Full wwPDB X-ray Structure Validation Report (i)

Aug 1, 2016 – 02:34 PM 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

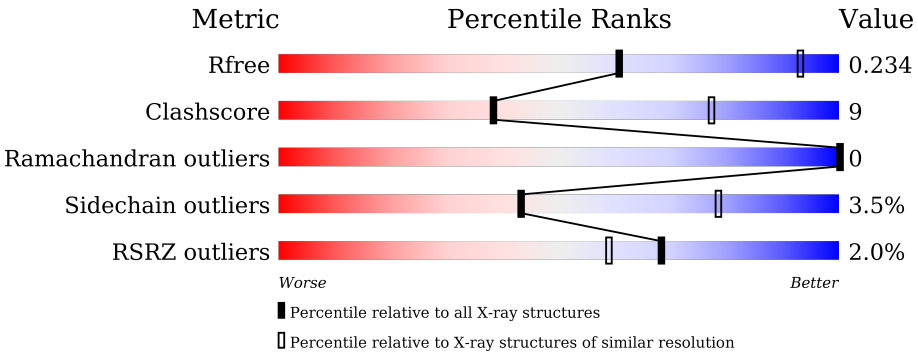
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	162	3% 69% 14% 17%
1	B	162	2% 68% 17% 15%
1	C	162	2% 67% 18% 15%
1	D	162	2% 64% 17% • 19%
1	E	162	3% 62% 20% 18%
1	K	162	% 64% 19% 17%

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Mol	Chain	Length	Quality of chain
1	L	162	3% 68% 15% 16%
1	M	162	4% 64% 20% 14%
1	N	162	4% 67% 14% 17%
1	O	162	% 65% 15% 20%
1	U	162	% 67% 15% 17%
1	V	162	2% 65% 18% 16%
1	W	162	2% 66% 15% 19%
1	X	162	2% 64% 17% 19%
1	Y	162	% 66% 17% 17%
1	e	162	4% 80% 18%
1	f	162	3% 80% 17%
1	g	162	4% 78% 20%
1	h	162	4% 79% 18%
1	i	162	6% 81% 17%
2	F	138	% 78% 15% 5%
2	G	138	82% 12% 5%
2	H	138	80% 13% 5%
2	I	138	% 83% 10% 5%
2	J	138	% 78% 15% 5%
2	P	138	80% 13% 5%
2	Q	138	% 84% 9% 5%
2	R	138	% 81% 12% 5%
2	S	138	2% 81% 12% 5%
2	T	138	83% 11% 5%
2	Z	138	% 81% 12% 5%

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Mol	Chain	Length	Quality of chain
2	a	138	92% 5%
2	b	138	93% 5%
2	c	138	92% 5%
2	d	138	92% 5%
2	j	138	92% 5%
2	k	138	92% 5%
2	l	138	92% 5%
2	m	138	93% 5%
2	n	138	92% 5%

2 Entry composition

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1031	670	172	185	4			
1	E	133	Total	C	N	O	S	0	0	0
			1016	662	169	181	4			
1	C	137	Total	C	N	O	S	0	0	0
			1051	680	177	190	4			
1	B	137	Total	C	N	O	S	0	0	0
			1051	682	179	186	4			
1	D	132	Total	C	N	O	S	0	0	0
			1013	660	171	178	4			
1	K	135	Total	C	N	O	S	0	0	0
			1032	670	174	184	4			
1	L	136	Total	C	N	O	S	0	0	0
			1045	677	175	189	4			
1	N	134	Total	C	N	O	S	0	0	0
			1023	664	172	183	4			
1	M	139	Total	C	N	O	S	0	0	0
			1072	693	181	194	4			
1	O	130	Total	C	N	O	S	0	0	0
			993	648	166	175	4			
1	U	134	Total	C	N	O	S	0	0	0
			1018	661	171	182	4			
1	V	136	Total	C	N	O	S	0	0	0
			1036	672	175	185	4			
1	X	132	Total	C	N	O	S	0	0	0
			1013	659	170	180	4			
1	W	132	Total	C	N	O	S	0	0	0
			1009	657	170	178	4			
1	Y	135	Total	C	N	O	S	0	0	0
			1017	659	170	184	4			
1	e	133	Total	C	N	O	S	0	0	0
			1018	662	171	181	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	f	134	Total	C	N	O	S	0	0	0
			1027	667	172	184	4			
1	h	133	Total	C	N	O	S	0	0	0
			1008	657	168	179	4			
1	g	130	Total	C	N	O	S	0	0	0
			995	648	168	175	4			
1	i	135	Total	C	N	O	S	0	0	0
			1026	666	170	186	4			

There are 280 discrepancies between the modelled and reference sequences:

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

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

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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
N	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

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

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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
X	11	MET	-	expression tag	UNP A0A0A3CUI3
X	29	LEU	ARG	engineered mutation	UNP A0A0A3CUI3
X	30	GLU	LYS	engineered mutation	UNP A0A0A3CUI3
X	33	ALA	ASP	engineered mutation	UNP A0A0A3CUI3
X	40	ILE	VAL	engineered mutation	UNP A0A0A3CUI3
X	50	ALA	GLU	engineered mutation	UNP A0A0A3CUI3
X	165	LEU	-	expression tag	UNP A0A0A3CUI3
X	166	GLU	-	expression tag	UNP A0A0A3CUI3
X	167	HIS	-	expression tag	UNP A0A0A3CUI3
X	168	HIS	-	expression tag	UNP A0A0A3CUI3
X	169	HIS	-	expression tag	UNP A0A0A3CUI3
X	170	HIS	-	expression tag	UNP A0A0A3CUI3
X	171	HIS	-	expression tag	UNP A0A0A3CUI3
X	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

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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
e	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
e	165	LEU	-	expression tag	UNP A0A0A3CUI3
e	166	GLU	-	expression tag	UNP A0A0A3CUI3
e	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
e	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

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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	Atoms					ZeroOcc	AltConf	Trace
2	F	131	Total	C	N	O	S	0	0	0
			1000	649	160	185	6			
2	H	131	Total	C	N	O	S	0	0	0
			1004	651	160	187	6			
2	G	131	Total	C	N	O	S	0	0	0
			996	646	159	185	6			
2	I	131	Total	C	N	O	S	0	0	0
			1000	649	160	185	6			
2	J	131	Total	C	N	O	S	0	0	0
			1004	651	160	187	6			
2	P	131	Total	C	N	O	S	0	0	0
			1004	651	160	187	6			
2	Q	131	Total	C	N	O	S	0	0	0
			1004	651	160	187	6			
2	S	131	Total	C	N	O	S	0	0	0
			1000	649	160	185	6			
2	R	131	Total	C	N	O	S	0	0	0
			1008	653	160	189	6			
2	T	131	Total	C	N	O	S	0	0	0
			1004	651	160	187	6			
2	b	131	Total	C	N	O	S	0	0	0
			1000	649	160	185	6			
2	d	131	Total	C	N	O	S	0	0	0
			1004	651	160	187	6			
2	c	131	Total	C	N	O	S	0	0	0
			1000	649	160	185	6			
2	Z	131	Total	C	N	O	S	0	0	0
			1004	651	160	187	6			
2	a	131	Total	C	N	O	S	0	0	0
			1004	651	160	187	6			
2	j	131	Total	C	N	O	S	0	0	0
			1004	651	160	187	6			
2	k	131	Total	C	N	O	S	0	0	0
			1008	653	160	189	6			
2	m	131	Total	C	N	O	S	0	0	0
			1000	649	160	185	6			
2	l	131	Total	C	N	O	S	0	0	0
			996	647	160	183	6			
2	n	131	Total	C	N	O	S	0	0	0
			1000	649	160	185	6			

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
H	-1	MET	-	expression tag	UNP Q8RD55
H	0	GLY	-	expression tag	UNP Q8RD55
H	45	LYS	VAL	engineered mutation	UNP Q8RD55
H	47	ALA	ARG	engineered mutation	UNP Q8RD55
H	51	MET	GLU	engineered mutation	UNP Q8RD55
H	52	ARG	LYS	engineered mutation	UNP Q8RD55
H	55	ILE	LYS	engineered mutation	UNP Q8RD55
H	56	ALA	GLU	engineered mutation	UNP Q8RD55
H	59	ALA	GLN	engineered mutation	UNP Q8RD55
H	81	GLU	SER	engineered mutation	UNP Q8RD55
H	85	THR	GLU	engineered mutation	UNP Q8RD55
H	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
I	47	ALA	ARG	engineered mutation	UNP Q8RD55
I	51	MET	GLU	engineered mutation	UNP Q8RD55
I	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
I	56	ALA	GLU	engineered mutation	UNP Q8RD55
I	59	ALA	GLN	engineered mutation	UNP Q8RD55
I	81	GLU	SER	engineered mutation	UNP Q8RD55
I	85	THR	GLU	engineered mutation	UNP Q8RD55
I	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
P	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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Chain	Residue	Modelled	Actual	Comment	Reference
S	0	GLY	-	expression tag	UNP Q8RD55
S	45	LYS	VAL	engineered mutation	UNP Q8RD55
S	47	ALA	ARG	engineered mutation	UNP Q8RD55
S	51	MET	GLU	engineered mutation	UNP Q8RD55
S	52	ARG	LYS	engineered mutation	UNP Q8RD55
S	55	ILE	LYS	engineered mutation	UNP Q8RD55
S	56	ALA	GLU	engineered mutation	UNP Q8RD55
S	59	ALA	GLN	engineered mutation	UNP Q8RD55
S	81	GLU	SER	engineered mutation	UNP Q8RD55
S	85	THR	GLU	engineered mutation	UNP Q8RD55
S	86	PHE	TYR	engineered mutation	UNP Q8RD55
R	-1	MET	-	expression tag	UNP Q8RD55
R	0	GLY	-	expression tag	UNP Q8RD55
R	45	LYS	VAL	engineered mutation	UNP Q8RD55
R	47	ALA	ARG	engineered mutation	UNP Q8RD55
R	51	MET	GLU	engineered mutation	UNP Q8RD55
R	52	ARG	LYS	engineered mutation	UNP Q8RD55
R	55	ILE	LYS	engineered mutation	UNP Q8RD55
R	56	ALA	GLU	engineered mutation	UNP Q8RD55
R	59	ALA	GLN	engineered mutation	UNP Q8RD55
R	81	GLU	SER	engineered mutation	UNP Q8RD55
R	85	THR	GLU	engineered mutation	UNP Q8RD55
R	86	PHE	TYR	engineered mutation	UNP Q8RD55
T	-1	MET	-	expression tag	UNP Q8RD55
T	0	GLY	-	expression tag	UNP Q8RD55
T	45	LYS	VAL	engineered mutation	UNP Q8RD55
T	47	ALA	ARG	engineered mutation	UNP Q8RD55
T	51	MET	GLU	engineered mutation	UNP Q8RD55
T	52	ARG	LYS	engineered mutation	UNP Q8RD55
T	55	ILE	LYS	engineered mutation	UNP Q8RD55
T	56	ALA	GLU	engineered mutation	UNP Q8RD55
T	59	ALA	GLN	engineered mutation	UNP Q8RD55
T	81	GLU	SER	engineered mutation	UNP Q8RD55
T	85	THR	GLU	engineered mutation	UNP Q8RD55
T	86	PHE	TYR	engineered mutation	UNP Q8RD55
b	-1	MET	-	expression tag	UNP Q8RD55
b	0	GLY	-	expression tag	UNP Q8RD55
b	45	LYS	VAL	engineered mutation	UNP Q8RD55
b	47	ALA	ARG	engineered mutation	UNP Q8RD55
b	51	MET	GLU	engineered mutation	UNP Q8RD55
b	52	ARG	LYS	engineered mutation	UNP Q8RD55
b	55	ILE	LYS	engineered mutation	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
c	-1	MET	-	expression tag	UNP Q8RD55
c	0	GLY	-	expression tag	UNP Q8RD55
c	45	LYS	VAL	engineered mutation	UNP Q8RD55
c	47	ALA	ARG	engineered mutation	UNP Q8RD55
c	51	MET	GLU	engineered mutation	UNP Q8RD55
c	52	ARG	LYS	engineered mutation	UNP Q8RD55
c	55	ILE	LYS	engineered mutation	UNP Q8RD55
c	56	ALA	GLU	engineered mutation	UNP Q8RD55
c	59	ALA	GLN	engineered mutation	UNP Q8RD55
c	81	GLU	SER	engineered mutation	UNP Q8RD55
c	85	THR	GLU	engineered mutation	UNP Q8RD55
c	86	PHE	TYR	engineered mutation	UNP Q8RD55
Z	-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
Z	55	ILE	LYS	engineered mutation	UNP Q8RD55
Z	56	ALA	GLU	engineered mutation	UNP Q8RD55
Z	59	ALA	GLN	engineered mutation	UNP Q8RD55
Z	81	GLU	SER	engineered mutation	UNP Q8RD55
Z	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

