



Full wwPDB X-ray Structure Validation Report i

Dec 17, 2023 – 08:15 am GMT

PDB ID : 4ALN
Title : Crystal structure of S. aureus FabI (P32)
Authors : Schiebel, J.; Kisker, C.
Deposited on : 2012-03-04
Resolution : 3.05 Å(reported)

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

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

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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

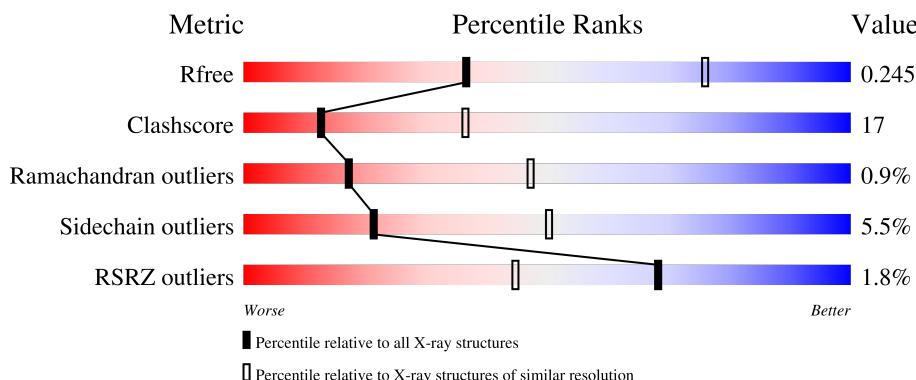
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

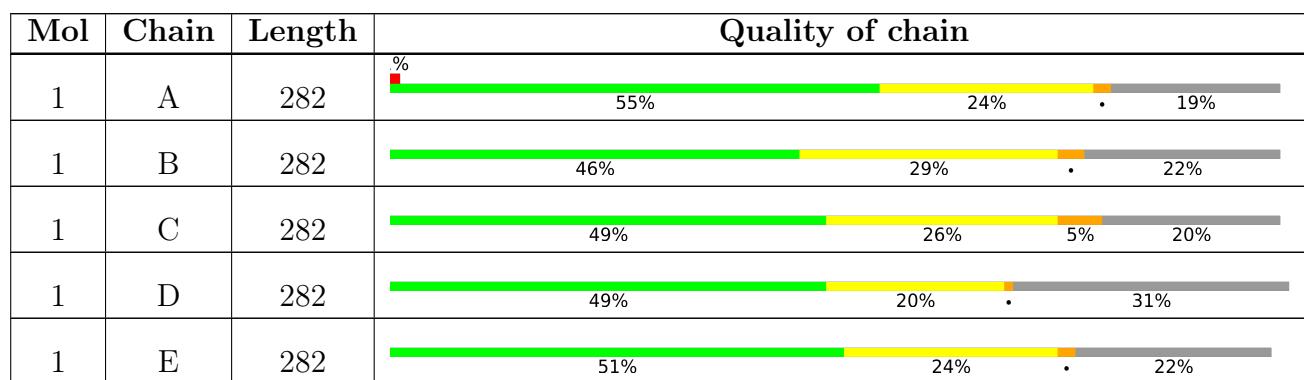
The reported resolution of this entry is 3.05 Å.

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.



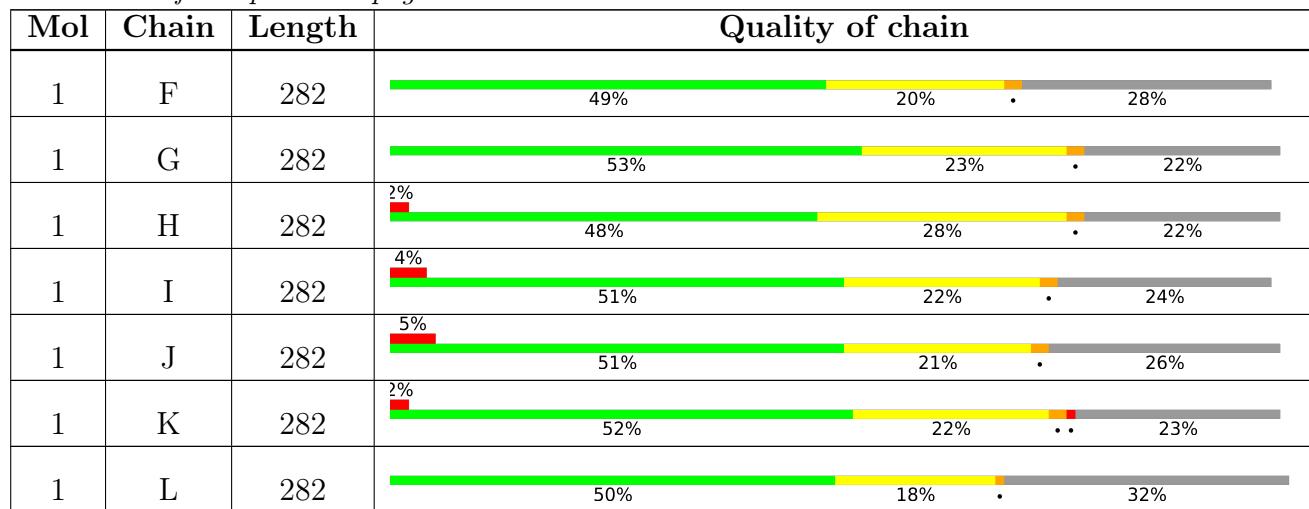
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



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2 Entry composition [\(i\)](#)

There are 2 unique types of molecules in this entry. The entry contains 20061 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 ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C 1769	N 1114	O 305	S 347	3	0	0
1	B	220	Total	C 1693	N 1067	O 293	S 330	3	0	0
1	C	225	Total	C 1739	N 1098	O 298	S 340	3	0	0
1	D	195	Total	C 1492	N 937	O 254	S 298	3	0	0
1	E	221	Total	C 1710	N 1079	O 292	S 336	3	0	0
1	F	203	Total	C 1558	N 982	O 265	S 308	3	0	0
1	G	221	Total	C 1710	N 1083	O 291	S 333	3	0	0
1	H	220	Total	C 1699	N 1072	O 290	S 334	3	0	0
1	I	214	Total	C 1654	N 1042	O 284	S 325	3	0	0
1	J	210	Total	C 1618	N 1017	O 279	S 319	3	0	0
1	K	218	Total	C 1690	N 1069	O 288	S 330	3	0	0
1	L	193	Total	C 1479	N 931	O 250	S 295	3	0	0

