Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2016 – 01:06 AM EDT

PDB ID	:	5IM5
Title	:	Crystal structure of designed two-component self-assembling icosahedral cage I53-40
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	:	3.70 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:

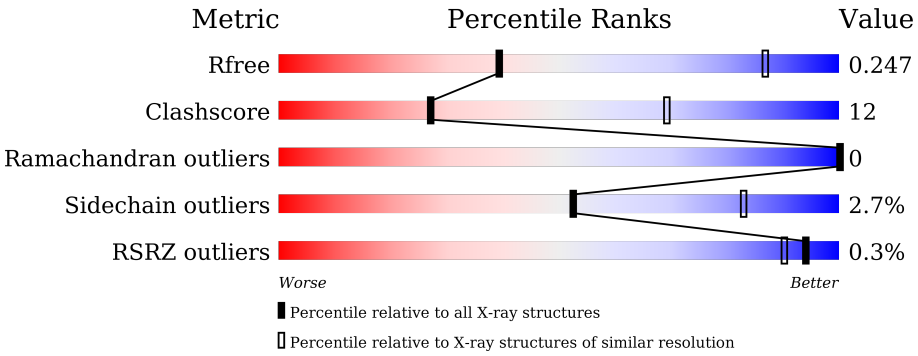
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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	156	64% 25% • 9%
1	B	156	64% 25% • 9%
1	C	156	64% 26% • 9%
1	D	156	59% 29% • 10%
1	E	156	% 65% 23% • 9%
1	F	156	62% 28% 10%

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Mol	Chain	Length	Quality of chain
1	G	156	63% 27% 9%
1	H	156	62% 28% 9%
1	I	156	65% 24% 9%
1	J	156	60% 29% 10%
1	K	156	65% 25% 9%
1	M	156	60% 28% 10%
1	O	156	62% 27% 10%
1	Q	156	62% 28% 9%
1	S	156	63% 25% 9%
2	1	219	83% 12% 5%
2	2	219	88% 7% 5%
2	3	219	84% 11% 5%
2	4	219	85% 10% 5%
2	L	219	86% 9% 5%
2	N	219	85% 9% 5%
2	P	219	83% 11% 5%
2	R	219	83% 12% 5%
2	T	219	86% 9% 5%
2	U	219	85% 9% 5%
2	V	219	84% 11% 5%
2	W	219	85% 9% 5%
2	X	219	86% 9% 5%
2	Y	219	85% 10% 5%
2	Z	219	87% 8% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39183 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 Designed Riboflavin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	142	Total	C	N	O	S	0	0	0
			1086	694	184	198	10			
1	M	141	Total	C	N	O	S	0	0	0
			1086	695	184	197	10			
1	O	141	Total	C	N	O	S	0	0	0
			1086	695	184	197	10			
1	Q	142	Total	C	N	O	S	0	0	0
			1086	694	184	198	10			
1	S	142	Total	C	N	O	S	0	0	0
			1086	694	184	198	10			
1	A	142	Total	C	N	O	S	0	0	0
			1086	694	184	198	10			
1	B	142	Total	C	N	O	S	0	0	0
			1086	694	184	198	10			
1	C	142	Total	C	N	O	S	0	0	0
			1086	694	184	198	10			
1	D	141	Total	C	N	O	S	0	0	0
			1086	695	184	197	10			
1	E	142	Total	C	N	O	S	0	0	0
			1086	694	184	198	10			
1	F	141	Total	C	N	O	S	0	0	0
			1082	692	183	197	10			
1	G	142	Total	C	N	O	S	0	0	0
			1086	694	184	198	10			
1	H	142	Total	C	N	O	S	0	0	0
			1086	694	184	198	10			
1	I	142	Total	C	N	O	S	0	0	0
			1086	694	184	198	10			
1	J	141	Total	C	N	O	S	0	0	0
			1082	692	183	197	10			

There are 165 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	20	ALA	ILE	engineered mutation	UNP Q58584
K	23	LEU	LYS	engineered mutation	UNP Q58584
K	24	THR	LYS	engineered mutation	UNP Q58584
K	27	MET	GLU	engineered mutation	UNP Q58584
K	28	GLU	LEU	engineered mutation	UNP Q58584
K	109	ALA	LYS	engineered mutation	UNP Q58584
K	112	LYS	ASP	engineered mutation	UNP Q58584
K	113	ILE	TRP	engineered mutation	UNP Q58584
K	116	ALA	LYS	engineered mutation	UNP Q58584
K	120	ILE	GLU	engineered mutation	UNP Q58584
K	124	LEU	GLU	engineered mutation	UNP Q58584
M	20	ALA	ILE	engineered mutation	UNP Q58584
M	23	LEU	LYS	engineered mutation	UNP Q58584
M	24	THR	LYS	engineered mutation	UNP Q58584
M	27	MET	GLU	engineered mutation	UNP Q58584
M	28	GLU	LEU	engineered mutation	UNP Q58584
M	109	ALA	LYS	engineered mutation	UNP Q58584
M	112	LYS	ASP	engineered mutation	UNP Q58584
M	113	ILE	TRP	engineered mutation	UNP Q58584
M	116	ALA	LYS	engineered mutation	UNP Q58584
M	120	ILE	GLU	engineered mutation	UNP Q58584
M	124	LEU	GLU	engineered mutation	UNP Q58584
O	20	ALA	ILE	engineered mutation	UNP Q58584
O	23	LEU	LYS	engineered mutation	UNP Q58584
O	24	THR	LYS	engineered mutation	UNP Q58584
O	27	MET	GLU	engineered mutation	UNP Q58584
O	28	GLU	LEU	engineered mutation	UNP Q58584
O	109	ALA	LYS	engineered mutation	UNP Q58584
O	112	LYS	ASP	engineered mutation	UNP Q58584
O	113	ILE	TRP	engineered mutation	UNP Q58584
O	116	ALA	LYS	engineered mutation	UNP Q58584
O	120	ILE	GLU	engineered mutation	UNP Q58584
O	124	LEU	GLU	engineered mutation	UNP Q58584
Q	20	ALA	ILE	engineered mutation	UNP Q58584
Q	23	LEU	LYS	engineered mutation	UNP Q58584
Q	24	THR	LYS	engineered mutation	UNP Q58584
Q	27	MET	GLU	engineered mutation	UNP Q58584
Q	28	GLU	LEU	engineered mutation	UNP Q58584
Q	109	ALA	LYS	engineered mutation	UNP Q58584
Q	112	LYS	ASP	engineered mutation	UNP Q58584
Q	113	ILE	TRP	engineered mutation	UNP Q58584
Q	116	ALA	LYS	engineered mutation	UNP Q58584
Q	120	ILE	GLU	engineered mutation	UNP Q58584

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	124	LEU	GLU	engineered mutation	UNP Q58584
S	20	ALA	ILE	engineered mutation	UNP Q58584
S	23	LEU	LYS	engineered mutation	UNP Q58584
S	24	THR	LYS	engineered mutation	UNP Q58584
S	27	MET	GLU	engineered mutation	UNP Q58584
S	28	GLU	LEU	engineered mutation	UNP Q58584
S	109	ALA	LYS	engineered mutation	UNP Q58584
S	112	LYS	ASP	engineered mutation	UNP Q58584
S	113	ILE	TRP	engineered mutation	UNP Q58584
S	116	ALA	LYS	engineered mutation	UNP Q58584
S	120	ILE	GLU	engineered mutation	UNP Q58584
S	124	LEU	GLU	engineered mutation	UNP Q58584
A	20	ALA	ILE	engineered mutation	UNP Q58584
A	23	LEU	LYS	engineered mutation	UNP Q58584
A	24	THR	LYS	engineered mutation	UNP Q58584
A	27	MET	GLU	engineered mutation	UNP Q58584
A	28	GLU	LEU	engineered mutation	UNP Q58584
A	109	ALA	LYS	engineered mutation	UNP Q58584
A	112	LYS	ASP	engineered mutation	UNP Q58584
A	113	ILE	TRP	engineered mutation	UNP Q58584
A	116	ALA	LYS	engineered mutation	UNP Q58584
A	120	ILE	GLU	engineered mutation	UNP Q58584
A	124	LEU	GLU	engineered mutation	UNP Q58584
B	20	ALA	ILE	engineered mutation	UNP Q58584
B	23	LEU	LYS	engineered mutation	UNP Q58584
B	24	THR	LYS	engineered mutation	UNP Q58584
B	27	MET	GLU	engineered mutation	UNP Q58584
B	28	GLU	LEU	engineered mutation	UNP Q58584
B	109	ALA	LYS	engineered mutation	UNP Q58584
B	112	LYS	ASP	engineered mutation	UNP Q58584
B	113	ILE	TRP	engineered mutation	UNP Q58584
B	116	ALA	LYS	engineered mutation	UNP Q58584
B	120	ILE	GLU	engineered mutation	UNP Q58584
B	124	LEU	GLU	engineered mutation	UNP Q58584
C	20	ALA	ILE	engineered mutation	UNP Q58584
C	23	LEU	LYS	engineered mutation	UNP Q58584
C	24	THR	LYS	engineered mutation	UNP Q58584
C	27	MET	GLU	engineered mutation	UNP Q58584
C	28	GLU	LEU	engineered mutation	UNP Q58584
C	109	ALA	LYS	engineered mutation	UNP Q58584
C	112	LYS	ASP	engineered mutation	UNP Q58584
C	113	ILE	TRP	engineered mutation	UNP Q58584

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Chain	Residue	Modelled	Actual	Comment	Reference
C	116	ALA	LYS	engineered mutation	UNP Q58584
C	120	ILE	GLU	engineered mutation	UNP Q58584
C	124	LEU	GLU	engineered mutation	UNP Q58584
D	20	ALA	ILE	engineered mutation	UNP Q58584
D	23	LEU	LYS	engineered mutation	UNP Q58584
D	24	THR	LYS	engineered mutation	UNP Q58584
D	27	MET	GLU	engineered mutation	UNP Q58584
D	28	GLU	LEU	engineered mutation	UNP Q58584
D	109	ALA	LYS	engineered mutation	UNP Q58584
D	112	LYS	ASP	engineered mutation	UNP Q58584
D	113	ILE	TRP	engineered mutation	UNP Q58584
D	116	ALA	LYS	engineered mutation	UNP Q58584
D	120	ILE	GLU	engineered mutation	UNP Q58584
D	124	LEU	GLU	engineered mutation	UNP Q58584
E	20	ALA	ILE	engineered mutation	UNP Q58584
E	23	LEU	LYS	engineered mutation	UNP Q58584
E	24	THR	LYS	engineered mutation	UNP Q58584
E	27	MET	GLU	engineered mutation	UNP Q58584
E	28	GLU	LEU	engineered mutation	UNP Q58584
E	109	ALA	LYS	engineered mutation	UNP Q58584
E	112	LYS	ASP	engineered mutation	UNP Q58584
E	113	ILE	TRP	engineered mutation	UNP Q58584
E	116	ALA	LYS	engineered mutation	UNP Q58584
E	120	ILE	GLU	engineered mutation	UNP Q58584
E	124	LEU	GLU	engineered mutation	UNP Q58584
F	20	ALA	ILE	engineered mutation	UNP Q58584
F	23	LEU	LYS	engineered mutation	UNP Q58584
F	24	THR	LYS	engineered mutation	UNP Q58584
F	27	MET	GLU	engineered mutation	UNP Q58584
F	28	GLU	LEU	engineered mutation	UNP Q58584
F	109	ALA	LYS	engineered mutation	UNP Q58584
F	112	LYS	ASP	engineered mutation	UNP Q58584
F	113	ILE	TRP	engineered mutation	UNP Q58584
F	116	ALA	LYS	engineered mutation	UNP Q58584
F	120	ILE	GLU	engineered mutation	UNP Q58584
F	124	LEU	GLU	engineered mutation	UNP Q58584
G	20	ALA	ILE	engineered mutation	UNP Q58584
G	23	LEU	LYS	engineered mutation	UNP Q58584
G	24	THR	LYS	engineered mutation	UNP Q58584
G	27	MET	GLU	engineered mutation	UNP Q58584
G	28	GLU	LEU	engineered mutation	UNP Q58584
G	109	ALA	LYS	engineered mutation	UNP Q58584

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Chain	Residue	Modelled	Actual	Comment	Reference
G	112	LYS	ASP	engineered mutation	UNP Q58584
G	113	ILE	TRP	engineered mutation	UNP Q58584
G	116	ALA	LYS	engineered mutation	UNP Q58584
G	120	ILE	GLU	engineered mutation	UNP Q58584
G	124	LEU	GLU	engineered mutation	UNP Q58584
H	20	ALA	ILE	engineered mutation	UNP Q58584
H	23	LEU	LYS	engineered mutation	UNP Q58584
H	24	THR	LYS	engineered mutation	UNP Q58584
H	27	MET	GLU	engineered mutation	UNP Q58584
H	28	GLU	LEU	engineered mutation	UNP Q58584
H	109	ALA	LYS	engineered mutation	UNP Q58584
H	112	LYS	ASP	engineered mutation	UNP Q58584
H	113	ILE	TRP	engineered mutation	UNP Q58584
H	116	ALA	LYS	engineered mutation	UNP Q58584
H	120	ILE	GLU	engineered mutation	UNP Q58584
H	124	LEU	GLU	engineered mutation	UNP Q58584
I	20	ALA	ILE	engineered mutation	UNP Q58584
I	23	LEU	LYS	engineered mutation	UNP Q58584
I	24	THR	LYS	engineered mutation	UNP Q58584
I	27	MET	GLU	engineered mutation	UNP Q58584
I	28	GLU	LEU	engineered mutation	UNP Q58584
I	109	ALA	LYS	engineered mutation	UNP Q58584
I	112	LYS	ASP	engineered mutation	UNP Q58584
I	113	ILE	TRP	engineered mutation	UNP Q58584
I	116	ALA	LYS	engineered mutation	UNP Q58584
I	120	ILE	GLU	engineered mutation	UNP Q58584
I	124	LEU	GLU	engineered mutation	UNP Q58584
J	20	ALA	ILE	engineered mutation	UNP Q58584
J	23	LEU	LYS	engineered mutation	UNP Q58584
J	24	THR	LYS	engineered mutation	UNP Q58584
J	27	MET	GLU	engineered mutation	UNP Q58584
J	28	GLU	LEU	engineered mutation	UNP Q58584
J	109	ALA	LYS	engineered mutation	UNP Q58584
J	112	LYS	ASP	engineered mutation	UNP Q58584
J	113	ILE	TRP	engineered mutation	UNP Q58584
J	116	ALA	LYS	engineered mutation	UNP Q58584
J	120	ILE	GLU	engineered mutation	UNP Q58584
J	124	LEU	GLU	engineered mutation	UNP Q58584

- Molecule 2 is a protein called Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosph ogluconate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	T	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	N	208	Total	C	N	O	S	0	0	0
			1523	971	256	288	8			
2	V	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	W	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	U	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	Y	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	Z	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	X	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	2	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	4	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	1	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	L	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	R	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			
2	3	208	Total	C	N	O	S	0	0	0
			1527	973	256	290	8			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	47	SER	ASP	engineered mutation	UNP A5KUH7
P	51	LYS	GLU	engineered mutation	UNP A5KUH7
P	54	MET	ARG	engineered mutation	UNP A5KUH7
P	58	SER	GLN	engineered mutation	UNP A5KUH7
P	74	VAL	GLU	engineered mutation	UNP A5KUH7
P	102	ILE	GLU	engineered mutation	UNP A5KUH7
P	210	GLY	-	expression tag	UNP A5KUH7
P	211	SER	-	expression tag	UNP A5KUH7
P	212	LEU	-	expression tag	UNP A5KUH7
P	213	GLU	-	expression tag	UNP A5KUH7

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Chain	Residue	Modelled	Actual	Comment	Reference
P	214	HIS	-	expression tag	UNP A5KUH7
P	215	HIS	-	expression tag	UNP A5KUH7
P	216	HIS	-	expression tag	UNP A5KUH7
P	217	HIS	-	expression tag	UNP A5KUH7
P	218	HIS	-	expression tag	UNP A5KUH7
P	219	HIS	-	expression tag	UNP A5KUH7
T	47	SER	ASP	engineered mutation	UNP A5KUH7
T	51	LYS	GLU	engineered mutation	UNP A5KUH7
T	54	MET	ARG	engineered mutation	UNP A5KUH7
T	58	SER	GLN	engineered mutation	UNP A5KUH7
T	74	VAL	GLU	engineered mutation	UNP A5KUH7
T	102	ILE	GLU	engineered mutation	UNP A5KUH7
T	210	GLY	-	expression tag	UNP A5KUH7
T	211	SER	-	expression tag	UNP A5KUH7
T	212	LEU	-	expression tag	UNP A5KUH7
T	213	GLU	-	expression tag	UNP A5KUH7
T	214	HIS	-	expression tag	UNP A5KUH7
T	215	HIS	-	expression tag	UNP A5KUH7
T	216	HIS	-	expression tag	UNP A5KUH7
T	217	HIS	-	expression tag	UNP A5KUH7
T	218	HIS	-	expression tag	UNP A5KUH7
T	219	HIS	-	expression tag	UNP A5KUH7
N	47	SER	ASP	engineered mutation	UNP A5KUH7
N	51	LYS	GLU	engineered mutation	UNP A5KUH7
N	54	MET	ARG	engineered mutation	UNP A5KUH7
N	58	SER	GLN	engineered mutation	UNP A5KUH7
N	74	VAL	GLU	engineered mutation	UNP A5KUH7
N	102	ILE	GLU	engineered mutation	UNP A5KUH7
N	210	GLY	-	expression tag	UNP A5KUH7
N	211	SER	-	expression tag	UNP A5KUH7
N	212	LEU	-	expression tag	UNP A5KUH7
N	213	GLU	-	expression tag	UNP A5KUH7
N	214	HIS	-	expression tag	UNP A5KUH7
N	215	HIS	-	expression tag	UNP A5KUH7
N	216	HIS	-	expression tag	UNP A5KUH7
N	217	HIS	-	expression tag	UNP A5KUH7
N	218	HIS	-	expression tag	UNP A5KUH7
N	219	HIS	-	expression tag	UNP A5KUH7
V	47	SER	ASP	engineered mutation	UNP A5KUH7
V	51	LYS	GLU	engineered mutation	UNP A5KUH7
V	54	MET	ARG	engineered mutation	UNP A5KUH7
V	58	SER	GLN	engineered mutation	UNP A5KUH7