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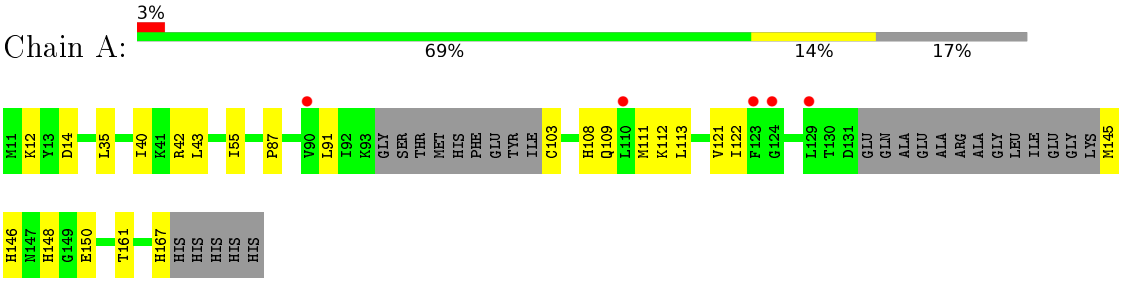
Chain	Residue	Modelled	Actual	Comment	Reference
m	56	ALA	GLU	engineered mutation	UNP Q8RD55
m	59	ALA	GLN	engineered mutation	UNP Q8RD55
m	81	GLU	SER	engineered mutation	UNP Q8RD55
m	85	THR	GLU	engineered mutation	UNP Q8RD55
m	86	PHE	TYR	engineered mutation	UNP Q8RD55
l	-1	MET	-	expression tag	UNP Q8RD55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

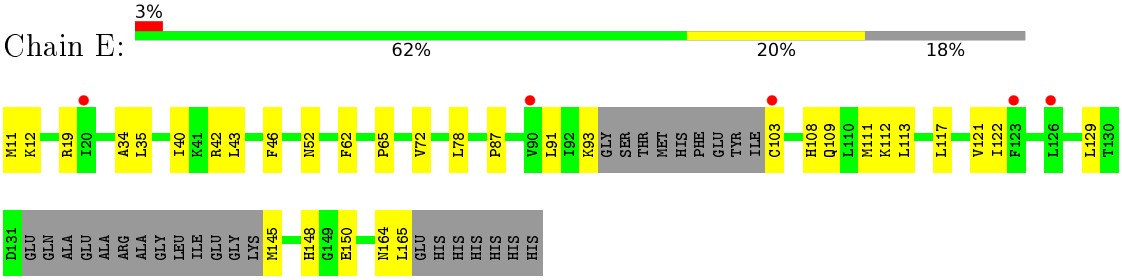
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain A:



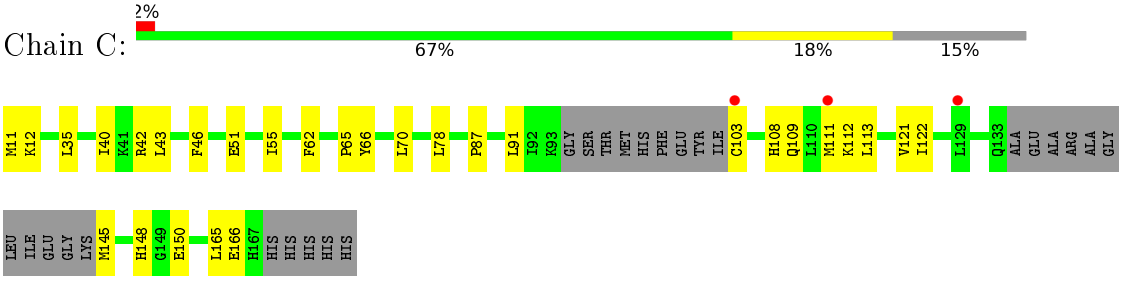
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain E:



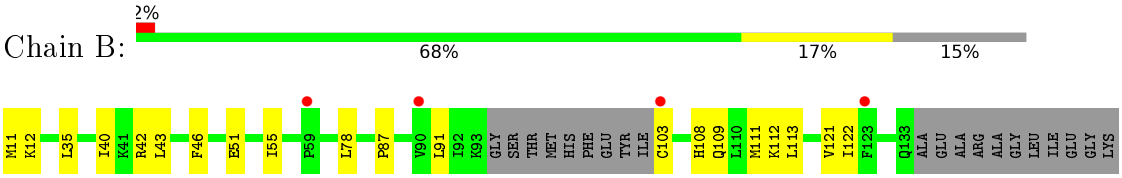
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

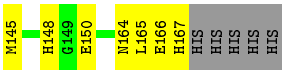
Chain C:



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

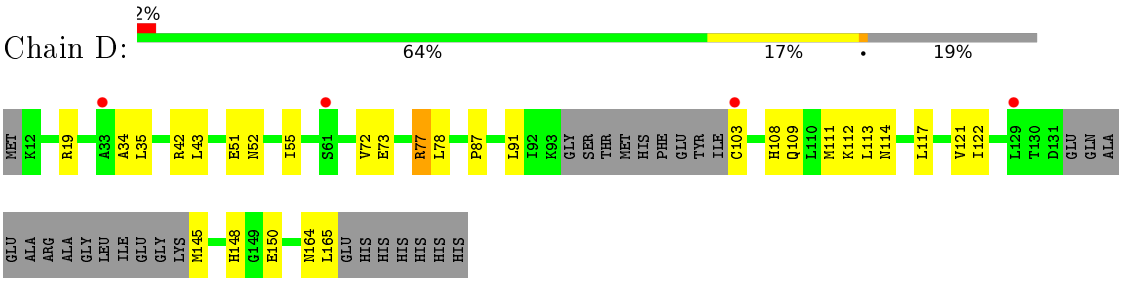
Chain B:





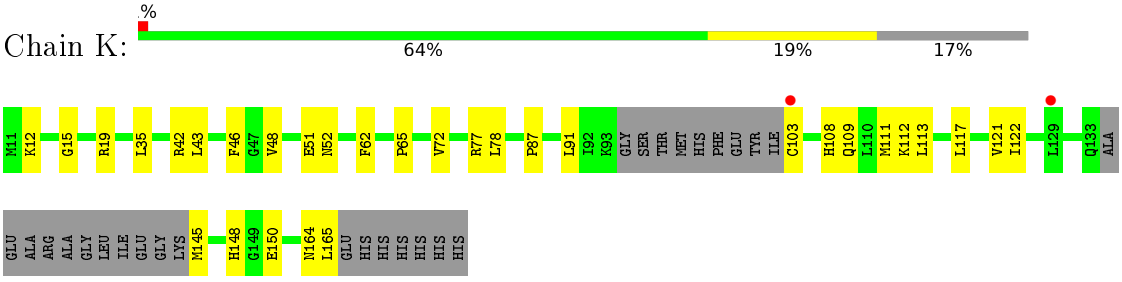
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain D:



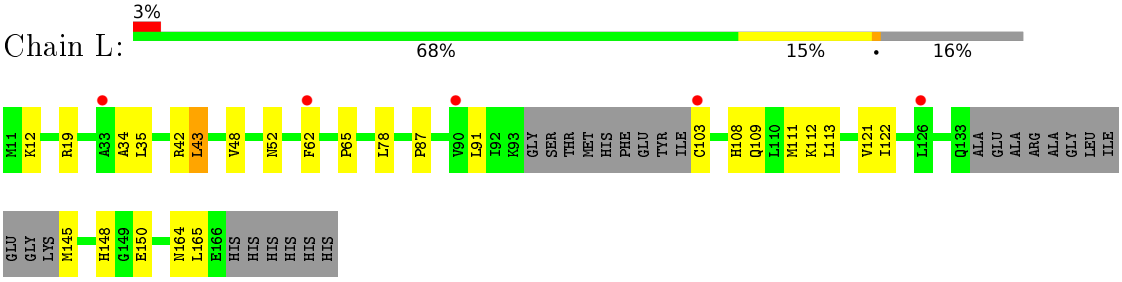
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain K:



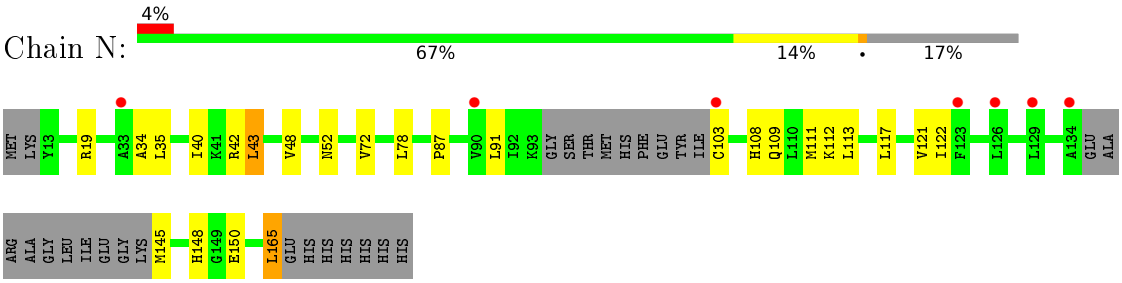
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain L:



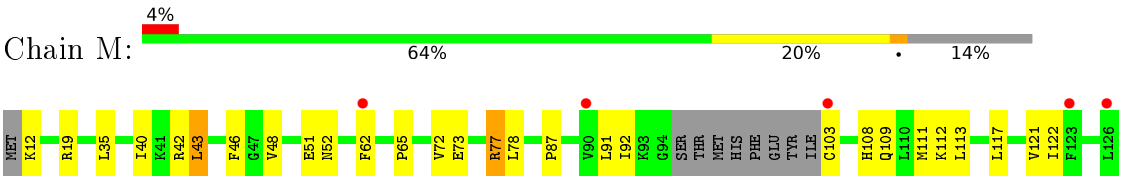
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

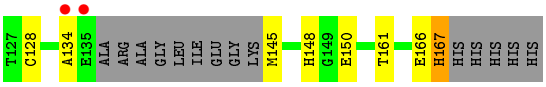
Chain N:



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

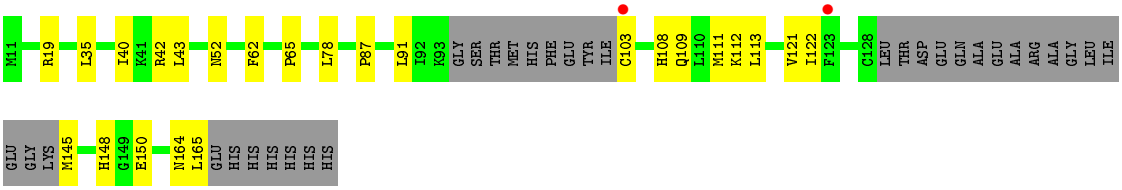
Chain M:





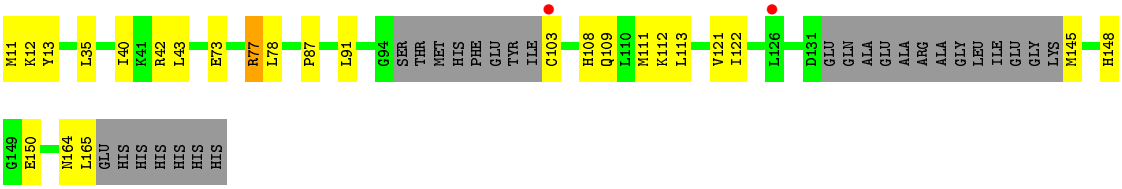
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain O:



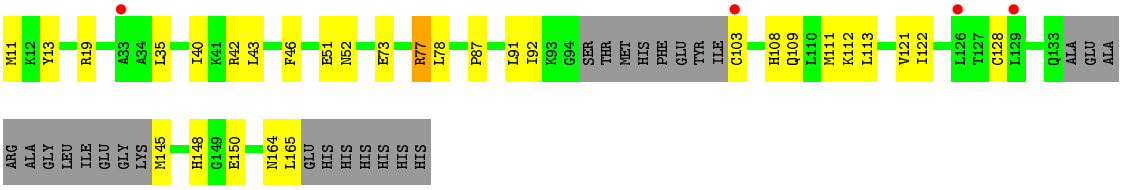
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain U:



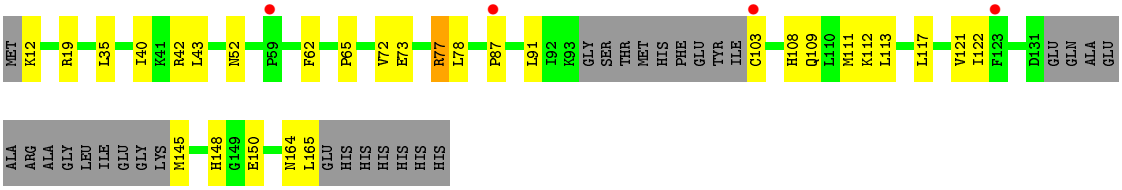
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain V:



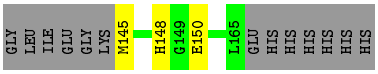
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain X:



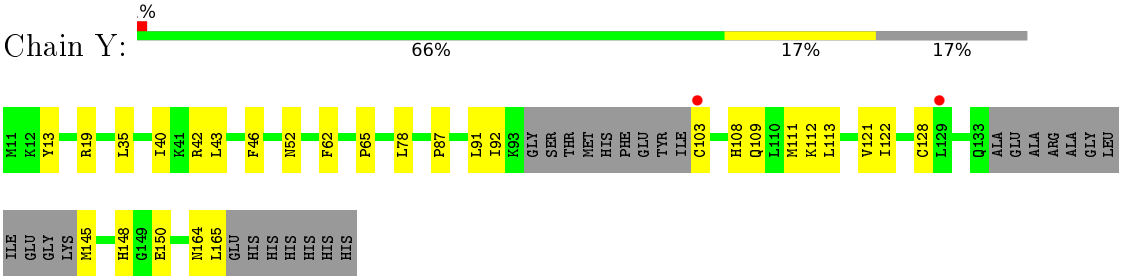
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain W:



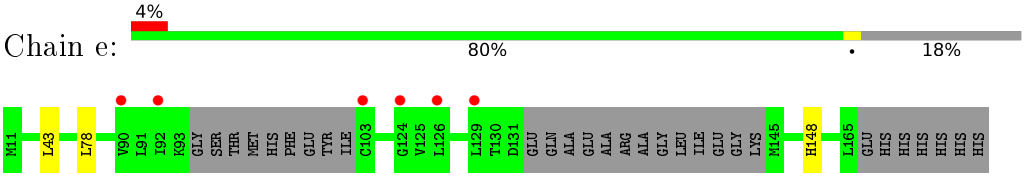
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Y:



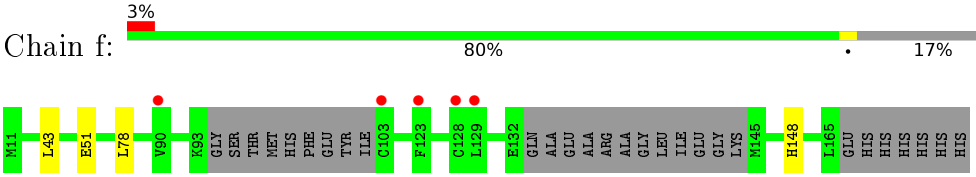
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain e:



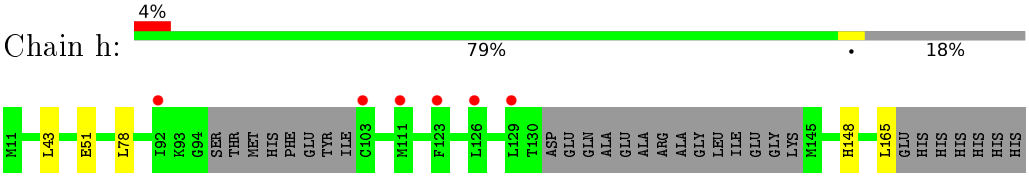
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain f:



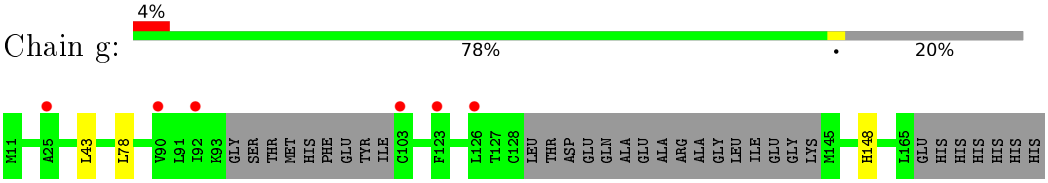
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain h:



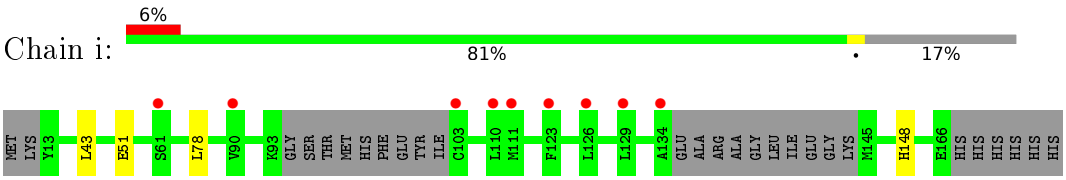
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain g:



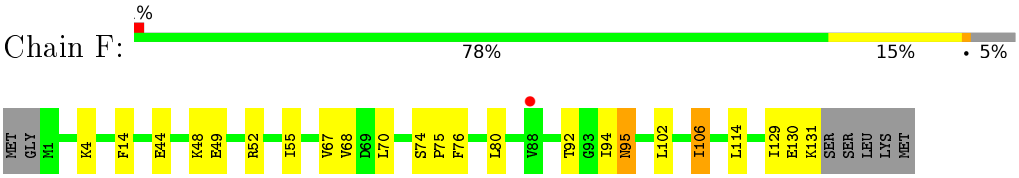
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain i:



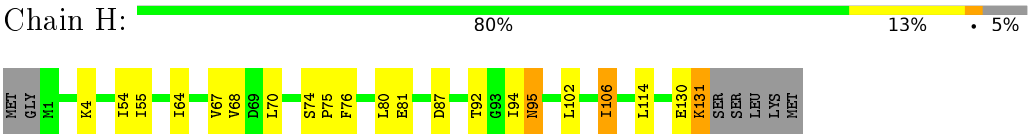
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain F:



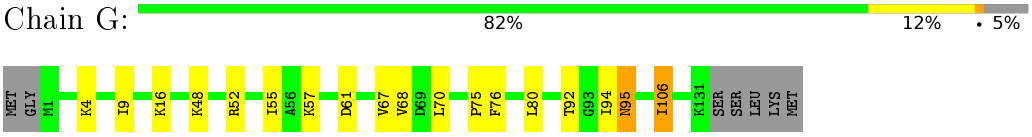
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain H:



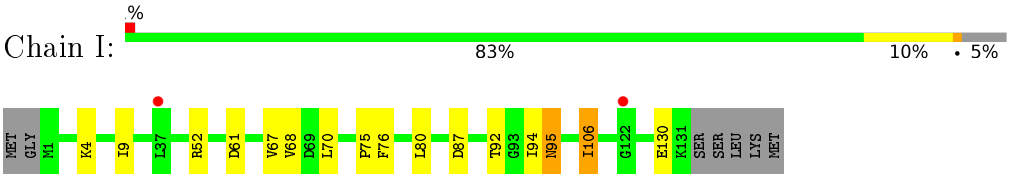
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain G:



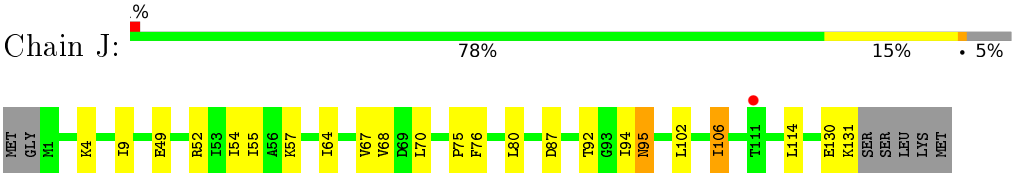
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain I:



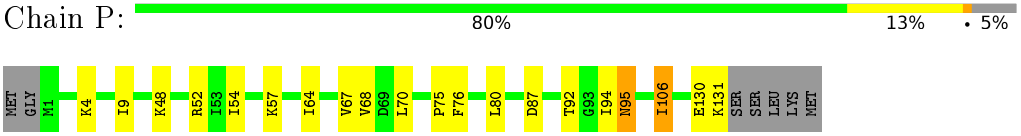
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain J:



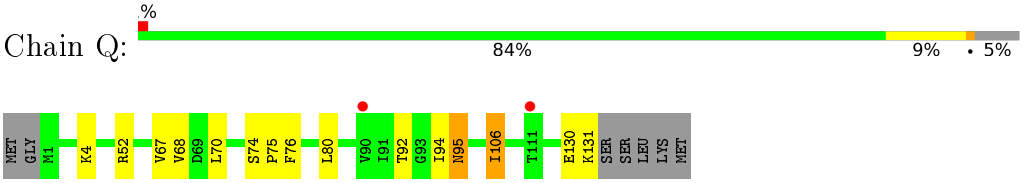
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain P:



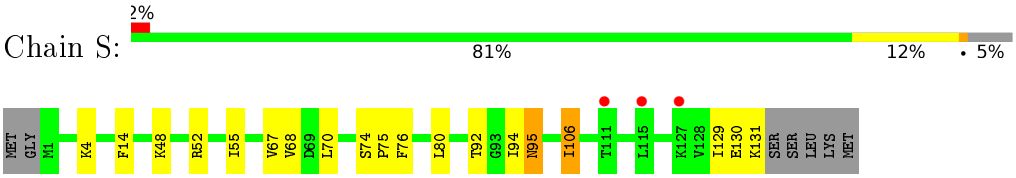
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain Q:



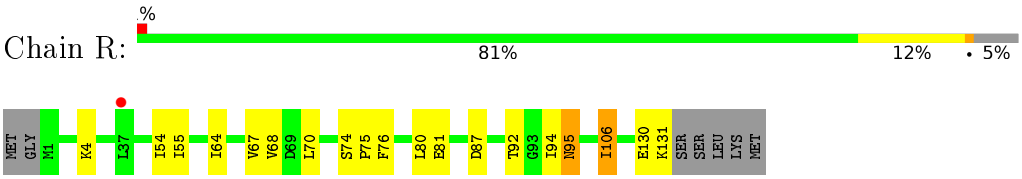
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain S:



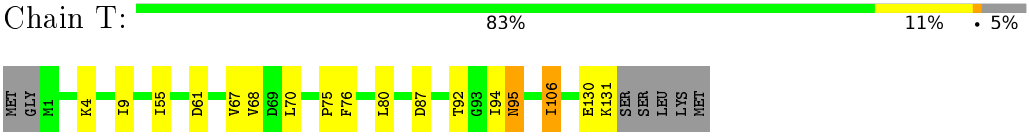
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain R:



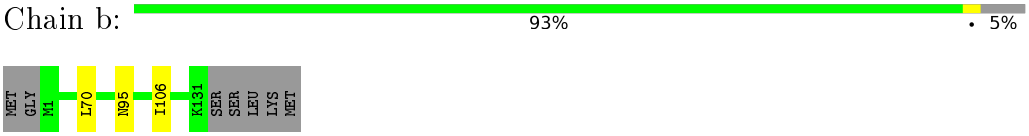
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain T:



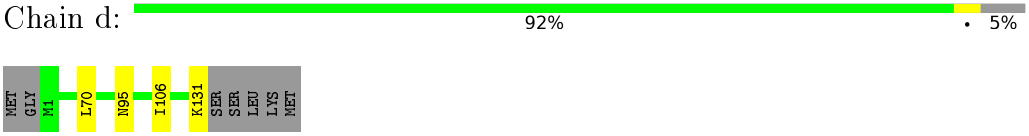
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain b:



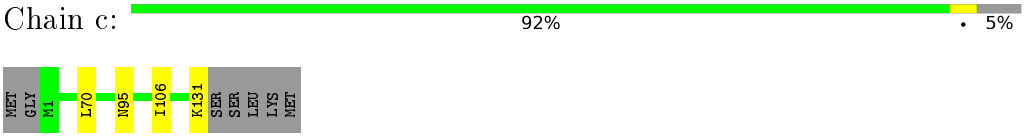
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain d:



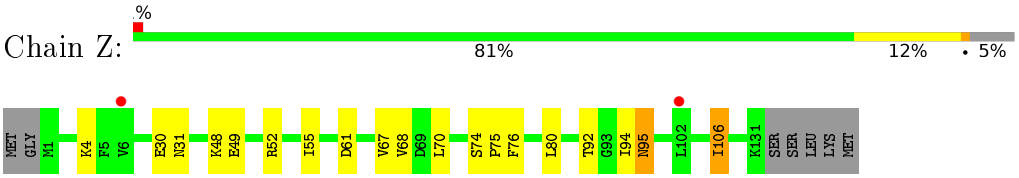
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain c:



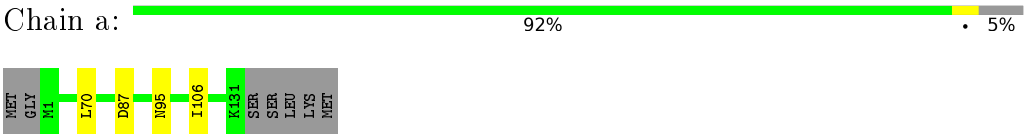
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain Z:



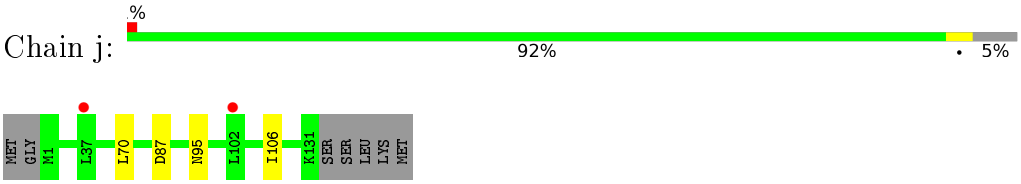
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain a:



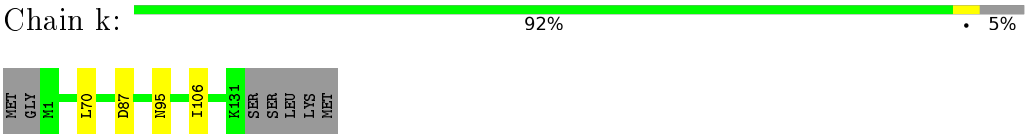
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain j:



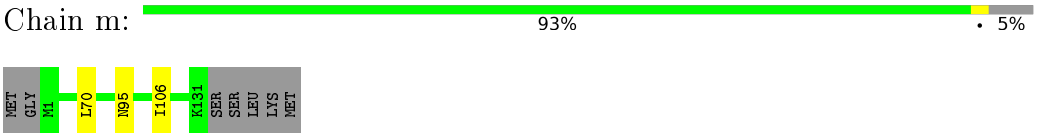
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain k:



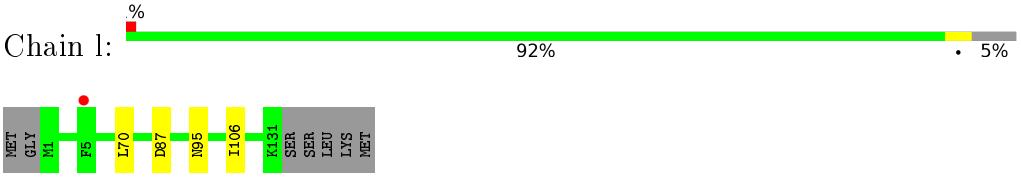
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain m:



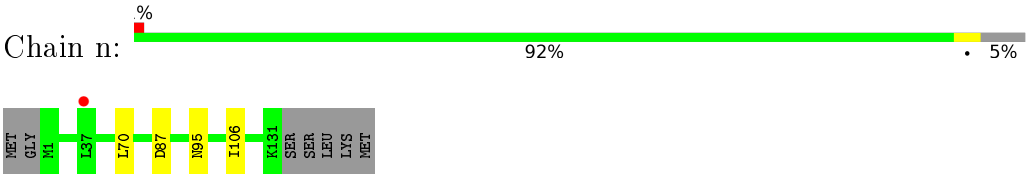
• Molecule 2: Phosphotransferase system, mannose/fructose-specific component IIA

Chain l:



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

Chain n:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	258.82Å 258.82Å 641.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	110.72 – 3.50 213.91 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (110.72-3.50) 99.1 (213.91-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.233 0.227 , 0.234	Depositor DCC
R_{free} test set	20029 reflections (10.00%)	DCC
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 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	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*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.000 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.000 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	Xtriage
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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.41	0/1049	0.49	0/1417
1	B	0.36	0/1069	0.50	0/1442
1	C	0.40	0/1069	0.52	0/1444
1	D	0.39	0/1030	0.51	0/1389
1	E	0.42	0/1033	0.50	0/1394
1	K	0.36	0/1049	0.49	0/1416
1	L	0.44	0/1062	0.51	0/1433
1	M	0.40	0/1090	0.51	0/1469
1	N	0.39	0/1040	0.50	0/1405
1	O	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	X	0.41	0/1030	0.50	0/1390
1	Y	0.38	0/1032	0.51	0/1393
1	e	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	H	0.54	0/1013	0.55	0/1361
2	I	0.51	0/1009	0.55	0/1356
2	J	0.54	0/1013	0.54	0/1361
2	P	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	T	0.55	0/1013	0.55	0/1361
2	Z	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	c	0.54	0/1009	0.56	0/1356

Mol	Chain	Bond lengths		Bond angles	
		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)

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	1031	0	1048	33	0
1	B	1051	0	1076	31	0
1	C	1051	0	1062	34	0
1	D	1013	0	1051	38	0
1	E	1016	0	1046	40	0
1	K	1032	0	1056	45	0
1	L	1045	0	1066	38	0
1	M	1072	0	1096	43	0
1	N	1023	0	1046	32	0
1	O	993	0	1024	30	0
1	U	1018	0	1038	32	0
1	V	1036	0	1059	38	0
1	W	1009	0	1040	30	0
1	X	1013	0	1044	32	0
1	Y	1017	0	1037	34	0
1	e	1018	0	1046	0	0
1	f	1027	0	1052	0	0
1	g	995	0	1024	0	0
1	h	1008	0	1034	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	i	1026	0	1041	0	0
2	F	1000	0	1074	26	0
2	G	996	0	1063	14	0
2	H	1004	0	1078	16	0
2	I	1000	0	1074	14	0
2	J	1004	0	1078	19	0
2	P	1004	0	1078	13	0
2	Q	1004	0	1078	13	0
2	R	1008	0	1082	12	0
2	S	1000	0	1074	25	0
2	T	1004	0	1078	15	0
2	Z	1004	0	1078	16	0
2	a	1004	0	1078	0	0
2	b	1000	0	1074	0	0
2	c	1000	0	1074	0	0
2	d	1004	0	1078	0	0
2	j	1004	0	1078	0	0
2	k	1008	0	1082	0	0
2	l	996	0	1070	0	0
2	m	1000	0	1074	0	0
2	n	1000	0	1074	0	0
All	All	40538	0	42503	546	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 9.