There are 325 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP Q7A6D8
A	-24	LYS	-	expression tag	UNP Q7A6D8
A	-23	HIS	-	expression tag	UNP Q7A6D8
A	-22	HIS	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	HIS	-	expression tag	UNP Q7A6D8
A	-20	HIS	-	expression tag	UNP Q7A6D8
A	-19	HIS	-	expression tag	UNP Q7A6D8
A	-18	HIS	-	expression tag	UNP Q7A6D8
A	-17	PRO	-	expression tag	UNP Q7A6D8
A	-16	MET	-	expression tag	UNP Q7A6D8
A	-15	SER	-	expression tag	UNP Q7A6D8
A	-14	ASP	-	expression tag	UNP Q7A6D8
A	-13	TYR	-	expression tag	UNP Q7A6D8
A	-12	ASP	-	expression tag	UNP Q7A6D8
A	-11	ILE	-	expression tag	UNP Q7A6D8
A	-10	PRO	-	expression tag	UNP Q7A6D8
A	-9	THR	-	expression tag	UNP Q7A6D8
A	-8	THR	-	expression tag	UNP Q7A6D8
A	-7	GLU	-	expression tag	UNP Q7A6D8
A	-6	ASN	-	expression tag	UNP Q7A6D8
A	-5	LEU	-	expression tag	UNP Q7A6D8
A	-4	TYR	-	expression tag	UNP Q7A6D8
A	-3	PHE	-	expression tag	UNP Q7A6D8
A	-2	GLN	-	expression tag	UNP Q7A6D8
A	-1	GLY	-	expression tag	UNP Q7A6D8
A	0	ALA	-	expression tag	UNP Q7A6D8
B	-25	MET	-	expression tag	UNP Q7A6D8
B	-24	LYS	-	expression tag	UNP Q7A6D8
B	-23	HIS	-	expression tag	UNP Q7A6D8
B	-22	HIS	-	expression tag	UNP Q7A6D8
B	-21	HIS	-	expression tag	UNP Q7A6D8
B	-20	HIS	-	expression tag	UNP Q7A6D8
B	-19	HIS	-	expression tag	UNP Q7A6D8
B	-18	HIS	-	expression tag	UNP Q7A6D8
B	-17	PRO	-	expression tag	UNP Q7A6D8
B	-16	MET	-	expression tag	UNP Q7A6D8
B	-15	SER	-	expression tag	UNP Q7A6D8
B	-14	ASP	-	expression tag	UNP Q7A6D8
B	-13	TYR	-	expression tag	UNP Q7A6D8
B	-12	ASP	-	expression tag	UNP Q7A6D8
B	-11	ILE	-	expression tag	UNP Q7A6D8
B	-10	PRO	-	expression tag	UNP Q7A6D8
B	-9	THR	-	expression tag	UNP Q7A6D8
B	-8	THR	-	expression tag	UNP Q7A6D8
B	-7	GLU	-	expression tag	UNP Q7A6D8
B	-6	ASN	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	LEU	-	expression tag	UNP Q7A6D8
B	-4	TYR	-	expression tag	UNP Q7A6D8
B	-3	PHE	-	expression tag	UNP Q7A6D8
B	-2	GLN	-	expression tag	UNP Q7A6D8
B	-1	GLY	-	expression tag	UNP Q7A6D8
B	0	ALA	-	expression tag	UNP Q7A6D8
C	-25	MET	-	expression tag	UNP Q7A6D8
C	-24	LYS	-	expression tag	UNP Q7A6D8
C	-23	HIS	-	expression tag	UNP Q7A6D8
C	-22	HIS	-	expression tag	UNP Q7A6D8
C	-21	HIS	-	expression tag	UNP Q7A6D8
C	-20	HIS	-	expression tag	UNP Q7A6D8
C	-19	HIS	-	expression tag	UNP Q7A6D8
C	-18	HIS	-	expression tag	UNP Q7A6D8
C	-17	PRO	-	expression tag	UNP Q7A6D8
C	-16	MET	-	expression tag	UNP Q7A6D8
C	-15	SER	-	expression tag	UNP Q7A6D8
C	-14	ASP	-	expression tag	UNP Q7A6D8
C	-13	TYR	-	expression tag	UNP Q7A6D8
C	-12	ASP	-	expression tag	UNP Q7A6D8
C	-11	ILE	-	expression tag	UNP Q7A6D8
C	-10	PRO	-	expression tag	UNP Q7A6D8
C	-9	THR	-	expression tag	UNP Q7A6D8
C	-8	THR	-	expression tag	UNP Q7A6D8
C	-7	GLU	-	expression tag	UNP Q7A6D8
C	-6	ASN	-	expression tag	UNP Q7A6D8
C	-5	LEU	-	expression tag	UNP Q7A6D8
C	-4	TYR	-	expression tag	UNP Q7A6D8
C	-3	PHE	-	expression tag	UNP Q7A6D8
C	-2	GLN	-	expression tag	UNP Q7A6D8
C	-1	GLY	-	expression tag	UNP Q7A6D8
C	0	ALA	-	expression tag	UNP Q7A6D8
D	-25	MET	-	expression tag	UNP Q7A6D8
D	-24	LYS	-	expression tag	UNP Q7A6D8
D	-23	HIS	-	expression tag	UNP Q7A6D8
D	-22	HIS	-	expression tag	UNP Q7A6D8
D	-21	HIS	-	expression tag	UNP Q7A6D8
D	-20	HIS	-	expression tag	UNP Q7A6D8
D	-19	HIS	-	expression tag	UNP Q7A6D8
D	-18	HIS	-	expression tag	UNP Q7A6D8
D	-17	PRO	-	expression tag	UNP Q7A6D8
D	-16	MET	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP Q7A6D8
D	-14	ASP	-	expression tag	UNP Q7A6D8
D	-13	TYR	-	expression tag	UNP Q7A6D8
D	-12	ASP	-	expression tag	UNP Q7A6D8
D	-11	ILE	-	expression tag	UNP Q7A6D8
D	-10	PRO	-	expression tag	UNP Q7A6D8
D	-9	THR	-	expression tag	UNP Q7A6D8
D	-8	THR	-	expression tag	UNP Q7A6D8
D	-7	GLU	-	expression tag	UNP Q7A6D8
D	-6	ASN	-	expression tag	UNP Q7A6D8
D	-5	LEU	-	expression tag	UNP Q7A6D8
D	-4	TYR	-	expression tag	UNP Q7A6D8
D	-3	PHE	-	expression tag	UNP Q7A6D8
D	-2	GLN	-	expression tag	UNP Q7A6D8
D	-1	GLY	-	expression tag	UNP Q7A6D8
D	0	ALA	-	expression tag	UNP Q7A6D8
E	-25	MET	-	expression tag	UNP Q7A6D8
E	-24	LYS	-	expression tag	UNP Q7A6D8
E	-23	HIS	-	expression tag	UNP Q7A6D8
E	-22	HIS	-	expression tag	UNP Q7A6D8
E	-21	HIS	-	expression tag	UNP Q7A6D8
E	-20	HIS	-	expression tag	UNP Q7A6D8
E	-19	HIS	-	expression tag	UNP Q7A6D8
E	-18	HIS	-	expression tag	UNP Q7A6D8
E	-17	PRO	-	expression tag	UNP Q7A6D8
E	-16	MET	-	expression tag	UNP Q7A6D8
E	-15	SER	-	expression tag	UNP Q7A6D8
E	-14	ASP	-	expression tag	UNP Q7A6D8
E	-13	TYR	-	expression tag	UNP Q7A6D8
E	-12	ASP	-	expression tag	UNP Q7A6D8
E	-11	ILE	-	expression tag	UNP Q7A6D8
E	-10	PRO	-	expression tag	UNP Q7A6D8
E	-9	THR	-	expression tag	UNP Q7A6D8
E	-8	THR	-	expression tag	UNP Q7A6D8
E	-7	GLU	-	expression tag	UNP Q7A6D8
E	-6	ASN	-	expression tag	UNP Q7A6D8
E	-5	LEU	-	expression tag	UNP Q7A6D8
E	-4	TYR	-	expression tag	UNP Q7A6D8
E	-3	PHE	-	expression tag	UNP Q7A6D8
E	-2	GLN	-	expression tag	UNP Q7A6D8
E	-1	GLY	-	expression tag	UNP Q7A6D8
E	0	ALA	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-25	MET	-	expression tag	UNP Q7A6D8
F	-24	LYS	-	expression tag	UNP Q7A6D8
F	-23	HIS	-	expression tag	UNP Q7A6D8
F	-22	HIS	-	expression tag	UNP Q7A6D8
F	-21	HIS	-	expression tag	UNP Q7A6D8
F	-20	HIS	-	expression tag	UNP Q7A6D8
F	-19	HIS	-	expression tag	UNP Q7A6D8
F	-18	HIS	-	expression tag	UNP Q7A6D8
F	-17	PRO	-	expression tag	UNP Q7A6D8
F	-16	MET	-	expression tag	UNP Q7A6D8
F	-15	SER	-	expression tag	UNP Q7A6D8
F	-14	ASP	-	expression tag	UNP Q7A6D8
F	-13	TYR	-	expression tag	UNP Q7A6D8
F	-12	ASP	-	expression tag	UNP Q7A6D8
F	-11	ILE	-	expression tag	UNP Q7A6D8
F	-10	PRO	-	expression tag	UNP Q7A6D8
F	-9	THR	-	expression tag	UNP Q7A6D8
F	-8	THR	-	expression tag	UNP Q7A6D8
F	-7	GLU	-	expression tag	UNP Q7A6D8
F	-6	ASN	-	expression tag	UNP Q7A6D8
F	-5	LEU	-	expression tag	UNP Q7A6D8
F	-4	TYR	-	expression tag	UNP Q7A6D8
F	-3	PHE	-	expression tag	UNP Q7A6D8
F	-2	GLN	-	expression tag	UNP Q7A6D8
F	-1	GLY	-	expression tag	UNP Q7A6D8
F	0	ALA	-	expression tag	UNP Q7A6D8
G	-25	MET	-	expression tag	UNP Q7A6D8
G	-24	LYS	-	expression tag	UNP Q7A6D8
G	-23	HIS	-	expression tag	UNP Q7A6D8
G	-22	HIS	-	expression tag	UNP Q7A6D8
G	-21	HIS	-	expression tag	UNP Q7A6D8
G	-20	HIS	-	expression tag	UNP Q7A6D8
G	-19	HIS	-	expression tag	UNP Q7A6D8
G	-18	HIS	-	expression tag	UNP Q7A6D8
G	-17	PRO	-	expression tag	UNP Q7A6D8
G	-16	MET	-	expression tag	UNP Q7A6D8
G	-15	SER	-	expression tag	UNP Q7A6D8
G	-14	ASP	-	expression tag	UNP Q7A6D8
G	-13	TYR	-	expression tag	UNP Q7A6D8
G	-12	ASP	-	expression tag	UNP Q7A6D8
G	-11	ILE	-	expression tag	UNP Q7A6D8
G	-10	PRO	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-9	THR	-	expression tag	UNP Q7A6D8
G	-8	THR	-	expression tag	UNP Q7A6D8
G	-7	GLU	-	expression tag	UNP Q7A6D8
G	-6	ASN	-	expression tag	UNP Q7A6D8
G	-5	LEU	-	expression tag	UNP Q7A6D8
G	-4	TYR	-	expression tag	UNP Q7A6D8
G	-3	PHE	-	expression tag	UNP Q7A6D8
G	-2	GLN	-	expression tag	UNP Q7A6D8
G	-1	GLY	-	expression tag	UNP Q7A6D8
G	0	ALA	-	expression tag	UNP Q7A6D8
H	-25	MET	-	expression tag	UNP Q7A6D8
H	-24	LYS	-	expression tag	UNP Q7A6D8
H	-23	HIS	-	expression tag	UNP Q7A6D8
H	-22	HIS	-	expression tag	UNP Q7A6D8
H	-21	HIS	-	expression tag	UNP Q7A6D8
H	-20	HIS	-	expression tag	UNP Q7A6D8
H	-19	HIS	-	expression tag	UNP Q7A6D8
H	-18	HIS	-	expression tag	UNP Q7A6D8
H	-17	PRO	-	expression tag	UNP Q7A6D8
H	-16	MET	-	expression tag	UNP Q7A6D8
H	-15	SER	-	expression tag	UNP Q7A6D8
H	-14	ASP	-	expression tag	UNP Q7A6D8
H	-13	TYR	-	expression tag	UNP Q7A6D8
H	-12	ASP	-	expression tag	UNP Q7A6D8
H	-11	ILE	-	expression tag	UNP Q7A6D8
H	-10	PRO	-	expression tag	UNP Q7A6D8
H	-9	THR	-	expression tag	UNP Q7A6D8
H	-8	THR	-	expression tag	UNP Q7A6D8
H	-7	GLU	-	expression tag	UNP Q7A6D8
H	-6	ASN	-	expression tag	UNP Q7A6D8
H	-5	LEU	-	expression tag	UNP Q7A6D8
H	-4	TYR	-	expression tag	UNP Q7A6D8
H	-3	PHE	-	expression tag	UNP Q7A6D8
H	-2	GLN	-	expression tag	UNP Q7A6D8
H	-1	GLY	-	expression tag	UNP Q7A6D8
H	0	ALA	-	expression tag	UNP Q7A6D8
H	1	MET	-	expression tag	UNP Q7A6D8
I	-25	MET	-	expression tag	UNP Q7A6D8
I	-24	LYS	-	expression tag	UNP Q7A6D8
I	-23	HIS	-	expression tag	UNP Q7A6D8
I	-22	HIS	-	expression tag	UNP Q7A6D8
I	-21	HIS	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-20	HIS	-	expression tag	UNP Q7A6D8
I	-19	HIS	-	expression tag	UNP Q7A6D8
I	-18	HIS	-	expression tag	UNP Q7A6D8
I	-17	PRO	-	expression tag	UNP Q7A6D8
I	-16	MET	-	expression tag	UNP Q7A6D8
I	-15	SER	-	expression tag	UNP Q7A6D8
I	-14	ASP	-	expression tag	UNP Q7A6D8
I	-13	TYR	-	expression tag	UNP Q7A6D8
I	-12	ASP	-	expression tag	UNP Q7A6D8
I	-11	ILE	-	expression tag	UNP Q7A6D8
I	-10	PRO	-	expression tag	UNP Q7A6D8
I	-9	THR	-	expression tag	UNP Q7A6D8
I	-8	THR	-	expression tag	UNP Q7A6D8
I	-7	GLU	-	expression tag	UNP Q7A6D8
I	-6	ASN	-	expression tag	UNP Q7A6D8
I	-5	LEU	-	expression tag	UNP Q7A6D8
I	-4	TYR	-	expression tag	UNP Q7A6D8
I	-3	PHE	-	expression tag	UNP Q7A6D8
I	-2	GLN	-	expression tag	UNP Q7A6D8
I	-1	GLY	-	expression tag	UNP Q7A6D8
I	0	ALA	-	expression tag	UNP Q7A6D8
J	-25	MET	-	expression tag	UNP Q7A6D8
J	-24	LYS	-	expression tag	UNP Q7A6D8
J	-23	HIS	-	expression tag	UNP Q7A6D8
J	-22	HIS	-	expression tag	UNP Q7A6D8
J	-21	HIS	-	expression tag	UNP Q7A6D8
J	-20	HIS	-	expression tag	UNP Q7A6D8
J	-19	HIS	-	expression tag	UNP Q7A6D8
J	-18	HIS	-	expression tag	UNP Q7A6D8
J	-17	PRO	-	expression tag	UNP Q7A6D8
J	-16	MET	-	expression tag	UNP Q7A6D8
J	-15	SER	-	expression tag	UNP Q7A6D8
J	-14	ASP	-	expression tag	UNP Q7A6D8
J	-13	TYR	-	expression tag	UNP Q7A6D8
J	-12	ASP	-	expression tag	UNP Q7A6D8
J	-11	ILE	-	expression tag	UNP Q7A6D8
J	-10	PRO	-	expression tag	UNP Q7A6D8
J	-9	THR	-	expression tag	UNP Q7A6D8
J	-8	THR	-	expression tag	UNP Q7A6D8
J	-7	GLU	-	expression tag	UNP Q7A6D8
J	-6	ASN	-	expression tag	UNP Q7A6D8
J	-5	LEU	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	TYR	-	expression tag	UNP Q7A6D8
J	-3	PHE	-	expression tag	UNP Q7A6D8
J	-2	GLN	-	expression tag	UNP Q7A6D8
J	-1	GLY	-	expression tag	UNP Q7A6D8
J	0	ALA	-	expression tag	UNP Q7A6D8
K	-25	MET	-	expression tag	UNP Q7A6D8
K	-24	LYS	-	expression tag	UNP Q7A6D8
K	-23	HIS	-	expression tag	UNP Q7A6D8
K	-22	HIS	-	expression tag	UNP Q7A6D8
K	-21	HIS	-	expression tag	UNP Q7A6D8
K	-20	HIS	-	expression tag	UNP Q7A6D8
K	-19	HIS	-	expression tag	UNP Q7A6D8
K	-18	HIS	-	expression tag	UNP Q7A6D8
K	-17	PRO	-	expression tag	UNP Q7A6D8
K	-16	MET	-	expression tag	UNP Q7A6D8
K	-15	SER	-	expression tag	UNP Q7A6D8
K	-14	ASP	-	expression tag	UNP Q7A6D8
K	-13	TYR	-	expression tag	UNP Q7A6D8
K	-12	ASP	-	expression tag	UNP Q7A6D8
K	-11	ILE	-	expression tag	UNP Q7A6D8
K	-10	PRO	-	expression tag	UNP Q7A6D8
K	-9	THR	-	expression tag	UNP Q7A6D8
K	-8	THR	-	expression tag	UNP Q7A6D8
K	-7	GLU	-	expression tag	UNP Q7A6D8
K	-6	ASN	-	expression tag	UNP Q7A6D8
K	-5	LEU	-	expression tag	UNP Q7A6D8
K	-4	TYR	-	expression tag	UNP Q7A6D8
K	-3	PHE	-	expression tag	UNP Q7A6D8
K	-2	GLN	-	expression tag	UNP Q7A6D8
K	-1	GLY	-	expression tag	UNP Q7A6D8
K	0	ALA	-	expression tag	UNP Q7A6D8
L	-25	MET	-	expression tag	UNP Q7A6D8
L	-24	LYS	-	expression tag	UNP Q7A6D8
L	-23	HIS	-	expression tag	UNP Q7A6D8
L	-22	HIS	-	expression tag	UNP Q7A6D8
L	-21	HIS	-	expression tag	UNP Q7A6D8
L	-20	HIS	-	expression tag	UNP Q7A6D8
L	-19	HIS	-	expression tag	UNP Q7A6D8
L	-18	HIS	-	expression tag	UNP Q7A6D8
L	-17	PRO	-	expression tag	UNP Q7A6D8
L	-16	MET	-	expression tag	UNP Q7A6D8
L	-15	SER	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-14	ASP	-	expression tag	UNP Q7A6D8
L	-13	TYR	-	expression tag	UNP Q7A6D8
L	-12	ASP	-	expression tag	UNP Q7A6D8
L	-11	ILE	-	expression tag	UNP Q7A6D8
L	-10	PRO	-	expression tag	UNP Q7A6D8
L	-9	THR	-	expression tag	UNP Q7A6D8
L	-8	THR	-	expression tag	UNP Q7A6D8
L	-7	GLU	-	expression tag	UNP Q7A6D8
L	-6	ASN	-	expression tag	UNP Q7A6D8
L	-5	LEU	-	expression tag	UNP Q7A6D8
L	-4	TYR	-	expression tag	UNP Q7A6D8
L	-3	PHE	-	expression tag	UNP Q7A6D8
L	-2	GLN	-	expression tag	UNP Q7A6D8
L	-1	GLY	-	expression tag	UNP Q7A6D8
L	0	ALA	-	expression tag	UNP Q7A6D8
A	2	VAL	LEU	engineered mutation	UNP Q7A6D8
B	2	VAL	LEU	engineered mutation	UNP Q7A6D8
C	2	VAL	LEU	engineered mutation	UNP Q7A6D8
D	2	VAL	LEU	engineered mutation	UNP Q7A6D8
E	2	VAL	LEU	engineered mutation	UNP Q7A6D8
F	2	VAL	LEU	engineered mutation	UNP Q7A6D8
G	2	VAL	LEU	engineered mutation	UNP Q7A6D8
H	2	VAL	LEU	engineered mutation	UNP Q7A6D8
I	2	VAL	LEU	engineered mutation	UNP Q7A6D8
J	2	VAL	LEU	engineered mutation	UNP Q7A6D8
K	2	VAL	LEU	engineered mutation	UNP Q7A6D8
L	2	VAL	LEU	engineered mutation	UNP Q7A6D8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	25	Total O 25 25	0	0
2	B	26	Total O 26 26	0	0
2	C	27	Total O 27 27	0	0
2	D	30	Total O 30 30	0	0
2	E	22	Total O 22 22	0	0
2	F	26	Total O 26 26	0	0