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Chain	Residue	Modelled	Actual	Comment	Reference
V	74	VAL	GLU	engineered mutation	UNP A5KUH7
V	102	ILE	GLU	engineered mutation	UNP A5KUH7
V	210	GLY	-	expression tag	UNP A5KUH7
V	211	SER	-	expression tag	UNP A5KUH7
V	212	LEU	-	expression tag	UNP A5KUH7
V	213	GLU	-	expression tag	UNP A5KUH7
V	214	HIS	-	expression tag	UNP A5KUH7
V	215	HIS	-	expression tag	UNP A5KUH7
V	216	HIS	-	expression tag	UNP A5KUH7
V	217	HIS	-	expression tag	UNP A5KUH7
V	218	HIS	-	expression tag	UNP A5KUH7
V	219	HIS	-	expression tag	UNP A5KUH7
W	47	SER	ASP	engineered mutation	UNP A5KUH7
W	51	LYS	GLU	engineered mutation	UNP A5KUH7
W	54	MET	ARG	engineered mutation	UNP A5KUH7
W	58	SER	GLN	engineered mutation	UNP A5KUH7
W	74	VAL	GLU	engineered mutation	UNP A5KUH7
W	102	ILE	GLU	engineered mutation	UNP A5KUH7
W	210	GLY	-	expression tag	UNP A5KUH7
W	211	SER	-	expression tag	UNP A5KUH7
W	212	LEU	-	expression tag	UNP A5KUH7
W	213	GLU	-	expression tag	UNP A5KUH7
W	214	HIS	-	expression tag	UNP A5KUH7
W	215	HIS	-	expression tag	UNP A5KUH7
W	216	HIS	-	expression tag	UNP A5KUH7
W	217	HIS	-	expression tag	UNP A5KUH7
W	218	HIS	-	expression tag	UNP A5KUH7
W	219	HIS	-	expression tag	UNP A5KUH7
U	47	SER	ASP	engineered mutation	UNP A5KUH7
U	51	LYS	GLU	engineered mutation	UNP A5KUH7
U	54	MET	ARG	engineered mutation	UNP A5KUH7
U	58	SER	GLN	engineered mutation	UNP A5KUH7
U	74	VAL	GLU	engineered mutation	UNP A5KUH7
U	102	ILE	GLU	engineered mutation	UNP A5KUH7
U	210	GLY	-	expression tag	UNP A5KUH7
U	211	SER	-	expression tag	UNP A5KUH7
U	212	LEU	-	expression tag	UNP A5KUH7
U	213	GLU	-	expression tag	UNP A5KUH7
U	214	HIS	-	expression tag	UNP A5KUH7
U	215	HIS	-	expression tag	UNP A5KUH7
U	216	HIS	-	expression tag	UNP A5KUH7
U	217	HIS	-	expression tag	UNP A5KUH7

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Chain	Residue	Modelled	Actual	Comment	Reference
U	218	HIS	-	expression tag	UNP A5KUH7
U	219	HIS	-	expression tag	UNP A5KUH7
Y	47	SER	ASP	engineered mutation	UNP A5KUH7
Y	51	LYS	GLU	engineered mutation	UNP A5KUH7
Y	54	MET	ARG	engineered mutation	UNP A5KUH7
Y	58	SER	GLN	engineered mutation	UNP A5KUH7
Y	74	VAL	GLU	engineered mutation	UNP A5KUH7
Y	102	ILE	GLU	engineered mutation	UNP A5KUH7
Y	210	GLY	-	expression tag	UNP A5KUH7
Y	211	SER	-	expression tag	UNP A5KUH7
Y	212	LEU	-	expression tag	UNP A5KUH7
Y	213	GLU	-	expression tag	UNP A5KUH7
Y	214	HIS	-	expression tag	UNP A5KUH7
Y	215	HIS	-	expression tag	UNP A5KUH7
Y	216	HIS	-	expression tag	UNP A5KUH7
Y	217	HIS	-	expression tag	UNP A5KUH7
Y	218	HIS	-	expression tag	UNP A5KUH7
Y	219	HIS	-	expression tag	UNP A5KUH7
Z	47	SER	ASP	engineered mutation	UNP A5KUH7
Z	51	LYS	GLU	engineered mutation	UNP A5KUH7
Z	54	MET	ARG	engineered mutation	UNP A5KUH7
Z	58	SER	GLN	engineered mutation	UNP A5KUH7
Z	74	VAL	GLU	engineered mutation	UNP A5KUH7
Z	102	ILE	GLU	engineered mutation	UNP A5KUH7
Z	210	GLY	-	expression tag	UNP A5KUH7
Z	211	SER	-	expression tag	UNP A5KUH7
Z	212	LEU	-	expression tag	UNP A5KUH7
Z	213	GLU	-	expression tag	UNP A5KUH7
Z	214	HIS	-	expression tag	UNP A5KUH7
Z	215	HIS	-	expression tag	UNP A5KUH7
Z	216	HIS	-	expression tag	UNP A5KUH7
Z	217	HIS	-	expression tag	UNP A5KUH7
Z	218	HIS	-	expression tag	UNP A5KUH7
Z	219	HIS	-	expression tag	UNP A5KUH7
X	47	SER	ASP	engineered mutation	UNP A5KUH7
X	51	LYS	GLU	engineered mutation	UNP A5KUH7
X	54	MET	ARG	engineered mutation	UNP A5KUH7
X	58	SER	GLN	engineered mutation	UNP A5KUH7
X	74	VAL	GLU	engineered mutation	UNP A5KUH7
X	102	ILE	GLU	engineered mutation	UNP A5KUH7
X	210	GLY	-	expression tag	UNP A5KUH7
X	211	SER	-	expression tag	UNP A5KUH7

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Chain	Residue	Modelled	Actual	Comment	Reference
X	212	LEU	-	expression tag	UNP A5KUH7
X	213	GLU	-	expression tag	UNP A5KUH7
X	214	HIS	-	expression tag	UNP A5KUH7
X	215	HIS	-	expression tag	UNP A5KUH7
X	216	HIS	-	expression tag	UNP A5KUH7
X	217	HIS	-	expression tag	UNP A5KUH7
X	218	HIS	-	expression tag	UNP A5KUH7
X	219	HIS	-	expression tag	UNP A5KUH7
2	47	SER	ASP	engineered mutation	UNP A5KUH7
2	51	LYS	GLU	engineered mutation	UNP A5KUH7
2	54	MET	ARG	engineered mutation	UNP A5KUH7
2	58	SER	GLN	engineered mutation	UNP A5KUH7
2	74	VAL	GLU	engineered mutation	UNP A5KUH7
2	102	ILE	GLU	engineered mutation	UNP A5KUH7
2	210	GLY	-	expression tag	UNP A5KUH7
2	211	SER	-	expression tag	UNP A5KUH7
2	212	LEU	-	expression tag	UNP A5KUH7
2	213	GLU	-	expression tag	UNP A5KUH7
2	214	HIS	-	expression tag	UNP A5KUH7
2	215	HIS	-	expression tag	UNP A5KUH7
2	216	HIS	-	expression tag	UNP A5KUH7
2	217	HIS	-	expression tag	UNP A5KUH7
2	218	HIS	-	expression tag	UNP A5KUH7
2	219	HIS	-	expression tag	UNP A5KUH7
4	47	SER	ASP	engineered mutation	UNP A5KUH7
4	51	LYS	GLU	engineered mutation	UNP A5KUH7
4	54	MET	ARG	engineered mutation	UNP A5KUH7
4	58	SER	GLN	engineered mutation	UNP A5KUH7
4	74	VAL	GLU	engineered mutation	UNP A5KUH7
4	102	ILE	GLU	engineered mutation	UNP A5KUH7
4	210	GLY	-	expression tag	UNP A5KUH7
4	211	SER	-	expression tag	UNP A5KUH7
4	212	LEU	-	expression tag	UNP A5KUH7
4	213	GLU	-	expression tag	UNP A5KUH7
4	214	HIS	-	expression tag	UNP A5KUH7
4	215	HIS	-	expression tag	UNP A5KUH7
4	216	HIS	-	expression tag	UNP A5KUH7
4	217	HIS	-	expression tag	UNP A5KUH7
4	218	HIS	-	expression tag	UNP A5KUH7
4	219	HIS	-	expression tag	UNP A5KUH7
1	47	SER	ASP	engineered mutation	UNP A5KUH7
1	51	LYS	GLU	engineered mutation	UNP A5KUH7

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Chain	Residue	Modelled	Actual	Comment	Reference
1	54	MET	ARG	engineered mutation	UNP A5KUH7
1	58	SER	GLN	engineered mutation	UNP A5KUH7
1	74	VAL	GLU	engineered mutation	UNP A5KUH7
1	102	ILE	GLU	engineered mutation	UNP A5KUH7
1	210	GLY	-	expression tag	UNP A5KUH7
1	211	SER	-	expression tag	UNP A5KUH7
1	212	LEU	-	expression tag	UNP A5KUH7
1	213	GLU	-	expression tag	UNP A5KUH7
1	214	HIS	-	expression tag	UNP A5KUH7
1	215	HIS	-	expression tag	UNP A5KUH7
1	216	HIS	-	expression tag	UNP A5KUH7
1	217	HIS	-	expression tag	UNP A5KUH7
1	218	HIS	-	expression tag	UNP A5KUH7
1	219	HIS	-	expression tag	UNP A5KUH7
L	47	SER	ASP	engineered mutation	UNP A5KUH7
L	51	LYS	GLU	engineered mutation	UNP A5KUH7
L	54	MET	ARG	engineered mutation	UNP A5KUH7
L	58	SER	GLN	engineered mutation	UNP A5KUH7
L	74	VAL	GLU	engineered mutation	UNP A5KUH7
L	102	ILE	GLU	engineered mutation	UNP A5KUH7
L	210	GLY	-	expression tag	UNP A5KUH7
L	211	SER	-	expression tag	UNP A5KUH7
L	212	LEU	-	expression tag	UNP A5KUH7
L	213	GLU	-	expression tag	UNP A5KUH7
L	214	HIS	-	expression tag	UNP A5KUH7
L	215	HIS	-	expression tag	UNP A5KUH7
L	216	HIS	-	expression tag	UNP A5KUH7
L	217	HIS	-	expression tag	UNP A5KUH7
L	218	HIS	-	expression tag	UNP A5KUH7
L	219	HIS	-	expression tag	UNP A5KUH7
R	47	SER	ASP	engineered mutation	UNP A5KUH7
R	51	LYS	GLU	engineered mutation	UNP A5KUH7
R	54	MET	ARG	engineered mutation	UNP A5KUH7
R	58	SER	GLN	engineered mutation	UNP A5KUH7
R	74	VAL	GLU	engineered mutation	UNP A5KUH7
R	102	ILE	GLU	engineered mutation	UNP A5KUH7
R	210	GLY	-	expression tag	UNP A5KUH7
R	211	SER	-	expression tag	UNP A5KUH7
R	212	LEU	-	expression tag	UNP A5KUH7
R	213	GLU	-	expression tag	UNP A5KUH7
R	214	HIS	-	expression tag	UNP A5KUH7
R	215	HIS	-	expression tag	UNP A5KUH7

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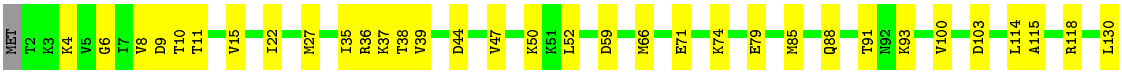
Chain	Residue	Modelled	Actual	Comment	Reference
R	216	HIS	-	expression tag	UNP A5KUH7
R	217	HIS	-	expression tag	UNP A5KUH7
R	218	HIS	-	expression tag	UNP A5KUH7
R	219	HIS	-	expression tag	UNP A5KUH7
3	47	SER	ASP	engineered mutation	UNP A5KUH7
3	51	LYS	GLU	engineered mutation	UNP A5KUH7
3	54	MET	ARG	engineered mutation	UNP A5KUH7
3	58	SER	GLN	engineered mutation	UNP A5KUH7
3	74	VAL	GLU	engineered mutation	UNP A5KUH7
3	102	ILE	GLU	engineered mutation	UNP A5KUH7
3	210	GLY	-	expression tag	UNP A5KUH7
3	211	SER	-	expression tag	UNP A5KUH7
3	212	LEU	-	expression tag	UNP A5KUH7
3	213	GLU	-	expression tag	UNP A5KUH7
3	214	HIS	-	expression tag	UNP A5KUH7
3	215	HIS	-	expression tag	UNP A5KUH7
3	216	HIS	-	expression tag	UNP A5KUH7
3	217	HIS	-	expression tag	UNP A5KUH7
3	218	HIS	-	expression tag	UNP A5KUH7
3	219	HIS	-	expression tag	UNP A5KUH7

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.

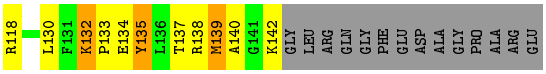
- Molecule 1: Designed Riboflavin synthase

Chain K:



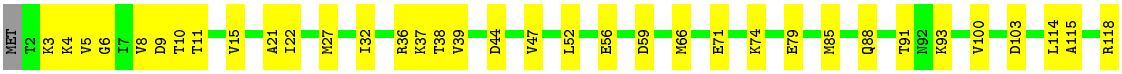
- Molecule 1: Designed Riboflavin synthase

Chain M:



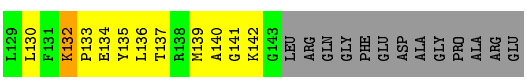
- Molecule 1: Designed Riboflavin synthase

Chain O:



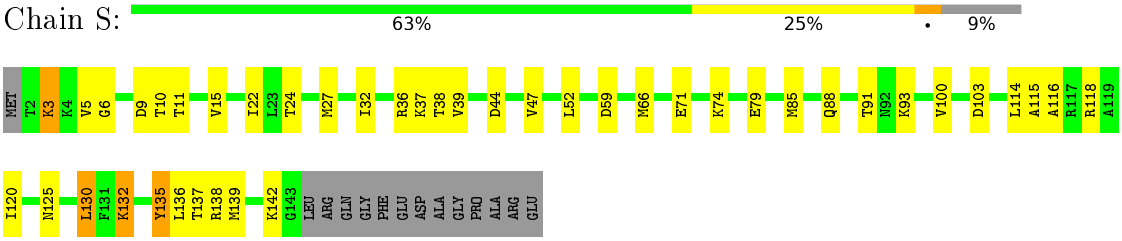
- Molecule 1: Designed Riboflavin synthase

Chain Q:



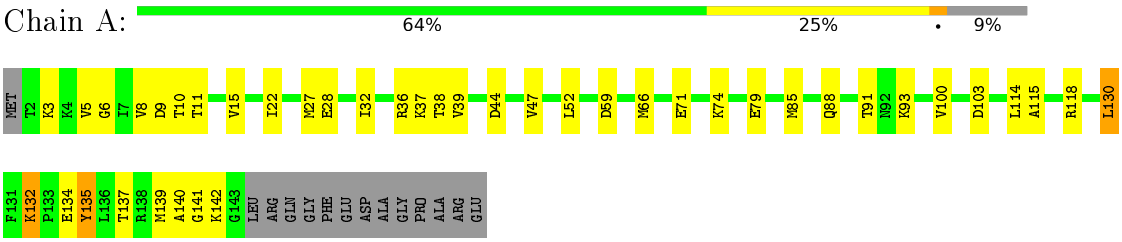
• Molecule 1: Designed Riboflavin synthase

Chain S:



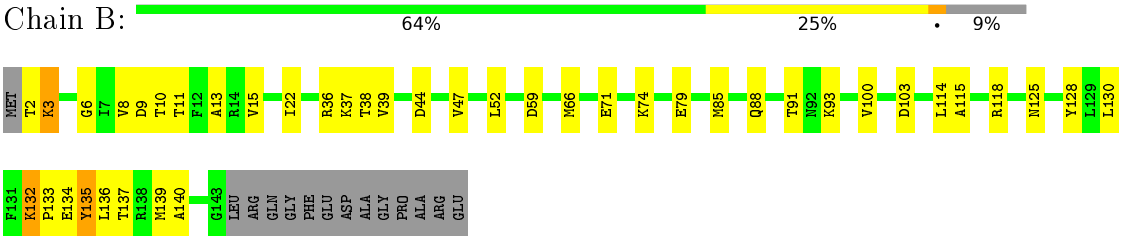
• Molecule 1: Designed Riboflavin synthase

Chain A:



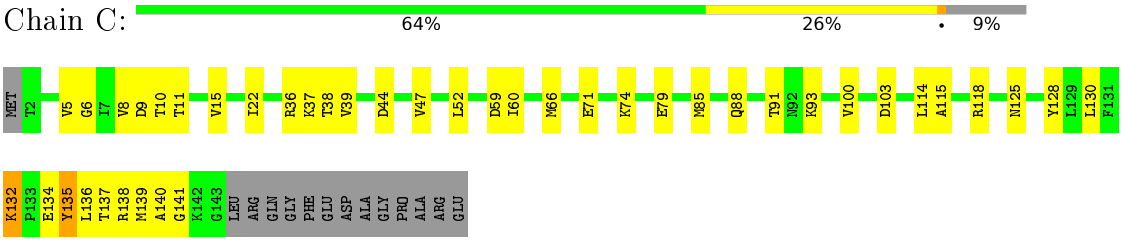
• Molecule 1: Designed Riboflavin synthase

Chain B:



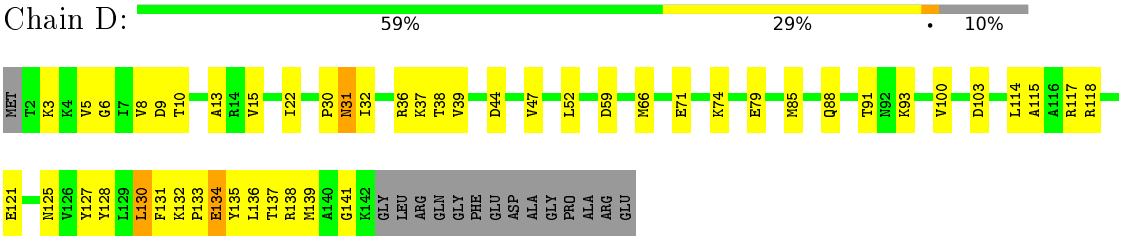
• Molecule 1: Designed Riboflavin synthase

Chain C:



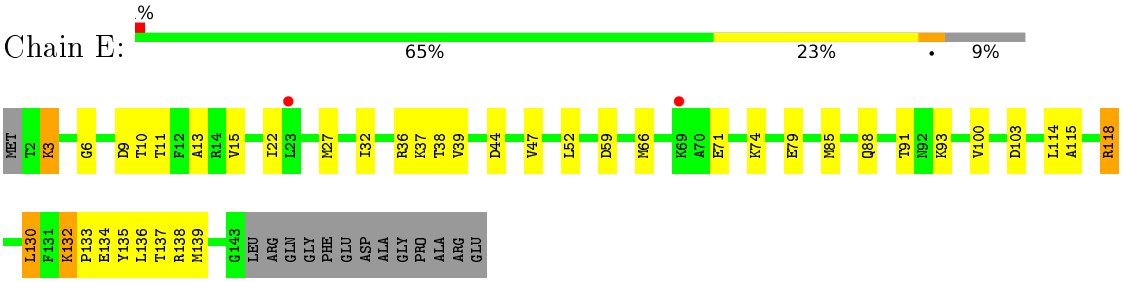
• Molecule 1: Designed Riboflavin synthase

Chain D:



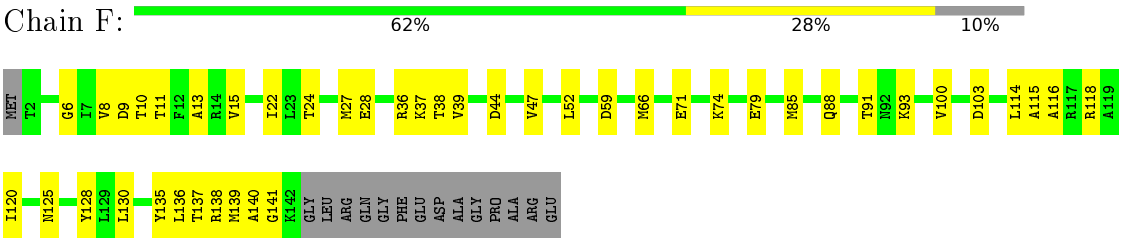
• Molecule 1: Designed Riboflavin synthase

Chain E:



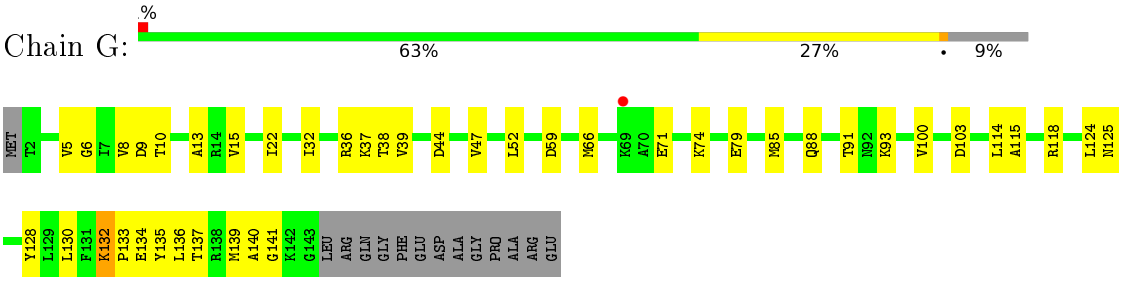
- Molecule 1: Designed Riboflavin synthase

Chain F:



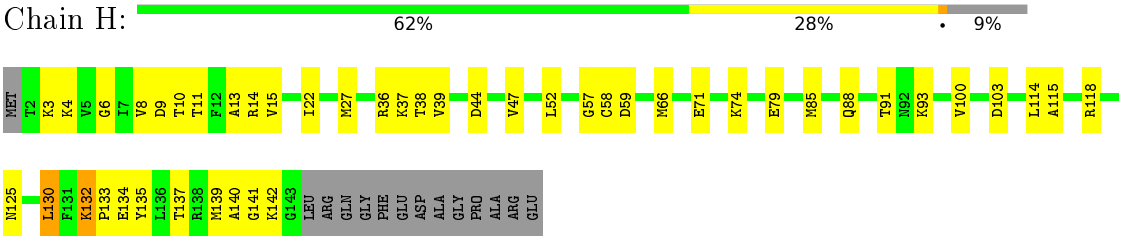
- Molecule 1: Designed Riboflavin synthase

Chain G:



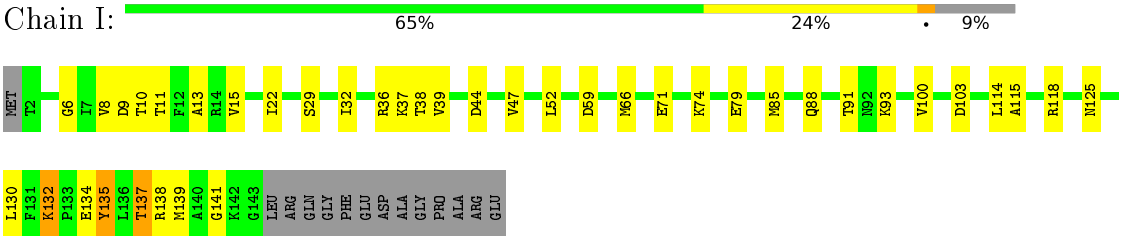
- Molecule 1: Designed Riboflavin synthase

Chain H:



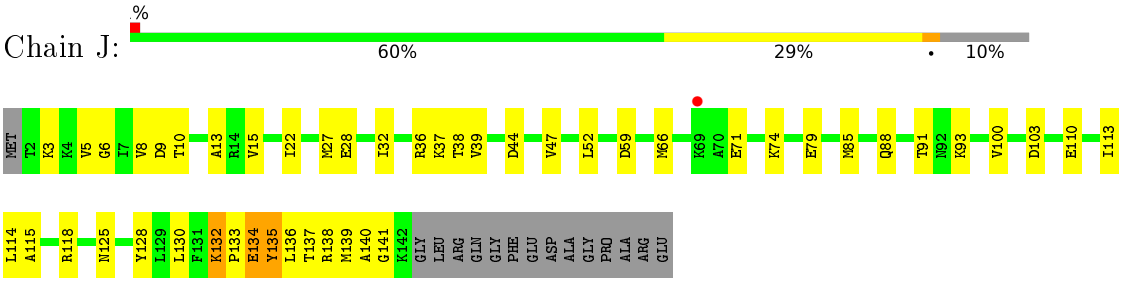
- Molecule 1: Designed Riboflavin synthase

Chain I:



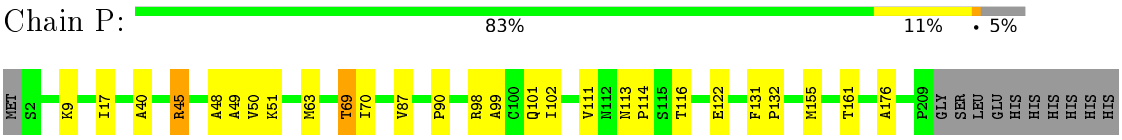
- Molecule 1: Designed Riboflavin synthase

Chain J:



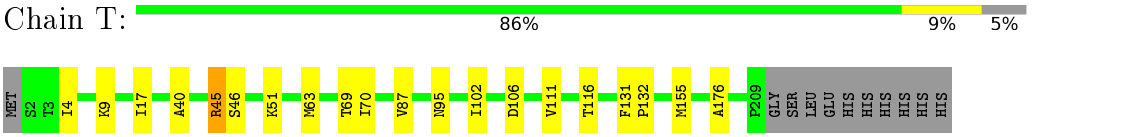
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain P:



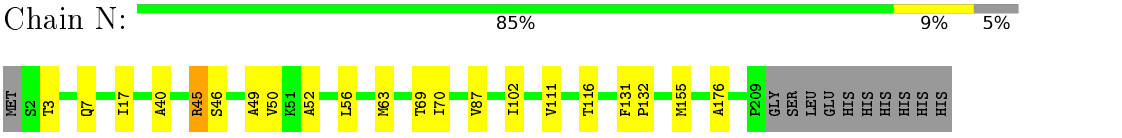
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain T:



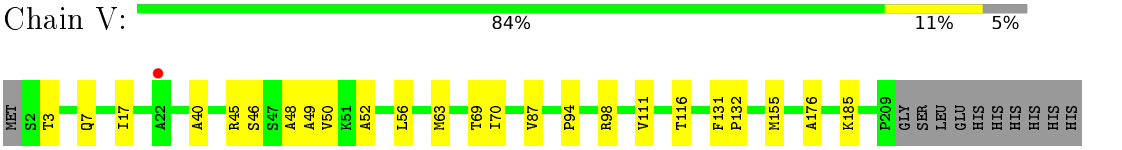
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain N:



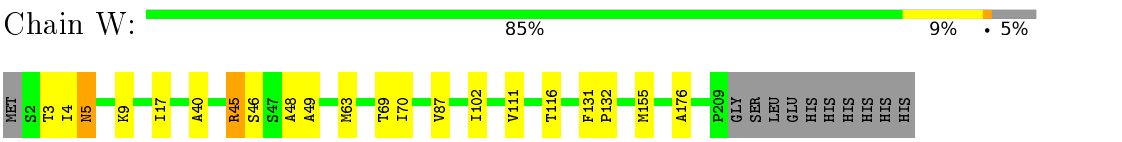
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain V:



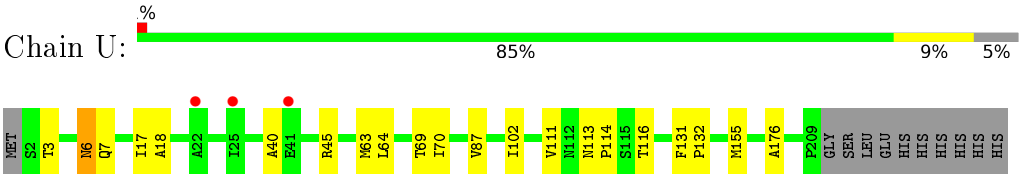
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain W:



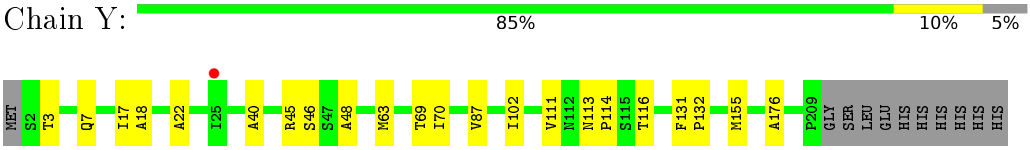
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain U:



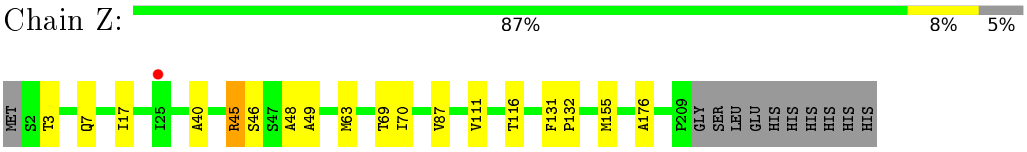
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain Y:



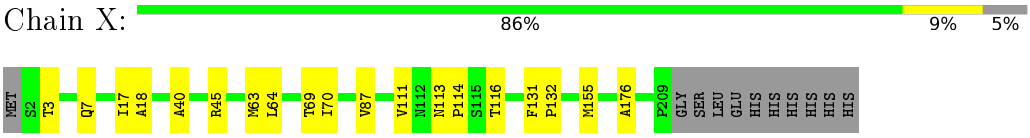
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain Z:



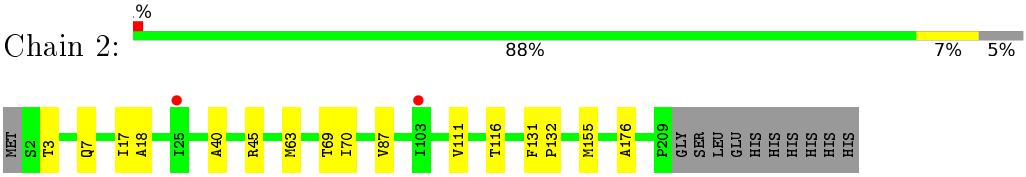
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain X:



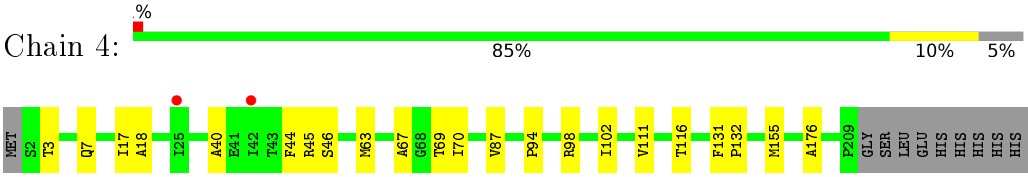
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain 2:



• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain 4:



• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

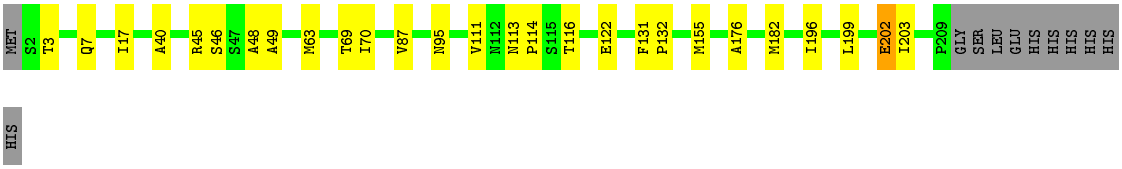
Chain 1:

• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain L:

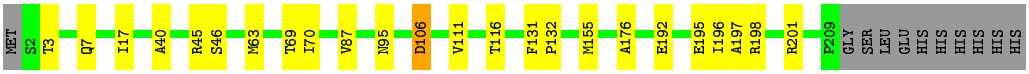
• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain R:



• Molecule 2: Designed Keto-hydroxyglutarate-aldolase/keto-deoxy-phosphogluconate aldolase

Chain 3:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	265.62Å 279.81Å 301.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	199.26 – 3.70 199.26 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (199.26-3.70) 99.0 (199.26-3.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.68Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.240 , 0.247 0.240 , 0.247	Depositor DCC
R_{free} test set	11800 reflections (10.00%)	DCC
Wilson B-factor (Å^2)	100.4	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	39183	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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	0.51	0/1100	0.73	4/1479 (0.3%)
1	B	0.58	0/1100	0.71	4/1479 (0.3%)
1	C	0.53	0/1100	0.72	4/1479 (0.3%)
1	D	0.56	0/1100	0.73	4/1478 (0.3%)
1	E	0.53	0/1100	0.72	4/1479 (0.3%)
1	F	0.54	0/1096	0.75	4/1474 (0.3%)
1	G	0.56	0/1100	0.73	4/1479 (0.3%)
1	H	0.54	0/1100	0.72	4/1479 (0.3%)
1	I	0.57	0/1100	0.73	4/1479 (0.3%)
1	J	0.54	0/1096	0.75	4/1474 (0.3%)
1	K	0.57	0/1100	0.73	4/1479 (0.3%)
1	M	0.56	0/1100	0.74	4/1478 (0.3%)
1	O	0.55	0/1100	0.74	4/1478 (0.3%)
1	Q	0.55	0/1100	0.72	4/1479 (0.3%)
1	S	0.54	0/1100	0.72	4/1479 (0.3%)
2	1	0.56	0/1551	0.63	0/2115
2	2	0.56	0/1551	0.62	0/2115
2	3	0.57	0/1551	0.62	0/2115
2	4	0.55	0/1551	0.62	0/2115
2	L	0.56	0/1551	0.62	0/2115
2	N	0.55	0/1547	0.61	0/2110
2	P	0.56	0/1551	0.65	0/2115
2	R	0.57	0/1551	0.63	0/2115
2	T	0.57	0/1551	0.63	0/2115
2	U	0.57	0/1551	0.62	0/2115
2	V	0.56	0/1551	0.62	0/2115
2	W	0.56	0/1551	0.63	0/2115
2	X	0.57	0/1551	0.62	0/2115
2	Y	0.56	0/1551	0.62	0/2115
2	Z	0.56	0/1551	0.62	0/2115
All	All	0.56	0/39753	0.67	60/53892 (0.1%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	9	ASP	CB-CG-OD1	6.32	123.99	118.30
1	S	9	ASP	CB-CG-OD1	6.27	123.94	118.30
1	E	9	ASP	CB-CG-OD1	6.18	123.86	118.30
1	E	59	ASP	CB-CG-OD1	6.17	123.85	118.30
1	Q	9	ASP	CB-CG-OD1	6.16	123.84	118.30
1	C	59	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	9	ASP	CB-CG-OD1	6.15	123.84	118.30
1	A	9	ASP	CB-CG-OD1	6.14	123.83	118.30
1	Q	59	ASP	CB-CG-OD1	6.14	123.83	118.30
1	G	9	ASP	CB-CG-OD1	6.12	123.81	118.30
1	K	9	ASP	CB-CG-OD1	6.12	123.80	118.30
1	S	59	ASP	CB-CG-OD1	6.12	123.80	118.30
1	G	59	ASP	CB-CG-OD1	6.10	123.79	118.30
1	F	9	ASP	CB-CG-OD1	6.08	123.77	118.30
1	M	9	ASP	CB-CG-OD1	6.07	123.77	118.30
1	K	59	ASP	CB-CG-OD1	6.06	123.76	118.30
1	M	59	ASP	CB-CG-OD1	6.04	123.74	118.30
1	D	59	ASP	CB-CG-OD1	6.04	123.73	118.30
1	D	9	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	59	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	59	ASP	CB-CG-OD1	6.02	123.72	118.30
1	J	59	ASP	CB-CG-OD1	6.02	123.72	118.30
1	I	9	ASP	CB-CG-OD1	6.02	123.71	118.30
1	H	59	ASP	CB-CG-OD1	6.01	123.71	118.30
1	O	9	ASP	CB-CG-OD1	5.93	123.64	118.30
1	H	9	ASP	CB-CG-OD1	5.93	123.63	118.30
1	F	59	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	9	ASP	CB-CG-OD1	5.82	123.54	118.30
1	M	103	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	103	ASP	CB-CG-OD1	5.81	123.53	118.30
1	O	59	ASP	CB-CG-OD1	5.78	123.50	118.30
1	I	59	ASP	CB-CG-OD1	5.75	123.47	118.30
1	H	103	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	103	ASP	CB-CG-OD1	5.71	123.44	118.30
1	O	103	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	103	ASP	CB-CG-OD1	5.66	123.39	118.30
1	K	44	ASP	CB-CG-OD1	5.65	123.39	118.30
1	Q	103	ASP	CB-CG-OD1	5.65	123.38	118.30
1	D	103	ASP	CB-CG-OD1	5.64	123.38	118.30
1	K	103	ASP	CB-CG-OD1	5.62	123.36	118.30
1	F	44	ASP	CB-CG-OD1	5.60	123.34	118.30
1	I	44	ASP	CB-CG-OD1	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	103	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	44	ASP	CB-CG-OD1	5.57	123.32	118.30
1	I	103	ASP	CB-CG-OD1	5.57	123.31	118.30
1	S	103	ASP	CB-CG-OD1	5.55	123.30	118.30
1	J	103	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	44	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	103	ASP	CB-CG-OD1	5.45	123.21	118.30
1	E	44	ASP	CB-CG-OD1	5.45	123.20	118.30
1	D	44	ASP	CB-CG-OD1	5.44	123.20	118.30
1	E	103	ASP	CB-CG-OD1	5.41	123.17	118.30
1	H	44	ASP	CB-CG-OD1	5.39	123.16	118.30
1	Q	44	ASP	CB-CG-OD1	5.39	123.15	118.30
1	J	44	ASP	CB-CG-OD1	5.36	123.12	118.30
1	O	44	ASP	CB-CG-OD1	5.33	123.10	118.30
1	S	44	ASP	CB-CG-OD1	5.33	123.10	118.30
1	G	44	ASP	CB-CG-OD1	5.32	123.09	118.30
1	M	44	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	44	ASP	CB-CG-OD1	5.26	123.03	118.30

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	1086	0	1141	59	0
1	B	1086	0	1141	61	0
1	C	1086	0	1141	54	0
1	D	1086	0	1149	62	0
1	E	1086	0	1141	63	0
1	F	1082	0	1138	51	0
1	G	1086	0	1141	46	0
1	H	1086	0	1141	63	0
1	I	1086	0	1141	55	0
1	J	1082	0	1138	64	0
1	K	1086	0	1141	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1086	0	1149	75	0
1	O	1086	0	1149	62	0
1	Q	1086	0	1141	64	0
1	S	1086	0	1141	62	0
2	1	1527	0	1585	20	0
2	2	1527	0	1585	8	0
2	3	1527	0	1585	15	1
2	4	1527	0	1585	15	0
2	L	1527	0	1585	11	0
2	N	1523	0	1581	22	0
2	P	1527	0	1585	16	1
2	R	1527	0	1585	16	0
2	T	1527	0	1585	15	0
2	U	1527	0	1585	13	0
2	V	1527	0	1585	16	0
2	W	1527	0	1585	12	0
2	X	1527	0	1585	9	0
2	Y	1527	0	1585	13	0
2	Z	1527	0	1585	13	0
All	All	39183	0	40904	959	1

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 12.

