



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:40 am BST

PDB ID : 5B01
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

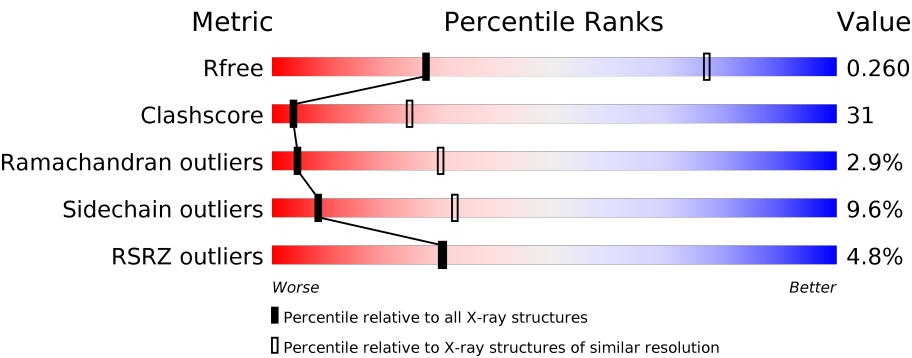
1 Overall quality at a glance i

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}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div><div>2%</div><div><div></div><div>46%</div><div>39%</div><div>•</div><div>11%</div></div></div>
1	B	294	<div><div>2%</div><div><div></div><div>45%</div><div>37%</div><div>6%</div><div>•</div><div>11%</div></div></div>
1	C	294	<div><div>3%</div><div><div></div><div>46%</div><div>38%</div><div>5%</div><div>11%</div></div></div>
1	D	294	<div><div>5%</div><div><div></div><div>44%</div><div>38%</div><div>7%</div><div>11%</div></div></div>
1	E	294	<div><div>3%</div><div><div></div><div>44%</div><div>40%</div><div>5%</div><div>11%</div></div></div>
1	F	294	<div><div>5%</div><div><div></div><div>45%</div><div>37%</div><div>6%</div><div>•</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	294	 6% 43% 40% 6% 11%
1	H	294	 6% 41% 41% 6% 11%
1	I	294	 6% 44% 40% 6% 11%
1	J	294	 4% 43% 40% 6% 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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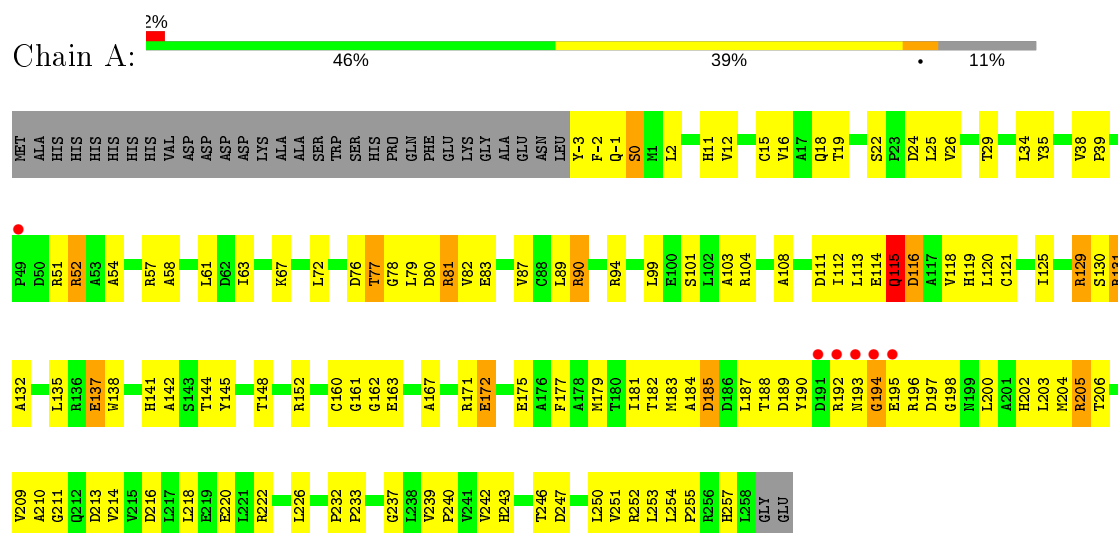
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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	PHE	-	expression tag	UNP A0A010
I	-1	GLN	-	expression tag	UNP A0A010
I	0	SER	-	expression tag	UNP A0A010
J	-33	MET	-	expression tag	UNP A0A010
J	-32	ALA	-	expression tag	UNP A0A010
J	-31	HIS	-	expression 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

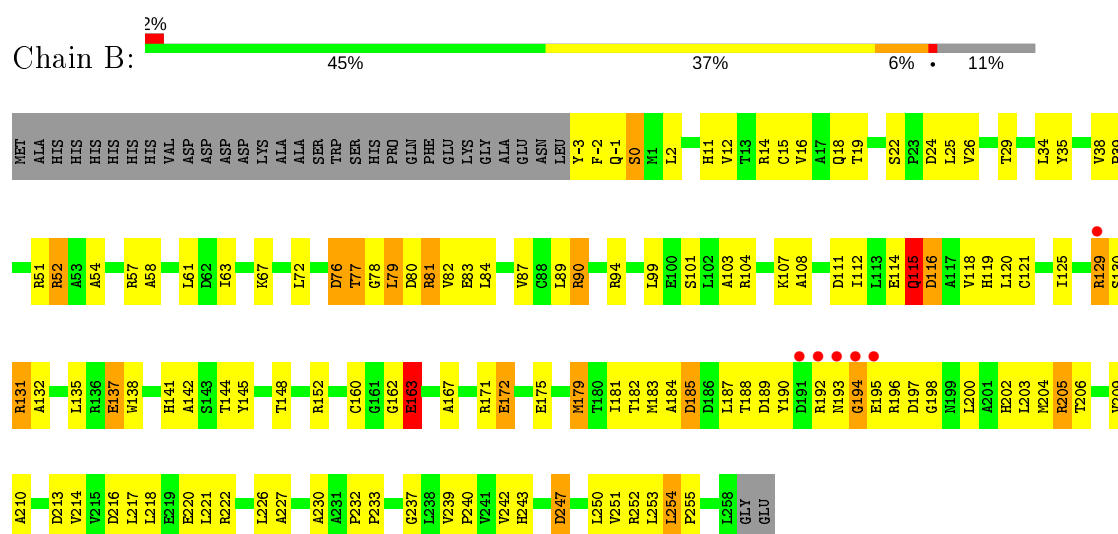
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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