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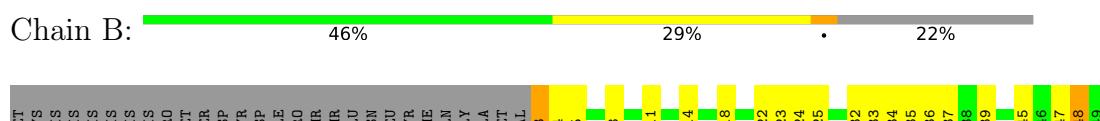
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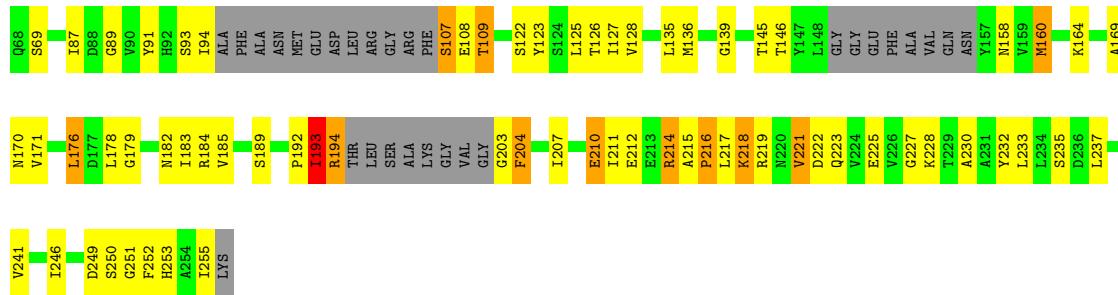
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	21	Total O 21 21	0	0
2	H	22	Total O 22 22	0	0
2	I	10	Total O 10 10	0	0
2	J	7	Total O 7 7	0	0
2	K	11	Total O 11 11	0	0
2	L	23	Total O 23 23	0	0

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.

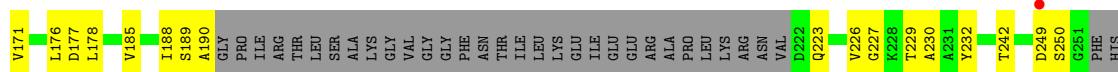
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]





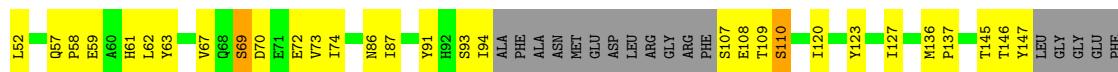
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain D:



ALA **ILE** **LYS**

Chain E:

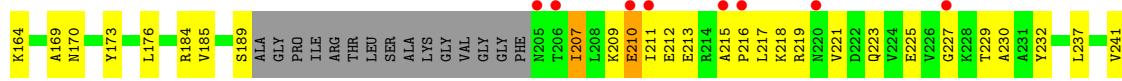


- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain F:

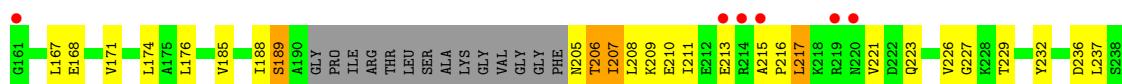






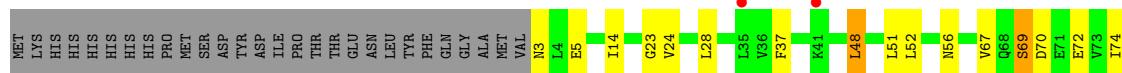
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain J: 5% • 51% 21% • 26%

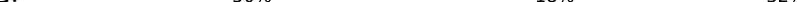


- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

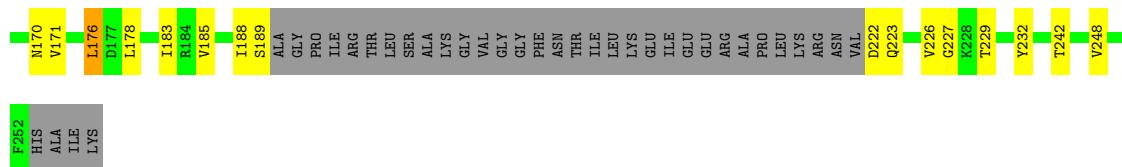
A horizontal progress bar representing the completion of Chain K. The bar is divided into four segments: a red segment at the far left labeled '2%', a long green segment labeled '52%', a yellow segment labeled '22%', and a grey segment on the right labeled '23%'. The total length of the bar corresponds to 100% completion.



- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain L:  50% 18% • 32%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	123.78Å 123.78Å 190.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.28 – 3.05 44.28 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.28-3.05) 99.3 (44.28-3.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.99 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R , R_{free}	0.203 , 0.246 0.202 , 0.245	Depositor DCC
R_{free} test set	3064 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.8	EDS
L-test for twinning ²	$< L > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.328 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
Reported twinning fraction	0.674 for H, K, L 0.326 for K, H, -L	Depositor
Outliers	0 of 61621 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20061	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [\(i\)](#)

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	0.78	0/1790	0.76	0/2414
1	B	0.82	0/1712	0.80	1/2307 (0.0%)
1	C	0.77	0/1760	0.82	1/2372 (0.0%)
1	D	0.80	0/1507	0.77	0/2031
1	E	0.75	0/1730	0.76	0/2330
1	F	0.82	0/1576	0.80	0/2125
1	G	0.77	0/1731	0.79	1/2333 (0.0%)
1	H	0.76	0/1719	0.78	2/2318 (0.1%)
1	I	0.60	0/1672	0.71	1/2253 (0.0%)
1	J	0.60	0/1635	0.66	0/2202
1	K	0.62	0/1710	0.71	1/2305 (0.0%)
1	L	0.65	0/1494	0.67	0/2012
All	All	0.73	0/20036	0.75	7/27002 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	176	LEU	CA-CB-CG	-7.93	97.07	115.30
1	H	18	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	K	176	LEU	CA-CB-CG	5.90	128.86	115.30
1	G	176	LEU	CA-CB-CG	-5.48	102.69	115.30
1	H	18	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	I	18	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	45	ARG	NE-CZ-NH1	5.12	122.86	120.30

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	1769	0	1779	64	0
1	B	1693	0	1716	70	0
1	C	1739	0	1754	78	0
1	D	1492	0	1497	53	0
1	E	1710	0	1722	55	0
1	F	1558	0	1558	54	0
1	G	1710	0	1723	69	0
1	H	1699	0	1713	64	0
1	I	1654	0	1672	53	0
1	J	1618	0	1635	49	0
1	K	1690	0	1706	51	0
1	L	1479	0	1486	41	0
2	A	25	0	0	1	0
2	B	26	0	0	0	0
2	C	27	0	0	1	0
2	D	30	0	0	0	0
2	E	22	0	0	1	0
2	F	26	0	0	3	0
2	G	21	0	0	0	0
2	H	22	0	0	1	0
2	I	10	0	0	2	0
2	J	7	0	0	0	0
2	K	11	0	0	0	0
2	L	23	0	0	0	0
All	All	20061	0	19961	659	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 17.

