



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:24 PM UTC

PDB ID : 5B01 / pdb_00005b01
Title : Structure of a prenyltransferase in its unbound form
Authors : Ko, T.-P.; Zhang, L.; Chen, C.-C.; Guo, R.-T.
Deposited on : 2015-10-27
Resolution : 3.45 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

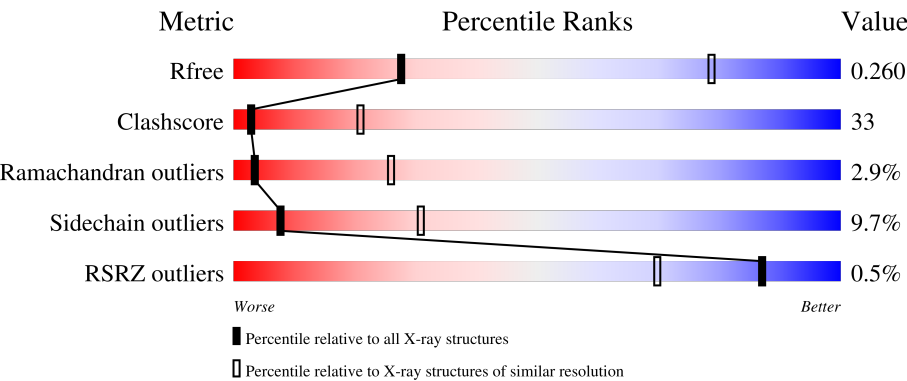
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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.

Mol	Chain	Length	Quality of chain
1	A	294	42%39%8%11%
1	B	294	41%36%11%11%
1	C	294	41%40%7%11%
1	D	294	% 39%38%12%.11%
1	E	294	41%37%11%11%

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Mol	Chain	Length	Quality of chain
1	F	294	% 41%38%10%11%
1	G	294	% 39%40%9%11%
1	H	294	39%40%10%11%
1	I	294	40%38%11%11%
1	J	294	40%39%10%11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20030 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 MoeN5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total 2003	C 1242	N 372	O 378	S 11	0	0	0
1	B	262	Total 2003	C 1242	N 372	O 378	S 11	0	0	0
1	C	262	Total 2003	C 1242	N 372	O 378	S 11	0	0	0
1	D	262	Total 2003	C 1242	N 372	O 378	S 11	0	0	0
1	E	262	Total 2003	C 1242	N 372	O 378	S 11	0	0	0
1	F	262	Total 2003	C 1242	N 372	O 378	S 11	0	0	0
1	G	262	Total 2003	C 1242	N 372	O 378	S 11	0	0	0
1	H	262	Total 2003	C 1242	N 372	O 378	S 11	0	0	0
1	I	262	Total 2003	C 1242	N 372	O 378	S 11	0	0	0
1	J	262	Total 2003	C 1242	N 372	O 378	S 11	0	0	0

There are 340 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP A0A010
A	-32	ALA	-	expression tag	UNP A0A010
A	-31	HIS	-	expression tag	UNP A0A010
A	-30	HIS	-	expression tag	UNP A0A010
A	-29	HIS	-	expression tag	UNP A0A010
A	-28	HIS	-	expression tag	UNP A0A010
A	-27	HIS	-	expression tag	UNP A0A010
A	-26	HIS	-	expression tag	UNP A0A010
A	-25	VAL	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	ASP	-	expression tag	UNP A0A010
A	-23	ASP	-	expression tag	UNP A0A010
A	-22	ASP	-	expression tag	UNP A0A010
A	-21	ASP	-	expression tag	UNP A0A010
A	-20	LYS	-	expression tag	UNP A0A010
A	-19	ALA	-	expression tag	UNP A0A010
A	-18	ALA	-	expression tag	UNP A0A010
A	-17	SER	-	expression tag	UNP A0A010
A	-16	TRP	-	expression tag	UNP A0A010
A	-15	SER	-	expression tag	UNP A0A010
A	-14	HIS	-	expression tag	UNP A0A010
A	-13	PRO	-	expression tag	UNP A0A010
A	-12	GLN	-	expression tag	UNP A0A010
A	-11	PHE	-	expression tag	UNP A0A010
A	-10	GLU	-	expression tag	UNP A0A010
A	-9	LYS	-	expression tag	UNP A0A010
A	-8	GLY	-	expression tag	UNP A0A010
A	-7	ALA	-	expression tag	UNP A0A010
A	-6	GLU	-	expression tag	UNP A0A010
A	-5	ASN	-	expression tag	UNP A0A010
A	-4	LEU	-	expression tag	UNP A0A010
A	-3	TYR	-	expression tag	UNP A0A010
A	-2	PHE	-	expression tag	UNP A0A010
A	-1	GLN	-	expression tag	UNP A0A010
A	0	SER	-	expression tag	UNP A0A010
B	-33	MET	-	expression tag	UNP A0A010
B	-32	ALA	-	expression tag	UNP A0A010
B	-31	HIS	-	expression tag	UNP A0A010
B	-30	HIS	-	expression tag	UNP A0A010
B	-29	HIS	-	expression tag	UNP A0A010
B	-28	HIS	-	expression tag	UNP A0A010
B	-27	HIS	-	expression tag	UNP A0A010
B	-26	HIS	-	expression tag	UNP A0A010
B	-25	VAL	-	expression tag	UNP A0A010
B	-24	ASP	-	expression tag	UNP A0A010
B	-23	ASP	-	expression tag	UNP A0A010
B	-22	ASP	-	expression tag	UNP A0A010
B	-21	ASP	-	expression tag	UNP A0A010
B	-20	LYS	-	expression tag	UNP A0A010
B	-19	ALA	-	expression tag	UNP A0A010
B	-18	ALA	-	expression tag	UNP A0A010
B	-17	SER	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	TRP	-	expression tag	UNP A0A010
B	-15	SER	-	expression tag	UNP A0A010
B	-14	HIS	-	expression tag	UNP A0A010
B	-13	PRO	-	expression tag	UNP A0A010
B	-12	GLN	-	expression tag	UNP A0A010
B	-11	PHE	-	expression tag	UNP A0A010
B	-10	GLU	-	expression tag	UNP A0A010
B	-9	LYS	-	expression tag	UNP A0A010
B	-8	GLY	-	expression tag	UNP A0A010
B	-7	ALA	-	expression tag	UNP A0A010
B	-6	GLU	-	expression tag	UNP A0A010
B	-5	ASN	-	expression tag	UNP A0A010
B	-4	LEU	-	expression tag	UNP A0A010
B	-3	TYR	-	expression tag	UNP A0A010
B	-2	PHE	-	expression tag	UNP A0A010
B	-1	GLN	-	expression tag	UNP A0A010
B	0	SER	-	expression tag	UNP A0A010
C	-33	MET	-	expression tag	UNP A0A010
C	-32	ALA	-	expression tag	UNP A0A010
C	-31	HIS	-	expression tag	UNP A0A010
C	-30	HIS	-	expression tag	UNP A0A010
C	-29	HIS	-	expression tag	UNP A0A010
C	-28	HIS	-	expression tag	UNP A0A010
C	-27	HIS	-	expression tag	UNP A0A010
C	-26	HIS	-	expression tag	UNP A0A010
C	-25	VAL	-	expression tag	UNP A0A010
C	-24	ASP	-	expression tag	UNP A0A010
C	-23	ASP	-	expression tag	UNP A0A010
C	-22	ASP	-	expression tag	UNP A0A010
C	-21	ASP	-	expression tag	UNP A0A010
C	-20	LYS	-	expression tag	UNP A0A010
C	-19	ALA	-	expression tag	UNP A0A010
C	-18	ALA	-	expression tag	UNP A0A010
C	-17	SER	-	expression tag	UNP A0A010
C	-16	TRP	-	expression tag	UNP A0A010
C	-15	SER	-	expression tag	UNP A0A010
C	-14	HIS	-	expression tag	UNP A0A010
C	-13	PRO	-	expression tag	UNP A0A010
C	-12	GLN	-	expression tag	UNP A0A010
C	-11	PHE	-	expression tag	UNP A0A010
C	-10	GLU	-	expression tag	UNP A0A010
C	-9	LYS	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP A0A010
C	-7	ALA	-	expression tag	UNP A0A010
C	-6	GLU	-	expression tag	UNP A0A010
C	-5	ASN	-	expression tag	UNP A0A010
C	-4	LEU	-	expression tag	UNP A0A010
C	-3	TYR	-	expression tag	UNP A0A010
C	-2	PHE	-	expression tag	UNP A0A010
C	-1	GLN	-	expression tag	UNP A0A010
C	0	SER	-	expression tag	UNP A0A010
D	-33	MET	-	expression tag	UNP A0A010
D	-32	ALA	-	expression tag	UNP A0A010
D	-31	HIS	-	expression tag	UNP A0A010
D	-30	HIS	-	expression tag	UNP A0A010
D	-29	HIS	-	expression tag	UNP A0A010
D	-28	HIS	-	expression tag	UNP A0A010
D	-27	HIS	-	expression tag	UNP A0A010
D	-26	HIS	-	expression tag	UNP A0A010
D	-25	VAL	-	expression tag	UNP A0A010
D	-24	ASP	-	expression tag	UNP A0A010
D	-23	ASP	-	expression tag	UNP A0A010
D	-22	ASP	-	expression tag	UNP A0A010
D	-21	ASP	-	expression tag	UNP A0A010
D	-20	LYS	-	expression tag	UNP A0A010
D	-19	ALA	-	expression tag	UNP A0A010
D	-18	ALA	-	expression tag	UNP A0A010
D	-17	SER	-	expression tag	UNP A0A010
D	-16	TRP	-	expression tag	UNP A0A010
D	-15	SER	-	expression tag	UNP A0A010
D	-14	HIS	-	expression tag	UNP A0A010
D	-13	PRO	-	expression tag	UNP A0A010
D	-12	GLN	-	expression tag	UNP A0A010
D	-11	PHE	-	expression tag	UNP A0A010
D	-10	GLU	-	expression tag	UNP A0A010
D	-9	LYS	-	expression tag	UNP A0A010
D	-8	GLY	-	expression tag	UNP A0A010
D	-7	ALA	-	expression tag	UNP A0A010
D	-6	GLU	-	expression tag	UNP A0A010
D	-5	ASN	-	expression tag	UNP A0A010
D	-4	LEU	-	expression tag	UNP A0A010
D	-3	TYR	-	expression tag	UNP A0A010
D	-2	PHE	-	expression tag	UNP A0A010
D	-1	GLN	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP A0A010
E	-33	MET	-	expression tag	UNP A0A010
E	-32	ALA	-	expression tag	UNP A0A010
E	-31	HIS	-	expression tag	UNP A0A010
E	-30	HIS	-	expression tag	UNP A0A010
E	-29	HIS	-	expression tag	UNP A0A010
E	-28	HIS	-	expression tag	UNP A0A010
E	-27	HIS	-	expression tag	UNP A0A010
E	-26	HIS	-	expression tag	UNP A0A010
E	-25	VAL	-	expression tag	UNP A0A010
E	-24	ASP	-	expression tag	UNP A0A010
E	-23	ASP	-	expression tag	UNP A0A010
E	-22	ASP	-	expression tag	UNP A0A010
E	-21	ASP	-	expression tag	UNP A0A010
E	-20	LYS	-	expression tag	UNP A0A010
E	-19	ALA	-	expression tag	UNP A0A010
E	-18	ALA	-	expression tag	UNP A0A010
E	-17	SER	-	expression tag	UNP A0A010
E	-16	TRP	-	expression tag	UNP A0A010
E	-15	SER	-	expression tag	UNP A0A010
E	-14	HIS	-	expression tag	UNP A0A010
E	-13	PRO	-	expression tag	UNP A0A010
E	-12	GLN	-	expression tag	UNP A0A010
E	-11	PHE	-	expression tag	UNP A0A010
E	-10	GLU	-	expression tag	UNP A0A010
E	-9	LYS	-	expression tag	UNP A0A010
E	-8	GLY	-	expression tag	UNP A0A010
E	-7	ALA	-	expression tag	UNP A0A010
E	-6	GLU	-	expression tag	UNP A0A010
E	-5	ASN	-	expression tag	UNP A0A010
E	-4	LEU	-	expression tag	UNP A0A010
E	-3	TYR	-	expression tag	UNP A0A010
E	-2	PHE	-	expression tag	UNP A0A010
E	-1	GLN	-	expression tag	UNP A0A010
E	0	SER	-	expression tag	UNP A0A010
F	-33	MET	-	expression tag	UNP A0A010
F	-32	ALA	-	expression tag	UNP A0A010
F	-31	HIS	-	expression tag	UNP A0A010
F	-30	HIS	-	expression tag	UNP A0A010
F	-29	HIS	-	expression tag	UNP A0A010
F	-28	HIS	-	expression tag	UNP A0A010
F	-27	HIS	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-26	HIS	-	expression tag	UNP A0A010
F	-25	VAL	-	expression tag	UNP A0A010
F	-24	ASP	-	expression tag	UNP A0A010
F	-23	ASP	-	expression tag	UNP A0A010
F	-22	ASP	-	expression tag	UNP A0A010
F	-21	ASP	-	expression tag	UNP A0A010
F	-20	LYS	-	expression tag	UNP A0A010
F	-19	ALA	-	expression tag	UNP A0A010
F	-18	ALA	-	expression tag	UNP A0A010
F	-17	SER	-	expression tag	UNP A0A010
F	-16	TRP	-	expression tag	UNP A0A010
F	-15	SER	-	expression tag	UNP A0A010
F	-14	HIS	-	expression tag	UNP A0A010
F	-13	PRO	-	expression tag	UNP A0A010
F	-12	GLN	-	expression tag	UNP A0A010
F	-11	PHE	-	expression tag	UNP A0A010
F	-10	GLU	-	expression tag	UNP A0A010
F	-9	LYS	-	expression tag	UNP A0A010
F	-8	GLY	-	expression tag	UNP A0A010
F	-7	ALA	-	expression tag	UNP A0A010
F	-6	GLU	-	expression tag	UNP A0A010
F	-5	ASN	-	expression tag	UNP A0A010
F	-4	LEU	-	expression tag	UNP A0A010
F	-3	TYR	-	expression tag	UNP A0A010
F	-2	PHE	-	expression tag	UNP A0A010
F	-1	GLN	-	expression tag	UNP A0A010
F	0	SER	-	expression tag	UNP A0A010
G	-33	MET	-	expression tag	UNP A0A010
G	-32	ALA	-	expression tag	UNP A0A010
G	-31	HIS	-	expression tag	UNP A0A010
G	-30	HIS	-	expression tag	UNP A0A010
G	-29	HIS	-	expression tag	UNP A0A010
G	-28	HIS	-	expression tag	UNP A0A010
G	-27	HIS	-	expression tag	UNP A0A010
G	-26	HIS	-	expression tag	UNP A0A010
G	-25	VAL	-	expression tag	UNP A0A010
G	-24	ASP	-	expression tag	UNP A0A010
G	-23	ASP	-	expression tag	UNP A0A010
G	-22	ASP	-	expression tag	UNP A0A010
G	-21	ASP	-	expression tag	UNP A0A010
G	-20	LYS	-	expression tag	UNP A0A010
G	-19	ALA	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-18	ALA	-	expression tag	UNP A0A010
G	-17	SER	-	expression tag	UNP A0A010
G	-16	TRP	-	expression tag	UNP A0A010
G	-15	SER	-	expression tag	UNP A0A010
G	-14	HIS	-	expression tag	UNP A0A010
G	-13	PRO	-	expression tag	UNP A0A010
G	-12	GLN	-	expression tag	UNP A0A010
G	-11	PHE	-	expression tag	UNP A0A010
G	-10	GLU	-	expression tag	UNP A0A010
G	-9	LYS	-	expression tag	UNP A0A010
G	-8	GLY	-	expression tag	UNP A0A010
G	-7	ALA	-	expression tag	UNP A0A010
G	-6	GLU	-	expression tag	UNP A0A010
G	-5	ASN	-	expression tag	UNP A0A010
G	-4	LEU	-	expression tag	UNP A0A010
G	-3	TYR	-	expression tag	UNP A0A010
G	-2	PHE	-	expression tag	UNP A0A010
G	-1	GLN	-	expression tag	UNP A0A010
G	0	SER	-	expression tag	UNP A0A010
H	-33	MET	-	expression tag	UNP A0A010
H	-32	ALA	-	expression tag	UNP A0A010
H	-31	HIS	-	expression tag	UNP A0A010
H	-30	HIS	-	expression tag	UNP A0A010
H	-29	HIS	-	expression tag	UNP A0A010
H	-28	HIS	-	expression tag	UNP A0A010
H	-27	HIS	-	expression tag	UNP A0A010
H	-26	HIS	-	expression tag	UNP A0A010
H	-25	VAL	-	expression tag	UNP A0A010
H	-24	ASP	-	expression tag	UNP A0A010
H	-23	ASP	-	expression tag	UNP A0A010
H	-22	ASP	-	expression tag	UNP A0A010
H	-21	ASP	-	expression tag	UNP A0A010
H	-20	LYS	-	expression tag	UNP A0A010
H	-19	ALA	-	expression tag	UNP A0A010
H	-18	ALA	-	expression tag	UNP A0A010
H	-17	SER	-	expression tag	UNP A0A010
H	-16	TRP	-	expression tag	UNP A0A010
H	-15	SER	-	expression tag	UNP A0A010
H	-14	HIS	-	expression tag	UNP A0A010
H	-13	PRO	-	expression tag	UNP A0A010
H	-12	GLN	-	expression tag	UNP A0A010
H	-11	PHE	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-10	GLU	-	expression tag	UNP A0A010
H	-9	LYS	-	expression tag	UNP A0A010
H	-8	GLY	-	expression tag	UNP A0A010
H	-7	ALA	-	expression tag	UNP A0A010
H	-6	GLU	-	expression tag	UNP A0A010
H	-5	ASN	-	expression tag	UNP A0A010
H	-4	LEU	-	expression tag	UNP A0A010
H	-3	TYR	-	expression tag	UNP A0A010
H	-2	PHE	-	expression tag	UNP A0A010
H	-1	GLN	-	expression tag	UNP A0A010
H	0	SER	-	expression tag	UNP A0A010
I	-33	MET	-	expression tag	UNP A0A010
I	-32	ALA	-	expression tag	UNP A0A010
I	-31	HIS	-	expression tag	UNP A0A010
I	-30	HIS	-	expression tag	UNP A0A010
I	-29	HIS	-	expression tag	UNP A0A010
I	-28	HIS	-	expression tag	UNP A0A010
I	-27	HIS	-	expression tag	UNP A0A010
I	-26	HIS	-	expression tag	UNP A0A010
I	-25	VAL	-	expression tag	UNP A0A010
I	-24	ASP	-	expression tag	UNP A0A010
I	-23	ASP	-	expression tag	UNP A0A010
I	-22	ASP	-	expression tag	UNP A0A010
I	-21	ASP	-	expression tag	UNP A0A010
I	-20	LYS	-	expression tag	UNP A0A010
I	-19	ALA	-	expression tag	UNP A0A010
I	-18	ALA	-	expression tag	UNP A0A010
I	-17	SER	-	expression tag	UNP A0A010
I	-16	TRP	-	expression tag	UNP A0A010
I	-15	SER	-	expression tag	UNP A0A010
I	-14	HIS	-	expression tag	UNP A0A010
I	-13	PRO	-	expression tag	UNP A0A010
I	-12	GLN	-	expression tag	UNP A0A010
I	-11	PHE	-	expression tag	UNP A0A010
I	-10	GLU	-	expression tag	UNP A0A010
I	-9	LYS	-	expression tag	UNP A0A010
I	-8	GLY	-	expression tag	UNP A0A010
I	-7	ALA	-	expression tag	UNP A0A010
I	-6	GLU	-	expression tag	UNP A0A010
I	-5	ASN	-	expression tag	UNP A0A010
I	-4	LEU	-	expression tag	UNP A0A010
I	-3	TYR	-	expression tag	UNP A0A010