All (546) 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:M:12:LYS:HB2	1:M:46:PHE:HE2	1.32	0.94
2:F:14:PHE:HE1	2:S:14:PHE:HE1	1.11	0.93
2:Q:52:ARG:HB2	2:Q:52:ARG:NH1	1.85	0.90
2:Z:49:GLU:HA	2:Z:52:ARG:HH21	1.37	0.90
1:U:91:LEU:HD13	1:U:103:CYS:HB3	1.52	0.89
1:Y:91:LEU:HD13	1:Y:103:CYS:HB3	1.53	0.88
1:M:91:LEU:HD13	1:M:103:CYS:HB3	1.53	0.88
2:G:48:LYS:O	2:G:52:ARG:HG3	1.75	0.86
1:E:11:MET:HA	1:E:46:PHE:HE1	1.42	0.85
1:B:91:LEU:HD13	1:B:103:CYS:HB3	1.59	0.84
1:W:93:LYS:HG3	1:W:129:LEU:HD23	1.60	0.84
1:D:91:LEU:HD13	1:D:103:CYS:HB3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:MET:HA	1:E:46:PHE:CE1	2.13	0.83
1:M:43:LEU:O	1:M:48:VAL:HG23	1.78	0.82
2:F:129:ILE:HD11	2:S:76:PHE:HE1	1.44	0.82
2:H:131:LYS:HA	2:H:131:LYS:NZ	1.95	0.80
1:Y:19:ARG:HA	1:Y:52:ASN:HB3	1.64	0.78
1:M:12:LYS:HB2	1:M:46:PHE:CE2	2.17	0.78
1:L:164:ASN:C	1:L:165:LEU:HD12	2.04	0.78
1:X:164:ASN:OD1	1:X:165:LEU:N	2.14	0.77
1:E:34:ALA:HB2	2:J:52:ARG:HE	1.48	0.77
1:B:91:LEU:CD1	1:B:103:CYS:HB3	2.15	0.77
2:F:14:PHE:CE1	2:S:14:PHE:HE1	2.00	0.76
1:D:91:LEU:CD1	1:D:103:CYS:HB3	2.15	0.76
1:E:164:ASN:OD1	1:E:165:LEU:N	2.18	0.76
2:Q:52:ARG:HB2	2:Q:52:ARG:HH11	1.47	0.76
2:F:76:PHE:HE1	2:S:129:ILE:HD11	1.49	0.76
1:D:34:ALA:CB	2:I:52:ARG:HH11	1.99	0.76
2:F:14:PHE:HE1	2:S:14:PHE:CE1	2.00	0.75
1:E:93:LYS:HG3	1:E:129:LEU:HD23	1.69	0.75
1:M:77:ARG:HG3	1:M:77:ARG:HH11	1.51	0.74
1:M:77:ARG:HG3	1:M:77:ARG:NH1	2.03	0.73
1:B:12:LYS:HG2	1:B:12:LYS:O	1.87	0.73
1:K:12:LYS:HD2	2:T:61:ASP:OD2	1.87	0.73
1:U:108:HIS:HE1	1:Y:108:HIS:HD2	1.37	0.73
1:V:73:GLU:O	1:V:77:ARG:HG2	1.89	0.72
1:K:108:HIS:HD2	1:L:108:HIS:HE1	1.38	0.72
1:Y:13:TYR:O	1:Y:46:PHE:HD2	1.72	0.72
2:F:130:GLU:O	2:F:131:LYS:HB2	1.88	0.72
1:V:165:LEU:HD12	1:V:165:LEU:O	1.89	0.71
1:C:108:HIS:HE1	1:B:108:HIS:HD2	1.36	0.71
1:N:34:ALA:HB2	2:S:52:ARG:HD3	1.73	0.70
2:J:4:LYS:HD2	2:J:106:ILE:HG13	1.74	0.70
2:H:4:LYS:HD2	2:H:106:ILE:HG13	1.74	0.70
2:S:4:LYS:HD2	2:S:106:ILE:HG13	1.74	0.70
2:R:4:LYS:HD2	2:R:106:ILE:HG13	1.74	0.70
2:P:4:LYS:HD2	2:P:106:ILE:HG13	1.74	0.69
1:K:109:GLN:HG3	1:L:111:MET:HG3	1.73	0.69
1:A:161:THR:HG23	1:A:167:HIS:ND1	2.08	0.69
2:G:4:LYS:HD2	2:G:106:ILE:HG13	1.74	0.69
1:E:12:LYS:HD2	2:I:61:ASP:OD2	1.92	0.69
1:Y:164:ASN:CG	1:Y:165:LEU:H	1.97	0.68
2:Z:4:LYS:HD2	2:Z:106:ILE:HG13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:MET:HG3	1:E:109:GLN:HG3	1.76	0.68
2:Q:4:LYS:HD2	2:Q:106:ILE:HG13	1.74	0.68
2:I:4:LYS:HD2	2:I:106:ILE:HG13	1.74	0.68
2:F:4:LYS:HD2	2:F:106:ILE:HG13	1.74	0.68
2:T:4:LYS:HD2	2:T:106:ILE:HG13	1.74	0.68
1:N:108:HIS:HD2	1:O:108:HIS:HE1	1.42	0.68
1:X:12:LYS:O	1:X:12:LYS:HG2	1.93	0.67
1:V:109:GLN:HG3	1:W:111:MET:HG3	1.74	0.67
1:K:108:HIS:CD2	1:L:108:HIS:HE1	2.12	0.67
2:F:129:ILE:HD11	2:S:76:PHE:CE1	2.26	0.67
2:H:130:GLU:O	2:H:131:LYS:HG2	1.94	0.67
1:C:108:HIS:CE1	1:B:108:HIS:HD2	2.14	0.66
1:C:66:TYR:CE2	1:C:70:LEU:HD11	2.31	0.66
1:A:111:MET:CG	1:E:109:GLN:HG3	2.25	0.66
1:X:111:MET:HG3	1:W:109:GLN:HG3	1.77	0.66
1:K:108:HIS:HD2	1:L:108:HIS:CE1	2.14	0.66
1:C:108:HIS:HE1	1:B:108:HIS:CD2	2.13	0.66
1:N:109:GLN:HG3	1:O:111:MET:HG3	1.77	0.66
2:H:131:LYS:HA	2:H:131:LYS:HZ3	1.57	0.66
1:K:12:LYS:HE2	2:T:61:ASP:CG	2.16	0.66
1:Y:92:ILE:CD1	1:Y:128:CYS:HB2	2.26	0.66
1:A:109:GLN:HG3	1:B:111:MET:HG3	1.78	0.65
1:N:108:HIS:HE1	1:M:108:HIS:HD2	1.44	0.65
1:D:34:ALA:HB2	2:I:52:ARG:HH11	1.60	0.65
1:K:77:ARG:CD	1:L:165:LEU:HD22	2.25	0.65
1:N:108:HIS:CD2	1:O:108:HIS:HE1	2.14	0.65
1:A:12:LYS:O	1:A:12:LYS:HG2	1.97	0.65
1:U:108:HIS:HE1	1:Y:108:HIS:CD2	2.15	0.65
1:V:109:GLN:HG3	1:W:111:MET:CG	2.27	0.65
1:C:91:LEU:HD13	1:C:103:CYS:HB3	1.77	0.65
2:F:76:PHE:CE1	2:S:129:ILE:HD11	2.32	0.65
1:U:108:HIS:HD2	1:V:108:HIS:HE1	1.42	0.65
1:C:108:HIS:HD2	1:D:108:HIS:HE1	1.43	0.64
1:L:43:LEU:O	1:L:48:VAL:HG23	1.97	0.64
1:X:109:GLN:HG3	1:Y:111:MET:HG3	1.77	0.64
1:L:109:GLN:HG3	1:M:111:MET:HG3	1.79	0.64
1:W:93:LYS:HG3	1:W:129:LEU:CD2	2.28	0.64
1:C:111:MET:HG3	1:B:109:GLN:HG3	1.80	0.64
1:O:164:ASN:CG	1:O:165:LEU:H	2.00	0.64
1:N:108:HIS:HD2	1:O:108:HIS:CE1	2.16	0.64
1:K:77:ARG:HD3	1:L:165:LEU:HD22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:77:ARG:HG3	1:V:77:ARG:NH1	2.11	0.63
2:Z:30:GLU:O	2:Z:31:ASN:HB2	1.98	0.63
1:K:108:HIS:CD2	1:L:108:HIS:CE1	2.86	0.63
1:U:111:MET:HG3	1:Y:109:GLN:HG3	1.79	0.63
1:E:42:ARG:HD3	1:E:150:GLU:HB3	1.86	0.63
1:K:109:GLN:HG3	1:L:111:MET:CG	2.29	0.63
1:U:109:GLN:HG3	1:V:111:MET:HG3	1.79	0.63
1:B:166:GLU:O	1:B:167:HIS:HB3	1.97	0.63
1:V:108:HIS:HD2	1:W:108:HIS:HE1	1.47	0.63
1:C:109:GLN:HG3	1:D:111:MET:HG3	1.81	0.63
1:L:91:LEU:HD13	1:L:103:CYS:HB3	1.81	0.63
1:N:111:MET:HG3	1:M:109:GLN:HG3	1.81	0.63
1:A:91:LEU:HD13	1:A:103:CYS:HB3	1.80	0.62
1:C:108:HIS:CE1	1:B:108:HIS:CD2	2.87	0.62
2:R:67:VAL:CG1	2:R:94:ILE:HB	2.29	0.62
1:X:108:HIS:HE1	1:W:108:HIS:HD2	1.47	0.62
1:D:165:LEU:HD12	1:D:165:LEU:C	2.20	0.62
2:H:67:VAL:CG1	2:H:94:ILE:HB	2.29	0.62
1:N:19:ARG:HA	1:N:52:ASN:HB3	1.82	0.62
1:U:108:HIS:CE1	1:Y:108:HIS:HD2	2.18	0.62
2:F:44:GLU:HA	2:F:44:GLU:OE2	1.99	0.62
1:E:91:LEU:HD13	1:E:103:CYS:HB3	1.81	0.62
1:O:91:LEU:HD13	1:O:103:CYS:HB3	1.82	0.62
2:P:130:GLU:O	2:P:131:LYS:HG2	1.99	0.62
2:R:130:GLU:OE1	2:R:130:GLU:HA	1.99	0.62
1:A:109:GLN:HG3	1:B:111:MET:CG	2.29	0.62
1:N:91:LEU:HD13	1:N:103:CYS:HB3	1.82	0.62
1:N:108:HIS:CD2	1:O:108:HIS:CE1	2.87	0.62
1:X:91:LEU:HD13	1:X:103:CYS:HB3	1.82	0.62
1:K:108:HIS:HE1	1:O:108:HIS:HD2	1.48	0.61
1:N:109:GLN:HG3	1:O:111:MET:CG	2.30	0.61
1:X:109:GLN:HG3	1:Y:111:MET:CG	2.29	0.61
1:K:12:LYS:HE2	2:T:61:ASP:OD1	2.00	0.61
1:V:164:ASN:O	1:V:165:LEU:C	2.39	0.61
1:V:108:HIS:HD2	1:W:108:HIS:CE1	2.19	0.61
1:C:108:HIS:CD2	1:D:108:HIS:HE1	2.18	0.61
1:V:91:LEU:HD13	1:V:103:CYS:HB3	1.81	0.61
1:W:91:LEU:HD13	1:W:103:CYS:HB3	1.82	0.61
1:X:108:HIS:HD2	1:Y:108:HIS:HE1	1.47	0.61
1:C:42:ARG:HD3	1:C:150:GLU:HB3	1.83	0.61
1:K:111:MET:HG3	1:O:109:GLN:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:77:ARG:HH11	1:V:77:ARG:HG3	1.65	0.61
1:X:111:MET:CG	1:W:109:GLN:HG3	2.31	0.61
1:X:19:ARG:HA	1:X:52:ASN:HB3	1.82	0.61
1:N:108:HIS:HE1	1:M:108:HIS:CD2	2.19	0.60
1:E:108:HIS:HE1	1:D:108:HIS:HD2	1.47	0.60
1:E:111:MET:HG3	1:D:109:GLN:HG3	1.82	0.60
1:K:109:GLN:CG	1:L:111:MET:HG3	2.31	0.60
1:K:91:LEU:HD13	1:K:103:CYS:HB3	1.81	0.60
1:O:42:ARG:HD3	1:O:150:GLU:HB3	1.84	0.60
1:L:108:HIS:HD2	1:M:108:HIS:HE1	1.49	0.60
1:L:109:GLN:HG3	1:M:111:MET:CG	2.32	0.60
1:U:108:HIS:HD2	1:V:108:HIS:CE1	2.18	0.60
2:Q:130:GLU:O	2:Q:131:LYS:HB2	2.02	0.60
1:V:77:ARG:HH11	1:V:77:ARG:CG	2.14	0.60
1:U:108:HIS:CD2	1:V:108:HIS:HE1	2.19	0.60
1:A:108:HIS:HD2	1:B:108:HIS:HE1	1.49	0.59
1:U:12:LYS:HD3	2:Z:61:ASP:OD2	2.01	0.59
1:K:42:ARG:HD3	1:K:150:GLU:HB3	1.84	0.59
1:X:108:HIS:HD2	1:Y:108:HIS:CE1	2.19	0.59
1:D:42:ARG:HD3	1:D:150:GLU:HB3	1.85	0.59
1:A:42:ARG:HD3	1:A:150:GLU:HB3	1.85	0.59
2:J:130:GLU:O	2:J:131:LYS:HG2	2.02	0.59
1:D:77:ARG:HB3	1:D:77:ARG:HH11	1.68	0.59
2:F:102:LEU:HD12	2:F:114:LEU:HD21	1.85	0.59
1:Y:42:ARG:HD3	1:Y:150:GLU:HB3	1.84	0.59
1:A:108:HIS:HE1	1:E:108:HIS:HD2	1.50	0.58
1:N:42:ARG:HD3	1:N:150:GLU:HB3	1.85	0.58
1:X:42:ARG:HD3	1:X:150:GLU:HB3	1.85	0.58
1:V:11:MET:HA	1:V:46:PHE:CE2	2.38	0.58
1:X:108:HIS:CE1	1:W:108:HIS:HD2	2.21	0.58
1:L:165:LEU:HD12	1:L:165:LEU:N	2.18	0.58
1:N:108:HIS:CE1	1:M:108:HIS:HD2	2.20	0.58
1:V:108:HIS:CD2	1:W:108:HIS:HE1	2.21	0.58
1:A:108:HIS:CE1	1:E:108:HIS:HD2	2.21	0.58
2:S:130:GLU:O	2:S:131:LYS:HB3	2.02	0.58
1:U:42:ARG:HD3	1:U:150:GLU:HB3	1.85	0.58
1:D:73:GLU:O	1:D:77:ARG:HG2	2.04	0.58
1:K:111:MET:CG	1:O:109:GLN:HG3	2.33	0.58
1:A:108:HIS:HE1	1:E:108:HIS:CD2	2.21	0.58
2:T:130:GLU:O	2:T:131:LYS:HG2	2.02	0.58
1:U:108:HIS:CE1	1:Y:108:HIS:CD2	2.92	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:HIS:HD2	1:D:108:HIS:CE1	2.21	0.57
1:L:108:HIS:HD2	1:M:108:HIS:CE1	2.23	0.57
1:A:108:HIS:CE1	1:E:108:HIS:CD2	2.93	0.57
1:D:34:ALA:CB	2:I:52:ARG:NH1	2.67	0.57
1:K:108:HIS:HE1	1:O:108:HIS:CD2	2.23	0.57
1:V:108:HIS:CD2	1:W:108:HIS:CE1	2.93	0.57
1:V:87:PRO:HD2	1:V:122:ILE:O	2.05	0.57
1:U:87:PRO:HD2	1:U:122:ILE:O	2.05	0.57
1:A:111:MET:HG3	1:E:109:GLN:CG	2.34	0.57
1:E:108:HIS:HE1	1:D:108:HIS:CD2	2.22	0.57
1:D:87:PRO:HD2	1:D:122:ILE:O	2.05	0.57
1:K:108:HIS:CE1	1:O:108:HIS:HD2	2.22	0.57
1:X:108:HIS:CD2	1:Y:108:HIS:CE1	2.93	0.57
1:B:87:PRO:HD2	1:B:122:ILE:O	2.05	0.57
2:H:102:LEU:HD12	2:H:114:LEU:HD21	1.86	0.57
1:M:77:ARG:CG	1:M:77:ARG:HH11	2.14	0.57
1:A:108:HIS:HD2	1:B:108:HIS:CE1	2.22	0.56
1:U:108:HIS:CD2	1:V:108:HIS:CE1	2.93	0.56
2:F:67:VAL:CG1	2:F:94:ILE:HB	2.36	0.56
1:L:42:ARG:HD3	1:L:150:GLU:HB3	1.86	0.56
1:X:108:HIS:HE1	1:W:108:HIS:CD2	2.22	0.56
1:A:108:HIS:CD2	1:B:108:HIS:HE1	2.22	0.56
1:E:87:PRO:HD2	1:E:122:ILE:O	2.05	0.56
1:L:87:PRO:HD2	1:L:122:ILE:O	2.06	0.56
2:J:102:LEU:HD12	2:J:114:LEU:HD21	1.86	0.56
1:L:108:HIS:CD2	1:M:108:HIS:HE1	2.23	0.56
1:Y:87:PRO:HD2	1:Y:122:ILE:O	2.05	0.56
1:A:87:PRO:HD2	1:A:122:ILE:O	2.05	0.56
2:J:130:GLU:O	2:J:131:LYS:HG3	3.19	0.56
1:V:164:ASN:CG	1:V:165:LEU:H	2.09	0.56
2:G:67:VAL:CG1	2:G:94:ILE:HB	2.36	0.56
1:E:93:LYS:HG3	1:E:129:LEU:CD2	2.36	0.56
1:N:109:GLN:CG	1:O:111:MET:HG3	2.36	0.56
1:W:93:LYS:CG	1:W:129:LEU:HD23	2.35	0.56
1:X:108:HIS:CD2	1:Y:108:HIS:HE1	2.22	0.56
2:Q:67:VAL:CG1	2:Q:94:ILE:HB	2.36	0.56
1:V:42:ARG:HD3	1:V:150:GLU:HB3	1.88	0.56
1:Y:91:LEU:CD1	1:Y:103:CYS:HB3	2.31	0.56
1:N:87:PRO:HD2	1:N:122:ILE:O	2.05	0.56
1:B:42:ARG:HD3	1:B:150:GLU:HB3	1.88	0.55
1:C:87:PRO:HD2	1:C:122:ILE:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:87:PRO:HD2	1:M:122:ILE:O	2.05	0.55
1:W:42:ARG:HD3	1:W:150:GLU:HB3	1.87	0.55
1:C:111:MET:CG	1:B:109:GLN:HG3	2.36	0.55
2:J:67:VAL:CG1	2:J:94:ILE:HB	2.36	0.55
1:O:87:PRO:HD2	1:O:122:ILE:O	2.06	0.55
2:R:67:VAL:HG11	2:R:94:ILE:HG12	1.88	0.55
1:V:109:GLN:CG	1:W:111:MET:HG3	2.35	0.55
1:W:87:PRO:HD2	1:W:122:ILE:O	2.05	0.55
2:I:67:VAL:CG1	2:I:94:ILE:HB	2.36	0.55
1:K:87:PRO:HD2	1:K:122:ILE:O	2.06	0.55
1:U:109:GLN:HG3	1:V:111:MET:CG	2.36	0.55
1:A:108:HIS:CD2	1:B:108:HIS:CE1	2.94	0.55
1:E:108:HIS:CE1	1:D:108:HIS:HD2	2.23	0.55
1:E:111:MET:CG	1:D:109:GLN:HG3	2.36	0.55
1:E:34:ALA:CB	2:J:52:ARG:HE	2.16	0.55
1:N:108:HIS:CE1	1:M:108:HIS:CD2	2.93	0.55
1:C:108:HIS:CD2	1:D:108:HIS:CE1	2.94	0.55
1:A:161:THR:CG2	1:A:167:HIS:ND1	2.68	0.55
2:J:76:PHE:CE2	2:J:80:LEU:HD11	2.42	0.55
1:X:87:PRO:HD2	1:X:122:ILE:O	2.05	0.55
1:M:91:LEU:CD1	1:M:103:CYS:HB3	2.32	0.55
2:S:67:VAL:CG1	2:S:94:ILE:HB	2.37	0.55
1:N:111:MET:CG	1:M:109:GLN:HG3	2.36	0.55
2:Q:76:PHE:CE2	2:Q:80:LEU:HD11	2.42	0.55
1:X:109:GLN:CG	1:Y:111:MET:HG3	2.37	0.55
2:Z:76:PHE:CE2	2:Z:80:LEU:HD11	2.42	0.55
1:C:109:GLN:HG3	1:D:111:MET:CG	2.37	0.54
2:H:67:VAL:HG11	2:H:94:ILE:HG12	1.90	0.54
1:K:164:ASN:ND2	1:K:165:LEU:HG	2.22	0.54
2:R:76:PHE:CE2	2:R:80:LEU:HD11	2.42	0.54
2:Z:67:VAL:CG1	2:Z:94:ILE:HB	2.37	0.54
1:E:12:LYS:O	1:E:12:LYS:HG2	2.05	0.54
2:F:76:PHE:CE2	2:F:80:LEU:HD11	2.43	0.54
2:T:67:VAL:CG1	2:T:94:ILE:HB	2.37	0.54
2:P:67:VAL:CG1	2:P:94:ILE:HB	2.36	0.54
1:X:108:HIS:CE1	1:W:108:HIS:CD2	2.95	0.54
2:P:48:LYS:O	2:P:52:ARG:HG3	2.08	0.54
1:Y:92:ILE:HD13	1:Y:128:CYS:HB2	1.89	0.54
1:K:77:ARG:HD2	1:L:165:LEU:HD22	1.90	0.54
2:R:130:GLU:O	2:R:131:LYS:HG2	2.08	0.54
1:E:108:HIS:CE1	1:D:108:HIS:CD2	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:76:PHE:CE2	2:I:80:LEU:HD11	2.43	0.54
2:H:67:VAL:HG11	2:H:94:ILE:CG1	2.38	0.54
1:N:34:ALA:CB	2:S:52:ARG:HD3	2.36	0.54
1:X:73:GLU:O	1:X:77:ARG:HG3	2.08	0.54
1:M:42:ARG:HD3	1:M:150:GLU:HB3	1.90	0.54
1:K:108:HIS:CE1	1:O:108:HIS:CD2	2.96	0.54
1:U:91:LEU:HD13	1:U:103:CYS:CB	2.32	0.54
2:G:76:PHE:CE2	2:G:80:LEU:HD11	2.43	0.53
2:H:76:PHE:CE2	2:H:80:LEU:HD11	2.43	0.53
2:S:76:PHE:CE2	2:S:80:LEU:HD11	2.43	0.53
1:N:109:GLN:OE1	1:N:112:LYS:HE2	2.09	0.53
2:P:76:PHE:CE2	2:P:80:LEU:HD11	2.43	0.53
2:S:48:LYS:O	2:S:52:ARG:HG3	2.08	0.53