All (659) 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:C:18:ARG:HH22	1:C:194:ARG:CB	1.57	1.17
1:C:18:ARG:NH2	1:C:194:ARG:HB2	1.63	1.11
1:B:18:ARG:HH22	1:B:194:ARG:HB3	0.97	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:GLY:HA2	1:D:136:MET:HE1	1.29	1.10
1:D:89:GLY:HA2	1:D:136:MET:CE	1.87	1.05
1:I:221:VAL:HG21	1:I:249:ASP:HA	1.37	1.04
1:G:157:TYR:HD1	1:G:158:ASN:N	1.60	1.00
1:C:18:ARG:HH22	1:C:194:ARG:HB2	0.82	0.96
1:K:217:LEU:HD13	1:K:219:ARG:HH21	1.29	0.96
1:B:18:ARG:NH2	1:B:194:ARG:HB3	1.82	0.94
1:G:147:TYR:CD1	1:G:148:LEU:HG	2.04	0.92
1:E:146:THR:HG22	1:E:189:SER:HA	1.52	0.92
1:A:146:THR:HG22	1:A:189:SER:HA	1.49	0.92
1:G:157:TYR:HD1	1:G:158:ASN:H	0.97	0.91
1:A:18:ARG:NH2	1:A:194:ARG:C	2.23	0.91
1:A:193:ILE:HG12	1:A:222:ASP:HA	1.53	0.90
1:A:107:SER:HA	1:A:110:SER:HB3	1.54	0.89
1:G:214:ARG:O	1:G:255:ILE:HD11	1.71	0.89
1:H:91:TYR:CE1	1:H:93:SER:HB2	2.07	0.88
1:K:91:TYR:CE1	1:K:93:SER:HB2	2.10	0.87
1:B:91:TYR:CE1	1:B:93:SER:HB2	2.11	0.86
1:A:192:PRO:O	1:A:193:ILE:HG13	1.77	0.84
1:F:146:THR:HG22	1:F:189:SER:HA	1.57	0.84
1:A:217:LEU:HB2	1:A:250:SER:HB3	1.59	0.83
1:K:24:VAL:HG21	1:K:91:TYR:CZ	2.14	0.83
1:G:147:TYR:HD1	1:G:148:LEU:HG	1.41	0.81
1:C:194:ARG:HA	1:C:204:PHE:CE2	2.15	0.81
1:I:217:LEU:HD13	1:L:242:THR:HG21	1.63	0.81
1:G:94:ILE:HG22	1:G:95:ALA:N	1.95	0.80
1:A:182:ASN:HA	2:A:2019:HOH:O	1.81	0.80
1:H:91:TYR:HE1	1:H:93:SER:HB2	1.46	0.80
1:B:146:THR:HG22	1:B:189:SER:HA	1.65	0.79
1:F:147:TYR:CD2	1:F:191:GLY:HA2	2.18	0.78
1:F:94:ILE:HA	2:F:2017:HOH:O	1.83	0.77
1:I:146:THR:HG22	1:I:189:SER:HA	1.64	0.77
1:G:94:ILE:CG2	1:G:95:ALA:N	2.46	0.77
1:D:91:TYR:CE2	1:D:93:SER:HB2	2.20	0.77
1:A:192:PRO:HG2	1:A:211:ILE:HG13	1.66	0.77
1:E:35:LEU:HB3	1:E:37:PHE:CE1	2.20	0.77
1:H:23:GLY:HA3	1:H:223:GLN:HB3	1.66	0.76
1:F:91:TYR:CE1	1:F:93:SER:HB2	2.21	0.76
1:J:211:ILE:HG23	1:J:215:ALA:HB2	1.66	0.76
1:H:211:ILE:HG23	1:H:215:ALA:HB2	1.67	0.76
1:G:39:TYR:OH	1:G:45:ARG:HD2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:TYR:CD1	1:G:158:ASN:N	2.49	0.75
1:I:119:ASP:OD1	1:J:111:ARG:NH1	2.19	0.75
1:L:91:TYR:CE1	1:L:93:SER:HB2	2.23	0.74
1:J:217:LEU:HB2	1:J:250:SER:HB3	1.67	0.74
1:L:146:THR:HG22	1:L:189:SER:HA	1.70	0.74
1:G:89:GLY:HA2	1:G:136:MET:HE1	1.69	0.74
1:C:194:ARG:HD3	1:C:194:ARG:N	2.03	0.73
1:H:89:GLY:HA2	1:H:136:MET:CE	2.18	0.73
1:I:157:TYR:CG	1:I:158:ASN:N	2.56	0.73
1:A:217:LEU:HD12	1:A:250:SER:HA	1.68	0.73
1:E:23:GLY:HA3	1:E:223:GLN:HB3	1.70	0.73
1:J:146:THR:HG22	1:J:189:SER:HA	1.71	0.73
1:K:212:GLU:HG2	1:K:219:ARG:HA	1.70	0.72
1:I:23:GLY:HA3	1:I:223:GLN:HB3	1.69	0.72
1:J:23:GLY:HA3	1:J:223:GLN:HB3	1.71	0.72
1:B:206:THR:HG23	1:B:207:ILE:H	1.54	0.72
1:D:190:ALA:O	1:D:249:ASP:HB3	1.90	0.72
1:E:179:GLY:HA2	1:H:217:LEU:HD23	1.72	0.71
1:G:217:LEU:HB2	1:G:250:SER:HB3	1.70	0.71
1:K:23:GLY:HA3	1:K:223:GLN:HB3	1.72	0.71
1:D:17:LYS:HE2	1:L:53:GLU:HA	1.72	0.70
1:H:214:ARG:O	1:H:255:ILE:HD11	1.90	0.70
1:H:39:TYR:CE2	1:H:45:ARG:HB2	2.25	0.70
1:I:221:VAL:HG12	1:I:225:GLU:OE1	1.92	0.70
1:A:214:ARG:O	1:A:255:ILE:HD11	1.91	0.70
1:A:18:ARG:HH21	1:A:194:ARG:C	1.94	0.69
1:L:23:GLY:HA3	1:L:223:GLN:HB3	1.73	0.69
1:C:91:TYR:CE2	1:C:93:SER:HB2	2.27	0.69
1:A:91:TYR:CE1	1:A:93:SER:HB2	2.28	0.69
1:A:208:LEU:O	1:A:212:GLU:HG3	1.92	0.69
1:D:89:GLY:CA	1:D:136:MET:CE	2.69	0.69
1:F:180:PRO:HG3	1:G:218:LYS:HE3	1.74	0.68
1:I:91:TYR:CE2	1:I:93:SER:HB2	2.29	0.68
1:I:221:VAL:CG2	1:I:249:ASP:HA	2.21	0.68
1:I:24:VAL:HG21	1:I:91:TYR:CZ	2.29	0.68
1:B:217:LEU:HD22	1:B:219:ARG:NH2	2.09	0.67
1:C:211:ILE:O	1:C:215:ALA:HB3	1.94	0.67
1:D:3:ASN:N	1:D:5:GLU:OE1	2.27	0.67
1:I:110:SER:HB2	2:I:2004:HOH:O	1.95	0.67
1:G:89:GLY:HA2	1:G:136:MET:CE	2.23	0.67
1:A:107:SER:HA	1:A:110:SER:CB	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:TYR:HE1	1:B:93:SER:HB2	1.57	0.67
1:J:5:GLU:HA	1:J:32:GLY:O	1.95	0.67
1:B:8:THR:HG23	1:B:34:LYS:HG3	1.76	0.67
1:C:193:ILE:C	1:C:194:ARG:HD3	2.16	0.67
1:G:91:TYR:CE2	1:G:93:SER:HB2	2.30	0.66
1:C:217:LEU:O	1:C:218:LYS:HB2	1.94	0.66
1:D:171:VAL:HG13	1:D:185:VAL:HG12	1.76	0.66
1:C:91:TYR:HE2	1:C:93:SER:HB2	1.61	0.66
1:J:24:VAL:HG21	1:J:91:TYR:CZ	2.30	0.66
1:K:217:LEU:HB3	1:K:219:ARG:HE	1.61	0.66
1:C:193:ILE:HB	1:C:194:ARG:HH11	1.60	0.65
1:D:39:TYR:OH	1:D:45:ARG:HD2	1.96	0.65
1:A:24:VAL:HG21	1:A:91:TYR:CZ	2.31	0.65
1:G:146:THR:HG22	1:G:189:SER:HA	1.78	0.65
1:K:70:ASP:O	1:K:74:ILE:HG13	1.95	0.65
1:J:205:ASN:C	1:J:207:ILE:H	1.98	0.65
1:B:23:GLY:HA3	1:B:223:GLN:HB3	1.78	0.65
1:E:157:TYR:N	2:E:2011:HOH:O	2.29	0.65
1:A:89:GLY:HA2	1:A:136:MET:HE1	1.79	0.65
1:K:205:ASN:HA	1:K:208:LEU:HB2	1.79	0.65
1:G:170:ASN:OD1	1:H:157:TYR:OH	2.14	0.65
1:E:255:ILE:O	1:E:256:LYS:HE3	1.96	0.65
1:C:158:ASN:OD1	1:C:158:ASN:N	2.30	0.64
1:A:94:ILE:CG2	1:A:95:ALA:N	2.60	0.64
1:G:127:ILE:HG23	1:G:128:VAL:N	2.13	0.64
1:I:217:LEU:CD1	1:L:242:THR:HG21	2.25	0.64
1:G:209:LYS:O	1:G:213:GLU:HB2	1.97	0.64
1:E:91:TYR:CE2	1:E:93:SER:HB2	2.33	0.64
1:J:91:TYR:CE1	1:J:93:SER:HB2	2.32	0.64
1:J:216:PRO:HG3	1:K:176:LEU:HD22	1.78	0.64
1:F:53:GLU:HA	1:L:50:LYS:NZ	2.13	0.64
1:F:89:GLY:HA2	1:F:136:MET:CE	2.28	0.64
1:E:214:ARG:O	1:E:255:ILE:HD11	1.99	0.63
1:G:23:GLY:HA3	1:G:223:GLN:HB3	1.80	0.63
1:H:221:VAL:HG11	1:H:248:VAL:O	1.98	0.63
1:C:107:SER:HB3	1:D:177:ASP:OD2	1.98	0.63
1:G:24:VAL:HG21	1:G:91:TYR:CZ	2.34	0.63
1:C:18:ARG:NH2	1:C:194:ARG:CB	2.42	0.62
1:F:89:GLY:HA2	1:F:136:MET:HE1	1.79	0.62
1:I:39:TYR:HB3	1:I:48:LEU:CD1	2.29	0.62
1:A:23:GLY:HA3	1:A:223:GLN:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:ALA:HB1	1:G:164:LYS:NZ	2.13	0.62
1:H:146:THR:HG22	1:H:189:SER:HA	1.82	0.62
1:C:24:VAL:HG21	1:C:91:TYR:CZ	2.35	0.62
1:C:107:SER:N	1:D:177:ASP:OD2	2.33	0.62
1:D:146:THR:HG22	1:D:189:SER:HA	1.81	0.62
1:C:107:SER:CB	1:D:177:ASP:OD2	2.48	0.61
1:K:91:TYR:HE1	1:K:93:SER:HB2	1.61	0.61
1:D:50:LYS:O	1:D:53:GLU:HB2	2.01	0.61
1:D:89:GLY:HA2	1:D:136:MET:HE2	1.80	0.61
1:G:94:ILE:O	1:G:95:ALA:HB2	2.00	0.61
1:H:8:THR:HG23	1:H:34:LYS:HG3	1.81	0.61
1:G:127:ILE:HG23	1:G:128:VAL:H	1.64	0.61
1:J:205:ASN:HB3	1:J:207:ILE:HD13	1.81	0.61
1:C:23:GLY:HA3	1:C:223:GLN:HB3	1.83	0.61
1:G:94:ILE:CG2	1:G:95:ALA:H	2.13	0.61
1:I:212:GLU:HA	1:I:218:LYS:O	2.01	0.61
1:E:35:LEU:HB3	1:E:37:PHE:HE1	1.65	0.60
1:H:70:ASP:O	1:H:74:ILE:HG13	2.01	0.60
1:A:94:ILE:HG22	1:A:95:ALA:N	2.15	0.60
1:F:23:GLY:HA3	1:F:223:GLN:HB3	1.83	0.60
1:H:89:GLY:HA2	1:H:136:MET:HE2	1.81	0.60
1:B:145:THR:HG22	1:B:146:THR:N	2.16	0.60
1:B:24:VAL:HA	1:B:227:GLY:HA2	1.82	0.60
1:F:147:TYR:HD2	1:F:191:GLY:HA2	1.63	0.59
1:H:89:GLY:HA2	1:H:136:MET:HE1	1.82	0.59
1:H:216:PRO:O	1:H:218:LYS:HD2	2.02	0.59
1:I:209:LYS:O	1:I:213:GLU:HB2	2.02	0.59
1:K:184:ARG:HD2	1:K:241:VAL:O	2.02	0.59
1:F:91:TYR:HE1	1:F:93:SER:HB2	1.64	0.59
1:L:24:VAL:HG21	1:L:91:TYR:CZ	2.37	0.59
1:D:17:LYS:CE	1:L:53:GLU:HA	2.32	0.59
1:E:221:VAL:CG1	1:E:222:ASP:N	2.65	0.59
1:A:229:THR:O	1:A:232:TYR:HB3	2.03	0.59
1:A:91:TYR:HE1	1:A:93:SER:HB2	1.65	0.59
1:B:212:GLU:HG3	1:B:220:ASN:HD22	1.68	0.59
1:D:11:ILE:CD1	1:D:35:LEU:HD22	2.32	0.59
1:A:206:THR:O	1:A:209:LYS:HB3	2.02	0.58
1:G:39:TYR:CE2	1:G:45:ARG:HB2	2.38	0.58
1:E:221:VAL:HG12	1:E:222:ASP:N	2.16	0.58
1:G:146:THR:HG23	1:G:147:TYR:N	2.17	0.58
1:D:23:GLY:HA3	1:D:223:GLN:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:O	1:A:218:LYS:NZ	2.36	0.58
1:E:94:ILE:HG21	1:E:120:ILE:HG22	1.85	0.58
1:E:70:ASP:O	1:E:74:ILE:HG13	2.03	0.57
1:F:109:THR:HG23	1:F:157:TYR:CD2	2.39	0.57
1:K:205:ASN:HA	1:K:208:LEU:HD12	1.86	0.57
1:B:60:ALA:HB1	1:B:62:LEU:CD2	2.34	0.57
1:C:251:GLY:HA2	1:C:253:HIS:CE1	2.39	0.57
1:I:216:PRO:HG2	1:I:251:GLY:O	2.04	0.57
1:I:219:ARG:NH2	1:I:225:GLU:OE2	2.37	0.57
1:I:89:GLY:HA2	1:I:136:MET:HE1	1.86	0.57
1:K:148:LEU:HD23	1:K:190:ALA:HB1	1.85	0.57
1:C:178:LEU:HB3	1:C:183:ILE:HB	1.85	0.57
1:C:194:ARG:HH12	1:C:223:GLN:HE22	1.53	0.57
1:A:89:GLY:HA2	1:A:136:MET:CE	2.34	0.57
1:J:188:ILE:HG21	1:J:226:VAL:HG13	1.86	0.57
1:A:192:PRO:CG	1:A:211:ILE:HG13	2.34	0.57
1:E:216:PRO:HG2	1:E:251:GLY:O	2.05	0.57
1:J:22:PHE:O	1:J:25:ALA:HB3	2.04	0.57
1:G:217:LEU:HD12	1:G:250:SER:HA	1.87	0.57
1:J:210:GLU:HG3	1:J:211:ILE:HD12	1.87	0.57
1:C:146:THR:HG22	1:C:189:SER:HA	1.86	0.56
1:D:22:PHE:O	1:D:25:ALA:HB3	2.05	0.56
1:E:22:PHE:O	1:E:25:ALA:HB3	2.04	0.56
1:D:39:TYR:CE2	1:D:45:ARG:HB2	2.39	0.56
1:E:146:THR:CG2	1:E:189:SER:HA	2.32	0.56
1:F:3:ASN:N	1:F:5:GLU:OE1	2.39	0.56
1:A:107:SER:CA	1:A:110:SER:HB3	2.32	0.56
1:K:146:THR:HG22	1:K:189:SER:HA	1.87	0.56
1:L:91:TYR:HE1	1:L:93:SER:HB2	1.70	0.56
1:I:216:PRO:HG3	1:L:176:LEU:HD22	1.86	0.56
1:A:155:GLN:HG2	1:A:156:ASN:H	1.71	0.56
1:C:122:SER:HB3	1:D:114:PHE:CZ	2.41	0.56
1:E:48:LEU:O	1:E:52:LEU:HG	2.06	0.56
1:H:5:GLU:HA	1:H:32:GLY:O	2.05	0.56
1:B:160:MET:O	1:B:164:LYS:HG2	2.05	0.55
1:K:211:ILE:O	1:K:215:ALA:HB3	2.06	0.55
1:H:69:SER:O	1:H:69:SER:OG	2.24	0.55
1:D:227:GLY:O	1:D:230:ALA:HB3	2.07	0.55
1:C:127:ILE:HG23	1:C:128:VAL:N	2.21	0.55
1:B:145:THR:CG2	1:B:146:THR:N	2.70	0.55
1:C:192:PRO:O	1:C:193:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:VAL:O	1:C:222:ASP:HB3	2.06	0.55
1:F:109:THR:HG23	1:F:157:TYR:HD2	1.71	0.55
1:H:214:ARG:HB3	1:H:255:ILE:HD12	1.87	0.55
1:H:24:VAL:O	1:H:28:LEU:HG	2.06	0.55
1:A:94:ILE:HG21	1:A:120:ILE:HG22	1.87	0.55
1:B:127:ILE:HG23	1:B:128:VAL:N	2.22	0.55
1:C:207:ILE:HG23	1:C:211:ILE:HD13	1.88	0.55
1:E:39:TYR:HB3	1:E:48:LEU:HD13	1.89	0.55
1:G:89:GLY:N	1:G:136:MET:HE2	2.22	0.55
1:H:11:ILE:HD11	1:H:35:LEU:HD22	1.88	0.55
1:J:239:SER:O	1:K:219:ARG:NH2	2.38	0.54
1:A:212:GLU:HG2	1:A:220:ASN:ND2	2.23	0.54
1:H:221:VAL:HG22	1:H:225:GLU:OE1	2.07	0.54
