS	2.9
1	А	129	LEU	2.9
1	0	11	MET	2.9
1	0	103	CYS	2.8
1	L	126	LEU	2.8
1	W	126	LEU	2.8
1	D	103	CYS	2.8
1	Ε	90	VAL	2.7
1	В	123	PHE	2.7
1	K	129	LEU	2.7
1	i	90	VAL	2.7
1	f	128	CYS	2.7
1	e	124	GLY	2.7
1	е	92	ILE	2.7
1	В	129	LEU	2.7
1	f	103	CYS	2.7
2	S	115	LEU	2.7
1	L	90	VAL	2.7
1	Е	123	PHE	2.6
1	g	126	LEU	2.6
1	A	90	VAL	2.6
1	i	126	LEU	2.6
1	Ε	103	CYS	2.6



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Mol	Chain	Res	Type	RSRZ
1	h	126	LEU	2.6
1	В	90	VAL	2.6
1	U	126	LEU	2.6
2	F	88	VAL	2.5
2	Ζ	102	LEU	2.5
2	G	92	THR	2.5
2	j	102	LEU	2.5
1	Х	87	PRO	2.5
1	V	129	LEU	2.5
2	n	37	LEU	2.5
1	W	90	VAL	2.5
1	V	126	LEU	2.5
1	L	103	CYS	2.5
2	S	127	LYS	2.5
1	g	123	PHE	2.4
1	N	126	LEU	2.4
1	А	124	GLY	2.4
2	k	65	ILE	2.4
2	k	118	ILE	2.4
2	Ζ	6	VAL	2.4
1	Y	129	LEU	2.4
1	N	33	ALA	2.4
1	Ν	90	VAL	2.4
1	А	110	LEU	2.4
1	В	59	PRO	2.4
2	Ι	37	LEU	2.4
1	i	103	CYS	2.4
2	J	90	VAL	2.4
1	L	33	ALA	2.4
1	L	129	LEU	2.3
1	D	33	ALA	2.3
1	f	90	VAL	2.3
2	j	37	LEU	2.3
2	Ι	127	LYS	2.3
1	f	123	PHE	2.3
1	i	61	SER	2.3
2	S	91	ILE	2.3
2	Q	90	VAL	2.3
1	М	126	LEU	2.3
1	Х	59	PRO	2.3
2	R	94	ILE	2.3
1	М	167	HIS	2.3



51M4

Mol	Chain	Res	Type	RSRZ
1	f	25	ALA	2.3
1	L	123	PHE	2.3
2	Q	111	THR	2.3
1	Е	129	LEU	2.3
2	k	102	LEU	2.3
1	D	61	SER	2.2
1	е	33	ALA	2.2
2	R	37	LEU	2.2
2	S	66	ILE	2.2
1	D	28	ASN	2.2
1	i	123	PHE	2.2
2	Q	127	LYS	2.2
1	М	90	VAL	2.2
2	b	126	ILE	2.2
2	a	37	LEU	2.2
1	h	123	PHE	2.2
1	D	123	PHE	2.2
2	d	92	THR	2.2
1	Е	126	LEU	2.2
1	С	126	LEU	2.2
1	U	90	VAL	2.2
2	Ι	91	ILE	2.2
2	с	65	ILE	2.2
1	h	111	MET	2.2
1	i	110	LEU	2.2
2	Т	37	LEU	2.2
1	V	33	ALA	2.2
1	g	92	ILE	2.2
1	W	25	ALA	2.1
2	Ζ	115	LEU	2.1
2	Р	118	ILE	2.1
2	Ζ	65	ILE	2.1
2	m	37	LEU	2.1
1	W	28	ASN	2.1
2	Z	95	ASN	2.1
1	C	90	VAL	2.1
2	F	111	THR	2.1
1	K	$12\overline{3}$	PHE	2.1
1	М	123	PHE	2.1
2	J	66	ILE	2.1
2	Ζ	111	THR	2.1
1	Х	126	LEU	2.1



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Mol	Chain	Res	Type	RSRZ	
1	W	129	LEU	2.1	
2	Р	66	ILE	2.1	
2	Ζ	89	LYS	2.1	
1	W	59	PRO	2.1	
1	g	25	ALA	2.1	
2	b	37	LEU	2.1	
2	R	127	LYS	2.1	
1	Х	27	TRP	2.1	
2	F	106	ILE	2.1	
2	Q	91	ILE	2.1	
1	D	124	GLY	2.1	
2	a	95	ASN	2.1	
2	k	127	LYS	2.1	
1	0	90	VAL	2.1	
1	е	89	GLY	2.1	
2	d	37	LEU	2.1	
2	S	64	ILE	2.1	
2	G	7	LEU	2.1	
2	F	97	PRO	2.0	
1	h	92	ILE	2.0	
1	Х	129	LEU	2.0	
2	d	86	PHE	2.0	
2	R	66	ILE	2.0	
2	m	95	ASN	2.0	
2	1	5	PHE	2.0	
1	А	128	CYS	2.0	
1	Х	90	VAL	2.0	
1	i	27	TRP	2.0	
1	i	111	MET	2.0	
1	L	124	GLY	2.0	
1	е	25	ALA	2.0	
2	F	66	ILE	2.0	
2	1	129	ILE	2.0	
2	S	90	VAL	2.0	
2	с	102	LEU	2.0	

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

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



6.3 Carbohydrates (i)

There are no monosaccharides 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.

