WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 12:10 AM EDT

PDB ID	:	2GLV
Title	:	Crystal structure of (3R)-Hydroxyacyl-Acyl Carrier Protein Dehydratase(FabZ) mutant(Y100A) from Helicobacter pylori
Authors	:	Zhang, L.; Liu, W.; Shen, X.; Jiang, H.
Deposited on	:	2006-04-05
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

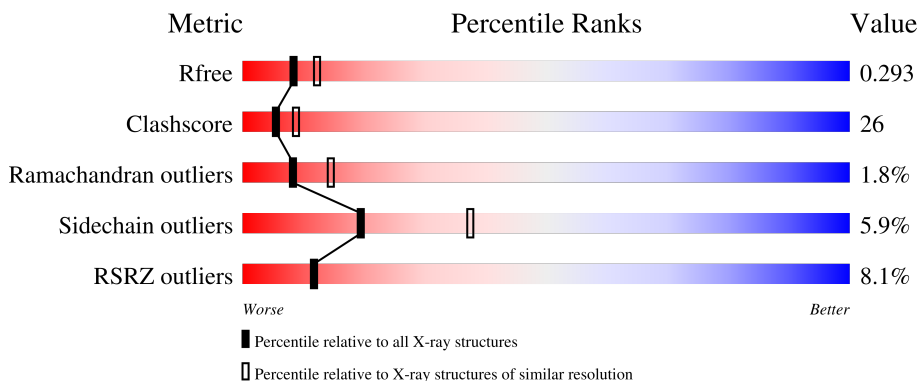|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.293
Clashscore		26
Ramachandran outliers		1.8%
Sidechain outliers		5.9%
RSRZ outliers		8.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	171	10% / 49% 37% · 11%
1	B	171	16% / 39% 41% 8% 12%
1	C	171	8% / 53% 33% ·· 11%
1	D	171	7% / 50% 35% · 12%
1	E	171	7% / 56% 30% ·· 12%

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Mol	Chain	Length	Quality of chain
1	F	171	3% 59% 27% 11%
1	G	171	3% 50% 32% 12%
1	H	171	11% 41% 39% 6% 13%
1	I	171	13% 46% 40% 11%
1	J	171	4% 45% 39% 5% 11%
1	K	171	2% 63% 24% 11%
1	L	171	2% 61% 24% 12%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 14745 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 (3R)-hydroxymyristoyl-acyl carrier protein dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1218	797	203	213	5			
1	B	150	Total	C	N	O	S	0	0	0
			1197	786	198	208	5			
1	C	152	Total	C	N	O	S	0	0	0
			1218	797	203	213	5			
1	D	151	Total	C	N	O	S	0	0	0
			1210	791	202	212	5			
1	E	151	Total	C	N	O	S	0	0	0
			1210	791	202	212	5			
1	F	152	Total	C	N	O	S	0	0	0
			1218	797	203	213	5			
1	G	150	Total	C	N	O	S	0	0	0
			1200	786	201	208	5			
1	H	148	Total	C	N	O	S	0	0	0
			1180	775	195	205	5			
1	I	152	Total	C	N	O	S	0	0	0
			1218	797	203	213	5			
1	J	152	Total	C	N	O	S	0	0	0
			1218	797	203	213	5			
1	K	152	Total	C	N	O	S	0	0	0
			1218	797	203	213	5			
1	L	151	Total	C	N	O	S	0	0	0
			1210	791	202	212	5			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q5G940
A	-10	ARG	-	expression tag	UNP Q5G940
A	-9	GLY	-	expression tag	UNP Q5G940
A	-8	SER	-	expression tag	UNP Q5G940
A	-7	HIS	-	expression tag	UNP Q5G940

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	expression tag	UNP Q5G940
A	-5	HIS	-	expression tag	UNP Q5G940
A	-4	HIS	-	expression tag	UNP Q5G940
A	-3	HIS	-	expression tag	UNP Q5G940
A	-2	HIS	-	expression tag	UNP Q5G940
A	-1	GLY	-	expression tag	UNP Q5G940
A	0	SER	-	expression tag	UNP Q5G940
A	100	ALA	TYR	engineered mutation	GB 56684725
B	-11	MET	-	expression tag	UNP Q5G940
B	-10	ARG	-	expression tag	UNP Q5G940
B	-9	GLY	-	expression tag	UNP Q5G940
B	-8	SER	-	expression tag	UNP Q5G940
B	-7	HIS	-	expression tag	UNP Q5G940
B	-6	HIS	-	expression tag	UNP Q5G940
B	-5	HIS	-	expression tag	UNP Q5G940
B	-4	HIS	-	expression tag	UNP Q5G940
B	-3	HIS	-	expression tag	UNP Q5G940
B	-2	HIS	-	expression tag	UNP Q5G940
B	-1	GLY	-	expression tag	UNP Q5G940
B	0	SER	-	expression tag	UNP Q5G940
B	100	ALA	TYR	engineered mutation	GB 56684725
C	-11	MET	-	expression tag	UNP Q5G940
C	-10	ARG	-	expression tag	UNP Q5G940
C	-9	GLY	-	expression tag	UNP Q5G940
C	-8	SER	-	expression tag	UNP Q5G940
C	-7	HIS	-	expression tag	UNP Q5G940
C	-6	HIS	-	expression tag	UNP Q5G940
C	-5	HIS	-	expression tag	UNP Q5G940
C	-4	HIS	-	expression tag	UNP Q5G940
C	-3	HIS	-	expression tag	UNP Q5G940
C	-2	HIS	-	expression tag	UNP Q5G940
C	-1	GLY	-	expression tag	UNP Q5G940
C	0	SER	-	expression tag	UNP Q5G940
C	100	ALA	TYR	engineered mutation	GB 56684725
D	-11	MET	-	expression tag	UNP Q5G940
D	-10	ARG	-	expression tag	UNP Q5G940
D	-9	GLY	-	expression tag	UNP Q5G940
D	-8	SER	-	expression tag	UNP Q5G940
D	-7	HIS	-	expression tag	UNP Q5G940
D	-6	HIS	-	expression tag	UNP Q5G940
D	-5	HIS	-	expression tag	UNP Q5G940
D	-4	HIS	-	expression tag	UNP Q5G940

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	HIS	-	expression tag	UNP Q5G940
D	-2	HIS	-	expression tag	UNP Q5G940
D	-1	GLY	-	expression tag	UNP Q5G940
D	0	SER	-	expression tag	UNP Q5G940
D	100	ALA	TYR	engineered mutation	GB 56684725
E	-11	MET	-	expression tag	UNP Q5G940
E	-10	ARG	-	expression tag	UNP Q5G940
E	-9	GLY	-	expression tag	UNP Q5G940
E	-8	SER	-	expression tag	UNP Q5G940
E	-7	HIS	-	expression tag	UNP Q5G940
E	-6	HIS	-	expression tag	UNP Q5G940
E	-5	HIS	-	expression tag	UNP Q5G940
E	-4	HIS	-	expression tag	UNP Q5G940
E	-3	HIS	-	expression tag	UNP Q5G940
E	-2	HIS	-	expression tag	UNP Q5G940
E	-1	GLY	-	expression tag	UNP Q5G940
E	0	SER	-	expression tag	UNP Q5G940
E	100	ALA	TYR	engineered mutation	GB 56684725
F	-11	MET	-	expression tag	UNP Q5G940
F	-10	ARG	-	expression tag	UNP Q5G940
F	-9	GLY	-	expression tag	UNP Q5G940
F	-8	SER	-	expression tag	UNP Q5G940
F	-7	HIS	-	expression tag	UNP Q5G940
F	-6	HIS	-	expression tag	UNP Q5G940
F	-5	HIS	-	expression tag	UNP Q5G940
F	-4	HIS	-	expression tag	UNP Q5G940
F	-3	HIS	-	expression tag	UNP Q5G940
F	-2	HIS	-	expression tag	UNP Q5G940
F	-1	GLY	-	expression tag	UNP Q5G940
F	0	SER	-	expression tag	UNP Q5G940
F	100	ALA	TYR	engineered mutation	GB 56684725
G	-11	MET	-	expression tag	UNP Q5G940
G	-10	ARG	-	expression tag	UNP Q5G940
G	-9	GLY	-	expression tag	UNP Q5G940
G	-8	SER	-	expression tag	UNP Q5G940
G	-7	HIS	-	expression tag	UNP Q5G940
G	-6	HIS	-	expression tag	UNP Q5G940
G	-5	HIS	-	expression tag	UNP Q5G940
G	-4	HIS	-	expression tag	UNP Q5G940
G	-3	HIS	-	expression tag	UNP Q5G940
G	-2	HIS	-	expression tag	UNP Q5G940
G	-1	GLY	-	expression tag	UNP Q5G940

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	expression tag	UNP Q5G940
G	100	ALA	TYR	engineered mutation	GB 56684725
H	-11	MET	-	expression tag	UNP Q5G940
H	-10	ARG	-	expression tag	UNP Q5G940
H	-9	GLY	-	expression tag	UNP Q5G940
H	-8	SER	-	expression tag	UNP Q5G940
H	-7	HIS	-	expression tag	UNP Q5G940
H	-6	HIS	-	expression tag	UNP Q5G940
H	-5	HIS	-	expression tag	UNP Q5G940
H	-4	HIS	-	expression tag	UNP Q5G940
H	-3	HIS	-	expression tag	UNP Q5G940
H	-2	HIS	-	expression tag	UNP Q5G940
H	-1	GLY	-	expression tag	UNP Q5G940
H	0	SER	-	expression tag	UNP Q5G940
H	100	ALA	TYR	engineered mutation	GB 56684725
I	-11	MET	-	expression tag	UNP Q5G940
I	-10	ARG	-	expression tag	UNP Q5G940
I	-9	GLY	-	expression tag	UNP Q5G940
I	-8	SER	-	expression tag	UNP Q5G940
I	-7	HIS	-	expression tag	UNP Q5G940
I	-6	HIS	-	expression tag	UNP Q5G940
I	-5	HIS	-	expression tag	UNP Q5G940
I	-4	HIS	-	expression tag	UNP Q5G940
I	-3	HIS	-	expression tag	UNP Q5G940
I	-2	HIS	-	expression tag	UNP Q5G940
I	-1	GLY	-	expression tag	UNP Q5G940
I	0	SER	-	expression tag	UNP Q5G940
I	100	ALA	TYR	engineered mutation	GB 56684725
J	-11	MET	-	expression tag	UNP Q5G940
J	-10	ARG	-	expression tag	UNP Q5G940
J	-9	GLY	-	expression tag	UNP Q5G940
J	-8	SER	-	expression tag	UNP Q5G940
J	-7	HIS	-	expression tag	UNP Q5G940
J	-6	HIS	-	expression tag	UNP Q5G940
J	-5	HIS	-	expression tag	UNP Q5G940
J	-4	HIS	-	expression tag	UNP Q5G940
J	-3	HIS	-	expression tag	UNP Q5G940
J	-2	HIS	-	expression tag	UNP Q5G940
J	-1	GLY	-	expression tag	UNP Q5G940
J	0	SER	-	expression tag	UNP Q5G940
J	100	ALA	TYR	engineered mutation	GB 56684725
K	-11	MET	-	expression tag	UNP Q5G940

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-10	ARG	-	expression tag	UNP Q5G940
K	-9	GLY	-	expression tag	UNP Q5G940
K	-8	SER	-	expression tag	UNP Q5G940
K	-7	HIS	-	expression tag	UNP Q5G940
K	-6	HIS	-	expression tag	UNP Q5G940
K	-5	HIS	-	expression tag	UNP Q5G940
K	-4	HIS	-	expression tag	UNP Q5G940
K	-3	HIS	-	expression tag	UNP Q5G940
K	-2	HIS	-	expression tag	UNP Q5G940
K	-1	GLY	-	expression tag	UNP Q5G940
K	0	SER	-	expression tag	UNP Q5G940
K	100	ALA	TYR	engineered mutation	GB 56684725
L	-11	MET	-	expression tag	UNP Q5G940
L	-10	ARG	-	expression tag	UNP Q5G940
L	-9	GLY	-	expression tag	UNP Q5G940
L	-8	SER	-	expression tag	UNP Q5G940
L	-7	HIS	-	expression tag	UNP Q5G940
L	-6	HIS	-	expression tag	UNP Q5G940
L	-5	HIS	-	expression tag	UNP Q5G940
L	-4	HIS	-	expression tag	UNP Q5G940
L	-3	HIS	-	expression tag	UNP Q5G940
L	-2	HIS	-	expression tag	UNP Q5G940
L	-1	GLY	-	expression tag	UNP Q5G940
L	0	SER	-	expression tag	UNP Q5G940
L	100	ALA	TYR	engineered mutation	GB 56684725

