



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:55 AM UTC

PDB ID : 6AP4 / pdb_00006ap4
Title : Crystal structure of the DNA polymerase III subunit beta from *Acinetobacter baumannii*
Authors : McGrath, A.E.; Oakley, A.J.
Deposited on : 2017-08-16
Resolution : 2.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

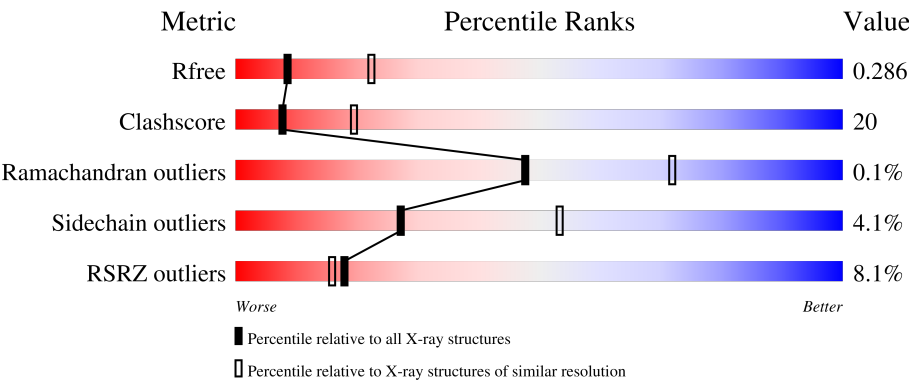
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	388	6% 64% 32% ..
1	B	388	3% 64% 32% ...
1	C	388	7% 66% 29% ..
1	D	388	5% 65% 30% ..
1	E	388	2% 70% 26% ..

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Mol	Chain	Length	Quality of chain
1	F	388	
1	G	388	
1	H	388	
1	I	388	
1	J	388	
1	K	388	
1	L	388	
1	M	388	
1	N	388	
1	O	388	
1	P	388	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46780 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 DNA polymerase III subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2938	1836	515	575	12			
1	B	382	Total	C	N	O	S	0	0	0
			2964	1852	518	582	12			
1	C	379	Total	C	N	O	S	0	0	0
			2942	1842	514	574	12			
1	D	382	Total	C	N	O	S	0	0	0
			2962	1853	520	578	11			
1	E	382	Total	C	N	O	S	0	0	0
			2965	1852	519	582	12			
1	F	379	Total	C	N	O	S	0	0	0
			2942	1839	515	576	12			
1	G	378	Total	C	N	O	S	0	0	0
			2941	1840	516	573	12			
1	H	383	Total	C	N	O	S	0	0	0
			2957	1848	517	580	12			
1	I	370	Total	C	N	O	S	0	0	0
			2874	1804	503	555	12			
1	J	384	Total	C	N	O	S	0	0	0
			2981	1862	525	582	12			
1	K	365	Total	C	N	O	S	0	1	0
			2830	1773	497	547	13			
1	L	356	Total	C	N	O	S	0	0	0
			2735	1710	476	537	12			
1	M	378	Total	C	N	O	S	0	0	0
			2929	1833	510	574	12			
1	N	372	Total	C	N	O	S	0	0	0
			2891	1812	507	560	12			
1	O	357	Total	C	N	O	S	0	0	0
			2768	1741	486	530	11			
1	P	377	Total	C	N	O	S	0	0	0
			2914	1823	508	571	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP V5V7W3
A	-4	HIS	-	expression tag	UNP V5V7W3
A	-3	HIS	-	expression tag	UNP V5V7W3
A	-2	HIS	-	expression tag	UNP V5V7W3
A	-1	HIS	-	expression tag	UNP V5V7W3
A	0	HIS	-	expression tag	UNP V5V7W3
B	-5	HIS	-	expression tag	UNP V5V7W3
B	-4	HIS	-	expression tag	UNP V5V7W3
B	-3	HIS	-	expression tag	UNP V5V7W3
B	-2	HIS	-	expression tag	UNP V5V7W3
B	-1	HIS	-	expression tag	UNP V5V7W3
B	0	HIS	-	expression tag	UNP V5V7W3
C	-5	HIS	-	expression tag	UNP V5V7W3
C	-4	HIS	-	expression tag	UNP V5V7W3
C	-3	HIS	-	expression tag	UNP V5V7W3
C	-2	HIS	-	expression tag	UNP V5V7W3
C	-1	HIS	-	expression tag	UNP V5V7W3
C	0	HIS	-	expression tag	UNP V5V7W3
D	-5	HIS	-	expression tag	UNP V5V7W3
D	-4	HIS	-	expression tag	UNP V5V7W3
D	-3	HIS	-	expression tag	UNP V5V7W3
D	-2	HIS	-	expression tag	UNP V5V7W3
D	-1	HIS	-	expression tag	UNP V5V7W3
D	0	HIS	-	expression tag	UNP V5V7W3
E	-5	HIS	-	expression tag	UNP V5V7W3
E	-4	HIS	-	expression tag	UNP V5V7W3
E	-3	HIS	-	expression tag	UNP V5V7W3
E	-2	HIS	-	expression tag	UNP V5V7W3
E	-1	HIS	-	expression tag	UNP V5V7W3
E	0	HIS	-	expression tag	UNP V5V7W3
F	-5	HIS	-	expression tag	UNP V5V7W3
F	-4	HIS	-	expression tag	UNP V5V7W3
F	-3	HIS	-	expression tag	UNP V5V7W3
F	-2	HIS	-	expression tag	UNP V5V7W3
F	-1	HIS	-	expression tag	UNP V5V7W3
F	0	HIS	-	expression tag	UNP V5V7W3
G	-5	HIS	-	expression tag	UNP V5V7W3
G	-4	HIS	-	expression tag	UNP V5V7W3
G	-3	HIS	-	expression tag	UNP V5V7W3
G	-2	HIS	-	expression tag	UNP V5V7W3
G	-1	HIS	-	expression tag	UNP V5V7W3
G	0	HIS	-	expression tag	UNP V5V7W3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP V5V7W3
H	-4	HIS	-	expression tag	UNP V5V7W3
H	-3	HIS	-	expression tag	UNP V5V7W3
H	-2	HIS	-	expression tag	UNP V5V7W3
H	-1	HIS	-	expression tag	UNP V5V7W3
H	0	HIS	-	expression tag	UNP V5V7W3
I	-5	HIS	-	expression tag	UNP V5V7W3
I	-4	HIS	-	expression tag	UNP V5V7W3
I	-3	HIS	-	expression tag	UNP V5V7W3
I	-2	HIS	-	expression tag	UNP V5V7W3
I	-1	HIS	-	expression tag	UNP V5V7W3
I	0	HIS	-	expression tag	UNP V5V7W3
J	-5	HIS	-	expression tag	UNP V5V7W3
J	-4	HIS	-	expression tag	UNP V5V7W3
J	-3	HIS	-	expression tag	UNP V5V7W3
J	-2	HIS	-	expression tag	UNP V5V7W3
J	-1	HIS	-	expression tag	UNP V5V7W3
J	0	HIS	-	expression tag	UNP V5V7W3
K	-5	HIS	-	expression tag	UNP V5V7W3
K	-4	HIS	-	expression tag	UNP V5V7W3
K	-3	HIS	-	expression tag	UNP V5V7W3
K	-2	HIS	-	expression tag	UNP V5V7W3
K	-1	HIS	-	expression tag	UNP V5V7W3
K	0	HIS	-	expression tag	UNP V5V7W3
L	-5	HIS	-	expression tag	UNP V5V7W3
L	-4	HIS	-	expression tag	UNP V5V7W3
L	-3	HIS	-	expression tag	UNP V5V7W3
L	-2	HIS	-	expression tag	UNP V5V7W3
L	-1	HIS	-	expression tag	UNP V5V7W3
L	0	HIS	-	expression tag	UNP V5V7W3
M	-5	HIS	-	expression tag	UNP V5V7W3
M	-4	HIS	-	expression tag	UNP V5V7W3
M	-3	HIS	-	expression tag	UNP V5V7W3
M	-2	HIS	-	expression tag	UNP V5V7W3
M	-1	HIS	-	expression tag	UNP V5V7W3
M	0	HIS	-	expression tag	UNP V5V7W3
N	-5	HIS	-	expression tag	UNP V5V7W3
N	-4	HIS	-	expression tag	UNP V5V7W3
N	-3	HIS	-	expression tag	UNP V5V7W3
N	-2	HIS	-	expression tag	UNP V5V7W3
N	-1	HIS	-	expression tag	UNP V5V7W3
N	0	HIS	-	expression tag	UNP V5V7W3

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	HIS	-	expression tag	UNP V5V7W3
O	-4	HIS	-	expression tag	UNP V5V7W3
O	-3	HIS	-	expression tag	UNP V5V7W3
O	-2	HIS	-	expression tag	UNP V5V7W3
O	-1	HIS	-	expression tag	UNP V5V7W3
O	0	HIS	-	expression tag	UNP V5V7W3
P	-5	HIS	-	expression tag	UNP V5V7W3
P	-4	HIS	-	expression tag	UNP V5V7W3
P	-3	HIS	-	expression tag	UNP V5V7W3
P	-2	HIS	-	expression tag	UNP V5V7W3
P	-1	HIS	-	expression tag	UNP V5V7W3
P	0	HIS	-	expression tag	UNP V5V7W3

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	14	Total O 14 14	0	0
3	B	14	Total O 14 14	0	0
3	C	15	Total O 15 15	0	0
3	D	30	Total O 30 30	0	0
3	E	47	Total O 47 47	0	0
3	F	11	Total O 11 11	0	0
3	G	22	Total O 22 22	0	0
3	H	8	Total O 8 8	0	0
3	I	5	Total O 5 5	0	0

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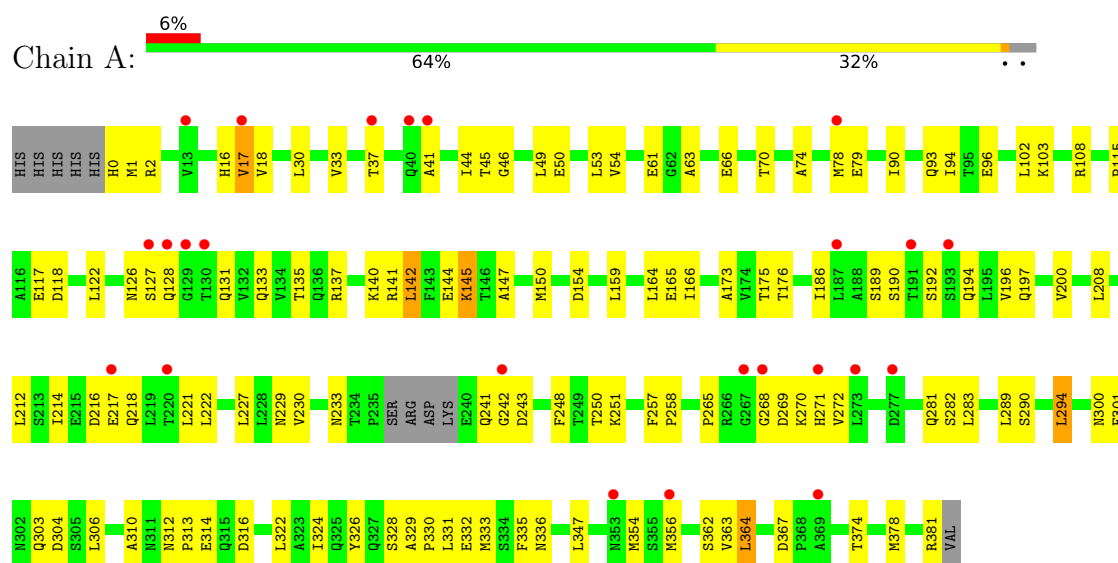
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	17	Total 17	O 17	0	0
3	K	9	Total 9	O 9	0	0
3	L	10	Total 10	O 10	0	0
3	M	18	Total 18	O 18	0	0
3	N	9	Total 9	O 9	0	0
3	O	6	Total 6	O 6	0	0
3	P	10	Total 10	O 10	0	0

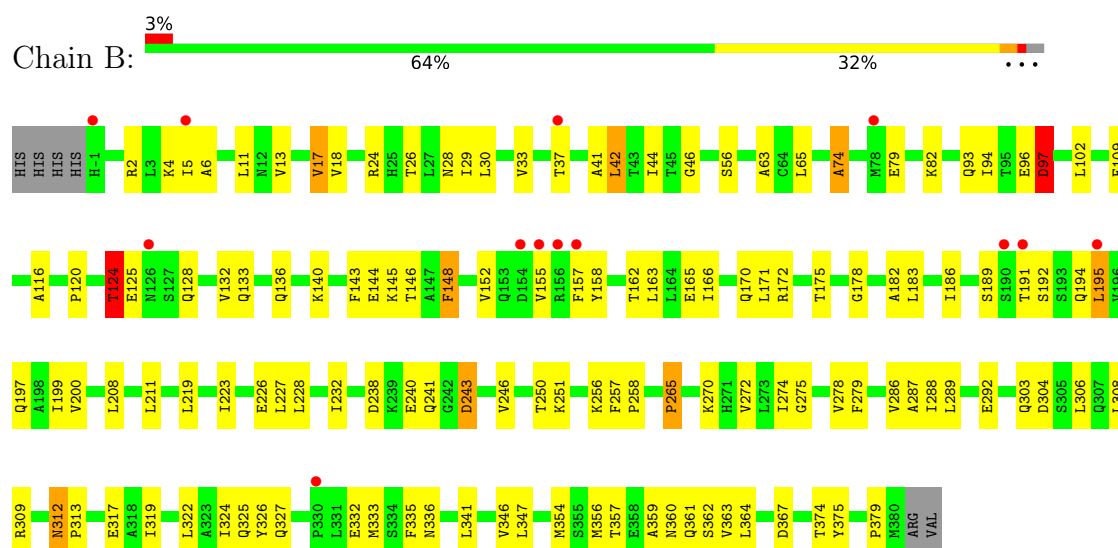
3 Residue-property plots [i](#)

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: DNA polymerase III subunit beta

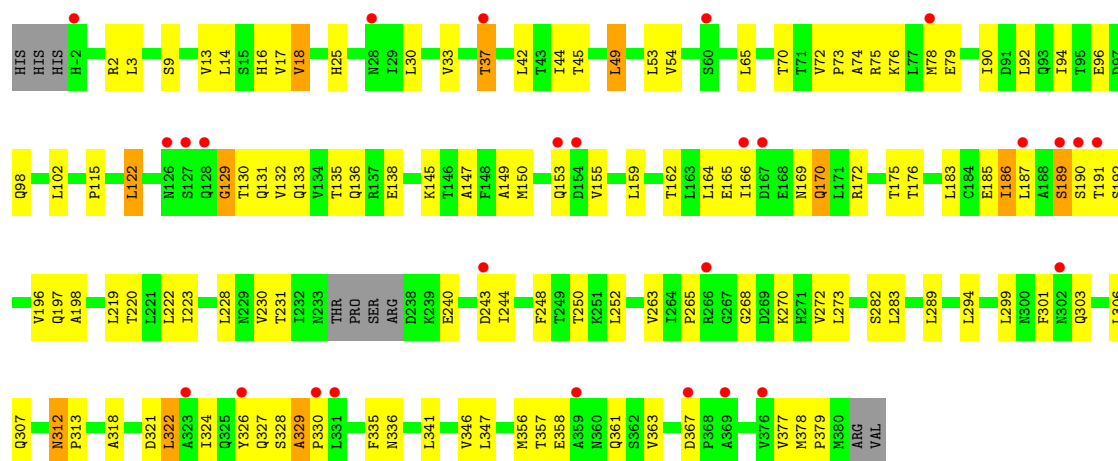


• Molecule 1: DNA polymerase III subunit beta

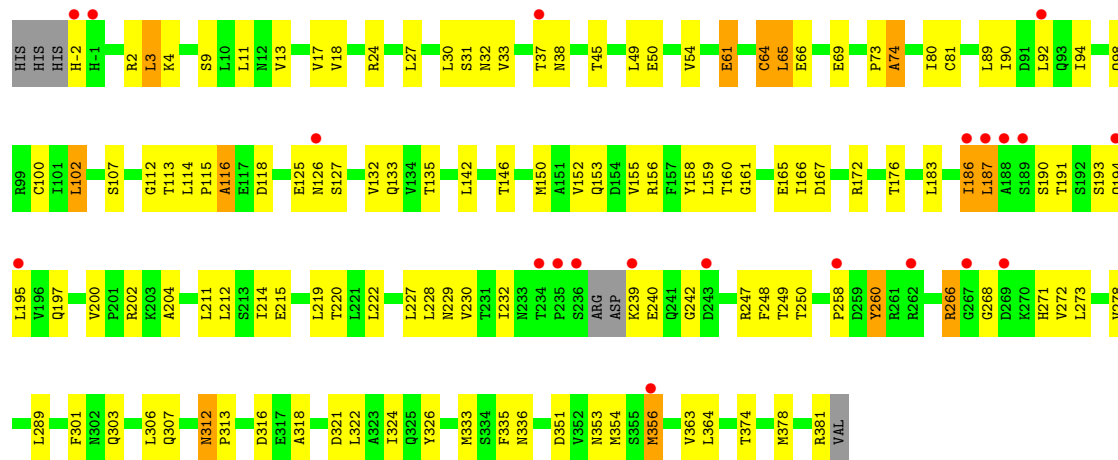


• Molecule 1: DNA polymerase III subunit beta

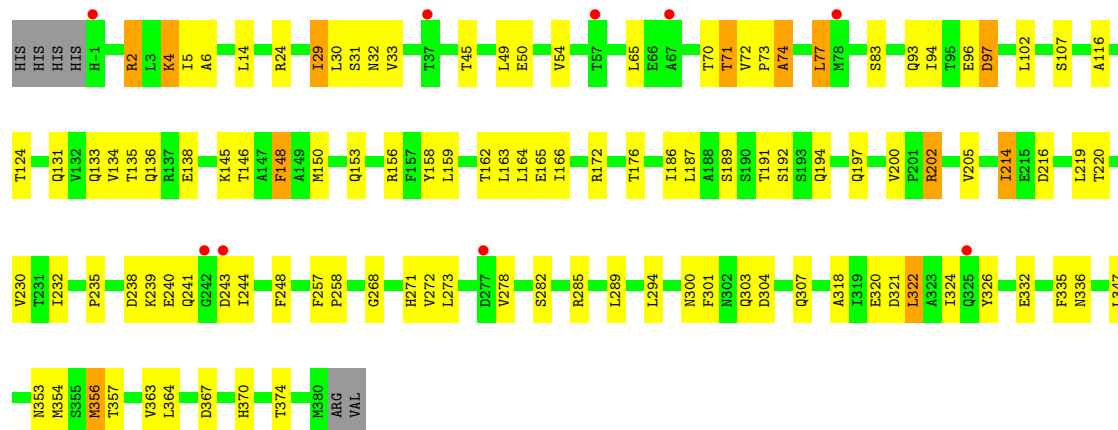




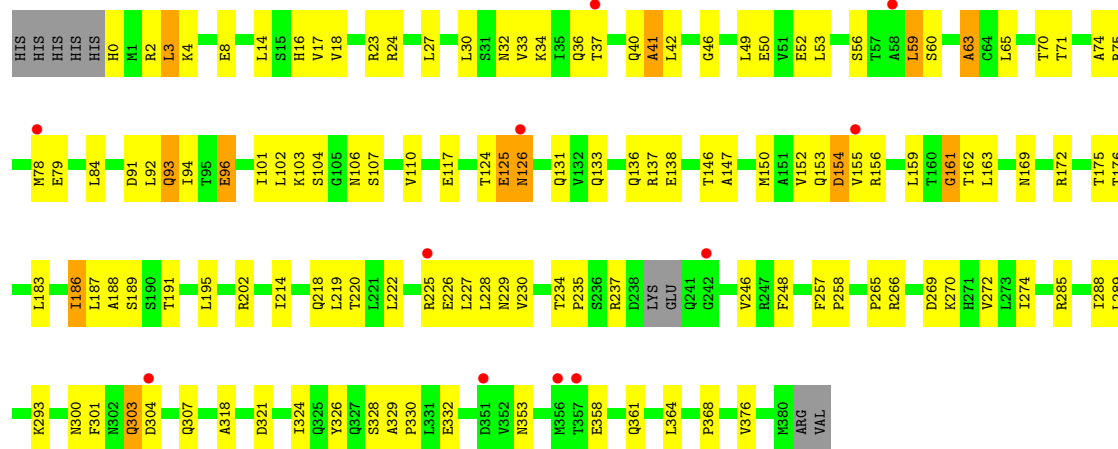
• Molecule 1: DNA polymerase III subunit beta



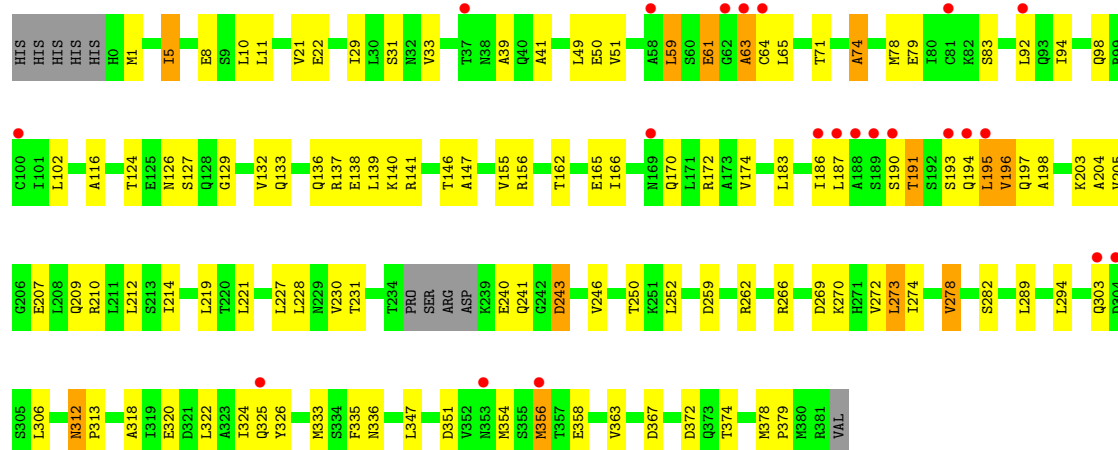
• Molecule 1: DNA polymerase III subunit beta



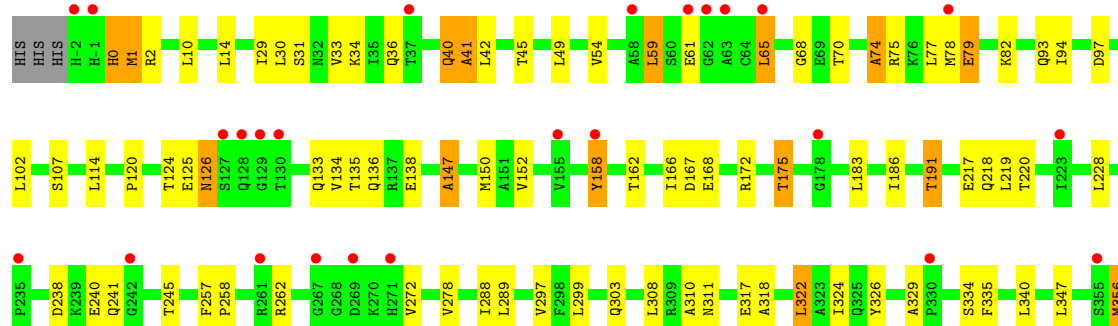
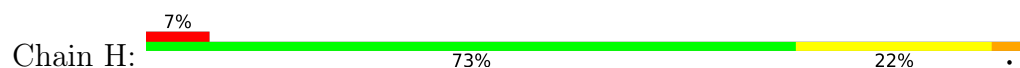
• Molecule 1: DNA polymerase III subunit beta