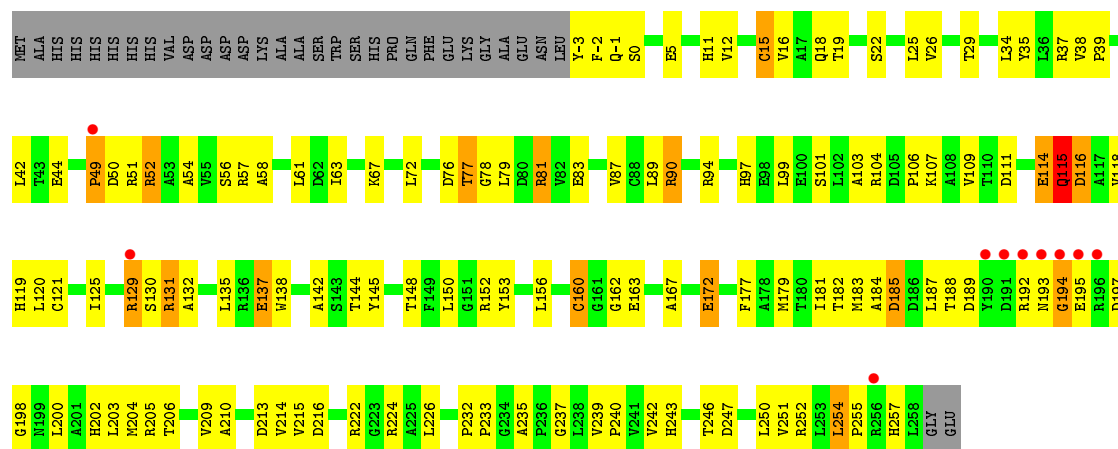


• Molecule 1: MoeN5

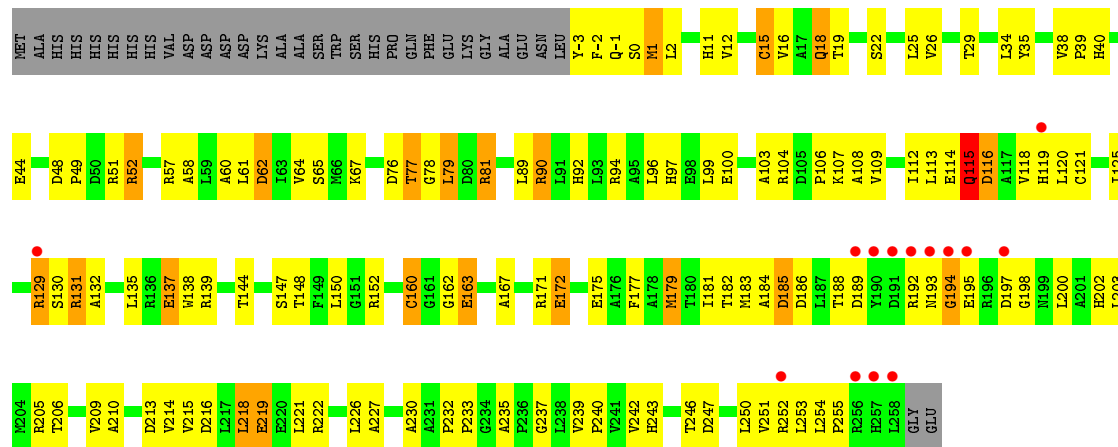


• Molecule 1: MoeN5

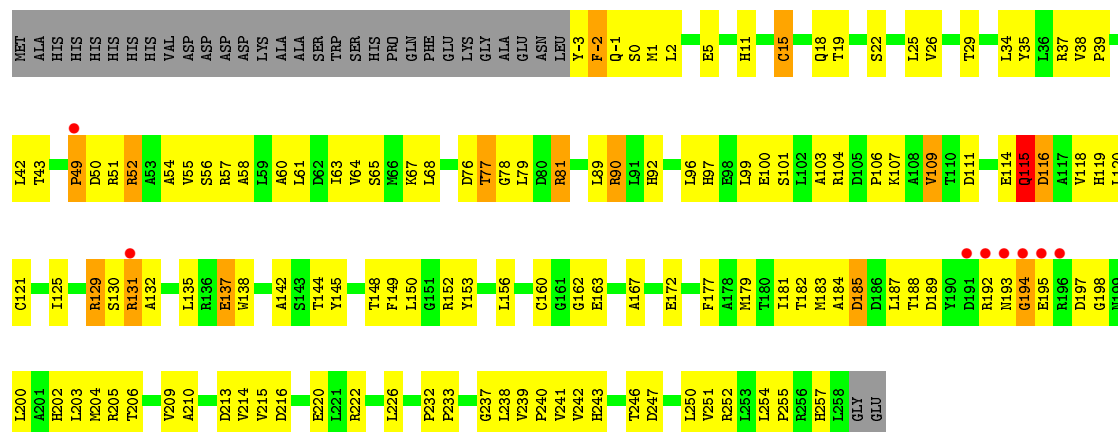
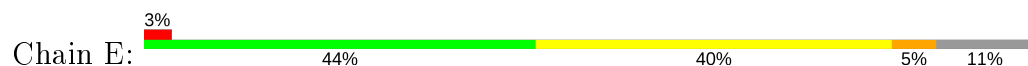




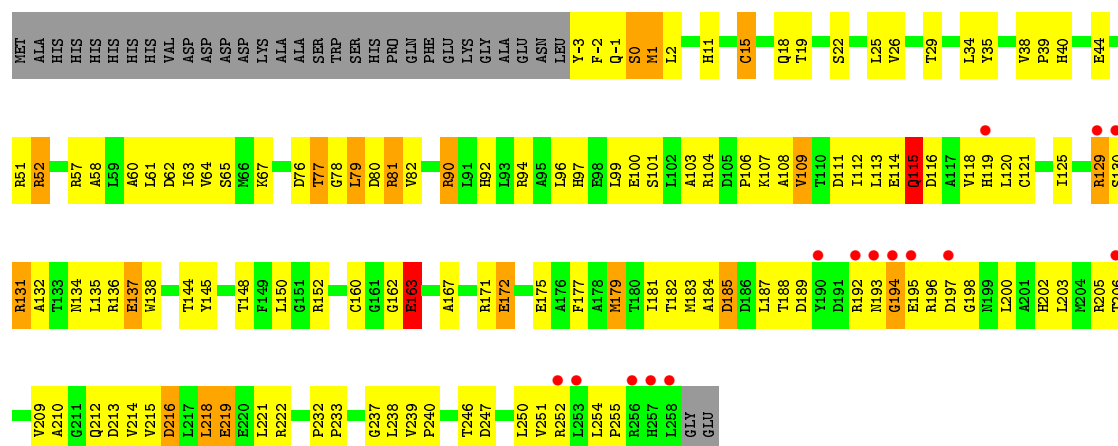
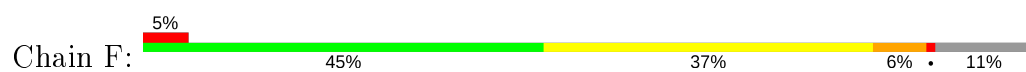
• Molecule 1: MoeN5



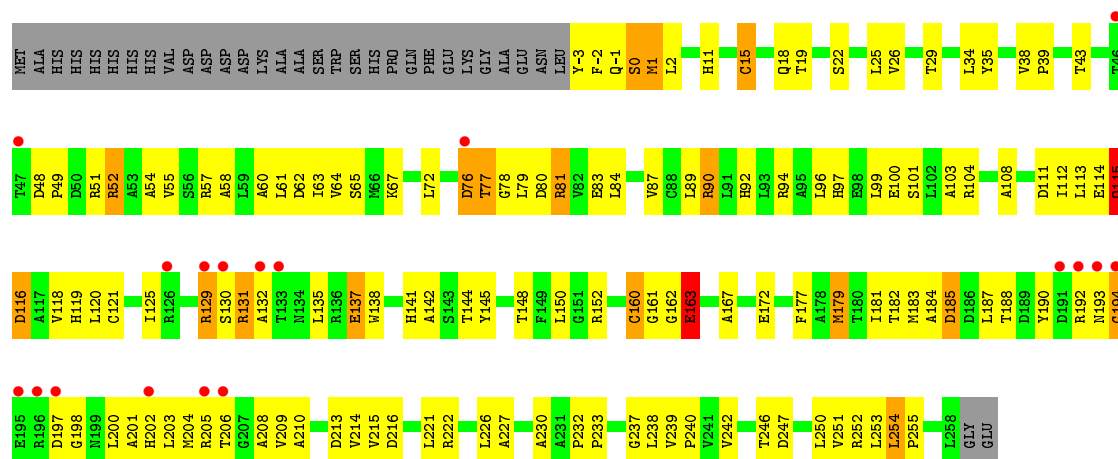
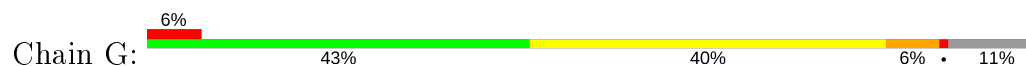
• Molecule 1: MoeN5