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0
2	B	1	Total 1	Cl 1	0	0
2	C	1	Total 1	Cl 1	0	0
2	D	1	Total 1	Cl 1	0	0
2	E	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0
2	G	2	Total 2	Cl 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	2	Total 2	Cl 2	0	0
2	K	2	Total 2	Cl 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total 14	O 14	0	0
3	B	17	Total 17	O 17	0	0
3	C	16	Total 16	O 16	0	0
3	D	15	Total 15	O 15	0	0
3	E	20	Total 20	O 20	0	0
3	F	21	Total 21	O 21	0	0
3	G	17	Total 17	O 17	0	0
3	H	14	Total 14	O 14	0	0
3	I	17	Total 17	O 17	0	0
3	J	19	Total 19	O 19	0	0
3	K	23	Total 23	O 23	0	0
3	L	25	Total 25	O 25	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
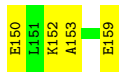
- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

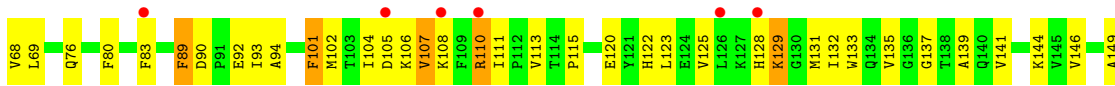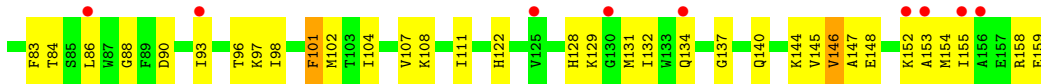- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase
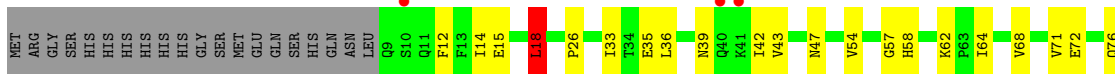
- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

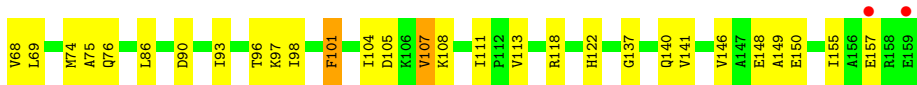- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

F83 T84 S85 L86 I93 T96 F101 M102 T103 I104 D105 K106 V107 K108 F109 R110 I111 P112 V113 T114 P115 R118 L119 E120 Y121 H122 L123 L126 K129 G130 M131 I132 W133 Q134 V135 G136 G137 T138 A139 Q140 V141 V145 V146 A147 E148 L151 K152 A153 M154 I155 A156 E157

R158 GLU

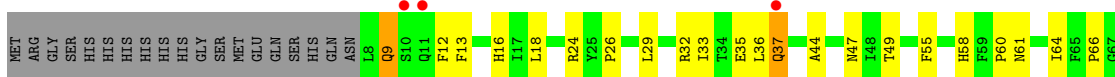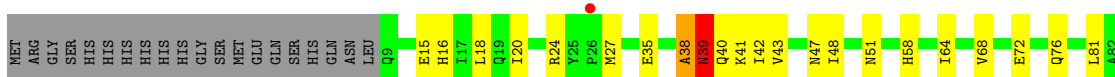• Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

Chain H:

11%				
41%		39%	6%	13%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET GLU GLN SER HIS GLN ASN LEU GLN S10 Q11 F12 F13 I14 I17 L18 R24 Y25 P26 M27 L28 L29 R32 I33 L36 Q37 Q40 K41 I42 V43 A44 N47 I48 G57 H58 F59 P60 N61 K62 P63 I64

F65 P66 G67 V68 L69 Q76 L81 A82 F83 T84 S85 L86 W87 G88 D90 P91 E92 I93 A94 K95 T96 K97 I98 V99 A100 F101 I104 D105 K106 V107 K108 F109 R110 I111 P115 L119 E120 Y121 H122 V125 L126 K127 H128 K129 G130 M131 W133 Q134 V135 G136 G137 T138

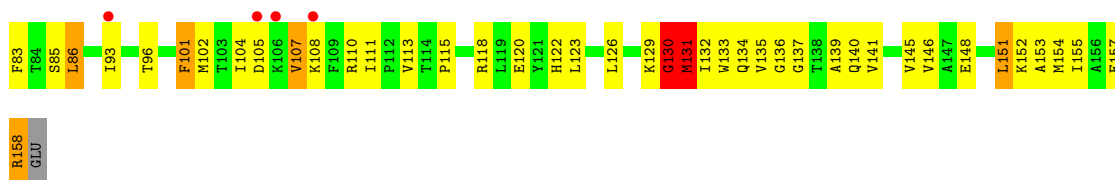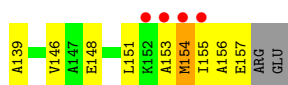A139 V146 A147 E148 L151 K152 A153 M154 I155 A156 E157 ARG GLU

• Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

Chain I:

13%				
46%		40%	•	11%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET GLU GLN SER HIS GLN ASN L8 Q9 S10 Q11 F12 F13 H16 I17 I20 R24 I33 T34 E35 L36 Q37 A38 N39 Q40 K41 I42 V43 N47 I48 N51 V54 H58 F59 P60 N61 K62 P63 I64 F65

P66 G67 V68 L69 F83 L86 W87 D90 P91 E92 I93 T96 K97 I98 V99 A100 F101 M102 T103 I104 D105 K106 V107 R110 I111 T114 P115 R118 L119 E120 Y121 H122 L123 E124 V125 L126 K127 H128 K129 G130 M131 I132 W133 Q134 V135 G136 G137 T138 A139 Q140 V141 D142 G143

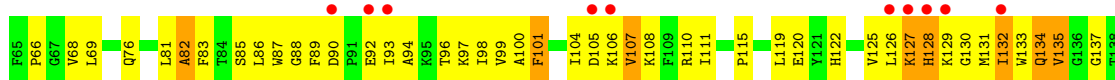K144 V145 V146 A147 E148 A149 K152 A153 M154 I155 A156 E157 R158 E159
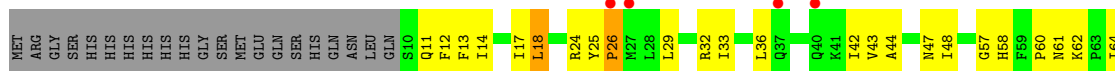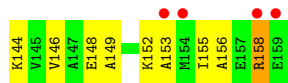
• Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

Chain J:

4%				
45%		39%	5%	11%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET GLU GLN SER HIS GLN ASN L8 Q9 S10 Q11 F12 F13 I14 E15 H16 H23 M27 L28 L29 I33 T34 E35 L36 Q37 A38 N39 Q40 K41 I42 V43 K46 N47 N51 E52 G57 H58 N61 K62 P63 I64

F65 P66 G67 V68 L69 I70 G73 M74 A75 Q76 L81 A82 F83 T84 S85 L86 W87 G88 K95 T96 K97 I98 V99 A100 F101 M102 T103 I104 D105 K106 V107 R110 T114 P115 L119 E120 Y121 H122 V125 L126 M131 I132 W133 Q134 V135 G136 G137 T138 A139 Q140 V145

V146 A147 E148 A149 E150 L151 K152 I155 A156 E157 R158 E159

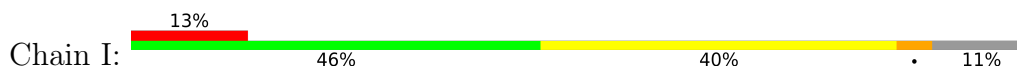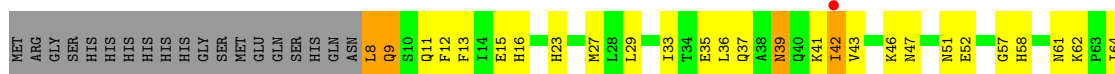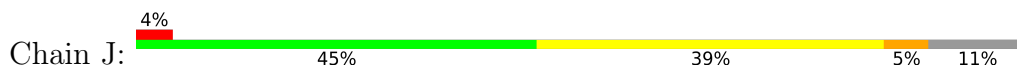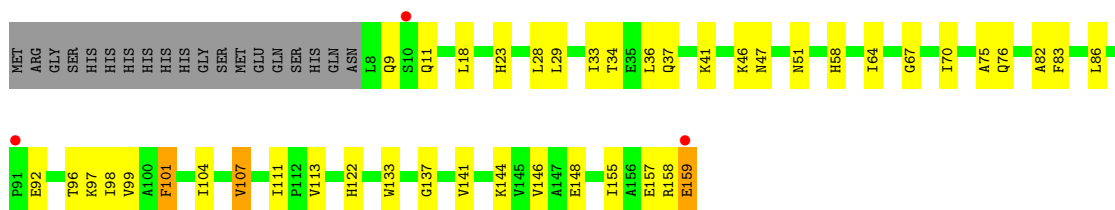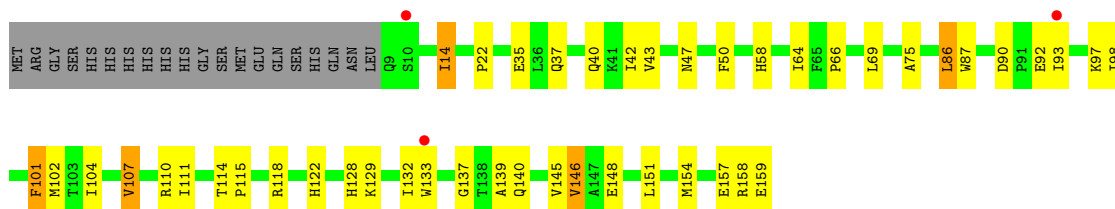• Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

Chain K:

• Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

Chain L:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	266.52Å 76.91Å 113.19Å 90.00° 102.25° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.36 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.50) 91.4 (48.36-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	1.36 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.293 0.241 , 0.293	Depositor DCC
R_{free} test set	3613 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 54.0	EDS
L-test for twinning[2]	$<\|L\|> = 0.51$, $<L^2> = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14745	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9244e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1   Standard geometry (i)

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

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	0.46	0/1248	0.68	0/1687
1	B	0.47	0/1227	0.69	0/1661
1	C	0.49	0/1248	0.68	0/1687
1	D	0.45	0/1240	0.69	0/1676
1	E	0.46	0/1240	0.69	1/1676 (0.1%)
1	F	0.45	0/1248	0.65	0/1687
1	G	0.60	3/1230 (0.2%)	0.81	3/1664 (0.2%)
1	H	0.47	0/1210	0.74	0/1638
1	I	0.46	0/1248	0.67	0/1687
1	J	0.44	0/1248	0.70	0/1687
1	K	0.45	0/1248	0.68	0/1687
1	L	0.45	0/1240	0.69	0/1676
All	All	0.47	3/14875 (0.0%)	0.70	4/20113 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	130	GLY	C-N	-11.97	1.06	1.34
1	G	38	ALA	C-N	-5.81	1.20	1.34
1	G	39	ASN	C-N	5.29	1.46	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	130	GLY	C-N-CA	10.39	147.68	121.70
1	G	130	GLY	O-C-N	-8.16	109.65	122.70
1	E	18	LEU	CA-CB-CG	5.56	128.09	115.30
1	G	130	GLY	CA-C-N	5.53	129.36	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	131	MET	Mainchain
1	G	39	ASN	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1218	0	1239	65	0
1	B	1197	0	1220	97	0
1	C	1218	0	1239	65	0
1	D	1210	0	1228	68	0
1	E	1210	0	1228	65	0
1	F	1218	0	1239	50	0
1	G	1200	0	1220	73	0
1	H	1180	0	1201	102	0
1	I	1218	0	1239	79	0
1	J	1218	0	1239	71	0
1	K	1218	0	1239	42	0
1	L	1210	0	1228	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	1	0
2	F	1	0	0	1	0
2	G	2	0	0	1	0
2	I	2	0	0	0	0
2	K	2	0	0	0	0
3	A	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	0	3	0
3	C	16	0	0	1	0
3	D	15	0	0	0	0
3	E	20	0	0	1	0
3	F	21	0	0	1	0
3	G	17	0	0	0	0
3	H	14	0	0	1	0
3	I	17	0	0	1	0
3	J	19	0	0	3	0
3	K	23	0	0	2	0
3	L	25	0	0	1	0
All	All	14745	0	14759	762	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 26.