All (959) 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:11:THR:HA	1:Q:140:ALA:HA	1.26	1.12
1:K:88:GLN:HB3	1:S:47:VAL:HG21	1.35	1.07
1:O:88:GLN:HB3	1:Q:47:VAL:HG21	1.38	1.03
2:4:18:ALA:HB1	2:4:45:ARG:HD2	1.39	1.02
1:B:47:VAL:HG21	1:D:88:GLN:HB3	1.42	1.01
1:A:47:VAL:HG21	1:B:88:GLN:HB3	1.46	0.98
1:K:47:VAL:HG21	1:M:88:GLN:HB3	1.46	0.96
1:G:47:VAL:HG21	1:I:88:GLN:HB3	1.48	0.95
1:F:88:GLN:HB3	1:J:47:VAL:HG21	1.49	0.94
1:F:47:VAL:HG21	1:G:88:GLN:HB3	1.47	0.94
1:H:88:GLN:HB3	1:I:47:VAL:HG21	1.47	0.94
2:T:4:ILE:HD11	2:T:106:ASP:OD2	1.68	0.93
1:C:47:VAL:HG21	1:E:88:GLN:HB3	1.46	0.93
1:A:88:GLN:HB3	1:E:47:VAL:HG21	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:VAL:HG21	1:J:88:GLN:HB3	1.52	0.92
1:M:47:VAL:HG21	1:Q:88:GLN:HB3	1.52	0.91
1:C:88:GLN:HB3	1:D:47:VAL:HG21	1.48	0.91
1:O:47:VAL:HG21	1:S:88:GLN:HB3	1.52	0.89
1:B:11:THR:HA	1:D:139:MET:O	1.73	0.88
2:1:22:ALA:HB2	2:1:48:ALA:HB1	1.56	0.88
1:G:71:GLU:O	1:G:74:LYS:HG2	1.75	0.87
1:K:71:GLU:O	1:K:74:LYS:HG2	1.75	0.87
1:A:71:GLU:O	1:A:74:LYS:HG2	1.75	0.86
1:H:71:GLU:O	1:H:74:LYS:HG2	1.75	0.86
1:E:71:GLU:O	1:E:74:LYS:HG2	1.75	0.86
1:S:71:GLU:O	1:S:74:LYS:HG2	1.76	0.86
1:O:71:GLU:O	1:O:74:LYS:HG2	1.75	0.85
1:C:71:GLU:O	1:C:74:LYS:HG2	1.75	0.85
1:B:71:GLU:O	1:B:74:LYS:HG2	1.75	0.85
1:Q:71:GLU:O	1:Q:74:LYS:HG2	1.75	0.85
1:H:139:MET:HE2	1:H:139:MET:HA	1.57	0.85
1:J:71:GLU:O	1:J:74:LYS:HG2	1.75	0.85
1:D:71:GLU:O	1:D:74:LYS:HG2	1.75	0.85
1:I:71:GLU:O	1:I:74:LYS:HG2	1.75	0.85
1:Q:5:VAL:HG23	1:Q:32:ILE:HD11	1.56	0.85
1:M:71:GLU:O	1:M:74:LYS:HG2	1.75	0.85
1:F:71:GLU:O	1:F:74:LYS:HG2	1.75	0.84
1:S:5:VAL:HG23	1:S:32:ILE:HD11	1.59	0.84
2:Y:22:ALA:HB2	2:Y:48:ALA:HB1	1.60	0.83
2:N:45:ARG:HD3	2:N:46:SER:N	1.93	0.83
1:H:135:TYR:CE1	1:H:139:MET:HG3	2.15	0.82
1:Q:2:THR:O	1:Q:3:LYS:HD2	1.80	0.81
1:B:139:MET:HA	1:B:139:MET:HE2	1.63	0.80
1:K:11:THR:HA	1:M:139:MET:O	1.81	0.80
1:K:88:GLN:HB3	1:S:47:VAL:CG2	2.10	0.79
1:A:5:VAL:HG23	1:A:32:ILE:HD11	1.62	0.79
1:S:3:LYS:HB2	1:S:3:LYS:HZ3	1.45	0.79
1:F:139:MET:HA	1:F:139:MET:HE2	1.65	0.79
1:O:91:THR:O	1:O:91:THR:HG22	1.83	0.79
1:S:91:THR:HG22	1:S:91:THR:O	1.83	0.78
1:J:91:THR:O	1:J:91:THR:HG22	1.84	0.78
1:O:88:GLN:HB3	1:Q:47:VAL:CG2	2.12	0.78
1:A:91:THR:HG22	1:A:91:THR:O	1.82	0.78
1:I:91:THR:HG22	1:I:91:THR:O	1.83	0.78
1:M:91:THR:O	1:M:91:THR:HG22	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:MET:HA	1:C:139:MET:HE2	1.64	0.78
1:A:141:GLY:HA2	1:E:13:ALA:O	1.83	0.78
1:E:27:MET:HA	2:4:102:ILE:HG21	1.65	0.78
1:K:91:THR:O	1:K:91:THR:HG22	1.84	0.78
1:G:91:THR:HG22	1:G:91:THR:O	1.84	0.78
1:B:91:THR:O	1:B:91:THR:HG22	1.83	0.77
1:D:91:THR:HG22	1:D:91:THR:O	1.84	0.77
1:C:91:THR:HG22	1:C:91:THR:O	1.83	0.77
1:E:71:GLU:C	1:E:74:LYS:HG2	2.05	0.77
1:G:71:GLU:C	1:G:74:LYS:HG2	2.05	0.77
1:H:4:LYS:HG3	1:H:58:CYS:HA	1.65	0.77
1:A:71:GLU:C	1:A:74:LYS:HG2	2.05	0.77
1:M:5:VAL:HG23	1:M:32:ILE:HD11	1.67	0.77
2:U:3:THR:O	2:U:7:GLN:HG3	1.84	0.77
1:C:71:GLU:C	1:C:74:LYS:HG2	2.05	0.77
1:D:71:GLU:C	1:D:74:LYS:HG2	2.05	0.77
1:H:14:ARG:HA	1:J:141:GLY:O	1.85	0.77
1:K:71:GLU:C	1:K:74:LYS:HG2	2.05	0.77
1:H:71:GLU:C	1:H:74:LYS:HG2	2.05	0.77
2:1:7:GLN:OE1	2:1:64:LEU:HD13	1.85	0.77
1:M:71:GLU:C	1:M:74:LYS:HG2	2.05	0.77
1:Q:71:GLU:C	1:Q:74:LYS:HG2	2.05	0.77
2:U:3:THR:C	2:U:7:GLN:HE21	1.88	0.76
1:B:71:GLU:HB2	1:B:74:LYS:HE2	1.67	0.76
1:F:71:GLU:C	1:F:74:LYS:HG2	2.06	0.76
1:M:71:GLU:HB2	1:M:74:LYS:HE2	1.67	0.76
1:S:71:GLU:HB2	1:S:74:LYS:HE2	1.67	0.76
1:J:71:GLU:HB2	1:J:74:LYS:HE2	1.67	0.76
1:C:71:GLU:HB2	1:C:74:LYS:HE2	1.68	0.76
1:D:71:GLU:HB2	1:D:74:LYS:HE2	1.68	0.76
1:H:140:ALA:HA	1:I:11:THR:HA	1.66	0.76
1:I:71:GLU:HB2	1:I:74:LYS:HE2	1.68	0.76
1:E:91:THR:O	1:E:91:THR:HG22	1.83	0.76
1:H:91:THR:O	1:H:91:THR:HG22	1.83	0.76
1:K:71:GLU:HB2	1:K:74:LYS:HE2	1.67	0.76
1:B:71:GLU:C	1:B:74:LYS:HG2	2.05	0.76
1:F:71:GLU:HB2	1:F:74:LYS:HE2	1.68	0.76
1:A:71:GLU:HB2	1:A:74:LYS:HE2	1.67	0.75
1:I:71:GLU:C	1:I:74:LYS:HG2	2.05	0.75
1:O:71:GLU:HB2	1:O:74:LYS:HE2	1.67	0.75
1:H:71:GLU:HB2	1:H:74:LYS:HE2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:71:GLU:HB2	1:Q:74:LYS:HE2	1.67	0.75
1:S:71:GLU:C	1:S:74:LYS:HG2	2.05	0.75
1:H:4:LYS:HD3	1:H:57:GLY:O	1.86	0.75
1:Q:91:THR:O	1:Q:91:THR:HG22	1.84	0.75
1:E:71:GLU:HB2	1:E:74:LYS:HE2	1.68	0.75
1:H:3:LYS:HG2	1:H:130:LEU:HG	1.68	0.75
1:O:138:ARG:C	1:O:139:MET:HE3	2.06	0.75
1:G:71:GLU:HB2	1:G:74:LYS:HE2	1.68	0.75
1:J:71:GLU:C	1:J:74:LYS:HG2	2.05	0.75
1:O:71:GLU:C	1:O:74:LYS:HG2	2.05	0.75
1:S:116:ALA:O	1:S:120:ILE:HG13	1.86	0.74
1:M:5:VAL:CG2	1:M:32:ILE:HD11	2.18	0.74
1:B:47:VAL:CG2	1:D:88:GLN:HB3	2.16	0.74
1:Q:135:TYR:HE1	1:Q:139:MET:HG3	1.52	0.74
1:H:139:MET:HA	1:H:139:MET:CE	2.19	0.73
1:H:135:TYR:HE1	1:H:139:MET:HG3	1.52	0.72
2:N:45:ARG:HD3	2:N:46:SER:CB	2.19	0.72
2:N:56:LEU:HD21	2:N:63:MET:SD	2.30	0.72
2:V:45:ARG:HH12	2:V:185:LYS:HE2	1.54	0.72
1:F:27:MET:HA	2:1:102:ILE:HG21	1.72	0.72
1:F:91:THR:HG22	1:F:91:THR:O	1.90	0.72
1:F:47:VAL:CG2	1:G:88:GLN:HB3	2.20	0.72
1:G:38:THR:OG1	1:I:137:THR:HA	1.90	0.72
1:C:47:VAL:CG2	1:E:88:GLN:HB3	2.20	0.71
1:O:139:MET:HE3	1:O:139:MET:N	2.05	0.71
1:I:139:MET:HA	1:I:139:MET:HE2	1.71	0.71
1:F:139:MET:HA	1:F:139:MET:CE	2.20	0.71
2:1:18:ALA:HB1	2:1:45:ARG:HD3	1.71	0.71
2:N:45:ARG:HH11	2:N:46:SER:CB	2.03	0.71
2:2:3:THR:HG22	2:2:7:GLN:HE21	1.56	0.71
1:E:139:MET:HA	1:E:139:MET:HE2	1.72	0.71
1:M:139:MET:HE2	1:M:139:MET:HA	1.73	0.71
1:M:138:ARG:C	1:M:139:MET:HE3	2.11	0.71
1:S:3:LYS:HG2	1:S:130:LEU:HG	1.73	0.70
2:Z:3:THR:HG22	2:Z:7:GLN:HE21	1.56	0.70
2:3:3:THR:HG22	2:3:7:GLN:HE21	1.56	0.70
1:G:124:LEU:O	1:G:128:TYR:HD1	1.74	0.70
1:K:139:MET:HB2	1:S:11:THR:HG22	1.72	0.70
2:N:3:THR:HG22	2:N:7:GLN:HE21	1.56	0.70
2:4:3:THR:HG22	2:4:7:GLN:HE21	1.56	0.70
1:E:139:MET:CE	1:E:139:MET:HA	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:MET:HA	1:D:139:MET:HE2	1.72	0.70
1:D:66:MET:HG2	1:D:100:VAL:O	1.92	0.70
2:V:45:ARG:HG3	2:V:46:SER:N	2.06	0.70
1:M:133:PRO:HD2	1:M:134:GLU:H	1.57	0.70
1:Q:139:MET:N	1:Q:139:MET:HE3	2.07	0.70
2:Y:3:THR:HG22	2:Y:7:GLN:HE21	1.57	0.70
1:A:47:VAL:CG2	1:B:88:GLN:HB3	2.20	0.70
1:S:139:MET:HE3	1:S:139:MET:N	2.06	0.69
1:M:66:MET:HG2	1:M:100:VAL:O	1.93	0.69
1:A:66:MET:HG2	1:A:100:VAL:O	1.93	0.69
1:I:66:MET:HG2	1:I:100:VAL:O	1.92	0.69
1:J:66:MET:HG2	1:J:100:VAL:O	1.93	0.69
1:K:139:MET:HA	1:K:139:MET:HE2	1.75	0.69
1:B:66:MET:HG2	1:B:100:VAL:O	1.93	0.69
1:C:66:MET:HG2	1:C:100:VAL:O	1.93	0.69
1:A:88:GLN:HB3	1:E:47:VAL:CG2	2.22	0.69
1:Q:66:MET:HG2	1:Q:100:VAL:O	1.93	0.69
2:V:3:THR:HG22	2:V:7:GLN:HE21	1.56	0.69
1:H:66:MET:HG2	1:H:100:VAL:O	1.93	0.69
1:H:141:GLY:HA2	1:I:13:ALA:O	1.92	0.69
1:F:120:ILE:HD13	2:1:77:LEU:HD23	1.75	0.69
1:S:66:MET:HG2	1:S:100:VAL:O	1.93	0.69
1:G:66:MET:HG2	1:G:100:VAL:O	1.93	0.69
1:S:5:VAL:CG2	1:S:32:ILE:HD11	2.23	0.69
1:K:47:VAL:CG2	1:M:88:GLN:HB3	2.21	0.68
1:O:66:MET:HG2	1:O:100:VAL:O	1.92	0.68
1:G:5:VAL:HG23	1:G:32:ILE:HD11	1.76	0.68
1:F:88:GLN:HB3	1:J:47:VAL:CG2	2.23	0.68
1:K:66:MET:HG2	1:K:100:VAL:O	1.93	0.68
2:L:3:THR:HG22	2:L:7:GLN:HE21	1.56	0.68
1:M:139:MET:HE3	1:M:139:MET:N	2.09	0.68
1:Q:128:TYR:HB2	1:Q:136:LEU:HD11	1.76	0.68
1:F:66:MET:HG2	1:F:100:VAL:O	1.93	0.68
1:S:27:MET:HA	2:P:102:ILE:HG21	1.74	0.68
1:E:66:MET:HG2	1:E:100:VAL:O	1.92	0.68
1:B:11:THR:CA	1:D:139:MET:O	2.42	0.68
2:L:18:ALA:HB1	2:L:45:ARG:HD2	1.76	0.68
1:H:88:GLN:HB3	1:I:47:VAL:CG2	2.23	0.67
2:X:18:ALA:HB1	2:X:45:ARG:HD2	1.75	0.67
2:X:3:THR:O	2:X:7:GLN:HG3	1.94	0.67
1:O:71:GLU:HB2	1:O:74:LYS:CE	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3:LYS:CG	1:S:130:LEU:HG	2.25	0.67
1:C:71:GLU:HB2	1:C:74:LYS:CE	2.25	0.67
1:D:71:GLU:HB2	1:D:74:LYS:CE	2.25	0.67
1:J:128:TYR:HB2	1:J:136:LEU:HD11	1.77	0.67
1:K:71:GLU:HB2	1:K:74:LYS:CE	2.25	0.67
1:C:128:TYR:CB	1:C:136:LEU:HD11	2.24	0.67
1:C:88:GLN:HB3	1:D:47:VAL:CG2	2.24	0.67
1:G:71:GLU:HB2	1:G:74:LYS:CE	2.25	0.67
1:I:71:GLU:HB2	1:I:74:LYS:CE	2.25	0.67
2:T:45:ARG:HG3	2:T:46:SER:N	2.09	0.67
1:J:71:GLU:HB2	1:J:74:LYS:CE	2.25	0.66
1:G:47:VAL:CG2	1:I:88:GLN:HB3	2.23	0.66
1:J:139:MET:N	1:J:139:MET:HE3	2.10	0.66
1:M:71:GLU:HB2	1:M:74:LYS:CE	2.25	0.66
2:V:45:ARG:NH1	2:V:185:LYS:HE2	2.10	0.66
1:J:5:VAL:HG23	1:J:32:ILE:HD11	1.76	0.66
2:1:18:ALA:HB1	2:1:45:ARG:CD	2.26	0.66
1:K:50:LYS:NZ	1:M:92:ASN:HD21	1.93	0.66
1:S:71:GLU:HB2	1:S:74:LYS:CE	2.25	0.66
1:H:47:VAL:CG2	1:J:88:GLN:HB3	2.26	0.66
2:U:18:ALA:HB1	2:U:45:ARG:HD2	1.76	0.66
1:A:71:GLU:HB2	1:A:74:LYS:CE	2.25	0.66
1:H:71:GLU:HB2	1:H:74:LYS:CE	2.25	0.66
1:S:135:TYR:HE1	1:S:139:MET:HG3	1.61	0.66
1:E:71:GLU:HB2	1:E:74:LYS:CE	2.25	0.66
1:Q:71:GLU:HB2	1:Q:74:LYS:CE	2.25	0.66
1:S:139:MET:HE2	1:S:139:MET:HA	1.78	0.66
1:A:141:GLY:CA	1:E:13:ALA:O	2.43	0.66
2:1:8:LEU:HD23	2:1:14:ILE:HD11	1.78	0.65
1:F:71:GLU:HB2	1:F:74:LYS:CE	2.25	0.65
1:G:124:LEU:O	1:G:128:TYR:CD1	2.49	0.65
2:2:18:ALA:HB1	2:2:45:ARG:HD2	1.76	0.65
1:H:135:TYR:CE1	1:H:139:MET:CG	2.79	0.65
1:B:71:GLU:HB2	1:B:74:LYS:CE	2.25	0.65
1:A:11:THR:HA	1:B:140:ALA:HA	1.76	0.65
1:J:139:MET:HA	1:J:139:MET:HE2	1.78	0.65
1:C:91:THR:CG2	1:C:91:THR:O	2.45	0.65
1:Q:135:TYR:CE1	1:Q:139:MET:CG	2.80	0.65
1:S:91:THR:CG2	1:S:91:THR:O	2.45	0.65
1:Q:139:MET:HA	1:Q:139:MET:HE2	1.77	0.65
1:F:116:ALA:O	1:F:120:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:THR:O	1:I:91:THR:CG2	2.45	0.64
2:1:56:LEU:HD21	2:1:63:MET:SD	2.38	0.64
1:C:128:TYR:HB2	1:C:136:LEU:HD11	1.78	0.64
1:A:91:THR:CG2	1:A:91:THR:O	2.45	0.64
1:S:3:LYS:NZ	1:S:3:LYS:HB2	2.12	0.64
1:J:91:THR:O	1:J:91:THR:CG2	2.46	0.64
1:D:30:PRO:HB2	1:D:31:ASN:OD1	1.97	0.64
1:O:91:THR:O	1:O:91:THR:CG2	2.45	0.64
1:M:47:VAL:CG2	1:Q:88:GLN:HB3	2.25	0.64
2:V:56:LEU:HD21	2:V:63:MET:SD	2.38	0.64
1:D:91:THR:CG2	1:D:91:THR:O	2.46	0.64
1:E:3:LYS:HG2	1:E:130:LEU:HG	1.77	0.64
1:H:91:THR:CG2	1:H:91:THR:O	2.45	0.64
1:O:47:VAL:CG2	1:S:88:GLN:HB3	2.24	0.64
1:A:139:MET:O	1:A:142:LYS:CB	2.46	0.63
1:A:5:VAL:CG2	1:A:32:ILE:HD11	2.28	0.63
1:E:91:THR:O	1:E:91:THR:CG2	2.45	0.63
1:G:91:THR:CG2	1:G:91:THR:O	2.46	0.63
1:M:133:PRO:CD	1:M:134:GLU:H	2.11	0.63
1:B:91:THR:O	1:B:91:THR:CG2	2.46	0.63
1:I:139:MET:N	1:I:139:MET:HE3	2.13	0.63
1:K:139:MET:HB2	1:S:11:THR:CG2	2.28	0.63
1:Q:91:THR:CG2	1:Q:91:THR:O	2.46	0.63
1:K:91:THR:O	1:K:91:THR:CG2	2.46	0.62
1:Q:135:TYR:CE1	1:Q:139:MET:HG3	2.34	0.62
1:F:91:THR:CG2	1:F:93:LYS:HD2	2.29	0.62
2:P:45:ARG:O	2:P:45:ARG:HD3	1.99	0.62
1:M:91:THR:CG2	1:M:91:THR:O	2.46	0.62
1:A:139:MET:HE2	1:A:139:MET:HA	1.81	0.62
1:J:71:GLU:O	1:J:74:LYS:HE2	2.00	0.62
1:D:31:ASN:OD1	1:D:31:ASN:N	2.34	0.61
1:K:11:THR:CA	1:M:139:MET:O	2.47	0.61
1:M:38:THR:CB	1:Q:137:THR:HA	2.30	0.61
1:M:13:ALA:O	1:Q:141:GLY:HA2	2.00	0.61
2:R:45:ARG:HG3	2:R:46:SER:N	2.15	0.61
1:D:138:ARG:C	1:D:139:MET:HE3	2.20	0.61
1:M:142:LYS:HG2	1:M:142:LYS:O	2.00	0.61
1:G:71:GLU:O	1:G:74:LYS:HE2	2.01	0.61
1:M:71:GLU:O	1:M:74:LYS:HE2	2.01	0.61
1:I:71:GLU:O	1:I:74:LYS:HE2	2.01	0.61
2:3:106:ASP:N	2:3:106:ASP:OD1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:O	1:A:74:LYS:HE2	2.01	0.61
1:K:22:ILE:HD11	1:K:36:ARG:HD2	1.83	0.61
1:A:10:THR:O	1:B:140:ALA:HA	2.00	0.61
1:D:71:GLU:O	1:D:74:LYS:HE2	2.01	0.61
1:C:22:ILE:HD11	1:C:36:ARG:HD2	1.83	0.61
1:C:71:GLU:O	1:C:74:LYS:HE2	2.01	0.61
1:O:71:GLU:O	1:O:74:LYS:HE2	2.01	0.61
1:D:139:MET:N	1:D:139:MET:HE3	2.15	0.60
1:F:71:GLU:O	1:F:74:LYS:HE2	2.00	0.60
1:O:138:ARG:C	1:O:139:MET:CE	2.69	0.60
1:B:71:GLU:O	1:B:74:LYS:HE2	2.01	0.60
1:K:71:GLU:O	1:K:74:LYS:HE2	2.01	0.60
1:O:22:ILE:HD11	1:O:36:ARG:HD2	1.83	0.60
1:D:22:ILE:HD11	1:D:36:ARG:HD2	1.83	0.60
1:I:22:ILE:HD11	1:I:36:ARG:HD2	1.83	0.60
1:S:22:ILE:HD11	1:S:36:ARG:HD2	1.83	0.60
1:A:91:THR:HG22	1:A:93:LYS:HD2	1.84	0.60
1:E:91:THR:HG22	1:E:93:LYS:HD2	1.84	0.60
1:G:38:THR:CB	1:I:137:THR:HA	2.30	0.60
1:D:3:LYS:HG2	1:D:130:LEU:HG	1.84	0.60
1:G:91:THR:HG22	1:G:93:LYS:HD2	1.84	0.60
1:I:91:THR:HG22	1:I:93:LYS:HD2	1.84	0.60
1:J:138:ARG:HB3	1:J:139:MET:HE3	1.83	0.60
1:J:22:ILE:HD11	1:J:36:ARG:HD2	1.83	0.60
1:M:5:VAL:HG22	1:M:60:ILE:HG22	1.82	0.60
1:F:22:ILE:HD11	1:F:36:ARG:HD2	1.83	0.60
1:M:22:ILE:HD11	1:M:36:ARG:HD2	1.83	0.60
1:Q:71:GLU:O	1:Q:74:LYS:HE2	2.01	0.60
1:Q:91:THR:HG22	1:Q:93:LYS:HD2	1.84	0.60
1:S:71:GLU:O	1:S:74:LYS:HE2	2.00	0.60
1:B:11:THR:CB	1:D:139:MET:O	2.49	0.60
1:H:71:GLU:O	1:H:74:LYS:HE2	2.01	0.60
1:S:91:THR:HG22	1:S:93:LYS:HD2	1.83	0.60
1:J:5:VAL:CG2	1:J:32:ILE:HD11	2.32	0.59
1:E:22:ILE:HD11	1:E:36:ARG:HD2	1.83	0.59
1:G:22:ILE:HD11	1:G:36:ARG:HD2	1.83	0.59
1:H:137:THR:HA	1:I:38:THR:OG1	2.03	0.59
1:M:10:THR:O	1:Q:140:ALA:HB1	2.03	0.59
1:Q:22:ILE:HD11	1:Q:36:ARG:HD2	1.83	0.59
1:M:91:THR:HG22	1:M:93:LYS:HD2	1.84	0.59
2:N:45:ARG:HD3	2:N:46:SER:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:TYR:HB2	1:D:136:LEU:HD11	1.85	0.59
1:F:141:GLY:O	1:J:13:ALA:O	2.20	0.59
1:F:91:THR:CG2	1:F:91:THR:O	2.51	0.59
1:H:133:PRO:CD	1:H:134:GLU:H	2.15	0.59
1:K:91:THR:HG22	1:K:93:LYS:HD2	1.84	0.59
1:E:71:GLU:O	1:E:74:LYS:HE2	2.01	0.59
1:H:13:ALA:O	1:J:141:GLY:O	2.21	0.59
1:O:139:MET:HE2	1:O:139:MET:HA	1.85	0.59
1:H:22:ILE:HD11	1:H:36:ARG:HD2	1.83	0.59
1:H:91:THR:HG22	1:H:93:LYS:HD2	1.84	0.59
1:A:22:ILE:HD11	1:A:36:ARG:HD2	1.83	0.59
1:B:91:THR:HG22	1:B:93:LYS:HD2	1.84	0.59
1:D:91:THR:HG22	1:D:93:LYS:HD2	1.84	0.59
1:A:85:MET:CE	1:E:79:GLU:HB3	2.33	0.58
1:B:22:ILE:HD11	1:B:36:ARG:HD2	1.83	0.58
1:O:27:MET:HA	2:Y:102:ILE:HG21	1.85	0.58
1:F:91:THR:HG22	1:F:93:LYS:HD2	1.85	0.58
1:E:91:THR:CG2	1:E:93:LYS:HD2	2.34	0.58
1:J:91:THR:HG22	1:J:93:LYS:HD2	1.84	0.58