• Molecule 1: DNA polymerase III subunit beta

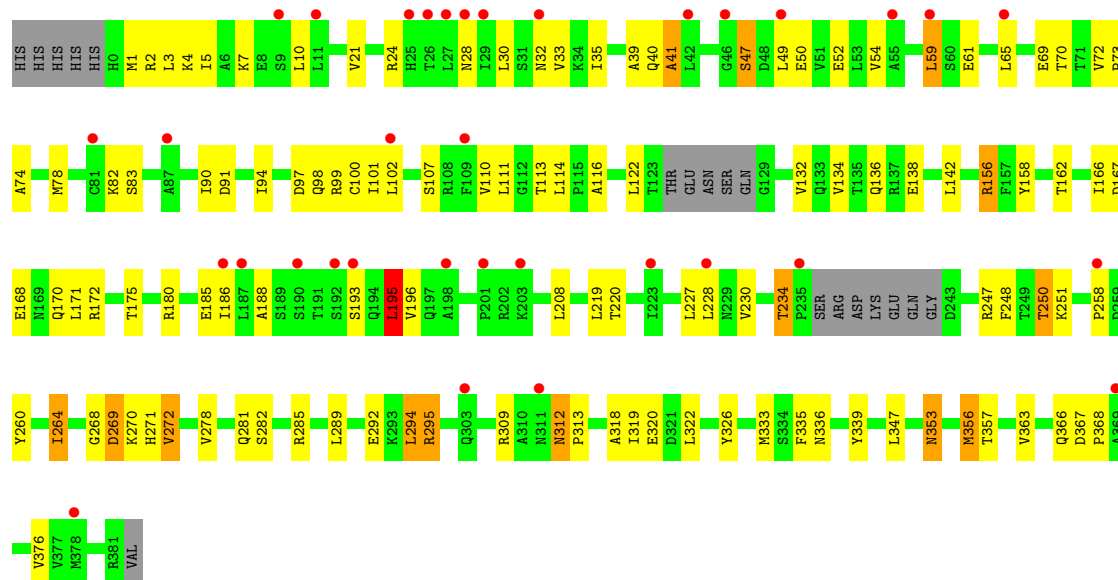


• Molecule 1: DNA polymerase III subunit beta

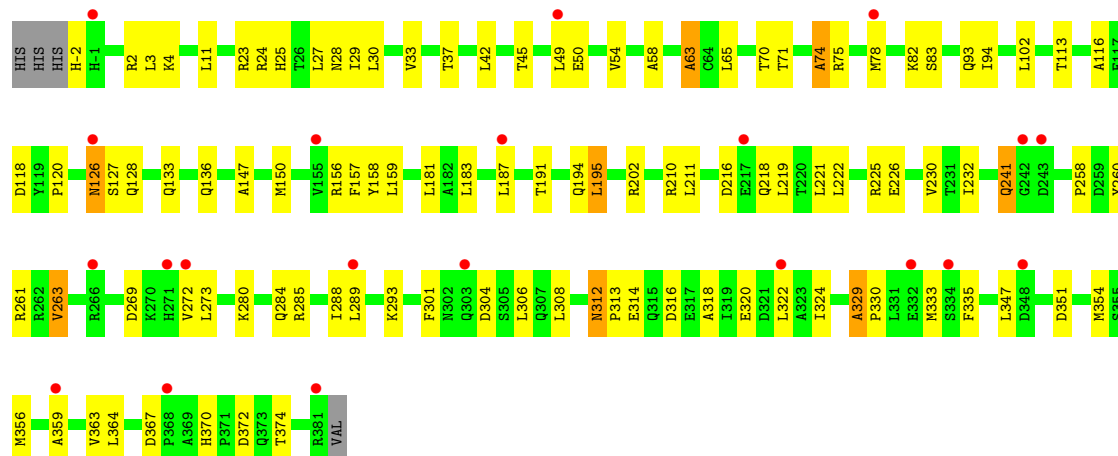




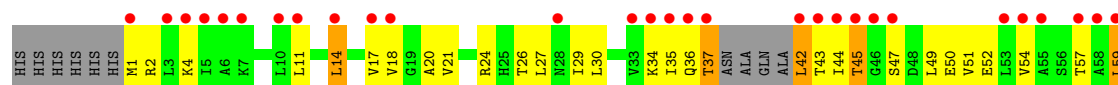
• Molecule 1: DNA polymerase III subunit beta

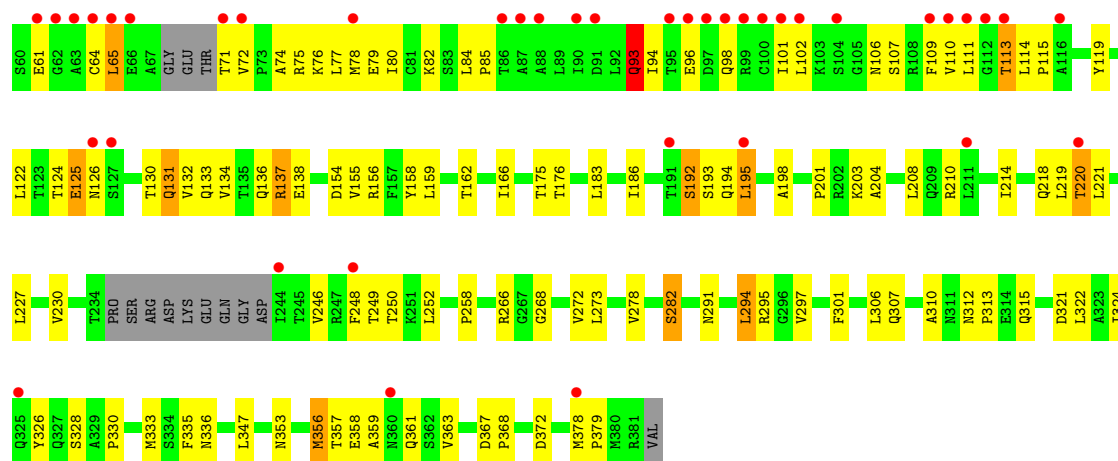


• Molecule 1: DNA polymerase III subunit beta



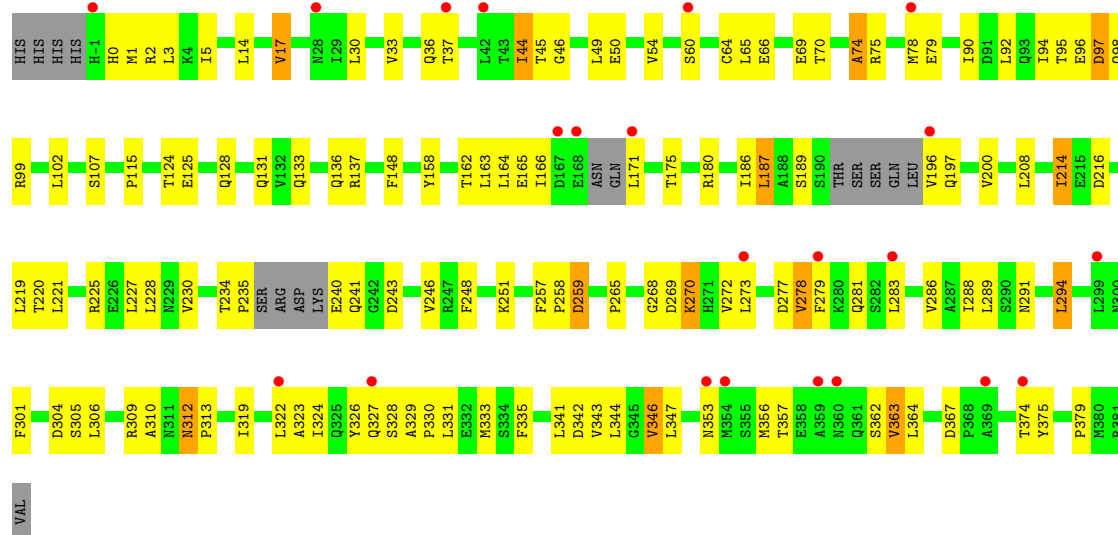
• Molecule 1: DNA polymerase III subunit beta



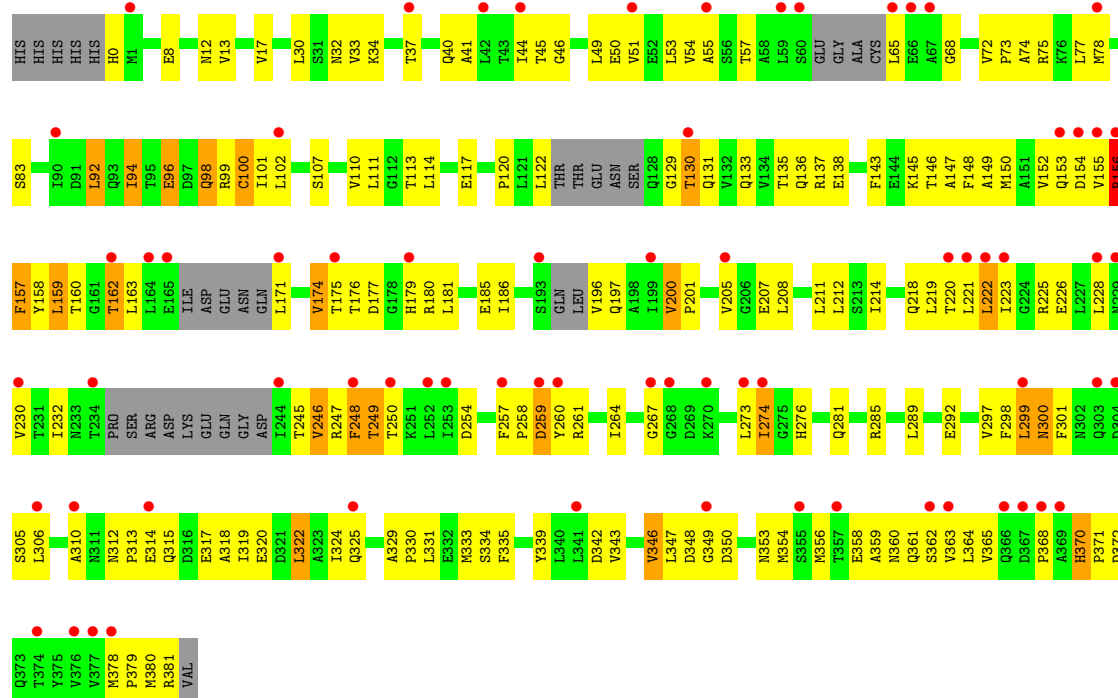




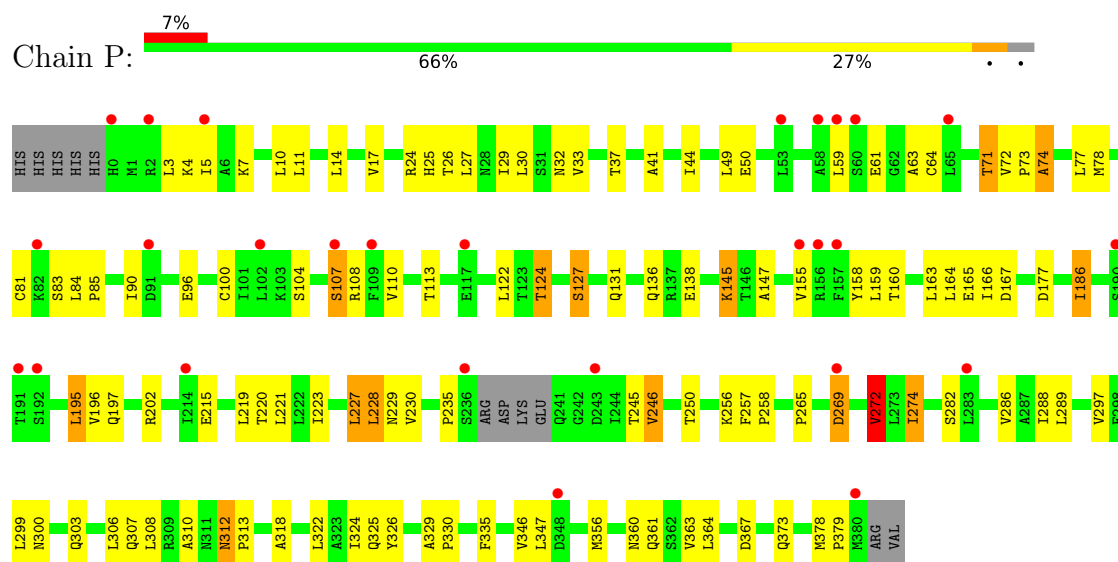
• Molecule 1: DNA polymerase III subunit beta



• Molecule 1: DNA polymerase III subunit beta



• Molecule 1: DNA polymerase III subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.71Å 328.60Å 147.50Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	164.30 – 2.95 164.30 – 2.95	Depositor EDS
% Data completeness (in resolution range)	92.5 (164.30-2.95) 92.8 (164.30-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.248 , 0.287 0.243 , 0.286	Depositor DCC
R_{free} test set	6719 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	46780	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.74	0/2972	1.03	18/4029 (0.4%)
1	B	0.75	0/3000	1.10	21/4070 (0.5%)
1	C	0.70	0/2977	1.07	21/4035 (0.5%)
1	D	0.80	0/2998	1.10	23/4066 (0.6%)
1	E	0.86	0/3001	1.09	17/4070 (0.4%)
1	F	0.73	0/2976	1.01	14/4035 (0.3%)
1	G	0.73	1/2974 (0.0%)	1.07	21/4030 (0.5%)
1	H	0.66	0/2994	1.04	20/4064 (0.5%)
1	I	0.71	1/2907 (0.0%)	1.08	22/3940 (0.6%)
1	J	0.73	0/3018	1.07	19/4094 (0.5%)
1	K	0.74	0/2860	1.10	23/3876 (0.6%)
1	L	0.65	0/2759	1.05	14/3736 (0.4%)
1	M	0.70	0/2963	1.04	14/4018 (0.3%)
1	N	0.66	0/2924	1.00	10/3961 (0.3%)
1	O	0.60	1/2797 (0.0%)	1.11	20/3786 (0.5%)
1	P	0.65	0/2948	1.05	18/3999 (0.5%)
All	All	0.72	3/47068 (0.0%)	1.06	295/63809 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	272	VAL	C-O	-7.11	1.15	1.23
1	O	300	ASN	CA-C	-6.09	1.45	1.52
1	G	129	GLY	C-O	-5.75	1.17	1.24