All (762) 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:A:8:LEU:HD13	1:A:9:GLN:H	1.13	1.05
1:H:126:LEU:HB2	1:H:134:GLN:HE22	1.22	1.01
1:H:129:LYS:HG2	1:H:132:ILE:HG23	1.43	1.00
1:B:102:MET:HE1	1:B:132:ILE:HG13	1.44	0.98
1:H:42:ILE:HG22	1:H:81:LEU:HD12	1.46	0.98
1:D:35:GLU:HB2	1:D:43:VAL:HG13	1.48	0.95
1:H:126:LEU:HB2	1:H:134:GLN:NE2	1.81	0.94
1:I:129:LYS:NZ	1:I:132:ILE:HB	1.82	0.93
1:B:13:PHE:H	1:B:16:HIS:HD2	1.15	0.92
1:F:93:ILE:O	1:F:96:THR:HG22	1.70	0.91
1:B:129:LYS:HG2	1:B:130:GLY:N	1.87	0.90
1:J:13:PHE:H	1:J:16:HIS:HD2	1.19	0.90
1:B:97:LYS:HD3	1:B:157:GLU:HG2	1.55	0.89
1:C:82:ALA:HB1	1:C:155:ILE:HD11	1.54	0.88
1:E:131:MET:HB2	1:E:155:ILE:HG12	1.55	0.87
1:I:101:PHE:HB3	1:I:153:ALA:HB2	1.55	0.86
1:K:98:ILE:HG23	1:K:158:ARG:HG3	1.57	0.86
1:G:158:ARG:HB3	1:G:158:ARG:CZ	2.06	0.85
1:C:129:LYS:NZ	1:C:129:LYS:HB3	1.92	0.85
1:I:13:PHE:H	1:I:16:HIS:HD2	1.20	0.85
1:A:58:HIS:HD2	1:A:64:ILE:O	1.59	0.84
1:H:98:ILE:C	1:H:156:ALA:HB3	1.98	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:98:ILE:HG22	1:J:156:ALA:HB3	1.60	0.83
1:A:8:LEU:CD1	1:A:9:GLN:H	1.92	0.83
1:B:8:LEU:HD22	1:B:38:ALA:HB2	1.61	0.81
1:G:158:ARG:HB3	1:G:158:ARG:NH1	1.95	0.81
1:H:154:MET:HG3	1:H:155:ILE:H	1.43	0.81
1:I:37:GLN:HB3	1:I:40:GLN:HB3	1.62	0.81
1:F:29:LEU:H	1:F:76:GLN:HE22	1.29	0.81
1:C:111:ILE:O	1:C:146:VAL:HG13	1.80	0.81
1:A:13:PHE:H	1:A:16:HIS:HD2	1.28	0.80
1:D:90:ASP:OD1	1:D:93:ILE:HG12	1.81	0.80
1:E:35:GLU:HB2	1:E:43:VAL:HB	1.64	0.80
1:K:29:LEU:H	1:K:76:GLN:HE22	1.30	0.80
1:A:11:GLN:C	1:A:11:GLN:HE21	1.86	0.79
1:B:38:ALA:O	1:B:40:GLN:N	2.15	0.79
1:F:13:PHE:H	1:F:16:HIS:HD2	1.31	0.79
1:C:62:LYS:NZ	1:D:159:GLU:HG2	1.97	0.79
1:G:39:ASN:HD21	1:G:85:SER:HB3	1.48	0.78
1:B:8:LEU:HD11	1:B:36:LEU:HG	1.66	0.78
1:B:102:MET:CE	1:B:132:ILE:HG13	2.14	0.77
1:I:129:LYS:HZ1	1:I:132:ILE:HB	1.48	0.77
1:A:8:LEU:O	1:A:9:GLN:HG2	1.84	0.77
1:A:47:ASN:HB3	1:F:47:ASN:HB3	1.67	0.77
1:C:29:LEU:H	1:C:76:GLN:HE22	1.32	0.76
1:G:39:ASN:ND2	1:G:85:SER:HB3	2.01	0.76
1:J:158:ARG:HH11	1:J:158:ARG:HB3	1.49	0.76
1:C:96:THR:HG23	1:C:97:LYS:HD2	1.66	0.76
1:D:40:GLN:O	1:D:125:VAL:HG23	1.86	0.76
1:A:8:LEU:HD13	1:A:9:GLN:N	1.97	0.75
1:B:110:ARG:NH2	1:B:148:GLU:OE2	2.18	0.75
1:H:132:ILE:O	1:H:132:ILE:HD13	1.86	0.75
1:I:13:PHE:H	1:I:16:HIS:CD2	2.05	0.75
1:D:58:HIS:HD2	1:D:64:ILE:O	1.68	0.75
1:D:48:ILE:HG22	1:D:115:PRO:HA	1.69	0.74
1:H:131:MET:HB2	1:H:155:ILE:CG2	2.17	0.74
1:E:131:MET:HB2	1:E:155:ILE:CG1	2.17	0.74
1:H:129:LYS:CG	1:H:132:ILE:HG23	2.18	0.74
1:L:111:ILE:O	1:L:146:VAL:HG22	1.87	0.74
1:I:98:ILE:HG23	1:I:156:ALA:HB3	1.69	0.74
1:H:98:ILE:HG22	1:H:99:VAL:H	1.52	0.73
1:B:131:MET:SD	1:B:155:ILE:HG22	2.28	0.73
1:H:98:ILE:HG22	1:H:99:VAL:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:GLN:HE21	1:H:134:GLN:C	1.91	0.73
1:G:102:MET:HE3	1:G:132:ILE:HG23	1.70	0.73
1:J:47:ASN:HB3	1:K:47:ASN:HB3	1.69	0.73
1:B:102:MET:CE	1:B:154:MET:HB2	2.19	0.73
1:D:129:LYS:HD3	1:D:129:LYS:H	1.52	0.73
1:E:33:ILE:HD12	1:E:42:ILE:HD11	1.70	0.72
1:K:104:ILE:HB	1:L:107:VAL:CG1	2.18	0.72
1:G:102:MET:CE	1:G:132:ILE:HG23	2.20	0.72
1:A:48:ILE:HG22	1:A:115:PRO:HA	1.72	0.72
1:H:155:ILE:HG23	1:H:155:ILE:O	1.90	0.72
1:L:102:MET:CE	1:L:154:MET:HB3	2.20	0.71
1:E:107:VAL:HG11	1:F:104:ILE:HB	1.71	0.71
1:I:101:PHE:CB	1:I:153:ALA:HB2	2.19	0.71
1:B:131:MET:O	1:B:154:MET:HA	1.91	0.71
1:C:62:LYS:HD3	1:D:159:GLU:O	1.89	0.71
1:H:129:LYS:NZ	1:H:132:ILE:HD12	2.05	0.71
1:A:90:ASP:HB3	1:A:93:ILE:HG22	1.73	0.71
1:J:98:ILE:HD13	1:J:99:VAL:H	1.55	0.71
1:B:107:VAL:HG22	1:B:149:ALA:CB	2.21	0.70
1:G:158:ARG:HD2	1:H:62:LYS:NZ	2.05	0.70
1:I:101:PHE:HA	1:I:153:ALA:HA	1.72	0.70
1:B:22:PRO:HG3	1:B:98:ILE:HG13	1.72	0.70
1:I:96:THR:O	1:I:97:LYS:HE3	1.90	0.70
1:A:11:GLN:HE21	1:A:12:PHE:N	1.89	0.70
1:C:104:ILE:HB	1:D:107:VAL:CG1	2.21	0.70
1:H:47:ASN:HB3	1:I:47:ASN:HB3	1.74	0.70
1:C:62:LYS:HZ2	1:D:159:GLU:HG2	1.55	0.70
1:L:58:HIS:HD2	1:L:64:ILE:O	1.74	0.70
1:D:111:ILE:O	1:D:146:VAL:HG13	1.91	0.70
1:E:107:VAL:CG1	1:F:104:ILE:HB	2.21	0.70
1:A:97:LYS:HD2	1:A:157:GLU:OE1	1.91	0.69
1:C:107:VAL:HA	1:C:148:GLU:O	1.92	0.69
1:B:102:MET:HE3	1:B:154:MET:HB2	1.74	0.69
1:D:131:MET:O	1:D:133:TRP:HD1	1.75	0.69
1:I:129:LYS:HG2	1:I:130:GLY:H	1.55	0.69
1:I:97:LYS:HD3	1:I:155:ILE:HG22	1.75	0.69
1:H:86:LEU:HD23	1:H:87:TRP:CH2	2.27	0.69
1:B:38:ALA:C	1:B:40:GLN:H	1.95	0.69
1:D:20:ILE:HG23	1:D:83:PHE:CD2	2.26	0.69
1:B:129:LYS:HD3	1:B:132:ILE:HB	1.73	0.68
1:K:11:GLN:HG3	1:K:33:ILE:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:HG3	1:A:158:ARG:O	1.94	0.68
1:B:107:VAL:HG22	1:B:149:ALA:HB2	1.73	0.68
1:A:37:GLN:HB3	1:A:40:GLN:HB2	1.76	0.68
1:C:22:PRO:HG3	1:C:98:ILE:HA	1.76	0.68
1:D:102:MET:HG3	1:D:153:ALA:HA	1.74	0.68
1:I:158:ARG:HG3	1:I:158:ARG:HH11	1.58	0.68
1:B:91:PRO:O	1:B:94:ALA:HB3	1.92	0.68
1:H:110:ARG:HH11	1:H:110:ARG:HG2	1.57	0.68
1:B:150:GLU:O	1:B:151:LEU:HD23	1.94	0.67
1:B:29:LEU:H	1:B:76:GLN:HE22	1.42	0.67
1:H:12:PHE:HB2	1:H:33:ILE:HB	1.76	0.67
1:I:129:LYS:HG2	1:I:130:GLY:N	2.09	0.67
1:C:131:MET:O	1:C:154:MET:HA	1.94	0.67
1:L:107:VAL:HA	1:L:148:GLU:O	1.94	0.67
1:C:12:PHE:HB2	1:C:33:ILE:HB	1.76	0.67
1:A:100:ALA:HB3	1:A:154:MET:HB3	1.76	0.67
1:E:158:ARG:O	1:E:159:GLU:HB3	1.94	0.66
1:G:107:VAL:HG13	1:H:104:ILE:HB	1.77	0.66
1:K:104:ILE:HB	1:L:107:VAL:HG13	1.78	0.66
1:L:102:MET:HE2	1:L:154:MET:HB3	1.77	0.66
1:K:86:LEU:HD13	1:K:133:TRP:HZ2	1.59	0.66
1:J:107:VAL:HG22	1:J:149:ALA:HB1	1.79	0.66
1:E:90:ASP:CG	1:E:93:ILE:HG12	2.17	0.65
1:H:126:LEU:CB	1:H:134:GLN:HE22	2.05	0.65
1:E:111:ILE:O	1:E:146:VAL:HG22	1.97	0.65
1:J:139:ALA:HB3	1:J:147:ALA:HB3	1.78	0.65
1:A:104:ILE:HB	1:B:107:VAL:HB	1.79	0.65
1:C:126:LEU:HB2	1:C:134:GLN:CG	2.27	0.65
1:I:99:VAL:HG12	1:I:99:VAL:O	1.96	0.65
1:H:131:MET:HB2	1:H:155:ILE:HB	1.78	0.65
1:A:15:GLU:O	1:A:19:GLN:HG3	1.97	0.65
1:A:11:GLN:HE21	1:A:11:GLN:CA	2.09	0.64
1:E:134:GLN:HG3	1:E:152:LYS:HD3	1.79	0.64
1:I:129:LYS:NZ	1:I:129:LYS:HB3	2.11	0.64
1:A:102:MET:HB2	1:A:152:LYS:O	1.98	0.64
1:B:155:ILE:O	1:B:155:ILE:CG2	2.45	0.64
1:G:104:ILE:HB	1:H:107:VAL:CG2	2.27	0.64
1:C:126:LEU:HD12	1:C:134:GLN:NE2	2.11	0.64
1:J:8:LEU:HD13	1:J:8:LEU:O	1.98	0.64
1:K:58:HIS:HD2	1:K:64:ILE:O	1.81	0.64
1:C:126:LEU:HB2	1:C:134:GLN:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:HD12	1:C:134:GLN:CD	2.18	0.64
1:J:158:ARG:HD2	3:J:175:HOH:O	1.97	0.64
1:L:90:ASP:OD1	1:L:92:GLU:HB2	1.98	0.64
1:G:47:ASN:HB3	1:L:47:ASN:HB3	1.78	0.64
1:E:104:ILE:HB	1:F:107:VAL:CG1	2.28	0.64
1:J:15:GLU:CD	1:J:15:GLU:H	2.01	0.63
1:B:41:LYS:HB3	1:B:124:GLU:HG3	1.80	0.63
1:C:96:THR:HG23	1:C:97:LYS:CD	2.28	0.63
1:H:120:GLU:HG2	1:H:122:HIS:NE2	2.13	0.63
1:C:39:ASN:ND2	1:C:133:TRP:HH2	1.96	0.63
1:D:133:TRP:O	1:D:152:LYS:HG3	1.98	0.63
1:L:98:ILE:HG23	1:L:158:ARG:HG2	1.79	0.63
1:H:110:ARG:HG2	1:H:110:ARG:NH1	2.14	0.62
1:F:9:GLN:HG2	1:F:12:PHE:CZ	2.34	0.62
1:I:12:PHE:HB3	1:I:16:HIS:HB2	1.80	0.62
1:I:138:THR:HG22	1:I:148:GLU:HB3	1.81	0.62
1:J:122:HIS:O	1:J:137:GLY:HA3	1.99	0.62
1:D:110:ARG:HH11	1:D:110:ARG:CB	2.12	0.62
1:H:33:ILE:HD12	1:H:42:ILE:HD11	1.81	0.62
1:C:104:ILE:HB	1:D:107:VAL:HG13	1.82	0.62
1:E:102:MET:HE3	1:E:132:ILE:HG23	1.81	0.62
1:C:68:VAL:HB	1:D:68:VAL:HB	1.82	0.62
1:I:129:LYS:HB3	1:I:129:LYS:HZ2	1.65	0.62
1:J:99:VAL:O	1:J:99:VAL:HG13	2.00	0.62
1:F:140:GLN:OE1	1:K:144:LYS:HE2	1.99	0.62
1:D:113:VAL:CG2	1:D:146:VAL:HG11	2.29	0.62
1:I:97:LYS:HG3	1:I:156:ALA:O	2.00	0.61
1:B:13:PHE:H	1:B:16:HIS:CD2	2.07	0.61
1:B:129:LYS:CG	1:B:130:GLY:N	2.60	0.61
1:D:123:LEU:HD22	1:D:135:VAL:CG2	2.29	0.61
1:I:48:ILE:HG22	1:I:115:PRO:HA	1.81	0.61
1:G:101:PHE:HB2	2:G:1008:CL:CL	2.37	0.61
1:J:29:LEU:H	1:J:76:GLN:HE22	1.48	0.61
1:C:29:LEU:H	1:C:76:GLN:NE2	1.99	0.61
1:G:158:ARG:HD2	1:H:62:LYS:HZ1	1.64	0.61
1:A:90:ASP:HB3	1:A:93:ILE:CG2	2.30	0.61
1:B:36:LEU:HD11	1:B:81:LEU:HD13	1.82	0.61
1:C:129:LYS:HB3	1:C:129:LYS:HZ3	1.64	0.61
1:A:36:LEU:HD21	1:A:84:THR:HG21	1.83	0.61
1:F:29:LEU:H	1:F:76:GLN:NE2	1.99	0.61
1:J:151:LEU:HD12	1:J:151:LEU:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:ASP:CG	1:L:93:ILE:HG13	2.20	0.61
1:A:122:HIS:O	1:A:137:GLY:HA3	2.01	0.61
1:E:155:ILE:O	1:E:155:ILE:HG13	2.01	0.61
1:A:111:ILE:HD11	1:A:144:LYS:HD2	1.82	0.60
1:D:90:ASP:CG	1:D:93:ILE:HG12	2.21	0.60
1:I:123:LEU:HD12	1:I:135:VAL:HG12	1.81	0.60
1:G:86:LEU:HG	1:G:131:MET:SD	2.41	0.60
1:H:87:TRP:CH2	1:H:97:LYS:HE2	2.36	0.60
1:I:97:LYS:HD3	1:I:155:ILE:CG2	2.30	0.60
1:A:100:ALA:O	1:A:154:MET:N	2.35	0.60
1:C:29:LEU:N	1:C:76:GLN:HE22	2.00	0.60