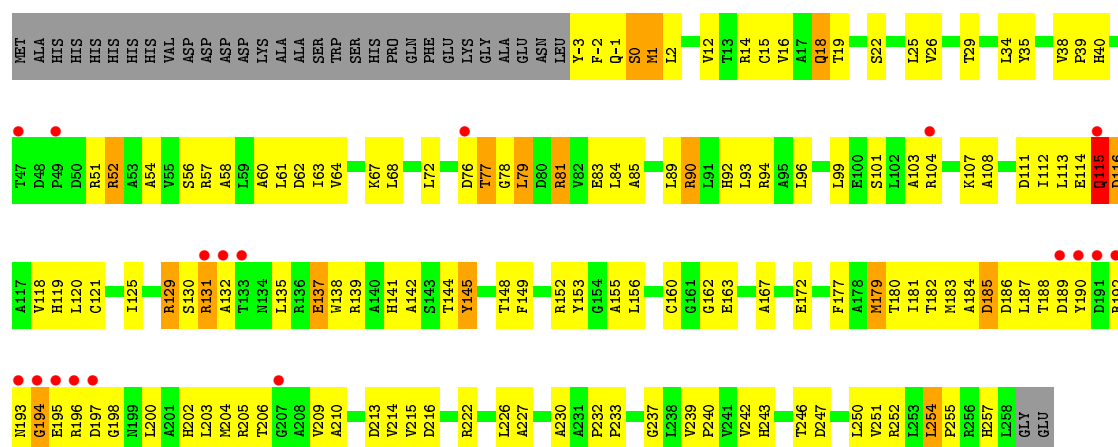
• Molecule 1: MoeN5



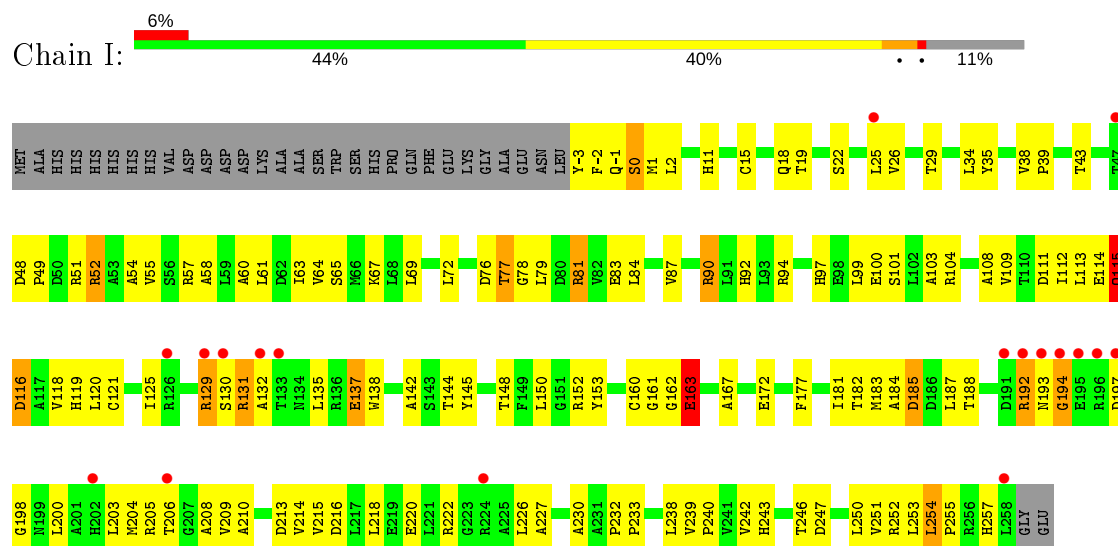
• Molecule 1: MoeN5



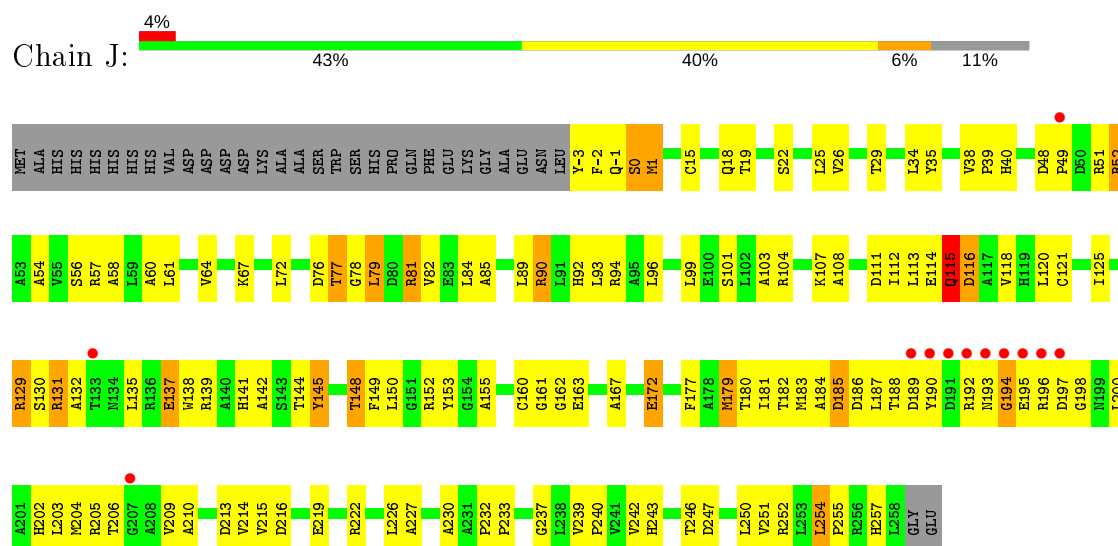
• Molecule 1: MoeN5



- Molecule 1: MoeN5



- Molecule 1: MoeN5



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 24.96 – 3.45	Depositor EDS
% Data completeness (in resolution range)	92.3 (25.00-3.45) 92.4 (24.96-3.45)	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)	0.31 , 45.1	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	0.83	1/2037 (0.0%)	0.92	0/2769
1	B	0.83	2/2037 (0.1%)	0.93	2/2769 (0.1%)
1	C	0.86	3/2037 (0.1%)	0.94	1/2769 (0.0%)
1	D	0.87	4/2037 (0.2%)	0.93	1/2769 (0.0%)
1	E	0.85	1/2037 (0.0%)	0.94	1/2769 (0.0%)
1	F	0.86	4/2037 (0.2%)	0.93	0/2769
1	G	0.70	3/2037 (0.1%)	0.86	0/2769
1	H	0.73	0/2037	0.88	1/2769 (0.0%)
1	I	0.69	1/2037 (0.0%)	0.85	0/2769
1	J	0.73	1/2037 (0.0%)	0.87	0/2769
All	All	0.80	20/20370 (0.1%)	0.91	6/27690 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	H	0	1
1	J	0	1
All	All	0	3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	219	GLU	CG-CD	8.31	1.64	1.51
1	F	219	GLU	CG-CD	8.12	1.64	1.51
1	C	15	CYS	CB-SG	-7.05	1.70	1.82
1	A	172	GLU	CG-CD	6.73	1.62	1.51
1	D	160	CYS	CB-SG	-6.69	1.70	1.82
1	D	15	CYS	CB-SG	-6.35	1.71	1.82
1	F	15	CYS	CB-SG	-5.84	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	160	CYS	CB-SG	-5.58	1.72	1.81
1	F	172	GLU	CG-CD	5.50	1.60	1.51
1	E	15	CYS	CB-SG	-5.49	1.72	1.81
1	C	160	CYS	CB-SG	-5.42	1.73	1.81
1	B	172	GLU	CG-CD	5.39	1.60	1.51
1	D	172	GLU	CG-CD	5.38	1.60	1.51
1	C	172	GLU	CG-CD	5.23	1.59	1.51
1	I	163	GLU	CB-CG	5.21	1.62	1.52
1	J	172	GLU	CG-CD	5.15	1.59	1.51
1	G	15	CYS	CB-SG	-5.10	1.73	1.81
1	B	163	GLU	CB-CG	5.08	1.61	1.52
1	G	163	GLU	CB-CG	5.06	1.61	1.52
1	F	163	GLU	CB-CG	5.03	1.61	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	D	62	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	247	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	224	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	E	89	LEU	CB-CG-CD2	-5.14	102.27	111.00
1	H	62	ASP	CB-CG-OD2	5.09	122.88	118.30

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	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2003	0	1989	132	0
1	C	2003	0	1989	118	0
1	D	2003	0	1989	135	0
1	E	2003	0	1989	132	0
1	F	2003	0	1989	135	0
1	G	2003	0	1989	134	0
1	H	2003	0	1989	129	0
1	I	2003	0	1989	130	0
1	J	2003	0	1989	130	0
All	All	20030	0	19890	1239	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 31.