1:B:18:ARG:NH2	1:B:194:ARG:HH11	2.05	0.54
1:L:39:TYR:OH	1:L:45:ARG:HD2	2.07	0.54
1:D:24:VAL:HG21	1:D:91:TYR:CZ	2.43	0.54
1:A:14:ILE:HD12	1:A:37:PHE:HD2	1.72	0.54
1:D:11:ILE:HD11	1:D:35:LEU:HD22	1.89	0.54
1:I:89:GLY:HA2	1:I:136:MET:CE	2.38	0.54
1:C:203:GLY:O	1:C:207:ILE:HD13	2.08	0.54
1:I:160:MET:O	1:I:164:LYS:HG2	2.07	0.54
1:D:39:TYR:HB3	1:D:48:LEU:HD13	1.90	0.54
1:B:242:THR:HG22	1:C:251:GLY:HA3	1.90	0.54
1:H:60:ALA:HB1	1:H:62:LEU:HD21	1.90	0.54
1:H:214:ARG:HB3	1:H:255:ILE:CD1	2.37	0.54
1:I:4:LEU:HB3	1:I:33:ALA:HB2	1.89	0.54
1:H:60:ALA:HB1	1:H:62:LEU:CD2	2.37	0.54
1:J:123:TYR:CE2	1:J:127:ILE:HB	2.42	0.54
1:C:48:LEU:O	1:C:52:LEU:HD13	2.07	0.54
1:F:222:ASP:HB2	2:F:2024:HOH:O	2.06	0.54
1:G:59:GLU:HG3	1:G:61:HIS:CE1	2.43	0.54
1:B:210:GLU:HG3	1:B:211:ILE:HD13	1.89	0.53
1:J:206:THR:HG22	1:J:206:THR:O	2.07	0.53
1:A:217:LEU:CD1	1:A:250:SER:HA	2.37	0.53
1:I:210:GLU:HA	1:I:213:GLU:HB3	1.90	0.53
1:B:48:LEU:O	1:B:52:LEU:HG	2.07	0.53
1:J:207:ILE:HG22	1:J:208:LEU:HD12	1.89	0.53
1:J:229:THR:O	1:J:232:TYR:HB3	2.08	0.53
1:B:127:ILE:HG23	1:B:128:VAL:H	1.73	0.53
1:E:211:ILE:O	1:E:215:ALA:HB3	2.08	0.53
1:F:24:VAL:HG21	1:F:91:TYR:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:VAL:HG13	1:H:185:VAL:HG12	1.90	0.53
1:K:87:ILE:HG12	1:K:135:LEU:HB2	1.91	0.53
1:C:89:GLY:HA2	1:C:136:MET:CE	2.39	0.53
1:B:209:LYS:HE3	1:B:213:GLU:OE2	2.09	0.53
1:C:89:GLY:HA2	1:C:136:MET:HE1	1.89	0.53
1:L:24:VAL:HA	1:L:227:GLY:HA2	1.91	0.53
1:B:50:LYS:O	1:B:53:GLU:HB2	2.10	0.52
1:B:89:GLY:HA2	1:B:136:MET:HE1	1.90	0.52
1:E:212:GLU:HG2	1:E:219:ARG:HA	1.92	0.52
1:F:147:TYR:HD2	1:F:191:GLY:CA	2.21	0.52
1:G:89:GLY:CA	1:G:136:MET:CE	2.86	0.52
1:G:173:TYR:CZ	1:H:161:GLY:HA3	2.44	0.52
1:H:4:LEU:HB3	1:H:33:ALA:HB2	1.90	0.52
1:K:217:LEU:HB2	1:K:250:SER:HB3	1.92	0.52
1:J:39:TYR:OH	1:J:45:ARG:HD2	2.09	0.52
1:B:11:ILE:HD12	1:B:35:LEU:HD13	1.91	0.52
1:G:39:TYR:HB3	1:G:48:LEU:CD1	2.40	0.52
1:G:91:TYR:HE2	1:G:93:SER:HB2	1.72	0.52
1:B:194:ARG:C	1:B:208:LEU:HD11	2.30	0.52
1:F:50:LYS:O	1:F:53:GLU:HB2	2.09	0.52
1:B:22:PHE:O	1:B:25:ALA:HB3	2.09	0.52
1:A:14:ILE:HD12	1:A:37:PHE:CD2	2.44	0.52
1:B:5:GLU:HA	1:B:32:GLY:O	2.09	0.52
1:C:160:MET:O	1:C:164:LYS:HG2	2.10	0.52
1:F:8:THR:HG23	1:F:34:LYS:HG3	1.92	0.52
1:G:67:VAL:O	1:H:111:ARG:NH2	2.38	0.52
1:H:221:VAL:HG21	1:H:249:ASP:CA	2.40	0.52
1:B:207:ILE:O	1:B:211:ILE:HG12	2.09	0.52
1:F:24:VAL:HA	1:F:227:GLY:HA2	1.92	0.52
1:H:227:GLY:O	1:H:230:ALA:HB3	2.10	0.52
1:A:146:THR:CG2	1:A:189:SER:HA	2.33	0.52
1:E:221:VAL:CG1	1:E:222:ASP:H	2.23	0.52
1:G:94:ILE:O	1:G:95:ALA:CB	2.57	0.52
1:F:146:THR:CG2	1:F:189:SER:HA	2.36	0.51
1:K:123:TYR:O	1:K:126:THR:N	2.43	0.51
1:H:39:TYR:CZ	1:H:64:GLN:HB2	2.46	0.51
1:C:127:ILE:HG23	1:C:128:VAL:H	1.75	0.51
1:D:60:ALA:HB1	1:D:62:LEU:CD2	2.41	0.51
1:G:5:GLU:HA	1:G:32:GLY:O	2.10	0.51
1:J:221:VAL:HG21	1:J:248:VAL:O	2.10	0.51
1:A:193:ILE:CG1	1:A:222:ASP:HA	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:GLY:CA	1:D:136:MET:HE2	2.39	0.51
1:I:91:TYR:HE2	1:I:93:SER:HB2	1.76	0.51
1:J:216:PRO:HG2	1:J:251:GLY:O	2.11	0.51
1:B:60:ALA:HB1	1:B:62:LEU:HD21	1.93	0.51
1:B:94:ILE:CG2	1:B:95:ALA:N	2.74	0.51
1:C:24:VAL:HA	1:C:227:GLY:HA2	1.93	0.51
1:D:69:SER:O	1:D:69:SER:OG	2.28	0.51
1:E:24:VAL:HA	1:E:227:GLY:HA2	1.93	0.51
1:B:67:VAL:HG21	1:B:94:ILE:CD1	2.41	0.50
1:F:53:GLU:HG2	1:L:50:LYS:HZ3	1.76	0.50
1:K:171:VAL:HG13	1:K:185:VAL:HG12	1.92	0.50
1:K:178:LEU:O	1:K:179:GLY:C	2.49	0.50
1:J:171:VAL:HG13	1:J:185:VAL:HG12	1.94	0.50
1:J:209:LYS:O	1:J:213:GLU:HB3	2.11	0.50
1:K:188:ILE:HG21	1:K:226:VAL:HG13	1.94	0.50
1:C:39:TYR:CE2	1:C:45:ARG:HB2	2.46	0.50
1:H:193:ILE:HB	1:H:221:VAL:O	2.11	0.50
1:K:185:VAL:O	1:K:243:GLY:N	2.35	0.50
1:A:192:PRO:C	1:A:193:ILE:HG13	2.31	0.50
1:K:24:VAL:HA	1:K:227:GLY:CA	2.41	0.50
1:K:208:LEU:HD23	1:K:220:ASN:HD22	1.76	0.50
1:B:89:GLY:HA2	1:B:136:MET:CE	2.41	0.50
1:B:171:VAL:HG13	1:B:185:VAL:HG12	1.93	0.50
1:H:40:ARG:HD3	2:H:2010:HOH:O	2.10	0.50
1:I:22:PHE:O	1:I:25:ALA:HB3	2.12	0.50
1:G:14:ILE:HG23	1:G:22:PHE:HB2	1.93	0.50
1:C:24:VAL:HA	1:C:227:GLY:CA	2.42	0.50
1:E:251:GLY:HA2	1:E:253:HIS:CE1	2.47	0.50
1:C:232:TYR:O	1:C:235:SER:OG	2.29	0.49
1:F:14:ILE:HG23	1:F:22:PHE:HB2	1.94	0.49
1:I:94:ILE:HG21	1:I:120:ILE:HG22	1.94	0.49
1:J:38:THR:HA	1:J:63:TYR:O	2.11	0.49
1:F:53:GLU:HA	1:L:50:LYS:HZ2	1.76	0.49
1:H:208:LEU:HD22	1:H:220:ASN:ND2	2.27	0.49
1:G:94:ILE:HG23	1:G:95:ALA:H	1.76	0.49
1:K:24:VAL:HA	1:K:227:GLY:HA2	1.94	0.49
1:B:24:VAL:HG21	1:B:91:TYR:CZ	2.48	0.49
1:D:91:TYR:HE2	1:D:93:SER:HB2	1.72	0.49
1:F:5:GLU:O	1:F:6:ASN:HB2	2.12	0.49
1:K:160:MET:O	1:K:164:LYS:HG2	2.11	0.49
1:E:236:ASP:O	1:E:239:SER:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:GLU:O	1:E:51:LEU:HG	2.12	0.49
1:L:114:PHE:O	1:L:117:ALA:HB3	2.13	0.49
1:D:127:ILE:HG23	1:D:128:VAL:N	2.28	0.49
1:D:188:ILE:HG21	1:D:226:VAL:HG13	1.95	0.49
1:E:217:LEU:HB2	1:E:250:SER:HB3	1.95	0.49
1:L:109:THR:HG22	1:L:109:THR:O	2.12	0.49
1:B:242:THR:CG2	1:C:251:GLY:HA3	2.43	0.49
1:I:184:ARG:HD2	1:I:241:VAL:O	2.13	0.49
1:H:47:GLU:O	1:H:51:LEU:HG	2.13	0.48
1:K:48:LEU:O	1:K:52:LEU:HD13	2.12	0.48
1:A:94:ILE:HG21	1:A:120:ILE:CG2	2.43	0.48
1:B:228:LYS:O	1:B:231:ALA:HB3	2.13	0.48
1:C:233:LEU:HD11	1:C:246:ILE:HD12	1.94	0.48
1:F:69:SER:OG	1:F:72:GLU:HG3	2.12	0.48
1:L:24:VAL:O	1:L:28:LEU:HG	2.13	0.48
1:B:24:VAL:HA	1:B:227:GLY:CA	2.44	0.48
1:C:171:VAL:HG13	1:C:185:VAL:HG12	1.95	0.48
1:D:169:ALA:O	1:D:170:ASN:C	2.52	0.48
1:E:62:LEU:HD22	1:E:62:LEU:N	2.28	0.48
1:E:86:ASN:OD1	1:E:137:PRO:HD3	2.13	0.48
1:I:185:VAL:O	1:I:243:GLY:N	2.39	0.48
1:L:160:MET:O	1:L:164:LYS:HG2	2.13	0.48
1:C:232:TYR:CD1	1:C:237:LEU:HB3	2.49	0.48
1:G:216:PRO:HD2	1:G:250:SER:O	2.13	0.48
1:I:229:THR:O	1:I:232:TYR:HB3	2.13	0.48
1:L:86:ASN:OD1	1:L:137:PRO:HD3	2.13	0.48
1:F:11:ILE:HD11	1:F:28:LEU:HD12	1.95	0.48
1:B:8:THR:HG23	1:B:34:LYS:CG	2.42	0.48
1:G:122:SER:HB3	1:H:114:PHE:CZ	2.49	0.48
1:A:37:PHE:CD1	1:A:37:PHE:N	2.82	0.48
1:C:214:ARG:C	1:C:255:ILE:HD11	2.34	0.48
1:E:107:SER:O	1:E:108:GLU:HG3	2.13	0.48
1:B:69:SER:OG	1:B:72:GLU:HG3	2.14	0.47
1:C:5:GLU:HA	1:C:32:GLY:O	2.14	0.47
1:E:11:ILE:HD12	1:E:35:LEU:HG	1.95	0.47
1:G:208:LEU:HD23	1:G:220:ASN:HD21	1.79	0.47
1:G:38:THR:HA	1:G:63:TYR:O	2.14	0.47
1:K:217:LEU:HD13	1:K:219:ARG:NH2	2.12	0.47
1:A:62:LEU:C	1:A:63:TYR:CD1	2.87	0.47
1:I:211:ILE:O	1:I:215:ALA:HB3	2.15	0.47
1:C:108:GLU:HG3	2:C:2020:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:THR:O	1:D:232:TYR:HB3	2.14	0.47
1:G:39:TYR:CZ	1:G:45:ARG:HD2	2.48	0.47
1:B:94:ILE:HG21	1:B:120:ILE:HG22	1.96	0.47
1:C:214:ARG:O	1:C:255:ILE:HD11	2.14	0.47
1:D:53:GLU:HA	1:F:17:LYS:HE3	1.95	0.47
1:J:205:ASN:C	1:J:207:ILE:N	2.67	0.47
1:H:218:LYS:HA	1:H:218:LYS:HE3	1.97	0.47
1:C:18:ARG:CZ	1:C:194:ARG:HB2	2.38	0.47
1:D:47:GLU:O	1:D:51:LEU:HG	2.15	0.47
1:I:122:SER:O	1:I:170:ASN:ND2	2.48	0.47
1:B:178:LEU:HB3	1:B:183:ILE:HB	1.98	0.47
1:G:171:VAL:HG13	1:G:185:VAL:HG12	1.97	0.47
1:B:3:ASN:N	1:B:5:GLU:OE1	2.48	0.46
1:G:3:ASN:N	1:G:5:GLU:OE1	2.48	0.46
1:A:188:ILE:HG21	1:A:226:VAL:HG13	1.96	0.46
1:F:5:GLU:HA	1:F:32:GLY:O	2.15	0.46
1:K:217:LEU:CB	1:K:219:ARG:HE	2.27	0.46
1:C:216:PRO:HD2	1:C:250:SER:O	2.15	0.46
1:F:11:ILE:HD12	1:F:35:LEU:HD13	1.98	0.46
1:A:38:THR:HA	1:A:63:TYR:O	2.15	0.46
1:E:24:VAL:HG21	1:E:91:TYR:CZ	2.50	0.46
1:E:91:TYR:HE2	1:E:93:SER:HB2	1.76	0.46
1:B:193:ILE:HG22	1:B:194:ARG:NH1	2.31	0.46
1:I:122:SER:HG	1:J:114:PHE:HZ	1.64	0.46
1:K:212:GLU:HG2	1:K:219:ARG:CA	2.42	0.46
1:K:228:LYS:O	1:K:231:ALA:HB3	2.16	0.46
1:A:24:VAL:HG21	1:A:91:TYR:CE2	2.51	0.46
1:B:14:ILE:HD12	1:B:37:PHE:CD2	2.51	0.46
1:G:122:SER:HB3	1:H:114:PHE:HZ	1.79	0.46
1:G:232:TYR:CD1	1:G:237:LEU:HB3	2.50	0.46
1:K:208:LEU:HD23	1:K:220:ASN:ND2	2.30	0.46
1:B:116:LEU:HD12	1:B:116:LEU:HA	1.78	0.46
1:E:59:GLU:HG3	1:E:61:HIS:CE1	2.50	0.46
1:G:203:GLY:O	1:G:206:THR:HG22	2.16	0.46
1:H:39:TYR:OH	1:H:45:ARG:HD2	2.15	0.46
1:C:235:SER:OG	1:C:237:LEU:HB2	2.16	0.46
1:E:59:GLU:HG3	1:E:61:HIS:NE2	2.31	0.46
1:A:67:VAL:HA	1:A:73:VAL:CG2	2.46	0.46
1:B:229:THR:O	1:B:232:TYR:HB3	2.16	0.46
1:G:232:TYR:HD1	1:G:237:LEU:HB3	1.81	0.46
1:C:221:VAL:HG11	1:C:249:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:C	1:D:137:PRO:HD3	2.36	0.45
1:F:39:TYR:OH	1:F:45:ARG:HD2	2.15	0.45
1:I:114:PHE:O	1:I:117:ALA:HB3	2.16	0.45
1:B:39:TYR:HB3	1:B:48:LEU:CD1	2.46	0.45
1:C:215:ALA:HB2	1:C:252:PHE:HD1	1.81	0.45
1:C:227:GLY:O	1:C:230:ALA:HB3	2.16	0.45
1:C:232:TYR:HD1	1:C:237:LEU:HB3	1.80	0.45
1:F:70:ASP:O	1:F:74:ILE:HG13	2.16	0.45
1:H:8:THR:HG23	1:H:34:LYS:CG	2.45	0.45
1:A:70:ASP:O	1:A:74:ILE:HG13	2.17	0.45
1:J:20:ILE:O	1:J:24:VAL:HG23	2.16	0.45
1:A:194:ARG:H	1:A:194:ARG:HG2	1.56	0.45
1:B:55:LEU:CD1	1:B:55:LEU:N	2.80	0.45
1:D:39:TYR:HB3	1:D:48:LEU:CD1	2.46	0.45
1:E:5:GLU:HA	1:E:32:GLY:O	2.16	0.45
1:G:127:ILE:CG2	1:G:128:VAL:N	2.80	0.45
1:I:5:GLU:HA	1:I:32:GLY:O	2.16	0.45
1:L:188:ILE:HG21	1:L:226:VAL:HG13	1.98	0.45
1:C:212:GLU:HG2	1:C:218:LYS:O	2.16	0.45
1:E:87:ILE:HD11	1:E:136:MET:HE3	1.98	0.45
1:F:94:ILE:HG21	1:F:120:ILE:HG22	1.99	0.45
1:G:229:THR:O	1:G:232:TYR:HB3	2.17	0.45
1:H:123:TYR:O	1:H:124:SER:C	2.55	0.45
1:I:227:GLY:O	1:I:230:ALA:HB3	2.16	0.45
1:E:227:GLY:O	1:E:230:ALA:HB3	2.17	0.45
1:H:147:TYR:HE1	1:H:192:PRO:HD3	1.82	0.45
1:L:171:VAL:HG13	1:L:185:VAL:HG12	1.98	0.45
1:A:221:VAL:O	1:A:222:ASP:HB3	2.16	0.45
1:C:193:ILE:C	1:C:194:ARG:CD	2.85	0.45
1:G:127:ILE:CG2	1:G:128:VAL:H	2.29	0.45
1:A:69:SER:OG	1:A:72:GLU:HG3	2.17	0.45
1:J:48:LEU:O	1:J:52:LEU:HD13	2.17	0.45
1:D:136:MET:N	1:D:137:PRO:HD3	2.32	0.44
1:H:89:GLY:CA	1:H:136:MET:HE2	2.46	0.44
1:H:221:VAL:HG21	1:H:249:ASP:HA	1.99	0.44
