



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2024 – 04:21 PM JST

PDB ID : 9JDT
Title : Crystal structure of reductase NaAD
Authors : Tang, J.; Liuqing, C.
Deposited on : 2024-09-01
Resolution : 3.26 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

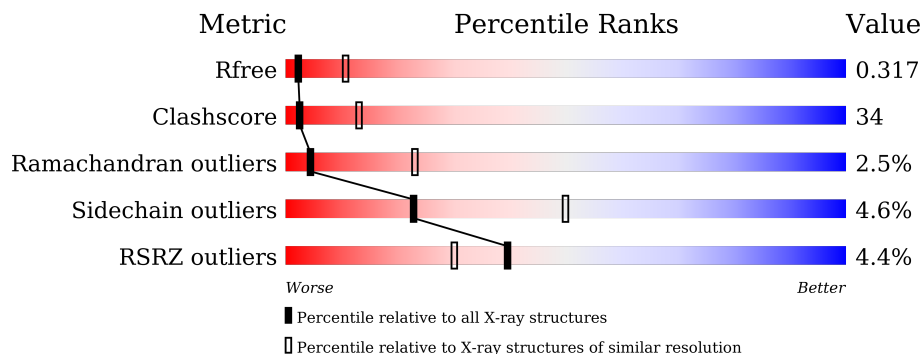
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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}	164625	1482 (3.30-3.22)
Clashscore	180529	1546 (3.30-3.22)
Ramachandran outliers	177936	1536 (3.30-3.22)
Sidechain outliers	177891	1535 (3.30-3.22)
RSRZ outliers	164620	1483 (3.30-3.22)

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	266	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">3% 39% 51% 6% .</p>
1	B	266	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">3% 44% 46% 6% . .</p>
1	C	266	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 42%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">6% 48% 42% 5% 5%</p>
1	D	266	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">5% 47% 45% . .</p>
1	E	266	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">7% 34% 55% 6% . .</p>
1	F	266	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">5% 38% 49% 8% .</p>

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Mol	Chain	Length	Quality of chain
1	G	266	<p>3% 45% 43% 7% . .</p>
1	H	266	<p>3% 50% 41% 5% .</p>
1	I	266	<p>2% 44% 47% 5% . .</p>
1	J	266	<p>2% 45% 44% 6% . .</p>
1	K	266	<p>5% 36% 52% 8% .</p>
1	L	266	<p>3% 46% 46% . .</p>
1	M	266	<p>6% 39% 48% 6% . .</p>
1	N	266	<p>7% 37% 51% 8% .</p>
1	O	266	<p>3% 45% 44% 5% . .</p>
1	P	266	<p>6% 39% 50% 6% . .</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29767 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 Short-chain dehydrogenase/reductase SDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	Total 1852	C 1161	N 325	O 352	S 14	0	0	0
1	B	257	Total 1860	C 1167	N 326	O 353	S 14	0	0	0
1	C	254	Total 1839	C 1152	N 323	O 350	S 14	0	0	0
1	D	256	Total 1852	C 1161	N 325	O 352	S 14	0	0	0
1	E	255	Total 1847	C 1158	N 324	O 351	S 14	0	0	0
1	F	255	Total 1847	C 1158	N 324	O 351	S 14	0	0	0
1	G	255	Total 1847	C 1158	N 324	O 351	S 14	0	0	0
1	H	256	Total 1852	C 1161	N 325	O 352	S 14	0	0	0
1	I	257	Total 1860	C 1167	N 326	O 353	S 14	0	0	0
1	J	256	Total 1852	C 1161	N 325	O 352	S 14	0	0	0
1	K	256	Total 1852	C 1161	N 325	O 352	S 14	0	0	0
1	L	256	Total 1852	C 1161	N 325	O 352	S 14	0	0	0
1	M	255	Total 1847	C 1158	N 324	O 351	S 14	0	0	0
1	N	256	Total 1852	C 1161	N 325	O 352	S 14	0	0	0
1	O	255	Total 1847	C 1158	N 324	O 351	S 14	0	0	0
1	P	255	Total 1847	C 1158	N 324	O 351	S 14	0	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A4XEP2
A	2	HIS	-	expression tag	UNP A4XEP2
A	3	HIS	-	expression tag	UNP A4XEP2
A	4	HIS	-	expression tag	UNP A4XEP2
A	5	HIS	-	expression tag	UNP A4XEP2
A	6	HIS	-	expression tag	UNP A4XEP2
A	7	HIS	-	expression tag	UNP A4XEP2
A	148	ALA	GLY	conflict	UNP A4XEP2
A	202	LEU	ILE	conflict	UNP A4XEP2
B	1	MET	-	initiating methionine	UNP A4XEP2
B	2	HIS	-	expression tag	UNP A4XEP2
B	3	HIS	-	expression tag	UNP A4XEP2
B	4	HIS	-	expression tag	UNP A4XEP2
B	5	HIS	-	expression tag	UNP A4XEP2
B	6	HIS	-	expression tag	UNP A4XEP2
B	7	HIS	-	expression tag	UNP A4XEP2
B	148	ALA	GLY	conflict	UNP A4XEP2
B	202	LEU	ILE	conflict	UNP A4XEP2
C	1	MET	-	initiating methionine	UNP A4XEP2
C	2	HIS	-	expression tag	UNP A4XEP2
C	3	HIS	-	expression tag	UNP A4XEP2
C	4	HIS	-	expression tag	UNP A4XEP2
C	5	HIS	-	expression tag	UNP A4XEP2
C	6	HIS	-	expression tag	UNP A4XEP2
C	7	HIS	-	expression tag	UNP A4XEP2
C	148	ALA	GLY	conflict	UNP A4XEP2
C	202	LEU	ILE	conflict	UNP A4XEP2
D	1	MET	-	initiating methionine	UNP A4XEP2
D	2	HIS	-	expression tag	UNP A4XEP2
D	3	HIS	-	expression tag	UNP A4XEP2
D	4	HIS	-	expression tag	UNP A4XEP2
D	5	HIS	-	expression tag	UNP A4XEP2
D	6	HIS	-	expression tag	UNP A4XEP2
D	7	HIS	-	expression tag	UNP A4XEP2
D	148	ALA	GLY	conflict	UNP A4XEP2
D	202	LEU	ILE	conflict	UNP A4XEP2
E	1	MET	-	initiating methionine	UNP A4XEP2
E	2	HIS	-	expression tag	UNP A4XEP2
E	3	HIS	-	expression tag	UNP A4XEP2
E	4	HIS	-	expression tag	UNP A4XEP2
E	5	HIS	-	expression tag	UNP A4XEP2
E	6	HIS	-	expression tag	UNP A4XEP2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	7	HIS	-	expression tag	UNP A4XEP2
E	148	ALA	GLY	conflict	UNP A4XEP2
E	202	LEU	ILE	conflict	UNP A4XEP2
F	1	MET	-	initiating methionine	UNP A4XEP2
F	2	HIS	-	expression tag	UNP A4XEP2
F	3	HIS	-	expression tag	UNP A4XEP2
F	4	HIS	-	expression tag	UNP A4XEP2
F	5	HIS	-	expression tag	UNP A4XEP2
F	6	HIS	-	expression tag	UNP A4XEP2
F	7	HIS	-	expression tag	UNP A4XEP2
F	148	ALA	GLY	conflict	UNP A4XEP2
F	202	LEU	ILE	conflict	UNP A4XEP2
G	1	MET	-	initiating methionine	UNP A4XEP2
G	2	HIS	-	expression tag	UNP A4XEP2
G	3	HIS	-	expression tag	UNP A4XEP2
G	4	HIS	-	expression tag	UNP A4XEP2
G	5	HIS	-	expression tag	UNP A4XEP2
G	6	HIS	-	expression tag	UNP A4XEP2
G	7	HIS	-	expression tag	UNP A4XEP2
G	148	ALA	GLY	conflict	UNP A4XEP2
G	202	LEU	ILE	conflict	UNP A4XEP2
H	1	MET	-	initiating methionine	UNP A4XEP2
H	2	HIS	-	expression tag	UNP A4XEP2
H	3	HIS	-	expression tag	UNP A4XEP2
H	4	HIS	-	expression tag	UNP A4XEP2
H	5	HIS	-	expression tag	UNP A4XEP2
H	6	HIS	-	expression tag	UNP A4XEP2
H	7	HIS	-	expression tag	UNP A4XEP2
H	148	ALA	GLY	conflict	UNP A4XEP2
H	202	LEU	ILE	conflict	UNP A4XEP2
I	1	MET	-	initiating methionine	UNP A4XEP2
I	2	HIS	-	expression tag	UNP A4XEP2
I	3	HIS	-	expression tag	UNP A4XEP2
I	4	HIS	-	expression tag	UNP A4XEP2
I	5	HIS	-	expression tag	UNP A4XEP2
I	6	HIS	-	expression tag	UNP A4XEP2
I	7	HIS	-	expression tag	UNP A4XEP2
I	148	ALA	GLY	conflict	UNP A4XEP2
I	202	LEU	ILE	conflict	UNP A4XEP2
J	1	MET	-	initiating methionine	UNP A4XEP2
J	2	HIS	-	expression tag	UNP A4XEP2
J	3	HIS	-	expression tag	UNP A4XEP2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	4	HIS	-	expression tag	UNP A4XEP2
J	5	HIS	-	expression tag	UNP A4XEP2
J	6	HIS	-	expression tag	UNP A4XEP2
J	7	HIS	-	expression tag	UNP A4XEP2
J	148	ALA	GLY	conflict	UNP A4XEP2
J	202	LEU	ILE	conflict	UNP A4XEP2
K	1	MET	-	initiating methionine	UNP A4XEP2
K	2	HIS	-	expression tag	UNP A4XEP2
K	3	HIS	-	expression tag	UNP A4XEP2
K	4	HIS	-	expression tag	UNP A4XEP2
K	5	HIS	-	expression tag	UNP A4XEP2
K	6	HIS	-	expression tag	UNP A4XEP2
K	7	HIS	-	expression tag	UNP A4XEP2
K	148	ALA	GLY	conflict	UNP A4XEP2
K	202	LEU	ILE	conflict	UNP A4XEP2
L	1	MET	-	initiating methionine	UNP A4XEP2
L	2	HIS	-	expression tag	UNP A4XEP2
L	3	HIS	-	expression tag	UNP A4XEP2
L	4	HIS	-	expression tag	UNP A4XEP2
L	5	HIS	-	expression tag	UNP A4XEP2
L	6	HIS	-	expression tag	UNP A4XEP2
L	7	HIS	-	expression tag	UNP A4XEP2
L	148	ALA	GLY	conflict	UNP A4XEP2
L	202	LEU	ILE	conflict	UNP A4XEP2
M	1	MET	-	initiating methionine	UNP A4XEP2
M	2	HIS	-	expression tag	UNP A4XEP2
M	3	HIS	-	expression tag	UNP A4XEP2
M	4	HIS	-	expression tag	UNP A4XEP2
M	5	HIS	-	expression tag	UNP A4XEP2
M	6	HIS	-	expression tag	UNP A4XEP2
M	7	HIS	-	expression tag	UNP A4XEP2
M	148	ALA	GLY	conflict	UNP A4XEP2
M	202	LEU	ILE	conflict	UNP A4XEP2
N	1	MET	-	initiating methionine	UNP A4XEP2
N	2	HIS	-	expression tag	UNP A4XEP2
N	3	HIS	-	expression tag	UNP A4XEP2
N	4	HIS	-	expression tag	UNP A4XEP2
N	5	HIS	-	expression tag	UNP A4XEP2
N	6	HIS	-	expression tag	UNP A4XEP2
N	7	HIS	-	expression tag	UNP A4XEP2
N	148	ALA	GLY	conflict	UNP A4XEP2
N	202	LEU	ILE	conflict	UNP A4XEP2

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Chain	Residue	Modelled	Actual	Comment	Reference
O	1	MET	-	initiating methionine	UNP A4XEP2
O	2	HIS	-	expression tag	UNP A4XEP2
O	3	HIS	-	expression tag	UNP A4XEP2
O	4	HIS	-	expression tag	UNP A4XEP2
O	5	HIS	-	expression tag	UNP A4XEP2
O	6	HIS	-	expression tag	UNP A4XEP2
O	7	HIS	-	expression tag	UNP A4XEP2
O	148	ALA	GLY	conflict	UNP A4XEP2
O	202	LEU	ILE	conflict	UNP A4XEP2
P	1	MET	-	initiating methionine	UNP A4XEP2
P	2	HIS	-	expression tag	UNP A4XEP2
P	3	HIS	-	expression tag	UNP A4XEP2
P	4	HIS	-	expression tag	UNP A4XEP2
P	5	HIS	-	expression tag	UNP A4XEP2
P	6	HIS	-	expression tag	UNP A4XEP2
P	7	HIS	-	expression tag	UNP A4XEP2
P	148	ALA	GLY	conflict	UNP A4XEP2
P	202	LEU	ILE	conflict	UNP A4XEP2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	13	Total O 13 13	0	0
2	B	11	Total O 11 11	0	0
2	C	7	Total O 7 7	0	0
2	D	8	Total O 8 8	0	0
2	E	13	Total O 13 13	0	0
2	F	4	Total O 4 4	0	0
2	G	9	Total O 9 9	0	0
2	H	7	Total O 7 7	0	0
2	I	11	Total O 11 11	0	0
2	J	12	Total O 12 12	0	0

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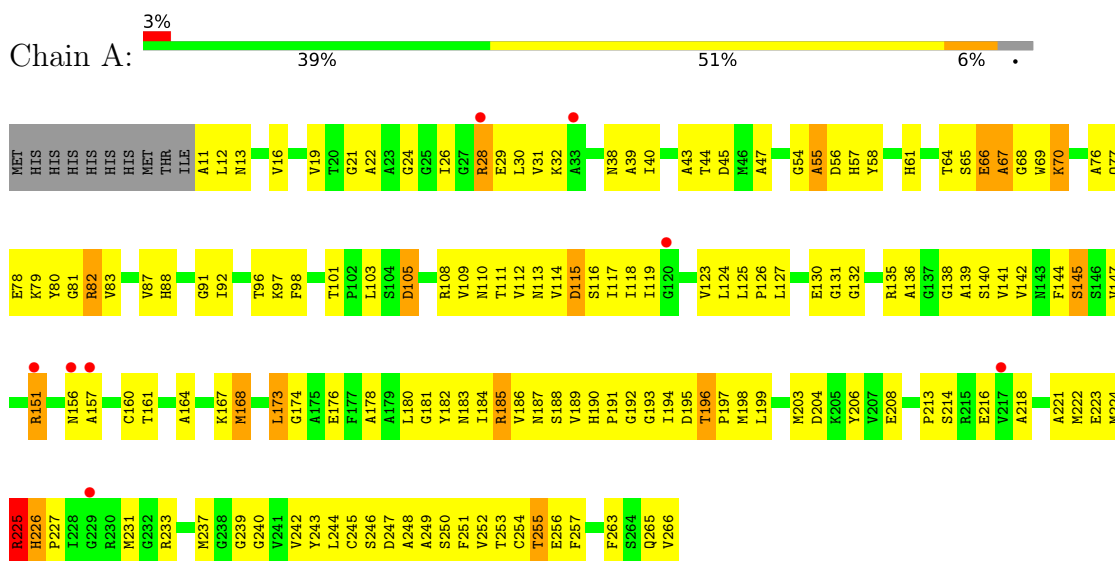
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	10	Total O 10 10	0	0
2	L	7	Total O 7 7	0	0
2	M	9	Total O 9 9	0	0
2	N	12	Total O 12 12	0	0
2	O	14	Total O 14 14	0	0
2	P	15	Total O 15 15	0	0

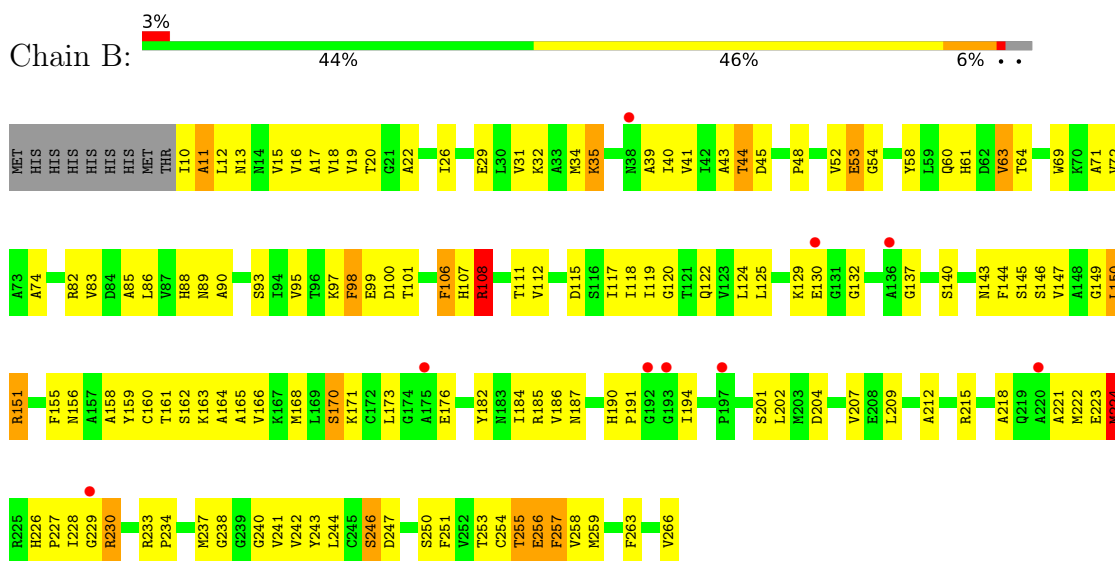
3 Residue-property plots [i](#)

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.

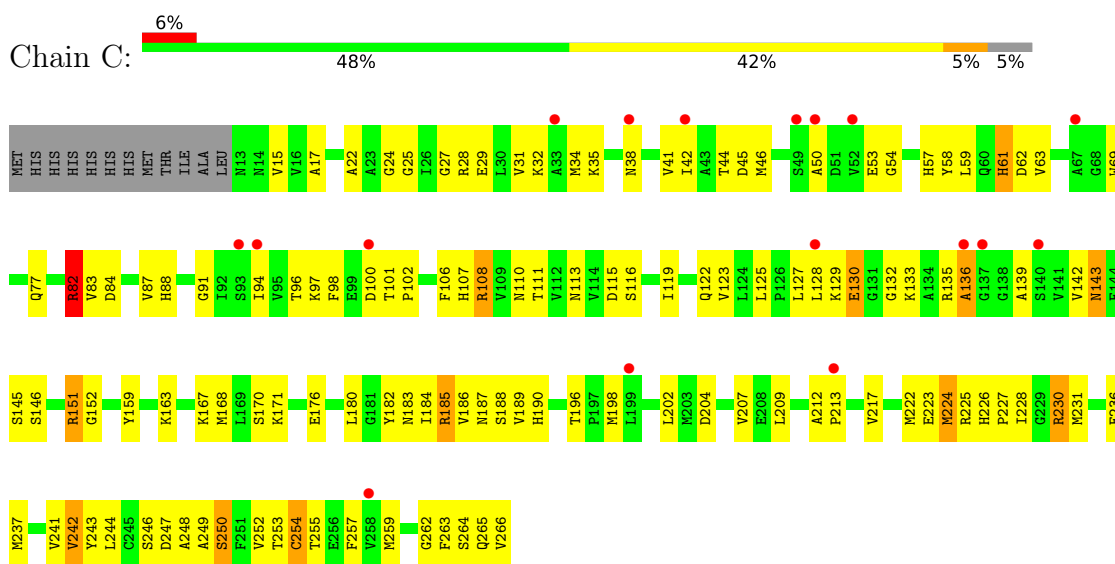
- Molecule 1: Short-chain dehydrogenase/reductase SDR



- Molecule 1: Short-chain dehydrogenase/reductase SDR



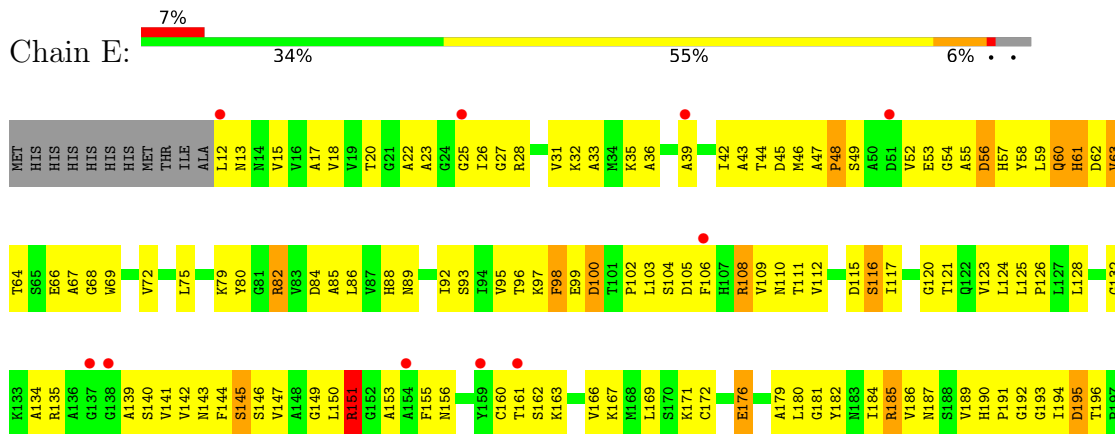
- Molecule 1: Short-chain dehydrogenase/reductase SDR



- Molecule 1: Short-chain dehydrogenase/reductase SDR

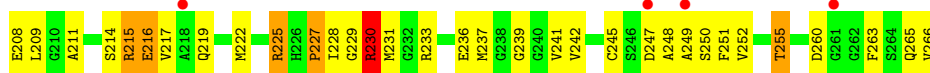
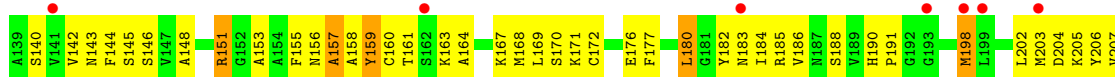
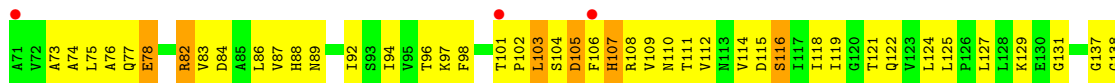


- Molecule 1: Short-chain dehydrogenase/reductase SDR

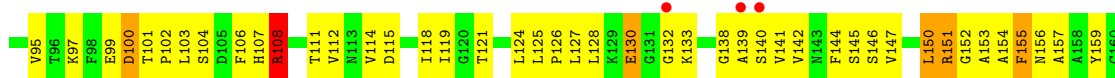
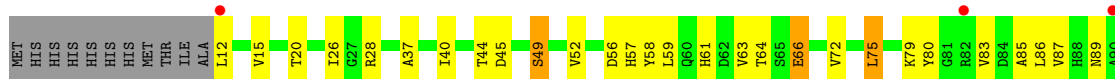




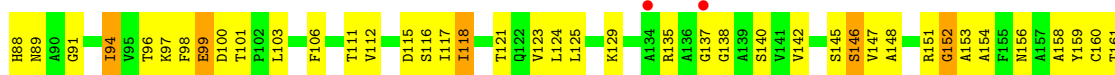
• Molecule 1: Short-chain dehydrogenase/reductase SDR

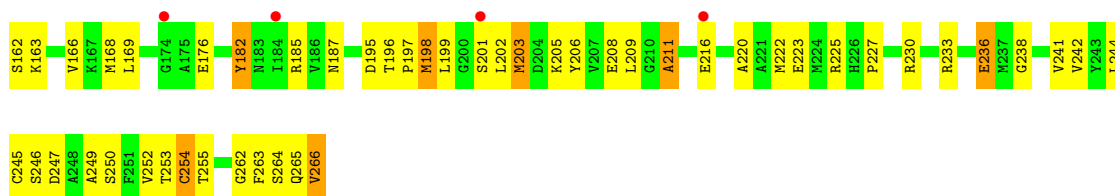


• Molecule 1: Short-chain dehydrogenase/reductase SDR

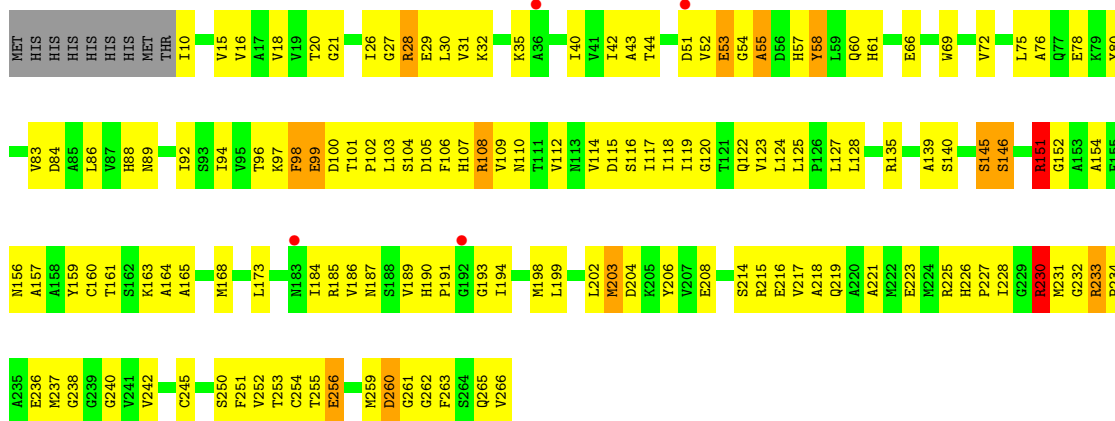
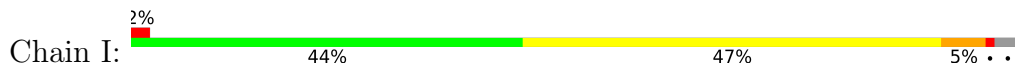


• Molecule 1: Short-chain dehydrogenase/reductase SDR

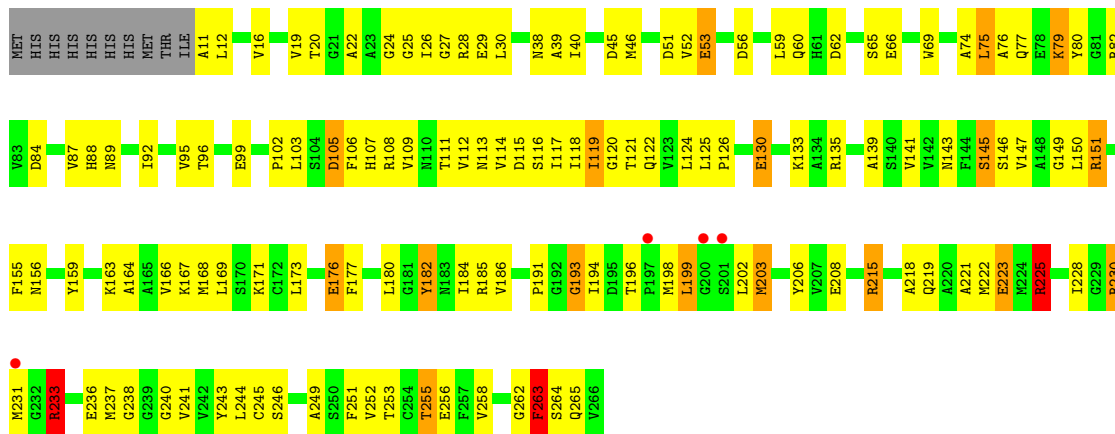
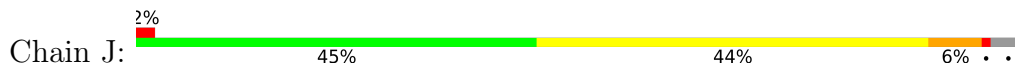




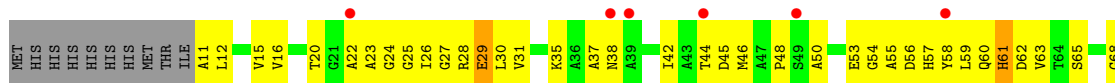
● Molecule 1: Short-chain dehydrogenase/reductase SDR