1:O:38:THR:OG1	1:S:137:THR:HA	2.04	0.58
1:Q:139:MET:O	1:Q:142:LYS:CB	2.52	0.58
1:K:38:THR:CB	1:M:137:THR:HA	2.34	0.58
1:B:91:THR:CG2	1:B:93:LYS:HD2	2.33	0.58
1:E:138:ARG:C	1:E:139:MET:HE3	2.23	0.58
1:I:135:TYR:HE1	1:I:139:MET:HG3	1.68	0.58
1:K:79:GLU:OE1	1:M:81:SER:HB3	2.04	0.58
1:O:91:THR:HG22	1:O:93:LYS:HD2	1.84	0.58
1:Q:29:SER:HB3	1:Q:30:PRO:HD2	1.84	0.58
1:D:133:PRO:HD2	1:D:134:GLU:H	1.69	0.58
1:A:91:THR:CG2	1:A:93:LYS:HD2	2.34	0.58
1:K:91:THR:CG2	1:K:93:LYS:HD2	2.34	0.58
1:I:100:VAL:HG21	1:I:115:ALA:HA	1.86	0.58
1:J:133:PRO:HD2	1:J:134:GLU:H	1.68	0.58
1:J:91:THR:CG2	1:J:93:LYS:HD2	2.34	0.58
1:M:38:THR:HG21	1:Q:140:ALA:HB2	1.86	0.58
1:S:139:MET:HA	1:S:139:MET:CE	2.34	0.58
1:H:11:THR:CG2	1:J:139:MET:HB2	2.34	0.58
1:J:139:MET:CE	1:J:139:MET:HA	2.33	0.58
1:M:91:THR:CG2	1:M:93:LYS:HD2	2.34	0.58
2:4:44:PHE:HE1	2:4:67:ALA:HB1	1.69	0.58
1:A:100:VAL:HG21	1:A:115:ALA:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:VAL:HG21	1:C:115:ALA:HA	1.86	0.58
1:G:91:THR:CG2	1:G:93:LYS:HD2	2.34	0.58
1:M:11:THR:HA	1:Q:140:ALA:CA	2.17	0.58
2:N:45:ARG:CD	2:N:46:SER:HB3	2.34	0.58
1:A:38:THR:OG1	1:B:137:THR:HA	2.04	0.57
1:D:100:VAL:HG21	1:D:115:ALA:HA	1.86	0.57
1:I:91:THR:CG2	1:I:93:LYS:HD2	2.34	0.57
1:S:100:VAL:HG21	1:S:115:ALA:HA	1.87	0.57
1:E:100:VAL:HG21	1:E:115:ALA:HA	1.86	0.57
1:G:100:VAL:HG21	1:G:115:ALA:HA	1.87	0.57
1:Q:139:MET:HA	1:Q:139:MET:CE	2.33	0.57
1:D:91:THR:CG2	1:D:93:LYS:HD2	2.34	0.57
1:A:71:GLU:O	1:A:74:LYS:CG	2.52	0.57
1:B:139:MET:HA	1:B:139:MET:CE	2.33	0.57
1:C:91:THR:HG22	1:C:93:LYS:HD2	1.84	0.57
1:J:100:VAL:HG21	1:J:115:ALA:HA	1.86	0.57
1:D:117:ARG:NE	1:D:121:GLU:OE2	2.35	0.57
1:C:11:THR:HG22	1:E:139:MET:HB2	1.85	0.57
1:F:137:THR:O	1:F:140:ALA:HB2	2.05	0.57
1:O:91:THR:CG2	1:O:93:LYS:HD2	2.35	0.57
1:M:5:VAL:HG22	1:M:60:ILE:CG2	2.35	0.57
1:H:100:VAL:HG21	1:H:115:ALA:HA	1.86	0.57
1:H:11:THR:HG22	1:J:139:MET:HB2	1.87	0.57
1:C:91:THR:CG2	1:C:93:LYS:HD2	2.35	0.56
1:H:91:THR:CG2	1:H:93:LYS:HD2	2.34	0.56
1:Q:100:VAL:HG21	1:Q:115:ALA:HA	1.86	0.56
1:S:91:THR:CG2	1:S:93:LYS:HD2	2.35	0.56
1:E:3:LYS:CG	1:E:130:LEU:HG	2.35	0.56
1:F:100:VAL:HG21	1:F:115:ALA:HA	1.86	0.56
1:M:11:THR:CA	1:Q:140:ALA:HA	2.17	0.56
2:Y:45:ARG:HG3	2:Y:46:SER:N	2.20	0.56
1:Q:91:THR:CG2	1:Q:93:LYS:HD2	2.35	0.56
1:B:71:GLU:O	1:B:74:LYS:CG	2.52	0.56
1:E:71:GLU:O	1:E:74:LYS:CG	2.52	0.56
1:H:133:PRO:HD2	1:H:134:GLU:H	1.70	0.56
1:M:100:VAL:HG21	1:M:115:ALA:HA	1.86	0.56
1:O:100:VAL:HG21	1:O:115:ALA:HA	1.86	0.56
2:V:46:SER:OG	2:V:48:ALA:HB3	2.05	0.56
1:B:100:VAL:HG21	1:B:115:ALA:HA	1.86	0.56
1:D:127:TYR:OH	1:D:132:LYS:HE2	2.06	0.56
1:B:132:LYS:HE3	1:B:134:GLU:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:48:ALA:O	2:P:49:ALA:C	2.44	0.56
1:S:135:TYR:CE1	1:S:139:MET:HG3	2.39	0.56
1:C:71:GLU:O	1:C:74:LYS:CG	2.52	0.55
1:K:100:VAL:HG21	1:K:115:ALA:HA	1.86	0.55
2:3:192:GLU:O	2:3:196:ILE:HG13	2.07	0.55
1:J:133:PRO:CD	1:J:134:GLU:H	2.20	0.55
2:N:45:ARG:HH11	2:N:46:SER:HB2	1.71	0.55
1:Q:71:GLU:O	1:Q:74:LYS:CG	2.52	0.55
1:C:139:MET:CA	1:C:139:MET:HE2	2.34	0.55
2:W:5:ASN:N	2:W:5:ASN:OD1	2.39	0.55
2:P:122:GLU:OE2	2:T:95:ASN:ND2	2.30	0.55
1:H:38:THR:CB	1:J:137:THR:HA	2.36	0.55
2:N:45:ARG:HH11	2:N:46:SER:HB3	1.72	0.55
1:O:71:GLU:O	1:O:74:LYS:CG	2.52	0.55
1:B:13:ALA:O	1:D:141:GLY:HA2	2.06	0.55
1:D:71:GLU:O	1:D:74:LYS:CG	2.52	0.55
1:K:71:GLU:O	1:K:74:LYS:CG	2.52	0.55
1:Q:5:VAL:CG2	1:Q:32:ILE:HD11	2.31	0.55
1:F:139:MET:CA	1:F:139:MET:CE	2.85	0.55
1:B:139:MET:CE	1:B:139:MET:CA	2.85	0.55
1:Q:128:TYR:CB	1:Q:136:LEU:HD11	2.36	0.55
2:L:38:PRO:C	2:L:63:MET:HG3	2.27	0.55
1:I:139:MET:HA	1:I:139:MET:CE	2.38	0.54
1:S:139:MET:CA	1:S:139:MET:CE	2.85	0.54
1:G:5:VAL:CG2	1:G:32:ILE:HD11	2.37	0.54
1:B:2:THR:O	1:B:3:LYS:HE2	2.07	0.54
1:C:137:THR:HA	1:D:38:THR:CB	2.37	0.54
2:N:45:ARG:NH1	2:N:46:SER:HB2	2.22	0.54
1:S:71:GLU:O	1:S:74:LYS:CG	2.52	0.54
1:O:133:PRO:CD	1:O:134:GLU:H	2.20	0.54
1:Q:135:TYR:HE1	1:Q:139:MET:CG	2.15	0.54
2:R:122:GLU:CD	2:3:95:ASN:HD22	2.10	0.54
1:D:139:MET:HA	1:D:139:MET:CE	2.38	0.54
1:E:132:LYS:HE3	1:E:134:GLU:HB2	1.90	0.54
1:B:139:MET:CA	1:B:139:MET:HE2	2.36	0.54
1:F:10:THR:HA	1:F:39:VAL:O	2.08	0.54
1:H:10:THR:HA	1:H:39:VAL:O	2.08	0.54
1:O:139:MET:CE	1:O:139:MET:HA	2.36	0.54
1:C:10:THR:HA	1:C:39:VAL:O	2.08	0.54
1:H:139:MET:CA	1:H:139:MET:CE	2.85	0.54
1:K:139:MET:HE2	1:K:139:MET:CA	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:138:ARG:C	1:S:139:MET:HE3	2.28	0.54
1:D:133:PRO:CD	1:D:134:GLU:H	2.21	0.54
1:F:71:GLU:O	1:F:74:LYS:CG	2.52	0.54
1:G:10:THR:HA	1:G:39:VAL:O	2.08	0.54
1:H:133:PRO:HG2	1:H:134:GLU:HG2	1.90	0.54
1:I:10:THR:HA	1:I:39:VAL:O	2.08	0.54
1:O:79:GLU:HB3	1:S:85:MET:CE	2.38	0.54
1:M:10:THR:O	1:Q:140:ALA:CB	2.56	0.54
1:F:11:THR:HA	1:G:139:MET:O	2.08	0.54
1:S:10:THR:HA	1:S:39:VAL:O	2.08	0.54
1:D:139:MET:CA	1:D:139:MET:CE	2.85	0.54
1:I:139:MET:CA	1:I:139:MET:CE	2.85	0.54
1:O:139:MET:CE	1:O:139:MET:CA	2.86	0.54
2:1:45:ARG:CG	2:1:46:SER:N	2.71	0.53
1:J:27:MET:HA	2:T:102:ILE:HG21	1.90	0.53
1:J:71:GLU:O	1:J:74:LYS:CG	2.52	0.53
1:M:139:MET:HA	1:M:139:MET:CE	2.37	0.53
1:Q:139:MET:CA	1:Q:139:MET:CE	2.85	0.53
2:R:3:THR:O	2:R:7:GLN:HG3	2.08	0.53
2:Z:45:ARG:HG3	2:Z:46:SER:N	2.23	0.53
1:C:139:MET:CA	1:C:139:MET:CE	2.85	0.53
1:C:11:THR:CG2	1:E:139:MET:HB2	2.38	0.53
1:J:10:THR:HA	1:J:39:VAL:O	2.08	0.53
1:I:135:TYR:HA	1:I:138:ARG:HD3	1.90	0.53
1:J:139:MET:CA	1:J:139:MET:CE	2.86	0.53
1:K:10:THR:HA	1:K:39:VAL:O	2.08	0.53
1:A:38:THR:CB	1:B:137:THR:HA	2.38	0.53
1:A:10:THR:HA	1:A:39:VAL:O	2.08	0.53
1:B:10:THR:HA	1:B:39:VAL:O	2.08	0.53
2:N:49:ALA:O	2:N:52:ALA:N	2.41	0.53
1:O:10:THR:HA	1:O:39:VAL:O	2.08	0.53
2:R:45:ARG:CG	2:R:46:SER:N	2.72	0.53
1:D:10:THR:HA	1:D:39:VAL:O	2.08	0.53
1:E:100:VAL:HG22	1:E:118:ARG:HH21	1.73	0.53
1:H:71:GLU:O	1:H:74:LYS:CG	2.52	0.53
2:P:122:GLU:CD	2:T:95:ASN:HD22	2.09	0.53
1:E:139:MET:CE	1:E:139:MET:CA	2.86	0.53
1:E:10:THR:HA	1:E:39:VAL:O	2.08	0.53
1:I:135:TYR:CE1	1:I:139:MET:HG3	2.44	0.53
1:C:139:MET:N	1:C:139:MET:HE3	2.24	0.53
1:M:139:MET:CA	1:M:139:MET:CE	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:VAL:HB	1:H:66:MET:HE1	1.90	0.53
1:O:5:VAL:HG23	1:O:32:ILE:HD11	1.89	0.53
1:B:135:TYR:HD1	1:B:135:TYR:O	1.92	0.53
1:A:139:MET:CE	1:A:139:MET:HA	2.40	0.52
1:B:139:MET:N	1:B:139:MET:HE3	2.24	0.52
1:D:139:MET:N	1:D:139:MET:CE	2.73	0.52
1:Q:139:MET:N	1:Q:139:MET:CE	2.73	0.52
1:Q:10:THR:HA	1:Q:39:VAL:O	2.08	0.52
1:C:139:MET:CE	1:C:139:MET:N	2.72	0.52
1:K:139:MET:CE	1:K:139:MET:N	2.72	0.52
1:K:50:LYS:HZ3	1:M:92:ASN:HD21	1.54	0.52
2:R:122:GLU:OE2	2:3:95:ASN:ND2	2.31	0.52
1:A:3:LYS:O	1:A:32:ILE:HG13	2.10	0.52
1:B:139:MET:N	1:B:139:MET:CE	2.73	0.52
1:H:27:MET:HA	2:W:102:ILE:HG21	1.90	0.52
1:M:4:LYS:HG2	1:M:33:LYS:HB2	1.92	0.52
1:M:71:GLU:O	1:M:74:LYS:CG	2.52	0.52
1:O:15:VAL:H	1:O:66:MET:HE1	1.74	0.52
1:B:11:THR:HG22	1:D:139:MET:O	2.09	0.52
1:F:79:GLU:HB3	1:G:85:MET:CE	2.40	0.52
2:P:98:ARG:O	2:P:101:GLN:N	2.43	0.52
2:V:49:ALA:O	2:V:50:VAL:C	2.48	0.52
1:O:21:ALA:O	1:O:22:ILE:C	2.47	0.52
1:S:139:MET:N	1:S:139:MET:CE	2.73	0.52
1:S:3:LYS:NZ	1:S:3:LYS:CB	2.73	0.52
1:B:3:LYS:HE2	1:B:3:LYS:HA	1.92	0.51
1:O:139:MET:CE	1:O:139:MET:N	2.73	0.51
1:C:139:MET:HA	1:C:139:MET:CE	2.36	0.51
1:J:32:ILE:HG23	1:J:32:ILE:O	2.09	0.51
1:M:133:PRO:CD	1:M:134:GLU:N	2.73	0.51
2:T:45:ARG:CG	2:T:46:SER:N	2.72	0.51
1:C:79:GLU:HB3	1:E:85:MET:CE	2.40	0.51
1:F:135:TYR:CD1	1:F:135:TYR:C	2.83	0.51
1:J:139:MET:N	1:J:139:MET:CE	2.73	0.51
1:A:139:MET:N	1:A:139:MET:CE	2.73	0.51
1:G:135:TYR:CD1	1:G:135:TYR:C	2.84	0.51
1:O:4:LYS:NZ	1:O:4:LYS:CB	2.73	0.51
2:3:3:THR:HG22	2:3:7:GLN:NE2	2.26	0.51
1:E:132:LYS:HG3	1:E:135:TYR:HB2	1.93	0.51
1:M:10:THR:HA	1:M:39:VAL:O	2.08	0.51
1:S:24:THR:OG1	1:S:120:ILE:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:15:VAL:HB	1:Q:66:MET:HE1	1.92	0.51
1:B:128:TYR:HB2	1:B:136:LEU:HD11	1.92	0.51
1:G:71:GLU:O	1:G:74:LYS:CG	2.52	0.51
1:Q:133:PRO:CD	1:Q:134:GLU:H	2.23	0.51
1:M:139:MET:N	1:M:139:MET:CE	2.73	0.51
1:M:38:THR:OG1	1:Q:137:THR:HA	2.11	0.51
2:4:18:ALA:CB	2:4:45:ARG:HD2	2.27	0.51
1:A:139:MET:HB2	1:E:11:THR:CG2	2.41	0.51
1:H:135:TYR:CD1	1:H:135:TYR:C	2.85	0.51
1:G:79:GLU:HB3	1:I:85:MET:CE	2.41	0.51
1:J:15:VAL:HB	1:J:66:MET:HE1	1.93	0.51
2:P:98:ARG:O	2:P:99:ALA:C	2.49	0.51
1:K:27:MET:HA	2:U:102:ILE:HG21	1.92	0.51
1:M:135:TYR:C	1:M:135:TYR:CD1	2.84	0.51
1:Q:133:PRO:HD2	1:Q:134:GLU:H	1.76	0.51
1:O:3:LYS:O	1:O:32:ILE:HG13	2.11	0.50
1:C:137:THR:HA	1:D:38:THR:OG1	2.12	0.50
1:F:38:THR:CB	1:G:137:THR:HA	2.41	0.50
1:I:139:MET:N	1:I:139:MET:CE	2.73	0.50
1:K:135:TYR:CD1	1:K:135:TYR:C	2.85	0.50
2:L:3:THR:HG22	2:L:7:GLN:NE2	2.26	0.50
1:A:142:LYS:O	1:E:11:THR:O	2.30	0.50
1:H:141:GLY:CA	1:I:13:ALA:O	2.59	0.50
1:I:71:GLU:O	1:I:74:LYS:CG	2.52	0.50
1:M:132:LYS:HG3	1:M:135:TYR:HB2	1.93	0.50
1:O:133:PRO:HG2	1:O:134:GLU:HG2	1.93	0.50
2:1:45:ARG:HG3	2:1:46:SER:N	2.26	0.50
1:A:135:TYR:CD1	1:A:135:TYR:C	2.85	0.50
1:I:135:TYR:CD1	1:I:135:TYR:C	2.84	0.50
1:G:128:TYR:HB3	1:G:136:LEU:HG	1.94	0.50
2:L:17:ILE:HD12	2:L:40:ALA:HB1	1.94	0.50
1:A:27:MET:HA	2:N:102:ILE:HG21	1.92	0.50
1:D:135:TYR:CD1	1:D:135:TYR:C	2.84	0.50
1:F:15:VAL:HB	1:F:66:MET:HE1	1.94	0.50
1:O:135:TYR:CD1	1:O:135:TYR:C	2.84	0.50
1:J:135:TYR:O	1:J:135:TYR:HD1	1.95	0.50
1:Q:135:TYR:C	1:Q:135:TYR:CD1	2.84	0.50
1:K:11:THR:CB	1:M:139:MET:O	2.60	0.50
1:G:15:VAL:HB	1:G:66:MET:HE1	1.94	0.50
1:M:79:GLU:HB3	1:Q:85:MET:CE	2.41	0.50
2:R:17:ILE:HD12	2:R:40:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:135:TYR:C	1:S:135:TYR:CD1	2.84	0.50
2:V:17:ILE:HD12	2:V:40:ALA:HB1	1.94	0.50
2:W:17:ILE:HD12	2:W:40:ALA:HB1	1.94	0.50
1:K:139:MET:CE	1:K:139:MET:CA	2.90	0.49
2:N:17:ILE:HD12	2:N:40:ALA:HB1	1.94	0.49
1:O:133:PRO:HD2	1:O:134:GLU:H	1.77	0.49
1:E:15:VAL:HB	1:E:66:MET:HE1	1.94	0.49
1:J:135:TYR:C	1:J:135:TYR:CD1	2.86	0.49
2:P:17:ILE:HD12	2:P:40:ALA:HB1	1.94	0.49
2:4:17:ILE:HD12	2:4:40:ALA:HB1	1.94	0.49
1:A:3:LYS:HG2	1:A:130:LEU:HG	1.94	0.49
1:S:135:TYR:CE1	1:S:139:MET:CG	2.95	0.49
2:Z:17:ILE:HD12	2:Z:40:ALA:HB1	1.94	0.49
1:A:139:MET:N	1:A:139:MET:HE3	2.27	0.49
2:N:3:THR:HG22	2:N:7:GLN:NE2	2.26	0.49
1:C:135:TYR:C	1:C:135:TYR:CD1	2.85	0.49
1:F:138:ARG:C	1:F:140:ALA:H	2.16	0.49
1:C:132:LYS:HE3	1:C:134:GLU:HB2	1.95	0.49
2:N:49:ALA:O	2:N:50:VAL:C	2.51	0.49
2:X:17:ILE:HD12	2:X:40:ALA:HB1	1.94	0.49
1:D:138:ARG:C	1:D:139:MET:CE	2.81	0.49
1:S:3:LYS:HG2	1:S:130:LEU:CG	2.42	0.49
2:Z:45:ARG:HD3	2:Z:46:SER:HB2	1.93	0.49
1:S:138:ARG:HB3	1:S:139:MET:HE3	1.94	0.49
1:D:127:TYR:HD2	1:D:128:TYR:CD1	2.30	0.49
1:A:141:GLY:C	1:E:13:ALA:O	2.52	0.49
1:K:15:VAL:HB	1:K:66:MET:HE1	1.94	0.49
2:T:4:ILE:CD1	2:T:106:ASP:OD2	2.51	0.49
2:Z:48:ALA:O	2:Z:49:ALA:C	2.51	0.49
1:A:15:VAL:HB	1:A:66:MET:HE1	1.95	0.48
1:O:133:PRO:CG	1:O:134:GLU:N	2.76	0.48
2:R:182:MET:O	2:R:196:ILE:HG23	2.12	0.48
2:2:3:THR:HG22	2:2:7:GLN:NE2	2.26	0.48
1:A:139:MET:CA	1:A:139:MET:CE	2.91	0.48
1:J:71:GLU:CB	1:J:74:LYS:HE2	2.41	0.48
1:D:128:TYR:CB	1:D:136:LEU:HD11	2.44	0.48
1:M:6:GLY:HA3	1:M:52:LEU:HD23	1.95	0.48
2:U:17:ILE:HD12	2:U:40:ALA:HB1	1.94	0.48
2:1:17:ILE:HD12	2:1:40:ALA:HB1	1.94	0.48
1:B:128:TYR:CB	1:B:136:LEU:HD11	2.43	0.48
2:Z:3:THR:HG22	2:Z:7:GLN:NE2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PRO:HG2	1:B:134:GLU:N	2.29	0.48
2:T:17:ILE:HD12	2:T:40:ALA:HB1	1.94	0.48
1:A:132:LYS:HE3	1:A:134:GLU:HB2	1.94	0.48
1:M:38:THR:CG2	1:Q:140:ALA:HB2	2.43	0.48
1:O:79:GLU:HB3	1:S:85:MET:HE1	1.95	0.48
2:1:70:ILE:HG13	2:1:87:VAL:HB	1.96	0.48
2:2:17:ILE:HD12	2:2:40:ALA:HB1	1.94	0.48
1:A:79:GLU:HB3	1:B:85:MET:CE	2.43	0.48
1:I:15:VAL:HB	1:I:66:MET:HE1	1.96	0.48
1:D:139:MET:CA	1:D:139:MET:HE2	2.43	0.48
1:E:32:ILE:O	1:E:32:ILE:HG23	2.13	0.48
1:F:11:THR:HA	1:G:140:ALA:HA	1.96	0.48
1:S:15:VAL:HB	1:S:66:MET:HE1	1.94	0.48
2:T:70:ILE:HG13	2:T:87:VAL:HB	1.96	0.48
2:U:7:GLN:OE1	2:U:64:LEU:HD13	2.13	0.48
2:V:45:ARG:CG	2:V:46:SER:N	2.76	0.48
2:Y:17:ILE:HD12	2:Y:40:ALA:HB1	1.94	0.48
2:4:44:PHE:CE1	2:4:67:ALA:HB1	2.49	0.48
1:K:139:MET:HE3	1:K:139:MET:N	2.29	0.48
1:M:15:VAL:HB	1:M:66:MET:HE1	1.95	0.48
1:H:133:PRO:CG	1:H:134:GLU:N	2.77	0.48
2:3:70:ILE:HG13	2:3:87:VAL:HB	1.96	0.47
1:E:3:LYS:HG2	1:E:130:LEU:CG	2.43	0.47
2:L:70:ILE:HG13	2:L:87:VAL:HB	1.96	0.47
2:R:70:ILE:HG13	2:R:87:VAL:HB	1.96	0.47
2:X:111:VAL:HG12	2:X:116:THR:HG22	1.96	0.47
2:Y:70:ILE:HG13	2:Y:87:VAL:HB	1.96	0.47
1:C:15:VAL:HB	1:C:66:MET:HE1	1.95	0.47
1:I:71:GLU:CB	1:I:74:LYS:HE2	2.42	0.47
2:V:70:ILE:HG13	2:V:87:VAL:HB	1.96	0.47
2:Z:70:ILE:HG13	2:Z:87:VAL:HB	1.96	0.47
2:4:70:ILE:HG13	2:4:87:VAL:HB	1.96	0.47
1:B:135:TYR:CD1	1:B:135:TYR:C	2.85	0.47
1:E:139:MET:HE3	1:E:139:MET:N	2.29	0.47
2:X:70:ILE:HG13	2:X:87:VAL:HB	1.96	0.47
2:Z:45:ARG:HG3	2:Z:46:SER:H	1.78	0.47
2:3:17:ILE:HD12	2:3:40:ALA:HB1	1.94	0.47
1:C:138:ARG:C	1:C:140:ALA:H	2.17	0.47
1:G:6:GLY:HA3	1:G:52:LEU:HD23	1.97	0.47
1:H:71:GLU:CB	1:H:74:LYS:HE2	2.42	0.47
2:U:111:VAL:HG12	2:U:116:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:70:ILE:HG13	2:W:87:VAL:HB	1.96	0.47
2:1:111:VAL:HG12	2:1:116:THR:HG22	1.97	0.47
2:2:111:VAL:HG12	2:2:116:THR:HG22	1.96	0.47
1:B:133:PRO:CG	1:B:134:GLU:N	2.77	0.47
1:B:71:GLU:CB	1:B:74:LYS:HE2	2.42	0.47
1:K:38:THR:OG1	1:M:137:THR:HA	2.14	0.47
2:R:111:VAL:HG12	2:R:116:THR:HG22	1.96	0.47
2:4:3:THR:HG22	2:4:7:GLN:NE2	2.26	0.47
1:A:11:THR:CG2	1:B:139:MET:HB2	2.45	0.47
1:G:136:LEU:HD23	1:G:136:LEU:HA	1.73	0.47
1:J:132:LYS:HG3	1:J:135:TYR:HB2	1.96	0.47