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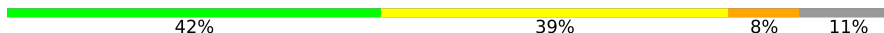
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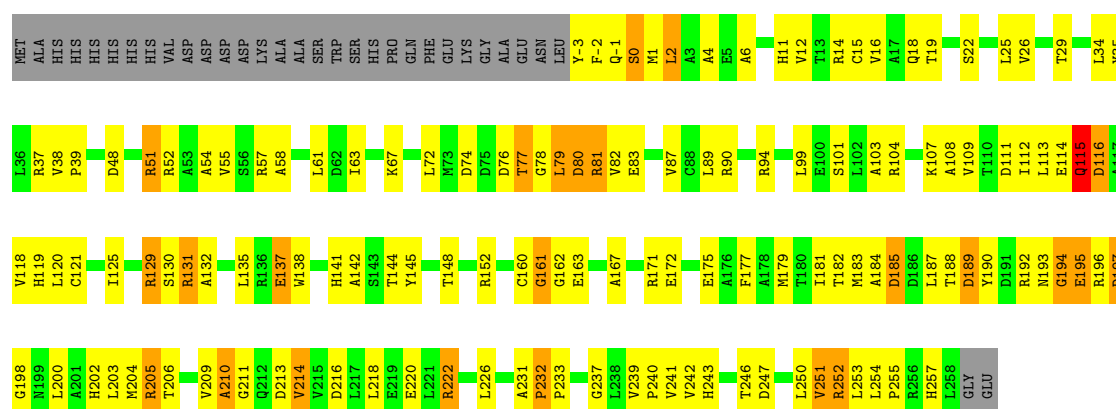
Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	PHE	-	expression tag	UNP A0A010
I	-1	GLN	-	expression tag	UNP A0A010
I	0	SER	-	expression tag	UNP A0A010
J	-33	MET	-	expression tag	UNP A0A010
J	-32	ALA	-	expression tag	UNP A0A010
J	-31	HIS	-	expression tag	UNP A0A010
J	-30	HIS	-	expression tag	UNP A0A010
J	-29	HIS	-	expression tag	UNP A0A010
J	-28	HIS	-	expression tag	UNP A0A010
J	-27	HIS	-	expression tag	UNP A0A010
J	-26	HIS	-	expression tag	UNP A0A010
J	-25	VAL	-	expression tag	UNP A0A010
J	-24	ASP	-	expression tag	UNP A0A010
J	-23	ASP	-	expression tag	UNP A0A010
J	-22	ASP	-	expression tag	UNP A0A010
J	-21	ASP	-	expression tag	UNP A0A010
J	-20	LYS	-	expression tag	UNP A0A010
J	-19	ALA	-	expression tag	UNP A0A010
J	-18	ALA	-	expression tag	UNP A0A010
J	-17	SER	-	expression tag	UNP A0A010
J	-16	TRP	-	expression tag	UNP A0A010
J	-15	SER	-	expression tag	UNP A0A010
J	-14	HIS	-	expression tag	UNP A0A010
J	-13	PRO	-	expression tag	UNP A0A010
J	-12	GLN	-	expression tag	UNP A0A010
J	-11	PHE	-	expression tag	UNP A0A010
J	-10	GLU	-	expression tag	UNP A0A010
J	-9	LYS	-	expression tag	UNP A0A010
J	-8	GLY	-	expression tag	UNP A0A010
J	-7	ALA	-	expression tag	UNP A0A010
J	-6	GLU	-	expression tag	UNP A0A010
J	-5	ASN	-	expression tag	UNP A0A010
J	-4	LEU	-	expression tag	UNP A0A010
J	-3	TYR	-	expression tag	UNP A0A010
J	-2	PHE	-	expression tag	UNP A0A010
J	-1	GLN	-	expression tag	UNP A0A010
J	0	SER	-	expression tag	UNP A0A010

3 Residue-property plots

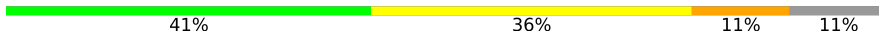
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

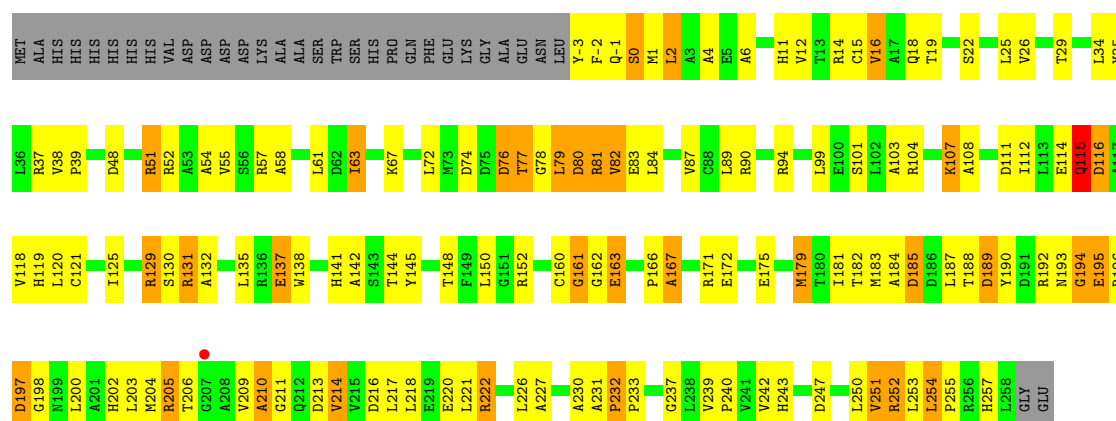
• Molecule 1: MoeN5

Chain A: 

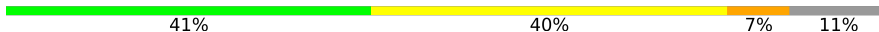


• Molecule 1: MoeN5

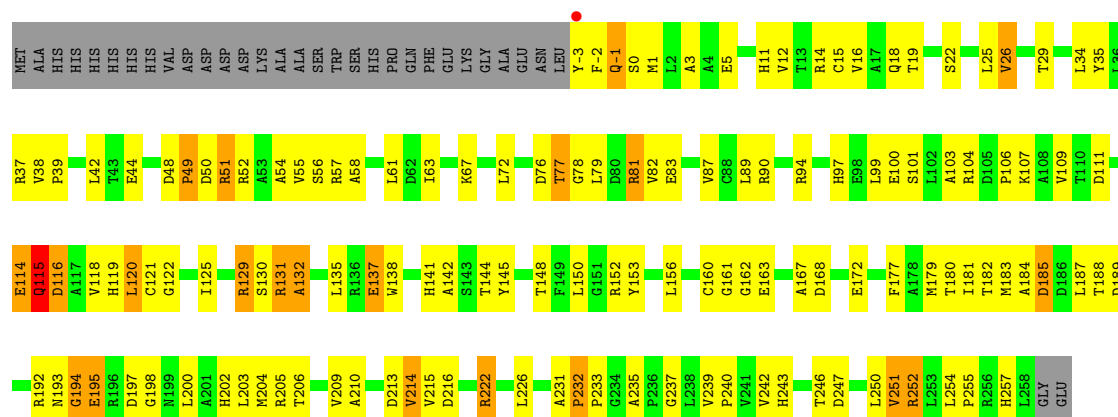
Chain B: 



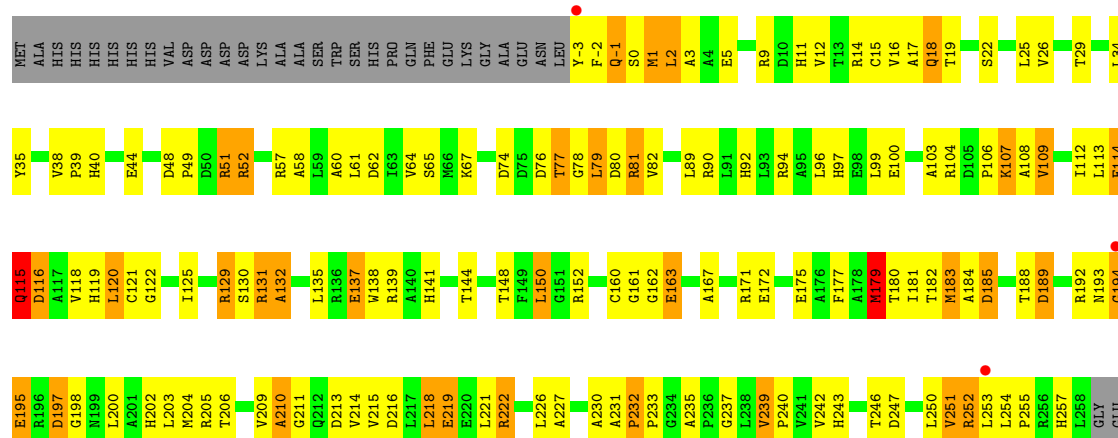
• Molecule 1: MoeN5

Chain C: 

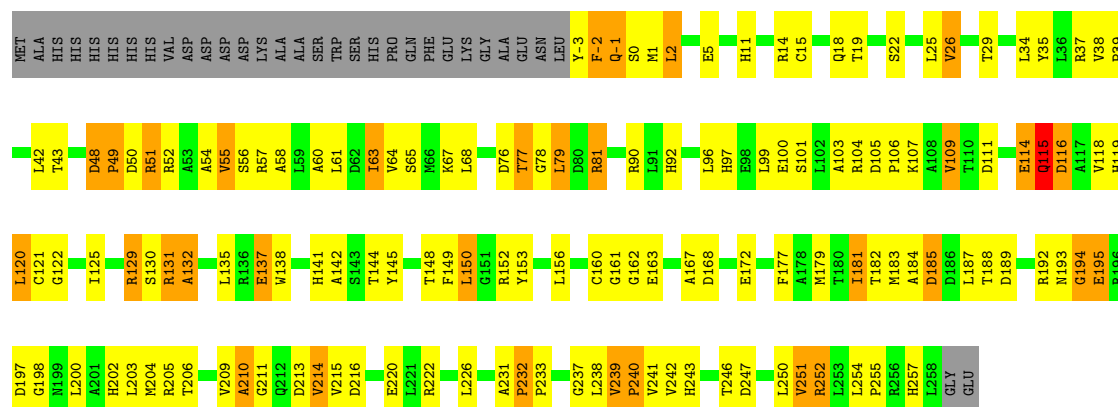




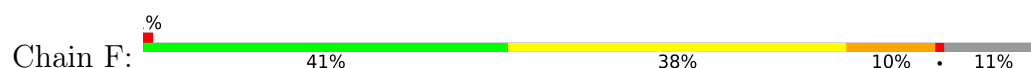
• Molecule 1: MoeN5

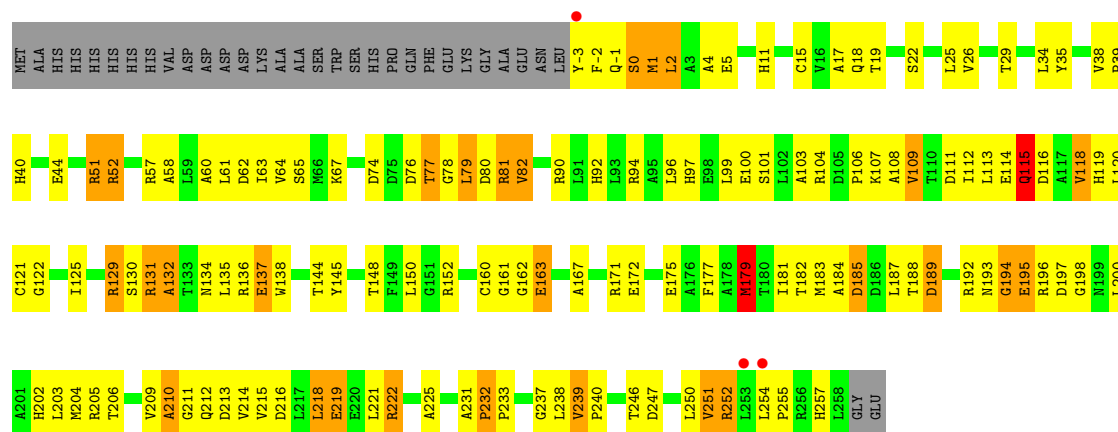


• Molecule 1: MoeN5

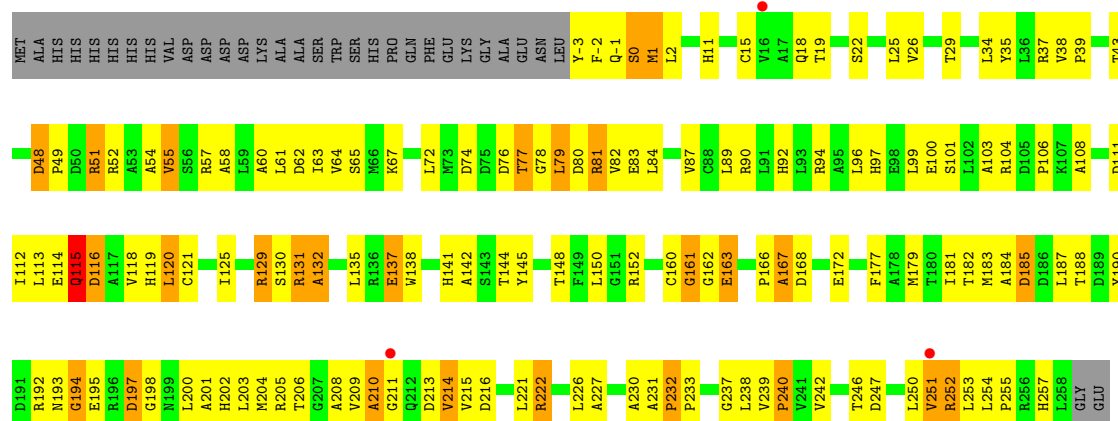


• Molecule 1: MoeN5

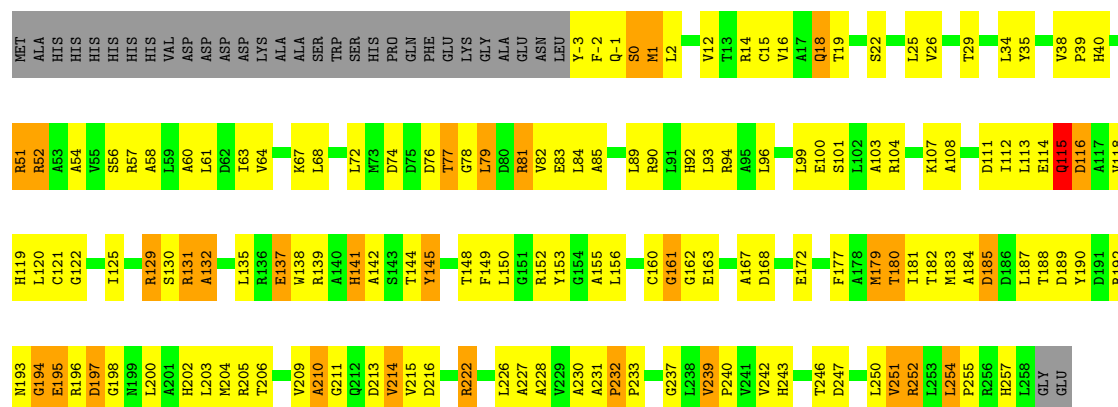




• Molecule 1: MoenN5



• Molecule 1: MoenN5



• Molecule 1: MoenN5



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	106.60Å 106.60Å 310.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.45 25.00 – 3.45	Depositor EDS
% Data completeness (in resolution range)	92.3 (25.00-3.45) 92.2 (25.00-3.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 3.46Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.261 0.225 , 0.260	Depositor DCC
R_{free} test set	2090 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	87.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20030	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.03	0/2037	1.32	22/2769 (0.8%)
1	B	1.04	1/2037 (0.0%)	1.34	22/2769 (0.8%)
1	C	1.03	2/2037 (0.1%)	1.33	22/2769 (0.8%)
1	D	1.04	3/2037 (0.1%)	1.33	24/2769 (0.9%)
1	E	1.04	1/2037 (0.0%)	1.33	25/2769 (0.9%)
1	F	1.04	3/2037 (0.1%)	1.34	19/2769 (0.7%)
1	G	0.85	0/2037	1.29	22/2769 (0.8%)
1	H	0.89	1/2037 (0.0%)	1.31	21/2769 (0.8%)
1	I	0.87	2/2037 (0.1%)	1.30	21/2769 (0.8%)
1	J	0.89	1/2037 (0.0%)	1.32	24/2769 (0.9%)
All	All	0.98	14/20370 (0.1%)	1.32	222/27690 (0.8%)

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	F	0	1
1	H	0	1
1	J	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	239	VAL	CA-CB	-9.41	1.47	1.53
1	H	179	MET	SD-CE	8.31	2.00	1.79
1	J	179	MET	SD-CE	8.29	2.00	1.79
1	F	239	VAL	CA-CB	-7.12	1.49	1.53
1	D	179	MET	SD-CE	5.75	1.94	1.79
1	B	63	ILE	CA-CB	-5.61	1.47	1.54
1	F	118	VAL	CA-CB	-5.61	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	179	MET	SD-CE	5.47	1.93	1.79
1	C	180	THR	CA-CB	5.23	1.61	1.53
1	I	239	VAL	CA-CB	-5.22	1.51	1.54
1	D	183	MET	SD-CE	-5.20	1.66	1.79
1	E	63	ILE	CA-CB	-5.07	1.48	1.54
1	I	66	MET	SD-CE	5.06	1.92	1.79
1	C	179	MET	SD-CE	5.01	1.92	1.79