1:B:216:PRO:HB2	1:C:179:GLY:HA3	2.00	0.44
1:F:147:TYR:HB3	1:F:191:GLY:H	1.82	0.44
1:B:167:LEU:HD12	1:B:167:LEU:O	2.17	0.44
1:D:14:ILE:HD12	1:D:37:PHE:CD2	2.52	0.44
1:E:108:GLU:C	1:E:110:SER:H	2.20	0.44
1:E:255:ILE:HG22	1:E:256:LYS:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:91:TYR:HE1	1:J:93:SER:HB2	1.81	0.44
1:A:209:LYS:O	1:A:213:GLU:HB2	2.16	0.44
1:K:86:ASN:OD1	1:K:137:PRO:HD3	2.18	0.44
1:A:217:LEU:HD12	1:A:250:SER:CA	2.43	0.44
1:B:123:TYR:O	1:B:124:SER:C	2.55	0.44
1:F:24:VAL:HA	1:F:227:GLY:CA	2.48	0.44
1:G:95:ALA:HB1	1:G:164:LYS:HZ3	1.80	0.44
1:K:3:ASN:N	1:K:5:GLU:OE1	2.50	0.44
1:J:251:GLY:HA3	1:K:242:THR:CG2	2.47	0.44
1:C:39:TYR:OH	1:C:45:ARG:HD2	2.17	0.44
1:E:38:THR:HA	1:E:63:TYR:O	2.17	0.44
1:F:127:ILE:HG23	1:F:128:VAL:N	2.32	0.44
1:F:160:MET:O	1:F:164:LYS:HG2	2.18	0.44
1:H:58:PRO:HB2	1:H:59:GLU:HG2	1.98	0.44
1:H:113:GLY:O	1:H:114:PHE:C	2.55	0.44
1:I:24:VAL:HA	1:I:227:GLY:HA2	1.99	0.44
1:J:206:THR:O	1:J:206:THR:CG2	2.66	0.44
1:L:14:ILE:HD12	1:L:37:PHE:CD2	2.53	0.44
1:L:123:TYR:O	1:L:126:THR:N	2.50	0.44
1:C:169:ALA:O	1:C:170:ASN:C	2.56	0.44
1:I:169:ALA:O	1:I:173:TYR:HD2	2.01	0.44
1:J:146:THR:CG2	1:J:189:SER:HA	2.42	0.44
1:L:38:THR:HA	1:L:63:TYR:O	2.17	0.44
1:A:24:VAL:HA	1:A:227:GLY:HA2	1.99	0.44
1:C:18:ARG:HH22	1:C:194:ARG:CA	2.26	0.44
1:D:60:ALA:HB1	1:D:62:LEU:HD21	1.99	0.44
1:I:67:VAL:HG21	1:I:94:ILE:HD11	2.00	0.44
1:K:87:ILE:HG12	1:K:135:LEU:CB	2.47	0.44
1:G:89:GLY:CA	1:G:136:MET:HE2	2.47	0.43
1:A:251:GLY:HA3	1:D:242:THR:HG22	2.00	0.43
1:B:36:VAL:HG22	1:B:61:HIS:HB2	2.01	0.43
1:B:69:SER:OG	1:B:69:SER:O	2.34	0.43
1:D:53:GLU:HB3	1:F:54:GLN:NE2	2.33	0.43
1:F:48:LEU:O	1:F:52:LEU:HG	2.18	0.43
1:F:184:ARG:HD2	1:F:241:VAL:O	2.18	0.43
1:I:57:GLN:HA	1:I:58:PRO:HD2	1.85	0.43
1:E:69:SER:OG	1:E:72:GLU:HG3	2.17	0.43
1:F:53:GLU:HA	1:L:50:LYS:HZ3	1.82	0.43
1:G:24:VAL:HG21	1:G:91:TYR:CE1	2.53	0.43
1:I:232:TYR:CD1	1:I:237:LEU:HB3	2.54	0.43
1:B:18:ARG:NH2	1:B:194:ARG:NH1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:CB	1:B:250:SER:HB3	2.48	0.43
1:B:218:LYS:HD2	1:B:218:LYS:HA	1.70	0.43
1:E:145:THR:HG22	1:E:146:THR:N	2.32	0.43
1:F:145:THR:HG22	1:F:146:THR:N	2.33	0.43
1:H:36:VAL:HG12	1:H:37:PHE:N	2.31	0.43
1:K:94:ILE:HG21	1:K:120:ILE:HG22	1.99	0.43
1:D:57:GLN:HA	1:D:58:PRO:HD2	1.87	0.43
1:J:236:ASP:O	1:J:239:SER:HB3	2.17	0.43
1:L:4:LEU:HB3	1:L:33:ALA:HB2	2.00	0.43
1:A:39:TYR:OH	1:A:45:ARG:HD2	2.18	0.43
1:A:47:GLU:O	1:A:51:LEU:HG	2.18	0.43
1:I:84:VAL:HG12	1:I:84:VAL:O	2.18	0.43
1:K:124:SER:O	1:K:128:VAL:HG23	2.19	0.43
1:L:94:ILE:HG21	1:L:120:ILE:HG22	2.01	0.43
1:L:229:THR:O	1:L:232:TYR:HB3	2.19	0.43
1:L:167:LEU:O	1:L:170:ASN:N	2.52	0.43
1:A:114:PHE:O	1:A:117:ALA:HB3	2.19	0.43
1:D:53:GLU:O	1:F:17:LYS:HD3	2.18	0.43
1:E:229:THR:O	1:E:232:TYR:HB3	2.18	0.43
1:H:236:ASP:O	1:H:239:SER:HB3	2.19	0.43
1:L:11:ILE:HD12	1:L:35:LEU:HD13	2.00	0.43
1:L:226:VAL:O	1:L:227:GLY:C	2.57	0.43
1:E:67:VAL:HA	1:E:73:VAL:CG2	2.48	0.43
1:G:24:VAL:HA	1:G:227:GLY:HA2	2.00	0.43
1:I:207:ILE:O	1:I:211:ILE:HD13	2.19	0.43
1:B:57:GLN:O	1:B:58:PRO:C	2.57	0.43
1:F:67:VAL:HA	1:F:73:VAL:CG2	2.48	0.43
1:G:146:THR:O	1:G:147:TYR:HB3	2.18	0.43
1:A:155:GLN:O	1:A:156:ASN:C	2.57	0.42
1:B:14:ILE:HD12	1:B:37:PHE:HD2	1.84	0.42
1:C:87:ILE:HG12	1:C:135:LEU:HB2	2.00	0.42
1:E:237:LEU:HD23	1:E:237:LEU:HA	1.82	0.42
1:I:16:ASN:OD1	1:I:18:ARG:HB2	2.19	0.42
1:B:227:GLY:O	1:B:230:ALA:HB3	2.19	0.42
1:I:221:VAL:HG11	1:I:250:SER:H	1.85	0.42
1:A:69:SER:O	1:A:70:ASP:C	2.57	0.42
1:C:225:GLU:O	1:C:228:LYS:HB2	2.19	0.42
1:A:36:VAL:C	1:A:37:PHE:CD1	2.93	0.42
1:D:17:LYS:HE2	1:L:53:GLU:CA	2.45	0.42
1:I:48:LEU:O	1:I:52:LEU:HG	2.19	0.42
1:J:37:PHE:CD1	1:J:37:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLN:O	1:B:119:ASP:C	2.58	0.42
1:B:222:ASP:OD1	1:B:225:GLU:HG3	2.19	0.42
1:C:210:GLU:HG2	1:C:211:ILE:HD12	2.01	0.42
1:E:24:VAL:HA	1:E:227:GLY:CA	2.49	0.42
1:H:24:VAL:HA	1:H:227:GLY:HA2	2.00	0.42
1:H:38:THR:HA	1:H:63:TYR:O	2.19	0.42
1:H:178:LEU:HB3	1:H:183:ILE:HB	2.01	0.42
1:I:24:VAL:HA	1:I:227:GLY:CA	2.50	0.42
1:K:178:LEU:HB3	1:K:183:ILE:HB	2.01	0.42
1:B:217:LEU:HB3	1:B:250:SER:HB3	2.01	0.42
1:G:87:ILE:HG12	1:G:135:LEU:HB3	2.01	0.42
1:G:87:ILE:HG12	1:G:135:LEU:CB	2.50	0.42
1:H:36:VAL:CG1	1:H:37:PHE:N	2.82	0.42
1:J:113:GLY:O	1:J:114:PHE:C	2.56	0.42
1:K:67:VAL:HG21	1:K:94:ILE:HD11	2.02	0.42
1:A:236:ASP:O	1:A:239:SER:HB3	2.19	0.42
1:C:18:ARG:HE	1:C:18:ARG:HB3	1.55	0.42
1:D:89:GLY:N	1:D:136:MET:HE2	2.33	0.42
1:F:146:THR:O	1:F:147:TYR:CB	2.66	0.42
1:H:55:LEU:N	1:H:55:LEU:HD23	2.35	0.42
1:H:57:GLN:O	1:H:58:PRO:C	2.58	0.42
1:J:232:TYR:CD1	1:J:237:LEU:HB3	2.54	0.42
1:A:50:LYS:O	1:A:53:GLU:HB2	2.19	0.42
1:C:146:THR:CG2	1:C:189:SER:HA	2.50	0.42
1:G:123:TYR:O	1:G:124:SER:C	2.57	0.42
1:G:160:MET:O	1:G:164:LYS:HG2	2.20	0.42
1:G:237:LEU:HD23	1:G:237:LEU:HA	1.76	0.42
1:H:11:ILE:HD12	1:H:35:LEU:HD13	2.00	0.42
1:J:112:GLU:OE1	1:J:112:GLU:N	2.37	0.42
1:K:123:TYR:CE2	1:K:127:ILE:HB	2.55	0.42
1:L:39:TYR:HB3	1:L:48:LEU:CD1	2.50	0.42
1:A:94:ILE:CG2	1:A:95:ALA:H	2.30	0.42
1:A:251:GLY:HA3	1:D:242:THR:CG2	2.50	0.42
1:C:39:TYR:HB3	1:C:48:LEU:CD1	2.50	0.42
1:C:89:GLY:N	1:C:136:MET:HE2	2.34	0.42
1:G:147:TYR:CD1	1:G:148:LEU:CG	2.91	0.42
1:J:123:TYR:O	1:J:126:THR:N	2.53	0.42
1:C:184:ARG:HD2	1:C:241:VAL:O	2.19	0.42
1:H:16:ASN:OD1	1:H:18:ARG:HB2	2.20	0.42
1:K:24:VAL:O	1:K:28:LEU:HG	2.20	0.42
1:C:123:TYR:O	1:C:126:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:TYR:CE2	1:E:127:ILE:HB	2.55	0.41
1:F:155:GLN:O	1:F:156:ASN:C	2.59	0.41
1:G:70:ASP:O	1:G:74:ILE:HG13	2.20	0.41
1:I:87:ILE:HG12	1:I:135:LEU:HB2	2.02	0.41
1:F:24:VAL:O	1:F:28:LEU:HG	2.20	0.41
1:J:236:ASP:OD1	1:K:228:LYS:NZ	2.27	0.41
1:C:107:SER:HB2	1:D:178:LEU:HD21	2.01	0.41
1:C:122:SER:HB3	1:D:114:PHE:HZ	1.82	0.41
1:C:125:LEU:O	1:C:126:THR:C	2.58	0.41
1:D:14:ILE:HD12	1:D:37:PHE:HD2	1.84	0.41
1:J:14:ILE:HD12	1:J:37:PHE:CD2	2.56	0.41
1:A:89:GLY:CA	1:A:136:MET:CE	2.98	0.41
1:B:47:GLU:O	1:B:51:LEU:HG	2.21	0.41
1:C:237:LEU:HD23	1:C:237:LEU:HA	1.77	0.41
1:G:67:VAL:HA	1:G:73:VAL:CG2	2.50	0.41
1:J:24:VAL:HA	1:J:227:GLY:HA2	2.02	0.41
1:K:14:ILE:HD12	1:K:37:PHE:CD2	2.55	0.41
1:L:94:ILE:HG21	1:L:120:ILE:CG2	2.50	0.41
1:B:221:VAL:HG13	1:B:222:ASP:N	2.36	0.41
1:D:24:VAL:HA	1:D:227:GLY:HA2	2.02	0.41
1:E:41:LYS:HD2	1:E:43:ARG:HD2	2.02	0.41
1:E:145:THR:CG2	1:E:146:THR:N	2.83	0.41
1:H:54:GLN:C	1:H:55:LEU:HD23	2.40	0.41
1:H:251:GLY:HA2	1:H:253:HIS:CE1	2.55	0.41
1:J:237:LEU:HD23	1:J:237:LEU:HA	1.85	0.41
1:K:147:TYR:HD1	1:K:148:LEU:H	1.68	0.41
1:B:4:LEU:HB3	1:B:33:ALA:HB2	2.01	0.41
1:E:69:SER:OG	1:E:69:SER:O	2.37	0.41
1:E:94:ILE:HG21	1:E:120:ILE:CG2	2.49	0.41
1:B:167:LEU:HD12	1:B:167:LEU:C	2.39	0.41
1:C:212:GLU:HA	1:C:218:LYS:O	2.21	0.41
1:I:47:GLU:O	1:I:51:LEU:HG	2.21	0.41
1:J:167:LEU:O	1:J:168:GLU:C	2.58	0.41
1:C:67:VAL:HG21	1:C:94:ILE:CD1	2.50	0.41
1:F:147:TYR:HD1	1:F:147:TYR:HA	1.60	0.41
1:G:37:PHE:HB2	1:G:62:LEU:HD13	2.03	0.41
1:L:178:LEU:HB3	1:L:183:ILE:HB	2.02	0.41
1:B:55:LEU:N	1:B:55:LEU:HD13	2.36	0.41
1:C:8:THR:HA	1:C:34:LYS:O	2.21	0.41
1:E:216:PRO:O	1:H:179:GLY:HA3	2.21	0.41
1:F:38:THR:HA	1:F:63:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:GLY:O	1:F:114:PHE:C	2.59	0.41
1:F:232:TYR:CD1	1:F:237:LEU:HB3	2.56	0.41
1:G:146:THR:CG2	1:G:189:SER:HA	2.49	0.41
1:G:178:LEU:HB3	1:G:183:ILE:HB	2.01	0.41
1:G:206:THR:O	1:G:209:LYS:HB3	2.20	0.41
1:H:158:ASN:OD1	1:H:160:MET:HB2	2.21	0.41
1:I:119:ASP:OD1	1:J:111:ARG:HD3	2.21	0.41
1:I:221:VAL:HG11	1:I:250:SER:N	2.35	0.41
1:K:207:ILE:HA	1:K:210:GLU:HB3	2.02	0.41
1:H:91:TYR:CE2	1:H:145:THR:OG1	2.72	0.41
1:J:89:GLY:HA2	1:J:136:MET:HE1	2.03	0.41
1:J:125:LEU:HG	1:J:174:LEU:CD1	2.50	0.41
1:L:5:GLU:O	1:L:6:ASN:HB2	2.21	0.41
1:L:248:VAL:O	1:L:248:VAL:HG12	2.21	0.41
1:A:46:LYS:O	1:A:50:LYS:HG2	2.21	0.40
1:C:145:THR:HG22	1:C:146:THR:N	2.35	0.40
1:D:47:GLU:O	1:D:50:LYS:HB2	2.21	0.40
1:E:57:GLN:HA	1:E:58:PRO:HD2	1.89	0.40
1:F:227:GLY:O	1:F:230:ALA:HB3	2.21	0.40
1:H:141:SER:HB3	1:H:234:LEU:HA	2.03	0.40
1:F:19:SER:HA	2:F:2002:HOH:O	2.20	0.40
1:I:218:LYS:HD3	2:I:2008:HOH:O	2.21	0.40
1:K:69:SER:OG	1:K:72:GLU:HG3	2.21	0.40
1:L:70:ASP:O	1:L:74:ILE:HG13	2.21	0.40
1:A:39:TYR:CD1	1:A:39:TYR:N	2.89	0.40
1:A:123:TYR:CE1	1:B:111:ARG:HA	2.56	0.40
1:C:11:ILE:HD11	1:C:35:LEU:HD22	2.04	0.40
1:C:139:GLY:HA3	1:C:182:ASN:O	2.21	0.40
1:D:8:THR:HG23	1:D:34:LYS:HG3	2.04	0.40
1:E:4:LEU:HB3	1:E:33:ALA:HB2	2.02	0.40
1:J:47:GLU:O	1:J:51:LEU:HG	2.22	0.40
1:J:57:GLN:HA	1:J:58:PRO:HD2	1.74	0.40
1:K:162:VAL:HG13	1:L:166:SER:O	2.21	0.40
1:L:14:ILE:HD12	1:L:37:PHE:HD2	1.87	0.40
1:F:65:ILE:HD11	1:F:76:GLY:HA3	2.03	0.40
1:I:24:VAL:HG21	1:I:91:TYR:CE1	2.57	0.40
1:B:221:VAL:HG21	1:B:249:ASP:HA	2.03	0.40
1:E:176:LEU:HD22	1:H:216:PRO:HG3	2.03	0.40
1:I:20:ILE:HA	1:I:223:GLN:HG3	2.02	0.40
1:K:148:LEU:CD2	1:K:190:ALA:HB1	2.51	0.40
1:K:227:GLY:O	1:K:230:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	221/282 (78%)	199 (90%)	19 (9%)	3 (1%)	11 36
1	B	212/282 (75%)	188 (89%)	23 (11%)	1 (0%)	29 60
1	C	217/282 (77%)	190 (88%)	21 (10%)	6 (3%)	5 21
1	D	187/282 (66%)	162 (87%)	25 (13%)	0	100 100
1	E	213/282 (76%)	188 (88%)	23 (11%)	2 (1%)	17 47
1	F	195/282 (69%)	176 (90%)	19 (10%)	0	100 100
1	G	213/282 (76%)	182 (85%)	29 (14%)	2 (1%)	17 47
1	H	212/282 (75%)	181 (85%)	26 (12%)	5 (2%)	6 23
1	I	206/282 (73%)	189 (92%)	17 (8%)	0	100 100
1	J	202/282 (72%)	175 (87%)	26 (13%)	1 (0%)	29 60
1	K	210/282 (74%)	179 (85%)	29 (14%)	2 (1%)	15 45
1	L	185/282 (66%)	170 (92%)	15 (8%)	0	100 100
All	All	2473/3384 (73%)	2179 (88%)	272 (11%)	22 (1%)	17 47