2:P:70:ILE:HG13	2:P:87:VAL:HB	1.96	0.47
2:U:70:ILE:HG13	2:U:87:VAL:HB	1.96	0.47
1:F:28:GLU:HA	1:F:28:GLU:OE1	2.15	0.47
1:H:132:LYS:HE3	1:H:134:GLU:HB2	1.95	0.47
1:M:3:LYS:O	1:M:32:ILE:HG13	2.15	0.47
1:M:5:VAL:HG13	1:M:60:ILE:HG23	1.97	0.47
2:N:111:VAL:HG12	2:N:116:THR:HG22	1.96	0.47
1:O:4:LYS:NZ	1:O:4:LYS:HB3	2.30	0.47
1:Q:2:THR:C	1:Q:3:LYS:HD2	2.35	0.47
1:S:71:GLU:CB	1:S:74:LYS:HE2	2.41	0.47
2:V:3:THR:HG22	2:V:7:GLN:NE2	2.26	0.47
2:Y:45:ARG:CG	2:Y:46:SER:N	2.77	0.47
2:Z:111:VAL:HG12	2:Z:116:THR:HG22	1.96	0.47
1:D:5:VAL:HG23	1:D:32:ILE:HD11	1.96	0.47
1:E:71:GLU:CB	1:E:74:LYS:HE2	2.42	0.47
1:J:6:GLY:HA3	1:J:52:LEU:HD23	1.97	0.47
1:K:71:GLU:CB	1:K:74:LYS:HE2	2.42	0.47
1:M:71:GLU:CB	1:M:74:LYS:HE2	2.41	0.47
2:P:111:VAL:HG12	2:P:116:THR:HG22	1.97	0.47
1:E:118:ARG:HG2	1:E:118:ARG:NH2	2.29	0.47
1:E:3:LYS:HG2	1:E:130:LEU:CD2	2.45	0.47
1:M:33:LYS:O	1:M:34:ILE:HD13	2.15	0.47
2:V:111:VAL:HG12	2:V:116:THR:HG22	1.96	0.47
2:3:111:VAL:HG12	2:3:116:THR:HG22	1.97	0.47
1:B:15:VAL:HB	1:B:66:MET:HE1	1.97	0.47
1:B:79:GLU:HB3	1:D:85:MET:CE	2.45	0.47
1:E:100:VAL:HG22	1:E:118:ARG:NH2	2.29	0.47
2:4:111:VAL:HG12	2:4:116:THR:HG22	1.96	0.47
1:C:71:GLU:CB	1:C:74:LYS:HE2	2.42	0.47
1:F:85:MET:CE	1:J:79:GLU:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:GLY:HA3	1:K:52:LEU:HD23	1.97	0.47
1:C:128:TYR:HB3	1:C:136:LEU:HD11	1.96	0.46
1:H:140:ALA:HA	1:I:10:THR:O	2.15	0.46
1:M:138:ARG:C	1:M:139:MET:CE	2.81	0.46
2:N:45:ARG:C	2:N:45:ARG:HD3	2.34	0.46
2:V:49:ALA:O	2:V:52:ALA:N	2.49	0.46
2:Y:3:THR:HG22	2:Y:7:GLN:NE2	2.26	0.46
1:B:133:PRO:CD	1:B:134:GLU:H	2.29	0.46
1:B:15:VAL:H	1:B:66:MET:HE1	1.81	0.46
1:E:6:GLY:HA3	1:E:52:LEU:HD23	1.97	0.46
1:H:133:PRO:CD	1:H:134:GLU:N	2.78	0.46
1:O:11:THR:O	1:S:142:LYS:O	2.34	0.46
2:W:48:ALA:O	2:W:49:ALA:C	2.53	0.46
2:2:70:ILE:HG13	2:2:87:VAL:HB	1.96	0.46
1:E:138:ARG:O	1:E:139:MET:HE2	2.15	0.46
2:L:111:VAL:HG12	2:L:116:THR:HG22	1.96	0.46
1:O:71:GLU:CB	1:O:74:LYS:HE2	2.41	0.46
1:A:71:GLU:CB	1:A:74:LYS:HE2	2.41	0.46
1:B:135:TYR:HD1	1:B:135:TYR:C	2.19	0.46
1:C:6:GLY:HA3	1:C:52:LEU:HD23	1.97	0.46
1:O:32:ILE:O	1:O:32:ILE:HG23	2.15	0.46
2:T:111:VAL:HG12	2:T:116:THR:HG22	1.96	0.46
1:F:128:TYR:HB3	1:F:136:LEU:HG	1.96	0.46
1:O:142:LYS:O	1:O:142:LYS:HG2	2.14	0.46
1:Q:6:GLY:HA3	1:Q:52:LEU:HD23	1.97	0.46
1:S:6:GLY:HA3	1:S:52:LEU:HD23	1.98	0.46
1:F:6:GLY:HA3	1:F:52:LEU:HD23	1.97	0.46
1:O:6:GLY:HA3	1:O:52:LEU:HD23	1.97	0.46
1:A:135:TYR:CD1	1:A:135:TYR:O	2.69	0.46
1:A:139:MET:HB2	1:E:11:THR:HG22	1.98	0.46
1:C:15:VAL:H	1:C:66:MET:HE1	1.81	0.46
1:H:85:MET:CE	1:I:79:GLU:HB3	2.45	0.46
1:Q:71:GLU:CB	1:Q:74:LYS:HE2	2.42	0.46
2:W:111:VAL:HG12	2:W:116:THR:HG22	1.97	0.46
2:Y:111:VAL:HG12	2:Y:116:THR:HG22	1.97	0.46
1:D:15:VAL:H	1:D:66:MET:HE1	1.80	0.46
1:H:6:GLY:HA3	1:H:52:LEU:HD23	1.97	0.46
1:H:38:THR:OG1	1:J:137:THR:HA	2.15	0.46
2:N:70:ILE:HG13	2:N:87:VAL:HB	1.96	0.46
2:Z:45:ARG:CG	2:Z:46:SER:N	2.78	0.46
1:A:137:THR:HA	1:E:38:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ARG:O	1:D:121:GLU:HG2	2.16	0.46
1:H:10:THR:O	1:J:140:ALA:HA	2.16	0.46
1:M:15:VAL:H	1:M:66:MET:HE1	1.81	0.46
2:4:94:PRO:O	2:4:98:ARG:HG3	2.16	0.46
1:I:132:LYS:HA	1:I:132:LYS:HD2	1.74	0.46
2:1:3:THR:O	2:1:7:GLN:HG3	2.17	0.45
1:B:6:GLY:HA3	1:B:52:LEU:HD23	1.97	0.45
1:I:134:GLU:O	1:I:138:ARG:HG3	2.16	0.45
2:U:3:THR:HG22	2:U:7:GLN:NE2	2.30	0.45
1:C:5:VAL:HG22	1:C:60:ILE:HG22	1.98	0.45
1:I:138:ARG:C	1:I:139:MET:HE3	2.36	0.45
1:M:4:LYS:HA	1:M:33:LYS:O	2.17	0.45
1:O:5:VAL:CG2	1:O:32:ILE:HD11	2.46	0.45
2:U:6:ASN:N	2:U:6:ASN:OD1	2.49	0.45
1:D:15:VAL:HB	1:D:66:MET:HE1	1.98	0.45
1:I:6:GLY:HA3	1:I:52:LEU:HD23	1.97	0.45
1:K:11:THR:HB	1:M:139:MET:O	2.17	0.45
1:C:128:TYR:HB3	1:C:136:LEU:HG	1.98	0.45
1:D:71:GLU:CB	1:D:74:LYS:HE2	2.42	0.45
1:I:15:VAL:H	1:I:66:MET:HE1	1.81	0.45
1:J:135:TYR:O	1:J:135:TYR:CD1	2.70	0.45
1:O:132:LYS:HA	1:O:132:LYS:HD2	1.74	0.45
2:V:94:PRO:O	2:V:98:ARG:HG3	2.15	0.45
2:3:195:GLU:HA	2:3:195:GLU:OE1	2.17	0.45
1:A:6:GLY:HA3	1:A:52:LEU:HD23	1.97	0.45
1:G:125:ASN:HA	1:G:125:ASN:HD22	1.62	0.45
1:Q:71:GLU:HA	1:Q:74:LYS:HD3	1.99	0.45
1:H:132:LYS:HA	1:H:132:LYS:HD2	1.75	0.45
1:O:138:ARG:O	1:O:139:MET:HE2	2.17	0.45
1:E:15:VAL:H	1:E:66:MET:HE1	1.82	0.45
1:H:4:LYS:CD	1:H:57:GLY:O	2.62	0.45
1:E:138:ARG:C	1:E:139:MET:CE	2.85	0.45
1:A:137:THR:HA	1:E:38:THR:CB	2.46	0.45
1:I:135:TYR:CE1	1:I:139:MET:CG	3.00	0.45
1:O:135:TYR:O	1:O:135:TYR:CD1	2.70	0.45
1:Q:135:TYR:O	1:Q:135:TYR:CD1	2.70	0.45
1:D:6:GLY:HA3	1:D:52:LEU:HD23	1.97	0.45
1:M:10:THR:O	1:Q:140:ALA:HA	2.17	0.45
1:E:132:LYS:HD2	1:E:132:LYS:HA	1.69	0.44
1:H:125:ASN:HA	1:H:125:ASN:HD22	1.62	0.44
1:J:3:LYS:O	1:J:32:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:50:VAL:O	2:P:51:LYS:C	2.54	0.44
1:K:137:THR:HA	1:S:38:THR:OG1	2.17	0.44
2:4:45:ARG:HG3	2:4:46:SER:N	2.31	0.44
1:F:135:TYR:CD1	1:F:135:TYR:O	2.70	0.44
1:H:137:THR:HA	1:I:38:THR:CB	2.46	0.44
1:H:79:GLU:HB3	1:J:85:MET:CE	2.47	0.44
1:S:71:GLU:HA	1:S:74:LYS:HD3	2.00	0.44
2:Z:45:ARG:HD3	2:Z:46:SER:CB	2.47	0.44
1:C:135:TYR:HD1	1:C:135:TYR:C	2.21	0.44
1:C:38:THR:OG1	1:E:137:THR:HA	2.16	0.44
1:E:37:LYS:HG3	1:E:52:LEU:HD11	2.00	0.44
2:L:122:GLU:CD	2:R:95:ASN:HD22	2.20	0.44
1:A:37:LYS:HG3	1:A:52:LEU:HD11	2.00	0.44
1:G:135:TYR:CD1	1:G:135:TYR:O	2.70	0.44
1:B:135:TYR:CD1	1:B:135:TYR:O	2.70	0.44
1:B:37:LYS:HG3	1:B:52:LEU:HD11	2.00	0.44
1:F:125:ASN:HA	1:F:125:ASN:HD22	1.62	0.44
1:G:15:VAL:H	1:G:66:MET:HE1	1.82	0.44
1:J:15:VAL:H	1:J:66:MET:HE1	1.82	0.44
1:K:71:GLU:HA	1:K:74:LYS:HD3	2.00	0.44
1:A:71:GLU:HA	1:A:74:LYS:HD3	2.00	0.44
1:K:15:VAL:H	1:K:66:MET:HE1	1.83	0.44
1:M:71:GLU:HA	1:M:74:LYS:HD3	2.00	0.44
1:O:4:LYS:HZ2	1:O:4:LYS:CB	2.31	0.44
1:A:15:VAL:H	1:A:66:MET:HE1	1.81	0.44
1:I:37:LYS:HG3	1:I:52:LEU:HD11	2.00	0.44
1:M:135:TYR:O	1:M:135:TYR:CD1	2.70	0.44
1:D:37:LYS:HG3	1:D:52:LEU:HD11	2.00	0.44
1:F:37:LYS:HG3	1:F:52:LEU:HD11	2.00	0.44
1:O:133:PRO:HG2	1:O:134:GLU:N	2.33	0.44
1:O:85:MET:CE	1:Q:79:GLU:HB3	2.48	0.44
1:S:15:VAL:H	1:S:66:MET:HE1	1.82	0.44
1:E:3:LYS:CE	1:E:3:LYS:HA	2.48	0.44
1:F:71:GLU:HA	1:F:74:LYS:HD3	2.00	0.44
1:I:138:ARG:HB2	1:I:139:MET:HE3	2.00	0.44
1:K:79:GLU:HB3	1:M:85:MET:CE	2.47	0.44
1:H:71:GLU:HA	1:H:74:LYS:HD3	2.00	0.43
1:J:135:TYR:C	1:J:135:TYR:HD1	2.21	0.43
1:C:135:TYR:HD1	1:C:135:TYR:O	2.00	0.43
1:J:125:ASN:HA	1:J:125:ASN:HD22	1.62	0.43
1:C:37:LYS:HG3	1:C:52:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:VAL:H	1:F:66:MET:HE1	1.82	0.43
1:I:125:ASN:HA	1:I:125:ASN:HD22	1.62	0.43
1:O:37:LYS:HG3	1:O:52:LEU:HD11	2.00	0.43
1:S:37:LYS:HG3	1:S:52:LEU:HD11	2.00	0.43
2:X:7:GLN:OE1	2:X:64:LEU:HD13	2.18	0.43
1:A:132:LYS:HD2	1:A:132:LYS:HA	1.75	0.43
1:C:135:TYR:O	1:C:135:TYR:CD1	2.71	0.43
1:G:37:LYS:HG3	1:G:52:LEU:HD11	2.00	0.43
1:I:138:ARG:CB	1:I:139:MET:HE3	2.48	0.43
1:M:37:LYS:HG3	1:M:52:LEU:HD11	1.99	0.43
1:E:71:GLU:HA	1:E:74:LYS:HD3	2.00	0.43
1:G:71:GLU:HA	1:G:74:LYS:HD3	2.00	0.43
1:I:135:TYR:HD1	1:I:135:TYR:C	2.22	0.43
1:K:132:LYS:HD2	1:K:132:LYS:HA	1.75	0.43
1:B:38:THR:CB	1:D:137:THR:HA	2.49	0.43
1:F:24:THR:OG1	1:F:120:ILE:HG23	2.19	0.43
1:O:4:LYS:HE2	1:O:56:GLU:O	2.17	0.43
1:D:71:GLU:HA	1:D:74:LYS:HD3	2.00	0.43
1:C:79:GLU:HB3	1:E:85:MET:HE1	2.00	0.43
1:K:37:LYS:HG3	1:K:52:LEU:HD11	1.99	0.43
1:O:125:ASN:HD22	1:O:125:ASN:HA	1.62	0.43
1:H:15:VAL:CB	1:H:66:MET:HE1	2.48	0.43
1:J:138:ARG:HB3	1:J:139:MET:CE	2.46	0.43
2:R:199:LEU:O	2:R:202:GLU:HG3	2.19	0.43
1:F:120:ILE:HD13	2:1:77:LEU:CD2	2.48	0.43
1:O:71:GLU:HA	1:O:74:LYS:HD3	2.00	0.43
1:C:128:TYR:HB3	1:C:136:LEU:CD1	2.49	0.43
1:H:37:LYS:HG3	1:H:52:LEU:HD11	2.00	0.43
1:H:15:VAL:H	1:H:66:MET:HE1	1.84	0.43
1:I:71:GLU:HA	1:I:74:LYS:HD3	1.99	0.43
1:J:133:PRO:CD	1:J:134:GLU:N	2.82	0.43
1:M:132:LYS:HD2	1:M:132:LYS:HA	1.75	0.43
1:M:133:PRO:CG	1:M:134:GLU:N	2.82	0.43
1:Q:37:LYS:HG3	1:Q:52:LEU:HD11	2.00	0.43
2:V:155:MET:HA	2:V:176:ALA:O	2.19	0.43
2:2:155:MET:HA	2:2:176:ALA:O	2.19	0.42
2:3:197:ALA:O	2:3:201:ARG:HG3	2.19	0.42
1:B:71:GLU:HA	1:B:74:LYS:HD3	2.00	0.42
1:C:141:GLY:HA2	1:D:13:ALA:O	2.19	0.42
1:E:133:PRO:O	1:E:136:LEU:HB2	2.18	0.42
1:J:28:GLU:OE1	1:J:28:GLU:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:ILE:HD11	2:T:51:LYS:HA	2.00	0.42
1:F:13:ALA:O	1:G:141:GLY:O	2.37	0.42
1:F:137:THR:HA	1:J:38:THR:CB	2.50	0.42
1:K:141:GLY:O	1:S:11:THR:O	2.37	0.42
1:M:132:LYS:HE3	1:M:134:GLU:HB2	2.01	0.42
2:N:45:ARG:CD	2:N:46:SER:N	2.73	0.42
2:T:155:MET:HA	2:T:176:ALA:O	2.19	0.42
2:W:155:MET:HA	2:W:176:ALA:O	2.19	0.42
1:A:28:GLU:HA	1:A:28:GLU:OE1	2.19	0.42
1:C:136:LEU:HA	1:C:136:LEU:HD23	1.78	0.42
1:C:71:GLU:HA	1:C:74:LYS:HD3	2.00	0.42
1:F:136:LEU:HD23	1:F:136:LEU:HA	1.78	0.42
1:O:142:LYS:HB3	1:Q:11:THR:O	2.20	0.42
1:Q:15:VAL:H	1:Q:66:MET:HE1	1.84	0.42
1:D:130:LEU:HB3	1:D:131:PHE:CD1	2.54	0.42
2:N:45:ARG:HD3	2:N:46:SER:CA	2.50	0.42
1:O:38:THR:CB	1:S:137:THR:HA	2.49	0.42
2:P:155:MET:HA	2:P:176:ALA:O	2.20	0.42
1:F:10:THR:O	1:G:140:ALA:HA	2.18	0.42
1:G:71:GLU:CB	1:G:74:LYS:HE2	2.42	0.42
2:Y:155:MET:HA	2:Y:176:ALA:O	2.20	0.42
1:F:71:GLU:CB	1:F:74:LYS:HE2	2.42	0.42
1:J:110:GLU:OE2	2:T:51:LYS:HD2	2.18	0.42
2:L:155:MET:HA	2:L:176:ALA:O	2.20	0.42
1:S:132:LYS:HD2	1:S:132:LYS:HA	1.75	0.42
2:X:155:MET:HA	2:X:176:ALA:O	2.20	0.42
2:Z:155:MET:HA	2:Z:176:ALA:O	2.20	0.42
1:G:133:PRO:O	1:G:136:LEU:HB2	2.20	0.42
1:J:37:LYS:HG3	1:J:52:LEU:HD11	2.00	0.42
2:R:155:MET:HA	2:R:176:ALA:O	2.20	0.42
2:Y:18:ALA:HB1	2:Y:45:ARG:HD3	2.01	0.42
2:3:45:ARG:HG3	2:3:46:SER:N	2.35	0.42
1:J:71:GLU:HA	1:J:74:LYS:HD3	2.01	0.42
1:K:135:TYR:CD1	1:K:135:TYR:O	2.73	0.42
2:L:131:PHE:CD1	2:L:132:PRO:HA	2.55	0.42
1:S:136:LEU:HD23	1:S:136:LEU:HA	1.89	0.42
2:1:131:PHE:CD1	2:1:132:PRO:HA	2.55	0.42
1:Q:15:VAL:CB	1:Q:66:MET:HE1	2.49	0.42
2:T:9:LYS:HE2	2:T:9:LYS:HB3	1.89	0.42
2:3:155:MET:HA	2:3:176:ALA:O	2.19	0.41
1:C:125:ASN:HD22	1:C:125:ASN:HA	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ASN:HA	1:D:125:ASN:HD22	1.62	0.41
1:K:10:THR:O	1:M:140:ALA:HA	2.20	0.41
2:N:155:MET:HA	2:N:176:ALA:O	2.20	0.41
2:W:45:ARG:CG	2:W:46:SER:N	2.82	0.41
2:1:18:ALA:HB1	2:1:45:ARG:HD2	2.01	0.41
1:C:85:MET:CE	1:D:79:GLU:HB3	2.50	0.41
1:K:4:LYS:HE2	1:K:35:ILE:HG13	2.02	0.41
2:R:131:PHE:CD1	2:R:132:PRO:HA	2.56	0.41
1:K:137:THR:HA	1:S:38:THR:CB	2.49	0.41
1:S:3:LYS:HA	1:S:3:LYS:HD3	1.90	0.41
2:W:9:LYS:HE2	2:W:9:LYS:HB3	1.88	0.41
2:3:131:PHE:CD1	2:3:132:PRO:HA	2.55	0.41
2:4:155:MET:HA	2:4:176:ALA:O	2.20	0.41
1:B:132:LYS:HE3	1:B:134:GLU:OE1	2.20	0.41
1:A:140:ALA:HA	1:E:10:THR:O	2.20	0.41
1:S:135:TYR:C	1:S:135:TYR:HD1	2.23	0.41
2:T:131:PHE:CD1	2:T:132:PRO:HA	2.56	0.41
2:U:155:MET:HA	2:U:176:ALA:O	2.20	0.41
2:4:131:PHE:CD1	2:4:132:PRO:HA	2.55	0.41
1:K:8:VAL:HA	1:K:37:LYS:O	2.21	0.41
1:M:135:TYR:HD1	1:M:135:TYR:C	2.23	0.41
1:O:133:PRO:CG	1:O:134:GLU:H	2.33	0.41
2:P:113:ASN:HB2	2:P:114:PRO:HD2	2.03	0.41
2:P:131:PHE:CD1	2:P:132:PRO:HA	2.56	0.41
1:Q:133:PRO:CG	1:Q:134:GLU:N	2.84	0.41
2:R:202:GLU:HG3	2:R:203:ILE:N	2.35	0.41
1:H:13:ALA:O	1:J:141:GLY:C	2.58	0.41
1:I:29:SER:OG	1:I:32:ILE:HB	2.20	0.41
2:X:131:PHE:CD1	2:X:132:PRO:HA	2.55	0.41
2:1:155:MET:HA	2:1:176:ALA:O	2.20	0.41
1:E:136:LEU:HD23	1:E:136:LEU:HA	1.87	0.41
1:H:142:LYS:O	1:I:11:THR:O	2.38	0.41
1:K:133:PRO:O	1:K:136:LEU:HB2	2.20	0.41
1:S:125:ASN:HD22	1:S:125:ASN:HA	1.62	0.41
2:U:131:PHE:CD1	2:U:132:PRO:HA	2.55	0.41
2:W:131:PHE:CD1	2:W:132:PRO:HA	2.55	0.41
2:Y:131:PHE:CD1	2:Y:132:PRO:HA	2.56	0.41
2:3:45:ARG:CG	2:3:46:SER:N	2.84	0.41
1:I:8:VAL:HA	1:I:37:LYS:O	2.21	0.41
2:N:131:PHE:CD1	2:N:132:PRO:HA	2.55	0.41
2:W:45:ARG:HG3	2:W:46:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:VAL:HA	1:D:37:LYS:O	2.21	0.41
2:P:69:THR:HA	2:P:90:PRO:HD3	2.01	0.41
2:R:48:ALA:O	2:R:49:ALA:C	2.58	0.41
2:U:113:ASN:HB2	2:U:114:PRO:HD2	2.03	0.41
2:2:131:PHE:CD1	2:2:132:PRO:HA	2.55	0.41
1:A:140:ALA:HA	1:E:11:THR:HA	2.01	0.41
2:R:113:ASN:HB2	2:R:114:PRO:HD2	2.03	0.41
2:V:131:PHE:CD1	2:V:132:PRO:HA	2.55	0.41
2:X:113:ASN:HB2	2:X:114:PRO:HD2	2.03	0.41
2:Y:113:ASN:HB2	2:Y:114:PRO:HD2	2.03	0.41
2:Z:131:PHE:CD1	2:Z:132:PRO:HA	2.56	0.41
1:A:8:VAL:HA	1:A:37:LYS:O	2.21	0.41
1:B:125:ASN:HA	1:B:125:ASN:HD22	1.62	0.41
1:K:85:MET:CE	1:S:79:GLU:HB3	2.52	0.41
1:K:50:LYS:HZ2	1:M:92:ASN:HD21	1.65	0.41
1:O:8:VAL:HA	1:O:37:LYS:O	2.21	0.41
1:Q:133:PRO:CD	1:Q:134:GLU:N	2.84	0.41
1:A:139:MET:CA	1:A:139:MET:HE2	2.49	0.40
1:B:37:LYS:CG	1:B:52:LEU:HD11	2.51	0.40
1:D:133:PRO:CD	1:D:134:GLU:N	2.84	0.40
1:E:15:VAL:CB	1:E:66:MET:HE1	2.52	0.40
1:J:8:VAL:HA	1:J:37:LYS:O	2.21	0.40
1:O:4:LYS:CE	1:O:56:GLU:O	2.70	0.40
2:P:9:LYS:HB3	2:P:9:LYS:HE2	1.88	0.40
2:4:44:PHE:CE1	2:4:70:ILE:HD11	2.56	0.40
1:B:8:VAL:HA	1:B:37:LYS:O	2.21	0.40
1:C:8:VAL:HA	1:C:37:LYS:O	2.21	0.40
1:G:132:LYS:HA	1:G:132:LYS:HD2	1.68	0.40
1:G:8:VAL:HA	1:G:37:LYS:O	2.21	0.40
1:Q:8:VAL:HA	1:Q:37:LYS:O	2.21	0.40
1:F:120:ILE:CD1	2:1:77:LEU:HD23	2.48	0.40
1:F:8:VAL:HA	1:F:37:LYS:O	2.21	0.40
2:L:113:ASN:HB2	2:L:114:PRO:HD2	2.03	0.40
1:Q:132:LYS:HA	1:Q:132:LYS:HD2	1.74	0.40
2:1:113:ASN:HB2	2:1:114:PRO:HD2	2.03	0.40
1:B:38:THR:OG1	1:D:137:THR:HA	2.22	0.40
1:B:11:THR:CG2	1:D:139:MET:O	2.68	0.40
1:H:8:VAL:HA	1:H:37:LYS:O	2.21	0.40
1:G:13:ALA:O	1:I:141:GLY:C	2.59	0.40
1:J:136:LEU:HA	1:J:136:LEU:HD23	1.89	0.40
1:J:15:VAL:CB	1:J:66:MET:HE1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:4:LYS:HZ2	1:O:4:LYS:HB2	1.86	0.40
2:W:3:THR:HG23	2:W:4:ILE:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:161:THR:CB	2:3:198:ARG:NH2[5_544]	2.11	0.09