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	231	ALA	CA-C-N	8.83	129.47	120.38
1	I	231	ALA	C-N-CA	8.83	129.47	120.38
1	G	231	ALA	CA-C-N	8.75	129.39	120.38
1	G	231	ALA	C-N-CA	8.75	129.39	120.38
1	E	231	ALA	CA-C-N	8.68	129.32	120.38
1	E	231	ALA	C-N-CA	8.68	129.32	120.38
1	B	231	ALA	CA-C-N	8.65	129.29	120.38
1	B	231	ALA	C-N-CA	8.65	129.29	120.38
1	J	231	ALA	CA-C-N	8.62	129.26	120.38
1	J	231	ALA	C-N-CA	8.62	129.26	120.38
1	B	214	VAL	N-CA-C	-8.60	102.17	110.42
1	C	231	ALA	CA-C-N	8.50	129.13	120.38
1	C	231	ALA	C-N-CA	8.50	129.13	120.38
1	H	231	ALA	CA-C-N	8.46	129.09	120.38
1	H	231	ALA	C-N-CA	8.46	129.09	120.38
1	F	51	ARG	N-CA-C	-8.44	102.04	111.07
1	A	214	VAL	N-CA-C	-8.43	102.33	110.42
1	C	251	VAL	N-CA-C	8.34	118.42	110.42
1	H	51	ARG	N-CA-C	-8.23	102.26	111.07
1	I	214	VAL	N-CA-C	-8.21	102.54	110.42
1	J	51	ARG	N-CA-C	-8.07	102.43	111.07
1	D	51	ARG	N-CA-C	-8.01	102.50	111.07
1	C	122	GLY	N-CA-C	-7.97	102.85	112.49
1	G	251	VAL	N-CA-C	7.90	117.96	110.30
1	I	251	VAL	N-CA-C	7.81	117.88	110.30
1	A	231	ALA	CA-C-N	7.75	128.36	120.38
1	A	231	ALA	C-N-CA	7.75	128.36	120.38
1	J	214	VAL	N-CA-C	-7.74	102.99	110.42
1	G	214	VAL	N-CA-C	-7.67	103.06	110.42
1	A	251	VAL	N-CA-C	7.57	117.64	110.30
1	H	214	VAL	N-CA-C	-7.53	103.19	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	251	VAL	N-CA-C	7.50	117.57	110.30
1	J	251	VAL	N-CA-C	7.45	117.53	110.30
1	D	231	ALA	CA-C-N	7.43	128.03	120.38
1	D	231	ALA	C-N-CA	7.43	128.03	120.38
1	A	51	ARG	N-CA-C	-7.42	103.12	111.07
1	B	51	ARG	N-CA-C	-7.39	103.16	111.07
1	D	214	VAL	N-CA-C	-7.29	103.42	110.42
1	C	51	ARG	N-CA-C	-7.26	103.30	111.07
1	F	214	VAL	N-CA-C	-7.26	103.45	110.42
1	I	51	ARG	N-CA-C	-7.24	103.32	111.07
1	B	251	VAL	N-CA-C	7.22	117.30	110.30
1	F	231	ALA	CA-C-N	7.21	127.81	120.38
1	F	231	ALA	C-N-CA	7.21	127.81	120.38
1	E	51	ARG	N-CA-C	-7.17	103.39	111.07
1	G	51	ARG	N-CA-C	-7.16	103.41	111.07
1	D	251	VAL	N-CA-C	7.08	117.17	110.30
1	E	122	GLY	N-CA-C	-7.00	104.02	112.49
1	I	161	GLY	N-CA-C	6.83	121.98	114.40
1	G	161	GLY	N-CA-C	6.71	121.85	114.40
1	E	251	VAL	N-CA-C	6.70	116.85	110.42
1	C	232	PRO	N-CA-C	6.67	118.83	110.70
1	C	195	GLU	N-CA-C	-6.60	99.08	109.50
1	E	232	PRO	N-CA-C	6.58	118.73	110.70
1	B	161	GLY	N-CA-C	6.58	121.70	114.40
1	F	251	VAL	N-CA-C	6.56	116.66	110.30
1	B	232	PRO	N-CA-C	6.54	118.68	110.70
1	E	214	VAL	N-CA-C	-6.47	104.21	110.42
1	C	214	VAL	N-CA-C	-6.47	104.21	110.42
1	I	122	GLY	N-CA-C	-6.37	104.78	112.49
1	E	55	VAL	N-CA-C	-6.37	104.29	110.72
1	I	195	GLU	N-CA-C	-6.36	99.45	109.50
1	J	161	GLY	N-CA-C	6.34	121.44	114.40
1	C	161	GLY	N-CA-C	6.34	121.44	114.40
1	G	195	GLU	N-CA-C	-6.33	99.50	109.50
1	F	252	ARG	N-CA-C	6.32	121.12	113.41
1	B	252	ARG	N-CA-C	6.30	121.10	113.41
1	E	252	ARG	N-CA-C	6.30	121.09	113.41
1	C	55	VAL	N-CA-C	-6.29	104.37	110.72
1	A	195	GLU	N-CA-C	-6.28	99.58	109.50
1	J	195	GLU	N-CA-C	-6.27	99.59	109.50
1	H	195	GLU	N-CA-C	-6.26	99.61	109.50
1	A	161	GLY	N-CA-C	6.26	121.34	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	VAL	N-CA-C	-6.23	104.42	110.72
1	E	161	GLY	N-CA-C	6.22	121.31	114.40
1	A	252	ARG	N-CA-C	6.22	120.99	113.41
1	F	122	GLY	N-CA-C	-6.21	104.97	112.49
1	B	195	GLU	N-CA-C	-6.20	99.70	109.50
1	H	232	PRO	N-CA-C	6.19	118.26	110.70
1	E	195	GLU	N-CA-C	-6.18	99.73	109.50
1	J	74	ASP	N-CA-C	-6.12	104.69	111.36
1	D	232	PRO	N-CA-C	6.12	118.16	110.70
1	C	252	ARG	N-CA-C	6.12	120.87	113.41
1	D	195	GLU	N-CA-C	-6.08	99.89	109.50
1	H	239	VAL	CA-C-O	6.08	122.77	118.69
1	B	189	ASP	N-CA-C	6.05	119.76	112.38
1	D	180	THR	N-CA-C	-6.05	104.76	111.36
1	I	222	ARG	N-CA-C	-6.05	104.76	111.71
1	H	82	VAL	N-CA-C	6.01	116.13	110.30
1	J	222	ARG	N-CA-C	-5.97	104.77	111.28
1	D	210	ALA	N-CA-C	5.95	118.35	109.25
1	G	232	PRO	N-CA-C	5.92	117.93	110.70
1	F	232	PRO	N-CA-C	5.92	117.92	110.70
1	F	195	GLU	N-CA-C	-5.90	100.17	109.50
1	D	122	GLY	N-CA-C	-5.84	105.42	112.49
1	J	82	VAL	N-CA-C	5.84	115.96	110.30
1	I	48	ASP	CA-C-N	5.84	125.70	119.28
1	I	48	ASP	C-N-CA	5.84	125.70	119.28
1	B	74	ASP	N-CA-C	-5.83	105.00	111.36
1	E	181	ILE	CB-CA-C	-5.82	104.19	112.22
1	J	122	GLY	N-CA-C	-5.81	105.46	112.49
1	B	55	VAL	N-CA-C	-5.81	104.85	110.72
1	C	48	ASP	CA-C-N	5.80	125.66	119.28
1	C	48	ASP	C-N-CA	5.80	125.66	119.28
1	C	26	VAL	N-CA-C	-5.79	104.87	110.72
1	J	232	PRO	N-CA-C	5.78	117.75	110.70
1	A	232	PRO	N-CA-C	5.78	117.75	110.70
1	H	168	ASP	N-CA-C	5.77	117.57	111.28
1	D	252	ARG	N-CA-C	5.75	120.42	113.41
1	F	210	ALA	N-CA-C	5.73	118.02	109.25
1	I	252	ARG	N-CA-C	5.73	120.40	113.41
1	H	222	ARG	N-CA-C	-5.70	105.15	111.71
1	J	14	ARG	N-CA-C	-5.70	104.97	111.07
1	D	132	ALA	N-CA-C	5.69	118.05	110.53
1	B	2	LEU	N-CA-C	-5.68	106.51	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	48	ASP	CA-C-N	5.68	125.53	119.28
1	J	48	ASP	C-N-CA	5.68	125.53	119.28
1	H	132	ALA	N-CA-C	5.66	117.85	110.43
1	H	161	GLY	N-CA-C	5.66	120.69	114.40
1	E	2	LEU	N-CA-C	-5.63	106.25	113.23
1	F	222	ARG	N-CA-C	-5.63	105.24	111.71
1	F	132	ALA	N-CA-C	5.62	117.94	110.53
1	H	74	ASP	N-CA-C	-5.61	105.25	111.36
1	E	168	ASP	N-CA-C	5.57	117.35	111.28
1	G	222	ARG	N-CA-C	-5.57	105.31	111.71
1	C	222	ARG	N-CA-C	-5.57	105.21	111.28
1	C	14	ARG	N-CA-C	-5.56	105.12	111.07
1	D	115	GLN	N-CA-C	5.56	122.64	110.80
1	E	48	ASP	CA-C-N	5.55	125.38	119.28
1	E	48	ASP	C-N-CA	5.55	125.38	119.28
1	C	132	ALA	N-CA-C	5.54	117.85	110.53
1	I	74	ASP	N-CA-C	-5.54	105.33	111.36
1	E	239	VAL	CB-CA-C	-5.53	108.49	114.35
1	G	74	ASP	N-CA-C	-5.51	105.35	111.36
1	F	225	ALA	N-CA-C	5.51	116.98	110.97
1	A	222	ARG	N-CA-C	-5.49	105.29	111.28
1	I	197	ASP	N-CA-C	5.48	118.29	107.98
1	E	210	ALA	N-CA-C	5.48	117.64	109.25
1	G	252	ARG	N-CA-C	5.48	120.09	113.41
1	A	115	GLN	N-CA-C	5.47	122.44	110.80
1	A	48	ASP	CA-C-N	5.45	125.28	119.28
1	A	48	ASP	C-N-CA	5.45	125.28	119.28
1	F	161	GLY	N-CA-C	5.45	120.45	114.40
1	E	26	VAL	N-CA-C	-5.45	105.06	110.62
1	F	115	GLN	N-CA-C	5.45	122.40	110.80
1	D	222	ARG	N-CA-C	-5.43	105.47	111.71
1	A	210	ALA	N-CA-C	5.43	117.55	109.25
1	H	122	GLY	N-CA-C	-5.42	105.93	112.49
1	B	16	VAL	CB-CA-C	-5.42	104.94	112.04
1	B	115	GLN	N-CA-C	5.42	122.34	110.80
1	E	132	ALA	N-CA-C	5.42	117.68	110.53
1	B	80	ASP	N-CA-C	5.41	117.53	109.59
1	B	222	ARG	N-CA-C	-5.41	105.39	111.28
1	J	80	ASP	N-CA-C	5.39	117.52	109.59
1	F	74	ASP	N-CA-C	-5.39	105.49	111.36
1	G	240	PRO	CA-C-N	5.38	127.34	120.56
1	G	240	PRO	C-N-CA	5.38	127.34	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	240	PRO	CA-C-N	5.37	127.33	120.56
1	I	240	PRO	C-N-CA	5.37	127.33	120.56
1	J	180	THR	N-CA-C	-5.37	105.51	111.36
1	D	239	VAL	CB-CA-C	-5.36	108.67	114.35
1	H	100	GLU	N-CA-C	5.35	117.86	111.71
1	G	168	ASP	N-CA-C	5.33	117.08	111.28
1	D	82	VAL	N-CA-C	5.32	115.46	110.30
1	D	161	GLY	N-CA-C	5.31	120.30	114.40
1	F	82	VAL	N-CA-C	5.29	115.43	110.30
1	J	239	VAL	CA-C-O	5.29	122.23	118.69
1	J	197	ASP	N-CA-C	5.29	117.92	107.98
1	D	197	ASP	N-CA-C	5.28	117.91	107.98
1	F	2	LEU	N-CA-C	-5.28	106.69	113.23
1	H	180	THR	N-CA-C	-5.28	105.61	111.36
1	G	197	ASP	N-CA-C	5.27	117.88	107.98
1	C	-1	GLN	N-CA-C	-5.26	99.60	110.80
1	A	189	ASP	N-CA-C	5.26	118.79	112.38
1	I	55	VAL	N-CA-C	-5.26	105.41	110.72
1	B	48	ASP	CA-C-N	5.25	125.06	119.28
1	B	48	ASP	C-N-CA	5.25	125.06	119.28
1	G	48	ASP	CA-C-N	5.25	125.06	119.28
1	G	48	ASP	C-N-CA	5.25	125.06	119.28
1	B	197	ASP	N-CA-C	5.24	117.84	107.98
1	J	132	ALA	N-CA-C	5.24	117.30	110.43
1	A	197	ASP	N-CA-C	5.23	117.82	107.98
1	J	100	GLU	N-CA-C	5.23	117.72	111.71
1	F	189	ASP	N-CA-C	5.23	119.14	112.87
1	J	115	GLN	N-CA-C	5.22	121.93	110.80
1	A	2	LEU	N-CA-C	-5.22	106.75	113.23
1	A	74	ASP	N-CA-C	-5.22	105.67	111.36
1	D	189	ASP	N-CA-C	5.22	119.13	112.87
1	H	197	ASP	N-CA-C	5.21	117.77	107.98
1	G	115	GLN	N-CA-C	5.20	121.88	110.80
1	G	210	ALA	N-CA-C	5.19	117.19	109.25
1	G	55	VAL	N-CA-C	-5.19	105.48	110.72
1	G	82	VAL	N-CA-C	5.18	115.33	110.30
1	J	228	ALA	N-CA-C	5.17	117.00	111.36
1	C	100	GLU	N-CA-C	5.17	117.66	111.71
1	A	80	ASP	N-CA-C	5.16	117.17	109.59
1	H	210	ALA	N-CA-C	5.15	117.13	109.25
1	I	115	GLN	N-CA-C	5.14	121.75	110.80
1	E	240	PRO	CA-C-N	5.14	127.04	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	240	PRO	C-N-CA	5.14	127.04	120.56
1	C	82	VAL	N-CA-C	5.13	115.28	110.30
1	I	168	ASP	N-CA-C	5.13	116.87	111.28
1	D	-1	GLN	N-CA-C	-5.11	99.92	110.80
1	D	2	LEU	N-CA-C	-5.11	106.89	113.23
1	B	210	ALA	N-CA-C	5.10	117.06	109.25
1	G	132	ALA	N-CA-C	5.10	117.11	110.43
1	I	232	PRO	N-CA-C	5.09	116.91	110.70
1	D	74	ASP	N-CA-C	-5.08	105.82	111.36
1	B	82	VAL	N-CA-C	5.08	115.23	110.30
1	E	115	GLN	N-CA-C	5.08	121.63	110.80
1	E	14	ARG	N-CA-C	-5.08	105.64	111.07
1	A	241	VAL	CB-CA-C	-5.07	105.48	111.97
1	C	168	ASP	N-CA-C	5.07	116.81	111.28
1	H	252	ARG	N-CA-C	5.07	119.60	113.41
1	I	256	ARG	N-CA-C	5.07	116.81	111.28
1	C	3	ALA	N-CA-C	-5.07	105.84	111.36
1	D	14	ARG	N-CA-C	-5.05	105.67	111.07
1	D	3	ALA	N-CA-C	-5.05	105.86	111.36
1	A	14	ARG	N-CA-C	-5.04	105.68	111.07
1	J	168	ASP	N-CA-C	5.04	116.77	111.28
1	H	228	ALA	N-CA-C	5.03	116.84	111.36
1	E	-1	GLN	N-CA-C	-5.03	100.09	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	145	TYR	Sidechain
1	H	145	TYR	Sidechain
1	J	145	TYR	Sidechain

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	2003	0	1989	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2003	0	1989	141	0
1	C	2003	0	1989	122	0
1	D	2003	0	1989	143	0
1	E	2003	0	1989	137	0
1	F	2003	0	1989	138	0
1	G	2003	0	1989	143	0
1	H	2003	0	1989	135	0
1	I	2003	0	1989	137	0
1	J	2003	0	1989	134	0
All	All	20030	0	19890	1299	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 33.