All (295) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	193	SER	N-CA-C	11.70	123.59	111.07
1	C	74	ALA	N-CA-C	11.43	123.30	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	PHE	N-CA-C	10.93	123.27	111.36
1	H	74	ALA	N-CA-C	10.48	122.28	111.07
1	C	312	ASN	CA-C-N	10.46	130.79	119.28
1	C	312	ASN	C-N-CA	10.46	130.79	119.28
1	G	63	ALA	N-CA-C	10.38	122.60	111.28
1	D	64	CYS	N-CA-C	9.98	122.16	111.28
1	J	347	LEU	N-CA-C	9.97	122.15	111.28
1	L	74	ALA	N-CA-C	9.80	121.56	111.07
1	J	312	ASN	CA-C-N	9.68	129.93	119.28
1	J	312	ASN	C-N-CA	9.68	129.93	119.28
1	B	312	ASN	CA-C-N	9.57	129.32	119.56
1	B	312	ASN	C-N-CA	9.57	129.32	119.56
1	J	74	ALA	N-CA-C	9.52	121.26	111.07
1	M	195	LEU	N-CA-C	9.48	124.33	111.24
1	G	98	GLN	N-CA-C	9.29	124.21	111.39
1	A	118	ASP	N-CA-C	9.19	121.29	111.28
1	I	102	LEU	N-CA-C	9.11	123.37	108.52
1	K	193	SER	N-CA-C	8.97	121.14	111.36
1	D	116	ALA	N-CA-C	8.88	121.92	111.71
1	M	312	ASN	CA-C-N	8.81	128.83	119.05
1	M	312	ASN	C-N-CA	8.81	128.83	119.05
1	P	312	ASN	CA-C-N	8.66	128.67	119.05
1	P	312	ASN	C-N-CA	8.66	128.67	119.05
1	N	312	ASN	CA-C-N	8.65	128.80	119.28
1	N	312	ASN	C-N-CA	8.65	128.80	119.28
1	L	215	GLU	N-CA-C	8.61	121.16	108.60
1	M	17	VAL	N-CA-C	8.56	119.37	110.72
1	B	148	PHE	N-CA-C	8.50	120.54	111.28
1	O	200	VAL	CA-C-N	8.49	128.53	119.78
1	O	200	VAL	C-N-CA	8.49	128.53	119.78
1	H	0	HIS	N-CA-C	8.27	122.16	110.50
1	L	216	ASP	N-CA-C	8.22	122.76	112.24
1	A	17	VAL	N-CA-C	8.21	123.92	112.50
1	J	116	ALA	N-CA-C	8.21	121.15	111.71
1	F	154	ASP	N-CA-C	8.17	122.68	111.90
1	I	294	LEU	N-CA-C	7.99	120.07	111.36
1	B	63	ALA	N-CA-C	7.96	119.58	111.07
1	K	266	ARG	N-CA-C	7.87	119.94	111.36
1	A	241	GLN	N-CA-C	7.81	122.16	111.39
1	B	116	ALA	N-CA-C	7.64	120.49	111.71
1	G	195	LEU	N-CA-C	7.64	122.21	111.52
1	O	349	GLY	N-CA-C	7.53	121.86	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	40	GLN	N-CA-C	7.53	119.57	111.36
1	H	329	ALA	CA-C-N	7.52	127.53	119.78
1	H	329	ALA	C-N-CA	7.52	127.53	119.78
1	G	193	SER	N-CA-C	7.51	121.09	110.50
1	F	147	ALA	N-CA-C	7.50	119.45	111.28
1	D	268	GLY	N-CA-C	7.43	125.42	114.95
1	E	116	ALA	N-CA-C	7.43	120.25	111.71
1	B	336	ASN	N-CA-C	-7.34	98.80	109.59
1	J	157	PHE	N-CA-C	7.34	119.28	111.28
1	I	28	ASN	N-CA-C	7.31	121.11	111.75
1	K	203	LYS	N-CA-C	7.28	119.22	111.28
1	F	155	VAL	N-CA-C	-7.26	97.65	109.12
1	F	234	THR	CA-C-N	7.24	128.16	120.12
1	F	234	THR	C-N-CA	7.24	128.16	120.12
1	E	31	SER	N-CA-C	-7.20	104.07	112.92
1	I	122	LEU	N-CA-C	-7.17	99.21	109.96
1	F	63	ALA	N-CA-C	7.14	119.06	111.28
1	B	74	ALA	N-CA-C	7.09	118.65	111.07
1	K	109	PHE	N-CA-C	7.08	120.93	109.40
1	P	378	MET	CA-C-N	7.06	127.02	120.03
1	P	378	MET	C-N-CA	7.06	127.02	120.03
1	E	191	THR	N-CA-C	7.05	119.04	111.36
1	L	347	LEU	N-CA-C	7.04	118.95	111.28
1	C	18	VAL	N-CA-C	7.02	119.86	111.09
1	M	243	ASP	N-CA-C	6.99	120.09	110.24
1	N	97	ASP	N-CA-C	-6.99	101.12	110.55
1	P	107	SER	N-CA-C	6.98	120.61	109.24
1	E	74	ALA	N-CA-C	6.97	118.53	111.07
1	H	378	MET	CA-C-N	6.96	127.41	120.52
1	H	378	MET	C-N-CA	6.96	127.41	120.52
1	K	192	SER	N-CA-C	6.96	120.78	110.48
1	M	74	ALA	N-CA-C	6.95	118.50	111.07
1	A	192	SER	N-CA-C	6.92	119.84	111.82
1	G	356	MET	N-CA-C	6.90	120.22	109.52
1	I	195	LEU	N-CA-C	6.88	120.47	110.28
1	K	26	THR	N-CA-C	-6.88	103.86	111.36
1	H	31	SER	N-CA-C	-6.88	103.84	111.82
1	G	74	ALA	N-CA-C	6.87	118.42	111.07
1	D	193	SER	N-CA-C	6.82	118.71	111.28
1	A	74	ALA	N-CA-C	6.81	118.36	111.07
1	A	63	ALA	N-CA-C	-6.79	103.96	111.36
1	J	329	ALA	CA-C-N	6.79	126.75	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	329	ALA	C-N-CA	6.79	126.75	119.76
1	C	336	ASN	N-CA-C	-6.74	98.25	108.96
1	D	356	MET	N-CA-C	6.73	120.11	109.81
1	C	189	SER	N-CA-C	6.70	118.58	111.28
1	L	329	ALA	CA-C-N	6.69	126.72	119.90
1	L	329	ALA	C-N-CA	6.69	126.72	119.90
1	I	74	ALA	N-CA-C	6.67	118.55	111.28
1	E	200	VAL	CA-C-N	6.65	128.15	119.84
1	E	200	VAL	C-N-CA	6.65	128.15	119.84
1	K	114	LEU	CA-C-N	6.65	128.15	119.84
1	K	114	LEU	C-N-CA	6.65	128.15	119.84
1	O	249	THR	N-CA-C	6.63	119.71	108.90
1	D	242	GLY	N-CA-C	6.61	123.40	112.30
1	E	50	GLU	N-CA-C	-6.59	104.42	113.18
1	M	336	ASN	N-CA-C	-6.59	99.17	109.25
1	D	107	SER	N-CA-C	6.59	121.03	109.96
1	D	312	ASN	CA-C-N	6.57	126.70	119.87
1	D	312	ASN	C-N-CA	6.57	126.70	119.87
1	J	241	GLN	N-CA-C	-6.55	104.06	111.14
1	G	126	ASN	N-CA-C	6.55	118.98	110.53
1	H	29	ILE	N-CA-C	6.53	119.22	111.05
1	G	116	ALA	N-CA-C	6.51	119.20	111.71
1	D	17	VAL	N-CA-C	6.50	122.84	113.16
1	O	147	ALA	N-CA-C	6.49	118.35	111.28
1	F	41	ALA	N-CA-C	6.48	119.03	109.24
1	C	17	VAL	N-CA-C	6.47	120.11	111.44
1	E	238	ASP	N-CA-C	-6.47	97.82	108.49
1	E	336	ASN	N-CA-C	-6.44	99.40	109.25
1	K	44	ILE	N-CA-C	6.44	117.34	108.84
1	K	356	MET	N-CA-C	6.42	119.63	109.81
1	D	336	ASN	N-CA-C	-6.41	99.56	109.76
1	M	170	GLN	N-CA-C	6.41	119.86	109.40
1	H	217	GLU	N-CA-C	-6.40	100.81	110.28
1	I	41	ALA	N-CA-C	6.39	117.93	108.60
1	H	40	GLN	N-CA-C	6.39	118.32	111.36
1	E	370	HIS	CA-C-N	6.36	125.98	119.56
1	E	370	HIS	C-N-CA	6.36	125.98	119.56
1	B	97	ASP	N-CA-C	-6.35	100.88	110.28
1	D	378	MET	CA-C-N	6.34	126.31	120.03
1	D	378	MET	C-N-CA	6.34	126.31	120.03
1	G	50	GLU	N-CA-C	-6.34	105.44	113.43
1	P	147	ALA	N-CA-C	6.31	118.69	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	61	GLU	N-CA-C	6.31	118.16	111.28
1	A	41	ALA	N-CA-C	6.31	118.77	109.24
1	O	114	LEU	CA-C-N	6.29	126.24	119.76
1	O	114	LEU	C-N-CA	6.29	126.24	119.76
1	I	101	ILE	N-CA-C	6.29	117.17	107.99
1	K	72	VAL	CA-C-N	6.29	127.70	119.84
1	K	72	VAL	C-N-CA	6.29	127.70	119.84
1	A	147	ALA	N-CA-C	6.27	118.11	111.28
1	E	192	SER	N-CA-C	6.26	119.43	110.10
1	O	41	ALA	N-CA-C	6.26	118.29	108.96
1	K	336	ASN	N-CA-C	-6.21	99.75	109.25
1	O	156	ARG	N-CA-C	-6.19	97.34	108.48
1	K	294	LEU	N-CA-C	6.18	118.10	111.36
1	I	234	THR	N-CA-C	6.18	123.46	109.81
1	P	74	ALA	N-CA-C	6.18	117.68	111.07
1	H	147	ALA	N-CA-C	6.17	118.52	111.11
1	D	74	ALA	N-CA-C	6.17	117.69	110.97
1	G	147	ALA	N-CA-C	6.16	118.00	111.28
1	I	292	GLU	N-CA-C	6.16	117.66	111.07
1	B	292	GLU	N-CA-C	6.16	117.99	111.28
1	O	259	ASP	N-CA-C	6.13	119.09	109.96
1	E	148	PHE	N-CA-C	6.08	119.80	112.38
1	D	31	SER	N-CA-C	-6.08	105.87	113.28
1	K	74	ALA	N-CA-C	6.07	117.69	111.14
1	O	370	HIS	CA-C-N	6.07	125.69	119.56
1	O	370	HIS	C-N-CA	6.07	125.69	119.56
1	M	147	ALA	N-CA-C	6.05	117.88	111.28
1	H	65	LEU	N-CA-C	-6.02	105.96	113.55
1	K	50	GLU	N-CA-C	-6.01	105.98	113.55
1	C	243	ASP	N-CA-C	6.00	118.66	110.55
1	I	50	GLU	N-CA-C	6.00	117.61	111.14
1	P	50	GLU	N-CA-C	-5.99	106.00	113.55
1	G	336	ASN	N-CA-C	-5.98	100.10	109.25
1	B	124	THR	CB-CA-C	-5.98	101.69	111.68
1	O	146	THR	N-CA-C	5.98	120.70	113.17
1	J	50	GLU	N-CA-C	-5.96	106.03	113.55
1	I	336	ASN	N-CA-C	-5.96	100.13	109.25
1	J	63	ALA	N-CA-C	5.92	117.40	111.07
1	C	147	ALA	N-CA-C	5.92	117.73	111.28
1	N	74	ALA	N-CA-C	5.91	118.23	111.02
1	G	41	ALA	N-CA-C	5.91	117.77	108.96
1	N	50	GLU	N-CA-C	-5.89	106.00	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	266	ARG	N-CA-C	5.89	117.78	111.36
1	N	294	LEU	N-CA-C	5.87	117.76	111.36
1	K	107	SER	N-CA-C	5.86	119.19	109.46
1	J	126	ASN	N-CA-C	5.83	118.79	110.10
1	A	50	GLU	N-CA-C	-5.82	106.10	113.43
1	O	350	ASP	N-CA-C	5.79	117.60	111.28
1	N	3	LEU	N-CA-C	5.79	118.90	109.24
1	N	327	GLN	N-CA-C	-5.79	104.93	113.61
1	B	17	VAL	N-CA-C	5.78	118.74	112.96
1	C	150	MET	N-CA-C	5.77	118.60	110.23
1	B	28	ASN	N-CA-C	5.77	117.57	111.28
1	C	3	LEU	N-CA-C	5.75	118.59	109.50
1	I	312	ASN	CA-C-N	5.75	125.42	119.56
1	I	312	ASN	C-N-CA	5.75	125.42	119.56
1	J	211	LEU	N-CA-C	5.73	117.60	111.36
1	P	272	VAL	N-CA-C	5.72	117.67	108.85
1	D	146	THR	N-CA-C	5.71	120.38	113.41
1	M	50	GLU	N-CA-C	-5.70	106.97	114.04
1	O	292	GLU	N-CA-C	5.69	117.48	111.28
1	G	246	VAL	N-CA-C	5.68	116.04	107.75
1	G	356	MET	N-CA-CB	-5.68	101.67	111.55
1	K	361	GLN	N-CA-C	5.67	118.20	110.55
1	O	107	SER	N-CA-C	5.67	118.87	109.46
1	I	272	VAL	CB-CA-C	-5.66	102.75	110.90
1	M	232	ILE	N-CA-C	5.65	116.00	107.75
1	I	195	LEU	N-CA-CB	-5.64	101.67	109.97
1	K	359	ALA	CA-C-N	5.64	128.11	120.44
1	K	359	ALA	C-N-CA	5.64	128.11	120.44
1	O	254	ASP	N-CA-C	5.64	117.43	111.28
1	H	1	MET	N-CA-C	5.64	118.50	110.10
1	P	17	VAL	N-CA-C	5.63	118.31	112.90
1	J	263	VAL	N-CA-C	5.62	116.40	110.72
1	G	156	ARG	N-CA-C	-5.62	98.57	108.23
1	F	154	ASP	CB-CA-C	-5.62	102.84	111.66
1	B	195	LEU	N-CA-C	5.61	118.59	110.28
1	G	294	LEU	N-CA-C	5.60	117.46	111.36
1	D	118	ASP	N-CA-C	-5.59	106.41	113.18
1	G	312	ASN	CA-C-N	5.57	125.67	119.87
1	G	312	ASN	C-N-CA	5.57	125.67	119.87
1	C	170	GLN	N-CA-C	5.56	118.53	109.24
1	A	294	LEU	N-CA-C	5.56	118.27	111.82
1	H	41	ALA	N-CA-C	5.56	117.52	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	147	ALA	N-CA-C	5.54	118.04	111.33
1	P	346	VAL	N-CA-C	5.52	117.42	112.17
1	F	125	GLU	N-CA-C	-5.52	99.05	110.80
1	F	161	GLY	N-CA-C	5.50	119.13	111.10
1	H	114	LEU	CA-C-N	5.49	126.71	119.84
1	H	114	LEU	C-N-CA	5.49	126.71	119.84
1	A	336	ASN	N-CA-C	-5.49	101.04	109.76
1	J	288	ILE	CB-CA-C	-5.48	104.86	112.04
1	P	41	ALA	N-CA-C	5.48	117.17	108.79
1	A	127	SER	N-CA-C	5.47	117.25	111.28
1	C	328	SER	N-CA-C	5.45	117.11	110.41
1	J	118	ASP	N-CA-C	-5.43	106.66	113.28
1	D	211	LEU	N-CA-C	5.42	117.27	111.36
1	M	356	MET	N-CA-C	5.42	118.41	109.85
1	J	118	ASP	N-CA-CB	5.41	118.95	110.46
1	D	118	ASP	N-CA-CB	5.40	119.48	110.41
1	J	127	SER	N-CA-C	5.39	117.24	111.36
1	A	362	SER	N-CA-C	5.39	117.49	110.43
1	L	346	VAL	N-CA-C	5.38	116.15	110.72
1	C	329	ALA	CA-C-N	5.38	126.22	119.98
1	C	329	ALA	C-N-CA	5.38	126.22	119.98
1	L	261	ARG	N-CA-C	5.37	117.88	111.71
1	L	329	ALA	N-CA-C	5.36	117.78	110.01
1	D	18	VAL	N-CA-C	5.34	119.52	112.04
1	G	29	ILE	N-CA-C	5.34	117.72	111.05
1	G	146	THR	N-CA-C	5.34	119.90	113.17
1	L	301	PHE	N-CA-C	5.33	117.42	108.73
1	F	376	VAL	N-CA-C	5.32	115.78	108.12
1	A	131	GLN	N-CA-C	5.31	118.14	110.28
1	K	20	ALA	N-CA-C	5.30	119.60	113.18
1	L	380	MET	CA-C-O	-5.29	115.45	120.90
1	C	76	LYS	N-CA-C	-5.27	105.53	111.28
1	H	361	GLN	N-CA-C	5.27	118.12	110.17
1	A	378	MET	CA-C-N	5.26	125.24	120.03
1	A	378	MET	C-N-CA	5.26	125.24	120.03
1	E	29	ILE	N-CA-C	5.26	117.63	111.05
1	B	192	SER	N-CA-C	5.25	117.85	110.23
1	L	278	VAL	N-CA-C	-5.25	104.33	111.89
1	F	266	ARG	N-CA-C	5.25	117.08	111.36
1	I	97	ASP	N-CA-CB	5.25	118.55	110.79
1	I	156	ARG	N-CA-C	-5.24	99.22	108.23
1	O	130	THR	N-CA-C	5.24	117.06	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	61	GLU	CB-CA-C	-5.23	110.57	116.63
1	C	377	VAL	N-CA-C	5.22	115.41	108.11
1	H	79	GLU	N-CA-C	-5.21	105.51	111.14
1	D	50	GLU	N-CA-C	-5.21	107.58	114.04
1	P	96	GLU	N-CA-C	5.20	116.95	111.28
1	C	244	ILE	N-CA-CB	5.20	118.75	112.10
1	O	157	PHE	N-CA-C	5.19	119.94	111.37
1	N	17	VAL	N-CA-C	5.18	119.59	113.22
1	B	41	ALA	N-CA-C	5.17	117.11	108.99
1	N	60	SER	N-CA-C	5.17	117.83	109.40
1	I	47	SER	N-CA-C	5.15	116.90	108.76
1	D	260	TYR	N-CA-C	5.14	116.89	111.28
1	F	186	ILE	N-CA-C	5.14	115.77	108.42
1	E	146	THR	N-CA-C	5.14	120.40	113.72
1	E	278	VAL	N-CA-C	-5.13	105.49	110.42
1	C	129	GLY	N-CA-C	5.12	125.32	113.18
1	L	41	ALA	N-CA-C	5.12	116.97	109.24
1	A	145	LYS	N-CA-C	5.12	117.75	111.82
1	C	294	LEU	N-CA-C	5.11	116.92	111.36
1	A	233	ASN	N-CA-C	-5.10	100.42	108.73
1	P	227	LEU	N-CA-C	5.08	116.91	109.24
1	F	235	PRO	N-CA-C	5.08	120.29	114.20
1	K	93	GLN	N-CA-C	5.08	117.08	110.53
1	I	269	ASP	N-CA-C	5.07	116.89	111.36
1	B	152	VAL	N-CA-C	5.07	115.29	110.53
1	C	243	ASP	CA-C-O	-5.07	115.83	121.81
1	M	18	VAL	N-CA-C	5.06	119.18	111.89
1	H	61	GLU	N-CA-C	5.05	118.71	112.54
1	H	97	ASP	N-CA-C	-5.05	103.39	110.50
1	B	94	ILE	N-CA-C	5.04	115.11	107.80
1	B	200	VAL	N-CA-C	5.04	113.41	107.77
1	O	248	PHE	N-CA-C	5.03	116.47	108.67
1	P	145	LYS	N-CA-C	5.03	116.84	111.36
1	M	190	SER	N-CA-C	5.02	118.32	111.39
1	P	127	SER	CB-CA-C	-5.02	110.81	116.63
1	P	246	VAL	N-CA-C	5.02	115.13	108.11
1	E	156	ARG	N-CA-C	-5.01	99.61	108.23
1	B	265	PRO	CB-CA-C	-5.00	106.85	111.40
1	J	147	ALA	N-CA-C	5.00	116.73	111.28
1	B	29	ILE	N-CA-C	5.00	117.30	111.05
1	K	27	LEU	N-CA-C	5.00	116.46	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2938	0	2992	117	0
1	B	2964	0	3009	119	0
1	C	2942	0	2990	106	0
1	D	2962	0	3006	112	0
1	E	2965	0	3011	95	0
1	F	2942	0	2998	125	0
1	G	2941	0	3001	99	0
1	H	2957	0	2986	108	0
1	I	2874	0	2939	114	0
1	J	2981	0	3025	99	0
1	K	2830	0	2874	136	0
1	L	2735	0	2772	164	0
1	M	2929	0	2975	105	0
1	N	2891	0	2948	153	0
1	O	2768	0	2839	191	0
1	P	2914	0	2963	98	0
2	C	1	0	0	0	0
2	J	1	0	0	0	0
3	A	14	0	0	0	0
3	B	14	0	0	1	0
3	C	15	0	0	0	0
3	D	30	0	0	1	0
3	E	47	0	0	2	0
3	F	11	0	0	1	0
3	G	22	0	0	1	0
3	H	8	0	0	0	0
3	I	5	0	0	0	0
3	J	17	0	0	0	0
3	K	9	0	0	1	0
3	L	10	0	0	0	0
3	M	18	0	0	0	0
3	N	9	0	0	1	0
3	O	6	0	0	0	0
3	P	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	46780	0	47328	1874	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1874) 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:O:276:HIS:CD2	1:O:347:LEU:HD11	1.53	1.40
1:G:92:LEU:HG	1:G:102:LEU:CD2	1.62	1.28
1:O:276:HIS:CD2	1:O:347:LEU:CD1	2.23	1.19
1:H:1:MET:CE	1:H:70:THR:HG22	1.73	1.19
1:C:162:THR:HG22	1:C:175:THR:CG2	1.72	1.18
1:D:4:LYS:NZ	1:D:89:LEU:HB3	1.60	1.17
1:J:308:LEU:HD11	1:J:322:LEU:HD21	1.22	1.16
1:O:98:GLN:HG2	1:O:113:THR:O	1.44	1.15
1:I:4:LYS:HE2	1:I:91:ASP:OD2	1.43	1.15
1:L:137:ARG:HB2	1:L:215:GLU:HA	1.28	1.15
1:L:303:GLN:OE1	1:L:327:GLN:HA	1.46	1.15
1:I:166:ILE:CG2	1:I:196:VAL:HG22	1.77	1.14
1:B:346:VAL:HG11	1:B:375:TYR:OH	1.45	1.13
1:B:272:VAL:CG2	1:B:356:MET:HE1	1.79	1.11
1:P:7:LYS:CD	1:P:84:LEU:HB2	1.81	1.11
1:K:14:LEU:CD1	1:K:78:MET:SD	2.39	1.10
1:B:272:VAL:HG23	1:B:356:MET:HE1	1.29	1.10
1:K:132:VAL:HG21	1:K:166:ILE:HD11	1.15	1.10
1:L:301:PHE:CE2	1:L:356:MET:HE1	1.87	1.10
1:I:5:ILE:HD12	1:I:10:LEU:HB2	1.33	1.10
1:J:78:MET:HE3	1:J:82:LYS:HE3	1.33	1.10
1:H:1:MET:HE1	1:H:70:THR:HG22	1.16	1.09
1:L:367:ASP:OD1	1:L:368:PRO:HD2	1.50	1.09
1:G:92:LEU:HG	1:G:102:LEU:HD23	1.19	1.09
1:C:162:THR:HG22	1:C:175:THR:HG22	1.30	1.08
1:N:36:GLN:HG2	1:N:69:GLU:HG2	1.27	1.08
1:M:262:ARG:HB2	1:M:262:ARG:HH11	1.18	1.07
1:C:136:GLN:HG2	1:C:219:LEU:HD11	1.35	1.06
1:J:312:ASN:HB2	1:J:313:PRO:HD2	1.32	1.06
1:K:14:LEU:HD13	1:K:78:MET:SD	1.95	1.06
1:G:172:ARG:HD3	1:G:183:LEU:HD11	1.38	1.05
1:K:132:VAL:HG21	1:K:166:ILE:CD1	1.86	1.05
1:N:36:GLN:HG2	1:N:69:GLU:CG	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:ILE:HG21	1:I:196:VAL:HG22	1.37	1.04
1:K:378[A]:MET:SD	1:K:379:PRO:HD2	1.97	1.04
1:P:167:ASP:HB2	1:P:195:LEU:HD23	1.39	1.04
1:G:221:LEU:HD23	1:G:230:VAL:CG2	1.87	1.03
1:D:150:MET:HE3	1:D:160:THR:O	1.59	1.02
1:B:143:PHE:CE2	1:B:208:LEU:HD23	1.94	1.02
1:J:312:ASN:HB2	1:J:313:PRO:CD	1.88	1.02
1:N:33:VAL:HG23	1:N:74:ALA:HB2	1.41	1.01
1:N:279:PHE:CE1	1:N:283:LEU:HD21	1.94	1.01
1:C:312:ASN:HB2	1:C:313:PRO:HD2	1.38	1.01
1:C:270:LYS:H	1:C:270:LYS:HD2	1.17	1.01
1:K:132:VAL:CG2	1:K:166:ILE:CD1	2.39	1.01
1:H:133:GLN:HB3	1:H:218:GLN:HE21	1.21	1.00
1:H:33:VAL:HG13	1:H:74:ALA:HB2	1.44	0.99
1:J:273:LEU:HD21	1:J:351:ASP:HB3	1.40	0.99