All (1239) 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:HB3	1:I:81:ARG:HH11	1.06	1.18
1:A:81:ARG:CB	1:A:81:ARG:HH11	1.58	1.16
1:E:81:ARG:CB	1:E:81:ARG:HH11	1.58	1.14
1:H:81:ARG:HB3	1:H:81:ARG:HH11	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:HH11	1:D:81:ARG:HB3	1.02	1.12
1:E:81:ARG:HB3	1:E:81:ARG:HH11	1.05	1.11
1:B:81:ARG:HB3	1:B:81:ARG:HH11	1.14	1.10
1:C:81:ARG:CB	1:C:81:ARG:HH11	1.64	1.08
1:H:81:ARG:CB	1:H:81:ARG:HH11	1.64	1.08
1:F:81:ARG:HH11	1:F:81:ARG:HB3	1.00	1.07
1:J:81:ARG:HB3	1:J:81:ARG:HH11	1.10	1.07
1:I:81:ARG:CB	1:I:81:ARG:HH11	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:CB	1:J:81:ARG:HH11	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:D:219:GLU:CD	1:F:219:GLU:CD	2.20	1.00
1:A:81:ARG:HB3	1:A:81:ARG:HH11	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:NH1	1:F:81:ARG:HB3	1.84	0.92
1:D:81:ARG:NH1	1:D:81:ARG:HB3	1.84	0.91
1:J:51:ARG:NH2	1:J:162:GLY:HA2	1.84	0.90
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:NH1	1:C:81:ARG:HB3	1.87	0.89
1:H:51:ARG:NH2	1:H:162:GLY:HA2	1.88	0.88
1:H:81:ARG:NH1	1:H:81:ARG:HB3	1.89	0.88
1:D:219:GLU:OE2	1:F:219:GLU:HG2	1.72	0.88
1:D:219:GLU:OE1	1:F:219:GLU:OE1	1.93	0.87
1:I:-3:TYR:C	1:I:-1:GLN:H	1.78	0.87
1:G:-3:TYR:C	1:G:-1:GLN:H	1.78	0.87
1:F:104:ARG:HD3	1:F:163:GLU:HG3	1.54	0.86
1:A:-3:TYR:C	1:A:-1:GLN:H	1.76	0.86
1:B:-3:TYR:C	1:B:-1:GLN:H	1.80	0.86
1:G:51:ARG:HH21	1:G:162:GLY:CA	1.89	0.86
1:I:81:ARG:NH1	1:I:81:ARG:HB3	1.89	0.86
1:B:81:ARG:NH1	1:B:81:ARG:HB3	1.91	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:NH1	1:J:81:ARG:HB3	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:A:129:ARG:HH21	1:B:80:ASP:CG	1.81	0.84
1:J:-3:TYR:C	1:J:-1:GLN:H	1.80	0.83
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:H:-3:TYR:C	1:H:-1:GLN:H	1.80	0.82
1:C:114:GLU:O	1:C:116:ASP:N	2.12	0.81
1:C:-3:TYR:C	1:C:-1:GLN:H	1.83	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
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:HG22	1:F:19:THR:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:-3:TYR:C	1:E:-1:GLN:H	1.82	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:O	1:C:115:GLN:HG2	1.81	0.80
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:F:-3:TYR:C	1:F:-1:GLN:H	1.85	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:114:GLU:O	1:A:116:ASP:N	2.16	0.79
1:A:51:ARG:NH2	1:A:162:GLY:HA2	1.98	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:HG2	1:E:115:GLN:O	1.85	0.77
1:A:80:ASP:CG	1:B:129:ARG:HH21	1.88	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:HH11	1:B:252:ARG:HG2	1.50	0.77
1:G:81:ARG:HB3	1:G:81:ARG:NH1	1.98	0.77
1:I:119:HIS:NE2	1:I:144:THR:HG22	1.99	0.77
1:I:52:ARG:HG3	1:I:52:ARG:HH11	1.48	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:114:GLU:O	1:F:116:ASP:N	2.17	0.75
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: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:114:GLU:O	1:B:116:ASP:N	2.19	0.75
1:B:77:THR:OG1	1:B:79:LEU:HB2	1.87	0.75
1:D:-3:TYR:C	1:D:-1:GLN:H	1.88	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:CA	1:A:81:ARG:HH11	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: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
1:A:114:GLU:OE2	1:B:94:ARG:HD2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:25:LEU:O	1:H:29:THR:HG23	1.91	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: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: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: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
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:NH1	1:A:81:ARG:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CA	1:B:81:ARG:HH11	2.08	0.67
1:F:132:ALA:HB1	1:F:137:GLU:HB3	1.77	0.67
1:F:58:ALA:HB1	1:F:99:LEU:HD23	1.75	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: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:NH1	1:C:81:ARG:CB	2.49	0.66
1:H:52:ARG:HG3	1:H:52:ARG:HH11	1.59	0.66
1:G:115:GLN:HG2	1:G:115:GLN:O	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:E:119:HIS:NE2	1:E:144:THR:HG22	2.11	0.66
1:I:-3:TYR:C	1:I:-1:GLN:N	2.49	0.66
1:J:202:HIS:O	1:J:206:THR:HG22	1.96	0.66
1:A:81:ARG:CG	1:A:81:ARG:HH11	2.08	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
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:NH1	1:I:81:ARG:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:O	1:B:19:THR:HG22	1.99	0.63
1:J:52:ARG:HH11	1:J:52:ARG:HG3	1.62	0.63
1:A:202:HIS:O	1:A:206:THR:HG22	1.98	0.63
1:A:94:ARG:HD2	1:B:114:GLU:OE2	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:HG2	1:D:115:GLN:O	1.97	0.63
1:C:239:VAL:HB	1:C:240:PRO:HD3	1.79	0.63
1:F:108:ALA:O	1:F:112:ILE:HG13	1.97	0.63
1:B:115:GLN:HG2	1:B:115:GLN:O	1.98	0.63
1:H:81:ARG:HH11	1:H:81:ARG:CA	2.10	0.63
1:D:90:ARG:O	1:D:90:ARG:HD3	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:D:90:ARG:HD3	1:D:90:ARG:C	2.18	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:HG22	1:C:19:THR:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:-3:TYR:C	1:H:-1:GLN:N	2.53	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:CG2	1:F:19:THR:O	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:NH1	1:F:81:ARG:CB	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:D:219:GLU:OE1	1:F:219:GLU:CD	2.37	0.61
1:F:252:ARG:HH11	1:F:252:ARG:HG2	1.66	0.61
1:A:19:THR:HG22	1:A:19:THR:O	1.99	0.61
1:D:19:THR:CG2	1:D:19:THR:O	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: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
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: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:HG2	1:A:115:GLN:O	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:G:11:HIS:CD2	1:G:57:ARG:HD3	2.37	0.60
1:J:120:LEU:O	1:J:120:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:177:PHE:O	1:D:181:ILE:HG12	2.01	0.60
1:D:52:ARG:HH11	1:D:52:ARG:HG3	1.67	0.60
1:C:132:ALA:HB1	1:C:137:GLU:HB3	1.83	0.59
1:E:-3:TYR:C	1:E:-1:GLN:N	2.55	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: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:NH1	1:J:81:ARG:CB	2.53	0.59
1:A:142:ALA:HA	1:A:145:TYR:CE2	2.37	0.59
1:I:19:THR:O	1:I:19:THR:HG22	2.02	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:HD3	1:F:67:LYS:O	2.02	0.59
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:CG2	1:E:19:THR:O	2.50	0.59
1:D:219:GLU:CD	1:F:219:GLU:OE1	2.38	0.59
1:A:252:ARG:NH1	1:A:252:ARG:HG2	2.17	0.59
1:D:252:ARG:HH11	1:D:252:ARG:HG2	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:115:GLN:HG2	1:F:115:GLN:O	2.02	0.58
1:F:177:PHE:O	1:F:181:ILE:HG12	2.03	0.58
1:F:51:ARG:HH21	1:F:162:GLY:HA2	1.61	0.58
1:D:81:ARG:NH1	1:D:81:ARG:CB	2.51	0.58
1:G:25:LEU:O	1:G:29:THR:HG23	2.03	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:F:135:LEU:N	1:F:209:VAL:HG22	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:181:ILE:O	1:C:184:ALA:HB3	2.04	0.58
1:C:22:SER:O	1:C:26:VAL:HG23	2.04	0.58
1:C:90:ARG:HD3	1:C:90:ARG:C	2.23	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: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:200:LEU:O	1:A:204:MET:HG3	2.04	0.57
1:A:22:SER:O	1:A:26:VAL:HG23	2.04	0.57
1:H:131:ARG:HD2	1:H:197:ASP:HB3	1.86	0.57
1:D:247:ASP:OD2	1:F:216:ASP:OD1	2.23	0.57
1:G:252:ARG:HH11	1:G:252:ARG:HG2	1.69	0.57
1:G:-3:TYR:C	1:G:-1:GLN:N	2.50	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: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:G:81:ARG:NH1	1:G:81:ARG:CB	2.55	0.56
1:A:210:ALA:HB3	1:A:213:ASP:OD2	2.06	0.56
1:B:-3:TYR:C	1:B:-1:GLN:N	2.52	0.56
1:H:203:LEU:HA	1:H:206:THR:CG2	2.36	0.56
1:E:81:ARG:CA	1:E:81:ARG:HH11	2.16	0.56
1:E:81:ARG:CG	1:E:81:ARG:HH11	2.18	0.56
1:E:90:ARG:C	1:E:90:ARG:HD3	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ALA:HA	1:B:145:TYR:CE2	2.41	0.56
1:D:219:GLU:CG	1:F:219:GLU:CD	2.74	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:C:131:ARG:HG3	1:C:198:GLY:HA3	1.88	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:G:19:THR:O	1:G:19:THR:HG22	2.06	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: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:B:90:ARG:HD3	1:B:90:ARG:C	2.27	0.55
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:239:VAL:HB	1:D:240:PRO:HD3	1.88	0.55
1:D:76:ASP:O	1:D:78:GLY:N	2.39	0.55
1:I:35:TYR:O	1:I:39:PRO:HD3	2.06	0.55
1:B:210:ALA:HB3	1:B:213:ASP:OD2	2.06	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:219:GLU:CD	1:F:219:GLU:CG	2.75	0.55
1:D:131:ARG:HD2	1:D:197:ASP:HB3	1.89	0.55
1:F:-3:TYR:C	1:F:-1:GLN:N	2.57	0.55
1:J:81:ARG:CA	1:J:81:ARG:HH11	2.19	0.55
1:A:19:THR:CG2	1:A:19:THR:O	2.54	0.55
1:E:42:LEU:HD21	1:E:150:LEU:HD21	1.89	0.55
1:G:215:VAL:HG22	1:G:254:LEU:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:ALA:O	1:G:61:LEU:HB2	2.07	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:F:90:ARG:HD3	1:F:90:ARG:C	2.27	0.55
1:G:131:ARG:HG3	1:G:198:GLY:HA3	1.89	0.55
1:C:19:THR:CG2	1:C:19:THR:O	2.54	0.54
1:F:58:ALA:CB	1:F:99:LEU:HD23	2.36	0.54
1:B:252:ARG:NH1	1:B:252:ARG:HG2	2.19	0.54
1:E:131:ARG:HG3	1:E:198:GLY:HA3	1.89	0.54
1:D:243:HIS:HB3	1:F:216:ASP:OD2	2.06	0.54
1:H:120:LEU:HD12	1:H:120:LEU:O	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: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:HD12	1:D:34:LEU:O	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:107:LYS:NZ	1:D:97:HIS:ND1	2.56	0.54
1:C:42:LEU:HD21	1:C:150:LEU:HD21	1.88	0.54
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: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:O	1:H:90:ARG:HD3	2.08	0.54
1:H:92:HIS:NE2	1:H:96:LEU:HD11	2.22	0.54
1:C:97:HIS:ND1	1:D:107:LYS:NZ	2.56	0.54
1:F:148:THR:O	1:F:152:ARG:HD3	2.08	0.54
1:H:90:ARG:HD3	1:H:90:ARG:C	2.28	0.54
1:F:189:ASP:HB3	1:F:195:GLU:OE2	2.06	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:J:182:THR:O	1:J:185:ASP:HB2	2.08	0.53
1:I:81:ARG:NH2	1:J:81:ARG:HH21	2.04	0.53
1:A:90:ARG:HD3	1:A:90:ARG:C	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:B:220:GLU:O	1:B:220:GLU:HG2	2.10	0.53
1:A:129:ARG:HH22	1:B:82:VAL:HB	1.73	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:G:131:ARG:HD2	1:G:197:ASP:HB3	1.91	0.52
1:H:182:THR:O	1:H:185:ASP:HB2	2.09	0.52
1:H:131:ARG:HG3	1:H:198:GLY:HA3	1.91	0.52