All (1299) 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:I:81:ARG:HH11	1:I:81:ARG:HB3	1.06	1.18
1:A:81:ARG:HH11	1:A:81:ARG:CB	1.58	1.16
1:E:81:ARG:CB	1:E:81:ARG:HH11	1.58	1.14
1:H:81:ARG:HH11	1:H:81:ARG:HB3	1.09	1.14
1:B:81:ARG:CB	1:B:81:ARG:HH11	1.62	1.12
1:C:81:ARG:HH11	1:C:81:ARG:HB3	1.05	1.12
1:D:81:ARG:HB3	1:D:81:ARG:HH11	1.02	1.12
1:E:81:ARG:HH11	1:E:81:ARG:HB3	1.05	1.11
1:B:81:ARG:HH11	1:B:81:ARG:HB3	1.14	1.10
1:D:219:GLU:CD	1:F:219:GLU:CD	2.20	1.09
1:C:81:ARG:HH11	1:C:81:ARG:CB	1.64	1.08
1:H:81:ARG:HH11	1:H:81:ARG:CB	1.64	1.08
1:F:81:ARG:HB3	1:F:81:ARG:HH11	1.00	1.07
1:J:81:ARG:HH11	1:J:81:ARG:HB3	1.10	1.07
1:I:81:ARG:HH11	1:I:81:ARG:CB	1.68	1.07
1:D:81:ARG:HH11	1:D:81:ARG:CB	1.67	1.07
1:F:81:ARG:HH11	1:F:81:ARG:CB	1.69	1.04
1:J:81:ARG:HH11	1:J:81:ARG:CB	1.69	1.04
1:G:81:ARG:HH11	1:G:81:ARG:HB3	1.16	1.04
1:G:81:ARG:HH11	1:G:81:ARG:CB	1.71	1.03
1:I:51:ARG:NH2	1:I:162:GLY:HA2	1.75	1.02
1:A:81:ARG:HH11	1:A:81:ARG:HB3	1.22	0.98
1:D:219:GLU:HG2	1:F:219:GLU:OE2	1.67	0.94
1:G:51:ARG:NH2	1:G:162:GLY:HA2	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:ARG:HB3	1:E:81:ARG:NH1	1.83	0.94
1:I:51:ARG:HH21	1:I:162:GLY:CA	1.81	0.92
1:F:81:ARG:HB3	1:F:81:ARG:NH1	1.84	0.92
1:I:-3:TYR:C	1:I:-1:GLN:H	1.78	0.92
1:G:-3:TYR:C	1:G:-1:GLN:H	1.78	0.92
1:D:81:ARG:HB3	1:D:81:ARG:NH1	1.84	0.91
1:A:-3:TYR:C	1:A:-1:GLN:H	1.76	0.90
1:J:51:ARG:NH2	1:J:162:GLY:HA2	1.84	0.90
1:B:-3:TYR:C	1:B:-1:GLN:H	1.80	0.89
1:D:104:ARG:HD3	1:D:163:GLU:HG3	1.53	0.89
1:A:81:ARG:HH21	1:B:81:ARG:HH21	1.20	0.89
1:C:81:ARG:HB3	1:C:81:ARG:NH1	1.87	0.89
1:A:129:ARG:HH21	1:B:80:ASP:CG	1.81	0.88
1:H:51:ARG:NH2	1:H:162:GLY:HA2	1.88	0.88
1:H:81:ARG:HB3	1:H:81:ARG:NH1	1.89	0.88
1:D:219:GLU:OE2	1:F:219:GLU:HG2	1.72	0.88
1:J:-3:TYR:C	1:J:-1:GLN:H	1.80	0.88
1:D:219:GLU:OE1	1:F:219:GLU:OE1	1.93	0.87
1:H:-3:TYR:C	1:H:-1:GLN:H	1.80	0.86
1:F:104:ARG:HD3	1:F:163:GLU:HG3	1.54	0.86
1:G:51:ARG:HH21	1:G:162:GLY:CA	1.89	0.86
1:I:81:ARG:HB3	1:I:81:ARG:NH1	1.89	0.86
1:B:81:ARG:HB3	1:B:81:ARG:NH1	1.91	0.85
1:C:-3:TYR:C	1:C:-1:GLN:H	1.83	0.85
1:E:-3:TYR:C	1:E:-1:GLN:H	1.82	0.85
1:G:104:ARG:HD3	1:G:163:GLU:HG3	1.56	0.85
1:I:104:ARG:HD3	1:I:163:GLU:HG3	1.59	0.85
1:C:104:ARG:HD3	1:C:163:GLU:HG3	1.57	0.84
1:J:81:ARG:HB3	1:J:81:ARG:NH1	1.92	0.84
1:D:135:LEU:H	1:D:209:VAL:HG22	1.43	0.84
1:E:104:ARG:HD3	1:E:163:GLU:HG3	1.59	0.84
1:I:34:LEU:O	1:I:38:VAL:HG23	1.77	0.84
1:I:51:ARG:HH21	1:I:162:GLY:HA2	1.33	0.84
1:A:81:ARG:HB3	1:A:81:ARG:NH1	1.91	0.84
1:F:-3:TYR:C	1:F:-1:GLN:H	1.85	0.84
1:E:77:THR:OG1	1:E:79:LEU:HB2	1.77	0.83
1:F:135:LEU:H	1:F:209:VAL:HG22	1.42	0.82
1:A:80:ASP:CG	1:B:129:ARG:HH21	1.88	0.81
1:C:114:GLU:O	1:C:116:ASP:N	2.12	0.81
1:H:34:LEU:O	1:H:38:VAL:HG23	1.81	0.81
1:G:51:ARG:HH21	1:G:162:GLY:HA2	1.40	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:114:GLU:O	1:J:116:ASP:N	2.14	0.81
1:A:252:ARG:HH11	1:A:252:ARG:HG2	1.46	0.81
1:F:19:THR:O	1:F:19:THR:HG22	1.81	0.80
1:G:204:MET:SD	1:G:214:VAL:HG21	2.21	0.80
1:A:104:ARG:HD3	1:A:163:GLU:HG3	1.63	0.80
1:B:188:THR:HG22	1:B:192:ARG:HH11	1.47	0.80
1:C:104:ARG:HG2	1:C:163:GLU:OE2	1.82	0.80
1:C:115:GLN:HG2	1:C:115:GLN:O	1.81	0.80
1:D:-3:TYR:C	1:D:-1:GLN:H	1.88	0.79
1:J:77:THR:OG1	1:J:79:LEU:HB2	1.83	0.79
1:A:-3:TYR:O	1:A:-1:GLN:N	2.15	0.79
1:J:51:ARG:HH21	1:J:162:GLY:CA	1.95	0.79
1:E:114:GLU:O	1:E:116:ASP:N	2.14	0.79
1:G:34:LEU:O	1:G:38:VAL:HG23	1.82	0.79
1:J:135:LEU:H	1:J:209:VAL:HG22	1.48	0.79
1:A:51:ARG:NH2	1:A:162:GLY:HA2	1.98	0.79
1:A:114:GLU:O	1:A:116:ASP:N	2.16	0.79
1:H:135:LEU:H	1:H:209:VAL:HG22	1.48	0.78
1:D:77:THR:OG1	1:D:79:LEU:HB2	1.83	0.78
1:A:2:LEU:HD13	1:J:219:GLU:OE2	1.82	0.78
1:C:77:THR:OG1	1:C:79:LEU:HB2	1.83	0.78
1:H:114:GLU:O	1:H:116:ASP:N	2.17	0.78
1:D:22:SER:O	1:D:26:VAL:HG23	1.83	0.78
1:J:34:LEU:O	1:J:38:VAL:HG23	1.83	0.78
1:F:51:ARG:NH2	1:F:162:GLY:HA2	1.99	0.78
1:H:-3:TYR:O	1:H:-1:GLN:N	2.17	0.78
1:G:77:THR:OG1	1:G:79:LEU:HB2	1.84	0.77
1:E:115:GLN:O	1:E:115:GLN:HG2	1.85	0.77
1:G:121:CYS:O	1:G:125:ILE:HG13	1.83	0.77
1:I:77:THR:OG1	1:I:79:LEU:HB2	1.84	0.77
1:B:252:ARG:HG2	1:B:252:ARG:HH11	1.50	0.77
1:G:81:ARG:HB3	1:G:81:ARG:NH1	1.98	0.77
1:I:52:ARG:HH11	1:I:52:ARG:HG3	1.48	0.77
1:I:119:HIS:NE2	1:I:144:THR:HG22	1.99	0.77
1:D:104:ARG:HG2	1:D:163:GLU:OE2	1.86	0.76
1:G:104:ARG:HG2	1:G:163:GLU:OE2	1.85	0.76
1:B:104:ARG:HG2	1:B:163:GLU:OE2	1.85	0.76
1:D:114:GLU:O	1:D:116:ASP:N	2.17	0.76
1:B:104:ARG:HD3	1:B:163:GLU:HG3	1.67	0.76
1:C:135:LEU:H	1:C:209:VAL:HG22	1.50	0.76
1:F:52:ARG:HG3	1:F:52:ARG:HH11	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:GLU:O	1:F:116:ASP:N	2.17	0.75
1:E:120:LEU:HD12	1:E:120:LEU:O	1.87	0.75
1:H:77:THR:OG1	1:H:79:LEU:HB2	1.85	0.75
1:D:19:THR:HG22	1:D:19:THR:O	1.87	0.75
1:I:81:ARG:NH2	1:J:81:ARG:NH2	2.34	0.75
1:E:135:LEU:H	1:E:209:VAL:HG22	1.51	0.75
1:F:188:THR:HG22	1:F:192:ARG:HH11	1.52	0.75
1:J:-3:TYR:O	1:J:-1:GLN:N	2.18	0.75
1:A:25:LEU:O	1:A:29:THR:HG23	1.87	0.75
1:D:250:LEU:O	1:D:255:PRO:HD3	1.87	0.75
1:I:114:GLU:O	1:I:116:ASP:N	2.20	0.75
1:B:77:THR:OG1	1:B:79:LEU:HB2	1.87	0.75
1:B:114:GLU:O	1:B:116:ASP:N	2.19	0.75
1:F:51:ARG:HH21	1:F:162:GLY:CA	1.99	0.75
1:G:22:SER:O	1:G:26:VAL:HG23	1.87	0.75
1:J:115:GLN:O	1:J:115:GLN:HG2	1.87	0.75
1:H:51:ARG:HH21	1:H:162:GLY:CA	2.00	0.74
1:F:104:ARG:HG2	1:F:163:GLU:OE2	1.86	0.74
1:G:114:GLU:O	1:G:116:ASP:N	2.19	0.74
1:I:-3:TYR:O	1:I:-1:GLN:N	2.19	0.74
1:D:51:ARG:NH2	1:D:162:GLY:HA2	2.03	0.74
1:E:81:ARG:HH21	1:F:81:ARG:NH2	1.86	0.74
1:E:114:GLU:OE2	1:F:94:ARG:HD2	1.86	0.74
1:E:34:LEU:O	1:E:38:VAL:HG23	1.87	0.74
1:I:121:CYS:O	1:I:125:ILE:HG13	1.88	0.74
1:A:188:THR:HG22	1:A:192:ARG:HH11	1.53	0.74
1:B:83:GLU:O	1:B:87:VAL:HG23	1.88	0.74
1:E:81:ARG:CB	1:E:81:ARG:NH1	2.44	0.74
1:G:-3:TYR:O	1:G:-1:GLN:N	2.20	0.74
1:J:51:ARG:NH2	1:J:162:GLY:CA	2.49	0.73
1:B:-3:TYR:O	1:B:-1:GLN:N	2.20	0.73
1:E:106:PRO:HB2	1:F:106:PRO:HB2	1.69	0.73
1:F:77:THR:OG1	1:F:79:LEU:HB2	1.87	0.73
1:B:51:ARG:NH2	1:B:162:GLY:HA2	2.03	0.73
1:A:81:ARG:HH11	1:A:81:ARG:CA	2.02	0.73
1:G:119:HIS:NE2	1:G:144:THR:HG22	2.03	0.73
1:A:135:LEU:H	1:A:209:VAL:HG22	1.53	0.73
1:J:104:ARG:HD3	1:J:163:GLU:HG3	1.71	0.72
1:A:204:MET:HE3	1:A:257:HIS:HB2	1.71	0.72
1:E:25:LEU:O	1:E:29:THR:HG23	1.89	0.72
1:H:210:ALA:HB3	1:H:213:ASP:OD2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:OE2	1:B:94:ARG:HD2	1.88	0.72
1:B:135:LEU:H	1:B:209:VAL:HG22	1.55	0.72
1:I:104:ARG:HG2	1:I:163:GLU:OE2	1.89	0.72
1:A:132:ALA:HB1	1:A:137:GLU:HB3	1.71	0.71
1:J:25:LEU:O	1:J:29:THR:HG23	1.90	0.71
1:A:77:THR:OG1	1:A:79:LEU:HB2	1.89	0.71
1:E:81:ARG:HH21	1:F:81:ARG:HH21	1.36	0.71
1:J:210:ALA:HB3	1:J:213:ASP:OD2	1.90	0.71
1:C:51:ARG:NH2	1:C:162:GLY:HA2	2.05	0.71
1:D:51:ARG:HH21	1:D:162:GLY:CA	2.03	0.71
1:I:204:MET:SD	1:I:214:VAL:HG21	2.30	0.71
1:H:202:HIS:O	1:H:206:THR:HG22	1.91	0.71
1:F:250:LEU:O	1:F:255:PRO:HD3	1.91	0.70
1:H:81:ARG:CB	1:H:81:ARG:NH1	2.48	0.70
1:I:-3:TYR:C	1:I:-1:GLN:N	2.49	0.70
1:H:25:LEU:O	1:H:29:THR:HG23	1.91	0.70
1:B:204:MET:HE3	1:B:257:HIS:HB2	1.74	0.70
1:D:188:THR:HG22	1:D:192:ARG:HH11	1.54	0.70
1:E:104:ARG:HG2	1:E:163:GLU:OE2	1.91	0.70
1:A:129:ARG:NH2	1:B:80:ASP:OD2	2.24	0.70
1:A:51:ARG:HH21	1:A:162:GLY:CA	2.05	0.70
1:A:81:ARG:HH21	1:B:81:ARG:NH2	1.90	0.70
1:C:204:MET:HE3	1:C:257:HIS:HB2	1.74	0.70
1:H:104:ARG:HD3	1:H:163:GLU:HG3	1.72	0.70
1:H:239:VAL:HB	1:H:240:PRO:HD3	1.73	0.70
1:C:114:GLU:OE2	1:D:94:ARG:HD2	1.92	0.69
1:C:25:LEU:O	1:C:29:THR:HG23	1.91	0.69
1:C:34:LEU:O	1:C:38:VAL:HG23	1.91	0.69
1:E:81:ARG:NH2	1:F:81:ARG:NH2	2.41	0.69
1:J:104:ARG:HG2	1:J:163:GLU:OE2	1.91	0.69
1:G:58:ALA:HB1	1:G:99:LEU:HD23	1.75	0.69
1:A:51:ARG:HH21	1:A:162:GLY:N	1.91	0.69
1:H:121:CYS:O	1:H:125:ILE:HG13	1.92	0.69
1:A:-3:TYR:C	1:A:-1:GLN:N	2.49	0.69
1:J:177:PHE:CE2	1:J:181:ILE:HD11	2.28	0.69
1:E:34:LEU:HD21	1:E:181:ILE:HD12	1.73	0.69
1:I:142:ALA:HA	1:I:145:TYR:CE2	2.28	0.69
1:I:204:MET:HE3	1:I:257:HIS:HB2	1.74	0.69
1:E:204:MET:HE3	1:E:257:HIS:HB2	1.75	0.68
1:H:51:ARG:NH2	1:H:162:GLY:CA	2.56	0.68
1:G:135:LEU:H	1:G:209:VAL:HG22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:GLU:CG	1:F:219:GLU:OE2	2.41	0.68
1:I:58:ALA:HB1	1:I:99:LEU:HD23	1.75	0.68
1:A:81:ARG:CB	1:A:81:ARG:NH1	2.43	0.68
1:B:25:LEU:O	1:B:29:THR:HG23	1.94	0.68
1:C:120:LEU:O	1:C:120:LEU:HD12	1.94	0.68
1:B:51:ARG:HH21	1:B:162:GLY:CA	2.07	0.68
1:D:-3:TYR:O	1:D:-1:GLN:N	2.27	0.68
1:G:204:MET:HE3	1:G:257:HIS:HB2	1.76	0.68
1:E:51:ARG:NH2	1:E:162:GLY:HA2	2.08	0.67
1:G:52:ARG:HG3	1:G:52:ARG:HH11	1.58	0.67
1:H:132:ALA:HB1	1:H:137:GLU:HB3	1.76	0.67
1:D:90:ARG:HD3	1:D:90:ARG:C	2.18	0.67
1:F:-3:TYR:O	1:F:-1:GLN:N	2.26	0.67
1:E:-3:TYR:O	1:E:-1:GLN:N	2.28	0.67
1:B:58:ALA:HB1	1:B:99:LEU:HD23	1.75	0.67
1:B:81:ARG:HH11	1:B:81:ARG:CA	2.08	0.67
1:F:58:ALA:HB1	1:F:99:LEU:HD23	1.75	0.67
1:F:132:ALA:HB1	1:F:137:GLU:HB3	1.77	0.67
1:B:132:ALA:HB1	1:B:137:GLU:HB3	1.76	0.67
1:I:22:SER:O	1:I:26:VAL:HG23	1.94	0.67
1:J:51:ARG:HH21	1:J:162:GLY:N	1.93	0.67
1:B:-3:TYR:C	1:B:-1:GLN:N	2.52	0.67
1:C:-3:TYR:O	1:C:-1:GLN:N	2.27	0.67
1:I:203:LEU:HB3	1:I:209:VAL:HG23	1.77	0.67
1:D:121:CYS:O	1:D:125:ILE:HG13	1.94	0.66
1:J:132:ALA:HB1	1:J:137:GLU:HB3	1.76	0.66
1:C:81:ARG:CB	1:C:81:ARG:NH1	2.49	0.66
1:H:52:ARG:HG3	1:H:52:ARG:HH11	1.59	0.66
1:G:115:GLN:O	1:G:115:GLN:HG2	1.93	0.66
1:H:58:ALA:HB1	1:H:99:LEU:HD23	1.77	0.66
1:F:22:SER:O	1:F:26:VAL:HG23	1.95	0.66
1:E:19:THR:HG22	1:E:19:THR:O	1.93	0.66
1:G:203:LEU:HB3	1:G:209:VAL:HG23	1.77	0.66
1:J:204:MET:HE3	1:J:257:HIS:HB2	1.76	0.66
1:E:119:HIS:NE2	1:E:144:THR:HG22	2.11	0.66
1:J:202:HIS:O	1:J:206:THR:HG22	1.96	0.66
1:A:81:ARG:HH11	1:A:81:ARG:CG	2.08	0.66
1:D:219:GLU:OE1	1:F:219:GLU:CD	2.37	0.66
1:A:58:ALA:HB1	1:A:99:LEU:HD23	1.78	0.66
1:I:188:THR:HG22	1:I:192:ARG:HH11	1.60	0.66
1:A:104:ARG:HG2	1:A:163:GLU:OE2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:CYS:O	1:B:125:ILE:HG13	1.96	0.66
1:D:108:ALA:O	1:D:112:ILE:HG13	1.96	0.65
1:G:142:ALA:HA	1:G:145:TYR:CE2	2.31	0.65
1:I:81:ARG:CB	1:I:81:ARG:NH1	2.52	0.65
1:D:34:LEU:O	1:D:38:VAL:HG23	1.97	0.65
1:C:106:PRO:HB2	1:D:106:PRO:HB2	1.77	0.65
1:G:177:PHE:O	1:G:181:ILE:HG12	1.96	0.65
1:I:135:LEU:H	1:I:209:VAL:HG22	1.61	0.65
1:B:51:ARG:HH21	1:B:162:GLY:N	1.94	0.65
1:J:121:CYS:O	1:J:125:ILE:HG13	1.96	0.65
1:C:202:HIS:O	1:C:206:THR:HG22	1.96	0.65
1:C:203:LEU:HA	1:C:206:THR:CG2	2.27	0.64
1:E:210:ALA:HB3	1:E:213:ASP:OD2	1.97	0.64
1:D:210:ALA:HB3	1:D:213:ASP:OD2	1.97	0.64
1:B:81:ARG:CB	1:B:81:ARG:NH1	2.47	0.64
1:F:210:ALA:HB3	1:F:213:ASP:OD2	1.96	0.64
1:H:204:MET:HE3	1:H:257:HIS:HB2	1.78	0.64
1:D:218:LEU:HD22	1:D:246:THR:HG23	1.78	0.64
1:I:114:GLU:OE2	1:J:94:ARG:HD2	1.98	0.64
1:F:121:CYS:O	1:F:125:ILE:HG13	1.97	0.64
1:H:108:ALA:O	1:H:112:ILE:HG13	1.98	0.64
1:J:58:ALA:HB1	1:J:99:LEU:HD23	1.79	0.64
1:B:200:LEU:O	1:B:204:MET:HG3	1.98	0.64
1:H:104:ARG:HG2	1:H:163:GLU:OE2	1.97	0.64
1:I:115:GLN:O	1:I:115:GLN:HG2	1.98	0.64
1:H:-3:TYR:C	1:H:-1:GLN:N	2.53	0.64
1:H:115:GLN:HG2	1:H:115:GLN:O	1.96	0.64
1:J:239:VAL:HB	1:J:240:PRO:HD3	1.80	0.64
1:B:19:THR:HG22	1:B:19:THR:O	1.99	0.63
1:J:52:ARG:HG3	1:J:52:ARG:HH11	1.62	0.63
1:A:94:ARG:HD2	1:B:114:GLU:OE2	1.98	0.63
1:A:202:HIS:O	1:A:206:THR:HG22	1.98	0.63
1:C:121:CYS:O	1:C:125:ILE:HG13	1.97	0.63
1:C:210:ALA:HB3	1:C:213:ASP:OD2	1.98	0.63
1:D:115:GLN:O	1:D:115:GLN:HG2	1.97	0.63
1:C:90:ARG:HD3	1:C:90:ARG:C	2.23	0.63
1:C:239:VAL:HB	1:C:240:PRO:HD3	1.79	0.63
1:D:219:GLU:CD	1:F:219:GLU:OE1	2.38	0.63
1:F:108:ALA:O	1:F:112:ILE:HG13	1.97	0.63
1:B:115:GLN:O	1:B:115:GLN:HG2	1.98	0.63
1:H:81:ARG:HH11	1:H:81:ARG:CA	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ARG:HD3	1:D:90:ARG:O	1.98	0.63
1:A:187:LEU:HD21	1:A:200:LEU:HD23	1.80	0.63
1:I:210:ALA:HB3	1:I:213:ASP:OD2	1.99	0.63
1:A:51:ARG:NH2	1:A:162:GLY:CA	2.62	0.63
1:A:81:ARG:NH2	1:B:81:ARG:HH21	1.94	0.63
1:D:219:GLU:OE2	1:F:219:GLU:CG	2.46	0.62
1:C:252:ARG:HH11	1:C:252:ARG:HG2	1.64	0.62
1:E:203:LEU:HA	1:E:206:THR:CG2	2.28	0.62
1:C:188:THR:HG22	1:C:192:ARG:HH11	1.63	0.62
1:F:25:LEU:O	1:F:29:THR:HG23	2.00	0.62
1:A:119:HIS:NE2	1:A:144:THR:HG22	2.15	0.62
1:C:19:THR:O	1:C:19:THR:HG22	1.99	0.62
1:F:34:LEU:O	1:F:38:VAL:HG23	2.00	0.62
1:I:113:LEU:HD23	1:I:152:ARG:NH2	2.15	0.62
1:J:131:ARG:HD2	1:J:197:ASP:HB3	1.82	0.62
1:A:81:ARG:NH2	1:B:81:ARG:NH2	2.48	0.62
1:B:204:MET:SD	1:B:214:VAL:HG21	2.39	0.62
1:D:58:ALA:HB1	1:D:99:LEU:HD23	1.82	0.62
1:E:239:VAL:HB	1:E:240:PRO:HD3	1.81	0.62
1:F:19:THR:O	1:F:19:THR:CG2	2.47	0.62
1:F:218:LEU:HD22	1:F:246:THR:HG23	1.82	0.62
1:G:188:THR:HG22	1:G:192:ARG:HH11	1.63	0.62
1:I:177:PHE:O	1:I:181:ILE:HG12	2.00	0.62
1:D:132:ALA:HB1	1:D:137:GLU:HB3	1.80	0.62
1:C:189:ASP:HB3	1:C:195:GLU:OE2	1.99	0.62
1:F:81:ARG:CB	1:F:81:ARG:NH1	2.53	0.62
1:G:83:GLU:O	1:G:87:VAL:HG23	2.00	0.61
1:I:81:ARG:HH21	1:J:81:ARG:NH2	1.96	0.61
1:C:51:ARG:HH21	1:C:162:GLY:CA	2.13	0.61
1:F:252:ARG:HH11	1:F:252:ARG:HG2	1.66	0.61
1:A:19:THR:O	1:A:19:THR:HG22	1.99	0.61
1:C:-3:TYR:C	1:C:-1:GLN:N	2.56	0.61
1:D:19:THR:O	1:D:19:THR:CG2	2.48	0.61
1:H:60:ALA:O	1:H:64:VAL:HG23	2.01	0.61
1:C:54:ALA:HA	1:C:57:ARG:CZ	2.31	0.61
1:E:90:ARG:HD3	1:E:90:ARG:C	2.26	0.61
1:I:177:PHE:CE2	1:I:181:ILE:HD11	2.36	0.61
1:A:-1:GLN:OE1	1:A:0:SER:N	2.34	0.61
1:A:203:LEU:HA	1:A:206:THR:CG2	2.30	0.61
1:A:120:LEU:O	1:A:120:LEU:HD12	2.01	0.61
1:G:132:ALA:HB1	1:G:137:GLU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:ILE:O	1:H:184:ALA:HB3	2.01	0.61
1:I:52:ARG:HG3	1:I:52:ARG:NH1	2.15	0.61
1:D:-3:TYR:C	1:D:-1:GLN:N	2.60	0.60
1:D:219:GLU:CG	1:F:219:GLU:CD	2.74	0.60
1:E:51:ARG:HH21	1:E:162:GLY:CA	2.13	0.60
1:E:252:ARG:HG2	1:E:252:ARG:HH11	1.66	0.60
1:E:121:CYS:O	1:E:125:ILE:HG13	2.01	0.60
1:E:200:LEU:O	1:E:204:MET:HG3	2.01	0.60
1:F:131:ARG:HD2	1:F:197:ASP:HB3	1.84	0.60
1:A:115:GLN:O	1:A:115:GLN:HG2	2.01	0.60
1:B:202:HIS:O	1:B:206:THR:HG22	2.01	0.60
1:A:108:ALA:O	1:A:112:ILE:HG13	2.00	0.60
1:B:90:ARG:HD3	1:B:90:ARG:C	2.27	0.60
1:G:11:HIS:CD2	1:G:57:ARG:HD3	2.37	0.60
1:J:120:LEU:HD12	1:J:120:LEU:O	2.02	0.60
1:J:250:LEU:O	1:J:255:PRO:HD3	2.00	0.60
1:F:202:HIS:O	1:F:206:THR:HG22	2.02	0.60
1:B:203:LEU:HA	1:B:206:THR:CG2	2.32	0.60
1:J:54:ALA:HA	1:J:57:ARG:CZ	2.31	0.60
1:A:138:TRP:CH2	1:A:183:MET:HG2	2.37	0.60
1:A:239:VAL:HB	1:A:240:PRO:HD3	1.84	0.60
1:D:52:ARG:HH11	1:D:52:ARG:HG3	1.67	0.60
1:D:177:PHE:O	1:D:181:ILE:HG12	2.01	0.60
1:C:132:ALA:HB1	1:C:137:GLU:HB3	1.83	0.59
1:I:60:ALA:O	1:I:64:VAL:HG23	2.01	0.59
1:B:138:TRP:CH2	1:B:183:MET:HG2	2.37	0.59
1:D:219:GLU:CD	1:F:219:GLU:CG	2.75	0.59
1:F:104:ARG:HD3	1:F:163:GLU:CG	2.29	0.59
1:I:132:ALA:HB1	1:I:137:GLU:HB3	1.84	0.59
1:J:60:ALA:O	1:J:64:VAL:HG23	2.01	0.59
1:J:81:ARG:CB	1:J:81:ARG:NH1	2.53	0.59
1:A:142:ALA:HA	1:A:145:TYR:CE2	2.37	0.59
1:F:90:ARG:C	1:F:90:ARG:HD3	2.27	0.59
1:B:108:ALA:O	1:B:112:ILE:HG13	2.02	0.59
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.85	0.59
1:I:25:LEU:O	1:I:29:THR:HG23	2.03	0.59
1:C:204:MET:SD	1:C:214:VAL:HG21	2.42	0.59
1:C:119:HIS:NE2	1:C:144:THR:HG22	2.17	0.59
1:D:202:HIS:O	1:D:206:THR:HG22	2.03	0.59
1:E:202:HIS:O	1:E:206:THR:HG22	2.03	0.59
1:F:67:LYS:O	1:F:67:LYS:HD3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:LEU:HD23	1:G:152:ARG:NH2	2.17	0.59
1:J:108:ALA:O	1:J:112:ILE:HG13	2.02	0.59
1:E:19:THR:O	1:E:19:THR:CG2	2.50	0.59
1:A:252:ARG:HG2	1:A:252:ARG:NH1	2.17	0.59
1:D:252:ARG:HG2	1:D:252:ARG:HH11	1.67	0.59
1:E:138:TRP:NE1	1:E:200:LEU:HB2	2.18	0.59
1:J:149:PHE:CE1	1:J:153:TYR:HE2	2.20	0.59
1:F:51:ARG:HH21	1:F:162:GLY:HA2	1.61	0.58
1:F:115:GLN:O	1:F:115:GLN:HG2	2.02	0.58
1:F:177:PHE:O	1:F:181:ILE:HG12	2.03	0.58
1:D:81:ARG:CB	1:D:81:ARG:NH1	2.51	0.58
1:G:25:LEU:O	1:G:29:THR:HG23	2.03	0.58
1:H:90:ARG:HD3	1:H:90:ARG:C	2.28	0.58
1:I:104:ARG:CZ	1:I:163:GLU:HA	2.34	0.58
1:G:239:VAL:HB	1:G:240:PRO:HD3	1.84	0.58
1:D:104:ARG:HD3	1:D:163:GLU:CG	2.29	0.58
1:A:90:ARG:C	1:A:90:ARG:HD3	2.28	0.58
1:F:135:LEU:N	1:F:209:VAL:HG22	2.17	0.58
1:G:222:ARG:HG2	1:G:226:LEU:HD12	1.84	0.58
1:E:138:TRP:CH2	1:E:183:MET:HG2	2.38	0.58
1:G:177:PHE:CE2	1:G:181:ILE:HD11	2.39	0.58
1:G:210:ALA:HB3	1:G:213:ASP:OD2	2.03	0.58
1:I:19:THR:HG22	1:I:19:THR:O	2.02	0.58
1:I:54:ALA:HA	1:I:57:ARG:CZ	2.34	0.58
1:C:138:TRP:CH2	1:C:183:MET:HG2	2.38	0.58
1:I:131:ARG:HG3	1:I:198:GLY:HA3	1.85	0.58
1:C:22:SER:O	1:C:26:VAL:HG23	2.04	0.58
1:C:181:ILE:O	1:C:184:ALA:HB3	2.04	0.58
1:E:132:ALA:HB1	1:E:137:GLU:HB3	1.84	0.58
1:B:51:ARG:NH2	1:B:162:GLY:CA	2.67	0.57
1:C:90:ARG:HD3	1:C:90:ARG:O	2.04	0.57
1:D:204:MET:HE3	1:D:257:HIS:HB2	1.85	0.57
1:E:97:HIS:ND1	1:F:107:LYS:NZ	2.51	0.57
1:F:52:ARG:HG3	1:F:52:ARG:NH1	2.19	0.57
1:I:239:VAL:HB	1:I:240:PRO:HD3	1.85	0.57
1:H:177:PHE:CE2	1:H:181:ILE:HD11	2.39	0.57
1:H:250:LEU:O	1:H:255:PRO:HD3	2.04	0.57
1:D:251:VAL:O	1:D:255:PRO:HG2	2.05	0.57
1:A:22:SER:O	1:A:26:VAL:HG23	2.04	0.57
1:A:200:LEU:O	1:A:204:MET:HG3	2.04	0.57
1:H:131:ARG:HD2	1:H:197:ASP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ASP:OD2	1:F:216:ASP:OD1	2.23	0.57
1:G:252:ARG:HG2	1:G:252:ARG:HH11	1.69	0.57
1:J:113:LEU:HD23	1:J:152:ARG:NH2	2.19	0.57
1:B:90:ARG:NH1	1:B:94:ARG:HB2	2.19	0.57
1:C:177:PHE:O	1:C:181:ILE:HG12	2.04	0.57
1:G:35:TYR:O	1:G:39:PRO:HD3	2.05	0.57
1:G:81:ARG:NH2	1:H:81:ARG:NH2	2.52	0.57
1:H:51:ARG:HH21	1:H:162:GLY:N	2.01	0.57
1:A:232:PRO:HA	1:A:233:PRO:C	2.29	0.57
1:B:-1:GLN:OE1	1:B:0:SER:N	2.38	0.57
1:B:187:LEU:HD21	1:B:200:LEU:HD23	1.85	0.57
1:I:222:ARG:HG2	1:I:226:LEU:HD12	1.87	0.57
1:E:135:LEU:HD23	1:E:135:LEU:C	2.30	0.56
1:G:81:ARG:CB	1:G:81:ARG:NH1	2.55	0.56
1:A:210:ALA:HB3	1:A:213:ASP:OD2	2.06	0.56
1:E:81:ARG:HH11	1:E:81:ARG:CA	2.16	0.56
1:E:81:ARG:HH11	1:E:81:ARG:CG	2.18	0.56
1:H:203:LEU:HA	1:H:206:THR:CG2	2.36	0.56
1:B:142:ALA:HA	1:B:145:TYR:CE2	2.41	0.56
1:G:58:ALA:CB	1:G:99:LEU:HD23	2.35	0.56
1:H:40:HIS:CE1	1:H:52:ARG:NH2	2.74	0.56
1:I:58:ALA:CB	1:I:99:LEU:HD23	2.35	0.56
1:J:67:LYS:HD3	1:J:67:LYS:O	2.06	0.56
1:G:54:ALA:HA	1:G:57:ARG:CZ	2.36	0.56
1:A:135:LEU:C	1:A:135:LEU:HD23	2.31	0.56
1:C:131:ARG:HG3	1:C:198:GLY:HA3	1.88	0.56
1:C:135:LEU:C	1:C:135:LEU:HD23	2.30	0.56
1:E:189:ASP:HB3	1:E:195:GLU:OE2	2.06	0.56
1:I:131:ARG:HD2	1:I:197:ASP:HB3	1.88	0.56
1:D:25:LEU:O	1:D:29:THR:HG23	2.06	0.56
1:D:90:ARG:C	1:D:90:ARG:CD	2.79	0.56
1:D:222:ARG:HB2	1:D:246:THR:HG21	1.87	0.56
1:E:52:ARG:HG3	1:E:52:ARG:HH11	1.70	0.56
1:B:135:LEU:HD23	1:B:135:LEU:C	2.30	0.56
1:D:113:LEU:HD23	1:D:152:ARG:NH2	2.21	0.56
1:E:103:ALA:HA	1:E:160:CYS:HA	1.88	0.56
1:D:177:PHE:CE2	1:D:181:ILE:HD11	2.41	0.55
1:F:203:LEU:HA	1:F:206:THR:CG2	2.36	0.55
1:D:76:ASP:O	1:D:78:GLY:N	2.39	0.55
1:D:239:VAL:HB	1:D:240:PRO:HD3	1.88	0.55
1:I:35:TYR:O	1:I:39:PRO:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ALA:HB3	1:B:213:ASP:OD2	2.06	0.55