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	221	VAL
1	G	95	ALA
1	A	95	ALA
1	C	109	THR
1	C	218	LYS
1	E	110	SER
1	G	213	GLU
1	H	109	THR
1	J	206	THR

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Mol	Chain	Res	Type
1	K	147	TYR
1	A	156	ASN
1	B	192	PRO
1	H	192	PRO
1	H	216	PRO
1	K	158	ASN
1	A	221	VAL
1	C	193	ILE
1	H	110	SER
1	H	218	LYS
1	C	221	VAL
1	C	216	PRO
1	C	24	VAL

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	191/234 (82%)	179 (94%)	12 (6%)	18 45
1	B	183/234 (78%)	172 (94%)	11 (6%)	19 46
1	C	188/234 (80%)	172 (92%)	16 (8%)	10 34
1	D	162/234 (69%)	154 (95%)	8 (5%)	25 55
1	E	185/234 (79%)	176 (95%)	9 (5%)	25 55
1	F	168/234 (72%)	159 (95%)	9 (5%)	22 51
1	G	184/234 (79%)	174 (95%)	10 (5%)	22 51
1	H	184/234 (79%)	176 (96%)	8 (4%)	29 59
1	I	180/234 (77%)	172 (96%)	8 (4%)	28 58
1	J	176/234 (75%)	169 (96%)	7 (4%)	31 62
1	K	183/234 (78%)	168 (92%)	15 (8%)	11 35
1	L	161/234 (69%)	156 (97%)	5 (3%)	40 68
All	All	2145/2808 (76%)	2027 (94%)	118 (6%)	21 50