1:K:132:VAL:CG2	1:K:166:ILE:HD11	1.92	0.99
1:N:98:GLN:HE22	1:N:115:PRO:HD3	1.25	0.99
1:B:257:PHE:CD2	1:B:258:PRO:HD2	1.97	0.98
1:H:133:GLN:HB3	1:H:218:GLN:NE2	1.77	0.98
1:O:135:THR:HG23	1:O:138:GLU:H	1.26	0.97
1:J:308:LEU:HD11	1:J:322:LEU:CD2	1.95	0.97
1:M:1:MET:SD	1:M:37:THR:HG22	2.04	0.97
1:I:195:LEU:CD1	1:I:195:LEU:H	1.77	0.97
1:O:276:HIS:NE2	1:O:347:LEU:HD11	1.78	0.97
1:P:312:ASN:HB2	1:P:313:PRO:HD2	1.44	0.96
1:L:350:ASP:O	1:L:351:ASP:OD1	1.81	0.96
1:E:300:ASN:OD1	1:E:332:GLU:HG3	1.64	0.96
1:H:378:MET:HB3	1:H:379:PRO:HD2	1.48	0.96
1:C:145:LYS:HD2	1:C:346:VAL:HG22	1.44	0.96
1:M:156:ARG:HG2	1:M:156:ARG:HH11	1.31	0.96
1:L:265:PRO:HG2	1:L:364:LEU:HD23	1.43	0.95
1:O:133:GLN:HB3	1:O:218:GLN:HE21	1.30	0.95
1:P:7:LYS:HD3	1:P:84:LEU:HB2	1.47	0.95
1:C:166:ILE:CG2	1:C:196:VAL:HG22	1.96	0.95
1:I:70:THR:HG21	1:I:94:ILE:HD11	1.48	0.95
1:P:312:ASN:HB2	1:P:313:PRO:CD	1.97	0.95
1:O:180:ARG:HD3	1:O:339:TYR:CD1	2.00	0.94
1:L:136:GLN:NE2	1:L:213:SER:HB3	1.82	0.94
1:M:312:ASN:HB2	1:M:313:PRO:HD2	1.50	0.94
1:H:1:MET:CE	1:H:70:THR:CG2	2.45	0.94
1:I:5:ILE:CD1	1:I:10:LEU:HB2	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:136:GLN:HG2	1:O:219:LEU:HD11	1.50	0.94
1:D:312:ASN:HB2	1:D:313:PRO:CD	1.97	0.94
1:P:7:LYS:HD2	1:P:84:LEU:HB2	1.45	0.94
1:K:4:LYS:HB3	1:K:64:CYS:HB2	1.50	0.94
1:O:335:PHE:HZ	1:O:363:VAL:HG21	1.30	0.93
1:O:145:LYS:HD3	1:O:346:VAL:HG22	1.49	0.93
1:J:33:VAL:HG13	1:J:74:ALA:HB2	1.51	0.93
1:I:138:GLU:HB3	1:I:186:ILE:HG21	1.50	0.93
1:I:195:LEU:O	1:I:195:LEU:HD22	1.68	0.93
1:B:272:VAL:HG23	1:B:356:MET:CE	1.99	0.92
1:H:136:GLN:HG2	1:H:219:LEU:HD11	1.51	0.92
1:K:14:LEU:HD12	1:K:78:MET:SD	2.07	0.92
1:O:33:VAL:HG13	1:O:74:ALA:HB2	1.48	0.92
1:J:308:LEU:CD1	1:J:322:LEU:CD2	2.47	0.92
1:G:132:VAL:HA	1:G:191:THR:HG22	1.51	0.91
1:L:142:LEU:CD1	1:L:171:LEU:HD22	2.00	0.91
1:K:138:GLU:HB3	1:K:186:ILE:HD12	1.49	0.91
1:O:137:ARG:NH1	1:O:137:ARG:HB3	1.85	0.91
1:M:312:ASN:HB2	1:M:313:PRO:CD	2.00	0.91
1:C:145:LYS:HA	1:C:346:VAL:HG21	1.50	0.91
1:F:59:LEU:HD12	1:F:60:SER:H	1.35	0.91
1:H:2:ARG:HD3	1:H:65:LEU:HD22	1.53	0.91
1:G:92:LEU:CG	1:G:102:LEU:CD2	2.48	0.91
1:O:276:HIS:HD2	1:O:347:LEU:HD11	1.19	0.91
1:F:59:LEU:HD11	1:F:63:ALA:HB1	1.52	0.90
1:D:4:LYS:HZ3	1:D:89:LEU:HB3	1.25	0.90
1:E:243:ASP:OD1	1:E:243:ASP:O	1.88	0.90
1:P:136:GLN:HG2	1:P:219:LEU:HD11	1.50	0.90
1:M:142:LEU:HD21	1:M:186:ILE:HB	1.51	0.90
1:H:262:ARG:NH1	1:H:262:ARG:HB3	1.86	0.90
1:F:59:LEU:HD11	1:F:63:ALA:CB	2.02	0.90
1:O:378:MET:SD	1:O:379:PRO:HD2	2.12	0.90
1:C:166:ILE:HG21	1:C:196:VAL:HG22	1.55	0.90
1:G:269:ASP:OD1	1:G:270:LYS:HG3	1.72	0.90
1:L:135:THR:HB	1:L:138:GLU:HG2	1.52	0.90
1:J:126:ASN:OD1	1:J:226:GLU:HG3	1.72	0.89
1:L:138:GLU:HB3	1:L:186:ILE:HG12	1.55	0.89
1:O:305:SER:O	1:O:324:ILE:HD11	1.72	0.89
1:D:150:MET:CE	1:D:160:THR:O	2.20	0.89
1:G:132:VAL:HG13	1:G:191:THR:CG2	2.03	0.89
1:I:166:ILE:CG2	1:I:196:VAL:CG2	2.50	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HD23	1:A:122:LEU:HD12	1.54	0.89
1:G:221:LEU:HD23	1:G:230:VAL:HG22	1.52	0.89
1:C:131:GLN:HG3	1:C:220:THR:CG2	2.03	0.88
1:B:274:ILE:HG12	1:B:324:ILE:HG22	1.55	0.88
1:N:98:GLN:NE2	1:N:115:PRO:HD3	1.88	0.88
1:F:4:LYS:HG3	1:F:65:LEU:HD11	1.54	0.88
1:P:299:LEU:HD22	1:P:308:LEU:HD22	1.55	0.88
1:G:172:ARG:CD	1:G:183:LEU:HD11	2.04	0.88
1:H:1:MET:HE1	1:H:70:THR:CG2	2.01	0.88
1:I:166:ILE:HG22	1:I:196:VAL:HG22	1.53	0.88
1:F:23:ARG:HG2	1:F:24:ARG:HG3	1.54	0.88
1:J:308:LEU:CD1	1:J:322:LEU:HD21	2.01	0.88
1:G:138:GLU:HB3	1:G:186:ILE:HD12	1.55	0.88
1:I:32:ASN:OD1	1:I:73:PRO:HA	1.74	0.88
1:N:95:THR:HG22	1:N:97:ASP:H	1.39	0.88
1:F:154:ASP:OD1	1:F:154:ASP:O	1.92	0.87
1:M:262:ARG:HH11	1:M:262:ARG:CB	1.87	0.87
1:O:136:GLN:CG	1:O:219:LEU:HD11	2.03	0.87
1:A:312:ASN:HB2	1:A:313:PRO:HD2	1.55	0.87
1:I:5:ILE:HD11	1:I:10:LEU:HD22	1.55	0.87
1:O:163:LEU:HD23	1:O:174:VAL:CG1	2.05	0.87
1:C:312:ASN:HB2	1:C:313:PRO:CD	2.03	0.87
1:H:322:LEU:H	1:H:322:LEU:HD12	1.40	0.87
1:L:301:PHE:HE2	1:L:356:MET:CE	1.87	0.87
1:A:166:ILE:CG2	1:A:196:VAL:HG22	2.04	0.87
1:H:257:PHE:CD2	1:H:258:PRO:HD2	2.09	0.87
1:O:133:GLN:HB3	1:O:218:GLN:NE2	1.89	0.87
1:B:124:THR:O	1:B:124:THR:OG1	1.88	0.86
1:B:312:ASN:HB2	1:B:313:PRO:HD2	1.57	0.86
1:O:137:ARG:HB3	1:O:137:ARG:HH11	1.38	0.86
1:I:70:THR:HG21	1:I:94:ILE:CD1	2.04	0.86
1:N:353:ASN:OD1	1:N:353:ASN:O	1.93	0.86
1:P:335:PHE:HZ	1:P:363:VAL:HG21	1.40	0.86
1:E:135:THR:OG1	1:E:138:GLU:HG3	1.75	0.86
1:O:276:HIS:NE2	1:O:347:LEU:CD1	2.37	0.85
1:G:136:GLN:HG2	1:G:219:LEU:HD11	1.58	0.85
1:L:301:PHE:CE2	1:L:356:MET:CE	2.58	0.85
1:C:329:ALA:HB1	1:C:330:PRO:HD2	1.56	0.85
1:J:280:LYS:O	1:J:284:GLN:HG3	1.76	0.85
1:D:4:LYS:HZ1	1:D:89:LEU:HB3	1.37	0.85
1:A:166:ILE:HG21	1:A:196:VAL:HG22	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:VAL:CG1	1:B:375:TYR:OH	2.24	0.84
1:L:37:THR:HG22	1:L:42:LEU:HD12	1.57	0.84
1:I:59:LEU:HD23	1:I:59:LEU:O	1.76	0.84
1:B:346:VAL:HG11	1:B:375:TYR:CZ	2.12	0.84
1:G:132:VAL:HG13	1:G:191:THR:HG21	1.59	0.84
1:N:279:PHE:O	1:N:283:LEU:HD23	1.75	0.84
1:D:356:MET:HG2	1:D:363:VAL:HG22	1.58	0.84
1:F:137:ARG:HB2	1:F:214:ILE:O	1.77	0.84
1:H:272:VAL:HG23	1:H:356:MET:HE1	1.60	0.84
1:I:132:VAL:HG21	1:I:166:ILE:HD13	1.59	0.84
1:L:301:PHE:HE2	1:L:356:MET:SD	2.01	0.84
1:O:136:GLN:HA	1:O:219:LEU:HD11	1.60	0.84
1:A:90:ILE:HG23	1:A:102:LEU:HD21	1.58	0.83
1:P:272:VAL:CG2	1:P:356:MET:HE1	2.07	0.83
1:A:331:LEU:HD23	1:A:356:MET:SD	2.18	0.83
1:P:165:GLU:HG2	1:P:195:LEU:HD21	1.58	0.83
1:N:0:HIS:CE1	1:N:96:GLU:HA	2.12	0.83
1:L:301:PHE:HE2	1:L:356:MET:HE1	1.41	0.83
1:L:301:PHE:O	1:L:330:PRO:HA	1.77	0.83
1:D:312:ASN:HB2	1:D:313:PRO:HD2	1.60	0.83
1:I:166:ILE:HG21	1:I:196:VAL:CG2	2.08	0.83
1:O:129:GLY:HA2	1:O:223:ILE:O	1.78	0.83
1:L:33:VAL:HG13	1:L:74:ALA:HB2	1.59	0.82
1:O:163:LEU:HB3	1:O:174:VAL:HG13	1.61	0.82
1:B:258:PRO:HB3	1:O:156:ARG:HE	1.43	0.82
1:I:335:PHE:HZ	1:I:363:VAL:HG21	1.44	0.82
1:I:195:LEU:CD1	1:I:195:LEU:N	2.41	0.82
1:K:35:ILE:CG2	1:K:37:THR:HG22	2.09	0.82
1:B:33:VAL:HG13	1:B:74:ALA:HB2	1.62	0.82
1:P:84:LEU:HD12	1:P:90:ILE:HD11	1.60	0.82
1:A:164:LEU:HD23	1:A:200:VAL:HG23	1.62	0.82
1:D:167:ASP:HB2	1:D:195:LEU:HD13	1.60	0.82
1:F:300:ASN:OD1	1:F:332:GLU:HG3	1.79	0.82
1:P:7:LYS:HD3	1:P:84:LEU:CB	2.09	0.82
1:B:312:ASN:HB2	1:B:313:PRO:CD	2.10	0.81
1:D:333:MET:SD	1:D:356:MET:SD	2.78	0.81
1:L:136:GLN:NE2	1:L:213:SER:CB	2.43	0.81
1:P:3:LEU:HD13	1:P:37:THR:HG21	1.61	0.81
1:B:166:ILE:HD11	1:B:223:ILE:HD12	1.62	0.81
1:D:301:PHE:CE2	1:D:356:MET:HE1	2.15	0.81
1:B:143:PHE:HE2	1:B:208:LEU:HD23	1.39	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:90:ILE:HG22	1:M:92:LEU:CD1	2.11	0.81
1:A:49:LEU:HD23	1:A:122:LEU:CD1	2.10	0.81
1:L:333:MET:HE3	1:L:359:ALA:HA	1.62	0.81
1:O:364:LEU:HD12	1:O:364:LEU:O	1.80	0.81
1:B:243:ASP:N	1:B:243:ASP:OD1	2.13	0.81
1:K:65:LEU:HD13	1:K:65:LEU:O	1.79	0.81
1:H:2:ARG:HG3	1:H:93:GLN:NE2	1.96	0.80
1:F:136:GLN:HG2	1:F:219:LEU:HD11	1.63	0.80
1:L:215:GLU:N	1:L:215:GLU:OE1	2.12	0.80
1:L:301:PHE:CE2	1:L:356:MET:SD	2.75	0.80
1:K:378[A]:MET:SD	1:K:379:PRO:CD	2.70	0.80
1:C:378:MET:SD	1:C:379:PRO:HD2	2.22	0.80
1:I:195:LEU:H	1:I:195:LEU:HD12	1.47	0.80
1:O:319:ILE:HD12	1:P:108:ARG:HD3	1.64	0.80
1:I:195:LEU:N	1:I:195:LEU:HD13	1.97	0.80
1:A:312:ASN:HB2	1:A:313:PRO:CD	2.10	0.79
1:I:312:ASN:HB2	1:I:313:PRO:HD2	1.63	0.79
1:G:33:VAL:HG13	1:G:74:ALA:HB2	1.64	0.79
1:N:64:CYS:SG	1:N:66:GLU:O	2.40	0.79
1:P:30:LEU:HD11	1:P:49:LEU:HG	1.64	0.79
1:N:186:ILE:HD12	1:N:186:ILE:O	1.83	0.78
1:F:307:GLN:HG3	1:F:321:ASP:OD1	1.82	0.78
1:G:312:ASN:HB2	1:G:313:PRO:CD	2.12	0.78
1:M:214:ILE:H	1:M:214:ILE:HD12	1.48	0.78
1:O:133:GLN:CB	1:O:218:GLN:HE21	1.96	0.78
1:P:138:GLU:HG2	1:P:186:ILE:HD12	1.65	0.78
1:F:353:ASN:ND2	1:F:368:PRO:HD3	1.98	0.78
1:M:354:MET:HE3	1:M:363:VAL:HG11	1.64	0.78
1:L:142:LEU:CD1	1:L:171:LEU:CD2	2.61	0.78
1:P:269:ASP:OD1	1:P:269:ASP:N	2.12	0.78
1:C:270:LYS:HD2	1:C:270:LYS:N	1.99	0.78
1:M:269:ASP:OD1	1:M:270:LYS:HG3	1.84	0.78
1:C:14:LEU:HD22	1:C:78:MET:HE1	1.65	0.78
1:N:278:VAL:HG12	1:N:322:LEU:HD11	1.65	0.78
1:O:163:LEU:HD23	1:O:174:VAL:HG11	1.64	0.78
1:B:143:PHE:HE2	1:B:208:LEU:CD2	1.97	0.77
1:C:272:VAL:HG23	1:C:356:MET:HE1	1.67	0.77
1:P:33:VAL:HG13	1:P:74:ALA:HB2	1.66	0.77
1:G:312:ASN:HB2	1:G:313:PRO:HD2	1.67	0.77
1:L:283:LEU:HD22	1:L:341:LEU:HG	1.67	0.77
1:O:136:GLN:CA	1:O:219:LEU:HD11	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:136:GLN:HA	1:O:219:LEU:CD1	2.15	0.77
1:O:353:ASN:ND2	1:O:368:PRO:HG3	2.00	0.77
1:P:4:LYS:HE2	1:P:63:ALA:HA	1.67	0.77
1:C:75:ARG:HD2	1:C:79:GLU:OE2	1.85	0.76
1:D:4:LYS:HZ1	1:D:89:LEU:CB	1.98	0.76
1:I:132:VAL:HG21	1:I:166:ILE:CD1	2.14	0.76
1:I:312:ASN:HB2	1:I:313:PRO:CD	2.15	0.76
1:L:45:THR:HG23	1:L:54:VAL:HG22	1.67	0.76
1:O:347:LEU:O	1:O:347:LEU:HD12	1.85	0.76
1:E:30:LEU:HD11	1:E:49:LEU:HG	1.65	0.76
1:D:61:GLU:OE1	1:D:61:GLU:N	2.17	0.76
1:I:166:ILE:HG22	1:I:196:VAL:CG2	2.15	0.76
1:D:166:ILE:HG13	1:D:191:THR:HG21	1.67	0.76
1:G:243:ASP:OD1	1:G:243:ASP:N	2.16	0.76
1:O:273:LEU:HB2	1:O:325:GLN:HB2	1.66	0.76
1:C:18:VAL:HB	1:C:78:MET:HE3	1.68	0.76
1:N:33:VAL:HG23	1:N:74:ALA:CB	2.15	0.76
1:C:162:THR:HG22	1:C:175:THR:HG21	1.67	0.75
1:G:5:ILE:HD13	1:G:10:LEU:HB2	1.68	0.75
1:N:166:ILE:HD12	1:N:196:VAL:HG22	1.67	0.75
1:G:136:GLN:HG2	1:G:219:LEU:CD1	2.17	0.75
1:N:234:THR:N	1:N:235:PRO:HD2	2.02	0.75
1:H:262:ARG:HB3	1:H:262:ARG:HH11	1.49	0.75
1:P:84:LEU:CD1	1:P:90:ILE:HD11	2.15	0.75
1:D:166:ILE:CG1	1:D:191:THR:HG21	2.16	0.75
1:H:322:LEU:HD12	1:H:322:LEU:N	2.00	0.75
1:H:367:ASP:OD1	1:H:368:PRO:HD2	1.86	0.75
1:K:137:ARG:HG3	1:K:214:ILE:O	1.86	0.75
1:O:331:LEU:HD11	1:O:359:ALA:HB2	1.68	0.75
1:E:303:GLN:OE1	1:E:303:GLN:N	2.18	0.75
1:K:132:VAL:HG22	1:K:166:ILE:CD1	2.17	0.75
1:M:156:ARG:HG2	1:M:156:ARG:NH1	1.99	0.75
1:C:96:GLU:H	1:C:96:GLU:CD	1.95	0.74
1:C:166:ILE:HG22	1:C:196:VAL:HG22	1.68	0.74
1:O:135:THR:HG22	1:O:138:GLU:CB	2.17	0.74
1:E:214:ILE:HD12	1:E:214:ILE:N	2.02	0.74
1:G:61:GLU:H	1:G:61:GLU:CD	1.95	0.74
1:O:40:GLN:NE2	1:O:40:GLN:H	1.85	0.74
1:O:129:GLY:CA	1:O:223:ILE:O	2.36	0.74
1:O:260:TYR:O	1:O:264:ILE:HD12	1.88	0.74
1:P:272:VAL:HG23	1:P:356:MET:CE	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:GLN:HE21	1:L:213:SER:HB3	1.52	0.74
1:M:272:VAL:HG22	1:M:326:TYR:CD1	2.22	0.74
1:M:214:ILE:HD12	1:M:214:ILE:N	2.03	0.74
1:O:335:PHE:CZ	1:O:363:VAL:HG21	2.20	0.74
1:L:185:GLU:OE1	1:L:185:GLU:N	2.20	0.74
1:P:167:ASP:CB	1:P:195:LEU:HD23	2.16	0.74
1:B:18:VAL:HG22	1:B:18:VAL:O	1.88	0.73
1:K:356:MET:HG2	1:K:363:VAL:HG22	1.70	0.73
1:M:303:GLN:OE1	1:M:303:GLN:N	2.16	0.73
1:L:136:GLN:HE22	1:L:213:SER:CB	2.00	0.73
1:O:135:THR:CG2	1:O:138:GLU:H	2.02	0.73
1:B:286:VAL:HG21	1:B:308:LEU:HB2	1.70	0.73
1:C:131:GLN:HG3	1:C:220:THR:HG22	1.70	0.73
1:C:145:LYS:CD	1:C:346:VAL:HG22	2.19	0.73
1:E:33:VAL:HG13	1:E:74:ALA:HB2	1.70	0.73
1:O:360:ASN:HB2	1:O:381:ARG:HD2	1.69	0.73
1:L:136:GLN:HG2	1:L:219:LEU:CD1	2.19	0.73
1:G:166:ILE:HG23	1:G:196:VAL:HG13	1.70	0.73
1:N:187:LEU:C	1:N:187:LEU:HD12	2.14	0.73
1:O:306:LEU:HB2	1:O:324:ILE:HD13	1.71	0.73
1:D:222:LEU:HB2	1:J:194:GLN:HE22	1.54	0.73
1:M:225:ARG:HD2	1:M:225:ARG:O	1.88	0.73
1:K:132:VAL:CG2	1:K:166:ILE:HD13	2.19	0.72
1:C:270:LYS:HB3	1:C:326:TYR:HE1	1.52	0.72
1:G:174:VAL:HG22	1:G:183:LEU:HD13	1.70	0.72
1:H:126:ASN:H	1:H:126:ASN:ND2	1.83	0.72
1:D:194:GLN:OE1	1:D:194:GLN:N	2.20	0.72
1:I:107:SER:HB3	1:J:320:GLU:OE1	1.88	0.72
1:K:132:VAL:HG22	1:K:166:ILE:HD13	1.70	0.72
1:L:137:ARG:HB2	1:L:215:GLU:CA	2.15	0.72
1:L:364:LEU:HD12	1:L:364:LEU:O	1.90	0.72
1:C:149:ALA:HB3	1:C:175:THR:OG1	1.89	0.72
1:N:33:VAL:CG2	1:N:74:ALA:HB2	2.16	0.72
1:F:59:LEU:CD1	1:F:63:ALA:CB	2.67	0.72
1:B:303:GLN:OE1	1:B:303:GLN:N	2.23	0.72
1:E:356:MET:HG3	1:E:363:VAL:HG13	1.71	0.72
1:H:134:VAL:HG23	1:H:138:GLU:OE1	1.89	0.72
1:F:65:LEU:H	1:F:65:LEU:HD12	1.53	0.72
1:G:92:LEU:HG	1:G:102:LEU:HD21	1.69	0.72
1:O:335:PHE:HZ	1:O:363:VAL:CG2	2.02	0.72
1:D:303:GLN:OE1	1:D:303:GLN:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347:LEU:HD22	1:H:367:ASP:HB2	1.70	0.72
1:L:37:THR:HG22	1:L:42:LEU:CD1	2.20	0.72
1:J:195:LEU:HD23	1:J:195:LEU:C	2.14	0.71
1:K:301:PHE:CE2	1:K:356:MET:HE1	2.24	0.71
1:M:262:ARG:HB2	1:M:262:ARG:NH1	2.01	0.71
1:N:333:MET:HE3	1:N:335:PHE:HE2	1.56	0.71
1:B:146:THR:O	1:B:175:THR:HG21	1.91	0.71
1:K:4:LYS:HB3	1:K:64:CYS:CB	2.20	0.71
1:L:65:LEU:HD12	1:L:65:LEU:N	2.04	0.71
1:H:1:MET:HB2	1:H:68:GLY:HA3	1.73	0.71
1:H:10:LEU:HD23	1:H:10:LEU:O	1.91	0.71
1:O:261:ARG:HD2	1:O:261:ARG:H	1.55	0.71
1:L:144:GLU:HG3	1:L:145:LYS:HD3	1.73	0.71
1:C:45:THR:HG23	1:C:54:VAL:HG22	1.73	0.71
1:M:278:VAL:CG1	1:M:322:LEU:HD22	2.21	0.71
1:C:136:GLN:HG2	1:C:219:LEU:CD1	2.18	0.71
1:C:347:LEU:HD22	1:C:367:ASP:HB2	1.72	0.71
1:I:156:ARG:HH11	1:L:262:ARG:HH21	1.39	0.71
1:H:75:ARG:HD2	1:H:79:GLU:OE1	1.89	0.70
1:K:4:LYS:O	1:K:64:CYS:HB2	1.91	0.70
1:B:272:VAL:HG21	1:B:356:MET:HE1	1.71	0.70
1:P:303:GLN:N	1:P:303:GLN:OE1	2.23	0.70
1:B:148:PHE:CE1	1:B:346:VAL:HG21	2.26	0.70
1:E:271:HIS:HD2	1:J:216:ASP:HB3	1.56	0.70
1:F:154:ASP:O	1:F:154:ASP:CG	2.34	0.70
1:K:133:GLN:HB3	1:K:218:GLN:HE21	1.54	0.70
1:L:30:LEU:HD21	1:L:49:LEU:HG	1.72	0.70
1:C:131:GLN:CG	1:C:220:THR:CG2	2.69	0.70
1:G:172:ARG:HD3	1:G:183:LEU:CD1	2.19	0.70
1:H:136:GLN:HG2	1:H:219:LEU:CD1	2.20	0.70
1:L:239:LYS:HG2	1:L:239:LYS:O	1.90	0.70
1:D:354:MET:HE3	1:D:363:VAL:HG11	1.74	0.70
1:H:311:ASN:HB3	1:H:317:GLU:HG3	1.72	0.70
1:D:165:GLU:HG2	1:D:195:LEU:HD11	1.73	0.70
1:F:153:GLN:HA	1:F:153:GLN:HE21	1.56	0.70
1:I:132:VAL:CG2	1:I:166:ILE:HD11	2.22	0.70
1:L:289:LEU:HD12	1:L:318:ALA:HB2	1.74	0.70
1:I:132:VAL:CG2	1:I:166:ILE:CD1	2.70	0.70
1:I:281:GLN:NE2	1:I:281:GLN:HA	2.06	0.70
1:N:131:GLN:CG	1:N:220:THR:HG23	2.22	0.70
1:O:276:HIS:HD2	1:O:347:LEU:CD1	1.81	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:GLU:CD	1:L:61:GLU:H	1.99	0.69
1:P:289:LEU:HD12	1:P:318:ALA:HB2	1.73	0.69
1:D:194:GLN:CD	1:D:194:GLN:H	1.99	0.69
1:J:273:LEU:CD2	1:J:351:ASP:HB3	2.17	0.69
1:N:279:PHE:CE1	1:N:283:LEU:CD2	2.75	0.69
1:D:187:LEU:HD13	1:D:187:LEU:C	2.18	0.69
1:N:98:GLN:HE22	1:N:115:PRO:CD	2.04	0.69
1:B:354:MET:HE2	1:B:363:VAL:HG11	1.73	0.69
1:G:132:VAL:HA	1:G:191:THR:CG2	2.21	0.69
1:K:42:LEU:HD12	1:K:42:LEU:N	2.08	0.69
1:C:169:ASN:H	1:C:191:THR:HG21	1.57	0.69
1:H:257:PHE:CG	1:H:258:PRO:HD2	2.27	0.69
1:N:312:ASN:HB2	1:N:313:PRO:HD2	1.73	0.69
1:O:339:TYR:O	1:O:343:VAL:HG23	1.92	0.69
1:P:124:THR:CG2	1:P:227:LEU:HD12	2.21	0.69
1:I:170:GLN:HE21	1:I:172:ARG:HH21	1.40	0.69
1:L:142:LEU:HD13	1:L:171:LEU:CD2	2.22	0.69
1:F:18:VAL:HG21	1:F:78:MET:HE3	1.74	0.69
1:G:141:ARG:NH1	1:G:372:ASP:OD2	2.23	0.69
1:I:281:GLN:HA	1:I:281:GLN:HE21	1.58	0.69
1:P:124:THR:HG22	1:P:227:LEU:HD12	1.74	0.69
1:E:304:ASP:HA	1:E:324:ILE:O	1.92	0.69
1:L:3:LEU:CD1	1:L:37:THR:HG21	2.23	0.69
1:N:163:LEU:HD22	1:N:257:PHE:CD2	2.27	0.69
1:O:222:LEU:HD23	1:O:222:LEU:C	2.18	0.69
1:A:217:GLU:OE2	1:A:218:GLN:O	2.10	0.68