1:I:232:PRO:HA	1:I:233:PRO:C	2.32	0.55
1:J:131:ARG:HG3	1:J:198:GLY:HA3	1.89	0.55
1:B:131:ARG:HD2	1:B:197:ASP:HB3	1.88	0.55
1:A:35:TYR:O	1:A:39:PRO:HD3	2.07	0.55
1:B:54:ALA:HA	1:B:57:ARG:CZ	2.37	0.55
1:D:203:LEU:HA	1:D:206:THR:CG2	2.35	0.55
1:H:113:LEU:HD23	1:H:152:ARG:NH2	2.22	0.55
1:H:252:ARG:HH11	1:H:252:ARG:HG2	1.71	0.55
1:A:226:LEU:HG	1:A:242:VAL:HG11	1.88	0.55
1:D:51:ARG:HH21	1:D:162:GLY:N	2.05	0.55
1:C:104:ARG:HD3	1:C:163:GLU:CG	2.31	0.55
1:E:215:VAL:HG22	1:E:254:LEU:CD1	2.37	0.55
1:D:131:ARG:HD2	1:D:197:ASP:HB3	1.89	0.55
1:J:81:ARG:HH11	1:J:81:ARG:CA	2.19	0.55
1:A:19:THR:O	1:A:19:THR:CG2	2.54	0.55
1:E:42:LEU:HD21	1:E:150:LEU:HD21	1.89	0.55
1:G:19:THR:HG22	1:G:19:THR:O	2.06	0.55
1:G:58:ALA:O	1:G:61:LEU:HB2	2.07	0.55
1:G:215:VAL:HG22	1:G:254:LEU:CD1	2.37	0.55
1:A:34:LEU:HD21	1:A:181:ILE:HD12	1.89	0.55
1:A:80:ASP:OD2	1:B:129:ARG:NH2	2.40	0.55
1:G:131:ARG:HG3	1:G:198:GLY:HA3	1.89	0.55
1:C:19:THR:O	1:C:19:THR:CG2	2.54	0.54
1:F:58:ALA:CB	1:F:99:LEU:HD23	2.36	0.54
1:B:252:ARG:HG2	1:B:252:ARG:NH1	2.19	0.54
1:D:243:HIS:HB3	1:F:216:ASP:OD2	2.06	0.54
1:E:131:ARG:HG3	1:E:198:GLY:HA3	1.89	0.54
1:H:120:LEU:O	1:H:120:LEU:HD12	2.08	0.54
1:I:76:ASP:O	1:I:78:GLY:N	2.40	0.54
1:D:135:LEU:N	1:D:209:VAL:HG22	2.18	0.54
1:A:130:SER:O	1:A:131:ARG:C	2.50	0.54
1:A:182:THR:O	1:A:185:ASP:HB2	2.07	0.54
1:B:19:THR:O	1:B:19:THR:CG2	2.55	0.54
1:C:148:THR:O	1:C:152:ARG:HD3	2.08	0.54
1:D:34:LEU:O	1:D:34:LEU:HD12	2.07	0.54
1:J:142:ALA:HA	1:J:145:TYR:CE2	2.43	0.54
1:J:181:ILE:O	1:J:184:ALA:HB3	2.07	0.54
1:C:42:LEU:HD21	1:C:150:LEU:HD21	1.88	0.54
1:C:97:HIS:ND1	1:D:107:LYS:NZ	2.56	0.54
1:C:107:LYS:NZ	1:D:97:HIS:ND1	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:GLU:OE2	1:H:94:ARG:HD2	2.07	0.54
1:H:190:TYR:HE2	1:H:196:ARG:HG3	1.73	0.54
1:B:232:PRO:HA	1:B:233:PRO:C	2.32	0.54
1:C:200:LEU:O	1:C:204:MET:HG3	2.08	0.54
1:D:90:ARG:NH1	1:D:94:ARG:HB2	2.23	0.54
1:C:51:ARG:HH21	1:C:162:GLY:N	2.06	0.54
1:G:104:ARG:HD3	1:G:163:GLU:CG	2.32	0.54
1:H:90:ARG:HD3	1:H:90:ARG:O	2.08	0.54
1:H:92:HIS:NE2	1:H:96:LEU:HD11	2.22	0.54
1:J:232:PRO:HA	1:J:233:PRO:C	2.33	0.54
1:F:148:THR:O	1:F:152:ARG:HD3	2.08	0.54
1:F:189:ASP:HB3	1:F:195:GLU:OE2	2.06	0.54
1:G:232:PRO:HA	1:G:233:PRO:C	2.32	0.54
1:I:215:VAL:HG22	1:I:254:LEU:CD1	2.38	0.54
1:B:148:THR:O	1:B:152:ARG:HD3	2.08	0.53
1:I:81:ARG:NH2	1:J:81:ARG:HH21	2.04	0.53
1:I:135:LEU:C	1:I:135:LEU:HD23	2.34	0.53
1:J:182:THR:O	1:J:185:ASP:HB2	2.08	0.53
1:B:81:ARG:HH11	1:B:81:ARG:CG	2.21	0.53
1:C:76:ASP:O	1:C:78:GLY:N	2.41	0.53
1:E:203:LEU:HA	1:E:206:THR:HG22	1.90	0.53
1:A:250:LEU:O	1:A:255:PRO:HD3	2.08	0.53
1:C:11:HIS:CD2	1:C:57:ARG:HD3	2.43	0.53
1:E:11:HIS:CD2	1:E:57:ARG:HD3	2.43	0.53
1:F:90:ARG:HD3	1:F:90:ARG:O	2.08	0.53
1:B:119:HIS:NE2	1:B:144:THR:HG22	2.24	0.53
1:F:51:ARG:HH21	1:F:162:GLY:N	2.06	0.53
1:B:120:LEU:HD12	1:B:120:LEU:O	2.09	0.53
1:B:182:THR:O	1:B:185:ASP:HB2	2.09	0.53
1:E:142:ALA:HA	1:E:145:TYR:CE2	2.43	0.53
1:I:81:ARG:HH21	1:J:81:ARG:HH21	1.57	0.53
1:J:19:THR:O	1:J:19:THR:HG22	2.08	0.53
1:A:129:ARG:NH2	1:B:80:ASP:CG	2.58	0.53
1:D:58:ALA:CB	1:D:99:LEU:HD23	2.39	0.53
1:E:131:ARG:HD2	1:E:197:ASP:HB3	1.91	0.53
1:E:193:ASN:O	1:E:194:GLY:C	2.52	0.53
1:C:138:TRP:NE1	1:C:200:LEU:HB2	2.23	0.53
1:D:226:LEU:HG	1:D:242:VAL:HG11	1.90	0.53
1:G:181:ILE:O	1:G:184:ALA:HB3	2.07	0.53
1:G:250:LEU:O	1:G:255:PRO:HD3	2.09	0.53
1:J:203:LEU:HA	1:J:206:THR:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:PHE:CE2	1:C:181:ILE:HD11	2.44	0.53
1:A:104:ARG:CZ	1:A:163:GLU:HA	2.39	0.53
1:A:129:ARG:HH22	1:B:82:VAL:HB	1.73	0.53
1:B:220:GLU:O	1:B:220:GLU:HG2	2.10	0.53
1:G:90:ARG:HD3	1:G:90:ARG:C	2.34	0.53
1:G:203:LEU:HA	1:G:206:THR:CG2	2.39	0.53
1:G:252:ARG:HH12	1:G:253:LEU:HD21	1.71	0.53
1:H:52:ARG:HG3	1:H:52:ARG:NH1	2.24	0.53
1:I:148:THR:O	1:I:152:ARG:HD3	2.09	0.53
1:B:250:LEU:O	1:B:255:PRO:HD3	2.08	0.52
1:I:250:LEU:O	1:I:255:PRO:HD3	2.09	0.52
1:F:222:ARG:HB2	1:F:246:THR:HG21	1.91	0.52
1:F:232:PRO:HA	1:F:233:PRO:C	2.34	0.52
1:G:131:ARG:HD2	1:G:197:ASP:HB3	1.91	0.52
1:H:131:ARG:HG3	1:H:198:GLY:HA3	1.91	0.52
1:H:182:THR:O	1:H:185:ASP:HB2	2.09	0.52
1:D:120:LEU:HD12	1:D:120:LEU:O	2.08	0.52
1:F:171:ARG:O	1:F:175:GLU:HG3	2.10	0.52
1:A:204:MET:SD	1:A:214:VAL:HG21	2.50	0.52
1:B:226:LEU:HG	1:B:242:VAL:HG11	1.91	0.52
1:E:120:LEU:HD12	1:E:120:LEU:C	2.34	0.52
1:G:76:ASP:O	1:G:78:GLY:N	2.42	0.52
1:H:142:ALA:HA	1:H:145:TYR:CE2	2.44	0.52
1:I:62:ASP:OD1	1:I:66:MET:HE3	2.10	0.52
1:F:193:ASN:O	1:F:194:GLY:C	2.52	0.52
1:A:25:LEU:CD2	1:A:87:VAL:HG21	2.40	0.52
1:E:188:THR:HG22	1:E:192:ARG:HH11	1.73	0.52
1:G:137:GLU:O	1:G:138:TRP:C	2.53	0.52
1:H:58:ALA:CB	1:H:99:LEU:HD23	2.39	0.52
1:A:83:GLU:O	1:A:87:VAL:HG23	2.10	0.52
1:D:135:LEU:HB2	1:D:209:VAL:HG13	1.91	0.52
1:E:181:ILE:O	1:E:184:ALA:HB3	2.09	0.52
1:I:65:SER:OG	1:I:92:HIS:HB2	2.09	0.52
1:J:89:LEU:HD12	1:J:89:LEU:O	2.09	0.52
1:C:142:ALA:HA	1:C:145:TYR:CE2	2.45	0.52
1:E:51:ARG:HH21	1:E:162:GLY:HA2	1.71	0.52
1:G:52:ARG:HG3	1:G:52:ARG:NH1	2.23	0.52
1:H:130:SER:O	1:H:131:ARG:C	2.53	0.52
1:J:22:SER:O	1:J:26:VAL:HG23	2.08	0.52
1:D:131:ARG:HG3	1:D:198:GLY:HA3	1.91	0.52
1:H:149:PHE:CE1	1:H:153:TYR:HE2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ASP:OD1	1:D:49:PRO:HD2	2.10	0.52
1:E:90:ARG:HD3	1:E:90:ARG:O	2.10	0.52
1:H:251:VAL:O	1:H:255:PRO:HG2	2.09	0.52
1:I:131:ARG:HG3	1:I:197:ASP:O	2.10	0.52
1:A:220:GLU:O	1:A:220:GLU:HG2	2.10	0.51
1:B:130:SER:O	1:B:131:ARG:C	2.53	0.51
1:C:193:ASN:O	1:C:194:GLY:C	2.53	0.51
1:D:219:GLU:HG2	1:F:219:GLU:CD	2.35	0.51
1:H:19:THR:O	1:H:19:THR:HG22	2.09	0.51
1:I:226:LEU:HG	1:I:242:VAL:HG11	1.91	0.51
1:H:190:TYR:CE2	1:H:196:ARG:HG3	2.45	0.51
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.75	0.51
1:A:171:ARG:O	1:A:175:GLU:HG3	2.09	0.51
1:B:193:ASN:O	1:B:194:GLY:C	2.52	0.51
1:B:203:LEU:HB3	1:B:209:VAL:HG23	1.92	0.51
1:F:251:VAL:O	1:F:255:PRO:HG2	2.09	0.51
1:H:204:MET:SD	1:H:214:VAL:HG21	2.51	0.51
1:J:179:MET:O	1:J:183:MET:HG3	2.10	0.51
1:B:135:LEU:HD23	1:B:135:LEU:O	2.11	0.51
1:D:67:LYS:O	1:D:67:LYS:HD3	2.11	0.51
1:E:76:ASP:O	1:E:78:GLY:N	2.44	0.51
1:G:182:THR:O	1:G:185:ASP:HB2	2.10	0.51
1:J:130:SER:O	1:J:131:ARG:C	2.53	0.51
1:C:90:ARG:C	1:C:90:ARG:CD	2.84	0.51
1:F:120:LEU:O	1:F:120:LEU:HD12	2.10	0.51
1:I:11:HIS:CD2	1:I:57:ARG:HD3	2.46	0.51
1:A:58:ALA:CB	1:A:99:LEU:HD23	2.40	0.51
1:B:22:SER:O	1:B:26:VAL:HG23	2.11	0.51
1:D:-1:GLN:O	1:D:2:LEU:N	2.21	0.51
1:D:222:ARG:NE	1:F:219:GLU:CD	2.69	0.51
1:E:222:ARG:HB2	1:E:246:THR:HG21	1.93	0.51
1:G:203:LEU:HA	1:G:206:THR:HG22	1.92	0.51
1:H:22:SER:O	1:H:26:VAL:HG23	2.10	0.51
1:I:19:THR:O	1:I:19:THR:CG2	2.58	0.51
1:J:138:TRP:CH2	1:J:183:MET:HG2	2.46	0.51
1:B:58:ALA:CB	1:B:99:LEU:HD23	2.40	0.51
1:F:-3:TYR:C	1:F:-1:GLN:N	2.57	0.51
1:F:76:ASP:O	1:F:78:GLY:N	2.43	0.51
1:G:48:ASP:OD1	1:G:49:PRO:HD2	2.11	0.51
1:G:104:ARG:CZ	1:G:163:GLU:HA	2.41	0.51
1:H:135:LEU:C	1:H:135:LEU:HD23	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:ARG:HD3	1:I:90:ARG:C	2.34	0.51
1:I:206:THR:HG23	1:I:208:ALA:H	1.75	0.51
1:C:103:ALA:HA	1:C:160:CYS:HA	1.93	0.51
1:D:58:ALA:O	1:D:61:LEU:HB2	2.11	0.51
1:H:193:ASN:O	1:H:194:GLY:C	2.54	0.51
1:A:90:ARG:NH1	1:A:94:ARG:HB2	2.26	0.51
1:B:34:LEU:HD21	1:B:181:ILE:HD12	1.93	0.51
1:F:90:ARG:NH1	1:F:94:ARG:HB2	2.26	0.51
1:F:135:LEU:C	1:F:135:LEU:HD23	2.36	0.51
1:G:19:THR:O	1:G:19:THR:CG2	2.59	0.51
1:I:83:GLU:O	1:I:87:VAL:HG23	2.11	0.51
1:I:142:ALA:HA	1:I:145:TYR:CD2	2.46	0.51
1:J:183:MET:O	1:J:187:LEU:HG	2.10	0.51
1:J:193:ASN:O	1:J:194:GLY:C	2.54	0.51
1:B:35:TYR:O	1:B:39:PRO:HD3	2.11	0.51
1:E:179:MET:O	1:E:183:MET:HG3	2.10	0.51
1:J:89:LEU:HD12	1:J:93:LEU:HG	1.93	0.51
1:J:204:MET:SD	1:J:214:VAL:HG21	2.51	0.51
1:A:54:ALA:HA	1:A:57:ARG:CZ	2.41	0.50
1:H:90:ARG:C	1:H:90:ARG:CD	2.85	0.50
1:A:131:ARG:HD2	1:A:197:ASP:HB3	1.92	0.50
1:D:182:THR:O	1:D:185:ASP:HB2	2.10	0.50
1:D:193:ASN:O	1:D:194:GLY:C	2.53	0.50
1:E:54:ALA:HA	1:E:57:ARG:CZ	2.41	0.50
1:F:40:HIS:CE1	1:F:52:ARG:NH2	2.79	0.50
1:F:90:ARG:C	1:F:90:ARG:CD	2.84	0.50
1:G:108:ALA:O	1:G:112:ILE:HG13	2.10	0.50
1:C:215:VAL:HG22	1:C:254:LEU:CD1	2.41	0.50
1:G:-3:TYR:C	1:G:-1:GLN:N	2.50	0.50
1:I:104:ARG:HD3	1:I:163:GLU:CG	2.34	0.50
1:A:203:LEU:HA	1:A:206:THR:HG22	1.92	0.50
1:C:203:LEU:HA	1:C:206:THR:HG22	1.92	0.50
1:C:222:ARG:HG2	1:C:226:LEU:HD12	1.93	0.50
1:H:232:PRO:HA	1:H:233:PRO:C	2.34	0.50
1:I:138:TRP:CH2	1:I:183:MET:HG2	2.46	0.50
1:B:67:LYS:O	1:B:67:LYS:HD3	2.12	0.50
1:D:219:GLU:CD	1:F:219:GLU:HG2	2.36	0.50
1:D:232:PRO:HA	1:D:233:PRO:C	2.35	0.50
1:I:51:ARG:HH21	1:I:162:GLY:N	2.09	0.50
1:I:203:LEU:HA	1:I:206:THR:HG22	1.93	0.50
1:F:131:ARG:HG3	1:F:198:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:ASP:O	1:H:78:GLY:N	2.45	0.50
1:I:252:ARG:HH12	1:I:253:LEU:HD21	1.75	0.50
1:B:34:LEU:O	1:B:38:VAL:HG23	2.12	0.50
1:E:250:LEU:O	1:E:255:PRO:HD3	2.12	0.50
1:F:179:MET:HG2	1:F:221:LEU:HD11	1.93	0.50
1:G:39:PRO:HG3	1:G:63:ILE:HD12	1.94	0.50
1:G:138:TRP:CH2	1:G:183:MET:HG2	2.47	0.50
1:H:179:MET:O	1:H:183:MET:HG3	2.11	0.50
1:I:182:THR:O	1:I:185:ASP:HB2	2.11	0.50
1:I:203:LEU:HA	1:I:206:THR:CG2	2.42	0.50
1:J:52:ARG:HG3	1:J:52:ARG:NH1	2.26	0.50
1:J:137:GLU:O	1:J:138:TRP:C	2.55	0.50
1:B:203:LEU:HA	1:B:206:THR:HG22	1.93	0.50
1:D:138:TRP:NE1	1:D:200:LEU:HB2	2.27	0.50
1:D:189:ASP:HB3	1:D:195:GLU:OE2	2.12	0.50
1:G:226:LEU:HG	1:G:242:VAL:HG11	1.94	0.50
1:A:190:TYR:HE2	1:A:196:ARG:HG3	1.77	0.50
1:A:193:ASN:O	1:A:194:GLY:C	2.54	0.50
1:C:131:ARG:HD2	1:C:197:ASP:HB3	1.94	0.50
1:F:103:ALA:HA	1:F:160:CYS:HA	1.94	0.50
1:I:125:ILE:HD12	1:J:19:THR:O	2.12	0.50
1:I:181:ILE:O	1:I:184:ALA:HB3	2.11	0.50
1:J:135:LEU:C	1:J:135:LEU:HD23	2.37	0.49
1:J:135:LEU:N	1:J:209:VAL:HG22	2.22	0.49
1:A:82:VAL:HB	1:B:129:ARG:HH22	1.77	0.49
1:A:103:ALA:HA	1:A:160:CYS:HA	1.95	0.49
1:A:113:LEU:HD23	1:A:152:ARG:NH2	2.28	0.49
1:C:67:LYS:O	1:C:67:LYS:HD3	2.12	0.49
1:E:104:ARG:HD3	1:E:163:GLU:CG	2.34	0.49
1:H:200:LEU:O	1:H:204:MET:HG3	2.13	0.49
1:A:72:LEU:HD23	1:B:72:LEU:HD23	1.93	0.49
1:C:52:ARG:O	1:C:56:SER:HB2	2.11	0.49
1:D:92:HIS:NE2	1:D:96:LEU:HD11	2.28	0.49
1:G:65:SER:OG	1:G:92:HIS:HB2	2.12	0.49
1:A:81:ARG:NH1	1:A:81:ARG:CG	2.73	0.49
1:E:51:ARG:HH21	1:E:162:GLY:N	2.10	0.49
1:I:251:VAL:O	1:I:255:PRO:HG2	2.12	0.49
1:C:58:ALA:HB1	1:C:99:LEU:HD23	1.94	0.49
1:D:34:LEU:HD21	1:D:181:ILE:HD12	1.92	0.49
1:E:153:TYR:HA	1:E:156:LEU:HD12	1.94	0.49
1:F:34:LEU:O	1:F:34:LEU:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:ARG:HH11	1:G:81:ARG:CA	2.23	0.49
1:A:111:ASP:O	1:A:115:GLN:HB3	2.13	0.49
1:B:181:ILE:O	1:B:184:ALA:HB3	2.12	0.49
1:C:130:SER:O	1:C:131:ARG:C	2.55	0.49
1:H:54:ALA:HA	1:H:57:ARG:CZ	2.43	0.49
1:H:196:ARG:HG2	1:H:202:HIS:CG	2.47	0.49
1:C:81:ARG:HH11	1:C:81:ARG:CG	2.26	0.49
1:H:19:THR:O	1:H:19:THR:CG2	2.60	0.49
1:I:48:ASP:OD1	1:I:49:PRO:HD2	2.12	0.49
1:I:137:GLU:O	1:I:138:TRP:C	2.55	0.49
1:J:19:THR:O	1:J:19:THR:CG2	2.60	0.49
1:J:40:HIS:CE1	1:J:52:ARG:NH2	2.81	0.49
1:J:90:ARG:HD3	1:J:90:ARG:C	2.37	0.49
1:J:177:PHE:O	1:J:181:ILE:HG12	2.13	0.49
1:B:12:VAL:O	1:B:16:VAL:HG23	2.12	0.49
1:E:232:PRO:HA	1:E:233:PRO:C	2.36	0.49
1:F:177:PHE:CE2	1:F:181:ILE:HD11	2.48	0.49
1:H:138:TRP:CE3	1:H:138:TRP:C	2.91	0.49
1:I:58:ALA:O	1:I:61:LEU:HB2	2.13	0.49
1:J:48:ASP:OD1	1:J:49:PRO:HD2	2.12	0.49
1:C:107:LYS:HD2	1:C:111:ASP:OD1	2.13	0.49
1:C:232:PRO:HA	1:C:233:PRO:C	2.37	0.49
1:G:251:VAL:O	1:G:255:PRO:HG2	2.12	0.49
1:C:52:ARG:HG3	1:C:52:ARG:HH11	1.78	0.49
1:F:204:MET:HE3	1:F:257:HIS:HB2	1.95	0.49
1:I:54:ALA:HA	1:I:57:ARG:NH1	2.28	0.49
1:J:76:ASP:O	1:J:78:GLY:N	2.45	0.49
1:B:190:TYR:HE2	1:B:196:ARG:HG3	1.77	0.48
1:D:35:TYR:O	1:D:39:PRO:HD3	2.13	0.48
1:G:206:THR:HG23	1:G:208:ALA:H	1.77	0.48
1:I:97:HIS:ND1	1:J:107:LYS:NZ	2.60	0.48
1:A:80:ASP:CG	1:B:129:ARG:NH2	2.66	0.48
1:C:129:ARG:HA	1:C:129:ARG:HD3	1.64	0.48
1:F:135:LEU:HB2	1:F:209:VAL:HG13	1.95	0.48
1:I:130:SER:O	1:I:131:ARG:C	2.56	0.48
1:E:149:PHE:CE1	1:E:153:TYR:HE2	2.32	0.48
1:G:203:LEU:HB3	1:G:209:VAL:CG2	2.43	0.48
1:B:89:LEU:HD12	1:B:89:LEU:O	2.13	0.48
1:B:131:ARG:HG3	1:B:198:GLY:HA3	1.95	0.48
1:D:104:ARG:CZ	1:D:163:GLU:HA	2.42	0.48
1:E:114:GLU:OE2	1:F:94:ARG:CD	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:THR:HG22	1:H:192:ARG:HH11	1.78	0.48
1:I:135:LEU:HD23	1:I:135:LEU:O	2.13	0.48
1:B:237:GLY:O	1:B:240:PRO:HD2	2.13	0.48
1:E:39:PRO:HG3	1:E:63:ILE:HD12	1.96	0.48
1:F:138:TRP:NE1	1:F:200:LEU:HB2	2.28	0.48
1:G:130:SER:O	1:G:131:ARG:C	2.55	0.48
1:H:-1:GLN:OE1	1:H:0:SER:N	2.47	0.48
1:A:183:MET:O	1:A:187:LEU:HG	2.13	0.48
1:J:190:TYR:HE2	1:J:196:ARG:HG3	1.79	0.48
1:D:103:ALA:HA	1:D:160:CYS:HA	1.96	0.48
1:E:148:THR:O	1:E:152:ARG:HD3	2.14	0.48
1:H:227:ALA:O	1:H:230:ALA:HB3	2.13	0.48
1:I:120:LEU:HD12	1:I:120:LEU:O	2.13	0.48
1:J:92:HIS:NE2	1:J:96:LEU:HD11	2.28	0.48
1:E:130:SER:O	1:E:131:ARG:C	2.57	0.48
1:E:226:LEU:HG	1:E:242:VAL:HG11	1.95	0.48
1:F:113:LEU:HD23	1:F:152:ARG:NH2	2.28	0.48
1:G:247:ASP:O	1:G:251:VAL:HG23	2.13	0.48
1:J:58:ALA:CB	1:J:99:LEU:HD23	2.44	0.48
1:A:189:ASP:HB3	1:A:195:GLU:OE2	2.14	0.48
1:C:39:PRO:HG3	1:C:63:ILE:HD12	1.96	0.48
1:C:254:LEU:N	1:C:255:PRO:CD	2.77	0.48
1:D:148:THR:O	1:D:152:ARG:HD3	2.14	0.48
1:E:187:LEU:HD21	1:E:200:LEU:HD23	1.95	0.48
1:G:120:LEU:HD12	1:G:120:LEU:O	2.14	0.48
1:H:137:GLU:O	1:H:138:TRP:C	2.56	0.48
1:J:200:LEU:O	1:J:204:MET:HG3	2.14	0.48
1:A:252:ARG:NH1	1:A:252:ARG:CG	2.77	0.47
1:B:76:ASP:O	1:B:78:GLY:N	2.47	0.47
1:C:81:ARG:HH11	1:C:81:ARG:CA	2.23	0.47
1:C:104:ARG:CG	1:C:163:GLU:OE2	2.58	0.47
1:E:90:ARG:C	1:E:90:ARG:CD	2.87	0.47
1:E:204:MET:SD	1:E:214:VAL:HG21	2.54	0.47
1:I:252:ARG:HG2	1:I:252:ARG:HH11	1.79	0.47
1:A:34:LEU:O	1:A:38:VAL:HG23	2.14	0.47
1:A:81:ARG:NH1	1:A:81:ARG:CA	2.75	0.47
1:E:65:SER:OG	1:E:92:HIS:HB2	2.15	0.47
1:J:251:VAL:O	1:J:255:PRO:HG2	2.14	0.47
1:A:81:ARG:NH1	1:A:81:ARG:HA	2.29	0.47
1:C:5:GLU:HG3	1:C:37:ARG:HB2	1.96	0.47
1:D:252:ARG:HH12	1:D:253:LEU:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:HIS:CE1	1:F:52:ARG:HH21	2.33	0.47
1:G:60:ALA:O	1:G:64:VAL:HG23	2.14	0.47
1:J:203:LEU:HB3	1:J:209:VAL:HG23	1.96	0.47
1:B:179:MET:HG2	1:B:221:LEU:HD11	1.96	0.47
1:B:205:ARG:HH11	1:B:205:ARG:CG	2.27	0.47
1:C:34:LEU:HD21	1:C:181:ILE:HD12	1.95	0.47
1:D:11:HIS:CD2	1:D:57:ARG:HD3	2.49	0.47
1:F:104:ARG:CZ	1:F:163:GLU:HA	2.43	0.47
1:G:34:LEU:O	1:G:34:LEU:HD12	2.13	0.47
1:G:125:ILE:HD12	1:H:19:THR:O	2.14	0.47
1:H:103:ALA:HA	1:H:160:CYS:HA	1.96	0.47
1:H:135:LEU:N	1:H:209:VAL:HG22	2.22	0.47
1:H:187:LEU:HD21	1:H:200:LEU:HD23	1.96	0.47
1:A:137:GLU:O	1:A:138:TRP:C	2.58	0.47
1:E:135:LEU:HD23	1:E:135:LEU:O	2.15	0.47
1:H:89:LEU:HD12	1:H:93:LEU:HG	1.97	0.47
1:H:177:PHE:O	1:H:181:ILE:HG12	2.13	0.47
1:I:51:ARG:HD3	1:I:161:GLY:C	2.39	0.47
1:J:34:LEU:HD21	1:J:181:ILE:HD12	1.96	0.47
1:J:138:TRP:C	1:J:138:TRP:CE3	2.93	0.47
1:A:192:ARG:CZ	1:A:192:ARG:HB3	2.44	0.47
1:D:181:ILE:O	1:D:184:ALA:HB3	2.15	0.47
1:E:52:ARG:O	1:E:56:SER:HB2	2.14	0.47
1:H:226:LEU:HG	1:H:242:VAL:HG11	1.96	0.47
1:I:103:ALA:HA	1:I:160:CYS:HA	1.96	0.47
1:I:119:HIS:HD2	1:I:119:HIS:O	1.97	0.47
1:I:192:ARG:CZ	1:I:192:ARG:HB3	2.45	0.47
1:J:-1:GLN:OE1	1:J:0:SER:N	2.47	0.47
1:J:190:TYR:CE2	1:J:196:ARG:HG3	2.50	0.47
1:A:190:TYR:CE2	1:A:196:ARG:HG3	2.50	0.47
1:A:203:LEU:HB3	1:A:209:VAL:HG23	1.97	0.47
1:B:179:MET:O	1:B:183:MET:HG3	2.15	0.47
1:C:135:LEU:HD23	1:C:135:LEU:O	2.15	0.47
1:F:135:LEU:HD23	1:F:135:LEU:O	2.14	0.47
1:G:51:ARG:HH21	1:G:162:GLY:N	2.12	0.47
1:G:222:ARG:HB2	1:G:246:THR:HG21	1.96	0.47
1:H:81:ARG:NH1	1:H:81:ARG:CA	2.78	0.47
1:J:132:ALA:CB	1:J:137:GLU:HB3	2.44	0.47
1:J:226:LEU:HG	1:J:242:VAL:HG11	1.96	0.47
1:A:12:VAL:O	1:A:16:VAL:HG23	2.15	0.47
1:B:103:ALA:HA	1:B:160:CYS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ARG:NH2	1:D:81:ARG:NH2	2.63	0.47
1:C:115:GLN:O	1:C:115:GLN:CG	2.60	0.47
1:D:171:ARG:O	1:D:175:GLU:HG3	2.15	0.47
1:E:183:MET:O	1:E:187:LEU:HG	2.15	0.47
1:G:90:ARG:HD3	1:G:90:ARG:O	2.14	0.47
1:H:138:TRP:HE3	1:H:139:ARG:N	2.13	0.47
1:A:179:MET:O	1:A:183:MET:HG3	2.15	0.47
1:A:237:GLY:O	1:A:240:PRO:HD2	2.15	0.47
1:F:130:SER:O	1:F:131:ARG:C	2.58	0.47
1:G:72:LEU:HD13	1:G:84:LEU:HB3	1.96	0.47
1:G:148:THR:O	1:G:152:ARG:HD3	2.14	0.47
1:G:193:ASN:O	1:G:194:GLY:C	2.57	0.47
1:J:132:ALA:HB2	1:J:141:HIS:CD2	2.50	0.47
1:J:227:ALA:O	1:J:230:ALA:HB3	2.13	0.47
1:B:190:TYR:CE2	1:B:196:ARG:HG3	2.50	0.47
1:C:114:GLU:C	1:C:116:ASP:H	2.20	0.47
1:H:34:LEU:HD21	1:H:181:ILE:HD12	1.97	0.47
1:H:129:ARG:HA	1:H:129:ARG:HD3	1.62	0.47
1:A:67:LYS:O	1:A:67:LYS:HD3	2.14	0.46
1:B:132:ALA:CB	1:B:137:GLU:HB3	2.45	0.46
1:C:49:PRO:HG2	1:C:50:ASP:N	2.31	0.46
1:E:254:LEU:N	1:E:255:PRO:CD	2.78	0.46
1:G:192:ARG:HB3	1:G:192:ARG:CZ	2.44	0.46
1:I:203:LEU:HB3	1:I:209:VAL:CG2	2.45	0.46
1:I:222:ARG:HB2	1:I:246:THR:HG21	1.96	0.46
1:A:76:ASP:O	1:A:78:GLY:N	2.48	0.46
1:C:222:ARG:HB2	1:C:246:THR:HG21	1.95	0.46
1:D:129:ARG:HA	1:D:129:ARG:HD3	1.66	0.46
1:D:130:SER:O	1:D:131:ARG:C	2.58	0.46
1:E:107:LYS:NZ	1:F:97:HIS:ND1	2.63	0.46
1:F:35:TYR:O	1:F:39:PRO:HD3	2.15	0.46
1:F:132:ALA:CB	1:F:137:GLU:HB3	2.44	0.46
1:A:222:ARG:HG2	1:A:226:LEU:HD12	1.96	0.46
1:B:104:ARG:CZ	1:B:163:GLU:HA	2.45	0.46
1:A:132:ALA:CB	1:A:137:GLU:HB3	2.41	0.46
1:B:104:ARG:CG	1:B:163:GLU:OE2	2.60	0.46
1:B:183:MET:O	1:B:187:LEU:HG	2.16	0.46
1:B:205:ARG:HH11	1:B:205:ARG:HG3	1.80	0.46
1:C:90:ARG:NH1	1:C:94:ARG:HB2	2.29	0.46
1:G:135:LEU:HD23	1:G:135:LEU:C	2.39	0.46
1:A:181:ILE:O	1:A:184:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ARG:HH11	1:D:81:ARG:CA	2.25	0.46
1:G:1:MET:HE3	1:G:37:ARG:CZ	2.45	0.46
1:I:-1:GLN:O	1:I:2:LEU:N	2.26	0.46
1:A:142:ALA:HA	1:A:145:TYR:CD2	2.51	0.46
1:D:137:GLU:O	1:D:138:TRP:C	2.58	0.46
1:E:67:LYS:HD3	1:E:67:LYS:O	2.14	0.46
1:E:137:GLU:O	1:E:138:TRP:C	2.58	0.46
1:F:254:LEU:N	1:F:255:PRO:CD	2.79	0.46
1:G:89:LEU:HD12	1:G:89:LEU:O	2.16	0.46
1:J:35:TYR:O	1:J:39:PRO:HD3	2.16	0.46
1:J:103:ALA:HA	1:J:160:CYS:HA	1.98	0.46
1:D:219:GLU:CD	1:F:222:ARG:NE	2.74	0.46
1:E:119:HIS:HD2	1:E:119:HIS:O	1.99	0.46
1:F:137:GLU:O	1:F:138:TRP:C	2.59	0.46
1:F:182:THR:O	1:F:185:ASP:HB2	2.16	0.46
1:G:11:HIS:CD2	1:G:57:ARG:CD	2.99	0.46
1:I:119:HIS:CD2	1:I:119:HIS:C	2.94	0.46
1:J:215:VAL:HG22	1:J:254:LEU:CD1	2.46	0.46
1:E:5:GLU:HG3	1:E:37:ARG:HB2	1.96	0.46
1:E:58:ALA:HB1	1:E:99:LEU:HD23	1.98	0.46
1:F:92:HIS:NE2	1:F:96:LEU:HD11	2.30	0.46
1:G:103:ALA:HA	1:G:160:CYS:HA	1.97	0.46
1:H:183:MET:O	1:H:187:LEU:HG	2.16	0.46
1:I:90:ARG:HD3	1:I:90:ARG:O	2.16	0.46
1:I:129:ARG:HA	1:I:129:ARG:HD3	1.80	0.46
1:I:129:ARG:HH22	1:J:82:VAL:HB	1.81	0.46
1:I:193:ASN:O	1:I:194:GLY:C	2.59	0.46
1:A:51:ARG:HD3	1:A:161:GLY:C	2.40	0.46
1:C:135:LEU:N	1:C:209:VAL:HG22	2.25	0.46
1:D:52:ARG:HG3	1:D:52:ARG:NH1	2.31	0.46
1:D:135:LEU:C	1:D:135:LEU:HD23	2.41	0.46