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	17	LYS
1	A	38	THR
1	A	48	LEU
1	A	69	SER
1	A	96	PHE
1	A	109	THR
1	A	156	ASN
1	A	176	LEU
1	A	208	LEU
1	A	210	GLU
1	A	219	ARG
1	B	3	ASN
1	B	48	LEU
1	B	55	LEU
1	B	69	SER
1	B	96	PHE
1	B	176	LEU
1	B	194	ARG
1	B	205	ASN
1	B	217	LEU
1	B	220	ASN
1	B	222	ASP
1	C	3	ASN
1	C	30	GLN
1	C	48	LEU
1	C	51	LEU
1	C	55	LEU
1	C	69	SER
1	C	107	SER
1	C	109	THR
1	C	160	MET
1	C	176	LEU
1	C	193	ILE
1	C	194	ARG
1	C	204	PHE
1	C	210	GLU
1	C	214	ARG
1	C	219	ARG
1	D	48	LEU
1	D	69	SER
1	D	156	ASN

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Mol	Chain	Res	Type
1	D	157	TYR
1	D	159	VAL
1	D	160	MET
1	D	176	LEU
1	D	250	SER
1	E	17	LYS
1	E	30	GLN
1	E	35	LEU
1	E	38	THR
1	E	48	LEU
1	E	69	SER
1	E	109	THR
1	E	147	TYR
1	E	176	LEU
1	F	3	ASN
1	F	17	LYS
1	F	48	LEU
1	F	55	LEU
1	F	69	SER
1	F	147	TYR
1	F	160	MET
1	F	176	LEU
1	F	222	ASP
1	G	30	GLN
1	G	48	LEU
1	G	51	LEU
1	G	55	LEU
1	G	69	SER
1	G	96	PHE
1	G	147	TYR
1	G	157	TYR
1	G	176	LEU
1	G	204	PHE
1	H	3	ASN
1	H	48	LEU
1	H	59	GLU
1	H	69	SER
1	H	176	LEU
1	H	193	ILE
1	H	219	ARG
1	H	222	ASP
1	I	4	LEU

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Mol	Chain	Res	Type
1	I	48	LEU
1	I	69	SER
1	I	157	TYR
1	I	160	MET
1	I	176	LEU
1	I	207	ILE
1	I	210	GLU
1	J	48	LEU
1	J	55	LEU
1	J	69	SER
1	J	176	LEU
1	J	189	SER
1	J	207	ILE
1	J	217	LEU
1	K	48	LEU
1	K	51	LEU
1	K	56	ASN
1	K	69	SER
1	K	109	THR
1	K	147	TYR
1	K	148	LEU
1	K	158	ASN
1	K	160	MET
1	K	176	LEU
1	K	204	PHE
1	K	205	ASN
1	K	206	THR
1	K	219	ARG
1	K	222	ASP
1	L	38	THR
1	L	48	LEU
1	L	69	SER
1	L	176	LEU
1	L	222	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	156	ASN
1	A	220	ASN
1	B	92	HIS

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Mol	Chain	Res	Type
1	B	220	ASN
1	C	92	HIS
1	D	130	HIS
1	F	56	ASN
1	G	92	HIS
1	G	220	ASN
1	H	56	ASN
1	J	92	HIS

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	229/282 (81%)	0.12	3 (1%)	77	56	32, 57, 102, 114	0
1	B	220/282 (78%)	0.08	1 (0%)	91	79	30, 51, 94, 104	0
1	C	225/282 (79%)	0.07	0	100	100	33, 57, 98, 109	0
1	D	195/282 (69%)	0.06	1 (0%)	91	79	32, 49, 82, 102	0
1	E	221/282 (78%)	0.13	1 (0%)	91	79	36, 60, 109, 127	0
1	F	203/282 (71%)	0.10	0	100	100	33, 51, 87, 101	0
1	G	221/282 (78%)	0.10	0	100	100	33, 59, 110, 123	0
1	H	220/282 (78%)	0.19	6 (2%)	54	28	33, 55, 102, 137	0
1	I	214/282 (75%)	0.46	12 (5%)	24	10	55, 79, 118, 128	0
1	J	210/282 (74%)	0.37	15 (7%)	16	6	53, 72, 124, 143	0
1	K	218/282 (77%)	0.42	5 (2%)	60	36	51, 79, 125, 131	0
1	L	193/282 (68%)	0.26	1 (0%)	91	79	48, 69, 107, 122	0
All	All	2569/3384 (75%)	0.20	45 (1%)	68	45	30, 63, 111, 143	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	210	GLU	5.3
1	J	214	ARG	4.0
1	H	212	GLU	3.7
1	J	92	HIS	3.6
1	I	206	THR	3.6
1	I	205	ASN	3.6
1	J	50	LYS	3.4
1	J	219	ARG	3.2
1	H	211	ILE	3.1
1	I	210	GLU	3.0
1	I	33	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	215	ALA	3.0
1	J	68	GLN	2.9
1	J	21	ALA	2.9
1	K	221	VAL	2.8
1	H	207	ILE	2.7
1	A	95	ALA	2.7
1	K	35	LEU	2.7
1	A	15	ALA	2.5
1	K	41	LYS	2.4
1	J	36	VAL	2.4
1	J	61	HIS	2.4
1	B	68	GLN	2.4
1	J	215	ALA	2.4
1	I	220	ASN	2.3
1	J	220	ASN	2.3
1	J	161	GLY	2.3
1	H	209	LYS	2.3
1	J	160	MET	2.3
1	J	48	LEU	2.2
1	J	59	GLU	2.2
1	I	5	GLU	2.2
1	K	122	SER	2.2
1	I	227	GLY	2.2
1	I	35	LEU	2.2
1	I	211	ILE	2.2
1	I	62	LEU	2.1
1	I	216	PRO	2.1
1	E	206	THR	2.1
1	L	124	SER	2.1
1	K	210	GLU	2.0
1	J	213	GLU	2.0
1	D	249	ASP	2.0
1	H	206	THR	2.0
1	A	251	GLY	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 monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.