1:F:34:LYS:HE2	1:F:36:GLN:NE2	2.08	0.68
1:H:1:MET:HE2	1:H:70:THR:HG22	1.74	0.68
1:H:2:ARG:HG3	1:H:93:GLN:HE21	1.58	0.68
1:J:23:ARG:HH22	1:J:75:ARG:NH1	1.92	0.68
1:N:148:PHE:CE1	1:N:346:VAL:HG11	2.29	0.68
1:J:45:THR:HG23	1:J:54:VAL:HG22	1.75	0.68
1:N:90:ILE:HG23	1:N:102:LEU:HD21	1.75	0.68
1:E:273:LEU:HD21	1:J:187:LEU:HD12	1.75	0.68
1:I:59:LEU:HD23	1:I:59:LEU:C	2.18	0.68
1:H:2:ARG:CD	1:H:65:LEU:HD22	2.23	0.68
1:K:230:VAL:HG12	1:K:248:PHE:HB3	1.75	0.68
1:C:240:GLU:OE1	1:C:240:GLU:HA	1.92	0.68
1:N:187:LEU:HD12	1:N:187:LEU:O	1.94	0.68
1:L:142:LEU:HD11	1:L:171:LEU:HD22	1.75	0.68
1:P:257:PHE:CD2	1:P:258:PRO:HD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:ASN:CG	1:F:332:GLU:HG3	2.19	0.68
1:G:133:GLN:HB2	1:G:190:SER:CB	2.24	0.68
1:I:353:ASN:HD21	1:I:366:GLN:HB2	1.57	0.67
1:A:1:MET:HE3	1:A:94:ILE:HD11	1.75	0.67
1:C:37:THR:HG23	1:C:42:LEU:HD12	1.75	0.67
1:C:145:LYS:HD2	1:C:346:VAL:CG2	2.19	0.67
1:H:135:THR:OG1	1:H:138:GLU:HG3	1.93	0.67
1:M:303:GLN:H	1:M:303:GLN:CD	2.01	0.67
1:O:305:SER:O	1:O:324:ILE:CD1	2.41	0.67
1:D:278:VAL:HG12	1:D:322:LEU:HD11	1.76	0.67
1:I:32:ASN:OD1	1:I:73:PRO:CA	2.42	0.67
1:N:166:ILE:HD12	1:N:196:VAL:CG2	2.24	0.67
1:D:266:ARG:HH22	1:O:300:ASN:CG	2.03	0.67
1:N:165:GLU:HG3	1:N:197:GLN:HG2	1.75	0.67
1:F:304:ASP:HA	1:F:324:ILE:O	1.94	0.67
1:K:4:LYS:O	1:K:64:CYS:SG	2.52	0.67
1:O:180:ARG:HD3	1:O:339:TYR:CE1	2.29	0.67
1:O:299:LEU:HD12	1:O:299:LEU:N	2.10	0.67
1:P:257:PHE:CG	1:P:258:PRO:HD2	2.29	0.67
1:F:237:ARG:HD2	1:F:237:ARG:O	1.95	0.67
1:M:364:LEU:HD11	1:M:374:THR:HG23	1.77	0.67
1:N:136:GLN:HG2	1:N:219:LEU:HD11	1.77	0.67
1:K:77:LEU:HD23	1:K:77:LEU:O	1.95	0.67
1:A:303:GLN:OE1	1:A:303:GLN:N	2.21	0.67
1:I:2:ARG:HG2	1:I:65:LEU:HD12	1.78	0.67
1:N:227:LEU:HD23	1:N:251:LYS:HA	1.76	0.67
1:O:162:THR:HG23	1:O:205:VAL:HG21	1.76	0.67
1:O:176:THR:HB	1:O:181:LEU:HD13	1.77	0.67
1:A:90:ILE:HG23	1:A:102:LEU:CD2	2.23	0.66
1:B:79:GLU:HA	1:B:79:GLU:OE2	1.95	0.66
1:D:266:ARG:CG	1:D:266:ARG:HH11	2.08	0.66
1:H:150:MET:HG3	1:H:175:THR:HG22	1.77	0.66
1:C:145:LYS:HA	1:C:346:VAL:CG2	2.22	0.66
1:I:132:VAL:HG22	1:I:166:ILE:HD11	1.76	0.66
1:F:153:GLN:HA	1:F:153:GLN:NE2	2.11	0.66
1:C:145:LYS:CD	1:C:346:VAL:CG2	2.73	0.66
1:M:136:GLN:NE2	1:M:213:SER:OG	2.29	0.66
1:O:33:VAL:HG13	1:O:74:ALA:CB	2.25	0.66
1:A:96:GLU:H	1:A:96:GLU:CD	2.02	0.66
1:A:186:ILE:O	1:A:186:ILE:HG13	1.96	0.66
1:H:134:VAL:HG21	1:H:186:ILE:CD1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:VAL:HG22	1:H:326:TYR:CD1	2.30	0.66
1:H:14:LEU:HD11	1:H:77:LEU:HD23	1.76	0.66
1:J:289:LEU:HD22	1:J:316:ASP:CB	2.26	0.66
1:L:136:GLN:HE22	1:L:213:SER:HB2	1.61	0.66
1:L:217:GLU:OE1	1:L:217:GLU:HA	1.96	0.66
1:N:124:THR:HB	1:N:227:LEU:HD12	1.78	0.66
1:O:135:THR:CG2	1:O:138:GLU:CB	2.74	0.66
1:M:195:LEU:HD12	1:M:195:LEU:O	1.95	0.66
1:N:279:PHE:CD1	1:N:283:LEU:CD2	2.79	0.66
1:F:358:GLU:HB2	1:F:361:GLN:HG3	1.76	0.66
1:A:133:GLN:HB3	1:A:189:SER:HB3	1.77	0.66
1:A:142:LEU:HD13	1:A:186:ILE:HG23	1.78	0.66
1:B:360:ASN:O	1:B:379:PRO:HG3	1.96	0.66
1:F:59:LEU:HG	1:F:63:ALA:HB3	1.76	0.66
1:J:356:MET:HG2	1:J:363:VAL:HG22	1.77	0.66
1:M:315:GLN:HE21	1:N:99:ARG:NH1	1.94	0.66
1:E:271:HIS:CD2	1:J:216:ASP:HB3	2.30	0.65
1:H:70:THR:HG21	1:H:94:ILE:HD11	1.77	0.65
1:L:33:VAL:HG13	1:L:74:ALA:CB	2.26	0.65
1:O:17:VAL:HG21	1:O:46:GLY:N	2.11	0.65
1:O:17:VAL:HG23	1:O:53:LEU:HB2	1.79	0.65
1:A:140:LYS:NZ	1:A:212:LEU:O	2.29	0.65
1:D:3:LEU:HD12	1:D:3:LEU:O	1.96	0.65
1:M:89:LEU:N	1:M:89:LEU:HD12	2.12	0.65
1:P:3:LEU:CD1	1:P:37:THR:HG21	2.27	0.65
1:A:2:ARG:HG3	1:A:93:GLN:OE1	1.97	0.65
1:C:283:LEU:HD23	1:C:341:LEU:HG	1.77	0.65
1:G:92:LEU:CD2	1:G:102:LEU:HD21	2.25	0.65
1:G:132:VAL:HG22	1:G:191:THR:HG21	1.77	0.65
1:I:185:GLU:O	1:I:186:ILE:HD13	1.96	0.65
1:P:272:VAL:HG23	1:P:356:MET:HE1	1.76	0.65
1:J:312:ASN:CB	1:J:313:PRO:CD	2.62	0.65
1:L:65:LEU:N	1:L:65:LEU:CD1	2.60	0.65
1:L:199:ILE:CG2	1:L:253:ILE:HB	2.27	0.65
1:L:282:SER:O	1:L:286:VAL:HG12	1.95	0.65
1:G:278:VAL:HG12	1:G:322:LEU:HD11	1.79	0.65
1:H:33:VAL:HG13	1:H:74:ALA:CB	2.24	0.65
1:J:289:LEU:HD22	1:J:316:ASP:HB2	1.77	0.65
1:O:17:VAL:CG2	1:O:46:GLY:H	2.10	0.65
1:E:307:GLN:HG3	1:E:321:ASP:OD1	1.96	0.65
1:F:18:VAL:HG21	1:F:78:MET:CE	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:33:VAL:HG13	1:J:74:ALA:CB	2.26	0.65
1:K:137:ARG:CG	1:K:214:ILE:O	2.44	0.65
1:A:300:ASN:OD1	1:A:332:GLU:HG3	1.96	0.65
1:L:164:LEU:HD22	1:L:171:LEU:HD21	1.79	0.65
1:C:9:SER:O	1:C:13:VAL:HG23	1.97	0.65
1:C:187:LEU:HD12	1:C:187:LEU:O	1.97	0.65
1:G:306:LEU:HB2	1:G:324:ILE:HD13	1.78	0.65
1:M:168:GLU:OE1	1:M:168:GLU:HA	1.97	0.65
1:N:259:ASP:OD1	1:N:259:ASP:N	2.13	0.65
1:O:259:ASP:OD1	1:O:259:ASP:O	2.15	0.65
1:G:221:LEU:CD2	1:G:230:VAL:CG2	2.70	0.65
1:M:228:LEU:HD23	1:M:228:LEU:C	2.22	0.65
1:I:134:VAL:HG12	1:I:188:ALA:CB	2.27	0.64
1:A:165:GLU:HG3	1:A:197:GLN:HG2	1.79	0.64
1:A:166:ILE:CG2	1:A:196:VAL:CG2	2.75	0.64
1:F:269:ASP:OD1	1:F:270:LYS:HG3	1.97	0.64
1:L:298:PHE:C	1:L:299:LEU:HD12	2.22	0.64
1:A:17:VAL:CG2	1:A:46:GLY:N	2.61	0.64
1:F:150:MET:HE1	1:F:202:ARG:HA	1.78	0.64
1:K:137:ARG:HG3	1:K:214:ILE:C	2.22	0.64
1:N:131:GLN:NE2	1:N:220:THR:CG2	2.60	0.64
1:D:301:PHE:CD2	1:D:356:MET:HE1	2.32	0.64
1:F:59:LEU:HD12	1:F:60:SER:N	2.10	0.64
1:J:330:PRO:HG2	1:N:329:ALA:HB1	1.78	0.64
1:K:138:GLU:HB3	1:K:186:ILE:CD1	2.23	0.64
1:E:303:GLN:HA	1:E:326:TYR:O	1.98	0.64
1:M:83:SER:HB3	1:N:288:ILE:HD11	1.79	0.64
1:A:301:PHE:CE2	1:A:356:MET:HE1	2.33	0.64
1:O:149:ALA:HB3	1:O:175:THR:OG1	1.98	0.64
1:B:238:ASP:HB2	1:B:241:GLN:HB2	1.80	0.64
1:I:3:LEU:N	1:I:3:LEU:HD23	2.13	0.64
1:M:278:VAL:HG12	1:M:322:LEU:HD22	1.80	0.64
1:O:257:PHE:CD2	1:O:258:PRO:HD2	2.32	0.64
1:A:314:GLU:OE2	1:A:314:GLU:N	2.30	0.64
1:E:83:SER:HB3	1:F:288:ILE:HD11	1.79	0.64
1:L:137:ARG:HD3	1:L:215:GLU:HB3	1.80	0.64
1:M:262:ARG:HH11	1:M:262:ARG:CG	2.10	0.64
1:D:272:VAL:HG22	1:D:326:TYR:CD1	2.32	0.63
1:O:37:THR:HG22	1:O:68:GLY:O	1.98	0.63
1:O:281:GLN:HB3	1:O:285:ARG:HH12	1.62	0.63
1:P:272:VAL:HG21	1:P:356:MET:HE1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD23	1:A:200:VAL:CG2	2.28	0.63
1:K:42:LEU:HG	1:K:57:THR:O	1.98	0.63
1:K:47:SER:HB3	1:K:52:GLU:HA	1.81	0.63
1:E:214:ILE:HD12	1:E:214:ILE:H	1.61	0.63
1:J:136:GLN:HG2	1:J:219:LEU:HD11	1.79	0.63
1:L:135:THR:CB	1:L:138:GLU:HG2	2.25	0.63
1:O:334:SER:OG	1:O:380:MET:HE2	1.98	0.63
1:P:27:LEU:HG	1:P:29:ILE:HG22	1.79	0.63
1:A:49:LEU:CD2	1:A:122:LEU:HD12	2.27	0.63
1:J:263:VAL:HG11	1:K:155:VAL:HG13	1.80	0.63
1:K:98:GLN:HA	1:K:113:THR:HG22	1.80	0.63
1:M:33:VAL:CG2	1:M:44:ILE:HG22	2.29	0.63
1:C:289:LEU:HD12	1:C:318:ALA:HB2	1.80	0.63
1:C:307:GLN:HG3	1:C:321:ASP:OD1	1.99	0.63
1:G:78:MET:HE2	1:G:79:GLU:HG3	1.79	0.63
1:J:30:LEU:HD21	1:J:120:PRO:HG2	1.79	0.63
1:M:2:ARG:HG2	1:M:65:LEU:HD13	1.81	0.63
1:A:269:ASP:O	1:A:271:HIS:CD2	2.51	0.63
1:F:228:LEU:HD23	1:F:228:LEU:C	2.23	0.63
1:D:100:CYS:HB2	1:D:113:THR:CG2	2.29	0.63
1:H:30:LEU:HD11	1:H:49:LEU:HG	1.81	0.63
1:A:269:ASP:OD1	1:A:270:LYS:N	2.32	0.63
1:B:125:GLU:HA	1:D:187:LEU:HD21	1.80	0.63
1:F:2:ARG:HG3	1:F:65:LEU:HD13	1.80	0.63
1:H:134:VAL:HG21	1:H:186:ILE:HD11	1.81	0.63
1:M:221:LEU:HD22	1:M:230:VAL:HG22	1.80	0.63
1:N:186:ILE:HD12	1:N:186:ILE:C	2.24	0.63
1:B:191:THR:O	1:J:222:LEU:HD21	1.98	0.63
1:G:140:LYS:NZ	1:G:209:GLN:O	2.32	0.63
1:N:180:ARG:NH1	1:N:342:ASP:OD2	2.28	0.63
1:C:270:LYS:HB3	1:C:326:TYR:CE1	2.34	0.62
1:M:269:ASP:OD1	1:M:270:LYS:N	2.31	0.62
1:G:162:THR:HG23	1:G:205:VAL:HG21	1.81	0.62
1:I:47:SER:HB2	1:I:52:GLU:HA	1.81	0.62
1:H:79:GLU:OE2	1:H:79:GLU:HA	1.99	0.62
1:H:378:MET:N	1:H:378:MET:SD	2.71	0.62
1:M:30:LEU:HD11	1:M:49:LEU:HG	1.81	0.62
1:M:315:GLN:HE21	1:N:99:ARG:HH12	1.45	0.62
1:N:312:ASN:HB2	1:N:313:PRO:CD	2.30	0.62
1:O:17:VAL:CG2	1:O:46:GLY:N	2.63	0.62
1:A:1:MET:HE1	1:A:70:THR:HG22	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLY:HA2	1:C:357:THR:HG22	1.82	0.62
1:D:100:CYS:HB2	1:D:113:THR:HG21	1.80	0.62
1:D:239:LYS:HG3	1:D:239:LYS:O	1.98	0.62
1:E:322:LEU:HD12	1:E:322:LEU:N	2.14	0.62
1:H:45:THR:HG23	1:H:54:VAL:HG22	1.81	0.62
1:K:14:LEU:HB3	1:K:78:MET:SD	2.39	0.62
1:N:36:GLN:CG	1:N:69:GLU:CG	2.73	0.62
1:A:17:VAL:HG21	1:A:46:GLY:N	2.15	0.62
1:C:335:PHE:HZ	1:C:363:VAL:HG21	1.64	0.62
1:G:259:ASP:O	1:G:262:ARG:HG2	1.99	0.62
1:I:41:ALA:HA	1:I:59:LEU:HD22	1.80	0.62
1:K:306:LEU:HB2	1:K:324:ILE:HD13	1.81	0.62
1:E:24:ARG:HE	1:E:24:ARG:HA	1.64	0.62
1:N:98:GLN:NE2	1:N:115:PRO:CD	2.62	0.62
1:O:0:HIS:NE2	1:O:96:GLU:HB2	2.13	0.62
1:P:335:PHE:CZ	1:P:363:VAL:HG21	2.29	0.62
1:I:270:LYS:NZ	1:I:357:THR:O	2.32	0.62
1:E:2:ARG:HG2	1:E:65:LEU:HD12	1.82	0.62
1:G:59:LEU:HG	1:G:63:ALA:HB3	1.82	0.62
1:H:77:LEU:CD1	1:H:102:LEU:HD21	2.30	0.62
1:I:142:LEU:HD21	1:I:186:ILE:HG12	1.82	0.62
1:K:301:PHE:O	1:K:330:PRO:HA	2.00	0.62
1:E:294:LEU:N	1:E:294:LEU:HD12	2.15	0.62
1:O:155:VAL:HG21	1:O:159:LEU:HD12	1.81	0.62
1:E:354:MET:HB3	1:E:356:MET:HE3	1.82	0.62
1:F:8:GLU:OE2	1:F:8:GLU:N	2.30	0.62
1:N:235:PRO:HG3	1:N:243:ASP:HB2	1.81	0.62
1:A:221:LEU:HD12	1:A:230:VAL:HB	1.82	0.61
1:A:281:GLN:OE1	1:A:281:GLN:HA	2.00	0.61
1:K:11:LEU:HD11	1:K:82:LYS:HG2	1.80	0.61
1:P:166:ILE:HG23	1:P:166:ILE:O	2.00	0.61
1:J:314:GLU:N	1:J:314:GLU:OE2	2.33	0.61
1:O:117:GLU:OE1	1:O:117:GLU:N	2.20	0.61
1:F:32:ASN:CB	1:F:71:THR:HG22	2.30	0.61
1:M:278:VAL:HG12	1:M:322:LEU:CD2	2.31	0.61
1:N:131:GLN:NE2	1:N:220:THR:HG21	2.15	0.61
1:G:207:GLU:OE2	1:G:210:ARG:NH2	2.24	0.61
1:K:96:GLU:O	1:K:96:GLU:HG2	1.98	0.61
1:M:1:MET:SD	1:M:37:THR:CG2	2.86	0.61
1:N:277:ASP:O	1:N:281:GLN:HG2	2.01	0.61
1:E:158:TYR:CE1	1:E:258:PRO:HD3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:THR:HG23	1:H:191:THR:O	2.00	0.61
1:L:3:LEU:HD13	1:L:37:THR:HG21	1.82	0.61
1:A:364:LEU:HD21	1:A:374:THR:CG2	2.30	0.61
1:B:128:GLN:OE1	1:B:128:GLN:HA	2.01	0.61
1:K:136:GLN:HG2	1:K:219:LEU:HD11	1.81	0.61
1:B:166:ILE:HD11	1:B:223:ILE:CD1	2.31	0.61
1:L:169:ASN:HA	1:L:188:ALA:O	2.01	0.61
1:O:273:LEU:HD22	1:O:325:GLN:OE1	2.01	0.61
1:A:1:MET:HE3	1:A:94:ILE:CD1	2.31	0.61
1:K:96:GLU:N	1:K:96:GLU:OE1	2.34	0.61
1:D:150:MET:HE3	1:D:160:THR:C	2.25	0.61
1:K:162:THR:HG22	1:K:175:THR:CG2	2.31	0.61
1:B:4:LYS:HG3	1:B:65:LEU:HD21	1.82	0.60
1:B:265:PRO:HG2	1:B:364:LEU:HB2	1.83	0.60
1:O:135:THR:HG23	1:O:138:GLU:N	2.09	0.60
1:O:137:ARG:HH11	1:O:137:ARG:CB	2.12	0.60
1:B:33:VAL:HG13	1:B:74:ALA:CB	2.31	0.60
1:G:273:LEU:CD2	1:G:351:ASP:HB3	2.32	0.60
1:H:238:ASP:HB2	1:H:241:GLN:HB2	1.82	0.60
1:H:372:ASP:N	1:H:372:ASP:OD1	2.28	0.60
1:J:330:PRO:HG2	1:N:329:ALA:CB	2.31	0.60
1:L:135:THR:HB	1:L:138:GLU:CG	2.27	0.60
1:O:122:LEU:HD12	1:O:249:THR:HG22	1.83	0.60
1:A:17:VAL:HG22	1:A:46:GLY:HA3	1.83	0.60
1:D:364:LEU:HD11	1:D:374:THR:HG23	1.83	0.60
1:P:274:ILE:HG23	1:P:324:ILE:HG22	1.83	0.60
1:H:70:THR:HG21	1:H:94:ILE:CD1	2.31	0.60
1:M:152:VAL:O	1:M:202:ARG:NH2	2.34	0.60
1:N:279:PHE:CD1	1:N:283:LEU:HD21	2.37	0.60
1:D:152:VAL:HG12	1:D:153:GLN:HG2	1.84	0.60
1:F:30:LEU:HD11	1:F:49:LEU:HG	1.84	0.60
1:F:125:GLU:N	1:F:125:GLU:OE2	2.33	0.60
1:O:214:ILE:O	1:O:214:ILE:HG22	2.00	0.60
1:B:270:LYS:HD3	1:B:326:TYR:OH	2.01	0.60
1:B:274:ILE:HG21	1:B:279:PHE:HB2	1.84	0.60
1:D:165:GLU:CG	1:D:195:LEU:HD11	2.31	0.60
1:H:303:GLN:N	1:H:303:GLN:OE1	2.34	0.60
1:C:230:VAL:HG12	1:C:248:PHE:HB3	1.84	0.60
1:C:358:GLU:HB2	1:C:361:GLN:HG2	1.82	0.60
1:D:3:LEU:HD12	1:D:3:LEU:C	2.26	0.60
1:G:356:MET:HG2	1:G:363:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:283:LEU:HD21	1:L:337:ALA:HB1	1.84	0.60
1:N:17:VAL:CG2	1:N:46:GLY:N	2.65	0.60
1:N:214:ILE:HG12	1:N:214:ILE:O	2.02	0.59
1:A:166:ILE:HG21	1:A:196:VAL:CG2	2.31	0.59
1:B:278:VAL:HB	1:B:322:LEU:HD11	1.84	0.59
1:C:187:LEU:HD12	1:C:187:LEU:C	2.27	0.59
1:K:111:LEU:HD23	1:L:316:ASP:CG	2.27	0.59
1:L:335:PHE:HB3	1:L:340:LEU:HD11	1.83	0.59
1:N:326:TYR:CE1	1:N:328:SER:HB2	2.37	0.59
1:L:166:ILE:HG12	1:L:196:VAL:HG22	1.83	0.59
1:N:291:ASN:HB3	1:N:294:LEU:HB2	1.84	0.59
1:B:97:ASP:N	1:B:97:ASP:OD1	2.27	0.59
1:K:18:VAL:O	1:K:21:VAL:HG12	2.02	0.59
1:D:150:MET:HE2	3:D:405:HOH:O	2.02	0.59
1:E:5:ILE:HG13	1:E:6:ALA:N	2.17	0.59
1:F:169:ASN:O	1:F:188:ALA:O	2.20	0.59
1:H:125:GLU:H	1:H:125:GLU:CD	2.09	0.59
1:O:207:GLU:HA	1:O:207:GLU:OE2	2.01	0.59
1:B:171:LEU:HB3	1:B:186:ILE:HD11	1.83	0.59
1:K:77:LEU:HD23	1:K:77:LEU:C	2.28	0.59
1:O:133:GLN:CB	1:O:218:GLN:NE2	2.62	0.59
1:B:30:LEU:HD21	1:B:120:PRO:HG2	1.84	0.59
1:E:321:ASP:C	1:E:322:LEU:HD12	2.28	0.59
1:N:131:GLN:HG3	1:N:220:THR:HG23	1.85	0.59
1:A:79:GLU:OE1	1:A:79:GLU:HA	2.02	0.59
1:A:269:ASP:O	1:A:271:HIS:HD2	1.86	0.59
1:H:278:VAL:HG12	1:H:322:LEU:HD23	1.84	0.59
1:H:378:MET:HB3	1:H:379:PRO:CD	2.28	0.59
1:K:35:ILE:HG22	1:K:37:THR:HG22	1.84	0.59
1:N:30:LEU:HD11	1:N:49:LEU:HG	1.85	0.59
1:F:270:LYS:HD3	1:F:326:TYR:OH	2.03	0.59
1:G:51:VAL:HG22	1:G:204:ALA:HB2	1.84	0.59
1:K:134:VAL:HG21	1:K:186:ILE:HD11	1.83	0.59
1:F:133:GLN:HB3	1:F:218:GLN:HE21	1.68	0.59
1:K:347:LEU:HD22	1:K:367:ASP:HB2	1.85	0.59
1:N:131:GLN:HG3	1:N:220:THR:CG2	2.33	0.59
1:O:196:VAL:HG12	1:O:197:GLN:N	2.16	0.59
1:L:135:THR:HG22	1:L:137:ARG:H	1.68	0.58
1:A:354:MET:HE3	1:A:363:VAL:HG11	1.85	0.58
1:H:183:LEU:HD23	1:H:183:LEU:C	2.28	0.58
1:I:39:ALA:HB1	1:I:61:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:43:THR:O	1:K:43:THR:HG22	2.02	0.58
1:K:357:THR:OG1	1:K:358:GLU:N	2.33	0.58
1:M:286:VAL:HG12	1:M:310:ALA:HB2	1.86	0.58
1:C:283:LEU:CD2	1:C:341:LEU:HG	2.32	0.58
1:O:133:GLN:CG	1:O:218:GLN:NE2	2.67	0.58
1:P:138:GLU:HB3	1:P:186:ILE:HG21	1.84	0.58
1:F:52:GLU:C	1:F:53:LEU:HD12	2.28	0.58
1:I:168:GLU:HG3	1:I:168:GLU:O	2.04	0.58
1:J:158:TYR:CE1	1:J:258:PRO:CD	2.86	0.58
1:O:159:LEU:HD13	1:O:177:ASP:HA	1.84	0.58
1:B:145:LYS:HD2	1:B:346:VAL:HG13	1.85	0.58
1:G:165:GLU:HG3	1:G:197:GLN:HG2	1.86	0.58
1:H:30:LEU:HD21	1:H:120:PRO:HG2	1.85	0.58
1:K:4:LYS:O	1:K:64:CYS:CB	2.51	0.58
1:O:317:GLU:HB3	1:P:110:VAL:HG22	1.85	0.58
1:C:132:VAL:HG22	1:C:166:ILE:HD12	1.84	0.58
1:J:23:ARG:HH22	1:J:75:ARG:HH11	1.52	0.58
1:L:64:CYS:SG	1:L:66:GLU:O	2.61	0.58
1:O:273:LEU:HG	1:O:353:ASN:OD1	2.04	0.58
1:P:223:ILE:HD12	1:P:228:LEU:HD13	1.84	0.58
1:A:96:GLU:OE1	1:A:96:GLU:N	2.23	0.58
1:D:90:ILE:HG22	1:D:92:LEU:CD1	2.34	0.58
1:H:364:LEU:HD11	1:H:374:THR:CG2	2.33	0.58
1:N:128:GLN:HE22	1:N:225:ARG:HE	1.50	0.58
1:N:133:GLN:HB2	1:N:189:SER:HB2	1.85	0.58
1:H:335:PHE:HZ	1:H:363:VAL:HG21	1.69	0.58
1:I:180:ARG:NH1	1:I:339:TYR:CE1	2.72	0.58
1:I:353:ASN:C	1:I:353:ASN:HD22	2.10	0.58
1:M:33:VAL:HG22	1:M:44:ILE:HG22	1.85	0.58
1:O:362:SER:OG	1:O:378:MET:HE1	2.03	0.58
1:I:134:VAL:HG12	1:I:188:ALA:HB1	1.85	0.58
1:K:291:ASN:HB3	1:K:294:LEU:HB2	1.86	0.58
1:P:136:GLN:HG2	1:P:219:LEU:CD1	2.29	0.58
1:D:381:ARG:CZ	1:D:381:ARG:HB2	2.33	0.57
1:M:167:ASP:HB3	1:M:172:ARG:HH12	1.68	0.57
1:B:289:LEU:HD22	1:B:289:LEU:N	2.19	0.57
1:D:381:ARG:HB2	1:D:381:ARG:NH2	2.19	0.57
1:M:12:ASN:ND2	1:M:241:GLN:NE2	2.51	0.57
1:M:214:ILE:H	1:M:214:ILE:CD1	2.16	0.57
1:O:17:VAL:HG21	1:O:46:GLY:H	1.66	0.57
1:E:97:ASP:OD1	1:E:97:ASP:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:ARG:HH12	1:J:75:ARG:NH1	2.02	0.57