1:D:120:LEU:O	1:D:120:LEU:HD12	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: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:A:232:PRO:HA	1:A:233:PRO:C	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:LEU:HD23	1:E:135:LEU:C	2.30	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: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
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:HG2	1:A:220:GLU:O	2.10	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:171:ARG:O	1:A:175:GLU:HG3	2.09	0.51
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.75	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:A:135:LEU:HD23	1:A:135:LEU:C	2.31	0.51
1:B:135:LEU:O	1:B:135:LEU:HD23	2.11	0.51
1:C:135:LEU:HD23	1:C:135:LEU:C	2.30	0.51
1:D:67:LYS:HD3	1:D:67:LYS:O	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: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:90:ARG:CD	1:D:90:ARG:C	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:SER:O	1:H:26:VAL:HG23	2.10	0.51
1:I:19:THR:CG2	1:I:19:THR:O	2.58	0.51
1:J:138:TRP:CH2	1:J:183:MET:HG2	2.46	0.51
1:B:135:LEU:C	1:B:135:LEU:HD23	2.30	0.51
1:B:58:ALA:CB	1:B:99:LEU:HD23	2.40	0.51
1:F:76:ASP:O	1:F:78:GLY:N	2.43	0.51
1:G:104:ARG:CZ	1:G:163:GLU:HA	2.41	0.51
1:G:48:ASP:OD1	1:G:49:PRO:HD2	2.11	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: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:G:19:THR:CG2	1:G:19:THR:O	2.59	0.51
1:I:142:ALA:HA	1:I:145:TYR:CD2	2.46	0.51
1:I:83:GLU:O	1:I:87:VAL:HG23	2.11	0.51
1:J:183:MET:O	1:J:187:LEU:HG	2.10	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:204:MET:SD	1:J:214:VAL:HG21	2.51	0.51
1:J:-3:TYR:C	1:J:-1:GLN:N	2.52	0.51
1:J:89:LEU:HD12	1:J:93:LEU:HG	1.93	0.51
1:A:54:ALA:HA	1:A:57:ARG:CZ	2.41	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: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: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: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:I:138:TRP:CH2	1:I:183:MET:HG2	2.46	0.50
1:B:67:LYS:HD3	1:B:67:LYS:O	2.12	0.50
1:I:203:LEU:HA	1:I:206:THR:HG22	1.93	0.50
1:I:232:PRO:HA	1:I:233:PRO:C	2.32	0.50
1:I:51:ARG:HH21	1:I:162:GLY:N	2.09	0.50
1:F:131:ARG:HG3	1:F:198:GLY:HA3	1.93	0.50
1:H:76:ASP:O	1:H:78:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:TRP:CH2	1:G:183:MET:HG2	2.47	0.50
1:G:39:PRO:HG3	1:G:63:ILE:HD12	1.94	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:B:203:LEU:HA	1:B:206:THR:HG22	1.93	0.50
1:D:189:ASP:HB3	1:D:195:GLU:OE2	2.12	0.50
1:D:138:TRP:NE1	1:D:200:LEU:HB2	2.27	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: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:N	1:J:209:VAL:HG22	2.22	0.49
1:A:113:LEU:HD23	1:A:152:ARG:NH2	2.28	0.49
1:A:103:ALA:HA	1:A:160:CYS:HA	1.95	0.49
1:A:82:VAL:HB	1:B:129:ARG:HH22	1.77	0.49
1:C:67:LYS:HD3	1:C:67:LYS:O	2.12	0.49
1:E:104:ARG:HD3	1:E:163:GLU:CG	2.34	0.49
1:G:232:PRO:HA	1:G:233:PRO:C	2.32	0.49
1:H:200:LEU:O	1:H:204:MET:HG3	2.13	0.49
1:A:130:SER:O	1:A:131:ARG:C	2.50	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:B:232:PRO:HA	1:B:233:PRO:C	2.32	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
1:G:81:ARG:HH11	1:G:81:ARG:CA	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:196:ARG:HG2	1:H:202:HIS:CG	2.47	0.49
1:H:54:ALA:HA	1:H:57:ARG:CZ	2.43	0.49
1:C:81:ARG:CG	1:C:81:ARG:HH11	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:J:177:PHE:O	1:J:181:ILE:HG12	2.13	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:B:12:VAL:O	1:B:16:VAL:HG23	2.12	0.49
1:A:129:ARG:NH2	1:B:80:ASP:CG	2.58	0.49
1:F:177:PHE:CE2	1:F:181:ILE:HD11	2.48	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:G:251:VAL:O	1:G:255:PRO:HG2	2.12	0.49
1:I:135:LEU:HD23	1:I:135:LEU:C	2.34	0.49
1:C:52:ARG:HH11	1:C:52:ARG:HG3	1.78	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:C:129:ARG:HD3	1:C:129:ARG:HA	1.64	0.48
1:F:135:LEU:HB2	1:F:209:VAL:HG13	1.95	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:131:ARG:HG3	1:B:198:GLY:HA3	1.95	0.48
1:B:89:LEU:O	1:B:89:LEU:HD12	2.13	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
1:H:188:THR:HG22	1:H:192:ARG:HH11	1.78	0.48
1:I:135:LEU:O	1:I:135:LEU:HD23	2.13	0.48
1:B:237:GLY:O	1:B:240:PRO:HD2	2.13	0.48
1:E:193:ASN:O	1:E:194:GLY:C	2.52	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:H:-1:GLN:OE1	1:H:0:SER:N	2.47	0.48
1:J:232:PRO:HA	1:J:233:PRO:C	2.33	0.48
1:A:183:MET:O	1:A:187:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:PRO:HA	1:F:233:PRO:C	2.34	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:O	1:I:120:LEU:HD12	2.13	0.48
1:J:92:HIS:NE2	1:J:96:LEU:HD11	2.28	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:G:90:ARG:HD3	1:G:90:ARG:C	2.34	0.48
1:J:204:MET:CE	1:J:257:HIS:HB2	2.44	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:254:LEU:N	1:C:255:PRO:CD	2.77	0.48
1:C:39:PRO:HG3	1:C:63:ILE:HD12	1.96	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:J:200:LEU:O	1:J:204:MET:HG3	2.14	0.48
1:A:252:ARG:CG	1:A:252:ARG:NH1	2.77	0.47
1:B:76:ASP:O	1:B:78:GLY:N	2.47	0.47
1:C:104:ARG:CG	1:C:163:GLU:OE2	2.58	0.47
1:C:81:ARG:CA	1:C:81:ARG:HH11	2.23	0.47
1:E:204:MET:SD	1:E:214:VAL:HG21	2.54	0.47
1:I:252:ARG:HH11	1:I:252:ARG:HG2	1.79	0.47
1:I:97:HIS:ND1	1:J:107:LYS:NZ	2.60	0.47
1:A:34:LEU:O	1:A:38:VAL:HG23	2.14	0.47
1:A:81:ARG:CA	1:A:81:ARG:NH1	2.75	0.47
1:E:120:LEU:C	1:E:120:LEU:HD12	2.34	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
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:205:ARG:CG	1:B:205:ARG:HH11	2.27	0.47
1:B:179:MET:HG2	1:B:221:LEU:HD11	1.96	0.47
1:C:34:LEU:HD21	1:C:181:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:193:ASN:O	1:F:194:GLY:C	2.52	0.47
1:G:125:ILE:HD12	1:H:19:THR:O	2.14	0.47
1:G:137:GLU:O	1:G:138:TRP:C	2.53	0.47
1:G:34:LEU:O	1:G:34:LEU:HD12	2.13	0.47
1:H:103:ALA:HA	1:H:160:CYS:HA	1.96	0.47
1:H:187:LEU:HD21	1:H:200:LEU:HD23	1.96	0.47
1:H:135:LEU:N	1:H:209:VAL:HG22	2.22	0.47
1:C:-3:TYR:C	1:C:-1:GLN:N	2.56	0.47
1:E:135:LEU:O	1:E:135:LEU:HD23	2.15	0.47
1:H:177:PHE:O	1:H:181:ILE:HG12	2.13	0.47
1:H:89:LEU:HD12	1:H:93:LEU:HG	1.97	0.47
1:J:34:LEU:HD21	1:J:181:ILE:HD12	1.96	0.47
1:A:192:ARG:HB3	1:A:192:ARG:CZ	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:130:SER:O	1:H:131:ARG:C	2.53	0.47
1:H:226:LEU:HG	1:H:242:VAL:HG11	1.96	0.47
1:I:119:HIS:O	1:I:119:HIS:HD2	1.97	0.47
1:I:103:ALA:HA	1:I:160:CYS:HA	1.96	0.47
1:I:192:ARG:CZ	1:I:192:ARG:HB3	2.45	0.47
1:J:190:TYR:CE2	1:J:196:ARG:HG3	2.50	0.47
1:J:-1:GLN:OE1	1:J:0:SER:N	2.47	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:F:131:ARG:HG2	1:F:131:ARG:O	2.14	0.47
1:F:135:LEU:HD23	1:F:135:LEU:O	2.14	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:A:190:TYR:CE2	1:A:196:ARG:HG3	2.50	0.47
1:C:135:LEU:O	1:C:135:LEU:HD23	2.15	0.47
1:G:51:ARG:HH21	1:G:162:GLY:N	2.12	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:130:SER:O	1:B:131:ARG:C	2.53	0.47
1:B:103:ALA:HA	1:B:160:CYS:HA	1.97	0.47
1:C:115:GLN:O	1:C:115:GLN:CG	2.60	0.47
1:C:193:ASN:O	1:C:194:GLY:C	2.53	0.47
1:C:81:ARG:NH2	1:D:81:ARG:NH2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ARG:O	1:D:175:GLU:HG3	2.15	0.47
1:D:219:GLU:HG2	1:F:219:GLU:CD	2.35	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:H:232:PRO:HA	1:H:233:PRO:C	2.34	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:G:148:THR:O	1:G:152:ARG:HD3	2.14	0.47
1:G:72:LEU:HD13	1:G:84:LEU:HB3	1.96	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:B:193:ASN:O	1:B:194:GLY:C	2.52	0.47
1:H:129:ARG:HD3	1:H:129:ARG:HA	1.62	0.47
1:H:34:LEU:HD21	1:H:181:ILE:HD12	1.97	0.47
1:A:67:LYS:HD3	1:A:67:LYS:O	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:J:130:SER:O	1:J:131:ARG:C	2.53	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:C:90:ARG:CD	1:C:90:ARG:C	2.84	0.46
1:D:129:ARG:HA	1:D:129:ARG:HD3	1.66	0.46
1:E:107:LYS:NZ	1:F:97:HIS:ND1	2.63	0.46
1:F:132:ALA:CB	1:F:137:GLU:HB3	2.44	0.46
1:F:35:TYR:O	1:F:39:PRO:HD3	2.15	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:D:222:ARG:NE	1:F:219:GLU:CD	2.69	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:H:135:LEU:HD23	1:H:135:LEU:C	2.36	0.46
1:I:90:ARG:C	1:I:90:ARG:HD3	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:O	1:A:184:ALA:HB3	2.15	0.46
1:D:81:ARG:HH11	1:D:81:ARG:CA	2.25	0.46
1:H:193:ASN:O	1:H:194:GLY:C	2.54	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:E:67:LYS:HD3	1:E:67:LYS:O	2.14	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:103:ALA:HA	1:J:160:CYS:HA	1.98	0.46
1:J:193:ASN:O	1:J:194:GLY:C	2.54	0.46
1:J:35:TYR:O	1:J:39:PRO:HD3	2.16	0.46
1:E:119:HIS:HD2	1:E:119:HIS:O	1.99	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: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:H:90:ARG:CD	1:H:90:ARG:C	2.85	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:90:ARG:O	1:I:90:ARG:HD3	2.16	0.46
1:C:135:LEU:N	1:C:209:VAL:HG22	2.25	0.46
1:D:193:ASN:O	1:D:194:GLY:C	2.53	0.46
1:D:52:ARG:HG3	1:D:52:ARG:NH1	2.31	0.46
1:F:90:ARG:C	1:F:90:ARG:CD	2.84	0.46
1:G:252:ARG:HH12	1:G:253:LEU:CD2	2.29	0.46
1:G:54:ALA:HA	1:G:57:ARG:NH1	2.31	0.46
1:H:67:LYS:HD3	1:H:67:LYS:O	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:F:135:LEU:HD23	1:F:135:LEU:C	2.36	0.46
1:J:135:LEU:O	1:J:135:LEU:HD23	2.16	0.46
1:D:100:GLU:HA	1:D:109:VAL:HG21	1.98	0.45
1:E:222:ARG:HG2	1:E:226:LEU:HD12	1.98	0.45
1:E:49:PRO:HG2	1:E:50:ASP:N	2.31	0.45
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:218:LEU:HD23	1:A:218:LEU:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:PRO:HA	1:D:233:PRO:C	2.35	0.45
1:D:40:HIS:CE1	1:D:52:ARG:NH2	2.84	0.45
1:F:181:ILE:O	1:F:184:ALA:HB3	2.16	0.45
1:D:219:GLU:CD	1:F:219:GLU:HG2	2.36	0.45
1:F:60:ALA:O	1:F:64:VAL:HG23	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:HA	1:B:72:LEU:HD12	1.76	0.45
1:C:42:LEU:HD21	1:C:150:LEU:CD2	2.46	0.45
1:E:107:LYS:HD2	1:E:111:ASP:OD1	2.17	0.45
1:E:11:HIS:CG	1:E:57:ARG:HD3	2.52	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: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:132:ALA:HB2	1:H:141:HIS:CD2	2.50	0.45
1:J:137:GLU:O	1:J:138:TRP:C	2.55	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: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:A:193:ASN:O	1:A:194:GLY:C	2.54	0.45
1:E:129:ARG:HD3	1:E:129:ARG:HA	1.65	0.45
1:E:251:VAL:O	1:E:255:PRO:HG2	2.16	0.45
1:F:138:TRP:CH2	1:F:183:MET:HG2	2.52	0.45
1:F:44:GLU:HG2	1:F:238:LEU:HG	1.98	0.45
1:G:190:TYR:HE2	1:G:202:HIS:HB2	1.81	0.45
1:H:142:ALA:HA	1:H:145:TYR:CD2	2.52	0.45
1:H:-1:GLN:O	1:H:2:LEU:N	2.27	0.45
1:J:148:THR:O	1:J:152:ARG:HD3	2.17	0.45