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	140/156 (90%)	137 (98%)	3 (2%)	0	100	100
1	B	140/156 (90%)	136 (97%)	4 (3%)	0	100	100
1	C	140/156 (90%)	136 (97%)	4 (3%)	0	100	100
1	D	139/156 (89%)	136 (98%)	3 (2%)	0	100	100
1	E	140/156 (90%)	137 (98%)	3 (2%)	0	100	100
1	F	139/156 (89%)	135 (97%)	4 (3%)	0	100	100
1	G	140/156 (90%)	136 (97%)	4 (3%)	0	100	100
1	H	140/156 (90%)	137 (98%)	3 (2%)	0	100	100
1	I	140/156 (90%)	136 (97%)	4 (3%)	0	100	100
1	J	139/156 (89%)	136 (98%)	3 (2%)	0	100	100
1	K	140/156 (90%)	136 (97%)	4 (3%)	0	100	100
1	M	139/156 (89%)	135 (97%)	4 (3%)	0	100	100
1	O	139/156 (89%)	134 (96%)	5 (4%)	0	100	100
1	Q	140/156 (90%)	136 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	140/156 (90%)	135 (96%)	5 (4%)	0	100	100
2	1	206/219 (94%)	203 (98%)	3 (2%)	0	100	100
2	2	206/219 (94%)	203 (98%)	3 (2%)	0	100	100
2	3	206/219 (94%)	203 (98%)	3 (2%)	0	100	100
2	4	206/219 (94%)	202 (98%)	4 (2%)	0	100	100
2	L	206/219 (94%)	203 (98%)	3 (2%)	0	100	100
2	N	206/219 (94%)	202 (98%)	4 (2%)	0	100	100
2	P	206/219 (94%)	202 (98%)	4 (2%)	0	100	100
2	R	206/219 (94%)	201 (98%)	5 (2%)	0	100	100
2	T	206/219 (94%)	203 (98%)	3 (2%)	0	100	100
2	U	206/219 (94%)	203 (98%)	3 (2%)	0	100	100
2	V	206/219 (94%)	202 (98%)	4 (2%)	0	100	100
2	W	206/219 (94%)	202 (98%)	4 (2%)	0	100	100
2	X	206/219 (94%)	203 (98%)	3 (2%)	0	100	100
2	Y	206/219 (94%)	203 (98%)	3 (2%)	0	100	100
2	Z	206/219 (94%)	202 (98%)	4 (2%)	0	100	100
All	All	5185/5625 (92%)	5075 (98%)	110 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/127 (91%)	110 (96%)	5 (4%)	35	74
1	B	115/127 (91%)	109 (95%)	6 (5%)	29	70
1	C	115/127 (91%)	110 (96%)	5 (4%)	35	74
1	D	116/127 (91%)	111 (96%)	5 (4%)	35	74
1	E	115/127 (91%)	110 (96%)	5 (4%)	35	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	115/127 (91%)	112 (97%)	3 (3%)	54 83
1	G	115/127 (91%)	110 (96%)	5 (4%)	35 74
1	H	115/127 (91%)	111 (96%)	4 (4%)	43 78
1	I	115/127 (91%)	109 (95%)	6 (5%)	29 70
1	J	115/127 (91%)	109 (95%)	6 (5%)	29 70
1	K	115/127 (91%)	109 (95%)	6 (5%)	29 70
1	M	116/127 (91%)	110 (95%)	6 (5%)	29 70
1	O	116/127 (91%)	111 (96%)	5 (4%)	35 74
1	Q	115/127 (91%)	111 (96%)	4 (4%)	43 78
1	S	115/127 (91%)	109 (95%)	6 (5%)	29 70
2	1	165/175 (94%)	164 (99%)	1 (1%)	90 96
2	2	165/175 (94%)	163 (99%)	2 (1%)	78 91
2	3	165/175 (94%)	162 (98%)	3 (2%)	66 89
2	4	165/175 (94%)	163 (99%)	2 (1%)	78 91
2	L	165/175 (94%)	164 (99%)	1 (1%)	90 96
2	N	164/175 (94%)	162 (99%)	2 (1%)	78 91
2	P	165/175 (94%)	162 (98%)	3 (2%)	66 89
2	R	165/175 (94%)	162 (98%)	3 (2%)	66 89
2	T	165/175 (94%)	162 (98%)	3 (2%)	66 89
2	U	165/175 (94%)	162 (98%)	3 (2%)	66 89
2	V	165/175 (94%)	164 (99%)	1 (1%)	90 96
2	W	165/175 (94%)	161 (98%)	4 (2%)	57 85
2	X	165/175 (94%)	163 (99%)	2 (1%)	78 91
2	Y	165/175 (94%)	163 (99%)	2 (1%)	78 91
2	Z	165/175 (94%)	162 (98%)	3 (2%)	66 89
All	All	4202/4530 (93%)	4090 (97%)	112 (3%)	52 83