1:J:304:ASP:HA	1:J:324:ILE:O	2.04	0.57
1:J:335:PHE:HZ	1:J:363:VAL:HG21	1.69	0.57
1:O:276:HIS:NE2	1:O:347:LEU:HD12	2.17	0.57
1:B:5:ILE:HG13	1:B:6:ALA:N	2.18	0.57
1:D:240:GLU:OE2	1:D:240:GLU:HA	2.04	0.57
1:D:266:ARG:HH22	1:O:300:ASN:ND2	2.03	0.57
1:H:299:LEU:HD13	1:H:335:PHE:HD2	1.69	0.57
1:K:85:PRO:HB3	1:L:281:GLN:HE22	1.69	0.57
1:L:283:LEU:HD22	1:L:341:LEU:CG	2.35	0.57
1:A:301:PHE:CZ	1:A:356:MET:HE1	2.39	0.57
1:D:183:LEU:C	1:D:183:LEU:HD23	2.29	0.57
1:A:304:ASP:HA	1:A:324:ILE:O	2.05	0.57
1:G:273:LEU:HD13	1:G:325:GLN:OE1	2.04	0.57
1:J:210:ARG:HB3	1:J:210:ARG:NH1	2.20	0.57
1:K:378[A]:MET:CE	1:K:379:PRO:HD2	2.35	0.57
1:N:17:VAL:O	1:N:17:VAL:HG22	2.03	0.57
1:N:301:PHE:O	1:N:330:PRO:HA	2.05	0.57
1:B:166:ILE:CD1	1:B:223:ILE:HD12	2.32	0.57
1:B:11:LEU:HD11	1:B:82:LYS:HG2	1.86	0.57
1:E:150:MET:HE1	1:E:202:ARG:HA	1.85	0.57
1:H:228:LEU:HD23	1:H:228:LEU:C	2.30	0.57
1:J:28:ASN:CG	1:L:28:ASN:HB3	2.30	0.57
1:J:58:ALA:HB3	1:J:241:GLN:HG3	1.87	0.57
1:L:350:ASP:O	1:L:351:ASP:CG	2.48	0.57
1:O:179:HIS:C	1:O:180:ARG:HG3	2.29	0.57
1:P:122:LEU:HD12	1:P:122:LEU:N	2.19	0.57
1:E:347:LEU:HD22	1:E:367:ASP:HB2	1.85	0.57
1:F:17:VAL:HG22	1:F:46:GLY:HA3	1.87	0.57
1:K:29:ILE:HG13	1:K:71:THR:HG21	1.87	0.57
1:N:95:THR:HG22	1:N:96:GLU:N	2.19	0.57
1:O:136:GLN:CA	1:O:219:LEU:CD1	2.80	0.57
1:O:138:GLU:CB	1:O:186:ILE:HG12	2.35	0.57
1:P:347:LEU:HD22	1:P:367:ASP:HB2	1.87	0.57
1:D:312:ASN:CB	1:D:313:PRO:CD	2.71	0.56
1:F:27:LEU:HD12	1:F:27:LEU:N	2.20	0.56
1:G:272:VAL:HG23	1:G:326:TYR:HB2	1.87	0.56
1:I:268:GLY:HA2	1:I:357:THR:HG22	1.85	0.56
1:J:156:ARG:HH12	1:K:154:ASP:HB2	1.70	0.56
1:P:131:GLN:HG3	1:P:220:THR:HG23	1.87	0.56
1:P:165:GLU:HG3	1:P:197:GLN:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:SER:HB3	1:E:194:GLN:HE22	1.69	0.56
1:F:18:VAL:CG2	1:F:78:MET:HE3	2.35	0.56
1:F:152:VAL:O	1:F:152:VAL:HG12	2.04	0.56
1:J:272:VAL:CG2	1:J:356:MET:HE1	2.35	0.56
1:M:331:LEU:HD23	1:M:356:MET:SD	2.45	0.56
1:O:55:ALA:HB2	1:O:246:VAL:HG22	1.87	0.56
1:P:145:LYS:HD2	1:P:373:GLN:OE1	2.05	0.56
1:A:166:ILE:HG22	1:A:196:VAL:CG2	2.35	0.56
1:B:327:GLN:HG3	1:B:327:GLN:O	2.04	0.56
1:D:4:LYS:NZ	1:D:89:LEU:CB	2.48	0.56
1:E:136:GLN:HG2	1:E:219:LEU:HD11	1.87	0.56
1:F:154:ASP:OD1	1:F:154:ASP:C	2.47	0.56
1:F:272:VAL:HG22	1:F:326:TYR:CD1	2.40	0.56
1:K:208:LEU:HD13	1:K:248:PHE:CD2	2.40	0.56
1:M:287:ALA:HB1	1:M:295:ARG:HH21	1.71	0.56
1:P:245:THR:HG23	1:P:245:THR:O	2.05	0.56
1:M:214:ILE:HG22	1:M:214:ILE:O	2.05	0.56
1:M:227:LEU:HD22	1:M:249:THR:HG22	1.87	0.56
1:E:273:LEU:CD2	1:J:187:LEU:HD12	2.35	0.56
1:I:136:GLN:HG2	1:I:219:LEU:HD11	1.88	0.56
1:K:227:LEU:HD23	1:K:249:THR:CG2	2.35	0.56
1:L:226:GLU:C	1:L:227:LEU:HD12	2.30	0.56
1:O:313:PRO:C	1:O:315:GLN:H	2.14	0.56
1:D:37:THR:HG22	1:D:64:CYS:SG	2.46	0.56
1:L:136:GLN:HG2	1:L:219:LEU:HG	1.87	0.56
1:E:162:THR:HG23	1:E:205:VAL:HG21	1.87	0.56
1:G:347:LEU:HD22	1:G:367:ASP:HB2	1.87	0.56
1:I:24:ARG:NH1	1:L:313:PRO:HG2	2.20	0.56
1:I:78:MET:HE1	1:I:82:LYS:HZ1	1.71	0.56
1:J:24:ARG:HH11	1:J:24:ARG:HB2	1.70	0.56
1:K:93:GLN:NE2	1:K:93:GLN:HA	2.20	0.56
1:P:32:ASN:HB3	1:P:71:THR:HG22	1.86	0.56
1:A:94:ILE:N	1:A:94:ILE:HD12	2.19	0.56
1:G:65:LEU:HD12	1:G:65:LEU:N	2.21	0.56
1:L:133:GLN:HB2	1:L:189:SER:HB2	1.87	0.56
1:O:163:LEU:HB3	1:O:174:VAL:CG1	2.33	0.56
1:D:220:THR:HG21	1:J:194:GLN:HG3	1.88	0.56
1:G:333:MET:HE1	1:G:363:VAL:CG2	2.36	0.56
1:M:90:ILE:HG22	1:M:92:LEU:HD12	1.86	0.56
1:N:162:THR:HB	1:N:200:VAL:HG23	1.87	0.56
1:B:17:VAL:CG2	1:B:46:GLY:N	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:36:GLN:HA	1:N:69:GLU:HG3	1.88	0.56
1:N:324:ILE:CD1	1:N:326:TYR:HB2	2.36	0.56
1:P:195:LEU:C	1:P:195:LEU:HD13	2.30	0.56
1:A:166:ILE:HG22	1:A:196:VAL:HG22	1.85	0.55
1:B:143:PHE:CE2	1:B:208:LEU:CD2	2.75	0.55
1:D:126:ASN:OD1	1:D:127:SER:N	2.39	0.55
1:G:132:VAL:CG1	1:G:191:THR:HG21	2.35	0.55
1:L:96:GLU:CD	1:L:96:GLU:H	2.13	0.55
1:L:297:VAL:CG1	1:L:337:ALA:HB2	2.36	0.55
1:N:125:GLU:HB2	1:N:128:GLN:HG3	1.87	0.55
1:O:158:TYR:CE1	1:O:258:PRO:HD3	2.40	0.55
1:A:1:MET:SD	1:A:37:THR:HG22	2.47	0.55
1:B:148:PHE:HE1	1:B:346:VAL:HG21	1.72	0.55
1:D:271:HIS:NE2	1:D:353:ASN:HB2	2.21	0.55
1:O:17:VAL:O	1:O:17:VAL:HG22	2.06	0.55
1:C:98:GLN:NE2	1:C:115:PRO:HD3	2.22	0.55
1:F:17:VAL:CG2	1:F:46:GLY:N	2.70	0.55
1:H:262:ARG:HH11	1:H:262:ARG:CB	2.19	0.55
1:J:30:LEU:HD11	1:J:49:LEU:HG	1.87	0.55
1:N:234:THR:N	1:N:235:PRO:CD	2.69	0.55
1:C:133:GLN:HG2	1:C:190:SER:HB2	1.88	0.55
1:E:136:GLN:NE2	1:E:232:ILE:HG23	2.21	0.55
1:I:78:MET:HE2	1:I:82:LYS:HD2	1.89	0.55
1:I:99:ARG:HH11	1:I:110:VAL:HG12	1.71	0.55
1:I:172:ARG:HD2	1:I:260:TYR:OH	2.06	0.55
1:I:98:GLN:HE22	1:I:114:LEU:C	2.14	0.55
1:N:362:SER:HA	1:N:379:PRO:HD3	1.89	0.55
1:C:172:ARG:HG2	1:C:185:GLU:HG2	1.89	0.55
1:K:59:LEU:N	1:K:59:LEU:HD12	2.20	0.55
1:N:14:LEU:HB3	1:N:78:MET:HE1	1.89	0.55
1:P:124:THR:HG22	1:P:227:LEU:CD1	2.36	0.55
1:C:329:ALA:CB	1:C:330:PRO:HD2	2.30	0.55
1:D:54:VAL:HG11	1:D:247:ARG:HH21	1.72	0.55
1:L:23:ARG:HB2	1:L:23:ARG:HH11	1.72	0.55
1:L:364:LEU:HD12	1:L:364:LEU:C	2.31	0.55
1:P:312:ASN:CB	1:P:313:PRO:CD	2.70	0.55
1:E:159:LEU:HD22	1:E:176:THR:HG23	1.87	0.55
1:N:326:TYR:CZ	1:N:328:SER:HB2	2.42	0.55
1:A:242:GLY:O	1:A:243:ASP:OD1	2.24	0.55
1:I:269:ASP:OD1	1:I:270:LYS:HG3	2.06	0.55
1:K:208:LEU:HD13	1:K:248:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:36:GLN:HG2	1:N:69:GLU:CD	2.31	0.55
1:N:306:LEU:HB2	1:N:324:ILE:HG21	1.89	0.55
1:P:14:LEU:HD23	1:P:44:ILE:HG21	1.88	0.55
1:D:54:VAL:HG11	1:D:247:ARG:NH2	2.23	0.54
1:G:230:VAL:HG12	1:G:231:THR:N	2.23	0.54
1:N:75:ARG:O	1:N:79:GLU:HG2	2.07	0.54
1:N:240:GLU:OE1	1:N:240:GLU:HA	2.07	0.54
1:A:49:LEU:HA	1:A:122:LEU:HD11	1.89	0.54
1:A:103:LYS:HE3	1:A:108:ARG:HH11	1.72	0.54
1:B:364:LEU:HD11	1:B:374:THR:CG2	2.37	0.54
1:L:301:PHE:N	1:L:331:LEU:O	2.31	0.54
1:O:133:GLN:CG	1:O:218:GLN:HE21	2.18	0.54
1:O:285:ARG:HG2	1:P:83:SER:HB2	1.89	0.54
1:C:131:GLN:CG	1:C:220:THR:HG23	2.37	0.54
1:K:335:PHE:HZ	1:K:363:VAL:HG21	1.72	0.54
1:P:223:ILE:CD1	1:P:228:LEU:HD13	2.37	0.54
1:B:158:TYR:C	1:B:158:TYR:CD1	2.85	0.54
1:H:158:TYR:CD1	1:H:158:TYR:C	2.85	0.54
1:L:298:PHE:CE1	1:L:334:SER:HB3	2.42	0.54
1:O:261:ARG:HD2	1:O:261:ARG:N	2.21	0.54
1:F:33:VAL:HG13	1:F:74:ALA:HB2	1.89	0.54
1:I:333:MET:HE1	1:I:363:VAL:CG2	2.37	0.54
1:K:45:THR:CG2	1:K:54:VAL:HG22	2.38	0.54
1:L:355:SER:HB2	1:L:364:LEU:HG	1.89	0.54
1:M:52:GLU:OE1	1:M:122:LEU:HD13	2.07	0.54
1:M:301:PHE:CD2	1:M:356:MET:HE1	2.41	0.54
1:I:309:ARG:HG3	1:I:319:ILE:HG12	1.89	0.54
1:P:7:LYS:HE2	1:P:85:PRO:O	2.06	0.54
1:E:243:ASP:OD1	1:E:243:ASP:C	2.51	0.54
1:L:199:ILE:HG21	1:L:253:ILE:HB	1.88	0.54
1:O:75:ARG:HD2	1:O:78:MET:HE2	1.88	0.54
1:C:33:VAL:HG22	1:C:44:ILE:CG2	2.38	0.54
1:L:248:PHE:CD1	1:L:248:PHE:C	2.85	0.54
1:L:335:PHE:CB	1:L:340:LEU:HD11	2.38	0.54
1:O:298:PHE:HD1	1:O:334:SER:HB2	1.73	0.54
1:B:17:VAL:HG22	1:B:46:GLY:HA3	1.89	0.54
1:B:286:VAL:HG21	1:B:308:LEU:CB	2.38	0.54
1:D:150:MET:HE3	1:D:161:GLY:HA2	1.89	0.54
1:D:230:VAL:HG12	1:D:248:PHE:HB3	1.88	0.54
1:F:14:LEU:HB3	1:F:78:MET:SD	2.47	0.54
1:L:329:ALA:HB1	1:L:330:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:362:SER:OG	1:O:378:MET:CE	2.56	0.54
1:B:257:PHE:CG	1:B:258:PRO:HD2	2.40	0.54
1:C:335:PHE:HZ	1:C:363:VAL:CG2	2.20	0.54
1:F:65:LEU:HD12	1:F:65:LEU:N	2.23	0.54
1:G:172:ARG:CG	1:G:183:LEU:HD11	2.37	0.54
1:L:65:LEU:CD1	1:L:65:LEU:H	2.21	0.54
1:L:166:ILE:O	1:L:166:ILE:HG13	2.08	0.54
1:L:299:LEU:HD12	1:L:299:LEU:N	2.24	0.54
1:B:26:THR:HB	1:O:314:GLU:CD	2.33	0.53
1:C:79:GLU:OE1	1:C:79:GLU:HA	2.08	0.53
1:D:9:SER:O	1:D:13:VAL:HG23	2.08	0.53
1:H:377:VAL:HG23	1:H:377:VAL:O	2.08	0.53
1:J:195:LEU:HD23	1:J:195:LEU:O	2.07	0.53
1:M:131:GLN:HG3	1:M:220:THR:HG23	1.90	0.53
1:O:130:THR:N	1:O:223:ILE:O	2.41	0.53
1:O:361:GLN:OE1	1:O:361:GLN:HA	2.07	0.53
1:E:94:ILE:HD12	1:E:94:ILE:N	2.22	0.53
1:F:131:GLN:HG3	1:F:220:THR:HG23	1.91	0.53
1:N:90:ILE:HG23	1:N:102:LEU:CD2	2.39	0.53
1:A:61:GLU:OE2	1:A:61:GLU:N	2.25	0.53
1:A:217:GLU:CD	1:A:218:GLN:O	2.51	0.53
1:B:172:ARG:HD3	1:B:183:LEU:HD11	1.91	0.53
1:C:16:HIS:O	1:C:53:LEU:HD13	2.08	0.53
1:C:49:LEU:HD13	1:C:122:LEU:HD11	1.90	0.53
1:I:285:ARG:NH2	1:I:320:GLU:OE2	2.36	0.53
1:O:196:VAL:CG1	1:O:197:GLN:N	2.70	0.53
1:E:96:GLU:OE1	1:E:96:GLU:HA	2.08	0.53
1:J:158:TYR:CE1	1:J:258:PRO:HD3	2.44	0.53
1:N:131:GLN:NE2	1:N:220:THR:HG23	2.24	0.53
1:A:364:LEU:HD21	1:A:374:THR:HG23	1.90	0.53
1:I:156:ARG:HH11	1:L:262:ARG:NH2	2.05	0.53
1:A:102:LEU:HD23	1:A:102:LEU:C	2.34	0.53
1:A:335:PHE:HZ	1:A:363:VAL:HG21	1.73	0.53
1:J:3:LEU:HD12	1:J:63:ALA:O	2.09	0.53
1:M:320:GLU:OE1	1:N:107:SER:HB3	2.08	0.53
1:N:235:PRO:HG3	1:N:243:ASP:CB	2.37	0.53
1:A:301:PHE:O	1:A:330:PRO:HA	2.09	0.53
1:B:155:VAL:HB	1:O:153:GLN:HE21	1.73	0.53
1:E:2:ARG:HG2	1:E:65:LEU:HB2	1.91	0.53
1:F:18:VAL:CG2	1:F:78:MET:CE	2.87	0.53
1:N:272:VAL:CG2	1:N:356:MET:HE1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:CG2	1:B:279:PHE:HB2	2.39	0.53
1:C:33:VAL:CG2	1:C:44:ILE:CG2	2.86	0.53
1:E:77:LEU:HD21	1:E:102:LEU:HD21	1.91	0.53
1:E:271:HIS:HD2	1:J:216:ASP:CB	2.19	0.53
1:H:34:LYS:HE2	1:H:36:GLN:HE21	1.74	0.53
1:D:150:MET:HE1	1:D:202:ARG:HA	1.91	0.53
1:F:124:THR:CG2	1:F:227:LEU:HD12	2.38	0.53
1:L:3:LEU:HD11	1:L:37:THR:HG21	1.90	0.53
1:M:312:ASN:CB	1:M:313:PRO:CD	2.72	0.53
1:N:131:GLN:HE21	1:N:220:THR:HG23	1.73	0.53
1:O:57:THR:HG23	1:O:57:THR:O	2.08	0.53
1:G:372:ASP:OD1	1:G:372:ASP:N	2.33	0.53
1:M:347:LEU:HD22	1:M:367:ASP:HB2	1.91	0.53
1:N:171:LEU:HB3	1:N:186:ILE:HD11	1.91	0.53
1:E:285:ARG:HD3	1:F:84:LEU:HD23	1.90	0.52
1:M:176:THR:HG23	1:M:180:ARG:O	2.09	0.52
1:P:272:VAL:HG23	1:P:356:MET:HE2	1.91	0.52
1:A:17:VAL:CG2	1:A:46:GLY:HA3	2.39	0.52
1:B:37:THR:HG22	1:B:42:LEU:HD12	1.91	0.52
1:B:335:PHE:CZ	1:B:363:VAL:HG21	2.45	0.52
1:B:361:GLN:OE1	1:B:361:GLN:HA	2.10	0.52
1:N:268:GLY:HA2	1:N:357:THR:HG22	1.92	0.52
1:C:129:GLY:HA3	1:C:222:LEU:HD11	1.91	0.52
1:C:272:VAL:HG21	1:C:301:PHE:CE1	2.44	0.52
1:I:228:LEU:HB3	1:I:250:THR:HG22	1.91	0.52
1:K:183:LEU:HD23	1:K:183:LEU:C	2.35	0.52
1:P:361:GLN:OE1	1:P:361:GLN:HA	2.09	0.52
1:C:282:SER:OG	1:C:322:LEU:CD1	2.57	0.52
1:F:59:LEU:CD1	1:F:63:ALA:HB3	2.38	0.52
1:G:65:LEU:N	1:G:65:LEU:CD1	2.72	0.52
1:G:272:VAL:HG12	1:G:354:MET:HB2	1.91	0.52
1:I:272:VAL:HG22	1:I:326:TYR:CD1	2.44	0.52
1:K:59:LEU:HD12	1:K:59:LEU:O	2.09	0.52
1:E:4:LYS:NZ	1:E:4:LYS:CB	2.73	0.52
1:E:214:ILE:HG22	1:E:214:ILE:O	2.09	0.52
1:E:235:PRO:HD3	3:E:418:HOH:O	2.09	0.52
1:G:378:MET:SD	1:G:379:PRO:HD2	2.50	0.52
1:N:36:GLN:CG	1:N:69:GLU:HG2	2.19	0.52
1:A:45:THR:HG23	1:A:54:VAL:HG22	1.91	0.52
1:H:1:MET:HE2	1:H:70:THR:CG2	2.34	0.52
1:I:282:SER:OG	1:I:322:LEU:HD11	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:353:ASN:O	1:I:353:ASN:ND2	2.43	0.52
1:M:291:ASN:HB3	1:M:294:LEU:HB2	1.91	0.52
1:P:122:LEU:N	1:P:122:LEU:CD1	2.73	0.52
1:A:166:ILE:HD11	1:A:190:SER:HB3	1.91	0.52
1:B:274:ILE:HG22	1:B:275:GLY:O	2.10	0.52
1:H:2:ARG:CG	1:H:93:GLN:NE2	2.71	0.52
1:I:285:ARG:HG2	1:J:83:SER:HB2	1.92	0.52
1:M:356:MET:HG2	1:M:363:VAL:HG22	1.91	0.52
1:H:77:LEU:HD11	1:H:102:LEU:HD21	1.91	0.52
1:J:241:GLN:OE1	1:J:241:GLN:HA	2.09	0.52
1:L:210:ARG:HG2	1:L:210:ARG:HH11	1.74	0.52
1:N:246:VAL:HG13	1:N:246:VAL:O	2.10	0.52
1:B:132:VAL:HG21	1:B:166:ILE:HG12	1.91	0.52
1:C:75:ARG:O	1:C:79:GLU:HG2	2.10	0.52
1:F:50:GLU:HG3	1:F:156:ARG:HH21	1.75	0.52
1:F:59:LEU:CG	1:F:63:ALA:HB3	2.40	0.52
1:L:367:ASP:CG	1:L:368:PRO:HD2	2.33	0.52
1:M:272:VAL:HG22	1:M:326:TYR:HD1	1.69	0.52
1:O:358:GLU:HA	1:O:358:GLU:OE2	2.09	0.52
1:O:372:ASP:OD1	1:O:372:ASP:N	2.36	0.52
1:F:14:LEU:HD13	1:F:78:MET:SD	2.50	0.52
1:J:24:ARG:HB2	1:J:24:ARG:NH1	2.24	0.52
1:L:23:ARG:HB2	1:L:23:ARG:NH1	2.25	0.52
1:L:299:LEU:N	1:L:299:LEU:CD1	2.73	0.52
1:A:257:PHE:CG	1:A:258:PRO:HD2	2.44	0.51
1:E:72:VAL:CG1	1:E:73:PRO:HD2	2.39	0.51
1:K:195:LEU:N	1:K:195:LEU:CD1	2.73	0.51
1:N:235:PRO:HG3	1:N:243:ASP:CA	2.40	0.51
1:O:257:PHE:CG	1:O:258:PRO:HD2	2.44	0.51
1:B:194:GLN:H	1:B:194:GLN:CD	2.18	0.51
1:P:25:HIS:CE1	1:P:30:LEU:HD12	2.44	0.51
1:A:347:LEU:HD22	1:A:367:ASP:HB2	1.92	0.51
1:B:325:GLN:O	1:B:325:GLN:HG2	2.10	0.51
1:F:172:ARG:HD3	1:F:183:LEU:HD11	1.91	0.51
1:G:22:GLU:HG3	1:G:203:LYS:NZ	2.25	0.51
1:P:14:LEU:HB3	1:P:78:MET:HE1	1.92	0.51
1:A:294:LEU:HD12	1:A:294:LEU:N	2.26	0.51
1:A:306:LEU:HB2	1:A:324:ILE:HD13	1.93	0.51
1:D:159:LEU:HD22	1:D:176:THR:HG23	1.93	0.51
1:E:187:LEU:HD23	1:E:187:LEU:C	2.36	0.51
1:E:239:LYS:HG3	1:E:239:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:334:SER:C	1:H:380:MET:HG2	2.35	0.51
1:L:136:GLN:HG2	1:L:219:LEU:CG	2.41	0.51
1:M:122:LEU:HD23	1:M:227:LEU:HD21	1.92	0.51
1:C:145:LYS:HD3	1:C:346:VAL:CG2	2.40	0.51
1:F:138:GLU:HB3	1:F:186:ILE:HG12	1.93	0.51
1:F:146:THR:HG22	1:F:175:THR:HG23	1.91	0.51
1:J:126:ASN:OD1	1:J:226:GLU:CG	2.53	0.51
1:K:65:LEU:N	1:K:65:LEU:CD1	2.73	0.51
1:N:45:THR:HG23	1:N:54:VAL:HG22	1.92	0.51
1:E:294:LEU:N	1:E:294:LEU:CD1	2.73	0.51
1:K:312:ASN:HB2	1:K:313:PRO:HD2	1.92	0.51
1:M:18:VAL:HG22	1:M:18:VAL:O	2.11	0.51
1:B:211:LEU:HD21	1:B:246:VAL:HG11	1.92	0.51
1:L:186:ILE:HD12	1:L:187:LEU:H	1.75	0.51
1:N:131:GLN:HE21	1:N:220:THR:CG2	2.24	0.51
1:B:18:VAL:O	1:B:18:VAL:CG2	2.59	0.51
1:D:98:GLN:NE2	1:D:115:PRO:HD3	2.26	0.51
1:E:165:GLU:HG3	1:E:197:GLN:HG2	1.93	0.51
1:H:10:LEU:HD23	1:H:10:LEU:C	2.32	0.51
1:K:35:ILE:HG21	1:K:37:THR:HG22	1.90	0.51
1:N:268:GLY:HA2	1:N:357:THR:CG2	2.41	0.51
1:O:8:GLU:OE1	1:O:8:GLU:N	2.37	0.51
1:A:18:VAL:HG11	1:A:78:MET:HG3	1.91	0.51
1:A:33:VAL:CG2	1:A:44:ILE:HG22	2.40	0.51
1:A:289:LEU:HD22	1:A:316:ASP:HB3	1.93	0.51
1:D:156:ARG:CZ	1:D:159:LEU:HD11	2.41	0.51
1:E:320:GLU:HG3	1:F:106:ASN:O	2.11	0.51
1:K:248:PHE:CE1	1:K:250:THR:OG1	2.62	0.51
1:P:228:LEU:HD12	1:P:229:ASN:N	2.26	0.51
1:A:257:PHE:CD2	1:A:258:PRO:HD2	2.46	0.50
1:E:268:GLY:HA2	1:E:357:THR:HG23	1.93	0.50
1:I:78:MET:HE1	1:I:82:LYS:NZ	2.25	0.50
1:J:136:GLN:NE2	1:J:232:ILE:HG23	2.25	0.50
1:O:32:ASN:HB3	1:O:72:VAL:O	2.10	0.50
1:O:333:MET:HG2	1:O:359:ALA:HA	1.92	0.50
1:P:297:VAL:HG22	1:P:310:ALA:HB2	1.93	0.50
1:G:92:LEU:HD21	1:G:102:LEU:HD21	1.93	0.50
1:G:166:ILE:HG23	1:G:166:ILE:O	2.12	0.50
1:L:163:LEU:HD23	1:L:199:ILE:HG12	1.93	0.50
1:N:286:VAL:HG12	1:N:310:ALA:HB2	1.94	0.50
1:G:139:LEU:HD23	1:G:212:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:158:TYR:CE1	1:I:258:PRO:HD3	2.46	0.50
1:L:79:GLU:OE1	1:L:79:GLU:HA	2.11	0.50
1:F:117:GLU:H	1:F:117:GLU:CD	2.19	0.50
1:K:42:LEU:N	1:K:42:LEU:CD1	2.73	0.50
1:M:138:GLU:HB3	1:M:186:ILE:HG12	1.94	0.50
1:B:257:PHE:CG	1:B:258:PRO:CD	2.95	0.50
1:C:306:LEU:HB2	1:C:324:ILE:HD13	1.92	0.50
1:K:273:LEU:HG	1:K:353:ASN:OD1	2.11	0.50
1:N:158:TYR:CE1	1:N:258:PRO:HD3	2.47	0.50
1:B:191:THR:O	1:J:222:LEU:CD2	2.59	0.50
1:B:272:VAL:HG22	1:B:326:TYR:CD1	2.47	0.50
1:L:18:VAL:HG21	1:L:78:MET:HE3	1.94	0.50
1:B:2:ARG:NH1	1:B:93:GLN:OE1	2.44	0.50
1:B:165:GLU:HG3	1:B:197:GLN:HG2	1.93	0.50
1:D:312:ASN:HB2	1:D:313:PRO:HD3	1.87	0.50