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.72	0.45
1:F:104:ARG:CG	1:F:163:GLU:OE2	2.62	0.45
1:D:216:ASP:OD1	1:F:247:ASP:OD2	2.35	0.45
1:I:25:LEU:CD2	1:I:87:VAL:HG21	2.46	0.45
1:J:135:LEU:C	1:J:135:LEU:HD23	2.37	0.45
1:A:222:ARG:HB2	1:A:246:THR:HG21	1.98	0.45
1:C:237:GLY:O	1:C:240:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:104:ARG:CZ	1:E:163:GLU:HA	2.47	0.45
1:E:81:ARG:NH2	1:F:81:ARG:HH21	2.04	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:E:22:SER:O	1:E:26:VAL:HG23	2.17	0.45
1:F:67:LYS:CD	1:F:67:LYS:O	2.65	0.45
1:H:215:VAL:HG22	1:H:254:LEU:CD1	2.46	0.45
1:A:119:HIS:O	1:A:119:HIS:HD2	2.00	0.44
1:A:131:ARG:HG3	1:A:198:GLY:HA3	2.00	0.44
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.72	0.44
1:B:81:ARG:CA	1:B:81:ARG:NH1	2.78	0.44
1:C:130:SER:O	1:C:131:ARG:C	2.55	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:192:ARG:HB3	1:B:192:ARG:CZ	2.47	0.44
1:B:243:HIS:O	1:B:247:ASP:HB2	2.18	0.44
1:B:81:ARG:NH1	1:B:81:ARG:HA	2.32	0.44
1:B:251:VAL:O	1:B:255:PRO:HG2	2.18	0.44
1:B:252:ARG:CG	1:B:252:ARG:NH1	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:O	1:H:135:LEU:HD23	2.16	0.44
1:H:138:TRP:CE3	1:H:138:TRP:C	2.91	0.44
1:H:138:TRP:NE1	1:H:200:LEU:HB2	2.31	0.44
1:I:137:GLU:O	1:I:138:TRP:C	2.55	0.44
1:J:129:ARG:HA	1:J:129:ARG:HD3	1.62	0.44
1:J:90:ARG:C	1:J:90:ARG:HD3	2.37	0.44
1:A:80:ASP:CG	1:B:129:ARG:NH2	2.66	0.44
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:C:232:PRO:HA	1:C:233:PRO:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:232:PRO:HA	1:E:233:PRO:C	2.36	0.44
1:F:237:GLY:O	1:F:240:PRO:HD2	2.17	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:G:81:ARG:HH21	1:H:81:ARG:NH2	2.15	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: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:I:220:GLU:O	1:I:220:GLU:HG2	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:187:LEU:HD21	1:J:200:LEU:HD23	1.99	0.44
1:J:76:ASP:OD1	1:J:77:THR:N	2.49	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:I:130:SER:O	1:I:131:ARG:C	2.56	0.44
1:C:187:LEU:HD21	1:C:200:LEU:HD23	1.99	0.44
1:G:130:SER:O	1:G:131:ARG:C	2.55	0.44
1:G:179:MET:HG2	1:G:221:LEU:HD11	2.00	0.44
1:I:34:LEU:HD12	1:I:34:LEU:O	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:HG2	1:E:220:GLU:O	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:204:MET:CE	1:A:257:HIS:HB2	2.47	0.43
1:A:205:ARG:CG	1:A:205:ARG:HH11	2.31	0.43
1:A:243:HIS:O	1:A:247:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HA	1:B:129:ARG:HD3	1.76	0.43
1:B:14:ARG:HB2	1:B:14:ARG:HE	1.56	0.43
1:B:25:LEU:CD2	1:B:87:VAL:HG21	2.48	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:O	1:H:89:LEU:HD12	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: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:D:12:VAL:O	1:D:16:VAL:HG23	2.18	0.43
1:F:129:ARG:HD3	1:F:129:ARG:HA	1.62	0.43
1:F:-1:GLN:O	1:F:2:LEU:N	2.25	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: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:237:GLY:O	1:H:240:PRO:HD2	2.19	0.43
1:H:35:TYR:O	1:H:39:PRO:HD3	2.17	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:I:67:LYS:HD3	1:I:67:LYS:O	2.19	0.43
1:A:121:CYS:O	1:A:125:ILE:HG13	2.18	0.43
1:A:-3:TYR:C	1:A:-1:GLN:N	2.49	0.43
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.88	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:E:130:SER:O	1:E:131:ARG:C	2.57	0.43
1:G:193:ASN:O	1:G:194:GLY:C	2.57	0.43
1:H:104:ARG:CZ	1:H:163:GLU:HA	2.48	0.43
1:C:243:HIS:O	1:C:247:ASP:HB2	2.19	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:E:52:ARG:HG3	1:E:52:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:J:-1:GLN:O	1:J:1:MET:N	2.51	0.43
1:J:90:ARG:O	1:J:90:ARG:HD3	2.19	0.43
1:C:203:LEU:CA	1:C:206:THR:HG22	2.49	0.43
1:E:90:ARG:C	1:E:90:ARG:CD	2.87	0.43
1:H:137:GLU:O	1:H:138:TRP:C	2.56	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: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:I:204:MET:CE	1:I:257:HIS:HB2	2.49	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:J:138:TRP:C	1:J:138:TRP:CE3	2.93	0.42
1:A:137:GLU:O	1:A:138:TRP:C	2.58	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:CG	1:E:115:GLN:O	2.61	0.42
1:G:135:LEU:N	1:G:209:VAL:HG22	2.30	0.42
1:G:67:LYS:HD3	1:G:67:LYS:O	2.19	0.42
1:I:51:ARG:HD3	1:I:161:GLY:C	2.39	0.42
1:J:72:LEU:HD13	1:J:84:LEU:HB3	2.00	0.42
1:A:251:VAL:O	1:A:255:PRO:HG2	2.20	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:C:250:LEU:O	1:C:255:PRO:HD3	2.20	0.42
1:D:104:ARG:HG3	1:D:104:ARG:H	1.63	0.42
1:D:138:TRP:HE3	1:D:139:ARG:N	2.17	0.42
1:D:243:HIS:CB	1:F:216:ASP:OD2	2.67	0.42
1:F:183:MET:HE1	1:F:214:VAL:HG13	2.01	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:111:ASP:O	1:H:115:GLN:HB3	2.19	0.42
1:H:19:THR:OG1	1:H:90:ARG:HG3	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:J:204:MET:HE1	1:J:257:HIS:HB2	2.02	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:B:61:LEU:HD23	1:B:61:LEU:HA	1.91	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:HB2	1:H:18:GLN:HE21	1.70	0.42
1:A:72:LEU:HA	1:A:72:LEU:HD12	1.86	0.42
1:C:131:ARG:HG3	1:C:198:GLY:CA	2.49	0.42
1:D:237:GLY:O	1:D:240:PRO:HD2	2.19	0.42
1:D:89:LEU:HD12	1:D:89:LEU:O	2.19	0.42
1:E:204:MET:CE	1:E:257:HIS:HB2	2.50	0.42
1:G:80:ASP:HB3	1:G:83:GLU:OE1	2.19	0.42
1:A:104:ARG:CG	1:A:163:GLU:OE2	2.64	0.42
1:C:119:HIS:O	1:C:119:HIS:HD2	2.02	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:F:130:SER:O	1:F:131:ARG:C	2.58	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
1:C:114:GLU:C	1:C:116:ASP:H	2.20	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:97:HIS:ND1	1:H:107:LYS:NZ	2.65	0.42
1:H:119:HIS:NE2	1:H:144:THR:HG22	2.35	0.42
1:H:72:LEU:HD13	1:H:84:LEU:HB3	2.01	0.42
1:H:22:SER:N	1:H:83:GLU:OE2	2.46	0.42
1:I:72:LEU:HD13	1:I:84:LEU:HB3	2.02	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:G:238:LEU:O	1:G:242:VAL:HG23	2.20	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:HD12	1:A:89:LEU:O	2.19	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:130:SER:O	1:D:131:ARG:C	2.58	0.41
1:D:131:ARG:HG2	1:D:131:ARG:O	2.16	0.41
1:E:-2:PHE:HZ	1:E:240:PRO:HB3	1.85	0.41
1:E:81:ARG:CG	1:E:81:ARG:NH1	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: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:G:135:LEU:HD23	1:G:135:LEU:C	2.39	0.41
1:I:11:HIS:CD2	1:I:57:ARG:CD	3.03	0.41
1:B:34:LEU:HD12	1:B:34:LEU:O	2.20	0.41
1:C:131:ARG:HG3	1:C:197:ASP:O	2.20	0.41
1:D:18:GLN:HB2	1:D:18:GLN:HE21	1.65	0.41
1:E:104:ARG:H	1:E:104:ARG:HG3	1.57	0.41
1:F:-1:GLN:OE1	1:F:0:SER:N	2.54	0.41
1:C:44:GLU:HG2	1:C:235:ALA:HB1	2.02	0.41
1:D:137:GLU:O	1:D:138:TRP:C	2.58	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:I:111:ASP:O	1:I:115:GLN:HB3	2.20	0.41
1:I:72:LEU:HD12	1:I:72:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:ARG:HG3	1:J:198:GLY:CA	2.51	0.41
1:I:72:LEU:HD23	1:J:72:LEU:HD23	2.02	0.41
1:A:51:ARG:HD3	1:A:161:GLY:C	2.40	0.41
1:B:81:ARG:NH1	1:B:81:ARG:CG	2.83	0.41
1:D:219:GLU:CD	1:F:222:ARG:NE	2.74	0.41
1:E:137:GLU:O	1:E:138:TRP:C	2.58	0.41
1:F:137:GLU:O	1:F:138:TRP:C	2.59	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:H:254:LEU:N	1:H:255:PRO:CD	2.83	0.41
1:I:119:HIS:CD2	1:I:119:HIS:C	2.94	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:NH1	1:A:52:ARG:HG3	2.35	0.41
1:C:11:HIS:CD2	1:C:57:ARG:CD	3.04	0.41
1:E:106:PRO:O	1:E:109:VAL:HG23	2.20	0.41
1:E:35:TYR:O	1:E:39:PRO:HD3	2.20	0.41
1:I:100:GLU:HA	1:I:109:VAL:HG21	2.02	0.41
1:I:55:VAL:HG21	1:I:161:GLY:HA2	2.02	0.41
1:I:193:ASN:O	1:I:194:GLY:C	2.59	0.41
1:J:149:PHE:CE1	1:J:153:TYR:CE2	3.05	0.41
1:C:142:ALA:HA	1:C:145:TYR:CD2	2.56	0.41
1:C:89:LEU:HD12	1:C:89:LEU:O	2.20	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:237:GLY:O	1:G:240:PRO:HD2	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:H:138:TRP:CE3	1:H:139:ARG:HA	2.56	0.41
1:I:69:LEU:HD11	1:J:85:ALA:HB1	2.02	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:I:142:ALA:HB1	1:I:182:THR:HG21	2.02	0.41
1:J:189:ASP:HB3	1:J:195:GLU:OE2	2.20	0.41
1:J:90:ARG:NH1	1:J:94:ARG:HB2	2.35	0.41
1:A:148:THR:O	1:A:152:ARG:HD3	2.20	0.41
1:D:62:ASP:O	1:D:65:SER:HB3	2.21	0.41
1:E:58:ALA:CB	1:E:99:LEU:HD23	2.51	0.41
1:F:39:PRO:HG3	1:F:63:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:58:ALA:O	1:J:61:LEU:HB2	2.21	0.41
1:A:-1:GLN:O	1:A:2:LEU:N	2.28	0.41
1:A:210:ALA:O	1:A:211:GLY:C	2.58	0.41
1:C:239:VAL:N	1:C:240:PRO:CD	2.84	0.41
1:E:129:ARG:HH22	1:F:82:VAL:HB	1.85	0.41
1:E:-1:GLN:O	1:E:1:MET:N	2.54	0.41
1:H:131:ARG:HG3	1:H:197:ASP:O	2.21	0.41
1:H:72:LEU:HD21	1:H:85:ALA:HB2	2.02	0.41
1:I:131:ARG:HG3	1:I:198:GLY:CA	2.48	0.41
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.89	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: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:132:ALA:CB	1:I:137:GLU:HB3	2.51	0.41
1:I:43:THR:HB	1:I:52:ARG:HG2	2.03	0.41
1:I:81:ARG:CA	1:I:81:ARG:HH11	2.29	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:D:183:MET:HE1	1:D:214:VAL:HG13	2.03	0.40
1:D:-3:TYR:C	1:D:-1:GLN:N	2.60	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
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:135:LEU:C	1:D:135:LEU:HD23	2.41	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:E:52:ARG:C	1:E:52:ARG:HD3	2.42	0.40
1:F:11:HIS:CD2	1:F:57:ARG:HD3	2.57	0.40
1:G:129:ARG:HA	1:G:129:ARG:HD3	1.73	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: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:J:51:ARG:HD3	1:J:161:GLY:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:HIS:NE2	1:E:96:LEU:HD11	2.36	0.40
1:G:190:TYR:CE2	1:G:202:HIS:HB2	2.55	0.40
1:I:218:LEU:HD23	1:I:218:LEU:HA	1.87	0.40
1:I:94:ARG:HD2	1:J:114:GLU:OE2	2.21	0.40
1:J:177:PHE:CZ	1:J:181:ILE:HD11	2.57	0.40
1:J:52:ARG:O	1:J:56:SER:HB2	2.22	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: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:206:THR:OG1	1:B:206:THR:O	2.35	0.40
1:C:137:GLU:O	1:C:138:TRP:C	2.60	0.40
1:C:204:MET:CE	1:C:257:HIS:HB2	2.52	0.40
1:C:61:LEU:HD23	1:C:61:LEU:HA	1.98	0.40
1:E:100:GLU:HA	1:E:109:VAL:HG21	2.03	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:129:ARG:HH21	1:F:80:ASP:CG	2.24	0.40
1:G:119:HIS:HD2	1:G:119:HIS:O	2.03	0.40
1:G:190:TYR:HB2	1:G:201:ALA:HB3	2.02	0.40
1:G:206:THR:O	1:G:206:THR:OG1	2.39	0.40
1:G:43:THR:HB	1:G:52:ARG:HG2	2.03	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