1:G:54:ALA:HA	1:G:57:ARG:NH1	2.31	0.46
1:G:252:ARG:HH12	1:G:253:LEU:CD2	2.29	0.46
1:H:67:LYS:O	1:H:67:LYS:HD3	2.16	0.46
1:J:254:LEU:HD23	1:J:254:LEU:HA	1.74	0.46
1:B:252:ARG:HH12	1:B:253:LEU:HD21	1.81	0.46
1:J:135:LEU:HD23	1:J:135:LEU:O	2.16	0.46
1:D:100:GLU:HA	1:D:109:VAL:HG21	1.98	0.45
1:E:49:PRO:HG2	1:E:50:ASP:N	2.31	0.45
1:E:222:ARG:HG2	1:E:226:LEU:HD12	1.98	0.45
1:I:1:MET:HE3	1:I:37:ARG:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:252:ARG:HG2	1:J:252:ARG:HH11	1.81	0.45
1:A:104:ARG:HD3	1:A:163:GLU:CG	2.38	0.45
1:A:210:ALA:O	1:A:211:GLY:C	2.58	0.45
1:A:218:LEU:HA	1:A:218:LEU:HD23	1.74	0.45
1:D:40:HIS:CE1	1:D:52:ARG:NH2	2.84	0.45
1:F:60:ALA:O	1:F:64:VAL:HG23	2.16	0.45
1:F:181:ILE:O	1:F:184:ALA:HB3	2.16	0.45
1:G:-1:GLN:OE1	1:G:0:SER:N	2.49	0.45
1:G:62:ASP:O	1:G:65:SER:HB3	2.16	0.45
1:A:135:LEU:HD23	1:A:135:LEU:O	2.16	0.45
1:B:72:LEU:HD12	1:B:72:LEU:HA	1.76	0.45
1:C:42:LEU:HD21	1:C:150:LEU:CD2	2.46	0.45
1:E:11:HIS:CG	1:E:57:ARG:HD3	2.52	0.45
1:E:107:LYS:HD2	1:E:111:ASP:OD1	2.17	0.45
1:H:12:VAL:O	1:H:16:VAL:HG23	2.16	0.45
1:H:204:MET:CE	1:H:257:HIS:HB2	2.46	0.45
1:J:204:MET:CE	1:J:257:HIS:HB2	2.44	0.45
1:B:52:ARG:HG3	1:B:52:ARG:HH11	1.82	0.45
1:E:177:PHE:O	1:E:181:ILE:HG12	2.17	0.45
1:E:182:THR:O	1:E:185:ASP:HB2	2.16	0.45
1:E:237:GLY:O	1:E:240:PRO:HD2	2.16	0.45
1:G:142:ALA:HA	1:G:145:TYR:CD2	2.52	0.45
1:H:114:GLU:C	1:H:116:ASP:H	2.23	0.45
1:H:132:ALA:HB2	1:H:141:HIS:CD2	2.50	0.45
1:D:60:ALA:O	1:D:64:VAL:HG23	2.16	0.45
1:I:11:HIS:CG	1:I:57:ARG:HD3	2.51	0.45
1:J:51:ARG:HD3	1:J:161:GLY:C	2.42	0.45
1:J:144:THR:HA	1:J:148:THR:OG1	2.17	0.45
1:A:104:ARG:HD3	1:A:163:GLU:OE2	2.17	0.45
1:E:129:ARG:HA	1:E:129:ARG:HD3	1.65	0.45
1:E:251:VAL:O	1:E:255:PRO:HG2	2.16	0.45
1:F:44:GLU:HG2	1:F:238:LEU:HG	1.98	0.45
1:F:138:TRP:CH2	1:F:183:MET:HG2	2.52	0.45
1:G:190:TYR:HE2	1:G:202:HIS:HB2	1.81	0.45
1:H:-1:GLN:O	1:H:2:LEU:N	2.27	0.45
1:H:142:ALA:HA	1:H:145:TYR:CD2	2.52	0.45
1:J:148:THR:O	1:J:152:ARG:HD3	2.17	0.45
1:A:254:LEU:HA	1:A:254:LEU:HD23	1.72	0.45
1:D:216:ASP:OD1	1:F:247:ASP:OD2	2.35	0.45
1:E:52:ARG:HD3	1:E:52:ARG:C	2.42	0.45
1:F:104:ARG:CG	1:F:163:GLU:OE2	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:LEU:CD2	1:I:87:VAL:HG21	2.46	0.45
1:A:222:ARG:HB2	1:A:246:THR:HG21	1.98	0.45
1:C:137:GLU:O	1:C:138:TRP:C	2.60	0.45
1:C:237:GLY:O	1:C:240:PRO:HD2	2.17	0.45
1:D:19:THR:OG1	1:D:90:ARG:HG3	2.17	0.45
1:G:104:ARG:CG	1:G:163:GLU:OE2	2.60	0.45
1:H:132:ALA:CB	1:H:137:GLU:HB3	2.44	0.45
1:H:222:ARG:HB2	1:H:246:THR:HG21	1.98	0.45
1:B:104:ARG:HD3	1:B:163:GLU:CG	2.43	0.45
1:C:120:LEU:HD12	1:C:120:LEU:C	2.42	0.45
1:C:153:TYR:HA	1:C:156:LEU:HD12	1.98	0.45
1:D:-1:GLN:O	1:D:1:MET:N	2.50	0.45
1:D:254:LEU:N	1:D:255:PRO:CD	2.79	0.45
1:E:81:ARG:NH2	1:F:81:ARG:HH21	2.04	0.45
1:E:104:ARG:CZ	1:E:163:GLU:HA	2.47	0.45
1:E:129:ARG:HH21	1:F:80:ASP:CG	2.24	0.45
1:H:39:PRO:HG3	1:H:63:ILE:HD12	1.99	0.45
1:J:152:ARG:O	1:J:155:ALA:HB3	2.16	0.45
1:B:210:ALA:O	1:B:211:GLY:C	2.60	0.45
1:E:22:SER:O	1:E:26:VAL:HG23	2.17	0.45
1:F:67:LYS:O	1:F:67:LYS:CD	2.65	0.45
1:H:215:VAL:HG22	1:H:254:LEU:CD1	2.46	0.45
1:A:119:HIS:HD2	1:A:119:HIS:O	2.00	0.44
1:A:131:ARG:HG3	1:A:198:GLY:HA3	2.00	0.44
1:B:81:ARG:NH1	1:B:81:ARG:CA	2.78	0.44
1:B:218:LEU:HA	1:B:218:LEU:HD23	1.72	0.44
1:D:11:HIS:CG	1:D:57:ARG:HD3	2.52	0.44
1:D:215:VAL:HG22	1:D:254:LEU:CD1	2.47	0.44
1:J:138:TRP:HE3	1:J:139:ARG:N	2.15	0.44
1:B:81:ARG:NH1	1:B:81:ARG:HA	2.32	0.44
1:B:192:ARG:CZ	1:B:192:ARG:HB3	2.47	0.44
1:B:243:HIS:O	1:B:247:ASP:HB2	2.18	0.44
1:B:251:VAL:O	1:B:255:PRO:HG2	2.18	0.44
1:B:252:ARG:NH1	1:B:252:ARG:CG	2.79	0.44
1:D:132:ALA:CB	1:D:137:GLU:HB3	2.48	0.44
1:F:119:HIS:NE2	1:F:144:THR:HG22	2.31	0.44
1:G:19:THR:OG1	1:G:90:ARG:HG3	2.18	0.44
1:H:135:LEU:HD23	1:H:135:LEU:O	2.16	0.44
1:H:138:TRP:NE1	1:H:200:LEU:HB2	2.31	0.44
1:J:129:ARG:HA	1:J:129:ARG:HD3	1.62	0.44
1:A:119:HIS:C	1:A:119:HIS:CD2	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:O	1:C:16:VAL:HG23	2.17	0.44
1:C:182:THR:O	1:C:185:ASP:HB2	2.18	0.44
1:D:51:ARG:NH2	1:D:162:GLY:CA	2.67	0.44
1:E:135:LEU:N	1:E:209:VAL:HG22	2.24	0.44
1:F:237:GLY:O	1:F:240:PRO:HD2	2.17	0.44
1:G:81:ARG:HH21	1:H:81:ARG:NH2	2.15	0.44
1:G:202:HIS:O	1:G:206:THR:HG22	2.18	0.44
1:H:203:LEU:HB3	1:H:209:VAL:HG23	1.98	0.44
1:I:-1:GLN:OE1	1:I:0:SER:N	2.50	0.44
1:J:111:ASP:O	1:J:115:GLN:HB3	2.18	0.44
1:B:137:GLU:O	1:B:138:TRP:C	2.60	0.44
1:C:35:TYR:O	1:C:39:PRO:HD3	2.18	0.44
1:F:62:ASP:O	1:F:65:SER:HB3	2.17	0.44
1:G:183:MET:O	1:G:187:LEU:HG	2.17	0.44
1:A:205:ARG:HG3	1:A:205:ARG:HH11	1.83	0.44
1:C:114:GLU:OE2	1:D:94:ARG:CD	2.63	0.44
1:H:148:THR:O	1:H:152:ARG:HD3	2.17	0.44
1:J:76:ASP:OD1	1:J:77:THR:N	2.49	0.44
1:J:187:LEU:HD21	1:J:200:LEU:HD23	1.99	0.44
1:F:210:ALA:O	1:F:211:GLY:C	2.59	0.44
1:F:239:VAL:HB	1:F:240:PRO:HD3	1.99	0.44
1:G:-1:GLN:O	1:G:2:LEU:N	2.25	0.44
1:B:144:THR:OG1	1:B:145:TYR:N	2.51	0.44
1:D:144:THR:HA	1:D:148:THR:OG1	2.18	0.44
1:F:100:GLU:HA	1:F:109:VAL:HG21	2.00	0.44
1:H:81:ARG:NH1	1:H:81:ARG:HA	2.32	0.44
1:I:119:HIS:NE2	1:I:144:THR:CG2	2.78	0.44
1:C:187:LEU:HD21	1:C:200:LEU:HD23	1.99	0.44
1:G:179:MET:HG2	1:G:221:LEU:HD11	2.00	0.44
1:I:34:LEU:O	1:I:34:LEU:HD12	2.18	0.44
1:J:138:TRP:NE1	1:J:200:LEU:HB2	2.33	0.44
1:A:129:ARG:NH2	1:B:80:ASP:OD1	2.51	0.43
1:C:222:ARG:HG2	1:C:226:LEU:CD1	2.47	0.43
1:C:254:LEU:HA	1:C:254:LEU:HD23	1.75	0.43
1:D:203:LEU:HB3	1:D:209:VAL:HG23	2.00	0.43
1:E:220:GLU:O	1:E:220:GLU:HG2	2.17	0.43
1:G:77:THR:HG1	1:G:79:LEU:HB2	1.79	0.43
1:H:40:HIS:CE1	1:H:52:ARG:HH21	2.36	0.43
1:A:205:ARG:HH11	1:A:205:ARG:CG	2.31	0.43
1:A:243:HIS:O	1:A:247:ASP:HB2	2.18	0.43
1:B:14:ARG:HE	1:B:14:ARG:HB2	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:CD2	1:B:87:VAL:HG21	2.48	0.43
1:B:129:ARG:HA	1:B:129:ARG:HD3	1.76	0.43
1:G:90:ARG:C	1:G:90:ARG:CD	2.91	0.43
1:A:131:ARG:HG3	1:A:197:ASP:O	2.18	0.43
1:D:203:LEU:HA	1:D:206:THR:HG22	1.99	0.43
1:D:227:ALA:O	1:D:230:ALA:HB3	2.18	0.43
1:G:11:HIS:CG	1:G:57:ARG:HD3	2.53	0.43
1:G:131:ARG:HG3	1:G:198:GLY:CA	2.48	0.43
1:H:89:LEU:HD12	1:H:89:LEU:O	2.18	0.43
1:I:183:MET:O	1:I:187:LEU:HG	2.17	0.43
1:I:200:LEU:O	1:I:204:MET:HG3	2.18	0.43
1:I:220:GLU:O	1:I:220:GLU:HG2	2.17	0.43
1:J:19:THR:OG1	1:J:90:ARG:HG3	2.18	0.43
1:A:38:VAL:N	1:A:39:PRO:CD	2.82	0.43
1:C:129:ARG:HH21	1:D:80:ASP:CG	2.27	0.43
1:D:12:VAL:O	1:D:16:VAL:HG23	2.18	0.43
1:F:-1:GLN:O	1:F:2:LEU:N	2.25	0.43
1:F:129:ARG:HD3	1:F:129:ARG:HA	1.62	0.43
1:I:90:ARG:C	1:I:90:ARG:CD	2.91	0.43
1:I:238:LEU:O	1:I:242:VAL:HG23	2.17	0.43
1:B:171:ARG:O	1:B:175:GLU:HG3	2.18	0.43
1:D:210:ALA:O	1:D:211:GLY:C	2.61	0.43
1:E:177:PHE:CE2	1:E:181:ILE:HD11	2.54	0.43
1:G:131:ARG:HG3	1:G:197:ASP:O	2.18	0.43
1:H:35:TYR:O	1:H:39:PRO:HD3	2.17	0.43
1:H:237:GLY:O	1:H:240:PRO:HD2	2.19	0.43
1:I:67:LYS:O	1:I:67:LYS:HD3	2.19	0.43
1:I:135:LEU:HB2	1:I:209:VAL:HG13	2.00	0.43
1:I:247:ASP:O	1:I:251:VAL:HG23	2.19	0.43
1:J:114:GLU:C	1:J:116:ASP:H	2.23	0.43
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.88	0.43
1:A:121:CYS:O	1:A:125:ILE:HG13	2.18	0.43
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.74	0.43
1:C:51:ARG:NH2	1:C:162:GLY:CA	2.72	0.43
1:C:57:ARG:CG	1:C:58:ALA:N	2.82	0.43
1:C:72:LEU:CD1	1:C:81:ARG:HH12	2.31	0.43
1:D:247:ASP:HB3	1:F:212:GLN:HE22	1.83	0.43
1:H:104:ARG:CZ	1:H:163:GLU:HA	2.48	0.43
1:B:51:ARG:HD3	1:B:161:GLY:C	2.43	0.43
1:B:138:TRP:C	1:B:138:TRP:CE3	2.96	0.43
1:C:243:HIS:O	1:C:247:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:ARG:HG3	1:E:52:ARG:NH1	2.34	0.43
1:E:144:THR:HA	1:E:148:THR:OG1	2.18	0.43
1:E:222:ARG:HG2	1:E:226:LEU:CD1	2.49	0.43
1:E:238:LEU:O	1:E:241:VAL:HB	2.19	0.43
1:F:11:HIS:CG	1:F:57:ARG:HD3	2.54	0.43
1:G:94:ARG:HD2	1:H:114:GLU:OE2	2.19	0.43
1:H:152:ARG:O	1:H:155:ALA:HB3	2.19	0.43
1:I:227:ALA:O	1:I:230:ALA:HB3	2.19	0.43
1:J:-1:GLN:O	1:J:1:MET:N	2.51	0.43
1:J:90:ARG:HD3	1:J:90:ARG:O	2.19	0.43
1:J:104:ARG:CZ	1:J:163:GLU:HA	2.48	0.43
1:J:188:THR:HG22	1:J:192:ARG:HH11	1.83	0.43
1:C:203:LEU:CA	1:C:206:THR:HG22	2.49	0.43
1:H:52:ARG:O	1:H:56:SER:HB2	2.18	0.43
1:B:11:HIS:CD2	1:B:57:ARG:HD3	2.53	0.43
1:E:132:ALA:CB	1:E:137:GLU:HB3	2.49	0.43
1:H:243:HIS:O	1:H:247:ASP:HB2	2.19	0.43
1:J:131:ARG:HG3	1:J:197:ASP:O	2.19	0.43
1:J:222:ARG:HB2	1:J:246:THR:HG21	2.01	0.43
1:B:111:ASP:O	1:B:115:GLN:HB3	2.18	0.43
1:B:193:ASN:O	1:B:193:ASN:CG	2.61	0.43
1:C:132:ALA:CB	1:C:137:GLU:HB3	2.49	0.43
1:F:81:ARG:HH11	1:F:81:ARG:CA	2.30	0.43
1:G:254:LEU:N	1:G:255:PRO:CD	2.82	0.43
1:H:58:ALA:O	1:H:61:LEU:HB2	2.18	0.43
1:C:83:GLU:O	1:C:87:VAL:HG23	2.19	0.42
1:F:-1:GLN:O	1:F:1:MET:N	2.52	0.42
1:G:55:VAL:HG21	1:G:161:GLY:HA2	2.01	0.42
1:H:76:ASP:OD1	1:H:77:THR:N	2.52	0.42
1:A:252:ARG:HH12	1:A:253:LEU:HD21	1.83	0.42
1:B:-1:GLN:O	1:B:2:LEU:N	2.27	0.42
1:B:58:ALA:O	1:B:61:LEU:HB2	2.19	0.42
1:C:247:ASP:O	1:C:251:VAL:HG23	2.19	0.42
1:D:119:HIS:NE2	1:D:144:THR:HG22	2.34	0.42
1:D:179:MET:HG2	1:D:221:LEU:HD11	2.00	0.42
1:E:115:GLN:O	1:E:115:GLN:CG	2.61	0.42
1:G:67:LYS:O	1:G:67:LYS:HD3	2.19	0.42
1:G:97:HIS:ND1	1:H:107:LYS:NZ	2.65	0.42
1:G:135:LEU:N	1:G:209:VAL:HG22	2.30	0.42
1:J:72:LEU:HD13	1:J:84:LEU:HB3	2.00	0.42
1:J:210:ALA:O	1:J:211:GLY:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:HG3	1:A:63:ILE:HD12	2.00	0.42
1:A:251:VAL:O	1:A:255:PRO:HG2	2.20	0.42
1:C:250:LEU:O	1:C:255:PRO:HD3	2.20	0.42
1:D:104:ARG:H	1:D:104:ARG:HG3	1.63	0.42
1:D:138:TRP:HE3	1:D:139:ARG:N	2.17	0.42
1:D:202:HIS:C	1:D:204:MET:N	2.76	0.42
1:D:243:HIS:CB	1:F:216:ASP:OD2	2.67	0.42
1:F:58:ALA:O	1:F:61:LEU:HB2	2.19	0.42
1:G:138:TRP:NE1	1:G:200:LEU:HB2	2.35	0.42
1:G:222:ARG:HG2	1:G:226:LEU:CD1	2.48	0.42
1:H:19:THR:OG1	1:H:90:ARG:HG3	2.19	0.42
1:H:111:ASP:O	1:H:115:GLN:HB3	2.19	0.42
1:I:104:ARG:CG	1:I:163:GLU:OE2	2.63	0.42
1:J:142:ALA:HA	1:J:145:TYR:CD2	2.54	0.42
1:J:254:LEU:N	1:J:255:PRO:CD	2.82	0.42
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.91	0.42
1:B:135:LEU:N	1:B:209:VAL:HG22	2.29	0.42
1:B:222:ARG:HG2	1:B:226:LEU:HD12	2.01	0.42
1:F:202:HIS:C	1:F:204:MET:N	2.76	0.42
1:F:203:LEU:HA	1:F:206:THR:HG22	2.00	0.42
1:G:135:LEU:HD23	1:G:135:LEU:O	2.20	0.42
1:H:18:GLN:HE21	1:H:18:GLN:HB2	1.70	0.42
1:I:166:PRO:O	1:I:167:ALA:C	2.62	0.42
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.86	0.42
1:C:131:ARG:HG3	1:C:198:GLY:CA	2.49	0.42
1:D:89:LEU:HD12	1:D:89:LEU:O	2.19	0.42
1:D:237:GLY:O	1:D:240:PRO:HD2	2.19	0.42
1:G:80:ASP:HB3	1:G:83:GLU:OE1	2.19	0.42
1:H:210:ALA:O	1:H:211:GLY:C	2.61	0.42
1:A:104:ARG:CG	1:A:163:GLU:OE2	2.64	0.42
1:C:119:HIS:HD2	1:C:119:HIS:O	2.02	0.42
1:D:76:ASP:O	1:D:77:THR:C	2.62	0.42
1:F:215:VAL:HG22	1:F:254:LEU:CD1	2.49	0.42
1:G:200:LEU:O	1:G:204:MET:HG3	2.19	0.42
1:H:189:ASP:HB3	1:H:195:GLU:OE2	2.19	0.42
1:A:177:PHE:CE2	1:A:181:ILE:HD11	2.55	0.42
1:D:104:ARG:CG	1:D:163:GLU:OE2	2.63	0.42
1:G:119:HIS:C	1:G:119:HIS:CD2	2.97	0.42
1:G:142:ALA:HB1	1:G:182:THR:HG21	2.01	0.42
1:I:108:ALA:O	1:I:112:ILE:HG13	2.20	0.42
1:J:237:GLY:O	1:J:240:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ALA:O	1:C:61:LEU:HB2	2.20	0.42
1:D:104:ARG:CD	1:D:163:GLU:HG3	2.38	0.42
1:E:243:HIS:O	1:E:247:ASP:HB2	2.19	0.42
1:G:111:ASP:O	1:G:115:GLN:HB3	2.19	0.42
1:H:22:SER:N	1:H:83:GLU:OE2	2.46	0.42
1:H:72:LEU:HD13	1:H:84:LEU:HB3	2.01	0.42
1:H:119:HIS:NE2	1:H:144:THR:HG22	2.35	0.42
1:I:72:LEU:HD13	1:I:84:LEU:HB3	2.02	0.42
1:J:-3:TYR:C	1:J:-1:GLN:N	2.52	0.42
1:B:39:PRO:HG3	1:B:63:ILE:HD12	2.01	0.42
1:D:90:ARG:HD3	1:D:90:ARG:HH11	1.72	0.42
1:E:119:HIS:CD2	1:E:119:HIS:C	2.98	0.42
1:G:238:LEU:O	1:G:242:VAL:HG23	2.20	0.42
1:H:183:MET:HE2	1:H:183:MET:HB3	1.89	0.42
1:I:63:ILE:HG12	1:I:153:TYR:CE2	2.55	0.42
1:J:138:TRP:HE3	1:J:139:ARG:HA	1.84	0.42
1:A:89:LEU:O	1:A:89:LEU:HD12	2.19	0.42
1:E:204:MET:HE3	1:E:257:HIS:CB	2.47	0.42
1:E:210:ALA:O	1:E:211:GLY:C	2.62	0.42
1:G:104:ARG:H	1:G:104:ARG:HG3	1.65	0.42
1:G:227:ALA:O	1:G:230:ALA:HB3	2.20	0.42
1:A:135:LEU:N	1:A:209:VAL:HG22	2.28	0.41
1:B:72:LEU:HD13	1:B:84:LEU:HB3	2.01	0.41
1:D:131:ARG:O	1:D:131:ARG:HG2	2.16	0.41
1:E:-2:PHE:HZ	1:E:240:PRO:HB3	1.85	0.41
1:E:81:ARG:NH1	1:E:81:ARG:CG	2.78	0.41
1:F:183:MET:O	1:F:187:LEU:HG	2.20	0.41
1:H:-1:GLN:O	1:H:1:MET:N	2.53	0.41
1:I:38:VAL:N	1:I:39:PRO:CD	2.83	0.41
1:A:114:GLU:C	1:A:116:ASP:H	2.25	0.41
1:C:94:ARG:HD2	1:D:114:GLU:OE2	2.20	0.41
1:E:11:HIS:CD2	1:E:57:ARG:CD	3.03	0.41
1:F:187:LEU:HD21	1:F:200:LEU:HD23	2.02	0.41
1:I:11:HIS:CD2	1:I:57:ARG:CD	3.03	0.41
1:J:204:MET:HE3	1:J:257:HIS:CB	2.47	0.41
1:A:193:ASN:O	1:A:193:ASN:CG	2.63	0.41
1:B:34:LEU:O	1:B:34:LEU:HD12	2.20	0.41
1:C:131:ARG:HG3	1:C:197:ASP:O	2.20	0.41
1:D:18:GLN:HE21	1:D:18:GLN:HB2	1.65	0.41
1:E:48:ASP:CG	1:E:49:PRO:HD2	2.45	0.41
1:E:104:ARG:H	1:E:104:ARG:HG3	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:ASP:OD1	1:E:105:ASP:C	2.64	0.41
1:F:-1:GLN:OE1	1:F:0:SER:N	2.54	0.41
1:F:4:ALA:O	1:F:5:GLU:C	2.62	0.41
1:I:131:ARG:HG3	1:I:197:ASP:C	2.46	0.41
1:J:90:ARG:C	1:J:90:ARG:CD	2.94	0.41
1:C:44:GLU:HG2	1:C:235:ALA:HB1	2.02	0.41
1:E:203:LEU:CA	1:E:206:THR:HG22	2.50	0.41
1:G:203:LEU:O	1:G:209:VAL:N	2.52	0.41
1:H:153:TYR:HA	1:H:156:LEU:HD12	2.02	0.41
1:H:204:MET:HE3	1:H:257:HIS:CB	2.48	0.41
1:I:72:LEU:HD12	1:I:72:LEU:HA	1.84	0.41
1:I:72:LEU:HD23	1:J:72:LEU:HD23	2.02	0.41
1:I:111:ASP:O	1:I:115:GLN:HB3	2.20	0.41
1:J:131:ARG:HG3	1:J:198:GLY:CA	2.51	0.41
1:B:81:ARG:NH1	1:B:81:ARG:CG	2.83	0.41
1:D:17:ALA:C	1:D:19:THR:H	2.29	0.41
1:F:254:LEU:HD23	1:F:254:LEU:HA	1.86	0.41
1:G:96:LEU:O	1:G:100:GLU:HB2	2.21	0.41
1:G:193:ASN:O	1:G:193:ASN:CG	2.63	0.41
1:G:210:ALA:O	1:G:211:GLY:C	2.62	0.41
1:H:254:LEU:N	1:H:255:PRO:CD	2.83	0.41
1:I:254:LEU:N	1:I:255:PRO:CD	2.84	0.41
1:J:138:TRP:CE3	1:J:139:ARG:HA	2.54	0.41
1:J:196:ARG:HG2	1:J:202:HIS:CG	2.56	0.41
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.35	0.41
1:A:138:TRP:C	1:A:138:TRP:CE3	2.99	0.41
1:C:11:HIS:CD2	1:C:57:ARG:CD	3.04	0.41
1:E:35:TYR:O	1:E:39:PRO:HD3	2.20	0.41
1:E:106:PRO:O	1:E:109:VAL:HG23	2.20	0.41
1:I:55:VAL:HG21	1:I:161:GLY:HA2	2.02	0.41
1:I:100:GLU:HA	1:I:109:VAL:HG21	2.02	0.41
1:J:149:PHE:CE1	1:J:153:TYR:CE2	3.05	0.41
1:C:89:LEU:HD12	1:C:89:LEU:O	2.20	0.41
1:C:142:ALA:HA	1:C:145:TYR:CD2	2.56	0.41
1:D:-3:TYR:C	1:D:-3:TYR:CD2	2.98	0.41
1:E:43:THR:CG2	1:E:55:VAL:HG12	2.51	0.41
1:F:196:ARG:HG2	1:F:196:ARG:O	2.21	0.41
1:G:38:VAL:N	1:G:39:PRO:CD	2.84	0.41
1:G:90:ARG:NH1	1:G:94:ARG:HB2	2.35	0.41
1:G:237:GLY:O	1:G:240:PRO:HD2	2.21	0.41
1:H:138:TRP:CE3	1:H:139:ARG:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:69:LEU:HD11	1:J:85:ALA:HB1	2.02	0.41
1:A:4:ALA:C	1:A:6:ALA:N	2.77	0.41
1:A:129:ARG:HD3	1:A:129:ARG:HA	1.81	0.41
1:A:138:TRP:HH2	1:A:183:MET:HG2	1.86	0.41
1:B:189:ASP:HB3	1:B:195:GLU:OE2	2.21	0.41
1:H:51:ARG:HD3	1:H:161:GLY:C	2.46	0.41
1:I:142:ALA:HB1	1:I:182:THR:HG21	2.02	0.41
1:J:90:ARG:NH1	1:J:94:ARG:HB2	2.35	0.41
1:J:189:ASP:HB3	1:J:195:GLU:OE2	2.20	0.41
1:A:-1:GLN:O	1:A:2:LEU:N	2.28	0.41
1:A:148:THR:O	1:A:152:ARG:HD3	2.20	0.41
1:C:239:VAL:N	1:C:240:PRO:CD	2.84	0.41
1:D:62:ASP:O	1:D:65:SER:HB3	2.21	0.41
1:E:-1:GLN:O	1:E:1:MET:N	2.54	0.41
1:E:58:ALA:CB	1:E:99:LEU:HD23	2.51	0.41
1:E:129:ARG:HH22	1:F:82:VAL:HB	1.85	0.41
1:E:202:HIS:C	1:E:204:MET:N	2.78	0.41
1:F:39:PRO:HG3	1:F:63:ILE:HD12	2.01	0.41
1:H:72:LEU:HD21	1:H:85:ALA:HB2	2.02	0.41
1:H:131:ARG:HG3	1:H:197:ASP:O	2.21	0.41
1:H:135:LEU:HB2	1:H:209:VAL:HG13	2.03	0.41
1:H:222:ARG:HG2	1:H:226:LEU:HD12	2.03	0.41
1:I:131:ARG:HG3	1:I:198:GLY:CA	2.48	0.41
1:J:58:ALA:O	1:J:61:LEU:HB2	2.21	0.41
1:B:1:MET:HE3	1:B:37:ARG:CZ	2.51	0.41
1:B:250:LEU:HA	1:B:250:LEU:HD23	1.89	0.41
1:D:5:GLU:CD	1:D:9:ARG:HH12	2.28	0.41
1:D:183:MET:HE2	1:D:183:MET:HB3	1.81	0.41
1:D:219:GLU:OE2	1:F:222:ARG:NH2	2.53	0.41
1:E:38:VAL:HG11	1:E:150:LEU:HD11	2.03	0.41
1:F:17:ALA:C	1:F:19:THR:H	2.29	0.41
1:F:134:ASN:OD1	1:F:136:ARG:HB3	2.21	0.41
1:H:14:ARG:HE	1:H:14:ARG:HB2	1.58	0.41
1:I:43:THR:HB	1:I:52:ARG:HG2	2.03	0.41
1:I:81:ARG:HH11	1:I:81:ARG:CA	2.29	0.41
1:I:132:ALA:CB	1:I:137:GLU:HB3	2.51	0.41
1:A:58:ALA:O	1:A:61:LEU:HB2	2.21	0.40
1:B:227:ALA:O	1:B:230:ALA:HB3	2.21	0.40
1:C:204:MET:HE3	1:C:257:HIS:CB	2.49	0.40
1:E:58:ALA:O	1:E:61:LEU:HB2	2.21	0.40
1:E:60:ALA:O	1:E:64:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:ASP:O	1:F:115:GLN:HB3	2.20	0.40
1:B:217:LEU:HD12	1:B:217:LEU:O	2.20	0.40
1:D:38:VAL:HG11	1:D:150:LEU:HD11	2.04	0.40
1:D:44:GLU:HG2	1:D:235:ALA:HB1	2.02	0.40
1:E:131:ARG:HG3	1:E:197:ASP:O	2.21	0.40
1:F:11:His:CD2	1:F:57:ARG:HD3	2.57	0.40
1:G:-1:GLN:O	1:G:1:MET:N	2.55	0.40
1:G:81:ARG:HH11	1:G:81:ARG:CG	2.28	0.40
1:G:129:ARG:HA	1:G:129:ARG:HD3	1.73	0.40
1:I:76:ASP:O	1:I:77:THR:C	2.65	0.40
1:I:243:HIS:O	1:I:247:ASP:HB2	2.21	0.40
1:J:104:ARG:CG	1:J:163:GLU:OE2	2.65	0.40
1:A:80:ASP:OD1	1:B:129:ARG:NH2	2.52	0.40
1:C:203:LEU:HB3	1:C:209:VAL:HG23	2.04	0.40
1:E:92:HIS:NE2	1:E:96:LEU:HD11	2.36	0.40
1:G:51:ARG:HD3	1:G:161:GLY:C	2.46	0.40
1:G:190:TYR:CE2	1:G:202:HIS:HB2	2.55	0.40
1:I:94:ARG:HD2	1:J:114:GLU:OE2	2.21	0.40
1:I:218:LEU:HA	1:I:218:LEU:HD23	1.87	0.40
1:J:52:ARG:O	1:J:56:SER:HB2	2.22	0.40
1:J:177:PHE:CZ	1:J:181:ILE:HD11	2.57	0.40
1:A:1:MET:HE3	1:A:37:ARG:CZ	2.51	0.40
1:B:4:ALA:C	1:B:6:ALA:N	2.77	0.40
1:C:52:ARG:C	1:C:52:ARG:HD3	2.46	0.40
1:C:226:LEU:HG	1:C:242:VAL:HG11	2.04	0.40
1:E:42:LEU:HD21	1:E:150:LEU:CD2	2.51	0.40
1:G:166:PRO:O	1:G:167:ALA:C	2.64	0.40
1:H:68:LEU:HD22	1:H:84:LEU:HD23	2.02	0.40
1:J:243:HIS:O	1:J:247:ASP:HB2	2.21	0.40
1:A:11:HIS:CD2	1:A:57:ARG:HD3	2.56	0.40
1:B:107:LYS:HA	1:B:107:LYS:HD3	1.84	0.40
1:B:166:PRO:O	1:B:167:ALA:C	2.65	0.40
1:B:206:THR:O	1:B:206:THR:OG1	2.35	0.40
1:C:61:LEU:HD23	1:C:61:LEU:HA	1.98	0.40
1:E:-1:GLN:O	1:E:2:LEU:N	2.30	0.40
1:E:68:LEU:HA	1:E:68:LEU:HD23	1.90	0.40
1:E:100:GLU:HA	1:E:109:VAL:HG21	2.03	0.40
1:G:43:THR:HB	1:G:52:ARG:HG2	2.03	0.40
1:G:119:HIS:HD2	1:G:119:HIS:O	2.03	0.40
1:G:138:TRP:C	1:G:138:TRP:CE3	2.99	0.40
1:G:190:TYR:HB2	1:G:201:ALA:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:THR:O	1:G:206:THR:OG1	2.39	0.40
1:H:149:PHE:CE1	1:H:153:TYR:CE2	3.09	0.40
1:I:135:LEU:N	1:I:209:VAL:HG22	2.31	0.40
1:I:193:ASN:O	1:I:193:ASN:CG	2.64	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	260/294 (88%)	223 (86%)	30 (12%)	7 (3%)	4	27
1	B	260/294 (88%)	224 (86%)	28 (11%)	8 (3%)	3	25
1	C	260/294 (88%)	223 (86%)	30 (12%)	7 (3%)	4	27
1	D	260/294 (88%)	222 (85%)	30 (12%)	8 (3%)	3	25
1	E	260/294 (88%)	225 (86%)	28 (11%)	7 (3%)	4	27
1	F	260/294 (88%)	220 (85%)	33 (13%)	7 (3%)	4	27
1	G	260/294 (88%)	217 (84%)	35 (14%)	8 (3%)	3	25
1	H	260/294 (88%)	220 (85%)	33 (13%)	7 (3%)	4	27
1	I	260/294 (88%)	220 (85%)	31 (12%)	9 (4%)	3	23
1	J	260/294 (88%)	222 (85%)	31 (12%)	7 (3%)	4	27
All	All	2600/2940 (88%)	2216 (85%)	309 (12%)	75 (3%)	3	26