1:L:108:HIS:CD2	1:M:108:HIS:CE1	2.96	0.53
1:C:111:MET:HG3	1:B:109:GLN:CG	2.38	0.53
1:N:43:LEU:O	1:N:48:VAL:HG23	2.08	0.53
2:T:76:PHE:CE2	2:T:80:LEU:HD11	2.43	0.53
1:U:111:MET:HG3	1:Y:109:GLN:CG	2.39	0.53
2:R:67:VAL:HG11	2:R:94:ILE:CG1	2.38	0.53
1:X:111:MET:HG3	1:W:109:GLN:CG	2.39	0.53
1:A:109:GLN:CG	1:B:111:MET:HG3	2.38	0.53
1:D:164:ASN:O	1:D:165:LEU:HD12	2.09	0.53
1:L:34:ALA:HB2	2:Q:52:ARG:HD3	1.91	0.53
1:E:93:LYS:CG	1:E:129:LEU:HD23	2.38	0.52
1:U:91:LEU:CD1	1:U:103:CYS:HB3	2.31	0.52
1:M:161:THR:HG23	1:M:167:HIS:CE1	2.45	0.52
1:M:73:GLU:O	1:M:77:ARG:HG2	2.09	0.52
1:L:109:GLN:CG	1:M:111:MET:HG3	2.39	0.52
1:N:165:LEU:C	1:N:165:LEU:HD12	2.30	0.52
1:M:166:GLU:O	1:M:167:HIS:CD2	2.63	0.52
1:M:19:ARG:HA	1:M:52:ASN:HB3	1.92	0.52
2:J:49:GLU:O	2:J:52:ARG:HB3	2.34	0.52
1:V:11:MET:HA	1:V:46:PHE:CZ	2.45	0.52
1:A:161:THR:CG2	1:A:167:HIS:CE1	2.93	0.52
1:A:111:MET:CG	1:E:109:GLN:CG	2.88	0.52
1:C:109:GLN:CG	1:D:111:MET:HG3	2.40	0.51
1:U:111:MET:CG	1:Y:109:GLN:HG3	2.39	0.51
1:K:42:ARG:O	1:K:46:PHE:HD1	1.93	0.51
1:U:109:GLN:CG	1:V:111:MET:HG3	2.40	0.51
1:X:164:ASN:OD1	1:X:165:LEU:HG	2.10	0.51
2:F:48:LYS:O	2:F:52:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:109:GLN:OE1	1:U:112:LYS:HE2	2.11	0.51
2:H:74:SER:N	2:H:75:PRO:CD	2.74	0.51
2:Z:30:GLU:O	2:Z:31:ASN:CB	2.58	0.51
1:X:164:ASN:CG	1:X:165:LEU:H	2.10	0.51
1:Y:91:LEU:HD13	1:Y:103:CYS:CB	2.35	0.51
1:K:19:ARG:HA	1:K:52:ASN:HB3	1.93	0.50
1:M:109:GLN:OE1	1:M:112:LYS:HE2	2.11	0.50
1:E:111:MET:HG3	1:D:109:GLN:CG	2.41	0.50
1:D:109:GLN:OE1	1:D:112:LYS:HE2	2.11	0.50
1:D:19:ARG:HA	1:D:52:ASN:HB3	1.93	0.50
1:K:109:GLN:CG	1:L:111:MET:CG	2.89	0.50
1:K:77:ARG:HB2	1:L:165:LEU:HD21	1.94	0.50
1:L:109:GLN:OE1	1:L:112:LYS:HE2	2.12	0.50
1:N:40:ILE:HD12	2:S:55:ILE:HD11	1.93	0.50
1:K:111:MET:HG3	1:O:109:GLN:CG	2.42	0.50
1:O:19:ARG:HA	1:O:52:ASN:HB3	1.94	0.50
1:D:34:ALA:HB1	2:I:52:ARG:NH1	2.27	0.50
2:F:74:SER:N	2:F:75:PRO:CD	2.75	0.49
1:C:109:GLN:OE1	1:C:112:LYS:HE2	2.12	0.49
1:N:111:MET:HG3	1:M:109:GLN:CG	2.41	0.49
1:B:91:LEU:CD1	1:B:103:CYS:CB	2.87	0.49
1:V:109:GLN:OE1	1:V:112:LYS:HE2	2.12	0.49
1:O:109:GLN:OE1	1:O:112:LYS:HE2	2.12	0.49
2:F:129:ILE:HD13	2:S:80:LEU:HD21	1.94	0.49
1:A:109:GLN:OE1	1:A:112:LYS:HE2	2.12	0.49
1:E:109:GLN:OE1	1:E:112:LYS:HE2	2.12	0.49
2:P:9:ILE:HG22	2:P:75:PRO:HB3	1.95	0.49
2:Q:74:SER:N	2:Q:75:PRO:CD	2.76	0.49
1:D:91:LEU:CD1	1:D:103:CYS:CB	2.88	0.49
1:C:66:TYR:CD1	1:D:114:ASN:HB3	2.48	0.48
2:R:74:SER:N	2:R:75:PRO:CD	2.76	0.48
1:W:19:ARG:HA	1:W:52:ASN:HB3	1.95	0.48
2:J:49:GLU:OE1	2:J:52:ARG:NH2	2.46	0.48
2:J:9:ILE:HG22	2:J:75:PRO:HB3	1.96	0.48
1:N:109:GLN:CG	1:O:111:MET:CG	2.91	0.48
1:U:11:MET:C	1:U:13:TYR:H	2.16	0.48
1:A:161:THR:HG21	1:A:167:HIS:CE1	2.49	0.48
2:S:74:SER:N	2:S:75:PRO:CD	2.76	0.48
1:A:109:GLN:CG	1:B:111:MET:CG	2.92	0.48
2:T:9:ILE:HG22	2:T:75:PRO:HB3	1.95	0.48
1:X:109:GLN:OE1	1:X:112:LYS:HE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLN:OE1	1:B:112:LYS:HE2	2.13	0.48
1:V:109:GLN:CG	1:W:111:MET:CG	2.91	0.48
2:F:76:PHE:CE1	2:S:129:ILE:CD1	2.96	0.47
2:Q:52:ARG:HB2	2:Q:52:ARG:CZ	2.43	0.47
1:K:164:ASN:CG	1:K:165:LEU:N	2.68	0.47
1:M:35:LEU:HD23	1:M:145:MET:O	2.14	0.47
1:V:92:ILE:CD1	1:V:128:CYS:HB2	2.44	0.47
1:N:109:GLN:OE1	1:N:112:LYS:CE	2.61	0.47
1:W:109:GLN:OE1	1:W:112:LYS:HE2	2.14	0.47
2:Z:74:SER:N	2:Z:75:PRO:CD	2.76	0.47
1:M:91:LEU:HD13	1:M:103:CYS:CB	2.34	0.47
1:E:164:ASN:O	1:E:165:LEU:HD23	4.85	0.47
1:K:42:ARG:HG3	1:K:46:PHE:HE1	1.80	0.47
1:M:92:ILE:CD1	1:M:128:CYS:HB2	2.44	0.47
1:V:19:ARG:HA	1:V:52:ASN:HB3	1.96	0.47
1:C:11:MET:HA	1:C:46:PHE:CE2	2.50	0.47
2:I:9:ILE:HG22	2:I:75:PRO:HB3	1.95	0.47
2:S:131:LYS:O	2:S:131:LYS:HG2	2.15	0.47
2:G:9:ILE:HG22	2:G:75:PRO:HB3	1.95	0.47
1:M:109:GLN:OE1	1:M:112:LYS:CE	2.63	0.47
1:M:40:ILE:HD12	2:R:55:ILE:HD11	1.97	0.47
2:F:130:GLU:O	2:F:131:LYS:CB	2.56	0.47
1:U:164:ASN:O	1:U:165:LEU:HB2	2.15	0.47
1:U:109:GLN:OE1	1:U:112:LYS:CE	2.63	0.47
1:V:35:LEU:HD23	1:V:145:MET:O	2.15	0.47
1:O:164:ASN:CG	1:O:165:LEU:N	2.68	0.46
1:E:19:ARG:HA	1:E:52:ASN:HB3	2.07	0.46
2:H:131:LYS:CA	2:H:131:LYS:NZ	2.73	0.46
1:B:55:ILE:HD11	1:V:40:ILE:HD12	217.98	0.46
2:F:76:PHE:HE1	2:S:129:ILE:CD1	2.23	0.46
1:K:109:GLN:OE1	1:K:112:LYS:HE2	2.15	0.46
1:Y:40:ILE:HD12	2:Z:55:ILE:HD11	1.97	0.46
1:C:40:ILE:HD12	2:H:55:ILE:HD11	1.98	0.46
1:B:40:ILE:HD12	2:G:55:ILE:HD11	1.96	0.46
1:C:91:LEU:CD1	1:C:103:CYS:HB3	2.46	0.46
1:D:109:GLN:OE1	1:D:112:LYS:CE	2.63	0.46
1:A:109:GLN:OE1	1:A:112:LYS:CE	2.64	0.46
1:C:12:LYS:HD2	2:G:61:ASP:OD2	2.16	0.46
1:D:35:LEU:HD23	1:D:145:MET:O	2.16	0.46
2:J:95:ASN:C	2:J:95:ASN:HD22	2.20	0.46
1:K:77:ARG:HD2	1:L:165:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:109:GLN:OE1	1:L:112:LYS:CE	2.64	0.46
1:Y:109:GLN:OE1	1:Y:112:LYS:HE2	2.15	0.46
1:A:40:ILE:HD12	2:F:55:ILE:HD11	1.98	0.45
1:X:109:GLN:CG	1:Y:111:MET:CG	2.92	0.45
1:B:35:LEU:HD23	1:B:145:MET:O	2.15	0.45
2:J:68:VAL:CG2	2:J:92:THR:HG22	2.47	0.45
2:Z:95:ASN:C	2:Z:95:ASN:HD22	2.20	0.45
2:I:68:VAL:CG2	2:I:92:THR:HG22	2.47	0.45
1:X:35:LEU:HD23	1:X:145:MET:O	2.17	0.45
1:K:77:ARG:CB	1:L:165:LEU:HD21	2.47	0.45
2:P:68:VAL:CG2	2:P:92:THR:HG22	2.47	0.45
1:B:164:ASN:OD1	1:B:165:LEU:N	2.49	0.45
1:E:109:GLN:OE1	1:E:112:LYS:CE	2.64	0.45
2:I:95:ASN:HD22	2:I:95:ASN:C	2.20	0.45
1:L:109:GLN:CG	1:M:111:MET:CG	2.95	0.45
1:V:164:ASN:CG	1:V:165:LEU:N	2.70	0.45
2:Z:48:LYS:O	2:Z:52:ARG:HG3	2.17	0.45
1:A:111:MET:SD	1:E:109:GLN:HG3	2.57	0.45
2:H:68:VAL:CG2	2:H:92:THR:HG22	2.47	0.45
2:Q:68:VAL:CG2	2:Q:92:THR:HG22	2.47	0.45
1:U:77:ARG:HH21	1:U:77:ARG:HG3	1.81	0.45
2:Z:67:VAL:HG11	2:Z:94:ILE:CG1	2.47	0.45
1:E:35:LEU:HD23	1:E:145:MET:O	2.17	0.45
2:F:67:VAL:HG11	2:F:94:ILE:CG1	2.47	0.45
2:J:67:VAL:HG11	2:J:94:ILE:CG1	2.47	0.45
1:O:109:GLN:OE1	1:O:112:LYS:CE	2.64	0.45
2:T:68:VAL:CG2	2:T:92:THR:HG22	2.47	0.45
1:Y:164:ASN:CG	1:Y:165:LEU:N	2.66	0.45
2:G:95:ASN:C	2:G:95:ASN:HD22	2.20	0.45
2:Q:95:ASN:C	2:Q:95:ASN:HD22	2.20	0.45
2:S:68:VAL:CG2	2:S:92:THR:HG22	2.47	0.45
2:S:95:ASN:C	2:S:95:ASN:HD22	2.20	0.45
2:T:95:ASN:C	2:T:95:ASN:HD22	2.20	0.45
1:Y:13:TYR:HB2	1:Y:46:PHE:CE2	2.52	0.45
1:M:92:ILE:HD13	1:M:128:CYS:HB2	1.99	0.45
1:N:35:LEU:HD23	1:N:145:MET:O	2.17	0.45
2:G:68:VAL:CG2	2:G:92:THR:HG22	2.47	0.45
1:L:165:LEU:N	1:L:165:LEU:CD1	2.79	0.45
1:V:109:GLN:OE1	1:V:112:LYS:CE	2.64	0.45
1:C:109:GLN:OE1	1:C:112:LYS:CE	2.65	0.44
1:C:55:ILE:HD11	1:W:40:ILE:HD12	207.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:35:LEU:HD23	1:O:145:MET:O	2.18	0.44
2:P:67:VAL:HG11	2:P:94:ILE:CG1	2.47	0.44
2:G:67:VAL:HG11	2:G:94:ILE:CG1	2.47	0.44
2:P:95:ASN:HD22	2:P:95:ASN:C	2.21	0.44
2:Z:68:VAL:CG2	2:Z:92:THR:HG22	2.47	0.44
1:B:109:GLN:OE1	1:B:112:LYS:CE	2.65	0.44
1:N:165:LEU:CD1	1:N:165:LEU:C	2.86	0.44
2:R:95:ASN:C	2:R:95:ASN:HD22	2.20	0.44
2:T:67:VAL:HG11	2:T:94:ILE:CG1	2.47	0.44
1:W:35:LEU:HD23	1:W:145:MET:O	2.16	0.44
1:Y:35:LEU:HD23	1:Y:145:MET:O	2.17	0.44
2:I:67:VAL:HG11	2:I:94:ILE:CG1	2.47	0.44
1:L:35:LEU:HD23	1:L:145:MET:O	2.16	0.44
1:K:77:ARG:CD	1:L:165:LEU:CD2	2.92	0.44
1:B:11:MET:HA	1:B:46:PHE:CE2	2.52	0.44
2:H:95:ASN:C	2:H:95:ASN:HD22	2.19	0.44
1:U:35:LEU:HD23	1:U:145:MET:O	2.16	0.44
1:U:91:LEU:CD1	1:U:103:CYS:CB	2.94	0.44
1:Y:91:LEU:CD1	1:Y:103:CYS:CB	2.95	0.44
1:E:40:ILE:HD12	2:J:55:ILE:HD11	2.03	0.44
1:K:35:LEU:HD23	1:K:145:MET:O	2.17	0.44
2:R:68:VAL:CG2	2:R:92:THR:HG22	2.47	0.44
2:S:67:VAL:HG11	2:S:94:ILE:HD13	2.00	0.44
2:F:68:VAL:CG2	2:F:92:THR:HG22	2.47	0.44
2:F:95:ASN:HD22	2:F:95:ASN:C	2.20	0.44
2:Q:67:VAL:HG11	2:Q:94:ILE:CG1	2.47	0.44
1:W:109:GLN:OE1	1:W:112:LYS:CE	2.66	0.44
1:X:111:MET:CG	1:W:109:GLN:CG	2.95	0.44
1:E:113:LEU:HB3	1:E:121:VAL:HG21	2.00	0.44
1:K:111:MET:CG	1:O:109:GLN:CG	2.96	0.44
1:K:164:ASN:CG	1:K:165:LEU:H	2.22	0.43
1:L:19:ARG:HA	1:L:52:ASN:HB3	1.99	0.43
1:X:109:GLN:OE1	1:X:112:LYS:CE	2.66	0.43
1:A:113:LEU:HB3	1:A:121:VAL:HG21	2.00	0.43
1:C:12:LYS:HG2	1:C:12:LYS:O	2.18	0.43
1:D:113:LEU:HB3	1:D:121:VAL:HG21	2.00	0.43
2:I:67:VAL:HG11	2:I:94:ILE:HD13	1.99	0.43
2:T:67:VAL:HG11	2:T:94:ILE:HD13	2.00	0.43
1:U:113:LEU:HB3	1:U:121:VAL:HG21	2.00	0.43
1:B:113:LEU:HB3	1:B:121:VAL:HG21	2.01	0.43
2:G:67:VAL:HG11	2:G:94:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:113:LEU:HB3	1:O:121:VAL:HG21	2.01	0.43
2:S:67:VAL:HG11	2:S:94:ILE:CG1	2.47	0.43
1:W:113:LEU:HB3	1:W:121:VAL:HG21	2.00	0.43
2:Z:49:GLU:CA	2:Z:52:ARG:HH21	2.20	0.43
1:M:113:LEU:HB3	1:M:121:VAL:HG21	2.01	0.43
1:X:113:LEU:HB3	1:X:121:VAL:HG21	2.01	0.43
1:A:14:ASP:HB3	1:A:167:HIS:NE2	2.33	0.43
1:D:165:LEU:CD1	1:D:165:LEU:C	2.86	0.43
1:M:91:LEU:CD1	1:M:103:CYS:CB	2.95	0.43
2:P:67:VAL:HG11	2:P:94:ILE:HD13	2.00	0.43
1:C:111:MET:CG	1:B:109:GLN:CG	2.96	0.43
1:C:165:LEU:O	1:C:166:GLU:C	2.57	0.43
2:J:67:VAL:HG11	2:J:94:ILE:HD13	2.00	0.43
2:F:49:GLU:O	2:F:52:ARG:HB2	2.18	0.43
1:V:113:LEU:HB3	1:V:121:VAL:HG21	2.00	0.43
1:C:35:LEU:HD23	1:C:145:MET:O	2.18	0.43
1:N:113:LEU:HB3	1:N:121:VAL:HG21	2.00	0.43
1:K:109:GLN:OE1	1:K:112:LYS:CE	2.67	0.43
1:K:91:LEU:CD1	1:K:103:CYS:HB3	2.49	0.43
1:U:11:MET:C	1:U:13:TYR:N	2.72	0.43
2:Z:67:VAL:HG11	2:Z:94:ILE:HD13	2.00	0.43
1:Y:109:GLN:OE1	1:Y:112:LYS:CE	2.66	0.42
1:C:42:ARG:O	1:C:46:PHE:HD1	2.02	0.42
1:K:113:LEU:HB3	1:K:121:VAL:HG21	2.00	0.42
2:F:67:VAL:HG11	2:F:94:ILE:HD13	2.00	0.42
2:Q:67:VAL:HG11	2:Q:94:ILE:HD13	2.00	0.42
1:M:62:PHE:O	1:M:65:PRO:HD2	2.20	0.42
1:O:40:ILE:HD12	2:T:55:ILE:HD11	2.01	0.42
1:V:91:LEU:CD1	1:V:103:CYS:HB3	2.49	0.42
1:Y:113:LEU:HB3	1:Y:121:VAL:HG21	2.01	0.42
1:E:62:PHE:O	1:E:65:PRO:HD2	2.22	0.42
2:G:16:LYS:HG2	2:G:16:LYS:O	2.20	0.42
1:D:55:ILE:HD11	1:X:40:ILE:HD12	165.70	0.42
1:C:109:GLN:CG	1:D:111:MET:CG	2.98	0.42
1:E:91:LEU:CD1	1:E:103:CYS:HB3	2.49	0.42
1:W:91:LEU:CD1	1:W:103:CYS:HB3	2.49	0.42
1:L:91:LEU:CD1	1:L:103:CYS:HB3	2.49	0.42
1:M:166:GLU:O	1:M:167:HIS:CB	2.68	0.42
1:O:62:PHE:O	1:O:65:PRO:HD2	2.19	0.42
2:T:67:VAL:HG11	2:T:94:ILE:HG12	2.02	0.42
2:H:102:LEU:CD1	2:H:114:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:HIS:O	1:A:150:GLU:HG3	2.20	0.41
1:C:62:PHE:O	1:C:65:PRO:HD2	2.21	0.41
2:P:67:VAL:HG11	2:P:94:ILE:HG12	2.03	0.41
1:K:62:PHE:O	1:K:65:PRO:HD2	2.20	0.41
1:M:92:ILE:HD11	1:M:134:ALA:HB2	2.01	0.41
1:A:35:LEU:HD23	1:A:145:MET:O	2.20	0.41
1:C:113:LEU:HB3	1:C:121:VAL:HG21	2.01	0.41
1:V:11:MET:C	1:V:13:TYR:H	2.24	0.41
2:F:102:LEU:CD1	2:F:114:LEU:HD21	2.50	0.41
2:J:67:VAL:HG11	2:J:94:ILE:HG12	2.02	0.41
2:R:54:ILE:HG23	2:R:64:ILE:HD13	2.03	0.41
2:S:67:VAL:HG11	2:S:94:ILE:HG12	2.03	0.41
2:I:67:VAL:HG11	2:I:94:ILE:HG12	2.03	0.41
1:U:109:GLN:CG	1:V:111:MET:CG	2.98	0.41
1:A:55:ILE:HD11	1:U:40:ILE:HD12	200.54	0.41
1:X:62:PHE:O	1:X:65:PRO:HD2	2.21	0.41
2:J:54:ILE:HG23	2:J:64:ILE:HD13	2.04	0.41
1:K:15:GLY:O	1:K:48:VAL:HG22	2.20	0.41
1:L:113:LEU:HB3	1:L:121:VAL:HG21	2.01	0.41
1:O:91:LEU:CD1	1:O:103:CYS:HB3	2.50	0.41
1:Y:62:PHE:O	1:Y:65:PRO:HD2	2.20	0.41
2:P:57:LYS:HD3	2:P:57:LYS:HA	1.90	0.41
1:W:62:PHE:O	1:W:65:PRO:HD2	2.21	0.41
1:K:42:ARG:HG3	1:K:46:PHE:CE1	2.55	0.41
1:N:111:MET:CG	1:M:109:GLN:CG	2.98	0.41
1:N:109:GLN:HG3	1:O:111:MET:SD	2.61	0.41
1:E:72:VAL:HG21	1:E:117:LEU:HD13	2.04	0.40
2:G:57:LYS:HD3	2:G:57:LYS:HA	1.90	0.40
2:H:54:ILE:HG23	2:H:64:ILE:HD13	2.03	0.40
1:U:73:GLU:O	1:U:77:ARG:HD2	2.21	0.40
2:Z:67:VAL:HG11	2:Z:94:ILE:HG12	2.02	0.40
1:E:111:MET:CG	1:D:109:GLN:CG	2.98	0.40
2:G:67:VAL:HG11	2:G:94:ILE:HG12	2.03	0.40
1:K:12:LYS:CD	2:T:61:ASP:OD2	2.63	0.40
1:M:72:VAL:HG21	1:M:117:LEU:HD13	2.04	0.40
2:P:54:ILE:HG23	2:P:64:ILE:HD13	2.03	0.40
1:X:72:VAL:HG21	1:X:117:LEU:HD13	2.04	0.40
2:J:57:LYS:HD3	2:J:57:LYS:HA	1.90	0.40
1:K:72:VAL:HG21	1:K:117:LEU:HD13	2.04	0.40
1:N:72:VAL:HG21	1:N:117:LEU:HD13	2.04	0.40
1:D:72:VAL:HG21	1:D:117:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:PHE:O	1:L:65:PRO:HD2	2.22	0.40