1:K:29:LEU:H	1:K:76:GLN:NE2	1.99	0.60
1:D:20:ILE:O	1:D:94:ALA:HB1	2.01	0.60
1:G:39:ASN:HD22	1:G:133:TRP:HH2	1.49	0.60
1:J:159:GLU:O	1:J:159:GLU:HG3	2.01	0.60
1:C:129:LYS:HB3	1:C:129:LYS:HZ2	1.65	0.60
1:F:141:VAL:HG23	1:F:146:VAL:HG21	1.83	0.60
1:I:58:HIS:HD2	1:I:64:ILE:O	1.83	0.60
1:I:158:ARG:HG3	1:I:158:ARG:NH1	2.16	0.60
1:J:35:GLU:HB3	1:J:43:VAL:HB	1.83	0.60
1:H:129:LYS:HZ2	1:H:132:ILE:HG21	1.67	0.60
1:F:29:LEU:N	1:F:76:GLN:HE22	1.98	0.60
1:A:96:THR:O	1:A:158:ARG:N	2.29	0.59
1:G:58:HIS:HD2	1:G:64:ILE:O	1.85	0.59
1:G:132:ILE:HG12	1:G:154:MET:HB3	1.83	0.59
1:J:39:ASN:O	1:J:39:ASN:ND2	2.34	0.59
1:C:125:VAL:O	1:C:126:LEU:HD23	2.02	0.59
1:D:58:HIS:CD2	1:D:64:ILE:O	2.52	0.59
1:H:131:MET:HB2	1:H:155:ILE:CB	2.31	0.59
1:K:104:ILE:HB	1:L:107:VAL:HG11	1.84	0.59
1:D:120:GLU:O	1:D:139:ALA:HA	2.03	0.59
1:E:111:ILE:HB	1:E:146:VAL:HG23	1.84	0.59
1:C:96:THR:HG23	1:C:97:LYS:CE	2.33	0.59
1:E:86:LEU:HD12	1:E:155:ILE:HD11	1.85	0.59
1:G:131:MET:O	1:G:154:MET:HA	2.03	0.59
1:F:32:ARG:O	1:F:44:ALA:HB1	2.03	0.59
1:B:92:GLU:O	1:B:93:ILE:C	2.41	0.59
1:I:58:HIS:HE1	3:J:170:HOH:O	1.85	0.59
1:K:107:VAL:HG13	1:L:104:ILE:O	2.02	0.59
1:J:150:GLU:C	1:J:151:LEU:HD12	2.23	0.59
1:G:123:LEU:HB3	1:G:135:VAL:HG11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:35:GLU:HB3	1:L:43:VAL:HB	1.85	0.58
1:B:85:SER:O	1:B:86:LEU:HG	2.03	0.58
1:G:107:VAL:CG1	1:H:104:ILE:HB	2.34	0.58
1:J:37:GLN:HG3	1:J:41:LYS:HZ2	1.67	0.58
1:J:42:ILE:HD13	1:J:43:VAL:N	2.18	0.58
1:B:17:ILE:HG23	1:B:21:LEU:HD12	1.85	0.58
1:K:29:LEU:N	1:K:76:GLN:HE22	2.00	0.58
1:B:61:ASN:N	1:B:61:ASN:HD22	2.00	0.58
1:A:138:THR:HG22	1:A:148:GLU:HB3	1.86	0.58
1:G:58:HIS:CD2	1:G:64:ILE:O	2.57	0.58
1:G:158:ARG:NH1	1:G:158:ARG:CB	2.66	0.58
1:H:29:LEU:H	1:H:76:GLN:HE22	1.50	0.58
1:F:58:HIS:HD2	1:F:64:ILE:O	1.87	0.58
1:I:126:LEU:HD12	1:I:134:GLN:HE22	1.69	0.58
1:C:42:ILE:HB	1:C:81:LEU:HD23	1.84	0.58
1:G:104:ILE:HB	1:H:107:VAL:HG22	1.85	0.58
1:E:102:MET:HE1	1:E:132:ILE:HG12	1.85	0.58
1:D:35:GLU:O	1:D:42:ILE:HG12	2.03	0.57
1:B:93:ILE:O	1:B:96:THR:HB	2.04	0.57
1:D:113:VAL:HG22	1:D:146:VAL:HG11	1.85	0.57
1:K:97:LYS:NZ	1:K:157:GLU:HG2	2.18	0.57
1:K:104:ILE:O	1:L:107:VAL:HG13	2.03	0.57
1:B:138:THR:HG22	1:B:148:GLU:HB3	1.86	0.57
1:K:111:ILE:O	1:K:146:VAL:HG13	2.05	0.57
1:B:129:LYS:HE2	1:B:131:MET:H	1.70	0.57
1:E:122:HIS:O	1:E:137:GLY:HA3	2.04	0.57
1:H:86:LEU:HB3	1:H:87:TRP:CE3	2.38	0.57
1:A:108:LYS:HZ2	1:A:148:GLU:CD	2.07	0.57
1:B:150:GLU:C	1:B:151:LEU:HD23	2.25	0.57
1:D:42:ILE:HD13	1:D:43:VAL:N	2.20	0.57
1:B:34:THR:OG1	1:B:43:VAL:HG12	2.04	0.57
1:C:83:PHE:HE2	1:C:97:LYS:HB2	1.69	0.57
1:A:108:LYS:HB2	1:A:108:LYS:NZ	2.19	0.57
1:B:36:LEU:HD11	1:B:81:LEU:CD1	2.35	0.57
1:F:113:VAL:HG22	1:F:146:VAL:HG11	1.87	0.57
1:H:108:LYS:HD2	1:H:110:ARG:CZ	2.35	0.57
1:H:132:ILE:HB	1:H:154:MET:SD	2.44	0.57
1:A:8:LEU:HD13	1:A:9:GLN:O	2.04	0.57
1:B:101:PHE:CE2	1:B:153:ALA:HB2	2.40	0.57
1:B:125:VAL:O	1:B:126:LEU:HD23	2.05	0.57
1:C:97:LYS:HD2	1:C:97:LYS:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:MET:HG3	1:E:154:MET:HG3	1.87	0.56
1:I:96:THR:O	1:I:97:LYS:HB2	2.04	0.56
1:J:101:PHE:CE2	1:J:104:ILE:HD11	2.40	0.56
1:H:60:PRO:O	1:H:61:ASN:HB2	2.05	0.56
1:K:141:VAL:HG23	1:K:146:VAL:HG21	1.88	0.56
1:H:87:TRP:CZ2	1:H:97:LYS:HE2	2.41	0.56
1:I:87:TRP:CZ3	1:I:155:ILE:HG21	2.41	0.56
1:C:42:ILE:HB	1:C:81:LEU:CD2	2.35	0.56
1:C:82:ALA:CB	1:C:155:ILE:HD11	2.32	0.56
1:F:35:GLU:OE1	1:F:37:GLN:NE2	2.38	0.56
1:L:102:MET:HE2	1:L:154:MET:N	2.21	0.56
1:J:96:THR:O	1:J:158:ARG:HG3	2.06	0.56
1:H:129:LYS:HZ1	1:H:132:ILE:HD12	1.68	0.56
1:D:110:ARG:HH11	1:D:110:ARG:HB2	1.69	0.55
1:B:75:ALA:HB1	1:B:101:PHE:CZ	2.42	0.55
1:J:8:LEU:O	1:J:9:GLN:O	2.25	0.55
1:B:155:ILE:O	1:B:155:ILE:HG23	2.07	0.55
1:E:83:PHE:HZ	1:E:97:LYS:O	1.89	0.55
1:G:42:ILE:HB	1:G:81:LEU:HD22	1.89	0.55
1:G:141:VAL:CG2	1:G:146:VAL:HG21	2.37	0.55
1:H:48:ILE:HG22	1:H:115:PRO:HA	1.89	0.55
1:H:98:ILE:O	1:H:156:ALA:HB3	2.07	0.55
1:I:122:HIS:O	1:I:137:GLY:HA3	2.07	0.55
1:K:113:VAL:CG2	1:K:146:VAL:HG11	2.36	0.55
1:A:11:GLN:NE2	1:A:12:PHE:N	2.55	0.55
1:D:47:ASN:HB3	1:E:47:ASN:HB3	1.88	0.55
1:I:104:ILE:HD12	1:J:107:VAL:HG11	1.89	0.55
1:A:97:LYS:HG2	1:A:155:ILE:HG22	1.86	0.55
1:B:131:MET:HA	1:B:131:MET:HE2	1.89	0.55
1:C:90:ASP:OD1	1:C:92:GLU:HG3	2.06	0.55
1:D:123:LEU:HD22	1:D:135:VAL:HG23	1.88	0.55
1:B:37:GLN:NE2	1:B:40:GLN:HG3	2.21	0.55
1:G:135:VAL:HG12	1:G:136:GLY:N	2.23	0.54
1:C:97:LYS:HG2	1:C:155:ILE:HG22	1.88	0.54
1:B:33:ILE:HD13	1:B:80:PHE:CD2	2.42	0.54
1:E:107:VAL:HG12	1:F:104:ILE:O	2.06	0.54
3:I:1020:HOH:O	1:J:58:HIS:HE1	1.90	0.54
1:H:96:THR:OG1	1:H:97:LYS:N	2.41	0.54
1:G:93:ILE:O	1:G:93:ILE:HG22	2.08	0.54
1:G:129:LYS:O	1:G:130:GLY:O	2.24	0.54
1:J:107:VAL:HG22	1:J:149:ALA:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:75:ALA:HB2	1:J:151:LEU:HD23	1.90	0.54
1:K:99:VAL:HG22	1:K:155:ILE:HD13	1.90	0.54
1:H:127:LYS:HG2	1:H:128:HIS:N	2.23	0.54
1:B:131:MET:C	1:B:132:ILE:HD12	2.27	0.53
1:F:122:HIS:O	1:F:137:GLY:HA3	2.08	0.53
1:I:17:ILE:HD11	1:I:33:ILE:HG13	1.90	0.53
1:A:13:PHE:H	1:A:16:HIS:CD2	2.18	0.53
1:B:131:MET:HA	1:B:131:MET:CE	2.38	0.53
1:H:154:MET:HG3	1:H:155:ILE:N	2.18	0.53
1:J:157:GLU:OE2	1:J:157:GLU:HA	2.09	0.53
1:E:58:HIS:HD2	1:E:64:ILE:O	1.90	0.53
1:B:120:GLU:O	1:B:139:ALA:HA	2.08	0.53
1:I:35:GLU:HG3	1:I:43:VAL:HB	1.90	0.53
1:K:107:VAL:HA	1:K:148:GLU:O	2.09	0.53
1:I:101:PHE:HD1	1:I:101:PHE:H	1.57	0.53
1:A:110:ARG:HG2	1:A:110:ARG:HH11	1.74	0.53
1:L:111:ILE:HB	1:L:146:VAL:HG23	1.90	0.53
1:B:86:LEU:CG	1:B:133:TRP:HZ2	2.22	0.53
1:D:16:HIS:HB3	1:D:89:PHE:CE1	2.44	0.53
1:D:42:ILE:HD13	1:D:42:ILE:C	2.29	0.53
1:B:132:ILE:HG22	1:B:132:ILE:O	2.09	0.53
1:C:126:LEU:HB2	1:C:134:GLN:CD	2.29	0.53
1:F:36:LEU:HD23	1:F:36:LEU:C	2.29	0.53
1:F:97:LYS:HG2	1:F:155:ILE:CG2	2.39	0.53
1:H:90:ASP:OD2	1:H:93:ILE:HD12	2.07	0.53
1:L:102:MET:CE	1:L:132:ILE:HG23	2.38	0.53
1:C:66:PRO:HB2	1:C:69:LEU:HG	1.90	0.53
1:L:93:ILE:HG22	1:L:97:LYS:HE2	1.91	0.53
1:L:102:MET:HE1	1:L:154:MET:HB3	1.90	0.53
1:L:157:GLU:C	1:L:159:GLU:H	2.12	0.53
1:K:36:LEU:C	1:K:36:LEU:HD23	2.28	0.52
1:L:139:ALA:O	1:L:146:VAL:HG12	2.09	0.52
1:D:17:ILE:HG23	1:D:21:LEU:HD12	1.91	0.52
1:H:129:LYS:HZ2	1:H:132:ILE:HD12	1.73	0.52
1:I:35:GLU:CG	1:I:43:VAL:HB	2.39	0.52
1:J:70:ILE:HG12	1:J:119:LEU:HD21	1.91	0.52
1:B:67:GLY:HA2	1:B:70:ILE:HD12	1.92	0.52
1:E:111:ILE:HB	1:E:146:VAL:CG2	2.39	0.52
1:E:111:ILE:HD12	1:E:111:ILE:N	2.25	0.52
1:I:36:LEU:HD23	1:I:37:GLN:N	2.25	0.52
1:E:104:ILE:HB	1:F:107:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:GLY:O	1:H:90:ASP:N	2.42	0.52
1:I:38:ALA:O	1:I:40:GLN:N	2.42	0.52
1:J:61:ASN:N	1:J:61:ASN:HD22	2.07	0.52
1:J:97:LYS:HA	1:J:156:ALA:O	2.09	0.52
1:B:38:ALA:C	1:B:40:GLN:N	2.63	0.52
1:B:87:TRP:HH2	1:B:155:ILE:HG21	1.75	0.52
1:G:108:LYS:HB2	1:G:148:GLU:HG2	1.90	0.52
1:H:86:LEU:HD13	1:H:133:TRP:HZ2	1.73	0.52
1:L:66:PRO:HD2	1:L:69:LEU:HD12	1.91	0.52
1:D:33:ILE:HD13	1:D:80:PHE:CE2	2.45	0.52
1:K:158:ARG:O	1:K:159:GLU:O	2.28	0.52
1:A:11:GLN:CA	1:A:11:GLN:NE2	2.72	0.52
1:H:86:LEU:HD23	1:H:87:TRP:CZ2	2.45	0.52
1:B:36:LEU:HD12	1:B:37:GLN:N	2.25	0.51
1:G:134:GLN:HB2	1:G:152:LYS:HG3	1.92	0.51
1:I:98:ILE:HG12	1:I:99:VAL:N	2.25	0.51
1:L:140:GLN:HG2	1:L:145:VAL:HA	1.92	0.51
1:E:107:VAL:HG13	1:F:104:ILE:H	1.75	0.51
1:E:131:MET:O	1:E:154:MET:HA	2.11	0.51
1:E:158:ARG:NH2	3:E:1023:HOH:O	2.42	0.51
1:I:86:LEU:HD12	1:I:155:ILE:CD1	2.40	0.51
1:C:24:ARG:O	1:D:57:GLY:HA3	2.10	0.51
1:K:141:VAL:CG2	1:K:146:VAL:HG21	2.40	0.51
1:B:36:LEU:HD12	1:B:37:GLN:H	1.75	0.51
1:H:122:HIS:O	1:H:137:GLY:HA3	2.11	0.51
1:A:108:LYS:HZ2	1:A:148:GLU:CG	2.24	0.51
1:D:34:THR:OG1	1:D:43:VAL:HG22	2.10	0.51
1:H:105:ASP:HB3	1:H:106:LYS:HG2	1.92	0.51
1:I:142:ASP:O	1:I:144:LYS:HG3	2.11	0.51
1:K:107:VAL:HG13	1:L:104:ILE:HB	1.91	0.51
1:L:118:ARG:NH2	3:L:174:HOH:O	2.42	0.51
1:A:108:LYS:HB3	1:A:148:GLU:HG2	1.93	0.51
1:G:101:PHE:HE1	1:G:151:LEU:HB2	1.76	0.51
1:L:110:ARG:NH1	1:L:145:VAL:HB	2.26	0.51
1:D:141:VAL:HG23	1:D:146:VAL:HG21	1.93	0.51
1:G:104:ILE:H	1:H:107:VAL:HG22	1.76	0.51
1:H:58:HIS:HD2	1:H:64:ILE:O	1.94	0.51
1:F:96:THR:O	1:F:97:LYS:HD2	2.12	0.50
1:E:71:VAL:HG11	1:E:104:ILE:HD13	1.93	0.50
1:G:48:ILE:HG22	1:G:115:PRO:HA	1.92	0.50
1:I:58:HIS:CD2	1:I:64:ILE:O	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:HIS:CD2	1:I:140:GLN:NE2	2.79	0.50
1:B:86:LEU:HG	1:B:133:TRP:HZ2	1.75	0.50
1:L:128:HIS:CD2	1:L:129:LYS:N	2.79	0.50
1:C:120:GLU:O	1:C:139:ALA:HA	2.11	0.50
1:D:37:GLN:CB	1:D:40:GLN:HB2	2.41	0.50