1:G:1:MET:HE2	1:G:94:ILE:HD13	1.94	0.50
1:H:134:VAL:CG2	1:H:186:ILE:CD1	2.90	0.50
1:O:145:LYS:HD3	1:O:346:VAL:CG2	2.30	0.50
1:G:10:LEU:HD12	1:G:10:LEU:O	2.12	0.50
1:K:272:VAL:HG22	1:K:326:TYR:CD1	2.46	0.50
1:N:17:VAL:HG22	1:N:46:GLY:HA3	1.93	0.50
1:N:272:VAL:O	1:N:353:ASN:HA	2.12	0.50
1:D:133:GLN:HB2	1:D:190:SER:HB2	1.93	0.50
1:E:166:ILE:HG23	1:E:166:ILE:O	2.11	0.50
1:H:42:LEU:CB	1:H:59:LEU:HD11	2.42	0.50
1:I:268:GLY:O	1:I:271:HIS:NE2	2.45	0.50
1:I:347:LEU:HD22	1:I:367:ASP:HB2	1.94	0.50
1:K:65:LEU:HD13	1:K:65:LEU:C	2.37	0.50
1:K:101:ILE:HD13	1:K:110:VAL:HG13	1.92	0.50
1:L:133:GLN:OE1	1:L:218:GLN:OE1	2.29	0.50
1:L:135:THR:HG22	1:L:137:ARG:N	2.27	0.50
1:M:228:LEU:HB3	1:M:250:THR:HG22	1.94	0.50
1:I:1:MET:HG2	1:I:3:LEU:HD22	1.94	0.49
1:J:260:TYR:CE1	1:J:261:ARG:HD2	2.47	0.49
1:K:111:LEU:HD23	1:L:316:ASP:OD2	2.12	0.49
1:L:322:LEU:HD12	1:L:322:LEU:C	2.36	0.49
1:N:33:VAL:CG2	1:N:74:ALA:CB	2.84	0.49
1:A:268:GLY:O	1:A:271:HIS:NE2	2.44	0.49
1:E:94:ILE:N	1:E:94:ILE:CD1	2.75	0.49
1:G:312:ASN:CB	1:G:313:PRO:CD	2.83	0.49
1:J:150:MET:HB2	1:J:202:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:301:PHE:CD2	1:L:356:MET:SD	3.05	0.49
1:O:34:LYS:HB3	1:O:45:THR:HG22	1.93	0.49
1:O:145:LYS:CD	1:O:346:VAL:HG22	2.31	0.49
1:C:282:SER:OG	1:C:322:LEU:HD11	2.12	0.49
1:E:214:ILE:N	1:E:214:ILE:CD1	2.73	0.49
1:F:41:ALA:HB2	1:H:40:GLN:HB3	1.93	0.49
1:J:183:LEU:HD23	1:J:183:LEU:C	2.36	0.49
1:K:201:PRO:HG2	1:K:250:THR:CG2	2.43	0.49
1:M:248:PHE:C	1:M:248:PHE:CD1	2.89	0.49
1:A:282:SER:CB	1:A:322:LEU:HD11	2.42	0.49
1:G:214:ILE:O	1:G:214:ILE:HG13	2.12	0.49
1:K:77:LEU:C	1:K:77:LEU:CD2	2.85	0.49
1:N:131:GLN:CG	1:N:220:THR:CG2	2.89	0.49
1:B:317:GLU:OE2	1:B:319:ILE:HD11	2.12	0.49
1:C:335:PHE:CZ	1:C:363:VAL:HG21	2.46	0.49
1:F:3:LEU:HD12	1:F:63:ALA:O	2.12	0.49
1:F:75:ARG:O	1:F:79:GLU:HG3	2.13	0.49
1:M:150:MET:HE3	1:M:161:GLY:HA2	1.95	0.49
1:N:235:PRO:HG3	1:N:243:ASP:HA	1.94	0.49
1:N:335:PHE:HZ	1:N:363:VAL:CG1	2.25	0.49
1:O:34:LYS:HB3	1:O:45:THR:CG2	2.43	0.49
1:O:289:LEU:HD12	1:O:318:ALA:HB2	1.94	0.49
1:B:335:PHE:CE1	1:B:363:VAL:HG21	2.47	0.49
1:D:266:ARG:CG	1:D:266:ARG:NH1	2.72	0.49
1:L:51:VAL:HG22	1:L:204:ALA:HB2	1.94	0.49
1:O:131:GLN:HA	1:O:221:LEU:O	2.11	0.49
1:D:202:ARG:O	1:D:202:ARG:HD2	2.12	0.49
1:I:172:ARG:HG3	1:I:185:GLU:HG2	1.93	0.49
1:J:272:VAL:HG23	1:J:356:MET:HE1	1.93	0.49
1:F:18:VAL:CB	1:F:78:MET:HE3	2.43	0.49
1:K:122:LEU:HB3	1:K:227:LEU:HD21	1.95	0.49
1:L:137:ARG:HB2	1:L:214:ILE:O	2.12	0.49
1:I:166:ILE:HG22	1:I:196:VAL:H	1.78	0.49
1:I:195:LEU:HD22	1:I:195:LEU:C	2.36	0.49
1:I:230:VAL:HG12	1:I:248:PHE:HB3	1.95	0.49
1:K:204:ALA:CB	1:K:250:THR:HG21	2.42	0.49
1:L:136:GLN:HG2	1:L:219:LEU:HD11	1.95	0.49
1:L:163:LEU:HB3	1:L:174:VAL:HG13	1.94	0.49
1:B:186:ILE:C	1:B:186:ILE:HD12	2.38	0.49
1:B:274:ILE:HG12	1:B:324:ILE:CG2	2.34	0.49
1:D:32:ASN:ND2	1:D:114:LEU:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:GLN:HG3	1:F:101:ILE:HB	1.95	0.49
1:H:134:VAL:HG22	1:H:138:GLU:HB2	1.95	0.49
1:I:24:ARG:HH12	1:L:313:PRO:HG2	1.77	0.49
1:K:59:LEU:HD12	1:K:59:LEU:H	1.78	0.49
1:M:59:LEU:HD22	1:M:63:ALA:CB	2.43	0.49
1:P:59:LEU:HD13	1:P:64:CYS:HB2	1.95	0.49
1:A:306:LEU:HB3	1:A:322:LEU:HB2	1.95	0.48
1:D:3:LEU:C	1:D:3:LEU:CD1	2.85	0.48
1:F:32:ASN:HB2	1:F:71:THR:CG2	2.42	0.48
1:K:301:PHE:CD2	1:K:356:MET:HE1	2.47	0.48
1:O:92:LEU:HG	1:O:102:LEU:HD22	1.95	0.48
1:B:227:LEU:HD23	1:B:251:LYS:HA	1.95	0.48
1:D:306:LEU:HB2	1:D:324:ILE:HD13	1.95	0.48
1:K:75:ARG:NH1	1:K:79:GLU:HG3	2.28	0.48
1:K:80:ILE:HG21	1:K:102:LEU:HD21	1.95	0.48
1:N:312:ASN:CB	1:N:313:PRO:CD	2.90	0.48
1:C:2:ARG:HG2	1:C:65:LEU:HD12	1.94	0.48
1:F:32:ASN:HB3	1:F:71:THR:HG22	1.94	0.48
1:H:1:MET:CE	1:H:70:THR:HG21	2.40	0.48
1:H:150:MET:HG3	1:H:175:THR:CG2	2.42	0.48
1:J:367:ASP:OD2	1:J:370:HIS:CD2	2.66	0.48
1:M:90:ILE:CG2	1:M:92:LEU:HD11	2.43	0.48
1:B:136:GLN:HG2	1:B:219:LEU:CD1	2.44	0.48
1:K:45:THR:HG22	1:K:54:VAL:HG22	1.95	0.48
1:O:222:LEU:C	1:O:222:LEU:CD2	2.85	0.48
1:A:16:HIS:O	1:A:53:LEU:HD23	2.14	0.48
1:A:282:SER:HB3	1:A:322:LEU:HD11	1.96	0.48
1:D:289:LEU:N	1:D:289:LEU:HD12	2.29	0.48
1:E:150:MET:HE2	1:E:202:ARG:HD2	1.95	0.48
1:L:297:VAL:HG13	1:L:337:ALA:HB2	1.95	0.48
1:O:298:PHE:CD1	1:O:334:SER:HB2	2.48	0.48
1:C:33:VAL:CG2	1:C:44:ILE:HG22	2.43	0.48
1:C:183:LEU:HD23	1:C:183:LEU:C	2.39	0.48
1:D:2:ARG:HA	1:D:92:LEU:O	2.13	0.48
1:E:4:LYS:NZ	1:E:4:LYS:HB2	2.29	0.48
1:E:273:LEU:HG	1:E:353:ASN:OD1	2.13	0.48
1:H:322:LEU:N	1:H:322:LEU:CD1	2.75	0.48
1:J:37:THR:HG22	1:J:42:LEU:HD12	1.94	0.48
1:J:181:LEU:HD13	1:J:263:VAL:HG21	1.96	0.48
1:O:145:LYS:HA	1:O:346:VAL:HG21	1.95	0.48
1:P:360:ASN:O	1:P:379:PRO:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:HD12	3:B:409:HOH:O	2.14	0.48
1:E:150:MET:HE1	1:E:202:ARG:CA	2.43	0.48
1:K:159:LEU:HD22	1:K:176:THR:HG23	1.96	0.48
1:O:353:ASN:HD22	1:O:368:PRO:HG3	1.78	0.48
1:A:17:VAL:HG22	1:A:17:VAL:O	2.14	0.48
1:A:290:SER:HB3	1:A:310:ALA:HB1	1.95	0.48
1:B:304:ASP:HA	1:B:324:ILE:O	2.14	0.48
1:E:272:VAL:HG21	1:E:301:PHE:CE1	2.48	0.48
1:I:136:GLN:HG2	1:I:219:LEU:CD1	2.44	0.48
1:L:163:LEU:HD13	1:L:163:LEU:C	2.38	0.48
1:A:78:MET:HE3	1:A:78:MET:C	2.39	0.48
1:A:222:LEU:HD12	1:A:229:ASN:HB3	1.96	0.48
1:B:309:ARG:NH2	1:B:332:GLU:OE2	2.46	0.48
1:C:49:LEU:HD13	1:C:49:LEU:O	2.14	0.48
1:C:169:ASN:H	1:C:191:THR:CG2	2.25	0.48
1:D:132:VAL:HA	1:D:190:SER:O	2.12	0.48
1:H:10:LEU:C	1:H:10:LEU:CD2	2.86	0.48
1:H:240:GLU:OE1	1:H:240:GLU:HA	2.13	0.48
1:L:163:LEU:CD2	1:L:199:ILE:HG12	2.44	0.48
1:M:262:ARG:NH1	1:M:262:ARG:CG	2.73	0.48
1:O:99:ARG:HA	1:O:111:LEU:O	2.13	0.48
1:O:226:GLU:O	1:O:226:GLU:HG2	2.13	0.48
1:P:303:GLN:N	1:P:303:GLN:CD	2.72	0.48
1:D:165:GLU:HG3	1:D:197:GLN:HG2	1.96	0.48
1:D:266:ARG:NH2	1:O:300:ASN:ND2	2.61	0.48
1:E:230:VAL:HG12	1:E:248:PHE:HB3	1.96	0.48
1:J:27:LEU:HG	1:J:29:ILE:HG22	1.94	0.48
1:K:210:ARG:HH11	1:K:210:ARG:HG3	1.79	0.48
1:K:297:VAL:HG12	1:K:310:ALA:HB2	1.95	0.48
1:N:2:ARG:HG2	1:N:65:LEU:HB3	1.95	0.48
1:O:77:LEU:CD1	1:O:102:LEU:HD11	2.44	0.48
1:O:143:PHE:HE2	1:O:208:LEU:HD13	1.79	0.48
1:O:301:PHE:CE1	1:O:356:MET:HE3	2.49	0.48
1:F:257:PHE:CG	1:F:258:PRO:HD2	2.49	0.47
1:A:154:ASP:OD1	1:P:158:TYR:OH	2.31	0.47
1:D:187:LEU:C	1:D:187:LEU:CD1	2.85	0.47
1:K:312:ASN:HB2	1:K:313:PRO:CD	2.44	0.47
1:E:32:ASN:HB3	1:E:71:THR:HG22	1.96	0.47
1:F:153:GLN:HE21	1:F:153:GLN:CA	2.19	0.47
1:H:303:GLN:N	1:H:303:GLN:CD	2.72	0.47
1:I:353:ASN:C	1:I:353:ASN:ND2	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:303:GLN:NE2	1:L:303:GLN:HA	2.30	0.47
1:N:343:VAL:HG23	1:N:375:TYR:CD2	2.48	0.47
1:O:83:SER:HB3	1:P:288:ILE:HD11	1.96	0.47
1:A:248:PHE:CD1	1:A:248:PHE:C	2.92	0.47
1:B:24:ARG:NH2	1:P:26:THR:HA	2.29	0.47
1:C:131:GLN:CD	1:C:220:THR:HG21	2.39	0.47
1:F:92:LEU:HD23	1:F:102:LEU:HG	1.95	0.47
1:H:152:VAL:HG23	1:H:152:VAL:O	2.14	0.47
1:J:372:ASP:OD1	1:J:372:ASP:N	2.45	0.47
1:K:84:LEU:HB3	1:K:85:PRO:HD2	1.95	0.47
1:K:330:PRO:CG	1:O:267:GLY:HA3	2.44	0.47
1:N:230:VAL:HG13	1:N:248:PHE:HB3	1.96	0.47
1:O:98:GLN:HG3	1:O:113:THR:OG1	2.14	0.47
1:O:248:PHE:C	1:O:248:PHE:CD1	2.92	0.47
1:P:167:ASP:HB2	1:P:195:LEU:CD2	2.27	0.47
1:E:134:VAL:HG21	1:E:186:ILE:HD11	1.96	0.47
1:G:333:MET:HE1	1:G:363:VAL:HG23	1.95	0.47
1:I:98:GLN:NE2	1:I:114:LEU:CA	2.78	0.47
1:I:312:ASN:CB	1:I:313:PRO:CD	2.84	0.47
1:J:308:LEU:CD1	1:J:322:LEU:HD22	2.41	0.47
1:L:92:LEU:HD23	1:L:102:LEU:HG	1.95	0.47
1:N:148:PHE:HE1	1:N:346:VAL:HG11	1.76	0.47
1:O:212:LEU:HD23	1:O:232:ILE:HD13	1.97	0.47
1:C:270:LYS:H	1:C:270:LYS:CD	2.01	0.47
1:D:33:VAL:HG13	1:D:74:ALA:HB2	1.96	0.47
1:F:163:LEU:HD22	1:F:257:PHE:CD1	2.50	0.47
1:G:94:ILE:HD12	1:G:94:ILE:N	2.29	0.47
1:H:138:GLU:HB3	1:H:186:ILE:CD1	2.43	0.47
1:K:322:LEU:HD23	3:K:405:HOH:O	2.13	0.47
1:L:289:LEU:CD1	1:L:318:ALA:HB2	2.41	0.47
1:M:89:LEU:N	1:M:89:LEU:CD1	2.77	0.47
1:N:65:LEU:HD13	1:N:65:LEU:C	2.38	0.47
1:O:135:THR:C	1:O:219:LEU:HD12	2.39	0.47
1:P:300:ASN:HB3	1:P:307:GLN:HB3	1.96	0.47
1:D:266:ARG:HH11	1:D:266:ARG:HG3	1.79	0.47
1:E:145:LYS:O	1:E:148:PHE:HE1	1.98	0.47
1:E:354:MET:HE2	1:E:363:VAL:HG11	1.96	0.47
1:J:4:LYS:HG3	1:J:4:LYS:O	2.15	0.47
1:K:36:GLN:HB2	1:K:43:THR:HG21	1.97	0.47
1:N:305:SER:C	1:N:324:ILE:HG12	2.39	0.47
1:O:94:ILE:CD1	1:O:100:CYS:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:314:GLU:OE1	1:O:314:GLU:N	2.43	0.47
1:B:96:GLU:OE1	1:B:96:GLU:HA	2.14	0.47
1:B:303:GLN:N	1:B:303:GLN:CD	2.72	0.47
1:C:327:GLN:CD	1:C:327:GLN:H	2.23	0.47
1:C:358:GLU:HB2	1:C:361:GLN:CG	2.44	0.47
1:M:3:LEU:HD13	1:M:37:THR:HG21	1.97	0.47
1:N:364:LEU:HD11	1:N:374:THR:HG23	1.96	0.47
1:D:37:THR:HG22	1:D:38:ASN:N	2.29	0.47
1:D:307:GLN:HG3	1:D:321:ASP:OD1	2.14	0.47
1:J:11:LEU:HD12	1:J:78:MET:SD	2.55	0.47
1:M:128:GLN:H	1:M:128:GLN:HG3	1.50	0.47
1:N:228:LEU:HD23	1:N:228:LEU:C	2.39	0.47
1:P:72:VAL:CG1	1:P:73:PRO:HD2	2.44	0.47
1:P:272:VAL:CG1	1:P:324:ILE:HD12	2.45	0.47
1:B:306:LEU:HB2	1:B:324:ILE:HD13	1.97	0.47
1:F:0:HIS:ND1	1:F:0:HIS:N	2.63	0.47
1:I:98:GLN:NE2	1:I:114:LEU:HA	2.30	0.47
1:J:221:LEU:HD23	1:J:230:VAL:HB	1.96	0.47
1:O:364:LEU:HD12	1:O:364:LEU:C	2.39	0.47
1:P:100:CYS:HB2	1:P:113:THR:CG2	2.45	0.47
1:B:278:VAL:HB	1:B:322:LEU:CD1	2.44	0.46
1:F:126:ASN:HD22	1:F:126:ASN:N	2.13	0.46
1:F:230:VAL:HG12	1:F:248:PHE:HB3	1.97	0.46
1:G:194:GLN:HB3	1:G:195:LEU:HD12	1.96	0.46
1:G:273:LEU:HB3	1:G:325:GLN:OE1	2.16	0.46
1:I:335:PHE:CZ	1:I:363:VAL:HG21	2.36	0.46
1:L:137:ARG:CB	1:L:215:GLU:HA	2.21	0.46
1:N:187:LEU:C	1:N:187:LEU:CD1	2.85	0.46
1:N:272:VAL:HG23	1:N:356:MET:HE1	1.97	0.46
1:A:289:LEU:HD22	1:A:316:ASP:CB	2.46	0.46
1:B:155:VAL:H	1:O:153:GLN:NE2	2.13	0.46
1:B:158:TYR:HB2	1:B:199:ILE:HD13	1.97	0.46
1:C:346:VAL:HG22	1:C:346:VAL:O	2.15	0.46
1:E:364:LEU:HD11	1:E:374:THR:CG2	2.45	0.46
1:F:230:VAL:CG1	1:F:248:PHE:HB3	2.45	0.46
1:G:21:VAL:HG11	1:G:31:SER:O	2.14	0.46
1:I:5:ILE:HD11	1:I:10:LEU:CD2	2.37	0.46
1:K:204:ALA:HB2	1:K:250:THR:HG21	1.97	0.46
1:L:174:VAL:HG23	1:L:181:LEU:HD21	1.96	0.46
1:L:174:VAL:HB	1:L:183:LEU:CD2	2.45	0.46
1:L:277:ASP:C	1:L:279:PHE:N	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:298:PHE:HB2	1:L:309:ARG:HG3	1.97	0.46
1:O:211:LEU:HD13	1:O:246:VAL:HG11	1.97	0.46
1:O:228:LEU:HB3	1:O:250:THR:HG22	1.97	0.46
1:O:305:SER:C	1:O:324:ILE:HG12	2.40	0.46
1:P:163:LEU:HD22	1:P:257:PHE:CD2	2.50	0.46
1:P:221:LEU:HD23	1:P:230:VAL:HB	1.98	0.46
1:A:303:GLN:N	1:A:303:GLN:CD	2.73	0.46
1:B:175:THR:HG22	1:B:182:ALA:HB3	1.96	0.46
1:C:327:GLN:CD	1:C:327:GLN:N	2.73	0.46
1:E:289:LEU:HD12	1:E:318:ALA:HB2	1.97	0.46
1:F:222:LEU:HB3	1:F:229:ASN:HB2	1.96	0.46
1:G:221:LEU:HD23	1:G:230:VAL:HG23	1.91	0.46
1:G:320:GLU:OE1	1:H:107:SER:HB3	2.15	0.46
1:H:168:GLU:HG3	1:H:168:GLU:O	2.14	0.46
1:K:134:VAL:HG12	1:K:221:LEU:CD1	2.46	0.46
1:K:301:PHE:CE1	1:K:306:LEU:HD13	2.50	0.46
1:L:358:GLU:HG3	1:L:360:ASN:H	1.79	0.46
1:N:304:ASP:HA	1:N:324:ILE:O	2.15	0.46
1:C:183:LEU:HD21	1:C:185:GLU:HG3	1.97	0.46
1:F:70:THR:HG21	1:F:94:ILE:HG12	1.96	0.46
1:F:125:GLU:N	1:F:125:GLU:CD	2.73	0.46
1:H:125:GLU:CD	1:H:125:GLU:N	2.73	0.46
1:H:147:ALA:HA	1:H:150:MET:HE2	1.97	0.46
1:J:128:GLN:NE2	1:J:225:ARG:HG3	2.30	0.46
1:L:331:LEU:HD23	1:L:356:MET:SD	2.56	0.46
1:O:179:HIS:O	1:O:180:ARG:HG3	2.15	0.46
1:A:17:VAL:CG2	1:A:46:GLY:CA	2.93	0.46
1:A:90:ILE:CG2	1:A:102:LEU:HD21	2.38	0.46
1:A:272:VAL:HG13	1:A:324:ILE:HD12	1.96	0.46
1:C:135:THR:HG23	1:C:138:GLU:H	1.79	0.46
1:D:187:LEU:HD13	1:D:187:LEU:O	2.15	0.46
1:D:335:PHE:HZ	1:D:363:VAL:HG21	1.80	0.46
1:G:1:MET:HE2	1:G:94:ILE:CD1	2.45	0.46
1:I:220:THR:HG23	1:I:220:THR:O	2.15	0.46
1:L:174:VAL:HG23	1:L:183:LEU:HG	1.97	0.46
1:D:125:GLU:OE2	1:D:227:LEU:N	2.48	0.46
1:G:241:GLN:CD	1:G:241:GLN:N	2.73	0.46
1:I:227:LEU:HD23	1:I:251:LYS:HA	1.98	0.46
1:I:264:ILE:HG13	1:I:376:VAL:HG21	1.98	0.46
1:K:162:THR:HG22	1:K:175:THR:HG21	1.96	0.46
1:O:94:ILE:O	1:O:94:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:378:MET:CG	1:O:379:PRO:HD2	2.45	0.46
1:A:303:GLN:CD	1:A:303:GLN:H	2.14	0.46
1:C:70:THR:HG21	1:C:94:ILE:CD1	2.46	0.46
1:H:78:MET:CE	1:H:82:LYS:HE3	2.46	0.46
1:J:156:ARG:HB2	1:J:159:LEU:HD23	1.98	0.46
1:N:33:VAL:CG1	1:N:44:ILE:HG22	2.46	0.46
1:N:279:PHE:CD1	1:N:283:LEU:HD23	2.50	0.46
1:O:312:ASN:HB2	1:O:313:PRO:HD2	1.98	0.46
1:A:326:TYR:CE1	1:A:328:SER:HB2	2.51	0.46
1:K:134:VAL:HG21	1:K:186:ILE:CD1	2.44	0.46
1:L:29:ILE:HG23	1:L:30:LEU:HD12	1.97	0.46
1:B:163:LEU:HD22	1:B:257:PHE:CD2	2.51	0.46
1:C:299:LEU:N	1:C:299:LEU:HD12	2.31	0.46
1:G:124:THR:HB	1:G:227:LEU:HD12	1.97	0.46
1:M:30:LEU:CD1	1:M:49:LEU:HG	2.44	0.46
1:M:176:THR:CG2	1:M:180:ARG:O	2.64	0.46
1:A:141:ARG:O	1:A:145:LYS:HG2	2.16	0.46
1:B:256:LYS:HE2	1:B:256:LYS:HB3	1.79	0.46
1:C:329:ALA:HB1	1:C:330:PRO:CD	2.38	0.46
1:F:126:ASN:ND2	1:F:126:ASN:H	2.13	0.46
1:F:326:TYR:CZ	1:F:328:SER:HB2	2.51	0.46
1:G:59:LEU:HG	1:G:63:ALA:CB	2.46	0.46
1:H:134:VAL:CG2	1:H:186:ILE:HD12	2.46	0.46
1:J:333:MET:HG2	1:J:359:ALA:HA	1.98	0.46
1:N:1:MET:HG3	1:N:37:THR:HG22	1.98	0.46
1:O:225:ARG:O	1:O:225:ARG:HG3	2.15	0.46
1:P:160:THR:O	1:P:202:ARG:HB2	2.16	0.46
1:E:354:MET:CE	1:E:363:VAL:HG11	2.46	0.45
1:F:265:PRO:HG2	1:F:364:LEU:HB2	1.98	0.45
1:F:307:GLN:NE2	3:F:401:HOH:O	2.49	0.45
1:J:195:LEU:C	1:J:195:LEU:CD2	2.85	0.45
1:J:289:LEU:HD22	1:J:316:ASP:HB3	1.97	0.45
1:K:34:LYS:HD2	1:K:119:TYR:CG	2.51	0.45
1:K:124:THR:C	1:K:126:ASN:H	2.24	0.45
1:L:30:LEU:HD11	1:L:120:PRO:CG	2.46	0.45
1:L:142:LEU:HD13	1:L:171:LEU:HD23	1.96	0.45
1:B:136:GLN:HG2	1:B:219:LEU:HD11	1.97	0.45
1:D:133:GLN:CG	1:D:190:SER:HB2	2.47	0.45
1:D:228:LEU:HB3	1:D:250:THR:HG22	1.98	0.45
1:F:153:GLN:NE2	1:F:153:GLN:CA	2.73	0.45
1:H:14:LEU:HD11	1:H:77:LEU:CD2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:163:LEU:HB3	1:L:174:VAL:CG1	2.46	0.45
1:N:346:VAL:HG21	1:N:375:TYR:CZ	2.51	0.45
1:E:14:LEU:HD11	1:E:77:LEU:HD12	1.98	0.45
1:G:49:LEU:HD23	1:G:49:LEU:HA	1.73	0.45
1:I:69:GLU:HG3	1:I:116:ALA:HB3	1.99	0.45
1:M:150:MET:HE1	1:M:202:ARG:HA	1.98	0.45
1:N:70:THR:HG21	1:N:94:ILE:CD1	2.47	0.45
1:P:159:LEU:HD23	1:P:177:ASP:HA	1.99	0.45
1:H:262:ARG:HB3	1:H:262:ARG:CZ	2.45	0.45
1:K:333:MET:HE2	1:K:333:MET:HB3	1.69	0.45
1:A:142:LEU:HG	1:A:173:ALA:HB2	1.99	0.45
1:C:159:LEU:HD22	1:C:176:THR:HG23	1.98	0.45
1:I:72:VAL:CG1	1:I:73:PRO:HD2	2.46	0.45
1:N:347:LEU:HD22	1:N:367:ASP:HB2	1.99	0.45
1:O:98:GLN:CG	1:O:113:THR:OG1	2.65	0.45
1:A:381:ARG:O	1:A:381:ARG:HG2	2.15	0.45
1:C:14:LEU:HB3	1:C:78:MET:HE1	1.98	0.45
1:C:228:LEU:HB2	1:C:252:LEU:HD21	1.99	0.45
1:F:49:LEU:HD23	1:F:49:LEU:HA	1.70	0.45
1:I:3:LEU:HD23	1:I:3:LEU:H	1.80	0.45
1:I:54:VAL:HG21	1:I:247:ARG:NH2	2.32	0.45
1:K:307:GLN:HG3	1:K:321:ASP:OD1	2.16	0.45
1:M:270:LYS:HE3	1:M:357:THR:O	2.16	0.45
1:O:171:LEU:C	1:O:171:LEU:HD12	2.42	0.45
1:B:211:LEU:HD23	1:B:232:ILE:HD12	1.97	0.45
1:D:167:ASP:HB2	1:D:195:LEU:CD1	2.37	0.45
1:L:61:GLU:CD	1:L:61:GLU:N	2.72	0.45
1:L:136:GLN:NE2	1:L:213:SER:H	2.15	0.45
1:P:37:THR:HG22	1:P:64:CYS:SG	2.57	0.45
1:F:126:ASN:N	1:F:126:ASN:ND2	2.60	0.45