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%)	5	31
1	B	260/294 (88%)	224 (86%)	28 (11%)	8 (3%)	4	29
1	C	260/294 (88%)	223 (86%)	30 (12%)	7 (3%)	5	31
1	D	260/294 (88%)	222 (85%)	30 (12%)	8 (3%)	4	29
1	E	260/294 (88%)	225 (86%)	28 (11%)	7 (3%)	5	31
1	F	260/294 (88%)	220 (85%)	33 (13%)	7 (3%)	5	31
1	G	260/294 (88%)	217 (84%)	35 (14%)	8 (3%)	4	29
1	H	260/294 (88%)	220 (85%)	33 (13%)	7 (3%)	5	31
1	I	260/294 (88%)	220 (85%)	31 (12%)	9 (4%)	3	26
1	J	260/294 (88%)	222 (85%)	31 (12%)	7 (3%)	5	31
All	All	2600/2940 (88%)	2216 (85%)	309 (12%)	75 (3%)	4	30

All (75) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	11	38
1	B	206/232 (89%)	185 (90%)	21 (10%)	7	30
1	C	206/232 (89%)	186 (90%)	20 (10%)	8	32
1	D	206/232 (89%)	187 (91%)	19 (9%)	9	34
1	E	206/232 (89%)	189 (92%)	17 (8%)	11	38
1	F	206/232 (89%)	185 (90%)	21 (10%)	7	30
1	G	206/232 (89%)	185 (90%)	21 (10%)	7	30
1	H	206/232 (89%)	185 (90%)	21 (10%)	7	30
1	I	206/232 (89%)	188 (91%)	18 (9%)	10	37
1	J	206/232 (89%)	183 (89%)	23 (11%)	6	25
All	All	2060/2320 (89%)	1862 (90%)	198 (10%)	8	32