1:H:66:PRO:HB2	1:H:69:LEU:HG	1.92	0.50
1:L:22:PRO:HB3	1:L:158:ARG:NH2	2.26	0.50
1:A:35:GLU:HB3	1:A:43:VAL:HB	1.94	0.50
1:G:102:MET:HE3	1:G:152:LYS:HG2	1.93	0.50
1:E:104:ILE:HB	1:F:107:VAL:HG13	1.93	0.50
1:G:104:ILE:N	1:H:107:VAL:HG22	2.27	0.50
1:I:13:PHE:N	1:I:16:HIS:HD2	1.99	0.50
1:B:33:ILE:HD13	1:B:80:PHE:CE2	2.47	0.50
1:B:75:ALA:HB1	1:B:101:PHE:CE1	2.47	0.50
1:G:113:VAL:CG2	1:G:146:VAL:HG11	2.42	0.50
1:G:141:VAL:HG23	1:G:146:VAL:HG21	1.93	0.50
1:F:75:ALA:HB2	1:F:101:PHE:CZ	2.47	0.50
1:F:101:PHE:HB2	2:F:1004:CL:CL	2.48	0.50
1:A:83:PHE:CZ	1:A:94:ALA:HB2	2.47	0.49
1:B:61:ASN:O	1:B:62:LYS:HB2	2.11	0.49
1:E:107:VAL:HA	1:E:148:GLU:O	2.12	0.49
1:G:107:VAL:HG13	1:H:104:ILE:O	2.11	0.49
1:F:36:LEU:HD23	1:F:37:GLN:N	2.26	0.49
1:F:141:VAL:CG2	1:F:146:VAL:HG21	2.42	0.49
1:G:39:ASN:ND2	1:G:85:SER:CB	2.74	0.49
1:E:86:LEU:CD1	1:E:155:ILE:HD11	2.42	0.49
1:H:96:THR:OG1	1:H:97:LYS:HG3	2.13	0.49
1:I:101:PHE:HB2	1:I:152:LYS:O	2.13	0.49
1:A:29:LEU:H	1:A:76:GLN:HE22	1.60	0.49
1:C:126:LEU:HD12	1:C:134:GLN:OE1	2.12	0.49
1:G:18:LEU:HD21	1:L:50:PHE:CZ	2.47	0.49
1:K:37:GLN:HE21	1:K:41:LYS:HE2	1.77	0.49
1:K:75:ALA:HB2	1:K:101:PHE:CZ	2.47	0.49
1:D:102:MET:HG3	1:D:153:ALA:CA	2.43	0.49
1:G:102:MET:HE1	1:G:153:ALA:C	2.33	0.49
1:H:108:LYS:NZ	1:H:110:ARG:HH22	2.10	0.49
1:H:131:MET:HB2	1:H:155:ILE:HG21	1.90	0.49
1:B:107:VAL:HG22	1:B:149:ALA:HB1	1.94	0.49
1:C:104:ILE:HB	1:D:107:VAL:HG11	1.93	0.49
1:H:132:ILE:HA	1:H:154:MET:HA	1.93	0.49
1:A:96:THR:O	1:A:158:ARG:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:CG2	1:B:152:LYS:HE3	2.42	0.49
1:H:98:ILE:HB	1:H:156:ALA:CB	2.43	0.49
1:I:111:ILE:HB	1:I:146:VAL:HG12	1.95	0.49
1:H:14:ILE:O	1:H:18:LEU:HD22	2.12	0.49
1:A:8:LEU:O	1:A:9:GLN:CG	2.58	0.49
1:C:32:ARG:HB3	1:C:45:TYR:CE1	2.47	0.49
1:E:102:MET:HE1	1:E:154:MET:HB2	1.95	0.49
1:K:83:PHE:CE1	1:K:155:ILE:HD12	2.48	0.49
1:C:134:GLN:HG3	1:C:134:GLN:O	2.12	0.48
1:F:107:VAL:HA	1:F:148:GLU:O	2.12	0.48
1:G:140:GLN:HG2	1:G:145:VAL:HA	1.95	0.48
1:I:24:ARG:O	1:J:57:GLY:HA3	2.13	0.48
1:I:129:LYS:HZ3	1:I:132:ILE:HB	1.69	0.48
1:J:98:ILE:HD13	1:J:99:VAL:N	2.26	0.48
1:J:158:ARG:HB3	1:J:158:ARG:NH1	2.24	0.48
1:K:97:LYS:HZ3	1:K:157:GLU:HG2	1.78	0.48
1:I:101:PHE:HA	1:I:153:ALA:CA	2.43	0.48
1:E:104:ILE:O	1:F:107:VAL:HG13	2.14	0.48
1:C:134:GLN:HE21	1:C:135:VAL:N	2.11	0.48
1:E:96:THR:O	1:E:97:LYS:HG2	2.13	0.48
1:E:128:HIS:CD2	1:E:129:LYS:N	2.82	0.48
1:I:59:PHE:CE2	1:J:98:ILE:HD11	2.49	0.48
1:B:88:GLY:O	1:B:90:ASP:N	2.47	0.48
1:G:102:MET:CE	1:G:152:LYS:HG2	2.43	0.48
1:A:90:ASP:CB	1:A:93:ILE:HG22	2.41	0.48
1:D:37:GLN:HB3	1:D:40:GLN:HB2	1.96	0.48
1:F:13:PHE:H	1:F:16:HIS:CD2	2.21	0.48
1:G:123:LEU:HB3	1:G:135:VAL:CG1	2.42	0.48
1:J:131:MET:HE2	1:J:155:ILE:O	2.14	0.48
1:E:158:ARG:O	1:E:158:ARG:HG2	2.14	0.48
1:I:107:VAL:HG22	1:I:149:ALA:CB	2.44	0.48
1:A:131:MET:C	1:A:132:ILE:HD12	2.33	0.48
1:C:74:MET:HB3	1:C:123:LEU:HD11	1.96	0.48
1:E:102:MET:CE	1:E:132:ILE:HG23	2.43	0.48
1:J:46:LYS:NZ	1:J:52:GLU:OE1	2.46	0.48
1:J:131:MET:HE3	1:J:155:ILE:CG2	2.44	0.48
1:K:82:ALA:O	1:K:86:LEU:HB2	2.14	0.48
1:A:72:GLU:HB2	1:B:68:VAL:HG21	1.96	0.47
1:B:112:PRO:HD3	3:B:1007:HOH:O	2.14	0.47
1:I:24:ARG:HG2	1:I:24:ARG:HH21	1.78	0.47
1:K:67:GLY:HA2	1:K:70:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:ILE:O	1:F:146:VAL:CG1	2.62	0.47
1:G:96:THR:HG22	1:G:96:THR:O	2.13	0.47
1:G:158:ARG:HD2	1:H:62:LYS:HZ3	1.78	0.47
1:I:66:PRO:HB2	1:I:69:LEU:HG	1.96	0.47
1:B:86:LEU:HG	1:B:133:TRP:CZ2	2.49	0.47
1:E:159:GLU:O	1:E:159:GLU:HG3	2.14	0.47
1:J:87:TRP:HH2	1:J:131:MET:CE	2.28	0.47
1:C:62:LYS:HZ1	1:D:159:GLU:HG2	1.79	0.47
1:D:33:ILE:HD13	1:D:80:PHE:CD2	2.50	0.47
1:D:131:MET:O	1:D:133:TRP:CD1	2.63	0.47
1:E:72:GLU:HG3	1:E:76:GLN:HE21	1.80	0.47
1:F:60:PRO:O	1:F:61:ASN:HB2	2.15	0.47
1:K:98:ILE:HG23	1:K:158:ARG:CG	2.37	0.47
1:B:61:ASN:N	1:B:61:ASN:ND2	2.63	0.47
1:D:125:VAL:HG21	1:D:133:TRP:HZ3	1.79	0.47
1:E:12:PHE:CE1	1:E:36:LEU:HD23	2.50	0.47
1:F:97:LYS:HG2	1:F:155:ILE:HG22	1.95	0.47
1:J:23:HIS:CE1	1:J:99:VAL:HG11	2.50	0.47
1:J:58:HIS:HD2	1:J:64:ILE:O	1.98	0.47
1:B:70:ILE:O	1:B:74:MET:HG3	2.14	0.47
1:B:90:ASP:OD1	1:B:92:GLU:HB2	2.15	0.47
1:D:128:HIS:O	1:D:132:ILE:O	2.33	0.47
1:H:82:ALA:O	1:H:85:SER:HB2	2.15	0.47
1:H:108:LYS:HD2	1:H:110:ARG:NH2	2.30	0.47
1:I:59:PHE:CZ	1:J:98:ILE:HD11	2.50	0.47
1:A:110:ARG:HG2	1:A:110:ARG:NH1	2.30	0.47
1:H:127:LYS:C	1:H:127:LYS:HD3	2.35	0.47
1:I:37:GLN:HG2	1:I:40:GLN:CD	2.35	0.47
1:A:42:ILE:CG2	1:A:123:LEU:HB2	2.46	0.47
1:A:99:VAL:HA	1:A:154:MET:O	2.16	0.47
1:B:58:HIS:HD2	1:B:64:ILE:O	1.98	0.47
1:E:96:THR:C	1:E:97:LYS:HG2	2.36	0.47
1:J:82:ALA:O	1:J:86:LEU:HD12	2.15	0.47
1:K:86:LEU:HD13	1:K:133:TRP:CZ2	2.46	0.47
1:A:66:PRO:HB2	1:A:69:LEU:HG	1.96	0.46
1:B:72:GLU:O	1:B:76:GLN:HG3	2.15	0.46
1:B:131:MET:SD	1:B:155:ILE:CG2	3.01	0.46
1:D:16:HIS:HB3	1:D:89:PHE:HE1	1.80	0.46
1:H:98:ILE:CG2	1:H:99:VAL:H	2.24	0.46
1:K:122:HIS:O	1:K:137:GLY:HA3	2.15	0.46
1:B:17:ILE:CG2	1:B:21:LEU:HD12	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:GLY:HA2	1:F:24:ARG:HB2	1.97	0.46
1:H:32:ARG:O	1:H:44:ALA:HB1	2.16	0.46
1:E:102:MET:CE	1:E:154:MET:HB2	2.46	0.46
1:B:102:MET:SD	1:B:154:MET:CB	3.03	0.46
1:H:42:ILE:CG2	1:H:81:LEU:HD12	2.30	0.46
1:H:131:MET:O	1:H:155:ILE:N	2.49	0.46
1:F:66:PRO:HB2	1:F:69:LEU:HG	1.98	0.46
1:C:32:ARG:O	1:C:44:ALA:HB1	2.14	0.46
1:D:37:GLN:O	1:D:38:ALA:C	2.53	0.46
1:D:122:HIS:O	1:D:137:GLY:HA3	2.15	0.46
1:D:125:VAL:HA	1:D:135:VAL:HG12	1.98	0.46
1:E:102:MET:HE2	1:E:153:ALA:C	2.36	0.46
1:L:102:MET:HE1	1:L:132:ILE:HG23	1.98	0.46
1:A:106:LYS:O	1:A:149:ALA:HA	2.16	0.46
1:E:107:VAL:HG13	1:F:104:ILE:N	2.31	0.46
1:A:15:GLU:CD	1:A:15:GLU:H	2.18	0.46
1:E:155:ILE:CG1	1:E:155:ILE:O	2.64	0.46
1:H:18:LEU:HD12	1:H:24:ARG:CZ	2.46	0.46
1:H:125:VAL:HA	1:H:135:VAL:HG12	1.97	0.46
1:B:129:LYS:HG2	1:B:130:GLY:H	1.78	0.45
1:J:42:ILE:HD13	1:J:42:ILE:C	2.36	0.45
1:J:87:TRP:HH2	1:J:131:MET:HE3	1.78	0.45
1:L:35:GLU:O	1:L:42:ILE:HA	2.16	0.45
1:C:30:VAL:HG23	1:C:76:GLN:HE21	1.82	0.45
1:K:107:VAL:CG1	1:L:104:ILE:HB	2.46	0.45
1:B:40:GLN:O	1:B:125:VAL:HG23	2.17	0.45
1:C:97:LYS:HG2	1:C:155:ILE:CG2	2.45	0.45
3:C:1020:HOH:O	1:D:58:HIS:HE1	1.98	0.45
1:J:12:PHE:HB3	1:J:16:HIS:HB2	1.98	0.45
1:J:102:MET:HE1	1:J:132:ILE:HG23	1.97	0.45
1:A:158:ARG:O	1:A:159:GLU:HB3	2.15	0.45
1:B:107:VAL:HA	1:B:148:GLU:O	2.17	0.45
1:B:85:SER:O	1:B:86:LEU:CG	2.64	0.45
1:E:140:GLN:HG2	1:E:145:VAL:HA	1.98	0.45
1:K:37:GLN:NE2	1:K:41:LYS:HE2	2.32	0.45
1:A:40:GLN:O	1:A:125:VAL:HG23	2.17	0.45
1:A:113:VAL:HG21	1:A:119:LEU:HD13	1.98	0.45
1:B:55:PHE:HB2	3:B:1006:HOH:O	2.16	0.45
1:B:129:LYS:CG	1:B:130:GLY:H	2.30	0.45
1:E:62:LYS:CD	1:F:98:ILE:HD13	2.47	0.45
1:E:134:GLN:CG	1:E:152:LYS:HD3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:GLU:HG3	1:H:93:ILE:N	2.31	0.45
1:H:110:ARG:NH2	1:H:148:GLU:OE2	2.49	0.45
1:I:87:TRP:CH2	1:I:155:ILE:HG21	2.52	0.45
1:C:103:THR:HG22	1:D:108:LYS:HG2	1.99	0.45
1:E:84:THR:HA	1:E:88:GLY:O	2.16	0.45
1:H:126:LEU:HD12	1:H:134:GLN:HE22	1.82	0.45
1:F:96:THR:HG23	1:F:157:GLU:OE2	2.16	0.45
1:B:101:PHE:CZ	1:B:153:ALA:HB2	2.51	0.45
1:H:97:LYS:HB3	1:H:156:ALA:O	2.16	0.45
1:C:29:LEU:HD22	1:C:46:LYS:HE3	1.99	0.45
1:I:125:VAL:HG12	1:I:125:VAL:O	2.16	0.45
1:A:107:VAL:HG13	1:A:149:ALA:HB2	1.99	0.44
1:H:83:PHE:CZ	1:H:94:ALA:HB2	2.52	0.44
1:I:34:THR:OG1	1:I:43:VAL:HG12	2.17	0.44
1:J:46:LYS:HE2	3:J:160:HOH:O	2.17	0.44
1:K:92:GLU:O	1:K:92:GLU:HG2	2.17	0.44
1:K:99:VAL:HG22	1:K:155:ILE:CD1	2.47	0.44
1:L:37:GLN:NE2	1:L:40:GLN:HG3	2.32	0.44
1:G:104:ILE:HB	1:H:107:VAL:HG21	1.99	0.44
1:E:84:THR:O	1:E:88:GLY:N	2.50	0.44
1:D:60:PRO:O	1:D:61:ASN:HB2	2.17	0.44
1:G:27:MET:O	1:G:76:GLN:NE2	2.51	0.44
1:J:140:GLN:HG2	1:J:145:VAL:HA	1.99	0.44
1:L:122:HIS:O	1:L:137:GLY:HA3	2.17	0.44
1:A:68:VAL:HG13	3:B:1012:HOH:O	2.17	0.44
1:C:129:LYS:NZ	1:C:129:LYS:CB	2.71	0.44
1:G:113:VAL:HG22	1:G:146:VAL:HG11	2.00	0.44
1:G:158:ARG:CB	1:G:158:ARG:HH11	2.30	0.44
1:H:104:ILE:HG22	1:H:107:VAL:CG1	2.48	0.44
1:C:138:THR:HG22	1:C:148:GLU:HG2	2.00	0.44
1:H:97:LYS:HA	1:H:157:GLU:HA	2.00	0.44
1:I:90:ASP:CG	1:I:93:ILE:HD12	2.37	0.44
1:J:9:GLN:NE2	1:J:11:GLN:O	2.36	0.44
1:G:68:VAL:HB	1:H:68:VAL:HB	2.00	0.44
1:G:157:GLU:O	1:G:158:ARG:HG2	2.18	0.44
1:B:49:THR:HB	1:C:47:ASN:O	2.17	0.44
1:D:141:VAL:CG2	1:D:146:VAL:HG21	2.48	0.44
1:G:135:VAL:HG12	1:G:136:GLY:H	1.81	0.44
1:B:20:ILE:HD13	1:B:83:PHE:CD2	2.53	0.43
1:B:20:ILE:HD11	1:B:89:PHE:HA	2.00	0.43
1:B:37:GLN:HB3	1:B:40:GLN:HB2	1.99	0.43