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	129/162 (80%)	127 (98%)	2 (2%)	0	100	100
1	B	131/162 (81%)	129 (98%)	2 (2%)	0	100	100
1	C	131/162 (81%)	128 (98%)	3 (2%)	0	100	100
1	D	126/162 (78%)	124 (98%)	2 (2%)	0	100	100
1	E	127/162 (78%)	125 (98%)	2 (2%)	0	100	100
1	K	129/162 (80%)	127 (98%)	2 (2%)	0	100	100
1	L	130/162 (80%)	127 (98%)	3 (2%)	0	100	100
1	M	133/162 (82%)	131 (98%)	2 (2%)	0	100	100
1	N	128/162 (79%)	126 (98%)	2 (2%)	0	100	100
1	O	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	X	126/162 (78%)	124 (98%)	2 (2%)	0	100	100
1	Y	129/162 (80%)	126 (98%)	3 (2%)	0	100	100
1	e	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	H	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	I	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	J	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	P	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	T	129/138 (94%)	128 (99%)	1 (1%)	0	100	100
2	Z	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	c	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
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 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	107/133 (80%)	105 (98%)	2 (2%)	65	87
1	B	109/133 (82%)	105 (96%)	4 (4%)	41	76
1	C	109/133 (82%)	105 (96%)	4 (4%)	41	76
1	D	106/133 (80%)	101 (95%)	5 (5%)	32	72
1	E	106/133 (80%)	103 (97%)	3 (3%)	51	82
1	K	107/133 (80%)	103 (96%)	4 (4%)	41	76
1	L	109/133 (82%)	105 (96%)	4 (4%)	41	76
1	M	112/133 (84%)	106 (95%)	6 (5%)	27	67
1	N	106/133 (80%)	102 (96%)	4 (4%)	40	76
1	O	103/133 (77%)	100 (97%)	3 (3%)	50	81
1	U	105/133 (79%)	101 (96%)	4 (4%)	40	76
1	V	107/133 (80%)	102 (95%)	5 (5%)	32	72
1	W	105/133 (79%)	101 (96%)	4 (4%)	40	76
1	X	106/133 (80%)	102 (96%)	4 (4%)	40	76
1	Y	105/133 (79%)	102 (97%)	3 (3%)	50	81
1	e	106/133 (80%)	103 (97%)	3 (3%)	51	82
1	f	107/133 (80%)	103 (96%)	4 (4%)	41	76
1	g	103/133 (77%)	100 (97%)	3 (3%)	50	81
1	h	104/133 (78%)	99 (95%)	5 (5%)	31	71
1	i	106/133 (80%)	102 (96%)	4 (4%)	40	76
2	F	112/120 (93%)	109 (97%)	3 (3%)	52	83
2	G	111/120 (92%)	108 (97%)	3 (3%)	52	83
2	H	113/120 (94%)	107 (95%)	6 (5%)	28	67
2	I	112/120 (93%)	107 (96%)	5 (4%)	34	73
2	J	113/120 (94%)	109 (96%)	4 (4%)	43	78
2	P	113/120 (94%)	109 (96%)	4 (4%)	43	78
2	Q	113/120 (94%)	110 (97%)	3 (3%)	52	83
2	R	114/120 (95%)	109 (96%)	5 (4%)	35	73
2	S	112/120 (93%)	109 (97%)	3 (3%)	52	83
2	T	113/120 (94%)	109 (96%)	4 (4%)	43	78
2	Z	113/120 (94%)	110 (97%)	3 (3%)	52	83
2	a	113/120 (94%)	109 (96%)	4 (4%)	43	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	b	112/120 (93%)	109 (97%)	3 (3%)	52 83
2	c	112/120 (93%)	108 (96%)	4 (4%)	42 77
2	d	113/120 (94%)	109 (96%)	4 (4%)	43 78
2	j	113/120 (94%)	109 (96%)	4 (4%)	43 78
2	k	114/120 (95%)	110 (96%)	4 (4%)	43 78
2	l	111/120 (92%)	107 (96%)	4 (4%)	42 77
2	m	112/120 (93%)	109 (97%)	3 (3%)	52 83
2	n	112/120 (93%)	108 (96%)	4 (4%)	42 77
All	All	4379/5060 (86%)	4224 (96%)	155 (4%)	43 78