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	114	LEU
1	K	118	ARG
1	K	130	LEU

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Mol	Chain	Res	Type
1	K	132	LYS
1	K	134	GLU
1	K	135	TYR
1	M	114	LEU
1	M	118	ARG
1	M	130	LEU
1	M	132	LYS
1	M	135	TYR
1	M	139	MET
1	O	114	LEU
1	O	118	ARG
1	O	130	LEU
1	O	132	LYS
1	O	134	GLU
1	Q	114	LEU
1	Q	118	ARG
1	Q	130	LEU
1	Q	132	LYS
1	S	3	LYS
1	S	114	LEU
1	S	118	ARG
1	S	130	LEU
1	S	132	LYS
1	S	135	TYR
1	A	114	LEU
1	A	118	ARG
1	A	130	LEU
1	A	132	LYS
1	A	135	TYR
1	B	3	LYS
1	B	114	LEU
1	B	118	ARG
1	B	130	LEU
1	B	132	LYS
1	B	135	TYR
1	C	114	LEU
1	C	118	ARG
1	C	130	LEU
1	C	132	LYS
1	C	135	TYR
1	D	31	ASN
1	D	114	LEU

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Mol	Chain	Res	Type
1	D	118	ARG
1	D	130	LEU
1	D	134	GLU
1	E	3	LYS
1	E	114	LEU
1	E	118	ARG
1	E	130	LEU
1	E	132	LYS
1	F	114	LEU
1	F	118	ARG
1	F	130	LEU
1	G	114	LEU
1	G	118	ARG
1	G	130	LEU
1	G	132	LYS
1	G	134	GLU
1	H	114	LEU
1	H	118	ARG
1	H	130	LEU
1	H	132	LYS
1	I	114	LEU
1	I	118	ARG
1	I	130	LEU
1	I	132	LYS
1	I	135	TYR
1	I	137	THR
1	J	114	LEU
1	J	118	ARG
1	J	130	LEU
1	J	132	LYS
1	J	134	GLU
1	J	135	TYR
2	P	45	ARG
2	P	63	MET
2	P	69	THR
2	T	45	ARG
2	T	63	MET
2	T	69	THR
2	N	45	ARG
2	N	69	THR
2	V	69	THR
2	W	5	ASN

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Mol	Chain	Res	Type
2	W	45	ARG
2	W	63	MET
2	W	69	THR
2	U	6	ASN
2	U	63	MET
2	U	69	THR
2	Y	63	MET
2	Y	69	THR
2	Z	45	ARG
2	Z	63	MET
2	Z	69	THR
2	X	63	MET
2	X	69	THR
2	2	63	MET
2	2	69	THR
2	4	63	MET
2	4	69	THR
2	1	69	THR
2	L	69	THR
2	R	63	MET
2	R	69	THR
2	R	202	GLU
2	3	63	MET
2	3	69	THR
2	3	106	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	125	ASN
1	M	92	ASN
1	M	125	ASN
1	O	125	ASN
1	Q	125	ASN
1	S	125	ASN
1	A	125	ASN
1	B	125	ASN
1	C	125	ASN
1	D	125	ASN
1	E	125	ASN
1	F	125	ASN
1	G	125	ASN

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Mol	Chain	Res	Type
1	H	125	ASN
1	I	125	ASN
1	J	125	ASN
2	T	7	GLN
2	N	7	GLN
2	V	7	GLN
2	U	7	GLN
2	Y	7	GLN
2	Z	7	GLN
2	2	7	GLN
2	4	7	GLN
2	L	7	GLN
2	R	7	GLN
2	3	7	GLN

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	142/156 (91%)	0.47	0 100 100	76, 93, 131, 145	0
1	B	142/156 (91%)	0.48	0 100 100	80, 98, 132, 155	0
1	C	142/156 (91%)	0.48	0 100 100	75, 89, 123, 142	0
1	D	141/156 (90%)	0.46	0 100 100	78, 96, 131, 147	0
1	E	142/156 (91%)	0.46	2 (1%) 78 64	76, 90, 127, 144	0
1	F	141/156 (90%)	0.38	0 100 100	78, 92, 130, 149	0
1	G	142/156 (91%)	0.48	1 (0%) 89 81	77, 94, 133, 151	0
1	H	142/156 (91%)	0.43	0 100 100	76, 93, 129, 149	0
1	I	142/156 (91%)	0.46	0 100 100	78, 94, 129, 153	0
1	J	141/156 (90%)	0.35	1 (0%) 89 81	72, 88, 126, 147	0
1	K	142/156 (91%)	0.37	0 100 100	77, 92, 137, 150	0
1	M	141/156 (90%)	0.34	0 100 100	75, 92, 130, 147	0
1	O	141/156 (90%)	0.46	0 100 100	76, 93, 126, 142	0
1	Q	142/156 (91%)	0.51	0 100 100	76, 91, 127, 149	0
1	S	142/156 (91%)	0.38	0 100 100	72, 90, 127, 148	0
2	1	208/219 (94%)	0.29	0 100 100	82, 103, 134, 142	0
2	2	208/219 (94%)	0.31	2 (0%) 84 72	82, 102, 134, 142	0
2	3	208/219 (94%)	0.32	0 100 100	69, 81, 104, 115	0
2	4	208/219 (94%)	0.33	2 (0%) 84 72	80, 99, 130, 140	0
2	L	208/219 (94%)	0.29	0 100 100	72, 91, 125, 136	0
2	N	208/219 (94%)	0.34	0 100 100	70, 93, 129, 143	0
2	P	208/219 (94%)	0.27	0 100 100	67, 82, 104, 114	0
2	R	208/219 (94%)	0.25	0 100 100	69, 83, 104, 117	0
2	T	208/219 (94%)	0.35	0 100 100	67, 80, 103, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	U	208/219 (94%)	0.27	3 (1%) 78 64	85, 109, 139, 152	0
2	V	208/219 (94%)	0.23	1 (0%) 91 86	82, 106, 137, 150	0
2	W	208/219 (94%)	0.22	0 100 100	81, 101, 131, 139	0
2	X	208/219 (94%)	0.26	0 100 100	86, 105, 133, 144	0
2	Y	208/219 (94%)	0.33	1 (0%) 91 86	84, 106, 133, 142	0
2	Z	208/219 (94%)	0.41	1 (0%) 91 86	85, 111, 144, 151	0
All	All	5245/5625 (93%)	0.35	14 (0%) 94 90	67, 96, 132, 155	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	25	ILE	3.4
2	Y	25	ILE	2.7
2	U	25	ILE	2.6
2	U	22	ALA	2.5
2	2	25	ILE	2.4
1	G	69	LYS	2.2
1	J	69	LYS	2.2
1	E	69	LYS	2.2
2	U	41	GLU	2.2
1	E	23	LEU	2.1
2	2	103	ILE	2.0
2	4	42	ILE	2.0
2	V	22	ALA	2.0
2	4	25	ILE	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.