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:114:THR:HB	1:J:115:PRO:CD	2.48	0.43
1:B:29:LEU:H	1:B:76:GLN:NE2	2.14	0.43
1:D:107:VAL:HB	1:D:149:ALA:CB	2.48	0.43
1:E:128:HIS:CD2	1:E:128:HIS:C	2.92	0.43
1:G:38:ALA:C	1:G:40:GLN:H	2.22	0.43
1:G:39:ASN:ND2	1:G:133:TRP:HH2	2.14	0.43
1:H:25:TYR:CE2	1:H:26:PRO:HB3	2.53	0.43
1:J:29:LEU:H	1:J:76:GLN:NE2	2.14	0.43
1:B:9:GLN:CD	1:B:10:SER:H	2.21	0.43
1:C:98:ILE:HD13	1:D:62:LYS:HD3	1.98	0.43
1:E:128:HIS:HD2	1:E:129:LYS:N	2.15	0.43
1:I:129:LYS:CG	1:I:130:GLY:H	2.21	0.43
1:A:13:PHE:CD1	1:A:13:PHE:N	2.86	0.43
1:D:129:LYS:HD3	1:D:129:LYS:N	2.21	0.43
1:G:24:ARG:O	1:H:57:GLY:HA3	2.18	0.43
1:I:129:LYS:HZ1	1:I:132:ILE:HD12	1.82	0.43
1:J:114:THR:HB	1:J:115:PRO:HD2	2.00	0.43
1:A:54:VAL:HG21	1:A:66:PRO:HG2	2.00	0.43
1:B:39:ASN:O	1:B:125:VAL:HG21	2.19	0.43
1:F:105:ASP:O	1:F:150:GLU:HB3	2.19	0.43
1:I:37:GLN:HG2	1:I:40:GLN:OE1	2.19	0.43
1:I:110:ARG:C	1:I:111:ILE:HG13	2.38	0.43
1:F:49:THR:O	1:F:55:PHE:CE1	2.72	0.43
1:G:111:ILE:O	1:G:146:VAL:HG13	2.19	0.43
1:L:129:LYS:HD3	1:L:129:LYS:HA	1.81	0.43
1:C:84:THR:O	1:C:88:GLY:N	2.27	0.43
1:D:106:LYS:HE3	1:D:150:GLU:OE2	2.19	0.43
1:J:95:LYS:NZ	1:J:95:LYS:HB3	2.34	0.43
3:K:1021:HOH:O	1:L:58:HIS:HE1	2.00	0.43
1:C:35:GLU:HB3	1:C:43:VAL:HB	2.00	0.43
1:E:108:LYS:O	1:E:147:ALA:HA	2.19	0.43
1:D:17:ILE:CG2	1:D:21:LEU:HD12	2.48	0.43
1:D:66:PRO:HB2	1:D:69:LEU:HG	2.01	0.43
1:E:101:PHE:HB2	2:E:1003:CL:CL	2.55	0.43
1:H:108:LYS:NZ	1:H:110:ARG:NH2	2.67	0.43
1:I:129:LYS:HZ1	1:I:132:ILE:CB	2.23	0.43
1:K:29:LEU:HD22	1:K:46:LYS:HE3	2.01	0.43
1:L:87:TRP:CH2	1:L:97:LYS:HE3	2.54	0.43
1:C:120:GLU:OE2	1:C:122:HIS:CE1	2.72	0.43
1:E:68:VAL:HB	1:F:68:VAL:HB	2.01	0.43
1:J:126:LEU:HG	1:J:136:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ILE:HG13	1:E:18:LEU:CD2	2.49	0.42
1:G:35:GLU:HB2	1:G:43:VAL:HB	2.01	0.42
1:G:96:THR:CG2	1:G:157:GLU:OE1	2.67	0.42
1:J:97:LYS:HD3	1:J:157:GLU:OE2	2.19	0.42
1:H:108:LYS:HZ3	1:H:110:ARG:HH22	1.66	0.42
1:L:102:MET:HE3	1:L:132:ILE:HG23	2.01	0.42
1:C:93:ILE:HG22	1:C:93:ILE:O	2.18	0.42
1:I:68:VAL:HB	1:J:68:VAL:HB	2.01	0.42
1:I:123:LEU:HB3	1:I:135:VAL:CG1	2.49	0.42
1:A:87:TRP:CD1	1:A:93:ILE:HD13	2.55	0.42
1:H:98:ILE:CG2	1:H:99:VAL:N	2.74	0.42
1:A:38:ALA:C	1:A:40:GLN:H	2.23	0.42
1:D:128:HIS:CD2	1:D:128:HIS:C	2.93	0.42
1:E:144:LYS:HB2	1:E:144:LYS:NZ	2.35	0.42
1:G:120:GLU:HG2	1:G:122:HIS:NE2	2.34	0.42
1:A:108:LYS:NZ	1:A:108:LYS:CB	2.83	0.42
1:G:16:HIS:O	1:G:20:ILE:HG12	2.20	0.42
1:G:120:GLU:O	1:G:139:ALA:HA	2.20	0.42
1:J:13:PHE:N	1:J:16:HIS:HD2	2.02	0.42
1:J:97:LYS:HB3	1:J:155:ILE:HG23	2.02	0.42
1:L:114:THR:HB	1:L:115:PRO:HD2	2.00	0.42
1:L:128:HIS:O	1:L:129:LYS:CD	2.67	0.42
1:B:58:HIS:CD2	1:B:64:ILE:O	2.72	0.42
1:F:90:ASP:OD1	1:F:90:ASP:C	2.58	0.42
1:I:120:GLU:O	1:I:139:ALA:HA	2.19	0.42
1:A:62:LYS:HD2	1:A:64:ILE:HD11	2.02	0.42
1:B:12:PHE:HB2	1:B:33:ILE:HB	2.02	0.42
1:B:20:ILE:HD13	1:B:83:PHE:HD2	1.84	0.42
1:G:104:ILE:CB	1:H:107:VAL:HG22	2.49	0.42
1:I:40:GLN:O	1:I:125:VAL:HG23	2.20	0.42
1:B:36:LEU:CD1	1:B:81:LEU:HD13	2.49	0.42
1:D:37:GLN:HB3	1:D:37:GLN:HE21	1.62	0.42
1:F:74:MET:CE	1:F:149:ALA:HB3	2.49	0.42
1:H:132:ILE:CG2	1:H:154:MET:SD	3.08	0.42
1:I:107:VAL:HA	1:I:148:GLU:O	2.20	0.42
1:J:106:LYS:HG3	1:J:150:GLU:OE2	2.19	0.42
1:J:133:TRP:O	1:J:152:LYS:HA	2.20	0.42
1:L:14:ILE:HD13	1:L:14:ILE:O	2.19	0.42
1:F:118:ARG:HB3	3:F:1013:HOH:O	2.18	0.42
1:G:72:GLU:HG3	1:G:76:GLN:HE21	1.83	0.42
1:H:13:PHE:O	1:H:17:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:ILE:HB	1:H:146:VAL:HG22	2.01	0.42
1:I:61:ASN:O	1:I:62:LYS:HB2	2.20	0.42
1:I:86:LEU:HD12	1:I:155:ILE:HD12	2.01	0.42
1:C:86:LEU:O	1:C:87:TRP:CG	2.73	0.41
1:G:58:HIS:HE1	3:H:166:HOH:O	2.03	0.41
1:I:20:ILE:HG23	1:I:83:PHE:CD2	2.55	0.41
1:C:15:GLU:HG3	1:C:16:HIS:N	2.35	0.41
1:E:158:ARG:O	1:E:159:GLU:CB	2.65	0.41
1:H:98:ILE:HB	1:H:156:ALA:HB3	2.02	0.41
1:H:130:GLY:O	1:H:133:TRP:NE1	2.53	0.41
1:I:125:VAL:O	1:I:126:LEU:C	2.58	0.41
1:I:133:TRP:O	1:I:152:LYS:HA	2.20	0.41
1:K:23:HIS:HB2	1:K:28:LEU:HD13	2.02	0.41
1:L:111:ILE:O	1:L:146:VAL:CG2	2.63	0.41
1:B:141:VAL:CG2	1:B:146:VAL:HG11	2.50	0.41
1:E:72:GLU:HG3	1:E:76:GLN:NE2	2.35	0.41
1:I:114:THR:HB	1:I:115:PRO:HD2	2.02	0.41
1:K:11:GLN:HG3	1:K:34:THR:HA	2.02	0.41
1:D:27:MET:O	1:D:76:GLN:NE2	2.52	0.41
1:G:83:PHE:CE2	1:G:155:ILE:HD12	2.55	0.41
1:I:87:TRP:HZ3	1:I:155:ILE:HG21	1.83	0.41
1:J:66:PRO:HB2	1:J:69:LEU:HG	2.02	0.41
1:A:108:LYS:O	1:A:147:ALA:HA	2.21	0.41
1:C:120:GLU:OE2	1:C:122:HIS:NE2	2.53	0.41
1:D:101:PHE:CE1	1:D:104:ILE:HG12	2.55	0.41
1:G:126:LEU:HD12	1:G:134:GLN:HG2	2.02	0.41
1:H:100:ALA:O	1:H:153:ALA:HA	2.20	0.41
1:H:151:LEU:C	1:H:151:LEU:HD12	2.41	0.41
1:L:114:THR:HB	1:L:115:PRO:CD	2.50	0.41
1:B:92:GLU:O	1:B:94:ALA:N	2.54	0.41
1:C:14:ILE:O	1:C:18:LEU:HD22	2.21	0.41
1:G:102:MET:HE3	1:G:152:LYS:HE3	2.02	0.41
1:G:110:ARG:C	1:G:111:ILE:HG13	2.41	0.41
1:H:62:LYS:O	1:H:64:ILE:HG12	2.21	0.41
1:B:102:MET:SD	1:B:154:MET:HB3	2.60	0.41
1:C:39:ASN:ND2	1:C:85:SER:HB3	2.36	0.41
1:C:107:VAL:HG22	1:D:104:ILE:HB	2.03	0.41
1:F:49:THR:O	1:F:55:PHE:HE1	2.03	0.41
1:F:111:ILE:O	1:F:146:VAL:HG13	2.20	0.41
1:A:42:ILE:HG22	1:A:123:LEU:HB2	2.02	0.41
1:B:97:LYS:HD3	1:B:157:GLU:CG	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LYS:HB2	1:D:144:LYS:HE3	1.78	0.41
1:E:108:LYS:HD2	1:E:148:GLU:OE2	2.21	0.41
1:F:33:ILE:HD13	1:F:44:ALA:CB	2.50	0.41
1:G:86:LEU:HD21	1:G:133:TRP:HE1	1.86	0.41
1:G:157:GLU:HG3	1:G:158:ARG:H	1.85	0.41
1:H:129:LYS:HG2	1:H:132:ILE:HD12	2.03	0.41
1:I:42:ILE:HG12	1:I:43:VAL:N	2.36	0.41
1:J:102:MET:CE	1:J:132:ILE:HG23	2.51	0.41
1:A:108:LYS:HD2	1:A:148:GLU:OE2	2.21	0.41
1:B:99:VAL:HG12	1:B:100:ALA:N	2.35	0.41
1:C:128:HIS:O	1:C:129:LYS:HB3	2.21	0.41
1:L:86:LEU:HD21	1:L:133:TRP:HE1	1.86	0.41
1:J:33:ILE:HG23	1:J:42:ILE:HD11	2.03	0.40
1:K:144:LYS:NZ	3:K:1029:HOH:O	2.54	0.40
1:L:22:PRO:CB	1:L:158:ARG:NH2	2.84	0.40
1:B:35:GLU:HB3	1:B:43:VAL:HB	2.03	0.40
1:D:42:ILE:O	1:D:42:ILE:HG23	2.22	0.40
1:E:14:ILE:HG23	1:E:15:GLU:N	2.36	0.40
1:F:108:LYS:HB2	1:F:148:GLU:HB2	2.02	0.40
1:G:38:ALA:O	1:G:40:GLN:N	2.55	0.40
1:H:98:ILE:HB	1:H:156:ALA:HB1	2.03	0.40
1:J:84:THR:O	1:J:88:GLY:N	2.51	0.40
1:H:81:LEU:C	1:H:81:LEU:HD23	2.41	0.40
1:K:158:ARG:O	1:K:159:GLU:C	2.60	0.40
1:L:75:ALA:HB2	1:L:101:PHE:CZ	2.56	0.40
1:L:158:ARG:O	1:L:159:GLU:C	2.60	0.40
1:G:122:HIS:O	1:G:137:GLY:HA3	2.21	0.40
1:I:24:ARG:HB2	1:J:57:GLY:HA2	2.04	0.40
1:J:69:LEU:HD23	1:J:69:LEU:HA	1.78	0.40
1:J:81:LEU:HD21	1:J:125:VAL:HG23	2.03	0.40
1:J:99:VAL:O	1:J:99:VAL:CG1	2.67	0.40
1:A:109:PHE:HD1	1:B:101:PHE:O	2.04	0.40
1:D:37:GLN:HB2	1:D:40:GLN:HB2	2.04	0.40
1:E:107:VAL:CG1	1:F:104:ILE:CB	2.97	0.40
1:E:159:GLU:O	1:E:159:GLU:CG	2.69	0.40
1:G:68:VAL:HG13	1:H:101:PHE:HE2	1.85	0.40
1:H:42:ILE:HG12	1:H:43:VAL:N	2.36	0.40
1:H:58:HIS:CD2	1:H:64:ILE:O	2.74	0.40
1:H:119:LEU:HD11	1:H:139:ALA:HB1	2.03	0.40
1:I:96:THR:O	1:I:96:THR:OG1	2.31	0.40
1:J:61:ASN:N	1:J:61:ASN:ND2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:73:GLY:HA3	1:J:121:TYR:CZ	2.56	0.40
1:L:98:ILE:CG2	1:L:158:ARG:HG2	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	150/171 (88%)	129 (86%)	21 (14%)	0	100	100
1	B	148/171 (86%)	123 (83%)	13 (9%)	12 (8%)	1	1
1	C	150/171 (88%)	134 (89%)	15 (10%)	1 (1%)	22	39
1	D	149/171 (87%)	133 (89%)	13 (9%)	3 (2%)	7	12
1	E	149/171 (87%)	131 (88%)	17 (11%)	1 (1%)	22	39
1	F	150/171 (88%)	138 (92%)	11 (7%)	1 (1%)	22	39
1	G	148/171 (86%)	136 (92%)	10 (7%)	2 (1%)	11	20
1	H	146/171 (85%)	125 (86%)	19 (13%)	2 (1%)	11	20
1	I	150/171 (88%)	130 (87%)	15 (10%)	5 (3%)	4	5
1	J	150/171 (88%)	136 (91%)	11 (7%)	3 (2%)	7	12
1	K	150/171 (88%)	140 (93%)	8 (5%)	2 (1%)	12	21
1	L	149/171 (87%)	138 (93%)	11 (7%)	0	100	100
All	All	1789/2052 (87%)	1593 (89%)	164 (9%)	32 (2%)	8	14