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

Mol	Chain	Res	Type
1	A	43	LEU
1	A	148	HIS
1	E	43	LEU
1	E	78	LEU
1	E	148	HIS
1	C	43	LEU
1	C	51	GLU
1	C	78	LEU
1	C	148	HIS
1	B	43	LEU
1	B	51	GLU
1	B	78	LEU
1	B	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	H	70	LEU
2	H	81	GLU
2	H	87	ASP
2	H	95	ASN
2	H	106	ILE

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Mol	Chain	Res	Type
2	H	131	LYS
2	G	70	LEU
2	G	95	ASN
2	G	106	ILE
2	I	70	LEU
2	I	87	ASP
2	I	95	ASN
2	I	106	ILE
2	I	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	M	43	LEU
1	M	51	GLU
1	M	77	ARG
1	M	78	LEU
1	M	148	HIS
1	M	167	HIS
1	O	43	LEU
1	O	78	LEU
1	O	148	HIS
2	P	70	LEU
2	P	87	ASP
2	P	95	ASN
2	P	106	ILE
2	Q	70	LEU
2	Q	95	ASN
2	Q	106	ILE
2	S	70	LEU

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Mol	Chain	Res	Type
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	T	70	LEU
2	T	87	ASP
2	T	95	ASN
2	T	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	X	43	LEU
1	X	77	ARG
1	X	78	LEU
1	X	148	HIS
1	W	43	LEU
1	W	51	GLU
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	c	70	LEU
2	c	95	ASN
2	c	106	ILE
2	c	131	LYS

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Mol	Chain	Res	Type
2	Z	70	LEU
2	Z	95	ASN
2	Z	106	ILE
2	a	70	LEU
2	a	87	ASP
2	a	95	ASN
2	a	106	ILE
1	e	43	LEU
1	e	78	LEU
1	e	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
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	l	70	LEU
2	l	87	ASP
2	l	95	ASN
2	l	106	ILE
2	n	70	LEU

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Mol	Chain	Res	Type
2	n	87	ASP
2	n	95	ASN
2	n	106	ILE

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

Mol	Chain	Res	Type
1	A	108	HIS
1	E	108	HIS
1	C	108	HIS
1	B	108	HIS
1	D	108	HIS
2	F	33	HIS
2	F	95	ASN
2	H	33	HIS
2	H	95	ASN
2	G	33	HIS
2	G	95	ASN
2	I	33	HIS
2	I	95	ASN
2	J	33	HIS
2	J	95	ASN
1	K	108	HIS
1	L	108	HIS
1	N	108	HIS
1	M	108	HIS
1	M	167	HIS
1	O	108	HIS
2	P	33	HIS
2	P	95	ASN
2	Q	95	ASN
2	S	33	HIS
2	S	95	ASN
2	R	33	HIS
2	R	95	ASN
2	T	33	HIS
2	T	95	ASN
1	U	108	HIS
1	V	108	HIS
1	X	108	HIS
1	W	108	HIS
1	Y	108	HIS

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Mol	Chain	Res	Type
2	b	33	HIS
2	b	95	ASN
2	d	33	HIS
2	d	95	ASN
2	c	33	HIS
2	c	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	l	33	HIS
2	l	95	ASN
2	n	33	HIS
2	n	95	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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			OWAB(Å^2)	Q<0.9
1	A	135/162 (83%)	0.65	5 (3%)	45	36	66, 93, 176, 231	0
1	B	137/162 (84%)	0.61	4 (2%)	55	45	55, 91, 168, 243	0
1	C	137/162 (84%)	0.53	3 (2%)	65	55	47, 73, 170, 239	0
1	D	132/162 (81%)	0.65	4 (3%)	54	43	47, 77, 158, 225	0
1	E	133/162 (82%)	0.75	5 (3%)	44	36	56, 86, 159, 236	0
1	K	135/162 (83%)	0.54	2 (1%)	76	67	55, 90, 167, 250	0
1	L	136/162 (83%)	0.65	5 (3%)	45	36	59, 89, 171, 245	0
1	M	139/162 (85%)	0.79	7 (5%)	32	25	58, 96, 192, 231	0
1	N	134/162 (82%)	0.79	7 (5%)	31	24	69, 98, 174, 256	0
1	O	130/162 (80%)	0.58	2 (1%)	76	67	64, 95, 154, 219	0
1	U	134/162 (82%)	0.60	2 (1%)	76	67	48, 77, 169, 229	0
1	V	136/162 (83%)	0.55	4 (2%)	55	45	44, 79, 178, 246	0
1	W	132/162 (81%)	0.61	3 (2%)	64	54	52, 82, 170, 226	0
1	X	132/162 (81%)	0.65	4 (3%)	54	43	61, 94, 168, 211	0
1	Y	135/162 (83%)	0.65	2 (1%)	76	67	58, 90, 179, 244	0
1	e	133/162 (82%)	0.66	6 (4%)	37	29	58, 91, 165, 222	0
1	f	134/162 (82%)	0.62	5 (3%)	45	36	64, 96, 173, 221	0
1	g	130/162 (80%)	0.68	6 (4%)	36	28	68, 96, 170, 203	0
1	h	133/162 (82%)	0.74	6 (4%)	37	29	60, 93, 161, 242	0
1	i	135/162 (83%)	0.67	9 (6%)	21	16	59, 87, 167, 245	0
2	F	131/138 (94%)	0.39	1 (0%)	87	80	78, 107, 158, 174	0
2	G	131/138 (94%)	0.41	0	100	100	66, 92, 146, 184	0
2	H	131/138 (94%)	0.37	0	100	100	55, 88, 149, 172	0
2	I	131/138 (94%)	0.37	2 (1%)	76	67	64, 97, 145, 176	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	J	131/138 (94%)	0.38	1 (0%) 87 80	73, 101, 146, 177	0
2	P	131/138 (94%)	0.38	0 100 100	69, 101, 146, 168	0
2	Q	131/138 (94%)	0.41	2 (1%) 76 67	72, 96, 140, 166	0
2	R	131/138 (94%)	0.32	1 (0%) 87 80	75, 102, 150, 170	0
2	S	131/138 (94%)	0.44	3 (2%) 64 54	80, 109, 156, 174	0
2	T	131/138 (94%)	0.30	0 100 100	65, 93, 146, 167	0
2	Z	131/138 (94%)	0.42	2 (1%) 76 67	72, 101, 152, 193	0
2	a	131/138 (94%)	0.33	0 100 100	65, 92, 149, 166	0
2	b	131/138 (94%)	0.34	0 100 100	62, 91, 142, 165	0
2	c	131/138 (94%)	0.36	0 100 100	66, 93, 146, 181	0
2	d	131/138 (94%)	0.37	0 100 100	78, 107, 157, 178	0
2	j	131/138 (94%)	0.38	2 (1%) 76 67	73, 99, 148, 163	0
2	k	131/138 (94%)	0.27	0 100 100	76, 103, 154, 183	0
2	l	131/138 (94%)	0.41	1 (0%) 87 80	80, 108, 151, 190	0
2	m	131/138 (94%)	0.38	0 100 100	66, 98, 151, 162	0
2	n	131/138 (94%)	0.37	1 (0%) 87 80	66, 88, 132, 147	0
All	All	5302/6000 (88%)	0.51	107 (2%) 68 59	44, 95, 160, 256	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	103	CYS	5.1
1	N	134	ALA	4.7
1	h	129	LEU	4.6
1	M	134	ALA	4.3
1	N	129	LEU	4.2
1	K	103	CYS	3.9
1	g	103	CYS	3.9
1	h	103	CYS	3.7
1	i	134	ALA	3.6
1	B	103	CYS	3.5
1	i	129	LEU	3.4
1	f	129	LEU	3.3
1	N	123	PHE	3.2
1	N	103	CYS	3.1
1	g	90	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	129	LEU	3.0
1	O	123	PHE	3.0
1	A	123	PHE	2.9
1	X	123	PHE	2.9
1	X	103	CYS	2.9
1	O	103	CYS	2.8
2	J	111	THR	2.8
1	E	90	VAL	2.8
1	C	111	MET	2.8
1	e	90	VAL	2.8
1	f	103	CYS	2.8
1	L	62	PHE	2.8
1	Y	103	CYS	2.7
1	e	103	CYS	2.7
1	C	129	LEU	2.7
1	e	126	LEU	2.7
1	E	123	PHE	2.7
2	S	111	THR	2.7
1	h	126	LEU	2.6
1	g	126	LEU	2.6
1	f	128	CYS	2.6
1	h	111	MET	2.6
2	I	122	GLY	2.5
1	C	103	CYS	2.5
1	N	126	LEU	2.5
1	N	33	ALA	2.5
1	e	129	LEU	2.5
1	A	90	VAL	2.5
1	W	103	CYS	2.5
1	i	90	VAL	2.5
1	V	103	CYS	2.5
1	W	126	LEU	2.4
1	h	123	PHE	2.4
1	g	123	PHE	2.4
1	N	90	VAL	2.4
1	X	87	PRO	2.4
1	A	110	LEU	2.4
1	L	126	LEU	2.4
1	i	126	LEU	2.4
1	L	90	VAL	2.4
1	B	123	PHE	2.4
1	U	103	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	90	VAL	2.4
2	F	88	VAL	2.4
1	E	103	CYS	2.3
1	e	92	ILE	2.3
2	n	37	LEU	2.3
1	M	126	LEU	2.3
1	M	90	VAL	2.3
2	S	115	LEU	2.3
1	A	124	GLY	2.2
1	e	124	GLY	2.2
1	E	126	LEU	2.2
1	U	126	LEU	2.2
1	L	103	CYS	2.2
1	g	25	ALA	2.2
2	j	37	LEU	2.2
1	A	129	LEU	2.2
1	V	126	LEU	2.2
2	I	37	LEU	2.2
2	j	102	LEU	2.2
1	M	135	GLU	2.2
1	Y	129	LEU	2.2
1	L	33	ALA	2.2
1	V	129	LEU	2.2
2	S	127	LYS	2.2
1	D	103	CYS	2.2
1	W	90	VAL	2.2
1	f	90	VAL	2.2
2	R	37	LEU	2.1
1	B	59	PRO	2.1
1	X	59	PRO	2.1
1	i	111	MET	2.1
1	g	92	ILE	2.1
1	i	61	SER	2.1
2	Q	111	THR	2.1
1	f	123	PHE	2.1
1	i	110	LEU	2.1
2	Z	102	LEU	2.1
1	K	129	LEU	2.1
1	D	33	ALA	2.1
1	i	103	CYS	2.1
2	l	5	PHE	2.1
1	M	123	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	i	123	PHE	2.0
1	D	61	SER	2.0
2	Q	90	VAL	2.0
2	Z	6	VAL	2.0
1	E	20	ILE	2.0
1	V	33	ALA	2.0
1	h	92	ILE	2.0
1	M	62	PHE	2.0

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 carbohydrates 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.