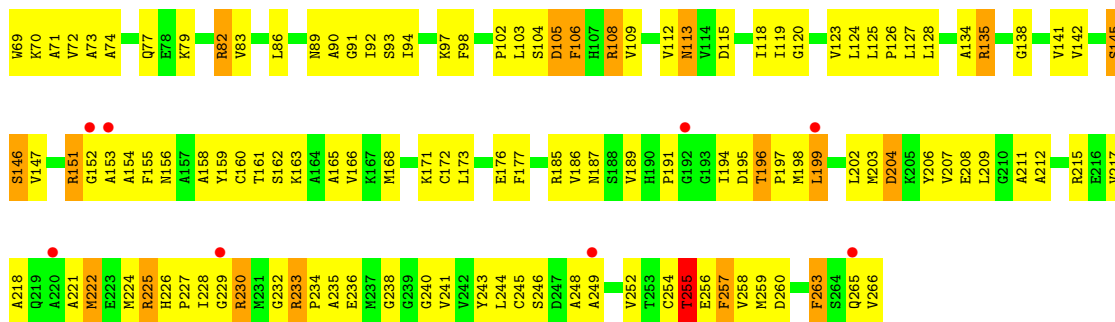


● Molecule 1: Short-chain dehydrogenase/reductase SDR

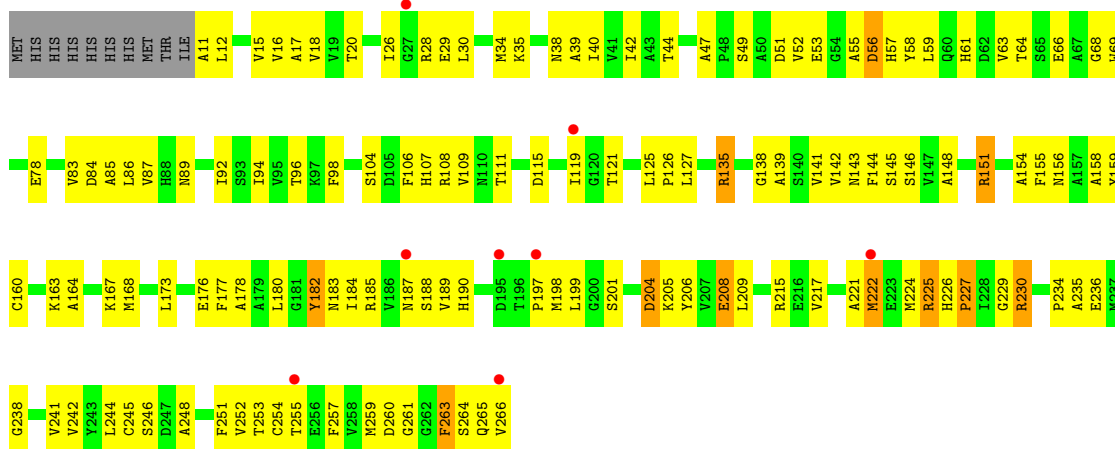


● Molecule 1: Short-chain dehydrogenase/reductase SDR

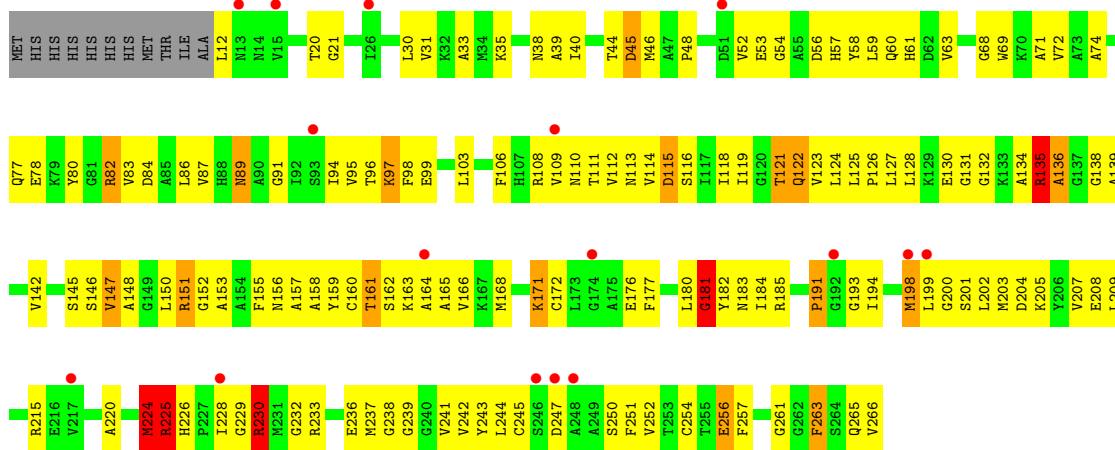




● Molecule 1: Short-chain dehydrogenase/reductase SDR

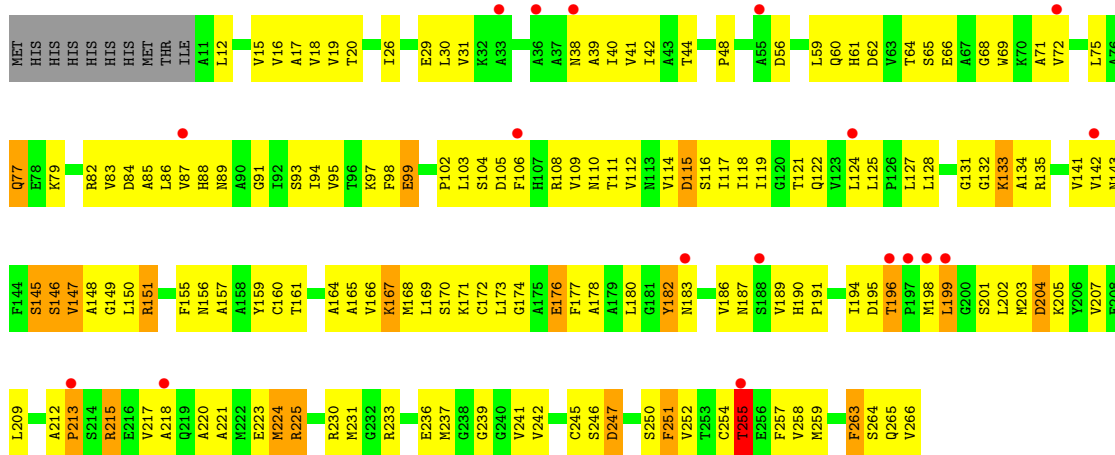


● Molecule 1: Short-chain dehydrogenase/reductase SDR

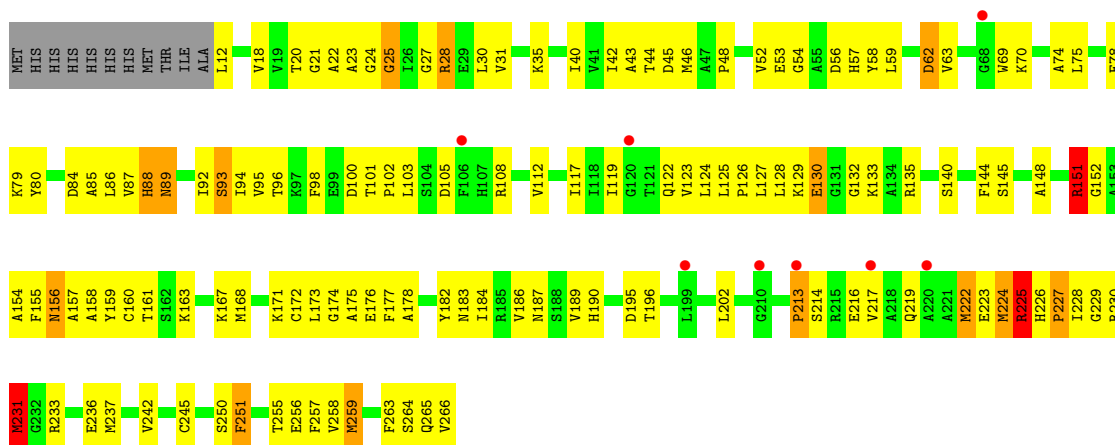


● Molecule 1: Short-chain dehydrogenase/reductase SDR





• Molecule 1: Short-chain dehydrogenase/reductase SDR



• Molecule 1: Short-chain dehydrogenase/reductase SDR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.32Å 121.77Å 276.15Å 90.00° 93.40° 90.00°	Depositor
Resolution (Å)	20.00 – 3.26 20.00 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-3.26) 81.0 (20.00-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 3.26Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.260 , 0.300 0.273 , 0.317	Depositor DCC
R_{free} test set	751 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtrriage
Anisotropy	0.452	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	29767	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8062e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.99	4/1881 (0.2%)	1.30	21/2548 (0.8%)
1	B	0.93	2/1889 (0.1%)	1.24	11/2559 (0.4%)
1	C	0.83	0/1868	1.23	16/2530 (0.6%)
1	D	0.91	2/1881 (0.1%)	1.25	18/2548 (0.7%)
1	E	1.01	5/1876 (0.3%)	1.31	19/2541 (0.7%)
1	F	1.03	8/1876 (0.4%)	1.24	14/2541 (0.6%)
1	G	1.03	8/1876 (0.4%)	1.35	19/2541 (0.7%)
1	H	0.97	8/1881 (0.4%)	1.18	10/2548 (0.4%)
1	I	0.91	6/1889 (0.3%)	1.16	9/2559 (0.4%)
1	J	1.00	7/1881 (0.4%)	1.35	20/2548 (0.8%)
1	K	0.95	5/1881 (0.3%)	1.31	24/2548 (0.9%)
1	L	0.93	4/1881 (0.2%)	1.22	13/2548 (0.5%)
1	M	0.91	5/1876 (0.3%)	1.21	12/2541 (0.5%)
1	N	1.00	7/1881 (0.4%)	1.26	19/2548 (0.7%)
1	O	0.96	5/1876 (0.3%)	1.22	14/2541 (0.6%)
1	P	1.00	8/1876 (0.4%)	1.27	20/2541 (0.8%)
All	All	0.96	84/30069 (0.3%)	1.26	259/40730 (0.6%)

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	A	0	1
1	B	0	4
1	C	0	2
1	D	0	1
1	E	0	3
1	F	0	3
1	G	0	4
1	H	0	2
1	I	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	4
1	K	0	1
1	L	0	3
1	M	0	8
1	O	0	2
1	P	0	2
All	All	0	44

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	176	GLU	CD-OE2	14.86	1.42	1.25
1	P	157	ALA	C-O	12.16	1.46	1.23
1	H	99	GLU	CD-OE2	10.82	1.37	1.25
1	N	29	GLU	CD-OE2	10.41	1.37	1.25
1	G	99	GLU	CD-OE2	10.08	1.36	1.25
1	F	66	GLU	CD-OE2	9.96	1.36	1.25
1	F	53	GLU	CD-OE2	9.81	1.36	1.25
1	G	66	GLU	CD-OE2	9.43	1.36	1.25
1	J	176	GLU	CD-OE2	9.40	1.35	1.25
1	D	66	GLU	CD-OE2	9.13	1.35	1.25
1	N	176	GLU	CD-OE1	8.97	1.35	1.25
1	F	53	GLU	CD-OE1	8.95	1.35	1.25
1	B	99	GLU	CD-OE2	7.95	1.34	1.25
1	N	176	GLU	CD-OE2	7.81	1.34	1.25
1	L	176	GLU	CD-OE1	7.78	1.34	1.25
1	L	53	GLU	CD-OE1	7.71	1.34	1.25
1	P	99	GLU	CD-OE1	7.62	1.34	1.25
1	I	208	GLU	CD-OE1	7.44	1.33	1.25
1	H	236	GLU	CD-OE2	7.25	1.33	1.25
1	J	256	GLU	CD-OE2	7.10	1.33	1.25
1	N	29	GLU	CD-OE1	7.07	1.33	1.25
1	F	66	GLU	CD-OE1	7.07	1.33	1.25
1	P	208	GLU	CD-OE2	7.06	1.33	1.25
1	O	78	GLU	CD-OE1	7.05	1.33	1.25
1	L	236	GLU	CD-OE1	6.97	1.33	1.25
1	I	53	GLU	CD-OE2	6.86	1.33	1.25
1	G	236	GLU	CD-OE1	6.83	1.33	1.25
1	O	176	GLU	CD-OE2	6.82	1.33	1.25
1	A	78	GLU	CD-OE1	6.79	1.33	1.25
1	P	66	GLU	CD-OE1	6.75	1.33	1.25
1	O	130	GLU	CD-OE1	6.65	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	176	GLU	CD-OE1	6.64	1.32	1.25
1	M	176	GLU	CD-OE2	6.62	1.32	1.25
1	A	66	GLU	CD-OE1	6.60	1.32	1.25
1	L	53	GLU	CD-OE2	6.43	1.32	1.25
1	G	99	GLU	CD-OE1	6.39	1.32	1.25
1	J	29	GLU	CD-OE2	6.30	1.32	1.25
1	P	208	GLU	CD-OE1	6.21	1.32	1.25
1	N	99	GLU	CD-OE1	6.21	1.32	1.25
1	G	66	GLU	CD-OE1	6.17	1.32	1.25
1	P	176	GLU	CD-OE1	6.16	1.32	1.25
1	B	53	GLU	CD-OE1	6.16	1.32	1.25
1	J	256	GLU	CD-OE1	6.07	1.32	1.25
1	F	78	GLU	CD-OE2	6.04	1.32	1.25
1	G	49	SER	CA-CB	6.03	1.61	1.52
1	I	230	ARG	NE-CZ	6.01	1.40	1.33
1	M	176	GLU	CD-OE1	5.99	1.32	1.25
1	P	66	GLU	CD-OE2	5.99	1.32	1.25
1	N	108	ARG	NE-CZ	5.96	1.40	1.33
1	F	208	GLU	CD-OE1	5.96	1.32	1.25
1	H	152	GLY	C-O	-5.90	1.14	1.23
1	G	130	GLU	CD-OE1	5.82	1.32	1.25
1	G	176	GLU	CD-OE1	5.81	1.32	1.25
1	I	256	GLU	CD-OE1	-5.64	1.19	1.25
1	E	61	HIS	CG-CD2	-5.59	1.26	1.35
1	M	256	GLU	CD-OE2	5.59	1.31	1.25
1	H	233	ARG	NE-CZ	5.59	1.40	1.33
1	K	225	ARG	NE-CZ	5.56	1.40	1.33
1	E	66	GLU	CD-OE2	5.53	1.31	1.25
1	K	208	GLU	CD-OE2	5.53	1.31	1.25
1	M	130	GLU	CD-OE2	5.52	1.31	1.25
1	F	216	GLU	CD-OE2	5.44	1.31	1.25
1	A	66	GLU	CD-OE2	5.43	1.31	1.25
1	O	78	GLU	CG-CD	5.40	1.60	1.51
1	J	107	HIS	CG-CD2	-5.34	1.26	1.35
1	K	176	GLU	CD-OE1	-5.27	1.19	1.25
1	I	78	GLU	CD-OE1	5.25	1.31	1.25
1	F	78	GLU	CD-OE1	5.25	1.31	1.25
1	H	29	GLU	CD-OE1	5.25	1.31	1.25
1	O	130	GLU	CD-OE2	5.24	1.31	1.25
1	J	223	GLU	CD-OE2	5.24	1.31	1.25
1	H	236	GLU	CG-CD	5.23	1.59	1.51
1	H	146	SER	CA-CB	-5.22	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	208	GLU	CD-OE1	5.17	1.31	1.25
1	I	78	GLU	CD-OE2	5.17	1.31	1.25
1	P	116	SER	CA-CB	-5.15	1.45	1.52
1	N	66	GLU	CD-OE1	-5.10	1.20	1.25
1	D	66	GLU	CD-OE1	5.09	1.31	1.25
1	J	130	GLU	CD-OE1	5.08	1.31	1.25
1	H	78	GLU	CD-OE2	5.06	1.31	1.25
1	K	29	GLU	CD-OE1	5.04	1.31	1.25
1	M	130	GLU	CG-CD	5.01	1.59	1.51
1	E	195	ASP	CG-OD2	5.01	1.36	1.25
1	A	130	GLU	CD-OE2	5.00	1.31	1.25

All (259) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	230	ARG	NE-CZ-NH1	14.93	127.77	120.30
1	G	233	ARG	NE-CZ-NH1	-13.65	113.48	120.30
1	J	151	ARG	NE-CZ-NH1	12.23	126.42	120.30
1	C	151	ARG	NE-CZ-NH1	-11.33	114.63	120.30
1	J	233	ARG	NE-CZ-NH2	-10.75	114.93	120.30
1	E	151	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	D	225	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	H	222	MET	CG-SD-CE	10.36	116.77	100.20
1	J	230	ARG	NE-CZ-NH2	-10.07	115.26	120.30
1	K	151	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	J	99	GLU	OE1-CD-OE2	9.91	135.20	123.30
1	O	151	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	D	82	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	B	247	ASP	CB-CG-OD1	-9.75	109.53	118.30
1	E	230	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	E	108	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	G	215	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	N	230	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	F	53	GLU	OE1-CD-OE2	9.32	134.48	123.30
1	N	224	MET	CG-SD-CE	9.26	115.02	100.20
1	M	225	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	D	100	ASP	CB-CG-OD2	-9.05	110.15	118.30
1	E	233	ARG	NE-CZ-NH1	-8.97	115.81	120.30
1	I	233	ARG	NE-CZ-NH2	8.87	124.73	120.30
1	C	151	ARG	CD-NE-CZ	8.81	135.93	123.60
1	L	78	GLU	OE1-CD-OE2	-8.73	112.83	123.30
1	M	224	MET	CG-SD-CE	8.72	114.15	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	151	ARG	NE-CZ-NH1	-8.67	115.96	120.30
1	L	208	GLU	OE1-CD-OE2	-8.65	112.92	123.30
1	P	230	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	E	66	GLU	OE1-CD-OE2	8.57	133.58	123.30
1	C	230	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	F	75	LEU	CB-CG-CD2	-8.46	96.61	111.00
1	F	176	GLU	OE1-CD-OE2	-8.46	113.15	123.30
1	J	223	GLU	OE1-CD-OE2	8.45	133.44	123.30
1	A	185	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	C	222	MET	CG-SD-CE	8.42	113.67	100.20
1	J	225	ARG	NE-CZ-NH1	-8.35	116.13	120.30
1	L	215	ARG	NE-CZ-NH1	-8.35	116.13	120.30
1	F	225	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	C	108	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	B	222	MET	CG-SD-CE	8.23	113.36	100.20
1	D	225	ARG	NH1-CZ-NH2	-8.20	110.38	119.40
1	L	151	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	O	251	PHE	CB-CG-CD2	8.12	126.48	120.80
1	H	176	GLU	OE1-CD-OE2	-8.09	113.60	123.30
1	G	108	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	G	230	ARG	NH1-CZ-NH2	-7.93	110.67	119.40
1	K	255	THR	OG1-CB-CG2	-7.87	91.90	110.00
1	M	230	ARG	NE-CZ-NH1	-7.79	116.41	120.30
1	N	255	THR	OG1-CB-CG2	7.74	127.80	110.00
1	H	100	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	D	225	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	E	222	MET	CG-SD-CE	7.65	112.44	100.20
1	K	233	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	A	168	MET	CG-SD-CE	7.50	112.21	100.20
1	B	98	PHE	CB-CG-CD1	7.50	126.05	120.80
1	A	195	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	108	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	N	99	GLU	OE1-CD-OE2	7.40	132.19	123.30
1	E	233	ARG	CD-NE-CZ	7.40	133.95	123.60
1	N	29	GLU	OE1-CD-OE2	7.39	132.17	123.30
1	J	233	ARG	NH1-CZ-NH2	7.39	127.53	119.40
1	C	46	MET	CG-SD-CE	7.38	112.00	100.20
1	M	53	GLU	OE1-CD-OE2	7.29	132.05	123.30
1	O	225	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	C	108	ARG	NH1-CZ-NH2	-7.19	111.49	119.40
1	G	100	ASP	CB-CG-OD1	-7.13	111.88	118.30
1	N	151	ARG	CB-CA-C	7.12	124.65	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	195	ASP	CB-CG-OD1	-7.04	111.97	118.30
1	K	108	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	J	233	ARG	NE-CZ-NH1	-7.03	116.79	120.30
1	J	51	ASP	CB-CG-OD2	6.97	124.57	118.30
1	E	75	LEU	CB-CG-CD2	6.95	122.82	111.00
1	B	98	PHE	CB-CG-CD2	-6.95	115.94	120.80
1	N	247	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	M	208	GLU	OE1-CD-OE2	6.93	131.62	123.30
1	M	135	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	D	230	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	C	151	ARG	NH1-CZ-NH2	6.87	126.96	119.40
1	O	62	ASP	CB-CG-OD2	6.87	124.48	118.30
1	D	204	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	A	28	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	A	66	GLU	OE1-CD-OE2	6.78	131.43	123.30
1	P	108	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	K	70	LYS	CD-CE-NZ	6.74	127.20	111.70
1	A	115	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	P	230	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	L	78	GLU	CG-CD-OE2	6.69	131.68	118.30
1	E	223	GLU	CG-CD-OE1	6.67	131.63	118.30
1	O	28	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	F	151	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	P	224	MET	CB-CG-SD	6.51	131.94	112.40
1	C	204	ASP	CB-CG-OD2	6.46	124.12	118.30
1	L	215	ARG	NH1-CZ-NH2	6.46	126.50	119.40
1	F	153	ALA	N-CA-CB	6.44	119.12	110.10
1	K	230	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	108	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	K	151	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	K	222	MET	CG-SD-CE	6.39	110.43	100.20
1	A	108	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	A	130	GLU	CG-CD-OE1	-6.37	105.56	118.30
1	F	208	GLU	OE1-CD-OE2	6.37	130.95	123.30
1	P	256	GLU	OE1-CD-OE2	-6.34	115.69	123.30
1	K	105	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	C	224	MET	CG-SD-CE	6.28	110.25	100.20
1	E	103	LEU	CB-CG-CD1	-6.27	100.34	111.00
1	N	255	THR	CA-CB-OG1	-6.27	95.84	109.00
1	O	53	GLU	OE1-CD-OE2	6.26	130.81	123.30
1	G	161	THR	OG1-CB-CG2	-6.24	95.65	110.00
1	G	236	GLU	OE1-CD-OE2	6.23	130.78	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	135	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	G	233	ARG	NH1-CZ-NH2	6.22	126.24	119.40
1	J	208	GLU	OE1-CD-OE2	6.21	130.75	123.30
1	F	62	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	E	223	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	M	115	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	56	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	A	108	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	99	GLU	OE1-CD-OE2	6.17	130.71	123.30
1	H	211	ALA	CB-CA-C	6.17	119.35	110.10
1	K	199	LEU	CB-CG-CD1	6.16	121.47	111.00
1	A	195	ASP	OD1-CG-OD2	6.14	134.98	123.30
1	N	263	PHE	CB-CG-CD1	6.12	125.08	120.80
1	K	209	LEU	CB-CG-CD2	6.11	121.39	111.00
1	O	222	MET	CG-SD-CE	6.11	109.97	100.20
1	E	176	GLU	CG-CD-OE1	-6.09	106.12	118.30
1	E	233	ARG	NH1-CZ-NH2	6.08	126.09	119.40
1	P	56	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	L	225	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	J	203	MET	CG-SD-CE	-6.06	90.51	100.20
1	L	215	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	F	66	GLU	OE1-CD-OE2	6.02	130.53	123.30
1	G	233	ARG	CD-NE-CZ	6.02	132.02	123.60
1	F	82	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	G	233	ARG	CA-CB-CG	6.01	126.63	113.40
1	O	251	PHE	CB-CG-CD1	-5.97	116.62	120.80
1	N	115	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	D	133	LYS	CD-CE-NZ	5.96	125.40	111.70
1	I	203	MET	CG-SD-CE	5.95	109.71	100.20
1	M	97	LYS	CD-CE-NZ	5.95	125.38	111.70
1	H	28	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	K	198	MET	CG-SD-CE	5.91	109.66	100.20
1	P	28	ARG	CD-NE-CZ	5.91	131.87	123.60
1	J	256	GLU	OE1-CD-OE2	5.90	130.38	123.30
1	L	135	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	K	257	PHE	N-CA-CB	5.88	121.18	110.60
1	N	196	THR	OG1-CB-CG2	-5.88	96.48	110.00
1	N	108	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	G	49	SER	N-CA-CB	5.87	119.31	110.50
1	A	57	HIS	CB-CA-C	5.84	122.08	110.40
1	J	198	MET	CG-SD-CE	5.83	109.52	100.20
1	D	251	PHE	CB-CG-CD2	5.81	124.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	121	THR	OG1-CB-CG2	-5.81	96.63	110.00
1	C	130	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	N	215	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	H	223	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	P	251	PHE	CB-CG-CD1	5.76	124.83	120.80
1	K	224	MET	CG-SD-CE	5.74	109.38	100.20
1	J	151	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	J	215	ARG	NE-CZ-NH1	-5.71	117.45	120.30
1	K	82	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	I	231	MET	CG-SD-CE	5.69	109.31	100.20
1	D	100	ASP	OD1-CG-OD2	5.68	134.09	123.30
1	K	225	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	J	79	LYS	CD-CE-NZ	5.67	124.73	111.70
1	G	222	MET	CG-SD-CE	5.66	109.26	100.20
1	N	251	PHE	CB-CG-CD1	5.64	124.75	120.80
1	M	225	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	I	260	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	A	108	ARG	NH1-CZ-NH2	5.61	125.58	119.40
1	N	99	GLU	CG-CD-OE2	-5.61	107.08	118.30
1	E	108	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
1	O	231	MET	CG-SD-CE	5.60	109.16	100.20
1	L	204	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	P	84	ASP	CB-CA-C	5.57	121.54	110.40
1	C	143	ASN	CB-CA-C	-5.56	99.28	110.40
1	B	224	MET	CG-SD-CE	5.55	109.08	100.20
1	I	98	PHE	CB-CG-CD1	5.55	124.68	120.80
1	K	97	LYS	CD-CE-NZ	5.53	124.43	111.70
1	A	224	MET	CG-SD-CE	5.52	109.03	100.20
1	P	130	GLU	OE1-CD-OE2	5.52	129.93	123.30
1	A	256	GLU	OE1-CD-OE2	-5.52	116.68	123.30
1	B	100	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	K	225	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	195	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	O	56	ASP	CB-CG-OD2	5.47	123.23	118.30
1	K	208	GLU	OE1-CD-OE2	5.47	129.87	123.30
1	P	128	LEU	CB-CG-CD1	5.46	120.29	111.00
1	D	204	ASP	CB-CG-OD1	-5.45	113.40	118.30
1	I	154	ALA	N-CA-CB	-5.44	102.48	110.10
1	I	98	PHE	CB-CG-CD2	-5.43	117.00	120.80
1	G	150	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	D	204	ASP	OD1-CG-OD2	5.40	133.57	123.30
1	F	159	TYR	CB-CG-CD2	5.40	124.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	GLU	CG-CD-OE1	-5.40	107.51	118.30
1	P	185	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	F	169	LEU	CB-CG-CD1	5.39	120.16	111.00
1	B	223	GLU	OE1-CD-OE2	5.38	129.76	123.30
1	M	225	ARG	CG-CD-NE	5.38	123.11	111.80
1	D	66	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	D	159	TYR	CB-CG-CD1	5.36	124.22	121.00
1	H	208	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	L	11	ALA	N-CA-CB	5.35	117.59	110.10
1	C	136	ALA	N-CA-CB	-5.35	102.61	110.10
1	O	225	ARG	NH1-CZ-NH2	5.35	125.28	119.40
1	M	122	GLN	CB-CA-C	-5.33	99.75	110.40
1	D	251	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	D	53	GLU	OE1-CD-OE2	5.32	129.68	123.30
1	N	133	LYS	CB-CA-C	5.30	121.01	110.40
1	N	251	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	K	230	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	L	151	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	P	198	MET	CG-SD-CE	5.28	108.64	100.20
1	J	46	MET	CG-SD-CE	5.26	108.62	100.20
1	P	56	ASP	OD1-CG-OD2	5.26	133.30	123.30
1	E	82	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	H	182	TYR	CB-CG-CD1	5.25	124.15	121.00
1	P	129	LYS	CD-CE-NZ	5.24	123.74	111.70
1	D	82	ARG	NH1-CZ-NH2	-5.22	113.65	119.40
1	O	224	MET	CG-SD-CE	5.21	108.54	100.20
1	A	225	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	C	230	ARG	N-CA-CB	-5.21	101.23	110.60
1	I	107	HIS	CA-CB-CG	5.20	122.45	113.60
1	K	225	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
1	N	263	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	A	105	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	P	156	ASN	O-C-N	-5.20	114.38	122.70
1	G	20	THR	OG1-CB-CG2	5.19	121.95	110.00
1	O	259	MET	CG-SD-CE	-5.19	91.90	100.20
1	H	99	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	C	45	ASP	CB-CA-C	5.18	120.77	110.40
1	E	253	THR	CA-CB-OG1	-5.18	98.12	109.00
1	G	108	ARG	NH1-CZ-NH2	5.18	125.09	119.40
1	G	20	THR	CA-CB-OG1	-5.17	98.14	109.00
1	A	108	ARG	CD-NE-CZ	5.17	130.84	123.60
1	P	208	GLU	OE1-CD-OE2	5.17	129.50	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	176	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	K	195	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	255	THR	CA-CB-OG1	-5.15	98.19	109.00
1	K	195	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	P	225	ARG	N-CA-CB	5.14	119.85	110.60
1	I	58	TYR	CB-CG-CD2	5.14	124.08	121.00
1	F	230	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	M	171	LYS	CD-CE-NZ	5.13	123.49	111.70
1	O	176	GLU	CG-CD-OE2	5.12	128.54	118.30
1	E	176	GLU	OE1-CD-OE2	5.11	129.43	123.30
1	B	161	THR	CA-CB-OG1	-5.10	98.28	109.00
1	K	135	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	J	105	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	F	198	MET	CG-SD-CE	5.07	108.32	100.20
1	A	151	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	N	225	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	L	208	GLU	CG-CD-OE2	5.05	128.39	118.30
1	G	223	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	A	28	ARG	NH1-CZ-NH2	5.03	124.93	119.40
1	J	51	ASP	OD1-CG-OD2	-5.02	113.76	123.30
1	E	256	GLU	OE1-CD-OE2	5.00	129.30	123.30
1	P	56	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	ARG	Sidechain
1	B	108	ARG	Sidechain
1	B	11	ALA	Peptide
1	B	230	ARG	Sidechain
1	B	233	ARG	Sidechain
1	C	185	ARG	Sidechain
1	C	82	ARG	Sidechain
1	D	28	ARG	Sidechain
1	E	151	ARG	Sidechain
1	E	185	ARG	Sidechain
1	E	233	ARG	Sidechain
1	F	215	ARG	Sidechain
1	F	230	ARG	Sidechain
1	F	233	ARG	Sidechain
1	G	108	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	G	215	ARG	Sidechain
1	G	231	MET	Peptide
1	G	233	ARG	Sidechain
1	H	230	ARG	Sidechain
1	H	28	ARG	Sidechain
1	I	108	ARG	Sidechain
1	I	151	ARG	Sidechain
1	I	230	ARG	Sidechain
1	I	28	ARG	Sidechain
1	J	156	ASN	Peptide
1	J	185	ARG	Sidechain
1	J	225	ARG	Sidechain
1	J	233	ARG	Sidechain
1	K	225	ARG	Sidechain
1	L	108	ARG	Sidechain
1	L	230	ARG	Sidechain
1	L	28	ARG	Sidechain
1	M	108	ARG	Sidechain
1	M	135	ARG	Sidechain
1	M	151	ARG	Sidechain
1	M	181	GLY	Peptide
1	M	185	ARG	Sidechain
1	M	225	ARG	Sidechain
1	M	230	ARG	Sidechain
1	M	82	ARG	Sidechain
1	O	151	ARG	Sidechain
1	O	225	ARG	Sidechain
1	P	108	ARG	Sidechain
1	P	225	ARG	Sidechain