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	ASN
1	B	92	GLU

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Mol	Chain	Res	Type
1	B	97	LYS
1	B	127	LYS
1	H	89	PHE
1	I	39	ASN
1	J	9	GLN
1	B	62	LYS
1	B	86	LEU
1	B	96	THR
1	B	130	GLY
1	D	129	LYS
1	F	9	GLN
1	G	130	GLY
1	I	86	LEU
1	B	89	PHE
1	C	129	LYS
1	G	51	ASN
1	K	51	ASN
1	B	51	ASN
1	E	39	ASN
1	I	51	ASN
1	J	62	LYS
1	K	9	GLN
1	D	51	ASN
1	H	82	ALA
1	I	9	GLN
1	I	62	LYS
1	J	51	ASN
1	B	40	GLN
1	D	89	PHE
1	B	93	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/147 (88%)	122 (94%)	8 (6%)	18	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	128/147 (87%)	123 (96%)	5 (4%)	32	57
1	C	130/147 (88%)	122 (94%)	8 (6%)	18	35
1	D	129/147 (88%)	122 (95%)	7 (5%)	22	42
1	E	129/147 (88%)	123 (95%)	6 (5%)	26	49
1	F	130/147 (88%)	124 (95%)	6 (5%)	27	50
1	G	128/147 (87%)	118 (92%)	10 (8%)	12	24
1	H	126/147 (86%)	114 (90%)	12 (10%)	8	17
1	I	130/147 (88%)	121 (93%)	9 (7%)	15	30
1	J	130/147 (88%)	121 (93%)	9 (7%)	15	30
1	K	130/147 (88%)	125 (96%)	5 (4%)	33	58
1	L	129/147 (88%)	123 (95%)	6 (5%)	26	49
All	All	1549/1764 (88%)	1458 (94%)	91 (6%)	19	37