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-2	PHE
1	A	77	THR
1	A	115	GLN

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Mol	Chain	Res	Type
1	A	167	ALA
1	A	194	GLY
1	B	-2	PHE
1	B	77	THR
1	B	115	GLN
1	B	194	GLY
1	C	-2	PHE
1	C	77	THR
1	C	115	GLN
1	C	194	GLY
1	D	-2	PHE
1	D	77	THR
1	D	115	GLN
1	D	194	GLY
1	E	-2	PHE
1	E	77	THR
1	E	115	GLN
1	E	194	GLY
1	F	-2	PHE
1	F	77	THR
1	F	115	GLN
1	F	194	GLY
1	G	-2	PHE
1	G	77	THR
1	G	115	GLN
1	G	194	GLY
1	H	-2	PHE
1	H	77	THR
1	H	115	GLN
1	H	194	GLY
1	I	-2	PHE
1	I	77	THR
1	I	115	GLN
1	I	194	GLY
1	J	-2	PHE
1	J	77	THR
1	J	115	GLN
1	J	194	GLY
1	A	0	SER
1	B	0	SER
1	B	167	ALA
1	C	0	SER

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Mol	Chain	Res	Type
1	C	167	ALA
1	D	0	SER
1	D	167	ALA
1	E	0	SER
1	E	167	ALA
1	F	167	ALA
1	G	0	SER
1	G	167	ALA
1	H	0	SER
1	H	167	ALA
1	I	167	ALA
1	J	0	SER
1	J	167	ALA
1	F	0	SER
1	I	0	SER
1	A	116	ASP
1	B	116	ASP
1	D	163	GLU
1	G	116	ASP
1	G	163	GLU
1	H	116	ASP
1	I	116	ASP
1	J	116	ASP
1	B	163	GLU
1	C	116	ASP
1	E	116	ASP
1	I	163	GLU
1	D	116	ASP
1	F	163	GLU
1	I	192	ARG