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1852	0	1857	145	0
1	B	1860	0	1868	120	1
1	C	1839	0	1841	118	1
1	D	1852	0	1857	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1847	0	1852	164	0
1	F	1847	0	1852	156	0
1	G	1847	0	1852	149	0
1	H	1852	0	1857	125	0
1	I	1860	0	1868	159	0
1	J	1852	0	1857	97	0
1	K	1852	0	1857	166	0
1	L	1852	0	1857	127	0
1	M	1847	0	1852	144	0
1	N	1852	0	1857	160	0
1	O	1847	0	1852	139	0
1	P	1847	0	1852	158	0
2	A	13	0	0	3	0
2	B	11	0	0	1	0
2	C	7	0	0	6	0
2	D	8	0	0	2	0
2	E	13	0	0	1	0
2	F	4	0	0	2	0
2	G	9	0	0	0	0
2	H	7	0	0	0	0
2	I	11	0	0	2	0
2	J	12	0	0	0	0
2	K	10	0	0	2	0
2	L	7	0	0	6	0
2	M	9	0	0	3	0
2	N	12	0	0	1	0
2	O	14	0	0	0	0
2	P	15	0	0	0	0
All	All	29767	0	29688	2005	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (2005) 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:P:157:ALA:O	1:P:160:CYS:N	1.75	1.19
1:A:54:GLY:HA2	2:A:311:HOH:O	1.46	1.13
1:N:165:ALA:HB1	1:P:161:THR:HG23	1.32	1.10
1:A:12:LEU:HB3	1:A:39:ALA:HB2	1.37	1.06
1:P:158:ALA:HA	1:P:161:THR:HB	1.31	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:MET:HA	1:K:206:TYR:HD2	1.17	1.03
1:G:237:MET:HA	1:G:259:MET:HE1	1.41	1.01
1:I:226:HIS:HD2	1:I:260:ASP:O	1.42	1.00
1:M:138:GLY:HA3	1:M:183:ASN:O	1.62	0.99
1:I:266:VAL:HG12	1:M:152:GLY:H	1.24	0.99
1:K:265:GLN:O	1:O:151:ARG:HB2	1.62	0.98
1:K:203:MET:HA	1:K:206:TYR:CD2	1.99	0.97
1:F:230:ARG:HG3	1:F:230:ARG:HH11	1.30	0.96
1:F:168:MET:HG3	1:H:161:THR:HG22	1.44	0.96
1:B:118:ILE:HG23	1:C:98:PHE:HE1	1.29	0.96
1:A:227:PRO:HG3	1:A:266:VAL:HG21	1.47	0.95
1:N:155:PHE:HA	1:P:176:GLU:OE2	1.67	0.94
1:A:203:MET:HB3	1:A:218:ALA:HB1	1.47	0.94
1:I:266:VAL:HG23	1:M:151:ARG:HH21	1.33	0.93
1:F:155:PHE:HE2	1:F:211:ALA:HB2	1.33	0.93
1:M:12:LEU:HB3	1:M:39:ALA:HB2	1.48	0.93
1:K:86:LEU:HD22	1:K:124:LEU:HD12	1.49	0.92
1:O:145:SER:HA	1:O:163:LYS:HD2	1.51	0.92
1:M:139:ALA:HB3	1:M:184:ILE:HG12	1.49	0.92
1:C:35:LYS:HG3	1:C:54:GLY:O	1.70	0.91
1:K:91:GLY:HA2	1:K:112:VAL:HG12	1.53	0.91
1:D:189:VAL:HA	1:D:257:PHE:O	1.71	0.90
1:L:187:ASN:OD1	1:L:188:SER:N	2.03	0.90
1:M:132:GLY:HA2	1:M:138:GLY:HA2	1.51	0.90
1:F:231:MET:HE2	2:F:301:HOH:O	1.71	0.90
1:M:99:GLU:OE2	1:O:182:TYR:HE2	1.55	0.90
1:I:226:HIS:CD2	1:I:260:ASP:O	2.25	0.90
1:K:134:ALA:O	1:K:135:ARG:HG3	1.72	0.89
1:G:151:ARG:HH21	1:G:153:ALA:HB2	1.37	0.89
1:C:82:ARG:CG	2:C:302:HOH:O	2.19	0.89
1:B:250:SER:OG	1:H:236:GLU:HG2	1.72	0.88
1:P:156:ASN:O	1:P:157:ALA:O	1.90	0.88
1:I:152:GLY:O	1:M:266:VAL:HB	1.72	0.87
1:K:196:THR:HB	1:K:197:PRO:HD2	1.55	0.87
1:F:112:VAL:O	1:F:116:SER:HB3	1.75	0.87
1:P:157:ALA:O	1:P:160:CYS:HB2	1.75	0.86
1:G:163:LYS:HA	1:G:166:VAL:HB	1.58	0.86
1:E:22:ALA:HA	1:E:27:GLY:HA3	1.58	0.85
1:H:227:PRO:HG2	1:H:262:GLY:HA3	1.59	0.85
1:I:266:VAL:HG12	1:M:152:GLY:N	1.90	0.85
1:O:130:GLU:OE1	1:O:133:LYS:HE3	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:139:ALA:O	1:M:184:ILE:HA	1.77	0.84
1:E:22:ALA:HA	1:E:27:GLY:CA	2.07	0.84
1:E:187:ASN:HB3	1:E:255:THR:HG22	1.60	0.84
1:N:176:GLU:OE2	1:P:155:PHE:HA	1.77	0.83
1:N:189:VAL:HA	1:N:257:PHE:O	1.78	0.83
1:K:196:THR:HB	1:K:197:PRO:CD	2.08	0.83
1:I:157:ALA:O	1:I:161:THR:HG23	1.76	0.83
1:O:130:GLU:OE1	1:O:133:LYS:CE	2.26	0.83
1:B:118:ILE:HG23	1:C:98:PHE:CE1	2.13	0.83
1:C:82:ARG:HG2	2:C:302:HOH:O	1.76	0.83
1:E:63:VAL:HB	1:E:116:SER:HB2	1.60	0.83
1:N:165:ALA:HB1	1:P:161:THR:CG2	2.08	0.83
1:A:173:LEU:HD21	1:D:98:PHE:CD1	2.14	0.82
1:E:82:ARG:NH2	1:E:134:ALA:HB3	1.94	0.82
1:I:10:ILE:HG22	1:I:10:ILE:O	1.78	0.82
1:N:83:VAL:O	1:N:131:GLY:HA3	1.79	0.82
1:L:44:THR:HB	1:L:61:HIS:HB2	1.61	0.82
1:F:231:MET:CE	2:F:301:HOH:O	2.27	0.82
1:B:32:LYS:HE2	1:B:53:GLU:HB3	1.62	0.82
1:C:82:ARG:CD	2:C:302:HOH:O	2.27	0.82
1:A:251:PHE:CD1	1:G:228:ILE:HD13	2.14	0.81
1:K:115:ASP:HA	1:K:118:ILE:HD12	1.62	0.81
1:G:86:LEU:HD22	1:G:128:LEU:HD11	1.62	0.81
1:H:253:THR:O	1:H:254:CYS:HB2	1.80	0.81
1:L:87:VAL:HA	1:L:142:VAL:O	1.81	0.81
1:B:204:ASP:O	1:B:207:VAL:HB	1.80	0.81
1:P:158:ALA:HA	1:P:161:THR:CB	2.10	0.81
1:N:221:ALA:HB1	1:N:225:ARG:NH2	1.94	0.81
1:E:97:LYS:HB2	1:E:100:ASP:HB2	1.62	0.81
1:N:16:VAL:HB	1:N:84:ASP:H	1.45	0.81
1:C:142:VAL:HG11	1:C:241:VAL:HG13	1.63	0.81
1:A:77:GLN:HA	1:A:81:GLY:HA2	1.63	0.81
1:I:237:MET:HA	1:I:259:MET:HE1	1.62	0.80
1:I:227:PRO:O	1:O:178:ALA:CB	2.28	0.80
1:G:151:ARG:HH21	1:G:153:ALA:CB	1.95	0.80
1:H:125:LEU:HG	1:H:129:LYS:HE3	1.62	0.80
1:F:215:ARG:O	1:F:219:GLN:HB2	1.81	0.79
1:N:91:GLY:HA2	1:N:112:VAL:HG12	1.64	0.79
1:D:171:LYS:HD3	1:E:265:GLN:HB3	1.63	0.79
1:K:259:MET:HA	1:M:252:VAL:HG22	1.62	0.79
1:B:101:THR:HG21	1:B:106:PHE:CD2	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:VAL:O	1:E:116:SER:HB3	1.82	0.79
1:I:190:HIS:NE2	1:I:256:GLU:HA	1.97	0.79
1:F:168:MET:HG3	1:H:161:THR:CG2	2.12	0.79
1:F:168:MET:SD	1:H:160:CYS:HB3	2.23	0.79
1:P:156:ASN:O	1:P:157:ALA:C	2.10	0.78
1:B:106:PHE:CE1	1:B:158:ALA:HA	2.17	0.78
1:E:115:ASP:OD2	1:G:107:HIS:NE2	2.16	0.78
1:F:31:VAL:HG21	1:F:52:VAL:CG1	2.14	0.78
1:C:77:GLN:OE1	1:C:127:LEU:HD21	1.82	0.78
1:A:248:ALA:HB1	1:G:239:GLY:HA3	1.66	0.78
1:F:114:VAL:HG11	1:H:106:PHE:CZ	2.19	0.78
1:E:155:PHE:HA	1:G:176:GLU:OE2	1.83	0.77
1:P:157:ALA:O	1:P:160:CYS:CA	2.32	0.77
1:P:106:PHE:CE1	1:P:161:THR:HG21	2.20	0.77
1:L:17:ALA:HA	1:L:85:ALA:O	1.84	0.77
1:O:156:ASN:O	1:O:159:TYR:N	2.18	0.77
1:D:185:ARG:HD3	1:D:250:SER:O	1.84	0.77
1:J:199:LEU:HA	1:J:202:LEU:HD12	1.66	0.77
1:E:180:LEU:HB2	1:E:182:TYR:CE2	2.20	0.76
1:P:145:SER:HB3	1:P:190:HIS:ND1	2.00	0.76
1:I:232:GLY:HA2	1:O:251:PHE:CE1	2.21	0.76
1:B:107:HIS:ND1	1:G:208:GLU:OE1	2.19	0.76
1:O:159:TYR:CE1	1:O:163:LYS:HG3	2.21	0.76
1:I:227:PRO:O	1:O:178:ALA:HB3	1.86	0.76
1:L:185:ARG:NH2	1:L:244:LEU:O	2.18	0.76
1:G:12:LEU:HD22	1:G:15:VAL:HG21	1.66	0.76
1:F:155:PHE:CE2	1:F:211:ALA:HB2	2.20	0.76
1:G:194:ILE:O	1:G:196:THR:N	2.19	0.75
1:P:192:GLY:O	1:P:194:ILE:HG12	1.86	0.75
1:D:203:MET:SD	1:D:219:GLN:HA	2.26	0.75
1:I:92:ILE:HG23	1:I:112:VAL:HG11	1.69	0.75
1:P:158:ALA:C	1:P:160:CYS:N	2.36	0.75
1:J:59:LEU:HD11	1:J:75:LEU:HD22	1.68	0.75
1:J:96:THR:O	1:J:155:PHE:HA	1.87	0.75
1:K:168:MET:SD	1:K:168:MET:O	2.44	0.75
1:F:168:MET:CE	1:H:148:ALA:O	2.36	0.74
1:P:106:PHE:HE1	1:P:161:THR:HG21	1.51	0.74
1:B:35:LYS:HG3	1:B:54:GLY:O	1.87	0.74
1:K:25:GLY:HA2	1:K:28:ARG:NH2	2.02	0.74
1:N:115:ASP:HA	1:N:118:ILE:HD12	1.68	0.74
1:G:49:SER:HA	1:G:58:TYR:CE2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:168:MET:SD	1:K:172:CYS:SG	2.86	0.74
1:M:94:ILE:HD12	1:M:109:VAL:HG22	1.69	0.74
1:O:266:VAL:HG23	1:O:266:VAL:O	1.88	0.74
1:I:232:GLY:CA	1:O:251:PHE:CE1	2.71	0.73
1:O:167:LYS:HD2	1:O:256:GLU:OE1	1.88	0.73
1:L:29:GLU:OE2	1:L:235:ALA:HB2	1.88	0.73
1:M:68:GLY:O	1:M:71:ALA:HB3	1.88	0.73
1:B:86:LEU:HD22	1:B:124:LEU:HD12	1.69	0.73
1:A:265:GLN:NE2	1:G:256:GLU:HG3	2.03	0.73
1:E:32:LYS:HG2	1:E:53:GLU:HB3	1.69	0.73
1:I:97:LYS:O	1:I:101:THR:N	2.21	0.73
1:G:45:ASP:O	1:G:61:HIS:N	2.21	0.73
1:C:25:GLY:O	1:C:29:GLU:HG2	1.89	0.73
1:D:238:GLY:O	1:D:242:VAL:HG23	1.89	0.73
1:N:86:LEU:HD13	1:N:124:LEU:HD12	1.70	0.73
1:P:55:ALA:HB1	1:P:57:HIS:O	1.88	0.73
1:L:260:ASP:HB2	1:L:263:PHE:CB	2.18	0.73
1:D:29:GLU:HG3	1:D:234:PRO:HB2	1.69	0.72
1:A:11:ALA:N	2:A:301:HOH:O	2.21	0.72
1:M:151:ARG:HD3	1:M:263:PHE:HE1	1.54	0.72
1:N:149:GLY:O	1:N:150:LEU:HD23	1.90	0.72
1:A:227:PRO:HG3	1:A:266:VAL:CG2	2.17	0.72
1:B:228:ILE:HD12	1:H:253:THR:HG22	1.71	0.72
1:F:13:ASN:OD1	1:F:38:ASN:HB2	1.90	0.72
1:L:26:ILE:HA	1:L:234:PRO:HB3	1.70	0.72
1:F:168:MET:HE1	1:H:148:ALA:O	1.89	0.72
1:N:180:LEU:HB3	1:N:182:TYR:CZ	2.25	0.72
1:I:238:GLY:O	1:I:242:VAL:HG23	1.88	0.72
1:P:252:VAL:HG12	1:P:255:THR:HG21	1.71	0.72
1:K:151:ARG:HB2	1:O:266:VAL:HA	1.72	0.72
1:B:63:VAL:HG21	1:B:90:ALA:HB1	1.71	0.72
1:M:91:GLY:HA2	1:M:112:VAL:HG12	1.72	0.72
1:J:95:VAL:HA	1:J:155:PHE:O	1.90	0.71
1:N:103:LEU:HD22	1:P:119:ILE:HD11	1.69	0.71
1:B:156:ASN:HB3	1:B:160:CYS:SG	2.30	0.71
1:M:180:LEU:O	1:M:182:TYR:N	2.23	0.71
1:N:221:ALA:HB1	1:N:225:ARG:CZ	2.20	0.71
1:P:157:ALA:O	1:P:160:CYS:CB	2.37	0.71
1:I:98:PHE:CE2	1:K:173:LEU:HD13	2.25	0.71
1:A:47:ALA:HB3	1:A:58:TYR:OH	1.90	0.71
1:B:238:GLY:O	1:B:242:VAL:HG23	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:HIS:HB2	1:G:208:GLU:HG2	1.73	0.71
1:D:95:VAL:HA	1:D:155:PHE:O	1.89	0.71
1:I:186:VAL:O	1:I:254:CYS:N	2.19	0.71
1:K:141:VAL:N	1:K:185:ARG:O	2.22	0.70
1:K:83:VAL:HG23	1:K:127:LEU:HD13	1.73	0.70
1:O:227:PRO:HG3	1:O:266:VAL:CG2	2.21	0.70
1:P:207:VAL:HA	1:P:212:ALA:O	1.90	0.70
1:L:266:VAL:O	1:P:151:ARG:CZ	2.40	0.70
1:D:20:THR:O	1:D:89:ASN:HB3	1.92	0.70
1:G:226:HIS:CE1	1:G:263:PHE:HD2	2.09	0.70
1:M:132:GLY:HA2	1:M:138:GLY:CA	2.21	0.70
1:H:96:THR:HA	1:H:209:LEU:HD11	1.73	0.70
1:I:118:ILE:HD13	1:K:103:LEU:CD1	2.20	0.70
1:E:56:ASP:HB2	1:E:57:HIS:CD2	2.27	0.70
1:I:160:CYS:HB3	1:K:168:MET:SD	2.32	0.70
1:N:75:LEU:HD11	1:N:79:LYS:HE3	1.74	0.70
1:L:222:MET:HA	1:L:225:ARG:HD2	1.72	0.69
1:E:69:TRP:O	1:E:72:VAL:HB	1.92	0.69
1:B:29:GLU:HG3	1:B:234:PRO:HB2	1.73	0.69
1:C:145:SER:HG	1:C:146:SER:H	1.37	0.69
1:J:24:GLY:O	1:J:28:ARG:NH1	2.25	0.69
1:E:93:SER:HB3	1:E:198:MET:SD	2.33	0.69
1:J:151:ARG:NH2	1:N:266:VAL:HB	2.07	0.69
1:A:221:ALA:O	1:A:225:ARG:HG3	1.92	0.69
1:E:32:LYS:HE2	1:E:53:GLU:HB3	1.73	0.69
1:N:122:GLN:NE2	1:P:101:THR:O	2.25	0.69
1:A:161:THR:HG22	1:D:169:LEU:HA	1.75	0.69
1:A:192:GLY:O	1:A:194:ILE:HG12	1.93	0.69
1:B:266:VAL:HG23	1:B:266:VAL:O	1.92	0.69
1:G:132:GLY:HA3	1:G:183:ASN:HB3	1.75	0.69
1:G:133:LYS:HB3	1:K:217:VAL:HG11	1.73	0.69
1:O:27:GLY:HA2	1:O:30:LEU:HD12	1.75	0.69
1:K:94:ILE:HD11	1:K:108:ARG:HH21	1.58	0.69
1:K:215:ARG:NH2	2:K:301:HOH:O	2.25	0.69
1:E:193:GLY:HA3	1:E:222:MET:SD	2.32	0.68
1:L:64:THR:HG22	1:L:111:THR:O	1.94	0.68
1:N:65:SER:O	1:N:69:TRP:HD1	1.75	0.68
1:N:114:VAL:HG22	1:N:166:VAL:HG23	1.73	0.68
1:D:66:GLU:HG3	1:D:123:VAL:HG21	1.75	0.68
1:D:145:SER:OG	1:D:146:SER:N	2.27	0.68
1:A:67:ALA:HA	1:A:70:LYS:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:THR:HA	1:D:115:ASP:HB2	1.74	0.68
1:I:96:THR:HG23	1:I:101:THR:OG1	1.93	0.68
1:N:97:LYS:HA	1:N:155:PHE:HD1	1.59	0.68
1:P:83:VAL:HG21	1:P:124:LEU:HD13	1.76	0.68
1:A:191:PRO:HB3	1:A:237:MET:SD	2.34	0.68
1:E:176:GLU:OE2	1:G:157:ALA:HB2	1.93	0.68
1:H:199:LEU:HA	1:H:202:LEU:HG	1.74	0.68
1:H:206:TYR:O	1:H:211:ALA:HB3	1.94	0.68
1:P:92:ILE:HD11	1:P:109:VAL:HG22	1.75	0.68
1:N:103:LEU:HD21	1:P:115:ASP:OD1	1.93	0.68
1:K:142:VAL:HG22	1:K:244:LEU:HD13	1.74	0.67
1:E:146:SER:HA	1:E:191:PRO:HD2	1.77	0.67
1:K:27:GLY:O	1:K:31:VAL:HG23	1.94	0.67
1:C:213:PRO:HD2	1:C:217:VAL:HG11	1.75	0.67
1:H:227:PRO:HG3	1:H:266:VAL:CG2	2.25	0.67
1:I:118:ILE:CD1	1:K:103:LEU:CD1	2.72	0.67
1:I:227:PRO:O	1:O:178:ALA:HB1	1.94	0.67
1:D:151:ARG:HD3	1:D:263:PHE:CE2	2.30	0.67
1:E:69:TRP:CD2	1:E:120:GLY:HA2	2.29	0.67
1:L:89:ASN:ND2	2:L:302:HOH:O	2.27	0.67
1:N:97:LYS:HE2	1:N:209:LEU:HD23	1.76	0.67
1:E:63:VAL:CB	1:E:116:SER:HB2	2.24	0.67
1:H:151:ARG:HH12	1:H:225:ARG:NE	1.93	0.67
1:B:101:THR:CG2	1:B:106:PHE:HD2	2.08	0.67
1:M:99:GLU:OE2	1:O:182:TYR:CE2	2.45	0.67
1:O:96:THR:HG23	1:O:101:THR:OG1	1.94	0.67
1:P:241:VAL:HA	1:P:244:LEU:HD12	1.76	0.67
1:O:223:GLU:O	1:O:225:ARG:N	2.28	0.67
1:B:150:LEU:HD12	1:B:190:HIS:ND1	2.10	0.67
1:F:96:THR:HG21	1:F:101:THR:HG22	1.74	0.67
1:F:216:GLU:HA	1:F:219:GLN:HB3	1.77	0.67
1:G:26:ILE:HG13	1:G:196:THR:HG21	1.77	0.67
1:H:227:PRO:HG3	1:H:266:VAL:HG21	1.77	0.67
1:K:185:ARG:NH1	1:K:244:LEU:O	2.27	0.67
1:L:52:VAL:HB	1:L:55:ALA:HB2	1.77	0.67
1:L:197:PRO:HD2	2:L:306:HOH:O	1.93	0.67
1:L:197:PRO:HG2	2:L:306:HOH:O	1.95	0.67
1:L:94:ILE:HG22	1:L:96:THR:HG22	1.77	0.66
1:D:253:THR:HG21	1:E:228:ILE:HD12	1.77	0.66
1:K:125:LEU:HB3	1:K:126:PRO:HD3	1.76	0.66
1:I:152:GLY:H	1:M:266:VAL:HG12	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:63:VAL:HG23	1:P:63:VAL:O	1.95	0.66
1:H:153:ALA:HB3	1:H:160:CYS:SG	2.36	0.66
1:N:16:VAL:H	1:N:84:ASP:HB2	1.59	0.66
1:F:145:SER:HB3	1:F:190:HIS:CD2	2.31	0.66
1:F:185:ARG:HD2	1:F:252:VAL:O	1.96	0.66
1:J:146:SER:O	1:J:149:GLY:N	2.29	0.66
1:K:196:THR:CB	1:K:197:PRO:CD	2.74	0.66
1:P:31:VAL:HG11	1:P:52:VAL:HG12	1.78	0.66
1:F:115:ASP:CG	1:H:103:LEU:HD11	2.16	0.66
1:E:63:VAL:CG2	1:E:116:SER:HB2	2.25	0.66
1:N:160:CYS:HB2	1:P:172:CYS:SG	2.36	0.66
1:A:76:ALA:O	1:A:81:GLY:N	2.29	0.66
1:O:223:GLU:C	1:O:225:ARG:H	1.99	0.66
1:K:196:THR:CB	1:K:197:PRO:HD2	2.26	0.66
1:M:82:ARG:HH21	1:M:131:GLY:HA2	1.61	0.66
1:F:247:ASP:C	1:F:249:ALA:H	1.99	0.65
1:H:94:ILE:O	1:H:94:ILE:HG22	1.94	0.65
1:I:94:ILE:HD12	1:I:105:ASP:CG	2.16	0.65
1:A:97:LYS:HE2	1:D:180:LEU:HD21	1.78	0.65
1:C:187:ASN:HB2	1:C:244:LEU:HD13	1.78	0.65
1:K:206:TYR:O	1:K:211:ALA:HB3	1.96	0.65
1:A:136:ALA:O	1:A:183:ASN:ND2	2.28	0.65
1:B:48:PRO:HA	1:B:60:GLN:HB2	1.78	0.65
1:C:151:ARG:HD3	1:C:264:SER:HA	1.77	0.65
1:J:92:ILE:HD11	1:J:109:VAL:HA	1.78	0.65
1:K:68:GLY:O	1:K:71:ALA:HB3	1.95	0.65
1:N:160:CYS:CB	1:P:172:CYS:SG	2.84	0.65
1:P:145:SER:CB	1:P:190:HIS:ND1	2.60	0.65
1:H:195:ASP:HA	1:H:199:LEU:HD23	1.79	0.65
1:J:26:ILE:HD11	1:J:194:ILE:HG21	1.76	0.65
1:P:16:VAL:HG11	1:P:80:TYR:CD2	2.31	0.65
1:B:97:LYS:HG3	1:B:209:LEU:HD22	1.79	0.65
1:I:118:ILE:HA	1:K:98:PHE:HZ	1.61	0.65
1:I:190:HIS:NE2	1:I:256:GLU:CA	2.59	0.65
1:J:262:GLY:O	1:J:264:SER:N	2.29	0.65
1:O:85:ALA:HA	1:O:140:SER:O	1.96	0.65
1:P:106:PHE:HE1	1:P:161:THR:CG2	2.10	0.65
1:G:144:PHE:O	1:G:166:VAL:HG11	1.97	0.65
1:F:97:LYS:O	1:F:101:THR:HG23	1.97	0.65
1:I:139:ALA:HB3	1:I:184:ILE:HA	1.79	0.65
1:L:16:VAL:HG22	1:L:40:ILE:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:MET:HA	1:F:206:TYR:HD2	1.62	0.65
1:K:185:ARG:HD2	1:K:249:ALA:O	1.96	0.65
1:M:74:ALA:HA	1:M:77:GLN:HB3	1.78	0.65
1:M:87:VAL:O	1:M:87:VAL:HG12	1.97	0.65
1:N:160:CYS:CB	1:P:172:CYS:HG	2.10	0.65
1:J:230:ARG:NH1	1:J:231:MET:O	2.29	0.65
1:O:155:PHE:C	1:O:157:ALA:H	2.01	0.65
1:H:158:ALA:O	1:H:162:SER:N	2.24	0.64
1:M:238:GLY:O	1:M:242:VAL:HG23	1.97	0.64
1:F:20:THR:O	1:F:89:ASN:HB3	1.95	0.64
1:K:232:GLY:HA3	1:M:251:PHE:CG	2.32	0.64
1:O:151:ARG:HD3	1:O:263:PHE:HE1	1.62	0.64
1:E:102:PRO:HD2	1:E:105:ASP:HB2	1.78	0.64
1:F:106:PHE:O	1:F:110:ASN:ND2	2.31	0.64
1:H:196:THR:HB	1:H:197:PRO:CD	2.28	0.64
1:M:145:SER:O	1:M:191:PRO:HD2	1.97	0.64
1:N:99:GLU:HB3	1:P:125:LEU:HD23	1.79	0.64
1:O:69:TRP:HB3	1:O:123:VAL:HG11	1.80	0.64
1:O:94:ILE:HG22	1:O:158:ALA:HB3	1.79	0.64
1:G:79:LYS:HB2	1:G:80:TYR:CE2	2.32	0.64
1:L:106:PHE:CE1	1:L:158:ALA:HA	2.33	0.64
1:O:213:PRO:HB2	1:O:217:VAL:HG21	1.79	0.64
1:P:29:GLU:HG3	1:P:234:PRO:HB2	1.80	0.64
1:D:185:ARG:CD	1:D:250:SER:O	2.46	0.64
1:E:185:ARG:NH1	1:E:244:LEU:O	2.29	0.64
1:G:12:LEU:CD2	1:G:15:VAL:HG21	2.27	0.64
1:I:89:ASN:CG	1:I:89:ASN:O	2.35	0.64
1:K:229:GLY:O	1:K:230:ARG:HB3	1.98	0.64
1:M:31:VAL:HG11	1:M:52:VAL:HG12	1.79	0.64
1:A:183:ASN:O	1:A:184:ILE:HG13	1.97	0.64
1:K:124:LEU:O	1:K:128:LEU:HG	1.97	0.64
1:M:182:TYR:HB3	1:M:184:ILE:HD12	1.79	0.64
1:K:44:THR:HB	1:K:61:HIS:HB3	1.80	0.64
1:K:142:VAL:HG22	1:K:244:LEU:CD1	2.28	0.64
1:K:145:SER:OG	1:K:146:SER:N	2.25	0.64
1:M:162:SER:HA	1:M:165:ALA:HB3	1.79	0.64
1:P:97:LYS:HG3	1:P:209:LEU:HD22	1.79	0.64
1:C:230:ARG:HH22	1:C:236:GLU:CD	2.01	0.64
1:G:237:MET:HA	1:G:259:MET:CE	2.23	0.64
1:H:18:VAL:HG22	1:H:42:ILE:HB	1.80	0.64
1:K:11:ALA:N	2:K:302:HOH:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:248:ALA:HB1	1:M:239:GLY:HA3	1.79	0.64
1:K:258:VAL:HG12	1:K:260:ASP:CG	2.18	0.64
1:A:21:GLY:HA2	1:A:45:ASP:OD2	1.97	0.64
1:C:167:LYS:O	1:C:170:SER:HB2	1.98	0.64
1:I:123:VAL:HG12	1:I:124:LEU:HD23	1.80	0.64
1:K:147:VAL:HG11	1:K:260:ASP:HB2	1.80	0.64
1:G:111:THR:HA	1:G:115:ASP:HB2	1.79	0.64
1:A:161:THR:HG22	1:D:169:LEU:CA	2.27	0.63
1:B:19:VAL:O	1:B:22:ALA:HB2	1.97	0.63
1:E:146:SER:OG	1:E:147:VAL:N	2.31	0.63
1:G:151:ARG:CZ	1:G:152:GLY:O	2.45	0.63
1:B:147:VAL:HG11	1:B:263:PHE:HB3	1.81	0.63
1:M:125:LEU:HB3	1:M:126:PRO:HD3	1.79	0.63
1:O:125:LEU:O	1:O:129:LYS:HG3	1.97	0.63
1:J:262:GLY:O	1:J:263:PHE:C	2.37	0.63
1:C:82:ARG:HD3	2:C:302:HOH:O	1.94	0.63
1:N:111:THR:HA	1:N:115:ASP:CG	2.19	0.63
1:O:226:HIS:O	1:O:229:GLY:N	2.30	0.63
1:F:102:PRO:C	1:F:104:SER:H	2.01	0.63
1:H:12:LEU:HD21	1:H:242:VAL:HG13	1.78	0.63
1:H:16:VAL:N	1:H:84:ASP:OD2	2.27	0.63
1:B:101:THR:HG21	1:B:106:PHE:HD2	1.63	0.63
1:B:159:TYR:CZ	1:B:163:LYS:HG3	2.33	0.63
1:C:265:GLN:HG3	1:F:255:THR:HA	1.79	0.63
1:K:113:ASN:HB2	1:K:162:SER:HB2	1.81	0.63
1:C:145:SER:OG	1:C:146:SER:N	2.31	0.63
1:C:152:GLY:CA	1:H:266:VAL:HG12	2.29	0.63
1:D:225:ARG:HD3	1:D:263:PHE:HE1	1.62	0.63
1:G:151:ARG:HD3	1:G:263:PHE:HE1	1.63	0.63
1:M:35:LYS:HG3	1:M:54:GLY:O	1.98	0.63
1:E:187:ASN:CB	1:E:255:THR:HG22	2.29	0.63
1:F:145:SER:O	1:F:191:PRO:HD3	1.99	0.63
1:F:168:MET:CG	1:H:161:THR:HG22	2.25	0.63
1:I:69:TRP:O	1:I:72:VAL:HB	1.98	0.63
1:L:261:GLY:HA2	1:N:251:PHE:O	1.99	0.63
1:B:125:LEU:HD12	1:B:184:ILE:HD13	1.81	0.62
1:D:265:GLN:OE1	1:E:171:LYS:HE2	1.99	0.62
1:G:199:LEU:HD21	1:G:231:MET:HE3	1.81	0.62
1:P:158:ALA:O	1:P:159:TYR:C	2.35	0.62
1:E:45:ASP:OD1	1:E:46:MET:N	2.32	0.62
1:J:173:LEU:HD22	1:J:177:PHE:CZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:102:PRO:HG2	1:K:105:ASP:OD2	1.99	0.62
1:G:169:LEU:O	1:G:172:CYS:N	2.33	0.62
1:H:135:ARG:NH2	1:H:245:CYS:O	2.32	0.62
1:K:26:ILE:HD11	1:K:194:ILE:HG21	1.81	0.62
1:M:46:MET:O	1:M:60:GLN:HG3	2.00	0.62
1:M:118:ILE:HG23	1:O:98:PHE:HE1	1.63	0.62
1:A:151:ARG:NE	1:E:266:VAL:C	2.53	0.62
1:B:240:GLY:O	1:B:243:TYR:HB3	1.99	0.62
1:D:156:ASN:HB2	1:D:160:CYS:SG	2.39	0.62
1:I:15:VAL:HG13	1:I:84:ASP:HB2	1.81	0.62
1:I:98:PHE:CE2	1:K:173:LEU:CD1	2.82	0.62
1:O:130:GLU:OE1	1:O:133:LYS:NZ	2.31	0.62
1:O:227:PRO:HG3	1:O:266:VAL:HG22	1.80	0.62
1:F:142:VAL:HG11	1:F:241:VAL:HG22	1.80	0.62
1:I:140:SER:OG	1:I:245:CYS:HA	1.98	0.62
1:J:69:TRP:CD2	1:J:120:GLY:HA2	2.35	0.62
1:E:117:ILE:CD1	1:E:166:VAL:HG13	2.29	0.62
1:A:222:MET:SD	1:A:231:MET:SD	2.97	0.62
1:D:109:VAL:O	1:D:109:VAL:HG12	1.98	0.62
1:K:30:LEU:HD23	1:K:238:GLY:HA2	1.80	0.62
1:I:103:LEU:HD11	1:K:115:ASP:OD1	2.00	0.62
1:M:135:ARG:O	1:M:136:ALA:C	2.37	0.62
1:D:205:LYS:NZ	2:D:302:HOH:O	2.30	0.62
1:P:42:ILE:HD11	1:P:80:TYR:HE2	1.64	0.62
1:C:145:SER:HG	1:C:190:HIS:CE1	2.17	0.62
1:D:146:SER:O	1:D:149:GLY:N	2.29	0.62
1:E:99:GLU:OE2	1:G:125:LEU:HD21	2.00	0.62
1:K:138:GLY:O	1:K:185:ARG:NH2	2.29	0.62
1:F:102:PRO:C	1:F:104:SER:N	2.53	0.61
1:N:155:PHE:CA	1:P:176:GLU:OE2	2.44	0.61
1:O:86:LEU:HD22	1:O:128:LEU:HD11	1.82	0.61
1:E:147:VAL:HG22	1:E:192:GLY:HA2	1.82	0.61
1:G:114:VAL:HG22	1:G:166:VAL:HG23	1.82	0.61
1:H:142:VAL:O	1:H:142:VAL:HG12	1.98	0.61
1:P:145:SER:HB3	1:P:190:HIS:CE1	2.35	0.61
1:L:29:GLU:HG3	1:L:234:PRO:HB2	1.82	0.61
1:L:266:VAL:HA	1:P:151:ARG:HB2	1.82	0.61
1:A:266:VAL:O	1:E:151:ARG:NE	2.33	0.61
1:B:93:SER:HA	1:B:159:TYR:CD1	2.35	0.61
1:C:189:VAL:HG21	1:C:241:VAL:HG22	1.82	0.61
1:K:152:GLY:O	1:O:266:VAL:HG12	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:44:THR:HB	1:L:61:HIS:CB	2.31	0.61
1:L:87:VAL:HG22	1:L:142:VAL:HB	1.81	0.61
1:N:62:ASP:HB3	1:N:65:SER:HB3	1.81	0.61
1:F:102:PRO:O	1:F:104:SER:N	2.33	0.61
1:L:260:ASP:HB2	1:L:263:PHE:HB3	1.83	0.61
1:N:59:LEU:HD13	1:N:72:VAL:HG13	1.82	0.61
1:P:12:LEU:HD21	1:P:245:CYS:HB2	1.81	0.61
1:B:63:VAL:HG21	1:B:90:ALA:CB	2.29	0.61
1:G:86:LEU:HB3	1:G:141:VAL:HG22	1.81	0.61
1:H:123:VAL:O	1:H:123:VAL:CG1	2.49	0.61
1:K:134:ALA:O	1:K:135:ARG:CG	2.48	0.61
1:A:242:VAL:O	1:A:246:SER:N	2.33	0.61
1:I:29:GLU:HG3	1:I:234:PRO:HB2	1.83	0.61
1:K:187:ASN:ND2	1:K:244:LEU:HD22	2.15	0.61
1:A:135:ARG:NH2	1:A:245:CYS:O	2.34	0.61
1:F:34:MET:HG2	1:F:242:VAL:HG22	1.83	0.61
1:I:199:LEU:HD12	1:I:202:LEU:HD12	1.83	0.61
1:L:16:VAL:HA	1:L:40:ILE:HB	1.81	0.61
1:L:242:VAL:O	1:L:246:SER:N	2.32	0.61
1:N:94:ILE:HG22	1:N:95:VAL:N	2.14	0.61
1:A:257:PHE:CE1	1:G:257:PHE:CE1	2.89	0.61
1:E:117:ILE:HD11	1:E:166:VAL:HG13	1.83	0.61
1:I:164:ALA:HB2	1:K:168:MET:CB	2.30	0.61
1:J:22:ALA:HA	1:J:27:GLY:HA3	1.83	0.61
1:J:164:ALA:HB2	1:L:168:MET:HE3	1.83	0.61
1:K:31:VAL:HG11	1:K:53:GLU:O	2.01	0.61
1:K:265:GLN:O	1:O:151:ARG:CB	2.44	0.61
1:E:45:ASP:O	1:E:60:GLN:HA	2.01	0.60
1:F:55:ALA:HB1	1:F:57:HIS:O	2.00	0.60
1:C:91:GLY:HA2	1:C:113:ASN:OD1	2.00	0.60
1:D:35:LYS:HG3	1:D:54:GLY:O	2.01	0.60
1:I:20:THR:O	1:I:89:ASN:HB3	2.01	0.60
1:A:266:VAL:C	1:E:151:ARG:HE	2.03	0.60
1:B:11:ALA:O	1:B:246:SER:HB2	2.01	0.60
1:D:128:LEU:HB3	1:D:184:ILE:HG21	1.81	0.60
1:E:187:ASN:OD1	1:E:252:VAL:HG12	2.01	0.60
1:M:82:ARG:NH2	1:M:84:ASP:OD1	2.34	0.60
1:K:257:PHE:CE1	1:M:257:PHE:HD2	2.19	0.60
1:M:148:ALA:HB1	1:M:160:CYS:SG	2.41	0.60
1:A:29:GLU:OE1	1:A:32:LYS:HD2	2.01	0.60
1:B:187:ASN:OD1	1:B:255:THR:HG22	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:THR:HA	1:C:115:ASP:OD2	2.01	0.60
1:G:151:ARG:NH2	1:G:152:GLY:O	2.33	0.60
1:I:214:SER:OG	1:I:217:VAL:HG23	2.01	0.60
1:B:221:ALA:HA	1:B:224:MET:SD	2.42	0.60
1:C:198:MET:O	1:C:202:LEU:HG	2.01	0.60
1:D:145:SER:HA	1:D:163:LYS:HD2	1.82	0.60
1:F:20:THR:HG21	1:F:69:TRP:CH2	2.36	0.60
1:G:167:LYS:O	1:G:171:LYS:HE3	2.02	0.60
1:I:164:ALA:CB	1:K:168:MET:HB3	2.31	0.60
1:J:219:GLN:HG2	1:J:223:GLU:OE1	2.02	0.60
1:L:26:ILE:O	1:L:30:LEU:N	2.32	0.60
1:M:163:LYS:O	1:M:166:VAL:HB	2.01	0.60
1:N:223:GLU:HG2	1:N:231:MET:HG3	1.83	0.60
1:O:23:ALA:HA	1:O:28:ARG:HG2	1.84	0.60
1:A:251:PHE:HD1	1:G:228:ILE:HD13	1.67	0.60
1:B:166:VAL:O	1:B:170:SER:OG	2.19	0.60
1:C:87:VAL:HA	1:C:142:VAL:HB	1.82	0.60
1:N:180:LEU:HB2	1:N:182:TYR:CE2	2.37	0.60
1:P:72:VAL:O	1:P:72:VAL:HG12	2.01	0.60
1:P:158:ALA:O	1:P:160:CYS:N	2.35	0.60
1:C:243:TYR:OH	1:F:239:GLY:HA3	2.00	0.60
1:F:31:VAL:HG21	1:F:52:VAL:HG13	1.83	0.60
1:G:226:HIS:HD2	1:G:260:ASP:O	1.85	0.60
1:H:123:VAL:O	1:H:123:VAL:HG12	2.00	0.60
1:K:146:SER:HA	1:K:191:PRO:HD2	1.83	0.60
1:P:142:VAL:CG1	1:P:189:VAL:HG23	2.32	0.60
1:A:151:ARG:CZ	1:E:266:VAL:C	2.70	0.60
1:F:110:ASN:O	1:F:114:VAL:HB	2.02	0.60
1:N:145:SER:O	1:N:146:SER:HB2	2.02	0.60
1:P:31:VAL:HG13	1:P:41:VAL:HG11	1.84	0.60
1:A:164:ALA:HA	1:A:167:LYS:HB3	1.84	0.59
1:I:98:PHE:CD2	1:K:173:LEU:HD22	2.37	0.59
1:K:252:VAL:HG13	1:K:255:THR:HG21	1.82	0.59
1:L:56:ASP:O	1:L:57:HIS:ND1	2.35	0.59
1:M:111:THR:O	1:M:116:SER:HB3	2.02	0.59
1:A:173:LEU:HD11	1:D:98:PHE:CZ	2.37	0.59
1:E:26:ILE:HD11	1:E:194:ILE:HG21	1.83	0.59
1:H:15:VAL:HG22	1:H:135:ARG:HD2	1.84	0.59
1:I:152:GLY:N	1:M:266:VAL:HG12	2.17	0.59
1:N:20:THR:O	1:N:89:ASN:HB3	2.02	0.59
1:H:56:ASP:HB2	1:H:57:HIS:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:91:GLY:CA	1:K:112:VAL:HG12	2.29	0.59
1:O:129:LYS:HE2	1:O:182:TYR:CG	2.37	0.59
1:O:227:PRO:CG	1:O:266:VAL:HG22	2.32	0.59
1:A:251:PHE:HB2	1:G:236:GLU:OE1	2.03	0.59
1:G:226:HIS:CE1	1:G:263:PHE:CD2	2.90	0.59
1:J:12:LEU:HB3	1:J:39:ALA:HB2	1.82	0.59
1:J:74:ALA:O	1:J:77:GLN:HB3	2.02	0.59
1:A:173:LEU:HD21	1:D:98:PHE:CE1	2.38	0.59
1:A:254:CYS:O	1:G:265:GLN:HG3	2.02	0.59
1:F:96:THR:CG2	1:F:101:THR:HG22	2.31	0.59
1:G:200:GLY:HA2	1:G:215:ARG:NH2	2.18	0.59
1:L:26:ILE:CA	1:L:234:PRO:HB3	2.32	0.59
1:L:185:ARG:HB3	1:L:253:THR:HB	1.83	0.59
1:E:246:SER:O	1:E:248:ALA:N	2.35	0.59
1:P:143:ASN:HB3	1:P:166:VAL:HG13	1.83	0.59
1:D:15:VAL:HG13	1:D:84:ASP:CB	2.32	0.59
1:E:18:VAL:HG22	1:E:42:ILE:HB	1.85	0.59
1:E:246:SER:C	1:E:248:ALA:H	2.06	0.59
1:J:30:LEU:HD13	1:J:241:VAL:HG21	1.84	0.59
1:F:44:THR:HB	1:F:61:HIS:HB3	1.85	0.59
1:I:228:ILE:CG2	1:I:261:GLY:HA3	2.32	0.59
1:N:166:VAL:O	1:N:169:LEU:HB3	2.03	0.59
1:N:176:GLU:O	1:N:180:LEU:HG	2.03	0.59
1:H:203:MET:O	1:H:206:TYR:HB2	2.02	0.59
1:E:69:TRP:HZ3	1:E:124:LEU:HD11	1.68	0.59
1:E:145:SER:HA	1:E:163:LYS:HD2	1.85	0.59
1:H:31:VAL:HG13	1:H:41:VAL:HG21	1.85	0.59
1:L:12:LEU:HB3	1:L:39:ALA:HB2	1.84	0.59
1:P:16:VAL:HG22	1:P:40:ILE:CD1	2.33	0.59
1:O:263:PHE:CD1	1:O:263:PHE:C	2.75	0.58
1:D:137:GLY:HA3	1:D:250:SER:HB2	1.85	0.58
1:E:112:VAL:O	1:E:116:SER:CB	2.51	0.58
1:H:20:THR:O	1:H:89:ASN:HB3	2.03	0.58
1:H:26:ILE:O	1:H:30:LEU:HG	2.03	0.58
1:K:135:ARG:NH2	1:K:245:CYS:O	2.35	0.58
1:L:58:TYR:C	1:L:59:LEU:HD12	2.23	0.58
1:M:56:ASP:O	1:M:57:HIS:CG	2.56	0.58
1:O:216:GLU:HA	1:O:219:GLN:HB3	1.85	0.58
1:F:44:THR:O	1:F:45:ASP:HB2	2.03	0.58
1:F:56:ASP:O	1:F:57:HIS:CG	2.56	0.58
1:H:198:MET:HG2	1:H:198:MET:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:253:THR:O	1:H:254:CYS:CB	2.49	0.58
1:N:48:PRO:HA	1:N:60:GLN:OE1	2.04	0.58
1:F:160:CYS:HB3	1:H:168:MET:SD	2.44	0.58
1:A:118:ILE:HG21	1:D:103:LEU:CD1	2.33	0.58
1:B:101:THR:CG2	1:B:106:PHE:CD2	2.84	0.58
1:H:140:SER:HB3	1:H:245:CYS:HA	1.84	0.58
1:C:152:GLY:C	1:H:266:VAL:HG12	2.24	0.58
1:C:241:VAL:O	1:C:244:LEU:N	2.37	0.58
1:F:260:ASP:HB2	1:F:263:PHE:HB3	1.85	0.58
1:H:115:ASP:HA	1:H:118:ILE:HD12	1.85	0.58
1:K:227:PRO:HG3	1:K:266:VAL:HG21	1.85	0.58
1:M:145:SER:C	1:M:191:PRO:HD2	2.24	0.58
1:O:96:THR:O	1:O:155:PHE:O	2.22	0.58
1:P:64:THR:HG22	1:P:111:THR:HG22	1.85	0.58
1:I:92:ILE:HG12	1:I:112:VAL:HB	1.86	0.58
1:L:49:SER:OG	2:L:301:HOH:O	2.17	0.58
1:H:185:ARG:NH2	1:H:246:SER:O	2.37	0.58
1:A:223:GLU:HG2	1:A:231:MET:HG3	1.85	0.58
1:I:27:GLY:HA2	1:I:30:LEU:HD12	1.86	0.58
1:A:257:PHE:HE1	1:G:257:PHE:CE1	2.22	0.57
1:E:180:LEU:HD12	1:E:182:TYR:HE2	1.69	0.57
1:F:182:TYR:O	1:F:184:ILE:N	2.37	0.57
1:E:13:ASN:HA	2:E:301:HOH:O	2.03	0.57
1:K:86:LEU:CD2	1:K:124:LEU:HD12	2.29	0.57
1:L:66:GLU:HA	1:L:119:ILE:HG21	1.85	0.57
1:P:146:SER:HB3	1:P:148:ALA:HB3	1.86	0.57
1:J:262:GLY:O	1:J:265:GLN:N	2.37	0.57
1:N:44:THR:HB	1:N:61:HIS:HB3	1.86	0.57
1:A:16:VAL:HG21	1:A:80:TYR:HB3	1.86	0.57
1:A:161:THR:CG2	1:D:169:LEU:HA	2.33	0.57
1:C:97:LYS:HD2	1:C:100:ASP:OD2	2.04	0.57
1:E:31:VAL:HG13	1:E:55:ALA:HB2	1.86	0.57
1:E:144:PHE:HA	1:E:189:VAL:HB	1.87	0.57
1:F:168:MET:HE3	1:H:148:ALA:O	2.04	0.57
1:L:260:ASP:OD2	1:L:264:SER:N	2.37	0.57
1:B:32:LYS:HE2	1:B:53:GLU:CB	2.33	0.57
1:F:161:THR:HA	1:H:168:MET:HG3	1.86	0.57
1:I:164:ALA:HB2	1:K:168:MET:HB3	1.86	0.57
1:N:16:VAL:O	1:N:85:ALA:N	2.32	0.57
1:A:132:GLY:HA2	1:A:183:ASN:HB3	1.85	0.57
1:G:203:MET:HA	1:G:206:TYR:HD2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:146:SER:H	1:I:190:HIS:HA	1.69	0.57
1:D:253:THR:CG2	1:E:228:ILE:HD12	2.34	0.57
1:J:159:TYR:CE1	1:J:163:LYS:HE2	2.39	0.57
1:K:42:ILE:HG12	1:K:57:HIS:HB2	1.86	0.57
1:M:48:PRO:HA	1:M:60:GLN:HB2	1.87	0.57
1:F:168:MET:SD	1:F:172:CYS:SG	3.03	0.57
1:K:69:TRP:CD2	1:K:120:GLY:HA2	2.40	0.57
1:N:146:SER:C	1:N:148:ALA:H	2.06	0.57
1:A:26:ILE:HD11	1:A:194:ILE:HG21	1.87	0.57
1:B:31:VAL:HG11	1:B:52:VAL:HG12	1.85	0.57
1:B:98:PHE:O	1:B:101:THR:HB	2.05	0.57
1:B:237:MET:HA	1:B:259:MET:CE	2.35	0.57
1:N:59:LEU:HD22	1:N:72:VAL:HA	1.87	0.57
1:N:102:PRO:HB2	1:N:104:SER:OG	2.05	0.57
1:N:150:LEU:O	1:N:151:ARG:HB3	2.05	0.57
1:O:219:GLN:O	1:O:222:MET:HB3	2.05	0.57
1:C:82:ARG:NH2	1:C:84:ASP:OD1	2.38	0.57
1:P:44:THR:HG22	1:P:59:LEU:HB2	1.87	0.57
1:C:115:ASP:O	1:C:116:SER:C	2.43	0.56
1:G:151:ARG:HD3	1:G:263:PHE:CE1	2.40	0.56
1:G:258:VAL:O	1:G:259:MET:HG3	2.05	0.56
1:H:26:ILE:HG13	1:H:196:THR:HG21	1.86	0.56
1:J:20:THR:OG1	1:J:88:HIS:HA	2.05	0.56
1:C:266:VAL:HB	1:H:151:ARG:NH2	2.20	0.56
1:D:151:ARG:NH2	1:D:152:GLY:O	2.36	0.56
1:G:121:THR:O	1:G:125:LEU:N	2.37	0.56
1:G:220:ALA:HA	1:G:223:GLU:HB2	1.87	0.56
1:K:115:ASP:OD1	1:K:118:ILE:HD12	2.05	0.56
1:L:205:LYS:HA	1:L:208:GLU:HB2	1.86	0.56
1:B:93:SER:HB3	1:B:202:LEU:HD11	1.87	0.56
1:B:244:LEU:HD11	1:B:257:PHE:CD2	2.40	0.56
1:D:169:LEU:O	1:D:172:CYS:HB2	2.05	0.56
1:D:171:LYS:NZ	1:D:256:GLU:OE1	2.31	0.56
1:K:44:THR:HG21	1:K:72:VAL:HG21	1.88	0.56
1:K:145:SER:O	1:K:163:LYS:HD2	2.06	0.56
1:N:19:VAL:HA	1:N:87:VAL:HB	1.87	0.56
1:P:194:ILE:HD13	1:P:232:GLY:HA3	1.85	0.56
1:B:43:ALA:O	1:B:58:TYR:HA	2.04	0.56
1:E:62:ASP:OD2	1:E:64:THR:OG1	2.23	0.56
1:H:111:THR:HA	1:H:115:ASP:HB2	1.86	0.56
1:J:115:ASP:HA	1:J:118:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:VAL:CG1	1:K:260:ASP:HB2	2.35	0.56
1:L:86:LEU:HD23	1:L:141:VAL:HG13	1.87	0.56
1:P:44:THR:HB	1:P:61:HIS:HB2	1.87	0.56
1:B:112:VAL:O	1:B:112:VAL:CG1	2.53	0.56
1:F:168:MET:CG	1:H:160:CYS:HB3	2.36	0.56
1:H:86:LEU:HD22	1:H:124:LEU:HD12	1.87	0.56
1:H:196:THR:HB	1:H:197:PRO:HD2	1.87	0.56
1:K:55:ALA:O	1:K:56:ASP:C	2.44	0.56
1:K:187:ASN:HD22	1:K:244:LEU:HD22	1.69	0.56
1:M:159:TYR:CZ	1:M:163:LYS:HE3	2.40	0.56
1:N:103:LEU:HD21	1:P:115:ASP:CG	2.26	0.56
1:N:161:THR:HG21	1:P:169:LEU:HB2	1.86	0.56
1:F:145:SER:HB3	1:F:190:HIS:NE2	2.20	0.56
1:F:222:MET:O	1:F:225:ARG:HB2	2.05	0.56
1:H:28:ARG:O	1:H:32:LYS:HE3	2.05	0.56
1:P:64:THR:CG2	1:P:111:THR:HG22	2.36	0.56
1:P:143:ASN:O	1:P:188:SER:HA	2.06	0.56
1:D:48:PRO:HA	1:D:60:GLN:CD	2.26	0.56
1:E:22:ALA:O	1:E:28:ARG:HA	2.05	0.56
1:L:115:ASP:O	1:L:119:ILE:HG13	2.05	0.56
1:P:158:ALA:C	1:P:160:CYS:H	2.08	0.56
1:G:87:VAL:HG22	1:G:142:VAL:HB	1.87	0.56
1:I:266:VAL:O	1:M:151:ARG:NH2	2.39	0.56
1:E:20:THR:O	1:E:89:ASN:HB3	2.06	0.56
1:H:71:ALA:O	1:H:74:ALA:HB3	2.05	0.56
1:K:227:PRO:HG3	1:K:266:VAL:CG2	2.36	0.56
1:K:232:GLY:HA3	1:M:251:PHE:CD1	2.41	0.56
1:P:199:LEU:HA	1:P:202:LEU:HD12	1.88	0.56
1:A:12:LEU:HB3	1:A:39:ALA:CB	2.25	0.55
1:C:186:VAL:O	1:C:254:CYS:N	2.38	0.55
1:G:222:MET:HG3	1:G:222:MET:O	2.06	0.55
1:H:19:VAL:O	1:H:22:ALA:HB2	2.05	0.55
1:I:69:TRP:CD2	1:I:120:GLY:HA2	2.40	0.55