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	11	GLN
1	A	37	GLN
1	A	62	LYS
1	A	98	ILE
1	A	101	PHE
1	A	151	LEU
1	A	158	ARG
1	B	9	GLN
1	B	41	LYS
1	B	105	ASP
1	B	110	ARG
1	B	128	HIS
1	C	18	LEU
1	C	36	LEU
1	C	81	LEU
1	C	96	THR
1	C	101	PHE
1	C	107	VAL
1	C	129	LYS
1	C	134	GLN
1	D	36	LEU

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Mol	Chain	Res	Type
1	D	42	ILE
1	D	92	GLU
1	D	101	PHE
1	D	105	ASP
1	D	107	VAL
1	D	110	ARG
1	E	18	LEU
1	E	26	PRO
1	E	54	VAL
1	E	98	ILE
1	E	101	PHE
1	E	146	VAL
1	F	18	LEU
1	F	26	PRO
1	F	37	GLN
1	F	86	LEU
1	F	101	PHE
1	F	107	VAL
1	G	15	GLU
1	G	41	LYS
1	G	86	LEU
1	G	101	PHE
1	G	105	ASP
1	G	107	VAL
1	G	118	ARG
1	G	131	MET
1	G	151	LEU
1	G	158	ARG
1	H	11	GLN
1	H	18	LEU
1	H	26	PRO
1	H	36	LEU
1	H	101	PHE
1	H	107	VAL
1	H	127	LYS
1	H	128	HIS
1	H	132	ILE
1	H	134	GLN
1	H	135	VAL
1	H	154	MET
1	I	8	LEU
1	I	37	GLN

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Mol	Chain	Res	Type
1	I	39	ASN
1	I	101	PHE
1	I	102	MET
1	I	105	ASP
1	I	118	ARG
1	I	128	HIS
1	I	158	ARG
1	J	8	LEU
1	J	27	MET
1	J	36	LEU
1	J	39	ASN
1	J	42	ILE
1	J	98	ILE
1	J	101	PHE
1	J	151	LEU
1	J	158	ARG
1	K	18	LEU
1	K	96	THR
1	K	101	PHE
1	K	107	VAL
1	K	159	GLU
1	L	14	ILE
1	L	86	LEU
1	L	101	PHE
1	L	107	VAL
1	L	146	VAL
1	L	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	11	GLN
1	A	16	HIS
1	A	19	GLN
1	A	39	ASN
1	A	40	GLN
1	A	51	ASN
1	A	58	HIS
1	A	61	ASN
1	A	76	GLN
1	B	16	HIS

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Mol	Chain	Res	Type
1	B	19	GLN
1	B	37	GLN
1	B	51	ASN
1	B	58	HIS
1	B	61	ASN
1	B	76	GLN
1	B	140	GLN
1	C	11	GLN
1	C	39	ASN
1	C	76	GLN
1	C	134	GLN
1	D	9	GLN
1	D	37	GLN
1	D	58	HIS
1	D	128	HIS
1	E	51	ASN
1	E	58	HIS
1	E	128	HIS
1	F	16	HIS
1	F	58	HIS
1	F	76	GLN
1	F	134	GLN
1	G	9	GLN
1	G	37	GLN
1	G	39	ASN
1	G	51	ASN
1	G	58	HIS
1	G	140	GLN
1	H	11	GLN
1	H	58	HIS
1	H	76	GLN
1	H	134	GLN
1	I	16	HIS
1	I	37	GLN
1	I	51	ASN
1	I	58	HIS
1	I	61	ASN
1	I	122	HIS
1	I	140	GLN
1	J	11	GLN
1	J	16	HIS
1	J	37	GLN

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Mol	Chain	Res	Type
1	J	39	ASN
1	J	40	GLN
1	J	51	ASN
1	J	58	HIS
1	J	61	ASN
1	J	76	GLN
1	J	134	GLN
1	K	11	GLN
1	K	37	GLN
1	K	58	HIS
1	K	76	GLN
1	K	134	GLN
1	L	37	GLN
1	L	51	ASN
1	L	58	HIS
1	L	128	HIS
1	L	134	GLN
1	L	140	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7　Other polymers (i)

There are no such residues in this entry.

5.8　Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	130:GLY	C	131:MET	N	1.06

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, 95th 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	152/171 (88%)	0.66	17 (11%)	5	4	29, 50, 69, 89	0
1	B	150/171 (87%)	1.08	28 (18%)	1	1	30, 52, 81, 86	0
1	C	152/171 (88%)	0.76	14 (9%)	9	9	27, 46, 71, 96	0
1	D	151/171 (88%)	0.68	12 (7%)	12	12	27, 44, 62, 81	0
1	E	151/171 (88%)	0.70	12 (7%)	12	12	28, 45, 67, 77	0
1	F	152/171 (88%)	0.38	5 (3%)	46	50	30, 41, 60, 79	0
1	G	150/171 (87%)	0.57	5 (3%)	46	50	26, 41, 57, 68	0
1	H	148/171 (86%)	0.78	18 (12%)	4	3	30, 43, 77, 85	0
1	I	152/171 (88%)	0.82	23 (15%)	2	1	27, 47, 73, 95	0
1	J	152/171 (88%)	0.54	6 (3%)	39	42	28, 42, 64, 82	0
1	K	152/171 (88%)	0.29	3 (1%)	65	68	29, 38, 60, 79	0
1	L	151/171 (88%)	0.45	3 (1%)	65	68	27, 39, 57, 81	0
All	All	1813/2052 (88%)	0.64	146 (8%)	12	12	26, 43, 70, 96	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	LEU	6.8
1	E	10	SER	6.1
1	C	93	ILE	5.5
1	G	93	ILE	5.3
1	E	130	GLY	5.0
1	B	87	TRP	4.8
1	C	159	GLU	4.8
1	E	134	GLN	4.7
1	B	92	GLU	4.6
1	C	134	GLN	4.3
1	A	105	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	93	ILE	4.2
1	B	93	ILE	4.1
1	D	108	LYS	4.1
1	L	93	ILE	4.1
1	D	83	PHE	4.1
1	B	153	ALA	3.9
1	I	96	THR	3.9
1	H	155	ILE	3.9
1	B	85	SER	3.8
1	I	158	ARG	3.8
1	B	132	ILE	3.8
1	B	101	PHE	3.7
1	B	83	PHE	3.6
1	I	10	SER	3.6
1	B	10	SER	3.6
1	A	145	VAL	3.6
1	K	10	SER	3.5
1	C	83	PHE	3.5
1	G	106	LYS	3.5
1	H	132	ILE	3.5
1	H	128	HIS	3.4
1	B	84	THR	3.3
1	C	105	ASP	3.3
1	I	87	TRP	3.3
1	H	154	MET	3.3
1	I	86	LEU	3.2
1	I	125	VAL	3.2
1	B	154	MET	3.1
1	H	153	ALA	3.1
1	J	101	PHE	3.1
1	A	108	LYS	3.0
1	B	152	LYS	3.0
1	I	143	GLY	3.0
1	D	105	ASP	3.0
1	B	86	LEU	2.9
1	B	129	LYS	2.9
1	I	92	GLU	2.9
1	H	40	GLN	2.9
1	I	40	GLN	2.9
1	A	106	LYS	2.9
1	G	105	ASP	2.9
1	A	40	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	155	ILE	2.8
1	B	106	LYS	2.7
1	D	41	LYS	2.7
1	I	83	PHE	2.7
1	D	110	ARG	2.7
1	F	10	SER	2.7
1	B	131	MET	2.7
1	B	128	HIS	2.7
1	A	83	PHE	2.7
1	J	110	ARG	2.7
1	B	40	GLN	2.7
1	A	125	VAL	2.6
1	E	153	ALA	2.6
1	C	152	LYS	2.6
1	E	86	LEU	2.6
1	D	26	PRO	2.6
1	F	159	GLU	2.6
1	C	106	LYS	2.6
1	E	41	LYS	2.6
1	H	127	LYS	2.5
1	J	159	GLU	2.5
1	D	126	LEU	2.5
1	C	131	MET	2.5
1	K	91	PRO	2.5
1	K	159	GLU	2.5
1	L	10	SER	2.5
1	I	154	MET	2.5
1	B	156	ALA	2.5
1	E	40	GLN	2.5
1	I	90	ASP	2.5
1	H	129	LYS	2.4
1	C	153	ALA	2.4
1	H	152	LYS	2.4
1	A	8	LEU	2.4
1	C	108	LYS	2.4
1	I	11	GLN	2.4
1	F	11	GLN	2.4
1	C	27	MET	2.4
1	I	93	ILE	2.4
1	H	90	ASP	2.4
1	G	26	PRO	2.4
1	A	142	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	11	GLN	2.4
1	A	10	SER	2.4
1	E	156	ALA	2.3
1	H	105	ASP	2.3
1	A	41	LYS	2.3
1	C	127	LYS	2.3
1	I	129	LYS	2.3
1	D	128	HIS	2.3
1	B	133	TRP	2.3
1	A	159	GLU	2.3
1	D	9	GLN	2.3
1	A	26	PRO	2.3
1	F	37	GLN	2.3
1	I	9	GLN	2.3
1	J	134	GLN	2.3
1	E	125	VAL	2.3
1	G	108	LYS	2.3
1	C	128	HIS	2.3
1	I	8	LEU	2.3
1	B	102	MET	2.2
1	I	101	PHE	2.2
1	B	127	LYS	2.2
1	B	96	THR	2.2
1	H	93	ILE	2.2
1	I	153	ALA	2.2
1	F	157	GLU	2.2
1	E	152	LYS	2.2
1	D	25	TYR	2.2
1	J	139	ALA	2.2
1	B	26	PRO	2.2
1	H	92	GLU	2.2
1	A	122	HIS	2.1
1	I	54	VAL	2.1
1	H	27	MET	2.1
1	I	48	ILE	2.1
1	J	42	ILE	2.1
1	C	154	MET	2.1
1	H	26	PRO	2.1
1	A	129	LYS	2.1
1	A	132	ILE	2.1
1	I	133	TRP	2.1
1	L	133	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	9	GLN	2.1
1	D	27	MET	2.1
1	H	37	GLN	2.1
1	D	40	GLN	2.0
1	A	127	LYS	2.0
1	H	106	LYS	2.0
1	H	126	LEU	2.0
1	B	55	PHE	2.0
1	I	159	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	I	1007	1/1	0.37	0.25	88,88,88,88	0
2	CL	I	1002	1/1	0.85	0.24	62,62,62,62	0
2	CL	A	1010	1/1	0.86	0.18	72,72,72,72	0
2	CL	G	1009	1/1	0.92	0.13	66,66,66,66	0
2	CL	D	1012	1/1	0.92	0.14	58,58,58,58	0
2	CL	G	1008	1/1	0.92	0.15	57,57,57,57	0
2	CL	E	1003	1/1	0.94	0.17	57,57,57,57	0
2	CL	B	1001	1/1	0.95	0.19	56,56,56,56	0
2	CL	K	1005	1/1	0.95	0.20	57,57,57,57	0
2	CL	K	1006	1/1	0.95	0.20	53,53,53,53	0
2	CL	C	1011	1/1	0.96	0.16	64,64,64,64	0
2	CL	F	1004	1/1	0.98	0.12	48,48,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.