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	206/232 (89%)	189 (92%)	17 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	206/232 (89%)	186 (90%)	20 (10%)	8	31
1	C	206/232 (89%)	187 (91%)	19 (9%)	8	32
1	D	206/232 (89%)	183 (89%)	23 (11%)	6	26
1	E	206/232 (89%)	186 (90%)	20 (10%)	8	31
1	F	206/232 (89%)	186 (90%)	20 (10%)	8	31
1	G	206/232 (89%)	187 (91%)	19 (9%)	8	32
1	H	206/232 (89%)	186 (90%)	20 (10%)	8	31
1	I	206/232 (89%)	185 (90%)	21 (10%)	7	28
1	J	206/232 (89%)	185 (90%)	21 (10%)	7	28
All	All	2060/2320 (89%)	1860 (90%)	200 (10%)	8	31

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	CYS
1	A	18	GLN
1	A	79	LEU
1	A	81	ARG
1	A	101	SER
1	A	107	LYS
1	A	109	VAL
1	A	115	GLN
1	A	118	VAL
1	A	129	ARG
1	A	131	ARG
1	A	137	GLU
1	A	141	HIS
1	A	172	GLU
1	A	185	ASP
1	A	205	ARG
1	A	216	ASP
1	B	15	CYS
1	B	18	GLN
1	B	76	ASP
1	B	79	LEU
1	B	81	ARG
1	B	101	SER
1	B	107	LYS
1	B	115	GLN

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Mol	Chain	Res	Type
1	B	118	VAL
1	B	129	ARG
1	B	131	ARG
1	B	137	GLU
1	B	141	HIS
1	B	150	LEU
1	B	172	GLU
1	B	179	MET
1	B	185	ASP
1	B	205	ARG
1	B	216	ASP
1	B	254	LEU
1	C	1	MET
1	C	15	CYS
1	C	18	GLN
1	C	49	PRO
1	C	81	ARG
1	C	101	SER
1	C	109	VAL
1	C	114	GLU
1	C	115	GLN
1	C	118	VAL
1	C	120	LEU
1	C	129	ARG
1	C	131	ARG
1	C	137	GLU
1	C	141	HIS
1	C	172	GLU
1	C	185	ASP
1	C	205	ARG
1	C	216	ASP
1	D	1	MET
1	D	15	CYS
1	D	18	GLN
1	D	52	ARG
1	D	79	LEU
1	D	81	ARG
1	D	107	LYS
1	D	109	VAL
1	D	114	GLU
1	D	115	GLN
1	D	118	VAL

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Mol	Chain	Res	Type
1	D	120	LEU
1	D	129	ARG
1	D	131	ARG
1	D	137	GLU
1	D	141	HIS
1	D	150	LEU
1	D	172	GLU
1	D	179	MET
1	D	185	ASP
1	D	205	ARG
1	D	218	LEU
1	D	219	GLU
1	E	15	CYS
1	E	18	GLN
1	E	49	PRO
1	E	79	LEU
1	E	81	ARG
1	E	101	SER
1	E	109	VAL
1	E	114	GLU
1	E	115	GLN
1	E	118	VAL
1	E	120	LEU
1	E	129	ARG
1	E	131	ARG
1	E	137	GLU
1	E	141	HIS
1	E	150	LEU
1	E	172	GLU
1	E	185	ASP
1	E	205	ARG
1	E	216	ASP
1	F	1	MET
1	F	15	CYS
1	F	18	GLN
1	F	52	ARG
1	F	79	LEU
1	F	81	ARG
1	F	101	SER
1	F	109	VAL
1	F	115	GLN
1	F	118	VAL

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Mol	Chain	Res	Type
1	F	129	ARG
1	F	131	ARG
1	F	137	GLU
1	F	150	LEU
1	F	172	GLU
1	F	179	MET
1	F	185	ASP
1	F	205	ARG
1	F	218	LEU
1	F	219	GLU
1	G	1	MET
1	G	15	CYS
1	G	18	GLN
1	G	79	LEU
1	G	81	ARG
1	G	101	SER
1	G	106	PRO
1	G	115	GLN
1	G	118	VAL
1	G	120	LEU
1	G	129	ARG
1	G	131	ARG
1	G	137	GLU
1	G	141	HIS
1	G	150	LEU
1	G	172	GLU
1	G	185	ASP
1	G	205	ARG
1	G	216	ASP
1	H	1	MET
1	H	15	CYS
1	H	18	GLN
1	H	52	ARG
1	H	79	LEU
1	H	81	ARG
1	H	101	SER
1	H	115	GLN
1	H	118	VAL
1	H	129	ARG
1	H	131	ARG
1	H	137	GLU
1	H	141	HIS

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Mol	Chain	Res	Type
1	H	150	LEU
1	H	172	GLU
1	H	180	THR
1	H	185	ASP
1	H	205	ARG
1	H	216	ASP
1	H	254	LEU
1	I	1	MET
1	I	15	CYS
1	I	18	GLN
1	I	52	ARG
1	I	79	LEU
1	I	81	ARG
1	I	101	SER
1	I	109	VAL
1	I	115	GLN
1	I	118	VAL
1	I	120	LEU
1	I	129	ARG
1	I	131	ARG
1	I	137	GLU
1	I	141	HIS
1	I	148	THR
1	I	150	LEU
1	I	172	GLU
1	I	185	ASP
1	I	205	ARG
1	I	216	ASP
1	J	1	MET
1	J	15	CYS
1	J	18	GLN
1	J	79	LEU
1	J	81	ARG
1	J	101	SER
1	J	109	VAL
1	J	115	GLN
1	J	118	VAL
1	J	129	ARG
1	J	131	ARG
1	J	137	GLU
1	J	141	HIS
1	J	148	THR

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Mol	Chain	Res	Type
1	J	150	LEU
1	J	172	GLU
1	J	180	THR
1	J	185	ASP
1	J	205	ARG
1	J	216	ASP
1	J	254	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	40	HIS
1	A	124	GLN
1	A	165	GLN
1	A	193	ASN
1	B	18	GLN
1	B	40	HIS
1	B	115	GLN
1	B	124	GLN
1	B	193	ASN
1	C	18	GLN
1	C	40	HIS
1	C	115	GLN
1	C	124	GLN
1	C	141	HIS
1	C	193	ASN
1	C	257	HIS
1	D	18	GLN
1	D	40	HIS
1	D	115	GLN
1	D	124	GLN
1	D	141	HIS
1	D	193	ASN
1	D	212	GLN
1	E	18	GLN
1	E	115	GLN
1	E	124	GLN
1	E	141	HIS
1	E	165	GLN
1	E	193	ASN
1	E	257	HIS

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Mol	Chain	Res	Type
1	F	18	GLN
1	F	40	HIS
1	F	115	GLN
1	F	124	GLN
1	F	141	HIS
1	F	165	GLN
1	F	193	ASN
1	F	212	GLN
1	G	18	GLN
1	G	40	HIS
1	G	115	GLN
1	G	124	GLN
1	G	141	HIS
1	G	193	ASN
1	G	257	HIS
1	H	18	GLN
1	H	40	HIS
1	H	115	GLN
1	H	124	GLN
1	H	141	HIS
1	H	165	GLN
1	H	193	ASN
1	I	18	GLN
1	I	40	HIS
1	I	115	GLN
1	I	124	GLN
1	I	141	HIS
1	I	193	ASN
1	J	18	GLN
1	J	40	HIS
1	J	115	GLN
1	J	124	GLN
1	J	141	HIS
1	J	165	GLN
1	J	193	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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

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	262/294 (89%)	-0.34	0 100 100	56, 83, 118, 151	0
1	B	262/294 (89%)	-0.35	1 (0%) 88 73	54, 84, 120, 152	0
1	C	262/294 (89%)	-0.48	1 (0%) 88 73	58, 81, 116, 156	0
1	D	262/294 (89%)	-0.30	3 (1%) 78 54	57, 84, 135, 164	0
1	E	262/294 (89%)	-0.47	0 100 100	53, 81, 120, 156	0
1	F	262/294 (89%)	-0.31	3 (1%) 78 54	57, 84, 132, 162	0
1	G	262/294 (89%)	0.02	3 (1%) 78 54	79, 115, 149, 164	0
1	H	262/294 (89%)	-0.19	0 100 100	76, 106, 147, 161	0
1	I	262/294 (89%)	-0.02	1 (0%) 88 73	84, 114, 148, 165	0
1	J	262/294 (89%)	-0.13	1 (0%) 88 73	74, 104, 148, 161	0
All	All	2620/2940 (89%)	-0.26	13 (0%) 87 70	53, 95, 143, 165	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	13	THR	3.6
1	B	207	GLY	2.7
1	G	16	VAL	2.6
1	F	254	LEU	2.6
1	I	231	ALA	2.5
1	C	-3	TYR	2.3
1	D	253	LEU	2.3
1	F	253	LEU	2.3
1	D	194	GLY	2.1
1	G	251	VAL	2.1
1	D	-3	TYR	2.1
1	G	211	GLY	2.0
1	F	-3	TYR	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 oligosaccharides 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.