1:I:103:LEU:CD1	1:K:115:ASP:OD1	2.54	0.55
1:I:204:ASP:OD1	1:I:215:ARG:HG3	2.06	0.55
1:K:12:LEU:HD22	1:K:15:VAL:HG21	1.88	0.55
1:C:231:MET:O	1:F:251:PHE:CE1	2.58	0.55
1:I:225:ARG:O	1:I:227:PRO:HD3	2.06	0.55
1:M:200:GLY:O	1:M:215:ARG:NH2	2.39	0.55
1:N:17:ALA:HA	1:N:85:ALA:HB3	1.88	0.55
1:N:26:ILE:O	1:N:30:LEU:HG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:263:PHE:CD1	1:P:263:PHE:C	2.80	0.55
1:A:151:ARG:CB	1:E:265:GLN:O	2.55	0.55
1:A:160:CYS:HB2	1:D:172:CYS:SG	2.45	0.55
1:E:17:ALA:O	1:E:18:VAL:HG23	2.06	0.55
1:E:176:GLU:O	1:E:179:ALA:HB3	2.06	0.55
1:F:161:THR:HG21	1:H:169:LEU:HD13	1.87	0.55
1:I:26:ILE:HG22	1:I:30:LEU:HG	1.88	0.55
1:L:61:HIS:CD2	1:L:63:VAL:HA	2.41	0.55
1:N:97:LYS:HA	1:N:155:PHE:CD1	2.40	0.55
1:O:155:PHE:O	1:O:157:ALA:N	2.39	0.55
1:E:144:PHE:CE2	1:E:189:VAL:HG11	2.42	0.55
1:E:146:SER:O	1:E:190:HIS:HB3	2.05	0.55
1:F:103:LEU:HG	1:F:107:HIS:NE2	2.22	0.55
1:N:110:ASN:O	1:N:114:VAL:HB	2.06	0.55
1:I:98:PHE:CZ	1:K:173:LEU:HD11	2.41	0.55
1:I:152:GLY:CA	1:M:266:VAL:HG12	2.36	0.55
1:K:240:GLY:O	1:K:243:TYR:HB3	2.07	0.55
1:O:93:SER:OG	1:O:159:TYR:CD2	2.44	0.55
1:F:63:VAL:O	1:F:69:TRP:NE1	2.39	0.55
1:I:43:ALA:O	1:I:58:TYR:HA	2.06	0.55
1:N:16:VAL:HB	1:N:84:ASP:N	2.19	0.55
1:A:168:MET:HG2	1:D:160:CYS:O	2.06	0.55
1:B:164:ALA:O	1:B:165:ALA:C	2.45	0.55
1:F:170:SER:HA	1:F:186:VAL:CG1	2.36	0.55
1:H:227:PRO:HG2	1:H:262:GLY:CA	2.33	0.55
1:K:119:ILE:O	1:K:123:VAL:HG23	2.06	0.55
1:L:217:VAL:HG12	1:L:217:VAL:O	2.06	0.55
1:N:252:VAL:HG13	1:N:255:THR:HG21	1.88	0.55
1:O:171:LYS:O	1:O:175:ALA:HB2	2.07	0.55
1:A:113:ASN:O	1:A:117:ILE:HD12	2.07	0.55
1:D:265:GLN:OE1	1:E:171:LYS:CE	2.55	0.55
1:K:226:HIS:HB3	1:K:228:ILE:HG22	1.89	0.55
1:N:133:LYS:O	1:N:135:ARG:N	2.39	0.55
1:N:180:LEU:CB	1:N:182:TYR:CZ	2.89	0.55
1:P:147:VAL:HG12	1:P:264:SER:HB3	1.89	0.55
1:P:169:LEU:O	1:P:170:SER:C	2.43	0.55
1:A:214:SER:HB2	1:A:216:GLU:OE2	2.07	0.55
1:B:115:ASP:HA	1:B:118:ILE:HD12	1.89	0.55
1:F:247:ASP:C	1:F:249:ALA:N	2.59	0.55
1:G:56:ASP:O	1:G:57:HIS:CD2	2.60	0.55
1:J:102:PRO:HD2	1:J:105:ASP:OD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:177:PHE:HB3	1:M:182:TYR:HB2	1.89	0.55
1:N:20:THR:HG21	1:N:69:TRP:CH2	2.42	0.55
1:O:95:VAL:HG23	1:O:202:LEU:HD22	1.89	0.55
1:A:80:TYR:O	1:A:82:ARG:HG2	2.07	0.55
1:F:102:PRO:HD2	1:F:105:ASP:OD2	2.06	0.55
1:N:65:SER:O	1:N:69:TRP:CD1	2.59	0.55
1:I:103:LEU:HD11	1:K:115:ASP:CG	2.27	0.54
1:K:59:LEU:HD13	1:K:72:VAL:HG13	1.89	0.54
1:P:48:PRO:HA	1:P:60:GLN:CD	2.28	0.54
1:I:18:VAL:HG21	1:I:86:LEU:HD12	1.89	0.54
1:I:118:ILE:CD1	1:K:103:LEU:HD13	2.36	0.54
1:L:260:ASP:HB2	1:L:263:PHE:HB2	1.88	0.54
1:O:124:LEU:HA	1:O:127:LEU:HD12	1.90	0.54
1:P:182:TYR:O	1:P:184:ILE:N	2.39	0.54
1:B:168:MET:HA	1:B:171:LYS:HG3	1.90	0.54
1:C:125:LEU:HA	1:C:128:LEU:HB2	1.89	0.54
1:E:201:SER:HA	1:E:204:ASP:CG	2.28	0.54
1:C:97:LYS:HE3	1:C:209:LEU:HD22	1.90	0.54
1:E:140:SER:CB	1:E:245:CYS:HA	2.37	0.54
1:I:160:CYS:HB3	1:K:168:MET:CG	2.38	0.54
1:K:44:THR:HG21	1:K:61:HIS:ND1	2.22	0.54
1:N:173:LEU:HB3	1:N:186:VAL:HG21	1.89	0.54
1:A:176:GLU:HG3	1:A:180:LEU:HD11	1.90	0.54
1:A:176:GLU:OE2	1:D:155:PHE:CD1	2.61	0.54
1:J:82:ARG:NE	1:J:84:ASP:OD2	2.41	0.54
1:M:172:CYS:SG	1:O:152:GLY:HA2	2.48	0.54
1:P:16:VAL:HG22	1:P:40:ILE:HD12	1.89	0.54
1:P:145:SER:OG	1:P:146:SER:N	2.41	0.54
1:B:162:SER:C	1:B:164:ALA:N	2.59	0.54
1:I:10:ILE:N	2:I:305:HOH:O	2.41	0.54
1:I:165:ALA:O	1:I:168:MET:N	2.41	0.54
1:J:164:ALA:O	1:J:167:LYS:HB3	2.08	0.54
1:K:35:LYS:HD3	1:K:54:GLY:O	2.08	0.54
1:N:182:TYR:N	1:N:182:TYR:CD1	2.74	0.54
1:O:195:ASP:HA	1:O:231:MET:SD	2.48	0.54
1:P:131:GLY:HA2	1:P:134:ALA:HB3	1.90	0.54
1:K:147:VAL:HG11	1:K:263:PHE:HB3	1.89	0.54
1:M:233:ARG:HH21	1:M:236:GLU:CD	2.11	0.54
1:N:98:PHE:N	1:P:176:GLU:OE1	2.40	0.54
1:G:79:LYS:HB2	1:G:80:TYR:CD2	2.42	0.54
1:J:40:ILE:HA	1:J:56:ASP:OD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:LEU:O	1:L:142:VAL:N	2.41	0.54
1:F:31:VAL:HG21	1:F:52:VAL:HG11	1.88	0.54
1:I:156:ASN:OD1	1:I:159:TYR:HB3	2.08	0.54
1:M:106:PHE:HZ	1:M:161:THR:OG1	1.90	0.54
1:M:110:ASN:O	1:M:114:VAL:N	2.37	0.54
1:M:243:TYR:O	1:M:245:CYS:N	2.41	0.54
1:N:190:HIS:HB2	1:N:258:VAL:HG13	1.90	0.54
1:P:176:GLU:O	1:P:180:LEU:N	2.41	0.54
1:B:229:GLY:O	1:B:230:ARG:HB3	2.08	0.54
1:E:44:THR:HB	1:E:61:HIS:CB	2.38	0.54
1:N:142:VAL:HG11	1:N:241:VAL:HG13	1.90	0.54
1:P:91:GLY:HA2	1:P:113:ASN:OD1	2.08	0.54
1:P:124:LEU:HD22	1:P:127:LEU:HD13	1.90	0.54
1:A:182:TYR:CE2	1:D:99:GLU:OE1	2.61	0.53
1:B:266:VAL:C	1:F:151:ARG:HE	2.12	0.53
1:I:198:MET:O	1:I:202:LEU:HG	2.08	0.53
1:L:248:ALA:HB1	1:N:239:GLY:HA3	1.90	0.53
1:M:30:LEU:O	1:M:33:ALA:N	2.40	0.53
1:N:12:LEU:HB2	1:N:39:ALA:HB2	1.88	0.53
1:N:176:GLU:OE1	1:P:97:LYS:HA	2.07	0.53
1:A:142:VAL:O	1:A:142:VAL:HG12	2.08	0.53
1:C:180:LEU:HD13	1:C:182:TYR:CZ	2.42	0.53
1:E:47:ALA:O	1:E:58:TYR:OH	2.22	0.53
1:H:142:VAL:HG11	1:H:241:VAL:HG13	1.90	0.53
1:L:180:LEU:O	1:L:182:TYR:CD1	2.61	0.53
1:O:89:ASN:HA	1:O:144:PHE:CD1	2.44	0.53
1:O:94:ILE:CG2	1:O:158:ALA:HB3	2.38	0.53
1:P:185:ARG:NE	1:P:249:ALA:O	2.41	0.53
1:B:191:PRO:HB3	1:B:194:ILE:HD11	1.90	0.53
1:C:187:ASN:OD1	1:C:252:VAL:HG12	2.07	0.53
1:D:129:LYS:HG2	1:D:184:ILE:HD11	1.89	0.53
1:D:156:ASN:CB	1:D:160:CYS:SG	2.97	0.53
1:M:118:ILE:HG23	1:O:98:PHE:CE1	2.42	0.53
1:E:139:ALA:HB3	1:E:184:ILE:HG12	1.91	0.53
1:L:15:VAL:HG13	1:L:84:ASP:HB2	1.91	0.53
1:O:237:MET:O	1:O:259:MET:HE1	2.09	0.53
1:P:96:THR:HA	1:P:209:LEU:HD11	1.90	0.53
1:A:188:SER:O	1:A:257:PHE:N	2.38	0.53
1:B:228:ILE:HD12	1:H:253:THR:CG2	2.36	0.53
1:C:88:HIS:HB2	1:C:143:ASN:HA	1.91	0.53
1:E:63:VAL:HB	1:E:116:SER:CB	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:THR:HG21	1:E:111:THR:HG22	1.91	0.53
1:F:83:VAL:O	1:F:131:GLY:HA3	2.08	0.53
1:N:115:ASP:O	1:N:118:ILE:N	2.42	0.53
1:N:161:THR:CG2	1:P:169:LEU:HB2	2.39	0.53
1:O:129:LYS:HE2	1:O:182:TYR:CD2	2.43	0.53
1:D:148:ALA:HB1	1:D:160:CYS:HA	1.91	0.53
1:G:194:ILE:HG22	1:G:196:THR:HG23	1.91	0.53
1:I:118:ILE:O	1:I:122:GLN:HB2	2.09	0.53
1:I:187:ASN:OD1	1:I:253:THR:HA	2.08	0.53
1:I:266:VAL:HG23	1:M:151:ARG:NH2	2.15	0.53
1:J:258:VAL:HG11	1:J:265:GLN:HE21	1.74	0.53
1:K:266:VAL:C	1:O:151:ARG:CZ	2.77	0.53
1:O:173:LEU:HB2	1:O:186:VAL:HG11	1.90	0.53
1:O:226:HIS:O	1:O:227:PRO:C	2.46	0.53
1:O:264:SER:OG	1:O:265:GLN:NE2	2.38	0.53
1:F:94:ILE:HD11	1:F:108:ARG:HH21	1.73	0.53
1:F:138:GLY:HA2	1:F:183:ASN:OD1	2.09	0.53
1:F:214:SER:OG	1:F:217:VAL:HG23	2.07	0.53
1:G:222:MET:HG3	1:G:231:MET:SD	2.48	0.53
1:H:151:ARG:HD3	1:H:263:PHE:CE2	2.43	0.53
1:K:12:LEU:HB2	1:K:37:ALA:HB1	1.90	0.53
1:P:25:GLY:O	1:P:234:PRO:HB3	2.08	0.53
1:C:227:PRO:HG3	1:C:266:VAL:HG22	1.90	0.53
1:F:19:VAL:HG22	1:F:87:VAL:HB	1.90	0.53
1:G:164:ALA:O	1:G:167:LYS:HB3	2.08	0.53
1:K:45:ASP:HB3	1:K:58:TYR:OH	2.09	0.53
1:M:30:LEU:HD13	1:M:241:VAL:HG11	1.91	0.53
1:N:172:CYS:SG	1:P:157:ALA:HA	2.48	0.53
1:O:40:ILE:HG21	1:O:80:TYR:CZ	2.44	0.53
1:C:265:GLN:CG	1:F:255:THR:HA	2.39	0.53
1:F:69:TRP:CH2	1:F:88:HIS:CE1	2.97	0.53
1:K:147:VAL:CG1	1:K:260:ASP:CB	2.87	0.53
1:M:56:ASP:O	1:M:57:HIS:CD2	2.62	0.53
1:M:109:VAL:HG21	1:M:158:ALA:HB1	1.91	0.53
1:M:109:VAL:O	1:M:113:ASN:ND2	2.42	0.53
1:B:101:THR:HG21	1:B:106:PHE:CE2	2.44	0.53
1:B:190:HIS:HB2	1:B:258:VAL:HA	1.90	0.53
1:G:97:LYS:HB2	1:G:100:ASP:HB2	1.91	0.53
1:I:60:GLN:NE2	2:I:303:HOH:O	2.34	0.53
1:B:88:HIS:HB2	1:B:143:ASN:OD1	2.09	0.52
1:G:59:LEU:HD22	1:G:72:VAL:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:TYR:HE2	1:G:252:VAL:HG21	1.74	0.52
1:I:42:ILE:HD13	1:I:75:LEU:HD23	1.91	0.52
1:I:265:GLN:HG3	1:O:255:THR:HA	1.90	0.52
1:J:168:MET:O	1:J:171:LYS:HB2	2.09	0.52
1:K:265:GLN:HG3	1:M:254:CYS:HB2	1.90	0.52
1:O:140:SER:CB	1:O:245:CYS:HA	2.39	0.52
1:B:17:ALA:CB	1:B:85:ALA:HB3	2.39	0.52
1:B:89:ASN:OD1	1:B:144:PHE:CE2	2.62	0.52
1:H:12:LEU:HD11	1:H:242:VAL:HG22	1.90	0.52
1:I:152:GLY:O	1:M:266:VAL:CB	2.53	0.52
1:K:151:ARG:CZ	1:K:263:PHE:CZ	2.93	0.52
1:D:74:ALA:HA	1:D:77:GLN:HB3	1.91	0.52
1:J:203:MET:O	1:J:206:TYR:HB2	2.10	0.52
1:A:26:ILE:O	1:A:30:LEU:HG	2.10	0.52
1:A:176:GLU:CG	1:A:180:LEU:HD11	2.39	0.52
1:D:29:GLU:HB3	1:D:235:ALA:HA	1.90	0.52
1:G:199:LEU:HD21	1:G:231:MET:CE	2.39	0.52
1:K:58:TYR:CD1	1:K:58:TYR:C	2.83	0.52
1:M:87:VAL:HG21	1:M:241:VAL:HG13	1.92	0.52
1:M:181:GLY:HA2	2:M:305:HOH:O	2.08	0.52
1:P:44:THR:HB	1:P:61:HIS:CB	2.39	0.52
1:G:243:TYR:CE2	1:G:252:VAL:HG21	2.45	0.52
1:J:191:PRO:HB3	1:J:237:MET:SD	2.49	0.52
1:M:132:GLY:CA	1:M:138:GLY:HA2	2.32	0.52
1:M:138:GLY:CA	1:M:183:ASN:O	2.46	0.52
1:A:24:GLY:O	1:A:28:ARG:HG3	2.09	0.52
1:A:225:ARG:O	1:A:263:PHE:CD2	2.63	0.52
1:D:82:ARG:NH2	1:D:135:ARG:HG3	2.25	0.52
1:F:230:ARG:HG3	1:F:230:ARG:NH1	2.05	0.52
1:H:199:LEU:C	1:H:201:SER:N	2.62	0.52
1:I:115:ASP:HA	1:I:118:ILE:HD12	1.91	0.52
1:P:20:THR:HA	1:P:44:THR:O	2.10	0.52
1:A:168:MET:HG2	1:D:160:CYS:C	2.30	0.52
1:C:198:MET:SD	2:C:305:HOH:O	2.58	0.52
1:D:15:VAL:HG13	1:D:84:ASP:HB2	1.92	0.52
1:D:150:LEU:HD21	1:D:256:GLU:OE2	2.09	0.52
1:F:94:ILE:O	1:F:94:ILE:HG22	2.09	0.52
1:G:101:THR:HG22	1:G:102:PRO:O	2.10	0.52
1:G:146:SER:HA	1:G:190:HIS:HA	1.92	0.52
1:L:83:VAL:HG23	1:L:127:LEU:HB3	1.91	0.52
1:L:187:ASN:HD22	1:L:244:LEU:HD22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:23:ALA:HA	1:O:28:ARG:CG	2.39	0.52
1:P:12:LEU:HD12	1:P:34:MET:HG2	1.92	0.52
1:P:23:ALA:HA	1:P:28:ARG:CG	2.39	0.52
1:B:162:SER:O	1:B:165:ALA:N	2.43	0.52
1:C:223:GLU:CG	1:C:231:MET:HG3	2.39	0.52
1:D:31:VAL:HG11	1:D:52:VAL:HG12	1.91	0.52
1:D:257:PHE:HE1	1:D:259:MET:HG3	1.75	0.52
1:J:151:ARG:HD3	1:J:263:PHE:HE1	1.75	0.52
1:L:141:VAL:HG12	1:L:143:ASN:HD21	1.75	0.52
1:N:31:VAL:HG13	1:N:41:VAL:HG11	1.92	0.52
1:N:164:ALA:O	1:N:167:LYS:HB3	2.09	0.52
1:P:125:LEU:N	1:P:126:PRO:HD2	2.25	0.52
1:A:204:ASP:O	1:A:208:GLU:N	2.34	0.52
1:A:247:ASP:C	1:A:249:ALA:H	2.13	0.52
1:I:66:GLU:HA	1:I:119:ILE:HG21	1.92	0.52
1:M:112:VAL:HG12	1:M:112:VAL:O	2.10	0.52
1:M:147:VAL:HA	1:M:150:LEU:HB2	1.91	0.52
1:M:243:TYR:C	1:M:245:CYS:H	2.12	0.52
1:O:93:SER:HA	1:O:159:TYR:HD2	1.75	0.52
1:D:44:THR:HG21	1:D:72:VAL:HG22	1.92	0.52
1:D:243:TYR:OH	1:E:259:MET:SD	2.66	0.52
1:E:179:ALA:C	1:E:181:GLY:H	2.12	0.52
1:F:25:GLY:HA2	1:F:28:ARG:HH12	1.75	0.52
1:O:223:GLU:C	1:O:225:ARG:N	2.63	0.52
1:P:48:PRO:HA	1:P:60:GLN:NE2	2.25	0.52
1:P:61:HIS:ND1	1:P:72:VAL:HG21	2.24	0.52
1:C:111:THR:O	1:C:115:ASP:HB2	2.10	0.51
1:C:223:GLU:HG2	1:C:231:MET:HG3	1.91	0.51
1:E:95:VAL:O	1:E:96:THR:HB	2.10	0.51
1:F:145:SER:OG	1:F:190:HIS:CE1	2.63	0.51
1:G:97:LYS:HD3	1:G:100:ASP:OD2	2.10	0.51
1:I:203:MET:SD	1:I:219:GLN:HG3	2.50	0.51
1:J:12:LEU:HD21	1:J:245:CYS:HB2	1.92	0.51
1:L:18:VAL:HG22	1:L:42:ILE:HB	1.91	0.51
1:N:12:LEU:CB	1:N:39:ALA:HB2	2.40	0.51
1:A:19:VAL:O	1:A:44:THR:N	2.41	0.51
1:D:171:LYS:HG2	1:D:254:CYS:O	2.10	0.51
1:F:125:LEU:HG	1:F:129:LYS:HE3	1.92	0.51
1:F:156:ASN:O	1:F:158:ALA:N	2.42	0.51
1:H:98:PHE:HA	1:H:101:THR:OG1	2.11	0.51
1:B:137:GLY:O	1:B:185:ARG:NE	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:PHE:CA	1:G:176:GLU:OE2	2.56	0.51
1:F:26:ILE:HD13	1:F:237:MET:HG3	1.92	0.51
1:F:87:VAL:HG12	1:F:87:VAL:O	2.10	0.51
1:H:44:THR:HB	1:H:61:HIS:HB3	1.93	0.51
1:L:221:ALA:HA	1:L:224:MET:HB2	1.92	0.51
1:N:86:LEU:HD13	1:N:124:LEU:CD1	2.40	0.51
1:C:248:ALA:C	1:C:250:SER:H	2.13	0.51
1:H:264:SER:OG	1:H:265:GLN:NE2	2.42	0.51
1:J:215:ARG:O	1:J:218:ALA:HB3	2.10	0.51
1:L:156:ASN:HB3	1:L:160:CYS:SG	2.50	0.51
1:A:252:VAL:HG12	1:A:255:THR:HG21	1.93	0.51
1:C:241:VAL:O	1:C:242:VAL:C	2.47	0.51
1:H:94:ILE:O	1:H:96:THR:HG22	2.10	0.51
1:M:156:ASN:O	1:M:158:ALA:N	2.43	0.51
1:M:229:GLY:O	1:M:230:ARG:HB3	2.10	0.51
1:P:119:ILE:O	1:P:122:GLN:HB2	2.11	0.51
1:G:130:GLU:HA	1:G:133:LYS:HD2	1.93	0.51
1:I:20:THR:HG22	1:I:44:THR:OG1	2.10	0.51
1:M:180:LEU:O	1:M:181:GLY:C	2.49	0.51
1:O:27:GLY:O	1:O:31:VAL:HG23	2.10	0.51
1:A:203:MET:O	1:A:204:ASP:C	2.49	0.51
1:B:117:ILE:CD1	1:B:166:VAL:HG22	2.40	0.51
1:C:250:SER:HB2	1:F:236:GLU:OE1	2.11	0.51
1:E:33:ALA:HA	1:E:36:ALA:HB3	1.93	0.51
1:I:98:PHE:O	1:I:100:ASP:N	2.44	0.51
1:J:233:ARG:HB2	1:J:236:GLU:HG3	1.92	0.51
1:L:260:ASP:OD2	1:L:265:GLN:HG2	2.11	0.51
1:M:40:ILE:HG21	1:M:80:TYR:CE1	2.45	0.51
1:N:114:VAL:HG11	1:P:106:PHE:CZ	2.46	0.51
1:P:143:ASN:HB2	1:P:170:SER:OG	2.10	0.51
1:B:45:ASP:O	1:B:60:GLN:HA	2.10	0.51
1:C:35:LYS:HG3	1:C:54:GLY:C	2.31	0.51
1:C:145:SER:OG	1:C:190:HIS:CE1	2.64	0.51
1:F:94:ILE:HD12	1:F:109:VAL:HG23	1.92	0.51
1:G:104:SER:O	1:G:108:ARG:N	2.44	0.51
1:I:97:LYS:HB2	1:I:100:ASP:HB2	1.92	0.51
1:J:52:VAL:O	1:J:53:GLU:C	2.48	0.51
1:L:106:PHE:HE1	1:L:158:ALA:HA	1.74	0.51
1:L:139:ALA:HB3	1:L:184:ILE:HG12	1.92	0.51
1:N:165:ALA:O	1:N:166:VAL:C	2.49	0.51
1:N:198:MET:HE2	1:N:199:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:PRO:HG3	1:C:266:VAL:CG2	2.41	0.51
1:I:250:SER:C	1:I:252:VAL:H	2.14	0.51
1:N:125:LEU:HA	1:N:128:LEU:HB2	1.93	0.51
1:D:15:VAL:HG13	1:D:84:ASP:HB3	1.91	0.51
1:E:149:GLY:O	1:G:168:MET:HE3	2.11	0.51
1:E:153:ALA:HB3	1:E:156:ASN:HB2	1.93	0.51
1:E:223:GLU:O	1:E:226:HIS:HB2	2.10	0.51
1:F:62:ASP:OD2	1:F:64:THR:OG1	2.28	0.51
1:F:247:ASP:O	1:F:249:ALA:N	2.43	0.51
1:J:125:LEU:HB3	1:J:126:PRO:HD3	1.92	0.51
1:P:125:LEU:N	1:P:126:PRO:CD	2.74	0.51
1:B:26:ILE:HG21	1:B:144:PHE:CZ	2.46	0.50
1:B:107:HIS:CB	1:G:208:GLU:HG2	2.40	0.50
1:G:144:PHE:O	1:G:166:VAL:CG1	2.58	0.50
1:I:118:ILE:HD12	1:K:103:LEU:CD1	2.41	0.50
1:I:251:PHE:HE1	1:O:230:ARG:O	1.94	0.50
1:B:26:ILE:HD13	1:B:144:PHE:HE2	1.76	0.50
1:M:60:GLN:OE1	2:M:301:HOH:O	2.18	0.50
1:M:146:SER:C	1:M:148:ALA:H	2.15	0.50
1:P:23:ALA:HA	1:P:28:ARG:HG3	1.93	0.50
1:B:44:THR:OG1	1:B:61:HIS:HB3	2.11	0.50
1:B:112:VAL:O	1:B:112:VAL:HG12	2.11	0.50
1:D:137:GLY:HA3	1:D:250:SER:CB	2.42	0.50
1:H:140:SER:CB	1:H:245:CYS:HA	2.41	0.50
1:H:162:SER:O	1:H:166:VAL:HG23	2.11	0.50
1:K:185:ARG:CD	1:K:249:ALA:O	2.60	0.50
1:P:249:ALA:HA	1:P:252:VAL:HG23	1.94	0.50
1:D:152:GLY:C	1:G:266:VAL:HG12	2.31	0.50
1:G:140:SER:OG	1:G:245:CYS:HA	2.11	0.50
1:K:146:SER:OG	1:K:191:PRO:O	2.29	0.50
1:L:185:ARG:HD2	1:L:252:VAL:O	2.11	0.50
1:O:148:ALA:HB1	1:O:160:CYS:SG	2.51	0.50
1:D:191:PRO:HA	1:D:259:MET:O	2.11	0.50
1:E:98:PHE:HB3	1:G:176:GLU:OE1	2.12	0.50
1:G:145:SER:HB3	1:G:190:HIS:CE1	2.47	0.50
1:G:226:HIS:CD2	1:G:260:ASP:O	2.65	0.50
1:I:98:PHE:C	1:I:100:ASP:N	2.63	0.50
1:I:118:ILE:HD13	1:K:103:LEU:HD13	1.89	0.50
1:I:225:ARG:HD3	1:I:263:PHE:CZ	2.46	0.50
1:I:236:GLU:CD	1:O:251:PHE:HB2	2.32	0.50
1:K:25:GLY:HA2	1:K:28:ARG:HH22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:89:ASN:CG	1:K:89:ASN:O	2.50	0.50
1:M:153:ALA:H	1:O:172:CYS:HG	1.60	0.50
1:P:189:VAL:HG12	1:P:191:PRO:HD3	1.93	0.50
1:A:193:GLY:O	1:G:251:PHE:HZ	1.94	0.50
1:B:71:ALA:O	1:B:74:ALA:HB3	2.12	0.50
1:B:146:SER:O	1:B:149:GLY:N	2.37	0.50
1:D:256:GLU:O	1:D:258:VAL:HG23	2.12	0.50
1:G:226:HIS:HB3	1:G:228:ILE:HG22	1.94	0.50
1:K:92:ILE:HG23	1:K:112:VAL:HG11	1.92	0.50
1:N:18:VAL:HG22	1:N:42:ILE:HD12	1.92	0.50
1:A:19:VAL:HA	1:A:87:VAL:HB	1.94	0.50
1:A:92:ILE:HD11	1:A:109:VAL:HA	1.94	0.50
1:C:142:VAL:HG11	1:C:241:VAL:CG1	2.39	0.50
1:G:12:LEU:HD21	1:G:245:CYS:HB2	1.93	0.50
1:H:187:ASN:OD1	1:H:253:THR:HA	2.11	0.50
1:H:247:ASP:O	1:H:250:SER:HB3	2.11	0.50
1:I:16:VAL:HG21	1:I:80:TYR:HB3	1.94	0.50
1:I:228:ILE:HG21	1:I:261:GLY:HA3	1.92	0.50
1:J:11:ALA:O	1:J:246:SER:HB3	2.12	0.50
1:K:162:SER:O	1:K:166:VAL:N	2.38	0.50
1:N:64:THR:HB	1:N:111:THR:HG22	1.94	0.50
1:O:63:VAL:O	1:O:69:TRP:NE1	2.45	0.50
1:A:112:VAL:O	1:A:116:SER:CB	2.59	0.50
1:A:265:GLN:HE22	1:G:256:GLU:HG3	1.75	0.50
1:D:129:LYS:CG	1:D:184:ILE:HD11	2.42	0.50
1:F:45:ASP:O	1:F:47:ALA:N	2.44	0.50
1:F:171:LYS:HB3	1:H:152:GLY:HA3	1.94	0.50
1:H:117:ILE:O	1:H:118:ILE:C	2.50	0.50
1:L:94:ILE:CG2	1:L:96:THR:HG22	2.41	0.50
1:P:81:GLY:O	1:P:127:LEU:HD23	2.12	0.50
1:A:83:VAL:N	1:A:127:LEU:O	2.33	0.50
1:C:17:ALA:O	1:C:41:VAL:HA	2.11	0.50
1:N:26:ILE:HG22	1:N:30:LEU:HD21	1.94	0.50
1:N:203:MET:HB3	1:N:218:ALA:HB1	1.94	0.50
1:A:69:TRP:CZ2	1:A:88:HIS:HE1	2.29	0.49
1:A:240:GLY:O	1:A:244:LEU:HG	2.11	0.49
1:F:140:SER:HB2	1:F:185:ARG:NH2	2.27	0.49
1:G:154:ALA:O	1:G:156:ASN:N	2.45	0.49
1:K:113:ASN:OD1	1:K:113:ASN:N	2.45	0.49
1:K:153:ALA:HB3	1:K:156:ASN:HB2	1.94	0.49
1:K:254:CYS:HB2	1:M:265:GLN:HG3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:187:ASN:ND2	1:L:244:LEU:HD22	2.27	0.49
1:O:156:ASN:HB3	1:O:159:TYR:HB3	1.93	0.49
1:G:215:ARG:O	1:G:219:GLN:N	2.33	0.49
1:L:121:THR:HG21	1:L:173:LEU:HD13	1.93	0.49
1:O:93:SER:HB3	1:O:202:LEU:HD11	1.94	0.49
1:O:159:TYR:CZ	1:O:163:LYS:HG3	2.45	0.49
1:E:160:CYS:O	1:G:168:MET:HG2	2.12	0.49
1:E:169:LEU:O	1:E:172:CYS:HB2	2.12	0.49
1:F:94:ILE:HD13	1:F:105:ASP:OD1	2.11	0.49
1:H:151:ARG:HD3	1:H:263:PHE:CZ	2.47	0.49
1:L:12:LEU:HD11	1:L:245:CYS:HB2	1.93	0.49
1:M:83:VAL:O	1:M:128:LEU:HA	2.12	0.49
1:M:168:MET:O	1:M:172:CYS:SG	2.67	0.49
1:B:266:VAL:O	1:B:266:VAL:CG2	2.58	0.49
1:C:189:VAL:HG22	1:C:257:PHE:HD2	1.78	0.49
1:E:32:LYS:HD3	1:E:53:GLU:OE2	2.12	0.49
1:E:62:ASP:C	1:E:64:THR:H	2.15	0.49
1:E:69:TRP:CE2	1:E:120:GLY:HA2	2.47	0.49
1:F:159:TYR:CE1	1:F:163:LYS:HE2	2.47	0.49
1:J:24:GLY:O	1:J:28:ARG:HG3	2.13	0.49
1:L:180:LEU:O	1:L:182:TYR:CE1	2.65	0.49
1:M:172:CYS:SG	1:O:152:GLY:CA	3.00	0.49
1:E:31:VAL:CG1	1:E:55:ALA:HB2	2.41	0.49
1:E:86:LEU:HD22	1:E:128:LEU:HD11	1.93	0.49
1:E:142:VAL:HG13	1:E:189:VAL:CG2	2.43	0.49
1:E:190:HIS:CG	1:E:258:VAL:HG22	2.47	0.49
1:E:237:MET:O	1:E:241:VAL:HG23	2.12	0.49
1:F:34:MET:CG	1:F:242:VAL:HG22	2.42	0.49
1:N:174:GLY:HA3	1:N:254:CYS:SG	2.53	0.49
1:P:18:VAL:N	1:P:85:ALA:O	2.34	0.49
1:B:26:ILE:HG21	1:B:144:PHE:CE2	2.47	0.49
1:C:266:VAL:HB	1:H:151:ARG:HH21	1.77	0.49
1:D:70:LYS:HE3	1:D:123:VAL:HG22	1.93	0.49
1:D:125:LEU:HA	1:D:128:LEU:HD12	1.95	0.49
1:E:88:HIS:NE2	1:E:121:THR:OG1	2.46	0.49
1:E:179:ALA:O	1:E:181:GLY:N	2.46	0.49
1:I:240:GLY:HA3	1:I:259:MET:SD	2.52	0.49
1:L:26:ILE:HA	1:L:234:PRO:CB	2.41	0.49
1:N:170:SER:HB3	1:N:186:VAL:HG12	1.94	0.49
1:N:225:ARG:NH2	2:N:302:HOH:O	2.43	0.49
1:P:146:SER:O	1:P:149:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:CZ	1:B:263:PHE:HE1	2.26	0.49
1:C:152:GLY:HA3	1:H:266:VAL:HG12	1.93	0.49
1:I:32:LYS:HG2	1:I:53:GLU:HB3	1.95	0.49
1:J:182:TYR:N	1:J:182:TYR:CD1	2.79	0.49
1:L:235:ALA:O	1:L:238:GLY:N	2.45	0.49
1:M:87:VAL:HG22	1:M:142:VAL:HB	1.94	0.49
1:M:226:HIS:CD2	1:M:263:PHE:HB2	2.47	0.49
1:O:159:TYR:CE1	1:O:163:LYS:CG	2.92	0.49
1:P:240:GLY:O	1:P:244:LEU:HG	2.13	0.49
1:B:95:VAL:HG23	1:B:202:LEU:HD22	1.95	0.49
1:E:199:LEU:HA	1:E:202:LEU:HB2	1.94	0.49
1:F:148:ALA:HB1	1:F:160:CYS:SG	2.53	0.49
1:H:15:VAL:HA	1:H:84:ASP:OD2	2.12	0.49
1:H:216:GLU:O	1:H:220:ALA:N	2.45	0.49
1:M:86:LEU:O	1:M:142:VAL:N	2.40	0.49
1:M:160:CYS:O	1:M:164:ALA:N	2.28	0.49
1:M:194:ILE:HD11	1:M:237:MET:SD	2.52	0.49
1:N:141:VAL:HB	1:N:186:VAL:HG22	1.93	0.49
1:N:241:VAL:O	1:N:245:CYS:SG	2.68	0.49
1:O:144:PHE:O	1:O:163:LYS:NZ	2.44	0.49
1:B:227:PRO:HG3	1:B:266:VAL:HG21	1.94	0.49
1:C:61:HIS:CD2	1:C:62:ASP:O	2.66	0.49
1:E:43:ALA:O	1:E:58:TYR:HA	2.12	0.49
1:E:44:THR:HB	1:E:61:HIS:HB3	1.94	0.49
1:E:110:ASN:O	1:E:111:THR:C	2.51	0.49
1:J:12:LEU:O	1:J:39:ALA:HB2	2.13	0.49
1:J:180:LEU:HD21	1:L:155:PHE:CZ	2.48	0.49
1:L:145:SER:HB3	1:L:190:HIS:ND1	2.27	0.49
1:O:18:VAL:HA	1:O:42:ILE:HB	1.95	0.49
1:A:69:TRP:CZ2	1:A:88:HIS:CE1	3.01	0.49
1:A:243:TYR:CZ	1:A:249:ALA:HB2	2.48	0.49
1:D:185:ARG:CZ	1:D:249:ALA:O	2.61	0.49
1:F:24:GLY:O	1:F:28:ARG:NH1	2.46	0.49
1:F:118:ILE:O	1:F:122:GLN:HB2	2.13	0.49
1:I:151:ARG:HB3	1:M:265:GLN:O	2.13	0.49
1:L:92:ILE:HD11	1:L:109:VAL:HA	1.95	0.49
1:N:156:ASN:HB3	1:N:160:CYS:SG	2.53	0.49
1:O:88:HIS:HB3	1:O:117:ILE:HG12	1.95	0.49
1:O:174:GLY:CA	1:O:186:VAL:HB	2.43	0.49
1:B:204:ASP:OD2	1:B:215:ARG:NH1	2.46	0.48
1:C:32:LYS:HE2	1:C:53:GLU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:ALA:O	1:F:76:ALA:HB3	2.13	0.48
1:I:218:ALA:HA	1:I:221:ALA:HB3	1.95	0.48
1:K:23:ALA:HB2	1:K:50:ALA:HB1	1.95	0.48
1:M:136:ALA:HB3	1:M:247:ASP:OD1	2.14	0.48
1:N:180:LEU:CB	1:N:182:TYR:CE2	2.96	0.48
1:B:162:SER:O	1:B:164:ALA:N	2.45	0.48
1:E:32:LYS:CG	1:E:53:GLU:HB3	2.39	0.48
1:E:176:GLU:HA	1:G:154:ALA:HB1	1.95	0.48
1:E:190:HIS:HB2	1:E:258:VAL:HG22	1.95	0.48
1:E:240:GLY:HA3	1:E:257:PHE:CE2	2.48	0.48
1:J:151:ARG:HH21	1:N:266:VAL:HB	1.74	0.48
1:P:43:ALA:HB3	1:P:58:TYR:HD1	1.76	0.48
1:A:77:GLN:O	1:A:81:GLY:N	2.46	0.48
1:E:112:VAL:C	1:E:116:SER:HB3	2.31	0.48
1:G:151:ARG:HH21	1:G:153:ALA:CA	2.26	0.48
1:I:76:ALA:CB	1:I:127:LEU:HD13	2.43	0.48
1:N:202:LEU:O	1:N:205:LYS:HB2	2.13	0.48
1:A:187:ASN:OD1	1:A:252:VAL:O	2.31	0.48
1:B:35:LYS:HA	1:B:39:ALA:HB3	1.95	0.48
1:D:217:VAL:O	1:D:221:ALA:HB2	2.13	0.48
1:N:77:GLN:HA	1:N:77:GLN:HE21	1.77	0.48
1:O:69:TRP:CB	1:O:123:VAL:HG11	2.42	0.48
1:A:138:GLY:N	1:A:183:ASN:HD21	2.11	0.48
1:A:140:SER:CB	1:A:245:CYS:HA	2.43	0.48
1:A:176:GLU:HG2	1:A:180:LEU:CD1	2.44	0.48
1:A:176:GLU:C	1:A:178:ALA:H	2.17	0.48
1:B:12:LEU:HD21	1:B:242:VAL:O	2.14	0.48
1:B:151:ARG:CZ	1:B:263:PHE:CE1	2.96	0.48
1:C:187:ASN:ND2	1:C:244:LEU:HD22	2.29	0.48
1:G:201:SER:O	1:G:204:ASP:HB2	2.12	0.48
1:G:255:THR:OG1	1:G:257:PHE:N	2.45	0.48
1:N:62:ASP:HB3	1:N:65:SER:CB	2.44	0.48
1:A:199:LEU:HD23	1:A:231:MET:SD	2.54	0.48
1:A:248:ALA:HB1	1:G:239:GLY:CA	2.40	0.48
1:B:176:GLU:OE2	1:C:97:LYS:HA	2.12	0.48
1:E:22:ALA:HA	1:E:27:GLY:C	2.34	0.48
1:E:186:VAL:O	1:E:254:CYS:N	2.45	0.48
1:E:246:SER:C	1:E:248:ALA:N	2.67	0.48
1:G:159:TYR:O	1:G:159:TYR:CD1	2.67	0.48
1:N:146:SER:HA	1:N:190:HIS:HA	1.96	0.48
1:N:187:ASN:OD1	1:N:252:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:69:TRP:CD1	1:O:119:ILE:HG22	2.48	0.48
1:P:145:SER:N	1:P:189:VAL:O	2.46	0.48
1:P:218:ALA:HA	1:P:221:ALA:HB3	1.96	0.48
1:A:221:ALA:HB1	1:A:225:ARG:HE	1.78	0.48
1:B:34:MET:HG2	1:B:242:VAL:HG22	1.95	0.48
1:C:187:ASN:CB	1:C:244:LEU:HD13	2.44	0.48
1:D:101:THR:HG21	1:D:106:PHE:CD1	2.48	0.48
1:F:156:ASN:O	1:F:157:ALA:C	2.50	0.48
1:I:118:ILE:HD13	1:K:103:LEU:HD12	1.94	0.48
1:I:232:GLY:N	1:O:251:PHE:CZ	2.82	0.48
1:I:232:GLY:N	1:O:251:PHE:CE1	2.81	0.48
1:L:148:ALA:HB1	1:L:160:CYS:HA	1.95	0.48
1:D:143:ASN:ND2	1:D:170:SER:OG	2.45	0.48
1:D:252:VAL:HG22	1:E:259:MET:HG2	1.95	0.48
1:G:44:THR:HG22	1:G:59:LEU:HB2	1.96	0.48
1:I:251:PHE:HD1	1:O:228:ILE:HD13	1.78	0.48
1:M:38:ASN:ND2	2:M:303:HOH:O	2.46	0.48
1:M:123:VAL:HG12	1:M:124:LEU:HD23	1.95	0.48
1:M:159:TYR:OH	1:M:163:LYS:HE3	2.13	0.48
1:P:111:THR:O	1:P:115:ASP:HB2	2.14	0.48
1:A:222:MET:HG3	1:A:223:GLU:HG3	1.95	0.48
1:D:58:TYR:CE1	1:D:59:LEU:O	2.67	0.48
1:E:12:LEU:HD12	1:E:242:VAL:HG13	1.96	0.48
1:F:252:VAL:HG13	1:F:255:THR:HG21	1.95	0.48
1:G:154:ALA:C	1:G:156:ASN:H	2.17	0.48
1:I:88:HIS:CE1	1:I:116:SER:O	2.67	0.48
1:L:251:PHE:CD2	1:N:237:MET:HE1	2.49	0.48
1:A:98:PHE:HZ	1:D:121:THR:HB	1.79	0.48
1:B:31:VAL:HG12	1:B:53:GLU:O	2.14	0.48
1:B:150:LEU:HD21	1:B:256:GLU:OE2	2.14	0.48
1:G:103:LEU:O	1:G:107:HIS:N	2.42	0.48
1:K:61:HIS:ND1	1:K:72:VAL:HG21	2.29	0.48
1:K:94:ILE:HD12	1:K:109:VAL:HG22	1.96	0.48
1:K:171:LYS:NZ	1:K:256:GLU:OE1	2.46	0.48
1:M:103:LEU:HD13	1:O:119:ILE:HG12	1.96	0.48
1:A:151:ARG:HB2	1:E:265:GLN:O	2.13	0.47
1:C:115:ASP:O	1:C:119:ILE:HG13	2.14	0.47
1:D:47:ALA:O	1:D:58:TYR:OH	2.30	0.47
1:E:35:LYS:HG3	1:E:54:GLY:HA3	1.96	0.47
1:F:214:SER:H	1:F:217:VAL:HB	1.79	0.47
1:H:69:TRP:HB3	1:H:123:VAL:HG11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:ASP:O	1:D:61:HIS:N	2.32	0.47
1:G:213:PRO:HD2	1:G:217:VAL:HG11	1.96	0.47
1:H:138:GLY:HA3	1:H:185:ARG:HE	1.78	0.47
1:I:86:LEU:HD22	1:I:128:LEU:HD11	1.94	0.47
1:L:12:LEU:HD12	1:L:242:VAL:HG13	1.96	0.47
1:F:13:ASN:O	1:F:14:ASN:HB2	2.15	0.47
1:F:86:LEU:HD22	1:F:124:LEU:HD12	1.96	0.47
1:G:44:THR:HB	1:G:61:HIS:CB	2.43	0.47
1:L:142:VAL:HG11	1:L:241:VAL:HG13	1.97	0.47
1:A:156:ASN:ND2	1:A:206:TYR:OH	2.47	0.47
1:C:31:VAL:HA	1:C:34:MET:HB2	1.96	0.47
1:C:236:GLU:CD	1:F:251:PHE:HB2	2.35	0.47
1:E:67:ALA:O	1:E:68:GLY:C	2.52	0.47
1:F:146:SER:HA	1:F:191:PRO:HD2	1.96	0.47
1:F:161:THR:HG21	1:H:169:LEU:CD1	2.43	0.47
1:I:83:VAL:HG23	1:I:127:LEU:HB3	1.97	0.47
1:J:16:VAL:H	1:J:84:ASP:HB2	1.78	0.47
1:J:20:THR:O	1:J:89:ASN:HB3	2.14	0.47
1:K:142:VAL:CG2	1:K:244:LEU:HD12	2.44	0.47
1:M:160:CYS:HA	1:M:163:LYS:HB2	1.97	0.47
1:B:155:PHE:HA	1:C:176:GLU:OE2	2.15	0.47
1:D:266:VAL:C	1:G:151:ARG:NH1	2.68	0.47
1:E:32:LYS:HG2	1:E:53:GLU:CB	2.39	0.47
1:I:18:VAL:CG2	1:I:86:LEU:HD12	2.44	0.47
1:K:161:THR:O	1:K:165:ALA:HB2	2.14	0.47
1:P:145:SER:OG	1:P:190:HIS:ND1	2.40	0.47
1:B:15:VAL:HG12	1:B:17:ALA:HB2	1.95	0.47
1:B:119:ILE:O	1:B:122:GLN:HB2	2.15	0.47
1:C:22:ALA:HA	1:C:27:GLY:HA3	1.96	0.47
1:F:56:ASP:O	1:F:57:HIS:CD2	2.67	0.47
1:G:95:VAL:HG23	1:G:202:LEU:HD13	1.95	0.47
1:I:223:GLU:OE1	1:I:230:ARG:HA	2.15	0.47
1:A:182:TYR:OH	1:D:99:GLU:OE1	2.27	0.47
1:B:16:VAL:HA	1:B:40:ILE:HB	1.95	0.47
1:B:212:ALA:CB	1:B:218:ALA:HB2	2.44	0.47
1:D:19:VAL:O	1:D:44:THR:N	2.39	0.47
1:D:83:VAL:O	1:D:131:GLY:HA3	2.15	0.47
1:D:206:TYR:HB3	1:D:211:ALA:HB3	1.96	0.47
1:F:170:SER:HA	1:F:186:VAL:HG11	1.97	0.47
1:F:180:LEU:C	1:F:182:TYR:H	2.18	0.47
1:G:159:TYR:HE1	1:G:163:LYS:HE2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:SER:O	1:I:163:LYS:HD2	2.14	0.47
1:J:62:ASP:O	1:J:65:SER:HB3	2.14	0.47
1:J:155:PHE:HE1	1:L:180:LEU:HD11	1.80	0.47
1:L:125:LEU:HB3	1:L:126:PRO:HD3	1.96	0.47
1:L:151:ARG:HD3	1:L:263:PHE:CE1	2.50	0.47
1:M:171:LYS:HG2	1:M:254:CYS:O	2.15	0.47
1:M:225:ARG:HB3	1:M:263:PHE:CE2	2.50	0.47
1:N:204:ASP:OD1	1:N:204:ASP:N	2.46	0.47
1:O:93:SER:HA	1:O:159:TYR:CD2	2.50	0.47
1:O:132:GLY:O	1:O:183:ASN:ND2	2.33	0.47
1:O:182:TYR:N	1:O:182:TYR:CD1	2.82	0.47
1:P:76:ALA:HB1	1:P:83:VAL:HG23	1.95	0.47
1:P:240:GLY:O	1:P:243:TYR:HB3	2.15	0.47
1:A:40:ILE:HG21	1:A:80:TYR:CZ	2.49	0.47
1:A:239:GLY:HA2	1:A:242:VAL:CG2	2.45	0.47
1:B:125:LEU:CD1	1:B:184:ILE:HD13	2.45	0.47
1:C:226:HIS:HB2	1:C:230:ARG:O	2.15	0.47
1:C:237:MET:HA	1:C:259:MET:HE1	1.97	0.47
1:M:146:SER:C	1:M:148:ALA:N	2.68	0.47
1:O:93:SER:OG	1:O:159:TYR:CE2	2.59	0.47
1:A:112:VAL:O	1:A:116:SER:HB3	2.15	0.47
1:C:167:LYS:HB2	1:C:190:HIS:HE1	1.79	0.47
1:C:230:ARG:NH2	1:C:236:GLU:OE1	2.48	0.47
1:G:168:MET:O	1:G:171:LYS:HB2	2.15	0.47
1:H:137:GLY:HA3	1:H:247:ASP:HB3	1.96	0.47
1:I:102:PRO:HD2	1:I:105:ASP:OD2	2.15	0.47
1:K:199:LEU:HA	1:K:202:LEU:HD12	1.96	0.47
1:L:182:TYR:CD1	1:L:182:TYR:N	2.78	0.47
1:M:164:ALA:HB2	1:O:168:MET:HG2	1.97	0.47
1:N:173:LEU:CB	1:N:186:VAL:HG21	2.45	0.47
1:P:119:ILE:O	1:P:122:GLN:N	2.48	0.47
1:C:152:GLY:O	1:H:266:VAL:HG12	2.15	0.47
1:C:170:SER:OG	1:C:188:SER:HB3	2.15	0.47
1:C:207:VAL:HG13	1:C:213:PRO:O	2.15	0.47
1:D:176:GLU:O	1:D:180:LEU:HG	2.14	0.47
1:F:41:VAL:O	1:F:56:ASP:HB2	2.14	0.47
1:F:145:SER:O	1:F:191:PRO:CD	2.61	0.47
1:G:40:ILE:HG21	1:G:80:TYR:CZ	2.50	0.47
1:G:57:HIS:CE1	1:G:79:LYS:HE3	2.50	0.47
1:G:85:ALA:HA	1:G:140:SER:O	2.15	0.47
1:G:147:VAL:O	1:G:150:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:125:LEU:HA	1:I:128:LEU:HB2	1.96	0.47
1:N:127:LEU:O	1:N:131:GLY:N	2.33	0.47
1:A:131:GLY:HA3	1:A:139:ALA:HB2	1.97	0.46
1:H:115:ASP:O	1:H:116:SER:C	2.52	0.46
1:H:145:SER:OG	1:H:146:SER:N	2.46	0.46
1:H:225:ARG:HD3	1:H:263:PHE:HE1	1.80	0.46
1:K:233:ARG:NH2	1:K:236:GLU:OE1	2.48	0.46
1:M:21:GLY:HA2	1:M:45:ASP:OD2	2.15	0.46
1:P:59:LEU:HD22	1:P:72:VAL:HG22	1.96	0.46
1:B:93:SER:HA	1:B:159:TYR:CE1	2.50	0.46
1:C:139:ALA:HB3	1:C:184:ILE:HG12	1.97	0.46
1:F:97:LYS:HE3	1:F:209:LEU:HD22	1.97	0.46
1:F:170:SER:OG	1:F:188:SER:HB3	2.15	0.46
1:F:207:VAL:O	1:F:209:LEU:N	2.48	0.46
1:I:118:ILE:HA	1:K:98:PHE:CZ	2.47	0.46
1:I:152:GLY:HA3	1:K:171:LYS:HB3	1.97	0.46
1:J:66:GLU:HA	1:J:119:ILE:HG21	1.97	0.46
1:J:145:SER:OG	1:J:146:SER:N	2.35	0.46
1:M:94:ILE:HD12	1:M:109:VAL:CG2	2.44	0.46
1:M:220:ALA:O	1:M:224:MET:HG3	2.16	0.46
1:B:108:ARG:HB2	1:G:208:GLU:HA	1.96	0.46
1:B:256:GLU:OE1	2:B:301:HOH:O	2.20	0.46
1:C:237:MET:SD	1:C:259:MET:HE1	2.54	0.46
1:D:26:ILE:HG13	1:D:196:THR:HG21	1.97	0.46
1:D:227:PRO:HG3	1:D:266:VAL:CG2	2.45	0.46
1:F:92:ILE:HG12	1:F:112:VAL:HG11	1.96	0.46
1:G:139:ALA:HB3	1:G:184:ILE:HG12	1.97	0.46
1:H:125:LEU:HG	1:H:129:LYS:CE	2.40	0.46
1:I:237:MET:CA	1:I:259:MET:HE1	2.41	0.46
1:L:35:LYS:O	1:L:38:ASN:N	2.46	0.46
1:C:69:TRP:O	1:C:123:VAL:HG11	2.16	0.46
1:F:115:ASP:O	1:F:118:ILE:N	2.48	0.46
1:H:185:ARG:NH1	1:H:244:LEU:O	2.38	0.46
1:I:168:MET:CG	1:K:160:CYS:HB3	2.45	0.46
1:K:248:ALA:HB1	1:M:239:GLY:CA	2.46	0.46
1:M:35:LYS:HD3	1:M:56:ASP:OD2	2.14	0.46
1:N:194:ILE:HG22	1:N:195:ASP:N	2.30	0.46
1:O:70:LYS:O	1:O:74:ALA:N	2.38	0.46
1:P:97:LYS:HB2	1:P:100:ASP:HB2	1.97	0.46
1:H:20:THR:OG1	1:H:88:HIS:HA	2.15	0.46
1:H:91:GLY:HA2	1:H:112:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:69:TRP:HE3	1:I:124:LEU:HD11	1.81	0.46
1:M:12:LEU:CB	1:M:39:ALA:HB2	2.34	0.46
1:F:111:THR:O	1:F:115:ASP:HB2	2.15	0.46
1:I:52:VAL:HB	1:I:55:ALA:HB2	1.98	0.46
1:K:83:VAL:CG2	1:K:127:LEU:HD13	2.44	0.46
1:K:159:TYR:CE1	1:K:163:LYS:HE3	2.51	0.46
1:L:167:LYS:HB2	1:L:190:HIS:HE1	1.81	0.46
1:L:254:CYS:C	1:N:265:GLN:HG3	2.35	0.46
1:M:63:VAL:HG23	1:M:116:SER:HB2	1.96	0.46
1:N:115:ASP:HA	1:N:118:ILE:CD1	2.42	0.46
1:O:12:LEU:HD21	1:O:245:CYS:HB2	1.98	0.46