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	CYS
1	A	18	GLN
1	A	24	ASP
1	A	52	ARG

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Mol	Chain	Res	Type
1	A	81	ARG
1	A	90	ARG
1	A	101	SER
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	24	ASP
1	B	52	ARG
1	B	76	ASP
1	B	79	LEU
1	B	81	ARG
1	B	90	ARG
1	B	101	SER
1	B	115	GLN
1	B	118	VAL
1	B	129	ARG
1	B	131	ARG
1	B	137	GLU
1	B	141	HIS
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	15	CYS
1	C	18	GLN
1	C	49	PRO
1	C	52	ARG
1	C	81	ARG
1	C	90	ARG
1	C	101	SER
1	C	109	VAL

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Mol	Chain	Res	Type
1	C	114	GLU
1	C	115	GLN
1	C	118	VAL
1	C	129	ARG
1	C	131	ARG
1	C	137	GLU
1	C	172	GLU
1	C	179	MET
1	C	185	ASP
1	C	205	ARG
1	C	216	ASP
1	C	254	LEU
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	90	ARG
1	D	115	GLN
1	D	118	VAL
1	D	129	ARG
1	D	131	ARG
1	D	137	GLU
1	D	147	SER
1	D	172	GLU
1	D	179	MET
1	D	185	ASP
1	D	186	ASP
1	D	205	ARG
1	D	218	LEU
1	E	15	CYS
1	E	18	GLN
1	E	49	PRO
1	E	52	ARG
1	E	81	ARG
1	E	90	ARG
1	E	101	SER
1	E	109	VAL
1	E	115	GLN
1	E	118	VAL
1	E	129	ARG

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Mol	Chain	Res	Type
1	E	131	ARG
1	E	137	GLU
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	90	ARG
1	F	101	SER
1	F	109	VAL
1	F	115	GLN
1	F	118	VAL
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	216	ASP
1	F	218	LEU
1	G	1	MET
1	G	15	CYS
1	G	18	GLN
1	G	52	ARG
1	G	76	ASP
1	G	81	ARG
1	G	90	ARG
1	G	101	SER
1	G	115	GLN
1	G	118	VAL
1	G	129	ARG
1	G	131	ARG
1	G	137	GLU
1	G	141	HIS
1	G	150	LEU

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Mol	Chain	Res	Type
1	G	172	GLU
1	G	179	MET
1	G	185	ASP
1	G	205	ARG
1	G	216	ASP
1	G	254	LEU
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	90	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	172	GLU
1	H	179	MET
1	H	180	THR
1	H	185	ASP
1	H	186	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	81	ARG
1	I	90	ARG
1	I	101	SER
1	I	115	GLN
1	I	118	VAL
1	I	129	ARG
1	I	131	ARG
1	I	137	GLU
1	I	150	LEU
1	I	172	GLU
1	I	185	ASP

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Mol	Chain	Res	Type
1	I	205	ARG
1	I	216	ASP
1	I	254	LEU
1	J	1	MET
1	J	15	CYS
1	J	18	GLN
1	J	52	ARG
1	J	79	LEU
1	J	81	ARG
1	J	90	ARG
1	J	101	SER
1	J	115	GLN
1	J	118	VAL
1	J	129	ARG
1	J	131	ARG
1	J	137	GLU
1	J	148	THR
1	J	150	LEU
1	J	172	GLU
1	J	179	MET
1	J	180	THR
1	J	185	ASP
1	J	186	ASP
1	J	205	ARG
1	J	216	ASP
1	J	254	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	40	HIS
1	B	18	GLN
1	B	40	HIS
1	C	18	GLN
1	C	40	HIS
1	D	18	GLN
1	D	40	HIS
1	D	212	GLN
1	E	18	GLN
1	F	18	GLN
1	F	40	HIS

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Mol	Chain	Res	Type
1	F	141	HIS
1	F	212	GLN
1	G	18	GLN
1	G	40	HIS
1	H	18	GLN
1	H	40	HIS
1	H	141	HIS
1	I	18	GLN
1	I	40	HIS
1	J	18	GLN
1	J	40	HIS
1	J	141	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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%)	-0.17	6 (2%) 60 58	56, 83, 118, 151	0
1	B	262/294 (89%)	-0.19	6 (2%) 60 58	54, 84, 120, 152	0
1	C	262/294 (89%)	-0.13	10 (3%) 40 39	58, 81, 116, 156	0
1	D	262/294 (89%)	0.04	14 (5%) 26 26	57, 84, 135, 164	0
1	E	262/294 (89%)	-0.09	8 (3%) 49 47	53, 81, 120, 156	0
1	F	262/294 (89%)	0.07	15 (5%) 23 23	57, 84, 132, 162	0
1	G	262/294 (89%)	0.28	18 (6%) 16 19	79, 115, 149, 164	0
1	H	262/294 (89%)	0.09	18 (6%) 16 19	76, 106, 147, 161	0
1	I	262/294 (89%)	0.29	18 (6%) 16 19	84, 114, 148, 165	0
1	J	262/294 (89%)	0.06	12 (4%) 32 31	74, 104, 148, 161	0
All	All	2620/2940 (89%)	0.03	125 (4%) 30 30	53, 95, 143, 165	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	191	ASP	6.2
1	D	257	HIS	6.1
1	D	193	ASN	6.1
1	I	195	GLU	5.7
1	F	193	ASN	5.7
1	F	257	HIS	5.2
1	J	196	ARG	5.1
1	D	192	ARG	5.0
1	D	194	GLY	5.0
1	H	133	THR	5.0
1	F	192	ARG	4.9
1	J	192	ARG	4.9
1	G	191	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	194	GLY	4.9
1	A	192	ARG	4.7
1	F	258	LEU	4.5
1	B	192	ARG	4.5
1	A	193	ASN	4.4
1	H	193	ASN	4.3
1	H	195	GLU	4.3
1	H	192	ARG	4.2
1	I	193	ASN	4.2
1	H	196	ARG	4.2
1	I	196	ARG	4.0
1	J	133	THR	4.0
1	G	192	ARG	3.9
1	B	193	ASN	3.9
1	J	193	ASN	3.9
1	A	195	GLU	3.8
1	G	193	ASN	3.8
1	F	256	ARG	3.8
1	D	258	LEU	3.7
1	G	132	ALA	3.7
1	F	194	GLY	3.7
1	G	196	ARG	3.6
1	E	191	ASP	3.5
1	E	193	ASN	3.5
1	H	190	TYR	3.5
1	G	76	ASP	3.5
1	E	192	ARG	3.4
1	H	194	GLY	3.4
1	G	129	ARG	3.3
1	H	115	GLN	3.3
1	F	129	ARG	3.2
1	I	191	ASP	3.2
1	D	129	ARG	3.2
1	F	195	GLU	3.2
1	I	129	ARG	3.2
1	H	189	ASP	3.2
1	D	256	ARG	3.2
1	D	252	ARG	3.2
1	I	192	ARG	3.1
1	I	132	ALA	3.1
1	E	196	ARG	3.1
1	B	195	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	207	GLY	3.0
1	G	195	GLU	3.0
1	D	190	TYR	2.9
1	A	191	ASP	2.9
1	B	191	ASP	2.9
1	B	194	GLY	2.9
1	G	47	THR	2.9
1	C	193	ASN	2.9
1	H	49	PRO	2.9
1	C	192	ARG	2.8
1	D	197	ASP	2.8
1	I	130	SER	2.8
1	D	195	GLU	2.8
1	H	197	ASP	2.8
1	J	197	ASP	2.8
1	E	195	GLU	2.7
1	B	129	ARG	2.7
1	H	132	ALA	2.7
1	I	194	GLY	2.7
1	E	194	GLY	2.7
1	G	197	ASP	2.7
1	J	189	ASP	2.7
1	J	195	GLU	2.6
1	E	49	PRO	2.6
1	C	190	TYR	2.6
1	H	191	ASP	2.6
1	I	47	THR	2.6
1	D	119	HIS	2.6
1	F	252	ARG	2.6
1	G	126	ARG	2.5
1	C	196	ARG	2.5
1	I	25	LEU	2.5
1	J	190	TYR	2.4
1	C	195	GLU	2.4
1	G	202	HIS	2.4
1	G	194	GLY	2.3
1	F	206	THR	2.3
1	E	131	ARG	2.3
1	F	197	ASP	2.3
1	C	256	ARG	2.3
1	J	194	GLY	2.3
1	I	197	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	131	ARG	2.3
1	J	191	ASP	2.2
1	D	191	ASP	2.2
1	I	258	LEU	2.2
1	H	207	GLY	2.2
1	I	202	HIS	2.2
1	F	119	HIS	2.2
1	I	126	ARG	2.2
1	J	49	PRO	2.2
1	I	224	ARG	2.2
1	C	194	GLY	2.2
1	A	49	PRO	2.2
1	I	133	THR	2.2
1	F	130	SER	2.1
1	H	104	ARG	2.1
1	C	49	PRO	2.1
1	G	206	THR	2.1
1	G	46	THR	2.1
1	G	130	SER	2.1
1	C	129	ARG	2.1
1	I	206	THR	2.1
1	G	205	ARG	2.1
1	D	189	ASP	2.1
1	H	76	ASP	2.0
1	H	47	THR	2.0
1	F	253	LEU	2.0
1	G	133	THR	2.0
1	F	190	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.