1:C:44:THR:HG22	1:C:59:LEU:HB2	1.98	0.46
1:D:227:PRO:HG2	1:D:262:GLY:O	2.16	0.46
1:E:218:ALA:C	1:E:220:ALA:H	2.18	0.46
1:G:196:THR:C	1:G:198:MET:H	2.19	0.46
1:I:214:SER:C	1:I:216:GLU:N	2.69	0.46
1:J:112:VAL:O	1:J:112:VAL:HG12	2.16	0.46
1:K:257:PHE:CE1	1:M:257:PHE:CD2	3.02	0.46
1:L:164:ALA:O	1:L:167:LYS:HB3	2.15	0.46
1:O:31:VAL:HG11	1:O:52:VAL:CG1	2.46	0.46
1:O:84:ASP:OD1	1:O:135:ARG:HG3	2.15	0.46
1:P:115:ASP:C	1:P:117:ILE:H	2.19	0.46
1:C:132:GLY:HA3	1:C:183:ASN:O	2.16	0.46
1:D:127:LEU:O	1:D:131:GLY:N	2.49	0.46
1:E:92:ILE:HD11	1:E:109:VAL:HA	1.98	0.46
1:F:159:TYR:CZ	1:F:163:LYS:HE3	2.50	0.46
1:F:229:GLY:O	1:F:230:ARG:HB3	2.16	0.46
1:I:104:SER:O	1:I:108:ARG:HB2	2.16	0.46
1:M:198:MET:O	1:M:202:LEU:HG	2.15	0.46
1:A:112:VAL:O	1:A:116:SER:OG	2.29	0.46
1:A:265:GLN:HG3	1:G:254:CYS:O	2.15	0.46
1:D:48:PRO:HA	1:D:60:GLN:NE2	2.31	0.46
1:D:180:LEU:HD23	1:D:180:LEU:HA	1.82	0.46
1:E:155:PHE:CD1	1:G:176:GLU:HG3	2.51	0.46
1:F:98:PHE:CZ	1:H:118:ILE:HA	2.50	0.46
1:F:202:LEU:O	1:F:205:LYS:N	2.49	0.46
1:G:83:VAL:HG23	1:G:127:LEU:CB	2.46	0.46
1:M:94:ILE:HG22	1:M:96:THR:HG22	1.97	0.46
1:O:233:ARG:N	1:O:236:GLU:OE2	2.49	0.46
1:P:35:LYS:HG3	1:P:54:GLY:CA	2.46	0.46
1:D:101:THR:HG22	1:D:102:PRO:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:THR:HA	1:E:44:THR:OG1	2.16	0.46
1:E:44:THR:HG22	1:E:59:LEU:HB2	1.98	0.46
1:E:64:THR:CG2	1:E:111:THR:HG22	2.46	0.46
1:E:162:SER:O	1:E:166:VAL:HG23	2.15	0.46
1:G:147:VAL:HA	1:G:150:LEU:HD12	1.98	0.46
1:I:44:THR:HB	1:I:61:HIS:HB2	1.97	0.46
1:I:266:VAL:CG1	1:M:152:GLY:N	2.71	0.46
1:J:45:ASP:O	1:J:60:GLN:HA	2.16	0.46
1:K:221:ALA:O	1:K:222:MET:C	2.55	0.46
1:M:203:MET:O	1:M:207:VAL:HG23	2.16	0.46
1:N:68:GLY:O	1:N:71:ALA:HB3	2.16	0.46
1:N:93:SER:HA	1:N:159:TYR:CD1	2.51	0.46
1:N:233:ARG:HB2	1:N:236:GLU:HG3	1.98	0.46
1:P:173:LEU:O	1:P:177:PHE:N	2.38	0.46
1:A:64:THR:O	1:A:119:ILE:HD12	2.16	0.45
1:A:79:LYS:O	1:A:80:TYR:CG	2.69	0.45
1:D:62:ASP:O	1:D:65:SER:HB3	2.16	0.45
1:F:103:LEU:HD12	1:H:118:ILE:HG21	1.96	0.45
1:F:143:ASN:O	1:F:188:SER:HA	2.15	0.45
1:G:227:PRO:HD3	1:G:262:GLY:O	2.15	0.45
1:H:17:ALA:O	1:H:42:ILE:N	2.48	0.45
1:J:88:HIS:CG	1:J:143:ASN:OD1	2.69	0.45
1:K:228:ILE:HG21	1:M:251:PHE:HE1	1.81	0.45
1:M:61:HIS:CE1	1:M:72:VAL:HG21	2.51	0.45
1:M:145:SER:HB2	1:M:166:VAL:CG1	2.46	0.45
1:O:35:LYS:HG3	1:O:54:GLY:O	2.16	0.45
1:C:227:PRO:CG	1:C:266:VAL:HG22	2.46	0.45
1:D:35:LYS:HG3	1:D:54:GLY:C	2.36	0.45
1:E:147:VAL:HG11	1:E:260:ASP:HB2	1.98	0.45
1:I:76:ALA:HB1	1:I:127:LEU:HD13	1.97	0.45
1:I:88:HIS:CE1	1:I:117:ILE:HA	2.51	0.45
1:I:92:ILE:HD11	1:I:109:VAL:HA	1.98	0.45
1:I:110:ASN:O	1:I:114:VAL:HB	2.15	0.45
1:I:232:GLY:CA	1:O:251:PHE:CZ	2.99	0.45
1:M:145:SER:O	1:M:163:LYS:NZ	2.38	0.45
1:N:16:VAL:N	1:N:84:ASP:HB2	2.30	0.45
1:N:201:SER:HA	1:N:215:ARG:CZ	2.46	0.45
1:O:155:PHE:C	1:O:157:ALA:N	2.66	0.45
1:O:227:PRO:HG3	1:O:266:VAL:HG21	1.98	0.45
1:P:180:LEU:C	1:P:182:TYR:H	2.19	0.45
1:A:125:LEU:N	1:A:126:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:THR:HG21	1:B:111:THR:HG22	1.97	0.45
1:G:142:VAL:HG22	1:G:244:LEU:HD13	1.98	0.45
1:K:141:VAL:HB	1:K:186:VAL:HG22	1.98	0.45
1:K:189:VAL:HG12	1:K:191:PRO:HD3	1.98	0.45
1:L:201:SER:O	1:L:204:ASP:N	2.40	0.45
1:L:227:PRO:O	1:N:178:ALA:HB1	2.16	0.45
1:N:111:THR:HA	1:N:115:ASP:HB2	1.98	0.45
1:N:167:LYS:HE3	1:N:171:LYS:HE3	1.98	0.45
1:P:12:LEU:O	1:P:39:ALA:HB2	2.17	0.45
1:P:157:ALA:O	1:P:161:THR:N	2.49	0.45
1:I:122:GLN:NE2	1:K:98:PHE:O	2.47	0.45
1:I:161:THR:O	1:I:164:ALA:HB3	2.16	0.45
1:J:76:ALA:O	1:J:80:TYR:N	2.36	0.45
1:J:88:HIS:NE2	1:J:141:VAL:HG13	2.31	0.45
1:J:182:TYR:N	1:J:182:TYR:HD1	2.14	0.45
1:M:112:VAL:O	1:M:112:VAL:CG1	2.64	0.45
1:C:244:LEU:HD11	1:C:257:PHE:CD2	2.51	0.45
1:D:129:LYS:HA	1:D:184:ILE:HD11	1.98	0.45
1:F:98:PHE:HZ	1:H:118:ILE:HA	1.81	0.45
1:F:146:SER:O	1:F:190:HIS:ND1	2.47	0.45
1:F:177:PHE:CE2	1:F:186:VAL:CG2	3.00	0.45
1:H:12:LEU:O	1:H:15:VAL:HB	2.16	0.45
1:I:10:ILE:HD11	1:O:242:VAL:HB	1.99	0.45
1:J:241:VAL:O	1:J:244:LEU:N	2.49	0.45
1:K:16:VAL:HG21	1:K:82:ARG:HG3	1.98	0.45
1:L:189:VAL:CG2	1:L:244:LEU:HD12	2.47	0.45
1:M:198:MET:O	1:M:201:SER:OG	2.33	0.45
1:O:182:TYR:C	1:O:184:ILE:HG13	2.37	0.45
1:O:195:ASP:CA	1:O:231:MET:SD	3.04	0.45
1:P:97:LYS:O	1:P:101:THR:N	2.50	0.45
1:C:237:MET:SD	1:C:259:MET:CE	3.05	0.45
1:D:101:THR:CG2	1:D:106:PHE:HD1	2.29	0.45
1:E:79:LYS:HB3	1:E:80:TYR:CD2	2.52	0.45
1:E:187:ASN:HB3	1:E:255:THR:CG2	2.39	0.45
1:G:15:VAL:O	1:G:40:ILE:N	2.47	0.45
1:H:22:ALA:HA	1:H:27:GLY:HA3	1.98	0.45
1:H:97:LYS:HG3	1:H:209:LEU:HD13	1.98	0.45
1:J:113:ASN:O	1:J:166:VAL:HG22	2.16	0.45
1:L:266:VAL:CA	1:P:151:ARG:HB2	2.46	0.45
1:N:105:ASP:O	1:N:109:VAL:HG23	2.17	0.45
1:P:18:VAL:CG1	1:P:86:LEU:HD12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:35:LYS:HD2	1:P:39:ALA:O	2.16	0.45
1:P:252:VAL:CG1	1:P:255:THR:HG21	2.43	0.45
1:D:29:GLU:CG	1:D:234:PRO:HB2	2.45	0.45
1:E:52:VAL:CG1	1:E:55:ALA:HB3	2.46	0.45
1:F:30:LEU:HD11	1:F:89:ASN:OD1	2.16	0.45
1:F:86:LEU:HD13	1:F:124:LEU:HD12	1.99	0.45
1:G:56:ASP:O	1:G:57:HIS:CG	2.70	0.45
1:G:125:LEU:HB3	1:G:126:PRO:HD3	1.99	0.45
1:G:132:GLY:HA2	1:G:138:GLY:HA2	1.98	0.45
1:G:146:SER:OG	1:G:147:VAL:N	2.50	0.45
1:I:84:ASP:HB3	1:I:135:ARG:HH11	1.81	0.45
1:L:139:ALA:O	1:L:184:ILE:HA	2.17	0.45
1:M:145:SER:HB2	1:M:166:VAL:HG11	1.99	0.45
1:A:135:ARG:NH2	1:A:247:ASP:OD1	2.44	0.45
1:B:201:SER:HA	1:B:204:ASP:OD2	2.17	0.45
1:C:101:THR:HG22	1:C:102:PRO:O	2.16	0.45
1:C:167:LYS:HD3	1:C:190:HIS:CE1	2.52	0.45
1:F:83:VAL:HG23	1:F:127:LEU:HD22	1.98	0.45
1:G:241:VAL:O	1:G:244:LEU:HB2	2.17	0.45
1:I:10:ILE:O	1:I:10:ILE:CG2	2.46	0.45
1:J:194:ILE:HG22	1:J:196:THR:HG23	1.98	0.45
1:K:23:ALA:HB2	1:K:50:ALA:CB	2.47	0.45
1:N:16:VAL:HG11	1:N:83:VAL:HA	1.99	0.45
1:N:173:LEU:HB3	1:N:177:PHE:CE2	2.52	0.45
1:O:187:ASN:OD1	1:O:255:THR:HG22	2.17	0.45
1:P:124:LEU:HD22	1:P:127:LEU:CD1	2.46	0.45
1:P:176:GLU:O	1:P:179:ALA:HB3	2.17	0.45
1:B:115:ASP:O	1:B:119:ILE:HG13	2.17	0.45
1:B:130:GLU:C	1:B:132:GLY:N	2.69	0.45
1:D:11:ALA:N	2:D:304:HOH:O	2.49	0.45
1:D:26:ILE:HG12	1:D:234:PRO:HA	1.98	0.45
1:D:82:ARG:NH2	1:D:84:ASP:OD1	2.49	0.45
1:D:237:MET:O	1:D:241:VAL:HG23	2.17	0.45
1:F:66:GLU:HA	1:F:119:ILE:HG21	1.99	0.45
1:I:98:PHE:O	1:I:99:GLU:C	2.54	0.45
1:J:255:THR:OG1	1:P:258:VAL:HG12	2.17	0.45
1:L:148:ALA:HB2	1:L:159:TYR:CE2	2.52	0.45
1:M:97:LYS:HE3	1:M:209:LEU:CD2	2.47	0.45
1:P:140:SER:HA	1:P:185:ARG:O	2.17	0.45
1:A:114:VAL:O	1:A:118:ILE:HG13	2.17	0.45
1:A:203:MET:HE2	1:A:222:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LYS:O	1:C:133:LYS:HG3	2.17	0.45
1:E:123:VAL:HG12	1:E:124:LEU:HD23	1.97	0.45
1:F:40:ILE:HA	1:F:56:ASP:OD2	2.16	0.45
1:F:45:ASP:O	1:F:46:MET:C	2.55	0.45
1:F:61:HIS:CE1	1:F:63:VAL:HG12	2.52	0.45
1:H:21:GLY:O	1:H:89:ASN:ND2	2.50	0.45
1:I:252:VAL:CG1	1:I:255:THR:HG21	2.47	0.45
1:K:26:ILE:CG1	1:K:234:PRO:HB3	2.45	0.45
1:K:185:ARG:NH1	1:K:249:ALA:O	2.50	0.45
1:M:147:VAL:O	1:M:151:ARG:O	2.35	0.45
1:P:105:ASP:O	1:P:109:VAL:HG23	2.17	0.45
1:A:151:ARG:HB3	1:E:265:GLN:O	2.17	0.44
1:A:185:ARG:HD3	1:A:250:SER:O	2.15	0.44
1:A:222:MET:O	1:A:226:HIS:CE1	2.71	0.44
1:B:18:VAL:HG11	1:B:72:VAL:HG11	1.99	0.44
1:C:227:PRO:HG2	1:C:262:GLY:O	2.17	0.44
1:G:12:LEU:HD11	1:G:245:CYS:HB2	2.00	0.44
1:J:26:ILE:HD13	1:J:237:MET:HG3	1.99	0.44
1:K:154:ALA:C	1:K:156:ASN:H	2.21	0.44
1:N:217:VAL:HA	1:N:220:ALA:HB3	1.99	0.44
1:O:24:GLY:O	1:O:25:GLY:C	2.55	0.44
1:P:146:SER:O	1:P:150:LEU:HG	2.17	0.44
1:P:162:SER:O	1:P:166:VAL:HG23	2.16	0.44
1:G:215:ARG:O	1:G:219:GLN:HB2	2.17	0.44
1:H:124:LEU:HD23	1:H:124:LEU:HA	1.78	0.44
1:I:35:LYS:HG3	1:I:54:GLY:HA3	1.98	0.44
1:J:112:VAL:O	1:J:112:VAL:CG1	2.64	0.44
1:K:53:GLU:C	1:K:55:ALA:H	2.20	0.44
1:P:16:VAL:HA	1:P:40:ILE:HB	1.98	0.44
1:I:15:VAL:HG13	1:I:84:ASP:CB	2.47	0.44
1:L:177:PHE:O	1:L:178:ALA:C	2.55	0.44
1:L:197:PRO:CG	2:L:306:HOH:O	2.58	0.44
1:M:193:GLY:O	1:M:232:GLY:N	2.44	0.44
1:A:88:HIS:CG	1:A:117:ILE:HG12	2.53	0.44
1:C:180:LEU:HD13	1:C:182:TYR:CE2	2.51	0.44
1:D:15:VAL:HG22	1:D:135:ARG:NE	2.32	0.44
1:E:150:LEU:HD23	1:E:167:LYS:HD2	1.99	0.44
1:K:20:THR:O	1:K:89:ASN:HB3	2.17	0.44
1:K:77:GLN:HB2	1:K:127:LEU:HD11	1.99	0.44
1:N:194:ILE:CG2	1:N:195:ASP:N	2.80	0.44
1:N:204:ASP:O	1:N:207:VAL:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:266:VAL:O	1:O:266:VAL:CG2	2.56	0.44
1:P:76:ALA:HB3	1:P:127:LEU:HD13	1.99	0.44
1:B:140:SER:HB2	1:B:185:ARG:NH2	2.33	0.44
1:E:20:THR:O	1:E:89:ASN:ND2	2.39	0.44
1:F:74:ALA:O	1:F:78:GLU:HB2	2.17	0.44
1:G:167:LYS:HG2	1:G:171:LYS:CE	2.47	0.44
1:I:88:HIS:NE2	1:I:117:ILE:HA	2.32	0.44
1:L:107:HIS:O	1:L:111:THR:N	2.48	0.44
1:N:115:ASP:O	1:N:116:SER:C	2.56	0.44
1:P:204:ASP:O	1:P:207:VAL:HB	2.17	0.44
1:A:239:GLY:HA2	1:A:242:VAL:HG23	1.99	0.44
1:D:22:ALA:HB3	1:D:45:ASP:HB2	1.99	0.44
1:D:97:LYS:HD3	1:D:99:GLU:CG	2.48	0.44
1:D:227:PRO:HG3	1:D:266:VAL:HG22	1.99	0.44
1:E:86:LEU:HD21	1:E:88:HIS:NE2	2.33	0.44
1:E:147:VAL:CG2	1:E:192:GLY:HA2	2.47	0.44
1:F:24:GLY:O	1:F:28:ARG:HG3	2.18	0.44
1:F:168:MET:SD	1:H:160:CYS:CB	3.02	0.44
1:G:163:LYS:O	1:G:167:LYS:N	2.46	0.44
1:K:159:TYR:CZ	1:K:163:LYS:HE3	2.53	0.44
1:N:114:VAL:HG12	1:N:118:ILE:HD11	1.99	0.44
1:P:147:VAL:HA	1:P:150:LEU:HB2	1.99	0.44
1:B:173:LEU:HB2	1:B:186:VAL:HG11	2.00	0.44
1:C:168:MET:HA	1:C:171:LYS:HD2	2.00	0.44
1:E:17:ALA:O	1:E:18:VAL:CG2	2.65	0.44
1:F:227:PRO:O	1:F:229:GLY:N	2.51	0.44
1:G:28:ARG:HD3	1:G:52:VAL:HA	2.00	0.44
1:I:97:LYS:O	1:I:100:ASP:C	2.56	0.44
1:J:173:LEU:HB2	1:J:186:VAL:HG11	1.99	0.44
1:M:148:ALA:O	1:M:160:CYS:SG	2.74	0.44
1:O:125:LEU:HA	1:O:128:LEU:HD12	1.99	0.44
1:A:141:VAL:HB	1:A:186:VAL:HA	2.00	0.44
1:B:253:THR:O	1:B:255:THR:N	2.51	0.44
1:C:24:GLY:O	1:C:28:ARG:HG3	2.18	0.44
1:C:225:ARG:NH2	2:C:303:HOH:O	2.51	0.44
1:D:220:ALA:HA	1:D:223:GLU:HB2	1.98	0.44
1:E:62:ASP:O	1:E:64:THR:N	2.50	0.44
1:F:25:GLY:HA2	1:F:28:ARG:NH1	2.31	0.44
1:G:115:ASP:HA	1:G:118:ILE:HD12	2.00	0.44
1:G:225:ARG:O	1:G:263:PHE:HA	2.18	0.44
1:I:44:THR:HB	1:I:61:HIS:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:204:ASP:OD1	1:K:215:ARG:HG3	2.18	0.44
1:N:82:ARG:NH1	1:N:134:ALA:HB3	2.33	0.44
1:P:230:ARG:HG3	1:P:231:MET:O	2.18	0.44
1:B:122:GLN:HG3	1:C:98:PHE:CZ	2.53	0.44
1:C:83:VAL:HG23	1:C:127:LEU:HB3	1.99	0.44
1:D:255:THR:OG1	1:D:256:GLU:N	2.51	0.44
1:D:265:GLN:OE1	1:E:171:LYS:NZ	2.47	0.44
1:F:20:THR:CG2	1:F:69:TRP:CH2	3.00	0.44
1:F:82:ARG:HH21	1:F:84:ASP:CG	2.22	0.44
1:K:106:PHE:CE1	1:K:158:ALA:HA	2.53	0.44
1:K:204:ASP:OD1	1:K:204:ASP:N	2.51	0.44
1:L:12:LEU:HD23	1:L:12:LEU:HA	1.86	0.44
1:N:94:ILE:CG2	1:N:95:VAL:N	2.79	0.44
1:N:189:VAL:HG12	1:N:191:PRO:HD3	1.99	0.44
1:O:22:ALA:O	1:O:28:ARG:HG2	2.18	0.44
1:A:138:GLY:H	1:A:183:ASN:HD21	1.64	0.43
1:C:17:ALA:HB3	1:C:41:VAL:HG22	1.99	0.43
1:F:170:SER:HA	1:F:186:VAL:HG12	2.00	0.43
1:G:12:LEU:HB2	1:G:37:ALA:HB1	2.00	0.43
1:G:140:SER:CB	1:G:245:CYS:HA	2.48	0.43
1:J:19:VAL:HG22	1:J:87:VAL:HB	2.00	0.43
1:J:76:ALA:O	1:J:79:LYS:N	2.51	0.43
1:J:130:GLU:OE1	1:J:133:LYS:NZ	2.36	0.43
1:L:12:LEU:HD21	1:L:245:CYS:C	2.38	0.43
1:L:64:THR:HG22	1:L:111:THR:C	2.37	0.43
1:D:109:VAL:O	1:D:109:VAL:CG1	2.66	0.43
1:E:12:LEU:HD13	1:E:39:ALA:HB2	2.00	0.43
1:E:42:ILE:HG23	1:E:57:HIS:HB2	2.00	0.43
1:F:164:ALA:O	1:F:167:LYS:HB3	2.18	0.43
1:L:26:ILE:HG22	1:L:30:LEU:HG	2.00	0.43
1:L:164:ALA:O	1:L:167:LYS:HE2	2.18	0.43
1:O:59:LEU:HD13	1:O:75:LEU:HD22	1.98	0.43
1:A:181:GLY:O	1:A:182:TYR:C	2.56	0.43
1:A:249:ALA:HB1	1:A:252:VAL:HB	2.00	0.43
1:B:162:SER:C	1:B:164:ALA:H	2.21	0.43
1:C:62:ASP:OD1	1:C:63:VAL:N	2.52	0.43
1:D:185:ARG:NE	1:D:250:SER:O	2.52	0.43
1:D:266:VAL:C	1:G:151:ARG:HD2	2.39	0.43
1:E:23:ALA:HA	1:E:28:ARG:HG2	2.00	0.43
1:E:88:HIS:N	1:E:142:VAL:O	2.50	0.43
1:H:199:LEU:C	1:H:201:SER:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:ARG:HD3	1:I:51:ASP:O	2.17	0.43
1:I:214:SER:C	1:I:216:GLU:H	2.20	0.43
1:J:221:ALA:O	1:J:225:ARG:HG3	2.19	0.43
1:K:12:LEU:HD23	1:K:246:SER:HA	2.00	0.43
1:M:118:ILE:O	1:M:122:GLN:HG3	2.18	0.43
1:N:16:VAL:CG1	1:N:83:VAL:HA	2.48	0.43
1:N:26:ILE:HD11	1:N:194:ILE:HG13	2.00	0.43
1:A:196:THR:C	1:A:198:MET:H	2.22	0.43
1:B:111:THR:HA	1:B:115:ASP:HB2	2.00	0.43
1:B:125:LEU:O	1:B:129:LYS:HG3	2.18	0.43
1:C:34:MET:HB3	1:C:41:VAL:HG21	1.99	0.43
1:D:57:HIS:NE2	1:D:80:TYR:OH	2.48	0.43
1:E:88:HIS:HB3	1:E:117:ILE:HG12	2.00	0.43
1:F:44:THR:HG21	1:F:61:HIS:ND1	2.32	0.43
1:H:159:TYR:CE1	1:H:163:LYS:HE2	2.54	0.43
1:I:226:HIS:HB3	1:I:228:ILE:HG22	2.01	0.43
1:J:20:THR:HG21	1:J:69:TRP:CH2	2.53	0.43
1:N:103:LEU:O	1:N:106:PHE:HB3	2.18	0.43
1:O:174:GLY:HA3	1:O:186:VAL:HB	2.00	0.43
1:C:145:SER:CB	1:C:190:HIS:CE1	3.01	0.43
1:C:266:VAL:O	1:H:151:ARG:CZ	2.66	0.43
1:C:266:VAL:O	1:H:151:ARG:NH1	2.51	0.43
1:E:12:LEU:HD23	1:E:12:LEU:HA	1.91	0.43
1:E:233:ARG:HE	1:E:233:ARG:HB2	1.57	0.43
1:G:151:ARG:NE	1:G:152:GLY:O	2.51	0.43
1:J:121:THR:O	1:J:125:LEU:N	2.51	0.43
1:K:173:LEU:O	1:K:177:PHE:CG	2.72	0.43
1:M:58:TYR:C	1:M:59:LEU:HD12	2.39	0.43
1:M:83:VAL:HG23	1:M:127:LEU:HB3	2.01	0.43
1:M:155:PHE:CD1	1:M:209:LEU:HD13	2.53	0.43
1:M:237:MET:O	1:M:241:VAL:HG23	2.19	0.43
1:N:115:ASP:O	1:N:119:ILE:HG13	2.18	0.43
1:O:125:LEU:N	1:O:126:PRO:CD	2.81	0.43
1:O:151:ARG:HD3	1:O:263:PHE:CE1	2.49	0.43
1:O:189:VAL:HG22	1:O:257:PHE:HB3	2.01	0.43
1:A:118:ILE:HG21	1:D:103:LEU:HD12	2.01	0.43
1:E:195:ASP:HB3	1:E:232:GLY:O	2.19	0.43
1:E:240:GLY:HA2	1:E:243:TYR:HB3	2.00	0.43
1:F:37:ALA:O	1:F:38:ASN:HB2	2.18	0.43
1:L:125:LEU:N	1:L:126:PRO:CD	2.81	0.43
1:N:40:ILE:HG23	1:N:56:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:SER:HB3	1:A:190:HIS:CD2	2.53	0.43
1:B:26:ILE:HA	1:B:234:PRO:HB3	2.01	0.43
1:E:180:LEU:HD21	1:G:155:PHE:CZ	2.54	0.43
1:F:27:GLY:O	1:F:31:VAL:HG23	2.18	0.43
1:F:168:MET:HG2	1:H:160:CYS:HB3	2.01	0.43
1:G:64:THR:CG2	1:G:112:VAL:HA	2.48	0.43
1:H:198:MET:O	1:H:202:LEU:N	2.52	0.43
1:J:151:ARG:O	1:J:151:ARG:HG3	2.19	0.43
1:J:164:ALA:HB2	1:L:168:MET:CE	2.46	0.43
1:K:103:LEU:HA	1:K:106:PHE:HB2	2.01	0.43
1:L:86:LEU:HB3	1:L:141:VAL:HA	2.01	0.43
1:L:266:VAL:C	1:P:151:ARG:NE	2.72	0.43
1:N:86:LEU:HD23	1:N:128:LEU:HD11	2.00	0.43
1:N:88:HIS:HB2	1:N:143:ASN:HA	2.01	0.43
1:N:156:ASN:CB	1:N:160:CYS:SG	3.06	0.43
1:N:194:ILE:CG2	1:N:195:ASP:H	2.32	0.43
1:A:138:GLY:HA2	1:A:183:ASN:ND2	2.34	0.43
1:A:176:GLU:O	1:A:180:LEU:HD12	2.19	0.43
1:B:209:LEU:HD23	1:B:209:LEU:HA	1.92	0.43
1:E:140:SER:HB3	1:E:245:CYS:HA	2.00	0.43
1:F:101:THR:O	1:F:102:PRO:C	2.56	0.43
1:F:140:SER:CB	1:F:245:CYS:HA	2.49	0.43
1:H:158:ALA:HA	1:H:161:THR:OG1	2.18	0.43
1:I:120:GLY:O	1:I:124:LEU:HG	2.18	0.43
1:J:103:LEU:HD21	1:L:115:ASP:HB3	1.99	0.43
1:J:249:ALA:HB1	1:J:252:VAL:HB	2.00	0.43
1:K:26:ILE:HG12	1:K:234:PRO:HB3	2.00	0.43
1:K:243:TYR:CZ	1:K:249:ALA:HB2	2.53	0.43
1:L:189:VAL:HA	1:L:257:PHE:O	2.19	0.43
1:N:141:VAL:O	1:N:186:VAL:HA	2.19	0.43
1:O:92:ILE:CG2	1:O:112:VAL:HG11	2.48	0.43
1:P:143:ASN:ND2	1:P:170:SER:HA	2.33	0.43
1:P:145:SER:CB	1:P:190:HIS:HD1	2.24	0.43
1:B:83:VAL:HG11	1:B:124:LEU:HD13	2.01	0.43
1:G:219:GLN:HG2	1:G:223:GLU:OE1	2.19	0.43
1:I:42:ILE:HA	1:I:57:HIS:HB2	2.00	0.43
1:J:113:ASN:O	1:J:166:VAL:CG2	2.66	0.43
1:L:30:LEU:HD11	1:L:144:PHE:CZ	2.54	0.43
1:M:228:ILE:HB	1:M:261:GLY:O	2.18	0.43
1:N:242:VAL:O	1:N:246:SER:N	2.44	0.43
1:O:44:THR:HA	1:O:59:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:91:GLY:HA2	1:P:112:VAL:HG12	1.99	0.43
1:A:103:LEU:HD11	1:D:118:ILE:HD12	2.00	0.43
1:C:135:ARG:NE	1:C:247:ASP:OD1	2.52	0.43
1:D:151:ARG:HD2	1:G:266:VAL:O	2.18	0.43
1:E:12:LEU:HD22	1:E:15:VAL:HG11	2.00	0.43
1:E:25:GLY:HA3	1:E:196:THR:HG22	2.00	0.43
1:E:142:VAL:HG13	1:E:189:VAL:HG23	2.01	0.43
1:E:207:VAL:HA	1:E:212:ALA:HB3	2.01	0.43
1:G:125:LEU:N	1:G:126:PRO:CD	2.82	0.43
1:G:228:ILE:HG12	1:G:230:ARG:HG2	2.00	0.43
1:H:154:ALA:O	1:H:156:ASN:N	2.49	0.43
1:I:88:HIS:HE1	1:I:120:GLY:HA3	1.83	0.43
1:I:189:VAL:HG12	1:I:191:PRO:HD3	2.00	0.43
1:I:227:PRO:HD2	1:I:263:PHE:N	2.34	0.43
1:L:138:GLY:HA3	1:L:183:ASN:O	2.18	0.43
1:L:163:LYS:O	1:L:164:ALA:C	2.57	0.43
1:M:145:SER:O	1:M:191:PRO:HG2	2.18	0.43
1:M:171:LYS:HZ1	1:M:256:GLU:HG2	1.83	0.43
1:P:32:LYS:HG2	1:P:53:GLU:O	2.18	0.43
1:A:109:VAL:O	1:A:110:ASN:C	2.57	0.42
1:J:122:GLN:HG3	1:L:98:PHE:CE2	2.54	0.42
1:L:61:HIS:CD2	1:L:68:GLY:HA3	2.54	0.42
1:L:266:VAL:O	1:P:151:ARG:NE	2.52	0.42
1:B:69:TRP:CE3	1:B:120:GLY:HA2	2.54	0.42
1:C:180:LEU:CD1	1:C:182:TYR:CE2	3.02	0.42
1:D:31:VAL:HG12	1:D:53:GLU:O	2.19	0.42
1:E:180:LEU:HD12	1:E:182:TYR:CE2	2.51	0.42
1:K:151:ARG:NH1	1:K:263:PHE:CZ	2.87	0.42
1:L:156:ASN:ND2	1:L:206:TYR:OH	2.47	0.42
1:N:88:HIS:CG	1:N:117:ILE:HG12	2.55	0.42
1:N:157:ALA:HA	1:P:172:CYS:SG	2.60	0.42
1:C:15:VAL:CG2	1:C:135:ARG:NH1	2.83	0.42
1:D:150:LEU:HA	1:D:167:LYS:HZ3	1.84	0.42
1:D:169:LEU:O	1:D:173:LEU:HG	2.19	0.42
1:E:63:VAL:O	1:E:116:SER:HA	2.20	0.42
1:E:117:ILE:HG21	1:E:169:LEU:HD23	2.01	0.42
1:F:102:PRO:HB2	1:F:104:SER:OG	2.18	0.42
1:I:98:PHE:C	1:I:100:ASP:H	2.23	0.42
1:J:147:VAL:HA	1:J:150:LEU:HB2	2.00	0.42
1:K:53:GLU:O	1:K:55:ALA:N	2.52	0.42
1:K:98:PHE:HE1	1:K:106:PHE:CZ	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:243:TYR:CD2	1:K:244:LEU:HD23	2.54	0.42
1:M:168:MET:HB3	1:O:161:THR:HG22	2.02	0.42
1:N:111:THR:HA	1:N:115:ASP:CB	2.48	0.42
1:O:20:THR:OG1	1:O:89:ASN:N	2.53	0.42
1:A:176:GLU:CG	1:A:180:LEU:CD1	2.97	0.42
1:D:167:LYS:HB2	1:D:190:HIS:HE1	1.83	0.42
1:D:257:PHE:CE2	1:E:257:PHE:HE1	2.36	0.42
1:E:176:GLU:HA	1:G:154:ALA:CB	2.48	0.42
1:J:139:ALA:O	1:J:184:ILE:HA	2.19	0.42
1:K:45:ASP:HB3	1:K:58:TYR:CZ	2.55	0.42
1:L:135:ARG:HH11	1:L:139:ALA:HA	1.85	0.42
1:L:226:HIS:O	1:L:229:GLY:N	2.49	0.42
1:M:204:ASP:O	1:M:205:LYS:C	2.57	0.42
1:N:64:THR:O	1:N:119:ILE:HD13	2.19	0.42
1:N:165:ALA:O	1:N:168:MET:N	2.52	0.42
1:O:130:GLU:OE2	1:O:133:LYS:HD2	2.19	0.42
1:E:32:LYS:CD	1:E:53:GLU:HB3	2.50	0.42
1:H:199:LEU:HD12	1:H:202:LEU:HB2	2.00	0.42
1:I:190:HIS:NE2	1:I:256:GLU:CB	2.83	0.42
1:L:244:LEU:HD21	1:L:257:PHE:CD1	2.55	0.42
1:N:146:SER:C	1:N:148:ALA:N	2.71	0.42
1:A:251:PHE:HD1	1:G:228:ILE:CD1	2.32	0.42
1:D:146:SER:HA	1:D:191:PRO:HD2	2.00	0.42
1:F:19:VAL:HA	1:F:87:VAL:O	2.20	0.42
1:F:41:VAL:HG12	1:F:42:ILE:N	2.35	0.42
1:O:102:PRO:HD2	1:O:105:ASP:HB2	2.01	0.42
1:A:31:VAL:HG11	1:A:55:ALA:HB2	2.02	0.42
1:B:226:HIS:HB3	1:B:228:ILE:HG22	2.02	0.42
1:E:82:ARG:NH2	1:E:134:ALA:CB	2.74	0.42
1:E:82:ARG:HH22	1:E:134:ALA:HB3	1.79	0.42
1:E:106:PHE:CG	1:G:118:ILE:HD13	2.55	0.42
1:H:142:VAL:O	1:H:142:VAL:CG1	2.66	0.42
1:I:173:LEU:HD21	1:K:98:PHE:CG	2.54	0.42
1:I:227:PRO:HG2	1:I:262:GLY:HA3	2.01	0.42
1:J:169:LEU:C	1:J:171:LYS:N	2.73	0.42
1:K:22:ALA:C	1:K:24:GLY:H	2.23	0.42
1:K:62:ASP:O	1:K:65:SER:N	2.53	0.42
1:L:20:THR:O	1:L:89:ASN:HB3	2.20	0.42
1:N:59:LEU:HD22	1:N:72:VAL:HG22	2.00	0.42
1:O:119:ILE:O	1:O:123:VAL:HG23	2.19	0.42
1:A:119:ILE:O	1:A:123:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:THR:HB	1:B:63:VAL:HG11	2.02	0.42
1:D:266:VAL:C	1:G:151:ARG:HH11	2.22	0.42
1:F:180:LEU:C	1:F:182:TYR:N	2.73	0.42
1:H:33:ALA:HB2	1:H:238:GLY:HA3	2.02	0.42
1:H:98:PHE:O	1:H:99:GLU:C	2.57	0.42
1:I:215:ARG:O	1:I:215:ARG:HG2	2.20	0.42
1:L:26:ILE:HA	1:L:29:GLU:HB2	2.02	0.42
1:L:187:ASN:HD21	1:L:257:PHE:HB2	1.85	0.42
1:O:154:ALA:O	1:O:156:ASN:N	2.49	0.42
1:A:251:PHE:HA	1:G:228:ILE:CD1	2.50	0.42
1:D:118:ILE:O	1:D:122:GLN:N	2.52	0.42
1:E:143:ASN:O	1:E:189:VAL:HB	2.20	0.42
1:F:161:THR:HA	1:H:168:MET:CG	2.48	0.42
1:H:137:GLY:O	1:H:247:ASP:HA	2.20	0.42
1:I:160:CYS:O	1:I:164:ALA:N	2.53	0.42
1:J:111:THR:O	1:J:115:ASP:HB2	2.20	0.42
1:J:176:GLU:HA	1:L:154:ALA:CB	2.49	0.42
1:K:12:LEU:HD21	1:K:245:CYS:C	2.40	0.42
1:L:252:VAL:HG22	1:N:259:MET:HA	2.02	0.42
1:M:30:LEU:CD1	1:M:87:VAL:HG11	2.49	0.42
1:N:199:LEU:HD12	1:N:202:LEU:HD12	2.01	0.42
1:P:16:VAL:HG22	1:P:40:ILE:HD13	2.01	0.42
1:A:88:HIS:CE1	1:A:117:ILE:HA	2.55	0.42
1:A:91:GLY:HA2	1:A:113:ASN:OD1	2.19	0.42
1:A:182:TYR:HE2	1:D:99:GLU:OE1	2.03	0.42
1:B:98:PHE:CZ	1:C:122:GLN:HG3	2.55	0.42
1:B:159:TYR:OH	1:B:163:LYS:HG3	2.20	0.42
1:C:25:GLY:HA3	1:C:196:THR:HG22	2.02	0.42
1:C:50:ALA:HB3	1:C:58:TYR:OH	2.20	0.42
1:C:247:ASP:O	1:C:250:SER:CB	2.68	0.42
1:H:146:SER:OG	1:H:147:VAL:N	2.53	0.42
1:H:185:ARG:HD2	1:H:252:VAL:O	2.20	0.42
1:J:114:VAL:O	1:J:117:ILE:HB	2.19	0.42
1:K:61:HIS:CD2	1:K:61:HIS:C	2.93	0.42
1:L:259:MET:HG2	1:N:252:VAL:HG22	2.02	0.42
1:N:117:ILE:O	1:N:121:THR:OG1	2.30	0.42
1:O:216:GLU:HA	1:O:219:GLN:CB	2.50	0.42
1:A:61:HIS:CD2	1:A:61:HIS:C	2.93	0.41
1:A:145:SER:N	1:A:189:VAL:O	2.52	0.41
1:B:145:SER:HB3	1:B:190:HIS:CD2	2.55	0.41
1:B:241:VAL:O	1:B:242:VAL:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:HB3	1:C:253:THR:HB	2.01	0.41
1:C:246:SER:OG	1:C:248:ALA:HB3	2.20	0.41
1:E:17:ALA:HA	1:E:85:ALA:HB3	2.02	0.41
1:G:200:GLY:HA2	1:G:215:ARG:HH22	1.85	0.41
1:H:137:GLY:O	1:H:185:ARG:NH2	2.51	0.41
1:H:201:SER:O	1:H:205:LYS:HG2	2.20	0.41
1:J:124:LEU:HD23	1:J:124:LEU:HA	1.89	0.41
1:L:242:VAL:O	1:L:245:CYS:N	2.50	0.41
1:M:31:VAL:HG11	1:M:52:VAL:CG1	2.48	0.41
1:N:102:PRO:HD2	1:N:105:ASP:OD2	2.20	0.41
1:O:43:ALA:HB3	1:O:57:HIS:O	2.19	0.41
1:P:106:PHE:HD1	1:P:158:ALA:HB2	1.84	0.41
1:A:139:ALA:HB3	1:A:184:ILE:HG12	2.01	0.41
1:B:45:ASP:HB3	1:B:58:TYR:OH	2.20	0.41
1:C:107:HIS:O	1:C:111:THR:N	2.46	0.41
1:D:225:ARG:HD3	1:D:263:PHE:CE1	2.50	0.41
1:J:263:PHE:C	1:J:263:PHE:CD1	2.94	0.41
1:K:142:VAL:HG13	1:K:189:VAL:HG23	2.02	0.41
1:L:197:PRO:CD	2:L:306:HOH:O	2.57	0.41
1:N:117:ILE:O	1:N:121:THR:CB	2.68	0.41
1:P:189:VAL:HA	1:P:257:PHE:HB3	2.02	0.41
1:D:257:PHE:CE1	1:D:259:MET:HG3	2.54	0.41
1:E:104:SER:O	1:E:108:ARG:HB2	2.20	0.41
1:E:141:VAL:HB	1:E:186:VAL:HG22	2.03	0.41
1:H:135:ARG:NH2	1:H:138:GLY:O	2.53	0.41
1:I:194:ILE:HD11	1:I:237:MET:CE	2.50	0.41
1:L:47:ALA:HB3	1:L:58:TYR:OH	2.19	0.41
1:N:202:LEU:HD23	1:N:202:LEU:HA	1.92	0.41
1:N:212:ALA:HB1	1:N:213:PRO:CD	2.50	0.41
1:A:98:PHE:CZ	1:D:121:THR:HB	2.54	0.41
1:D:48:PRO:HA	1:D:60:GLN:OE1	2.21	0.41
1:J:251:PHE:CZ	1:P:232:GLY:N	2.89	0.41
1:L:63:VAL:HB	1:L:69:TRP:HZ2	1.85	0.41
1:L:205:LYS:O	1:L:209:LEU:HG	2.20	0.41
1:M:134:ALA:O	1:M:135:ARG:HG3	2.20	0.41
1:N:15:VAL:HA	1:N:84:ASP:OD2	2.20	0.41
1:O:46:MET:CG	1:O:62:ASP:HA	2.50	0.41
1:O:69:TRP:C	1:O:123:VAL:HG11	2.40	0.41
1:P:26:ILE:HG22	1:P:30:LEU:HG	2.03	0.41
1:P:96:THR:HG23	1:P:101:THR:OG1	2.20	0.41
1:A:203:MET:HA	1:A:206:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:TYR:CZ	1:C:163:LYS:HE3	2.56	0.41
1:C:185:ARG:HG2	1:F:228:ILE:HD12	2.01	0.41
1:D:66:GLU:HG3	1:D:123:VAL:CG2	2.49	0.41
1:H:17:ALA:HA	1:H:85:ALA:O	2.21	0.41
1:I:236:GLU:HG2	1:O:250:SER:OG	2.20	0.41
1:M:45:ASP:O	1:M:60:GLN:HA	2.19	0.41
1:N:82:ARG:HH12	1:N:134:ALA:HB3	1.84	0.41
1:O:21:GLY:O	1:O:27:GLY:HA3	2.20	0.41
1:P:12:LEU:HG	1:P:242:VAL:HG13	2.03	0.41
1:A:83:VAL:HG21	1:A:124:LEU:HD22	2.02	0.41
1:B:20:THR:HG21	1:B:69:TRP:CH2	2.56	0.41
1:B:69:TRP:CE3	1:B:120:GLY:CA	3.04	0.41
1:C:130:GLU:HA	1:C:133:LYS:HB2	2.01	0.41
1:C:171:LYS:HE2	1:F:265:GLN:OE1	2.21	0.41
1:D:92:ILE:HD11	1:D:109:VAL:HA	2.01	0.41
1:L:251:PHE:CD2	1:N:237:MET:CE	3.03	0.41
1:L:251:PHE:HB2	1:N:236:GLU:CD	2.41	0.41
1:O:75:LEU:HG	1:O:79:LYS:HG3	2.01	0.41
1:O:190:HIS:HB2	1:O:258:VAL:HA	2.01	0.41
1:P:263:PHE:C	1:P:263:PHE:HD1	2.24	0.41
1:A:187:ASN:OD1	1:A:253:THR:HA	2.20	0.41
1:B:32:LYS:CE	1:B:53:GLU:HB3	2.42	0.41
1:B:237:MET:HA	1:B:259:MET:HE2	2.03	0.41
1:E:84:ASP:HB3	1:E:135:ARG:HH11	1.85	0.41
1:E:132:GLY:HA2	1:E:139:ALA:N	2.35	0.41
1:F:265:GLN:O	1:F:266:VAL:CG1	2.69	0.41
1:J:243:TYR:CE1	1:P:240:GLY:N	2.89	0.41
1:K:207:VAL:HA	1:K:212:ALA:O	2.21	0.41
1:L:251:PHE:HD2	1:N:237:MET:HE1	1.86	0.41
1:M:119:ILE:HG13	1:O:103:LEU:HD13	2.02	0.41
1:N:212:ALA:HB1	1:N:213:PRO:HD2	2.02	0.41
1:P:18:VAL:HG21	1:P:124:LEU:CD1	2.51	0.41
1:B:221:ALA:HA	1:B:224:MET:CE	2.50	0.41
1:C:159:TYR:CE1	1:C:163:LYS:HE3	2.56	0.41
1:D:18:VAL:O	1:D:87:VAL:N	2.53	0.41
1:E:72:VAL:HG12	1:E:124:LEU:HD21	2.03	0.41
1:F:103:LEU:O	1:F:107:HIS:NE2	2.54	0.41
1:F:265:GLN:O	1:F:266:VAL:HG13	2.21	0.41
1:G:12:LEU:HD21	1:G:245:CYS:CB	2.50	0.41
1:I:185:ARG:HD3	1:I:250:SER:O	2.21	0.41
1:I:203:MET:HA	1:I:206:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:147:VAL:HG21	1:N:263:PHE:HD2	1.85	0.41
1:N:155:PHE:CD1	1:P:176:GLU:OE2	2.73	0.41
1:O:45:ASP:HB3	1:O:58:TYR:OH	2.21	0.41
1:P:80:TYR:C	1:P:82:ARG:H	2.23	0.41
1:A:13:ASN:HB2	2:A:304:HOH:O	2.21	0.41
1:A:66:GLU:C	1:A:68:GLY:N	2.74	0.41
1:A:173:LEU:HB3	1:A:186:VAL:HG21	2.01	0.41
1:B:31:VAL:HG13	1:B:41:VAL:HG11	2.03	0.41
1:B:251:PHE:CG	1:B:251:PHE:O	2.74	0.41
1:D:66:GLU:HA	1:D:69:TRP:HB2	2.02	0.41
1:E:35:LYS:HG3	1:E:54:GLY:CA	2.51	0.41
1:E:69:TRP:HZ3	1:E:124:LEU:CD1	2.31	0.41
1:E:69:TRP:CE2	1:E:120:GLY:CA	3.04	0.41
1:F:73:ALA:O	1:F:77:GLN:N	2.43	0.41
1:G:233:ARG:N	1:G:236:GLU:OE2	2.54	0.41
1:I:21:GLY:O	1:I:27:GLY:HA3	2.20	0.41
1:J:167:LYS:O	1:J:171:LYS:HG3	2.21	0.41
1:J:251:PHE:CE1	1:P:231:MET:C	2.94	0.41
1:J:265:GLN:OE1	1:P:171:LYS:NZ	2.49	0.41
1:K:74:ALA:HA	1:K:77:GLN:HB3	2.03	0.41
1:K:142:VAL:CG2	1:K:244:LEU:CD1	2.97	0.41
1:L:139:ALA:HB3	1:L:184:ILE:HG23	2.02	0.41
1:N:132:GLY:HA3	1:N:183:ASN:O	2.21	0.41
1:N:143:ASN:OD1	1:N:143:ASN:N	2.54	0.41
1:N:170:SER:O	1:N:173:LEU:N	2.54	0.41
1:O:87:VAL:HG12	1:O:89:ASN:HB2	2.03	0.41
1:O:125:LEU:HG	1:O:129:LYS:HE3	2.03	0.41
1:O:227:PRO:HD2	1:O:263:PHE:HA	2.03	0.41
1:A:111:THR:HA	1:A:115:ASP:HB2	2.02	0.41
1:A:157:ALA:HA	1:D:172:CYS:HB3	2.03	0.41
1:C:94:ILE:HG22	1:C:96:THR:HG22	2.03	0.41
1:F:216:GLU:HA	1:F:219:GLN:CB	2.47	0.41
1:G:193:GLY:CA	1:G:199:LEU:HD13	2.50	0.41
1:H:15:VAL:HA	1:H:84:ASP:CG	2.41	0.41
1:I:35:LYS:HG3	1:I:54:GLY:CA	2.51	0.41
1:J:240:GLY:O	1:J:244:LEU:HG	2.20	0.41
1:L:12:LEU:HD12	1:L:242:VAL:HG22	2.02	0.41
1:M:151:ARG:HD3	1:M:263:PHE:CE1	2.44	0.41
1:N:111:THR:O	1:N:115:ASP:HB2	2.21	0.41
1:O:108:ARG:O	1:O:112:VAL:HG23	2.20	0.41
1:P:72:VAL:O	1:P:72:VAL:CG1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLY:HA3	1:A:254:CYS:SG	2.61	0.40
1:A:176:GLU:C	1:A:178:ALA:N	2.74	0.40
1:G:194:ILE:HG23	1:G:232:GLY:O	2.21	0.40
1:H:22:ALA:HA	1:H:27:GLY:CA	2.51	0.40
1:I:189:VAL:O	1:I:191:PRO:HD3	2.21	0.40
1:I:266:VAL:C	1:M:151:ARG:CZ	2.90	0.40
1:K:30:LEU:HD21	1:K:241:VAL:HG21	2.03	0.40
1:K:266:VAL:C	1:O:151:ARG:NH2	2.74	0.40
1:M:61:HIS:HE1	1:M:69:TRP:CZ3	2.40	0.40
1:M:95:VAL:O	1:M:96:THR:HB	2.20	0.40
1:O:177:PHE:CD2	1:O:184:ILE:HB	2.56	0.40
1:P:42:ILE:CD1	1:P:75:LEU:HD23	2.51	0.40
1:A:96:THR:HG23	1:A:101:THR:OG1	2.21	0.40
1:A:157:ALA:O	1:A:161:THR:HG23	2.21	0.40
1:A:173:LEU:CD2	1:D:98:PHE:CD1	2.96	0.40
1:C:132:GLY:O	1:C:183:ASN:HB3	2.21	0.40
1:D:205:LYS:C	1:D:207:VAL:H	2.24	0.40
1:F:23:ALA:HB2	1:F:50:ALA:HB3	2.03	0.40
1:F:229:GLY:O	1:F:230:ARG:CB	2.68	0.40
1:G:169:LEU:HG	1:G:173:LEU:HG	2.04	0.40
1:I:10:ILE:CD1	1:O:242:VAL:HB	2.51	0.40
1:J:155:PHE:CE1	1:L:180:LEU:HD11	2.56	0.40
1:J:194:ILE:HD11	1:J:237:MET:CE	2.51	0.40
1:K:63:VAL:HG11	1:K:90:ALA:HB3	2.03	0.40
1:K:73:ALA:HB2	1:K:124:LEU:HD23	2.04	0.40
1:L:34:MET:O	1:L:39:ALA:HB3	2.20	0.40
1:L:188:SER:O	1:L:257:PHE:HB3	2.21	0.40
1:O:20:THR:HG1	1:O:89:ASN:H	1.68	0.40
1:A:22:ALA:CB	1:A:43:ALA:HB1	2.51	0.40
1:C:106:PHE:O	1:C:110:ASN:ND2	2.55	0.40
1:C:228:ILE:HG23	1:C:230:ARG:HG2	2.04	0.40
1:D:69:TRP:CD2	1:D:120:GLY:HA2	2.56	0.40
1:D:257:PHE:CD1	1:D:257:PHE:C	2.95	0.40
1:E:161:THR:HG21	1:G:169:LEU:HB2	2.02	0.40
1:G:193:GLY:HA3	1:G:199:LEU:HD13	2.02	0.40
1:H:96:THR:CA	1:H:209:LEU:HD11	2.48	0.40
1:H:135:ARG:CZ	1:H:138:GLY:O	2.69	0.40
1:I:203:MET:HA	1:I:206:TYR:CD2	2.56	0.40
1:J:219:GLN:HA	1:J:222:MET:HB3	2.04	0.40
1:J:253:THR:HG22	1:P:228:ILE:HD12	2.02	0.40
1:J:265:GLN:HG3	1:P:255:THR:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:48:PRO:HA	1:K:60:GLN:HB2	2.02	0.40
1:K:57:HIS:NE2	1:K:79:LYS:HE3	2.36	0.40
1:M:20:THR:HG1	1:M:89:ASN:H	1.64	0.40
1:M:121:THR:O	1:M:122:GLN:C	2.60	0.40
1:P:65:SER:OG	1:P:68:GLY:N	2.42	0.40
1:C:42:ILE:HG23	1:C:57:HIS:O	2.21	0.40
1:E:176:GLU:O	1:E:180:LEU:HG	2.21	0.40
1:F:73:ALA:HA	1:F:76:ALA:HB3	2.03	0.40
1:F:137:GLY:HA3	1:F:250:SER:HB3	2.03	0.40
1:G:26:ILE:HG13	1:G:196:THR:CG2	2.50	0.40
1:G:59:LEU:HD11	1:G:75:LEU:HD22	2.02	0.40
1:I:28:ARG:O	1:I:31:VAL:N	2.55	0.40
1:I:40:ILE:HG21	1:I:80:TYR:CE1	2.56	0.40
1:J:108:ARG:HA	1:J:111:THR:HB	2.03	0.40
1:J:193:GLY:O	1:J:231:MET:HB3	2.20	0.40
1:M:98:PHE:O	1:O:122:GLN:NE2	2.54	0.40
1:M:171:LYS:NZ	1:M:256:GLU:HG2	2.37	0.40
1:M:194:ILE:HA	1:M:232:GLY:O	2.21	0.40
1:B:17:ALA:HB2	1:B:85:ALA:HB3	2.02	0.40
1:C:212:ALA:HB1	1:C:217:VAL:CG1	2.51	0.40
1:D:83:VAL:HG23	1:D:127:LEU:HB3	2.04	0.40
1:E:48:PRO:HB2	1:E:49:SER:H	1.67	0.40
1:E:156:ASN:HD21	1:E:206:TYR:HE1	1.70	0.40
1:F:20:THR:HG21	1:F:69:TRP:CZ2	2.56	0.40
1:G:86:LEU:CD1	1:G:124:LEU:HD13	2.52	0.40
1:G:169:LEU:O	1:G:170:SER:C	2.59	0.40
1:H:146:SER:OG	1:H:148:ALA:N	2.50	0.40
1:I:88:HIS:CG	1:I:117:ILE:HG12	2.56	0.40
1:J:125:LEU:N	1:J:126:PRO:CD	2.84	0.40
1:K:163:LYS:HA	1:K:166:VAL:HB	2.03	0.40
1:P:109:VAL:HG12	1:P:113:ASN:HD22	1.86	0.40
1:P:143:ASN:HD21	1:P:186:VAL:CG1	2.34	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:OE1	1:C:136:ALA:CB[1_455]	1.92	0.28

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	254/266 (96%)	203 (80%)	45 (18%)	6 (2%)	5	23
1	B	255/266 (96%)	213 (84%)	39 (15%)	3 (1%)	11	37
1	C	252/266 (95%)	214 (85%)	33 (13%)	5 (2%)	6	27
1	D	254/266 (96%)	213 (84%)	35 (14%)	6 (2%)	5	23
1	E	253/266 (95%)	215 (85%)	31 (12%)	7 (3%)	4	21
1	F	253/266 (95%)	207 (82%)	36 (14%)	10 (4%)	2	14
1	G	253/266 (95%)	224 (88%)	22 (9%)	7 (3%)	4	21
1	H	254/266 (96%)	216 (85%)	33 (13%)	5 (2%)	6	27
1	I	255/266 (96%)	223 (88%)	27 (11%)	5 (2%)	6	27
1	J	254/266 (96%)	225 (89%)	20 (8%)	9 (4%)	3	17
1	K	254/266 (96%)	212 (84%)	35 (14%)	7 (3%)	4	21
1	L	254/266 (96%)	214 (84%)	37 (15%)	3 (1%)	11	37
1	M	253/266 (95%)	206 (81%)	40 (16%)	7 (3%)	4	21
1	N	254/266 (96%)	214 (84%)	34 (13%)	6 (2%)	5	23
1	O	253/266 (95%)	214 (85%)	33 (13%)	6 (2%)	5	23
1	P	253/266 (95%)	207 (82%)	38 (15%)	8 (3%)	3	19
All	All	4058/4256 (95%)	3420 (84%)	538 (13%)	100 (2%)	4	23

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	63	VAL
1	F	38	ASN
1	F	45	ASP
1	F	157	ALA
1	G	195	ASP
1	H	118	ILE

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Mol	Chain	Res	Type
1	I	145	SER
1	I	146	SER
1	J	38	ASN
1	J	263	PHE
1	K	145	SER
1	K	218	ALA
1	N	213	PRO
1	P	156	ASN
1	P	157	ALA
1	P	183	ASN
1	A	38	ASN
1	E	247	ASP
1	F	103	LEU
1	F	116	SER
1	F	230	ARG
1	F	248	ALA
1	G	213	PRO
1	H	53	GLU
1	H	254	CYS
1	I	99	GLU
1	J	193	GLY
1	K	38	ASN
1	K	146	SER
1	K	196	THR
1	L	51	ASP
1	M	78	GLU
1	M	181	GLY
1	N	38	ASN
1	N	147	VAL
1	O	25	GLY
1	O	224	MET
1	A	55	ALA
1	A	67	ALA
1	A	145	SER
1	B	254	CYS
1	B	256	GLU
1	C	254	CYS
1	C	263	PHE
1	D	136	ALA
1	D	200	GLY
1	E	48	PRO
1	E	100	ASP

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Mol	Chain	Res	Type
1	F	14	ASN
1	F	227	PRO
1	G	89	ASN
1	G	197	PRO
1	H	249	ALA
1	L	146	SER
1	M	136	ALA
1	M	244	LEU
1	N	145	SER
1	N	146	SER
1	O	213	PRO
1	P	38	ASN
1	A	70	LYS
1	A	197	PRO
1	C	38	ASN
1	D	145	SER
1	D	232	GLY
1	E	60	GLN
1	F	46	MET
1	G	200	GLY
1	I	55	ALA
1	J	53	GLU
1	J	145	SER
1	M	157	ALA
1	O	48	PRO
1	O	156	ASN
1	P	159	TYR
1	P	210	GLY
1	C	249	ALA
1	E	145	SER
1	J	238	GLY
1	K	235	ALA
1	L	198	MET
1	N	167	LYS
1	O	88	HIS
1	C	242	VAL
1	D	206	TYR
1	G	155	PHE
1	J	116	SER
1	K	263	PHE
1	M	263	PHE
1	H	94	ILE

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Mol	Chain	Res	Type
1	J	25	GLY
1	J	119	ILE
1	B	63	VAL
1	P	48	PRO
1	D	147	VAL
1	M	147	VAL
1	P	63	VAL
1	E	234	PRO
1	G	119	ILE
1	I	193	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/198 (95%)	177 (94%)	11 (6%)	16	42
1	B	189/198 (96%)	175 (93%)	14 (7%)	11	33
1	C	187/198 (94%)	181 (97%)	6 (3%)	34	59
1	D	188/198 (95%)	182 (97%)	6 (3%)	34	59
1	E	188/198 (95%)	181 (96%)	7 (4%)	29	55
1	F	188/198 (95%)	179 (95%)	9 (5%)	21	48
1	G	188/198 (95%)	180 (96%)	8 (4%)	25	51
1	H	188/198 (95%)	180 (96%)	8 (4%)	25	51
1	I	189/198 (96%)	185 (98%)	4 (2%)	48	69
1	J	188/198 (95%)	181 (96%)	7 (4%)	29	55
1	K	188/198 (95%)	178 (95%)	10 (5%)	19	45
1	L	188/198 (95%)	179 (95%)	9 (5%)	21	48
1	M	188/198 (95%)	177 (94%)	11 (6%)	16	42
1	N	188/198 (95%)	178 (95%)	10 (5%)	19	45
1	O	188/198 (95%)	181 (96%)	7 (4%)	29	55
1	P	188/198 (95%)	177 (94%)	11 (6%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3009/3168 (95%)	2871 (95%)	138 (5%)	23 50

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	82	ARG
1	A	105	ASP
1	A	144	PHE
1	A	147	VAL
1	A	173	LEU
1	A	196	THR
1	A	213	PRO
1	A	226	HIS
1	A	233	ARG
1	A	255	THR
1	B	10	ILE
1	B	13	ASN
1	B	35	LYS
1	B	44	THR
1	B	82	ARG
1	B	106	PHE
1	B	150	LEU
1	B	151	ARG
1	B	170	SER
1	B	182	TYR
1	B	224	MET
1	B	246	SER
1	B	255	THR
1	B	257	PHE
1	C	61	HIS
1	C	82	ARG
1	C	108	ARG
1	C	224	MET
1	C	250	SER
1	C	255	THR
1	D	99	GLU
1	D	106	PHE
1	D	147	VAL
1	D	198	MET
1	D	222	MET
1	D	257	PHE

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Mol	Chain	Res	Type
1	E	56	ASP
1	E	98	PHE
1	E	116	SER
1	E	125	LEU
1	E	126	PRO
1	E	204	ASP
1	E	231	MET
1	F	105	ASP
1	F	107	HIS
1	F	121	THR
1	F	144	PHE
1	F	180	LEU
1	F	198	MET
1	F	204	ASP
1	F	230	ARG
1	F	255	THR
1	G	63	VAL
1	G	66	GLU
1	G	75	LEU
1	G	106	PHE
1	G	151	ARG
1	G	161	THR
1	G	257	PHE
1	G	258	VAL
1	H	38	ASN
1	H	57	HIS
1	H	63	VAL
1	H	182	TYR
1	H	198	MET
1	H	203	MET
1	H	255	THR
1	H	266	VAL
1	I	106	PHE
1	I	151	ARG
1	I	230	ARG
1	I	233	ARG
1	J	75	LEU
1	J	106	PHE
1	J	182	TYR
1	J	199	LEU
1	J	228	ILE
1	J	255	THR

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Mol	Chain	Res	Type
1	J	263	PHE
1	K	29	GLU
1	K	46	MET
1	K	61	HIS
1	K	93	SER
1	K	104	SER
1	K	106	PHE
1	K	113	ASN
1	K	155	PHE
1	K	204	ASP
1	K	255	THR
1	L	56	ASP
1	L	104	SER
1	L	182	TYR
1	L	199	LEU
1	L	222	MET
1	L	227	PRO
1	L	230	ARG
1	L	255	THR
1	L	263	PHE
1	M	44	THR
1	M	45	ASP
1	M	89	ASN
1	M	115	ASP
1	M	121	THR
1	M	161	THR
1	M	191	PRO
1	M	198	MET
1	M	199	LEU
1	M	224	MET
1	M	250	SER
1	N	77	GLN
1	N	182	TYR
1	N	196	THR
1	N	199	LEU
1	N	204	ASP
1	N	224	MET
1	N	247	ASP
1	N	250	SER
1	N	255	THR
1	N	264	SER
1	O	89	ASN

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Mol	Chain	Res	Type
1	O	93	SER
1	O	100	ASP
1	O	196	THR
1	O	214	SER
1	O	227	PRO
1	O	231	MET
1	P	26	ILE
1	P	46	MET
1	P	75	LEU
1	P	93	SER
1	P	96	THR
1	P	110	ASN
1	P	147	VAL
1	P	151	ARG
1	P	199	LEU
1	P	216	GLU
1	P	263	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	88	HIS
1	A	183	ASN
1	A	187	ASN
1	A	265	GLN
1	B	89	ASN
1	C	89	ASN
1	C	143	ASN
1	D	61	HIS
1	D	88	HIS
1	D	110	ASN
1	D	143	ASN
1	E	38	ASN
1	E	110	ASN
1	F	110	ASN
1	G	14	ASN
1	G	38	ASN
1	G	57	HIS
1	G	226	HIS
1	H	88	HIS
1	H	89	ASN

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Mol	Chain	Res	Type
1	H	143	ASN
1	I	88	HIS
1	I	89	ASN
1	I	226	HIS
1	J	61	HIS
1	J	89	ASN
1	J	156	ASN
1	L	88	HIS
1	L	143	ASN
1	M	38	ASN
1	M	57	HIS
1	M	61	HIS
1	M	89	ASN
1	M	113	ASN
1	M	265	GLN
1	N	38	ASN
1	N	77	GLN
1	N	156	ASN
1	O	89	ASN
1	P	110	ASN
1	P	143	ASN

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 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	256/266 (96%)	0.36	8 (3%) 51 38	4, 25, 62, 107	0
1	B	257/266 (96%)	0.32	9 (3%) 47 35	0, 25, 63, 128	0
1	C	254/266 (95%)	0.47	17 (6%) 25 20	4, 36, 90, 163	0
1	D	256/266 (96%)	0.53	12 (4%) 37 28	9, 37, 84, 130	0
1	E	255/266 (95%)	0.55	18 (7%) 23 19	1, 33, 94, 150	0
1	F	255/266 (95%)	0.54	14 (5%) 32 25	8, 32, 66, 89	0
1	G	255/266 (95%)	0.32	8 (3%) 51 38	0, 33, 76, 106	0
1	H	256/266 (96%)	0.43	8 (3%) 51 38	6, 33, 73, 119	0
1	I	257/266 (96%)	0.28	4 (1%) 70 57	5, 31, 61, 96	0
1	J	256/266 (96%)	0.27	4 (1%) 70 57	5, 26, 56, 95	0
1	K	256/266 (96%)	0.46	14 (5%) 32 25	4, 31, 71, 126	0
1	L	256/266 (96%)	0.37	8 (3%) 51 38	8, 33, 66, 123	0
1	M	255/266 (95%)	0.54	16 (6%) 27 22	10, 39, 82, 138	0
1	N	256/266 (96%)	0.53	18 (7%) 24 19	6, 36, 87, 159	0
1	O	255/266 (95%)	0.29	8 (3%) 51 38	7, 26, 57, 85	0
1	P	255/266 (95%)	0.49	16 (6%) 27 22	9, 31, 79, 117	0
All	All	4090/4256 (96%)	0.42	182 (4%) 39 30	0, 31, 74, 163	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	SER	5.4
1	A	120	GLY	5.2
1	M	13	ASN	4.5
1	N	213	PRO	4.3
1	E	51	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	261	GLY	4.1
1	F	101	THR	4.1
1	M	192	GLY	4.0
1	D	250	SER	3.8
1	C	50	ALA	3.8
1	P	159	TYR	3.8
1	P	136	ALA	3.8
1	L	197	PRO	3.7
1	F	193	GLY	3.7
1	K	39	ALA	3.7
1	N	197	PRO	3.6
1	A	229	GLY	3.6
1	H	137	GLY	3.6
1	I	51	ASP	3.5
1	C	137	GLY	3.5
1	B	130	GLU	3.5
1	A	157	ALA	3.5
1	D	31	VAL	3.5
1	B	197	PRO	3.4
1	E	222	MET	3.4
1	K	44	THR	3.4
1	H	216	GLU	3.4
1	P	219	GLN	3.4
1	C	33	ALA	3.4
1	P	211	ALA	3.3
1	J	197	PRO	3.3
1	B	192	GLY	3.3
1	E	159	TYR	3.1
1	P	74	ALA	3.1
1	F	249	ALA	3.1
1	C	199	LEU	3.1
1	E	106	PHE	3.1
1	N	218	ALA	3.1
1	G	12	LEU	3.1
1	O	68	GLY	3.0
1	P	198	MET	3.0
1	N	124	LEU	3.0
1	F	247	ASP	3.0
1	G	140	SER	3.0
1	D	210	GLY	3.0
1	G	132	GLY	3.0
1	E	204	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	106	PHE	2.9
1	H	201	SER	2.9
1	K	192	GLY	2.9
1	F	203	MET	2.9
1	G	223	GLU	2.9
1	H	134	ALA	2.9
1	H	45	ASP	2.9
1	K	199	LEU	2.9
1	D	39	ALA	2.9
1	L	266	VAL	2.8
1	E	218	ALA	2.8
1	E	161	THR	2.8
1	M	199	LEU	2.8
1	K	58	TYR	2.8
1	O	217	VAL	2.8
1	J	201	SER	2.7
1	M	246	SER	2.7
1	C	136	ALA	2.7
1	K	152	GLY	2.7
1	O	213	PRO	2.7
1	I	36	ALA	2.7
1	K	153	ALA	2.7
1	O	199	LEU	2.7
1	L	187	ASN	2.6
1	G	90	ALA	2.6
1	K	22	ALA	2.6
1	J	200	GLY	2.6
1	E	207	VAL	2.6
1	F	106	PHE	2.6
1	P	157	ALA	2.6
1	M	164	ALA	2.6
1	M	248	ALA	2.6
1	K	229	GLY	2.6
1	N	36	ALA	2.6
1	A	33	ALA	2.5
1	B	136	ALA	2.5
1	B	220	ALA	2.5
1	N	33	ALA	2.5
1	E	234	PRO	2.5
1	D	199	LEU	2.5
1	L	255	THR	2.5
1	E	137	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	213	PRO	2.5
1	M	93	SER	2.5
1	N	188	SER	2.5
1	K	38	ASN	2.5
1	E	25	GLY	2.5
1	N	255	THR	2.5
1	C	93	SER	2.5
1	K	249	ALA	2.5
1	E	213	PRO	2.4
1	M	228	ILE	2.4
1	N	196	THR	2.4
1	N	198	MET	2.4
1	P	77	GLN	2.4
1	C	94	ILE	2.4
1	F	199	LEU	2.4
1	K	220	ALA	2.4
1	O	210	GLY	2.4
1	M	217	VAL	2.4
1	F	162	SER	2.3
1	F	218	ALA	2.3
1	I	192	GLY	2.3
1	J	231	MET	2.3
1	L	119	ILE	2.3
1	G	82	ARG	2.3
1	M	198	MET	2.3
1	D	207	VAL	2.3
1	F	71	ALA	2.3
1	E	12	LEU	2.3
1	A	28	ARG	2.3
1	E	138	GLY	2.3
1	E	220	ALA	2.3
1	M	174	GLY	2.3
1	K	49	SER	2.3
1	F	183	ASN	2.2
1	N	183	ASN	2.2
1	P	197	PRO	2.2
1	G	206	TYR	2.2
1	L	222	MET	2.2
1	C	100	ASP	2.2
1	N	38	ASN	2.2
1	N	106	PHE	2.2
1	P	225	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	128	LEU	2.2
1	D	211	ALA	2.2
1	G	139	ALA	2.2
1	L	195	ASP	2.2
1	P	58	TYR	2.2
1	C	67	ALA	2.2
1	P	149	GLY	2.2
1	C	38	ASN	2.2
1	N	72	VAL	2.2
1	B	175	ALA	2.2
1	E	39	ALA	2.2
1	O	220	ALA	2.2
1	D	132	GLY	2.2
1	E	229	GLY	2.2
1	L	27	GLY	2.2
1	A	151	ARG	2.2
1	C	49	SER	2.2
1	P	14	ASN	2.2
1	C	258	VAL	2.2
1	M	15	VAL	2.2
1	N	55	ALA	2.1
1	D	138	GLY	2.1
1	O	120	GLY	2.1
1	H	184	ILE	2.1
1	C	52	VAL	2.1
1	F	141	VAL	2.1
1	D	218	ALA	2.1
1	M	51	ASP	2.1
1	C	42	ILE	2.1
1	D	61	HIS	2.1
1	N	199	LEU	2.1
1	E	154	ALA	2.1
1	P	12	LEU	2.1
1	A	217	VAL	2.1
1	D	36	ALA	2.1
1	M	26	ILE	2.1
1	B	229	GLY	2.1
1	H	174	GLY	2.1
1	A	156	ASN	2.1
1	N	87	VAL	2.1
1	H	71	ALA	2.1
1	P	158	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	265	GLN	2.1
1	I	183	ASN	2.1
1	M	247	ASP	2.1
1	B	193	GLY	2.0
1	M	109	VAL	2.0
1	N	142	VAL	2.0
1	B	38	ASN	2.0
1	F	198	MET	2.0
1	P	120	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.