1:F:274:ILE:HG12	1:F:324:ILE:HG22	1.99	0.45
1:J:133:GLN:HB3	1:J:218:GLN:NE2	2.32	0.45
1:K:248:PHE:CD1	1:K:248:PHE:C	2.95	0.45
1:M:33:VAL:HG22	1:M:44:ILE:CG2	2.47	0.45
1:O:260:TYR:HD1	1:O:264:ILE:CD1	2.30	0.45
1:P:223:ILE:HD12	1:P:223:ILE:N	2.32	0.45
1:A:96:GLU:CD	1:A:96:GLU:N	2.72	0.45
1:C:18:VAL:CB	1:C:78:MET:HE3	2.44	0.45
1:D:158:TYR:CE1	1:D:258:PRO:HD3	2.52	0.45
1:E:235:PRO:CD	3:E:418:HOH:O	2.64	0.45
1:F:169:ASN:C	1:F:188:ALA:O	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:PHE:HZ	1:G:363:VAL:HG21	1.82	0.45
1:I:7:LYS:HA	1:I:90:ILE:HD11	1.99	0.45
1:I:230:VAL:CG1	1:I:248:PHE:HB3	2.46	0.45
1:K:76:LYS:HD3	1:K:111:LEU:HD21	1.97	0.45
1:K:158:TYR:CE1	1:K:258:PRO:HD3	2.51	0.45
1:L:210:ARG:HG2	1:L:210:ARG:NH1	2.32	0.45
1:L:335:PHE:HB3	1:L:340:LEU:CD1	2.47	0.45
1:M:90:ILE:CG2	1:M:92:LEU:CD1	2.90	0.45
1:O:40:GLN:NE2	1:O:40:GLN:N	2.60	0.45
1:B:178:GLY:O	1:O:154:ASP:OD2	2.35	0.45
1:C:283:LEU:HD23	1:C:341:LEU:CG	2.46	0.45
1:F:257:PHE:CD1	1:F:258:PRO:HD2	2.51	0.45
1:G:166:ILE:HD12	1:G:170:GLN:O	2.17	0.45
1:M:122:LEU:HD12	1:M:122:LEU:N	2.31	0.45
1:N:70:THR:HG21	1:N:94:ILE:HD11	1.99	0.45
1:O:157:PHE:O	1:O:157:PHE:HD2	2.00	0.45
1:D:229:ASN:OD1	1:D:249:THR:HG23	2.17	0.44
1:E:303:GLN:N	1:E:303:GLN:CD	2.73	0.44
1:G:33:VAL:O	1:G:71:THR:HA	2.16	0.44
1:J:70:THR:HG21	1:J:94:ILE:CD1	2.47	0.44
1:N:221:LEU:HD23	1:N:230:VAL:HB	1.98	0.44
1:O:13:VAL:HG23	1:O:44:ILE:HD12	1.99	0.44
1:P:124:THR:HG21	1:P:227:LEU:HD12	2.00	0.44
1:C:301:PHE:HB3	1:C:326:TYR:CE2	2.52	0.44
1:C:326:TYR:O	1:C:326:TYR:CG	2.70	0.44
1:F:191:THR:O	1:F:191:THR:OG1	2.27	0.44
1:L:128:GLN:HB3	1:L:129:GLY:H	1.54	0.44
1:M:45:THR:HG23	1:M:54:VAL:HG22	1.99	0.44
1:N:240:GLU:HG3	1:N:240:GLU:O	2.17	0.44
1:N:301:PHE:N	1:N:331:LEU:O	2.38	0.44
1:O:30:LEU:HD21	1:O:49:LEU:HG	1.98	0.44
1:O:150:MET:HE3	1:O:150:MET:HB2	1.91	0.44
1:P:10:LEU:HD23	1:P:81:CYS:SG	2.57	0.44
1:P:215:GLU:OE2	1:P:235:PRO:HG3	2.17	0.44
1:A:326:TYR:CZ	1:A:328:SER:HB2	2.53	0.44
1:B:170:GLN:NE2	1:B:172:ARG:NH2	2.66	0.44
1:C:283:LEU:HD23	1:C:341:LEU:CD2	2.47	0.44
1:E:24:ARG:HA	1:E:24:ARG:NE	2.30	0.44
1:F:0:HIS:HE1	1:F:96:GLU:HG2	1.81	0.44
1:F:16:HIS:O	1:F:53:LEU:HD23	2.18	0.44
1:F:37:THR:HG22	1:F:42:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:THR:HA	1:F:175:THR:HG22	1.99	0.44
1:L:153:GLN:HA	1:L:160:THR:HG21	2.00	0.44
1:O:346:VAL:O	1:O:346:VAL:HG13	2.18	0.44
1:E:72:VAL:HG12	1:E:73:PRO:HD2	1.98	0.44
1:E:257:PHE:CG	1:E:258:PRO:HD2	2.53	0.44
1:F:56:SER:CB	1:H:40:GLN:OE1	2.66	0.44
1:G:39:ALA:HA	1:G:64:CYS:SG	2.58	0.44
1:N:309:ARG:NH2	3:N:401:HOH:O	2.50	0.44
1:O:98:GLN:HG2	1:O:113:THR:C	2.31	0.44
1:O:370:HIS:HA	1:O:371:PRO:HD2	1.85	0.44
1:D:172:ARG:HD2	1:D:260:TYR:OH	2.18	0.44
1:F:301:PHE:O	1:F:330:PRO:HA	2.17	0.44
1:G:273:LEU:HD23	1:G:351:ASP:HB3	1.99	0.44
1:H:42:LEU:HB3	1:H:59:LEU:HD11	1.98	0.44
1:I:132:VAL:HG22	1:I:166:ILE:CD1	2.43	0.44
1:K:282:SER:OG	1:K:322:LEU:HD11	2.18	0.44
1:K:353:ASN:ND2	1:K:368:PRO:HG3	2.32	0.44
1:N:90:ILE:HG22	1:N:92:LEU:HD12	1.98	0.44
1:B:333:MET:HE2	1:B:333:MET:HB3	1.86	0.44
1:C:98:GLN:HE21	1:C:115:PRO:HD3	1.82	0.44
1:N:95:THR:HG22	1:N:97:ASP:N	2.20	0.44
1:O:101:ILE:HG23	1:O:110:VAL:HG22	2.00	0.44
1:P:167:ASP:CA	1:P:195:LEU:HD23	2.47	0.44
1:A:0:HIS:O	1:A:66:GLU:HB3	2.18	0.44
1:B:24:ARG:HB3	1:P:24:ARG:HG2	1.99	0.44
1:B:194:GLN:OE1	1:B:194:GLN:N	2.40	0.44
1:B:364:LEU:HD11	1:B:374:THR:HG23	1.98	0.44
1:E:93:GLN:O	1:E:93:GLN:HG3	2.14	0.44
1:F:40:GLN:HE22	1:H:245:THR:HG23	1.82	0.44
1:H:308:LEU:N	1:H:308:LEU:HD12	2.33	0.44
1:L:136:GLN:OE1	1:L:232:ILE:HG23	2.18	0.44
1:L:148:PHE:CE2	1:L:346:VAL:HG21	2.52	0.44
1:M:300:ASN:OD1	1:M:332:GLU:HG3	2.17	0.44
1:N:1:MET:SD	1:N:37:THR:HG22	2.58	0.44
1:N:36:GLN:HE21	1:N:69:GLU:CD	2.26	0.44
1:O:136:GLN:CB	1:O:219:LEU:HD11	2.47	0.44
1:D:69:GLU:HG3	1:D:116:ALA:HB3	2.00	0.44
1:M:91:ASP:C	1:M:92:LEU:HD12	2.42	0.44
1:M:241:GLN:OE1	1:M:241:GLN:HA	2.17	0.44
1:O:301:PHE:CD1	1:O:356:MET:HE3	2.53	0.44
1:C:90:ILE:CG2	1:C:102:LEU:HD23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:GLN:N	1:D:194:GLN:CD	2.73	0.44
1:E:322:LEU:N	1:E:322:LEU:CD1	2.80	0.44
1:F:17:VAL:HG23	1:F:53:LEU:O	2.17	0.44
1:P:7:LYS:CD	1:P:84:LEU:CB	2.68	0.44
1:E:4:LYS:HG3	1:E:65:LEU:HD11	2.00	0.43
1:G:358:GLU:OE1	1:G:358:GLU:HA	2.18	0.43
1:I:281:GLN:NE2	1:I:281:GLN:CA	2.73	0.43
1:K:201:PRO:HG2	1:K:250:THR:HG21	1.98	0.43
1:L:75:ARG:O	1:L:79:GLU:HG2	2.17	0.43
1:L:164:LEU:HA	1:L:164:LEU:HD23	1.76	0.43
1:L:215:GLU:C	1:L:215:GLU:CD	2.85	0.43
1:L:358:GLU:HG2	1:L:360:ASN:OD1	2.18	0.43
1:B:175:THR:CG2	1:B:182:ALA:HB3	2.48	0.43
1:D:266:ARG:NH1	1:D:266:ARG:HG2	2.33	0.43
1:E:335:PHE:HZ	1:E:363:VAL:HG21	1.84	0.43
1:I:289:LEU:HD12	1:I:318:ALA:HB2	2.00	0.43
1:J:25:HIS:CE1	1:J:30:LEU:HD12	2.53	0.43
1:L:4:LYS:HE3	1:L:89:LEU:CD2	2.49	0.43
1:L:159:LEU:C	1:L:161:GLY:H	2.26	0.43
1:A:159:LEU:HD22	1:A:176:THR:HG23	2.01	0.43
1:B:140:LYS:O	1:B:144:GLU:HG3	2.18	0.43
1:B:171:LEU:HB3	1:B:186:ILE:CD1	2.48	0.43
1:D:-2:HIS:O	1:D:-2:HIS:CG	2.70	0.43
1:D:80:ILE:HG21	1:D:102:LEU:HD12	2.00	0.43
1:E:163:LEU:HD11	1:E:197:GLN:HB3	2.00	0.43
1:E:240:GLU:O	1:E:240:GLU:HG3	2.19	0.43
1:G:170:GLN:HG3	1:G:187:LEU:HD13	2.00	0.43
1:N:305:SER:N	1:N:324:ILE:HG13	2.33	0.43
1:O:148:PHE:CD2	1:O:342:ASP:HB3	2.53	0.43
1:O:297:VAL:HG12	1:O:310:ALA:HB2	2.00	0.43
1:O:299:LEU:N	1:O:299:LEU:CD1	2.80	0.43
1:C:131:GLN:CD	1:C:220:THR:CG2	2.92	0.43
1:D:65:LEU:HA	1:D:65:LEU:HD13	1.58	0.43
1:F:56:SER:HB3	1:H:40:GLN:OE1	2.18	0.43
1:F:101:ILE:HG12	1:F:110:VAL:HG22	2.01	0.43
1:G:127:SER:HB2	3:G:417:HOH:O	2.19	0.43
1:K:125:GLU:O	1:K:125:GLU:HG2	2.19	0.43
1:M:269:ASP:OD1	1:M:270:LYS:CG	2.61	0.43
1:N:257:PHE:CG	1:N:258:PRO:HD2	2.53	0.43
1:O:145:LYS:HA	1:O:346:VAL:CG2	2.49	0.43
1:D:65:LEU:HB3	1:D:66:GLU:H	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ARG:HE	1:D:172:ARG:HB2	1.53	0.43
1:E:248:PHE:CD1	1:E:248:PHE:C	2.96	0.43
1:J:102:LEU:HD23	1:J:102:LEU:C	2.44	0.43
1:L:135:THR:CG2	1:L:137:ARG:HB3	2.48	0.43
1:L:297:VAL:HG11	1:L:337:ALA:HB2	2.00	0.43
1:M:136:GLN:HE21	1:M:213:SER:H	1.65	0.43
1:M:187:LEU:HD23	1:M:187:LEU:HA	1.78	0.43
1:N:65:LEU:HD13	1:N:66:GLU:HG2	2.01	0.43
1:O:155:VAL:HB	1:O:156:ARG:CZ	2.48	0.43
1:O:356:MET:N	1:O:356:MET:SD	2.92	0.43
1:A:1:MET:HG3	1:A:37:THR:CG2	2.49	0.43
1:A:294:LEU:N	1:A:294:LEU:CD1	2.81	0.43
1:C:133:GLN:HB2	1:C:189:SER:HB3	2.00	0.43
1:C:356:MET:HG3	1:C:363:VAL:HG13	2.00	0.43
1:D:142:LEU:HD11	1:D:186:ILE:HD13	2.01	0.43
1:D:273:LEU:HD21	1:D:351:ASP:OD1	2.18	0.43
1:H:378:MET:CB	1:H:379:PRO:CD	2.92	0.43
1:M:227:LEU:HD22	1:M:249:THR:CG2	2.49	0.43
1:O:50:GLU:O	1:O:50:GLU:HG2	2.18	0.43
1:O:260:TYR:HD1	1:O:264:ILE:HD13	1.84	0.43
1:B:347:LEU:HD22	1:B:367:ASP:HB2	2.00	0.43
1:E:136:GLN:HE22	1:E:232:ILE:HG23	1.83	0.43
1:F:18:VAL:HB	1:F:78:MET:HE3	2.01	0.43
1:J:2:ARG:NH1	1:J:93:GLN:OE1	2.51	0.43
1:M:32:ASN:CB	1:M:71:THR:HG22	2.49	0.43
1:M:264:ILE:HA	1:M:265:PRO:HD3	1.92	0.43
1:P:329:ALA:HA	1:P:330:PRO:HD3	1.87	0.43
1:E:24:ARG:HE	1:E:24:ARG:CA	2.29	0.43
1:E:164:LEU:HD12	1:E:164:LEU:HA	1.93	0.43
1:F:17:VAL:HG22	1:F:46:GLY:CA	2.49	0.43
1:I:100:CYS:HB2	1:I:113:THR:CG2	2.49	0.43
1:K:65:LEU:CD1	1:K:65:LEU:H	2.31	0.43
1:K:134:VAL:HG12	1:K:221:LEU:HD13	2.01	0.43
1:L:37:THR:CG2	1:L:42:LEU:CD1	2.95	0.43
1:M:32:ASN:HB3	1:M:71:THR:HG22	2.00	0.43
1:M:59:LEU:HD22	1:M:63:ALA:HB1	1.99	0.43
1:M:278:VAL:CG1	1:M:322:LEU:CD2	2.91	0.43
1:O:333:MET:HE2	1:O:333:MET:HB3	1.90	0.43
1:A:1:MET:CE	1:A:70:THR:HG22	2.46	0.43
1:A:333:MET:HB3	1:A:333:MET:HE2	1.72	0.43
1:G:289:LEU:HD12	1:G:318:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:MET:HE2	1:H:82:LYS:NZ	2.34	0.43
1:H:135:THR:HA	1:H:218:GLN:HA	2.01	0.43
1:I:78:MET:HE3	1:I:78:MET:HB2	1.83	0.43
1:I:83:SER:HB2	1:J:285:ARG:HG2	2.00	0.43
1:I:142:LEU:CD2	1:I:186:ILE:HG12	2.48	0.43
1:I:356:MET:HE3	1:I:356:MET:HB2	1.71	0.43
1:M:33:VAL:CG2	1:M:44:ILE:CG2	2.97	0.43
1:M:312:ASN:HB2	1:M:313:PRO:HD3	1.96	0.43
1:N:166:ILE:CD1	1:N:196:VAL:CG2	2.96	0.43
1:P:272:VAL:HG22	1:P:326:TYR:CD1	2.53	0.43
1:D:45:THR:HG23	1:D:54:VAL:HG22	2.00	0.43
1:F:32:ASN:CB	1:F:71:THR:CG2	2.95	0.43
1:J:3:LEU:HD22	1:J:37:THR:HG21	2.01	0.43
1:J:71:THR:O	1:J:113:THR:HB	2.18	0.43
1:J:306:LEU:HB2	1:J:324:ILE:HG21	2.01	0.43
1:N:208:LEU:HD12	1:N:208:LEU:HA	1.87	0.43
1:A:33:VAL:CG2	1:A:44:ILE:CG2	2.96	0.42
1:B:155:VAL:H	1:O:153:GLN:HE21	1.66	0.42
1:D:289:LEU:HD23	1:D:316:ASP:HB3	2.01	0.42
1:E:272:VAL:HG13	1:E:324:ILE:HD12	2.01	0.42
1:F:30:LEU:HD23	1:F:30:LEU:HA	1.79	0.42
1:G:198:ALA:HB1	1:G:252:LEU:HD13	2.01	0.42
1:I:49:LEU:HA	1:I:49:LEU:HD12	1.43	0.42
1:L:283:LEU:HA	1:L:286:VAL:CG1	2.49	0.42
1:N:162:THR:HA	1:N:175:THR:HG22	2.01	0.42
1:O:13:VAL:CG2	1:O:44:ILE:HD12	2.48	0.42
1:P:59:LEU:CD1	1:P:64:CYS:HB2	2.49	0.42
1:P:256:LYS:HE2	1:P:256:LYS:HB3	1.91	0.42
1:A:303:GLN:HA	1:A:326:TYR:O	2.19	0.42
1:B:133:GLN:HB2	1:B:189:SER:HB3	2.01	0.42
1:D:27:LEU:HD12	1:D:30:LEU:HD12	2.01	0.42
1:D:30:LEU:HD11	1:D:49:LEU:HG	2.01	0.42
1:D:94:ILE:HD12	1:D:94:ILE:N	2.35	0.42
1:D:142:LEU:CD1	1:D:186:ILE:HD13	2.49	0.42
1:D:200:VAL:HG12	1:D:204:ALA:HB3	2.01	0.42
1:E:124:THR:O	1:E:124:THR:HG23	2.18	0.42
1:F:17:VAL:HG21	1:F:46:GLY:N	2.35	0.42
1:G:83:SER:HB3	1:H:288:ILE:HD11	2.01	0.42
1:L:163:LEU:HD12	1:L:165:GLU:HB2	2.00	0.42
1:N:171:LEU:HB3	1:N:186:ILE:CD1	2.49	0.42
1:N:289:LEU:O	1:N:312:ASN:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:281:GLN:HB3	1:O:285:ARG:NH1	2.31	0.42
1:F:2:ARG:HG3	1:F:65:LEU:HB2	2.01	0.42
1:J:258:PRO:HB3	1:K:156:ARG:CZ	2.49	0.42
1:K:208:LEU:HD12	1:K:208:LEU:HA	1.77	0.42
1:K:313:PRO:C	1:K:315:GLN:H	2.27	0.42
1:K:326:TYR:CE1	1:K:328:SER:HB2	2.55	0.42
1:L:42:LEU:HB2	1:L:59:LEU:HD13	2.01	0.42
1:L:163:LEU:CD1	1:L:165:GLU:HB2	2.49	0.42
1:L:174:VAL:HB	1:L:183:LEU:HD21	2.01	0.42
1:L:195:LEU:HB3	1:L:196:VAL:H	1.61	0.42
1:L:289:LEU:HD22	1:L:316:ASP:HB3	2.00	0.42
1:N:272:VAL:HG23	1:N:356:MET:CE	2.50	0.42
1:A:33:VAL:HG22	1:A:44:ILE:CG2	2.49	0.42
1:B:5:ILE:HG13	1:B:6:ALA:H	1.83	0.42
1:B:132:VAL:CG2	1:B:166:ILE:HG12	2.49	0.42
1:D:27:LEU:HD12	1:D:30:LEU:CD1	2.49	0.42
1:E:29:ILE:O	1:E:32:ASN:HB2	2.19	0.42
1:F:150:MET:HE3	1:F:161:GLY:HA2	2.00	0.42
1:K:11:LEU:HD11	1:K:82:LYS:CG	2.47	0.42
1:K:96:GLU:H	1:K:96:GLU:CD	2.28	0.42
1:K:131:GLN:HG3	1:K:220:THR:HG23	2.01	0.42
1:L:152:VAL:O	1:L:153:GLN:HG3	2.20	0.42
1:N:1:MET:CE	1:N:70:THR:HG22	2.49	0.42
1:N:124:THR:HB	1:N:227:LEU:CD1	2.47	0.42
1:O:30:LEU:HD11	1:O:120:PRO:CG	2.49	0.42
1:A:272:VAL:HG22	1:A:326:TYR:CD1	2.54	0.42
1:J:158:TYR:CZ	1:J:258:PRO:HD3	2.55	0.42
1:L:137:ARG:CB	1:L:214:ILE:O	2.67	0.42
1:L:148:PHE:CD2	1:L:346:VAL:HG21	2.53	0.42
1:L:299:LEU:HG	1:L:308:LEU:CD2	2.49	0.42
1:M:132:VAL:HB	1:M:221:LEU:HB2	2.01	0.42
1:P:306:LEU:HB2	1:P:324:ILE:HD13	2.02	0.42
1:A:312:ASN:CB	1:A:313:PRO:CD	2.83	0.42
1:C:25:HIS:CE1	1:C:30:LEU:HD12	2.54	0.42
1:C:165:GLU:HG3	1:C:197:GLN:HG2	2.00	0.42
1:C:186:ILE:HD12	1:C:187:LEU:H	1.85	0.42
1:E:354:MET:HE2	1:E:356:MET:CE	2.49	0.42
1:F:237:ARG:HH11	1:F:237:ARG:HG3	1.83	0.42
1:O:186:ILE:HD12	1:O:186:ILE:HA	1.95	0.42
1:A:115:PRO:HB3	1:A:117:GLU:HG2	2.01	0.42
1:B:102:LEU:HB2	1:B:109:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:CYS:SG	1:D:64:CYS:O	2.77	0.42
1:E:49:LEU:HD23	1:E:49:LEU:HA	1.82	0.42
1:F:32:ASN:HB2	1:F:71:THR:HG22	2.02	0.42
1:G:269:ASP:OD1	1:G:270:LYS:N	2.52	0.42
1:I:294:LEU:HD12	1:I:294:LEU:N	2.35	0.42
1:J:293:LYS:HD3	1:J:293:LYS:N	2.34	0.42
1:J:329:ALA:HA	1:J:330:PRO:HD3	1.77	0.42
1:K:2:ARG:HG2	1:K:94:ILE:N	2.34	0.42
1:K:295:ARG:HD2	1:K:295:ARG:HA	1.87	0.42
1:L:8:GLU:CD	1:L:8:GLU:H	2.25	0.42
1:N:1:MET:HG3	1:N:37:THR:CG2	2.50	0.42
1:O:354:MET:HG2	1:O:365:VAL:HG22	2.02	0.42
1:P:14:LEU:HD11	1:P:77:LEU:CD2	2.50	0.42
1:P:228:LEU:HB3	1:P:250:THR:HG22	2.01	0.42
1:B:195:LEU:HD12	1:B:195:LEU:O	2.19	0.42
1:D:289:LEU:HD13	1:D:318:ALA:HB2	2.02	0.42
1:H:299:LEU:HD13	1:H:335:PHE:CD2	2.51	0.42
1:K:75:ARG:CZ	1:K:79:GLU:HG3	2.50	0.42
1:K:198:ALA:HB1	1:K:252:LEU:HD13	2.02	0.42
1:M:122:LEU:N	1:M:122:LEU:CD1	2.82	0.42
1:N:17:VAL:CG2	1:N:17:VAL:O	2.68	0.42
1:H:297:VAL:HG22	1:H:310:ALA:HB2	2.02	0.42
1:I:295:ARG:HA	1:I:295:ARG:HD2	1.71	0.42
1:J:150:MET:HB2	1:J:202:ARG:HH12	1.85	0.42
1:K:30:LEU:HD11	1:K:49:LEU:HG	2.00	0.42
1:N:1:MET:HE1	1:N:70:THR:HG22	2.02	0.42
1:O:208:LEU:HD23	1:O:208:LEU:HA	1.90	0.42
1:A:329:ALA:HA	1:A:330:PRO:HD3	1.89	0.42
1:G:282:SER:OG	1:G:322:LEU:HD13	2.20	0.42
1:H:220:THR:HG23	1:H:220:THR:O	2.20	0.42
1:I:2:ARG:CG	1:I:65:LEU:HD12	2.47	0.42
1:I:162:THR:HA	1:I:175:THR:HG22	2.02	0.42
1:J:37:THR:HG22	1:J:42:LEU:CD1	2.50	0.42
1:J:70:THR:HG21	1:J:94:ILE:HD12	2.02	0.42
1:K:61:GLU:HA	1:K:64:CYS:SG	2.60	0.42
1:K:131:GLN:CG	1:K:220:THR:HG23	2.49	0.42
1:K:268:GLY:HA2	1:K:357:THR:HG22	2.00	0.42
1:L:132:VAL:HG11	1:L:171:LEU:HD12	2.00	0.42
1:L:145:LYS:HD2	1:L:346:VAL:HG12	2.01	0.42
1:A:33:VAL:HG22	1:A:44:ILE:HG22	2.03	0.41
1:D:73:PRO:HD3	1:D:112:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ASN:CB	1:D:313:PRO:HD3	2.46	0.41
1:H:138:GLU:HB3	1:H:186:ILE:HD12	2.02	0.41
1:J:364:LEU:HD11	1:J:374:THR:CG2	2.50	0.41
1:K:162:THR:HA	1:K:175:THR:HG22	2.02	0.41
1:N:234:THR:HB	1:N:235:PRO:HD3	2.01	0.41
1:O:72:VAL:CG1	1:O:73:PRO:HD2	2.50	0.41
1:B:287:ALA:O	1:B:288:ILE:C	2.61	0.41
1:D:322:LEU:HD12	1:D:322:LEU:HA	1.78	0.41
1:E:45:THR:HG23	1:E:54:VAL:HG22	2.02	0.41
1:F:225:ARG:NH1	1:F:226:GLU:OE1	2.52	0.41
1:H:364:LEU:HD11	1:H:374:THR:HG23	2.02	0.41
1:B:333:MET:HE3	1:B:359:ALA:O	2.21	0.41
1:C:49:LEU:HD13	1:C:122:LEU:CD1	2.50	0.41
1:C:198:ALA:HB2	1:C:223:ILE:CG2	2.51	0.41
1:G:137:ARG:HG2	1:G:137:ARG:NH1	2.35	0.41
1:I:166:ILE:O	1:I:166:ILE:HG23	2.20	0.41
1:I:166:ILE:HD12	1:I:171:LEU:HD13	2.02	0.41
1:J:263:VAL:HG11	1:K:155:VAL:CG1	2.47	0.41
1:M:228:LEU:HD23	1:M:228:LEU:O	2.20	0.41
1:N:95:THR:CG2	1:N:96:GLU:N	2.82	0.41
1:O:333:MET:HE1	1:O:363:VAL:CG2	2.50	0.41
1:P:265:PRO:HG2	1:P:364:LEU:HB2	2.00	0.41
1:A:140:LYS:O	1:A:144:GLU:HG3	2.19	0.41
1:C:72:VAL:CG1	1:C:73:PRO:HD2	2.51	0.41
1:F:27:LEU:N	1:F:27:LEU:CD1	2.83	0.41
1:H:134:VAL:HG23	1:H:186:ILE:HD12	2.01	0.41
1:I:24:ARG:HH12	1:L:313:PRO:CG	2.33	0.41
1:K:4:LYS:CB	1:K:64:CYS:HB2	2.34	0.41
1:K:51:VAL:HG22	1:K:204:ALA:HB2	2.03	0.41
1:L:140:LYS:NZ	1:L:209:GLN:O	2.53	0.41
1:A:150:MET:HG2	1:A:175:THR:HG22	2.02	0.41
1:A:227:LEU:HD23	1:A:251:LYS:HA	2.03	0.41
1:C:162:THR:CG2	1:C:175:THR:HG22	2.22	0.41
1:D:37:THR:CG2	1:D:38:ASN:N	2.83	0.41
1:G:136:GLN:HG2	1:G:219:LEU:CG	2.49	0.41
1:I:30:LEU:HD23	1:I:30:LEU:HA	1.71	0.41
1:J:28:ASN:CB	1:L:28:ASN:HB3	2.50	0.41
1:M:83:SER:CB	1:N:288:ILE:HD11	2.49	0.41
1:M:110:VAL:O	1:M:110:VAL:HG23	2.20	0.41
1:M:378:MET:HE2	1:M:378:MET:HB3	1.67	0.41
1:N:14:LEU:HB3	1:N:78:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:17:VAL:HG21	1:N:46:GLY:N	2.34	0.41
1:P:104:SER:O	1:P:107:SER:HB2	2.20	0.41
1:B:2:ARG:NH1	1:B:93:GLN:HB2	2.36	0.41
1:E:172:ARG:HE	1:E:172:ARG:HB2	1.61	0.41
1:J:354:MET:HE2	1:J:354:MET:HB3	1.92	0.41
1:M:151:ALA:HB2	1:M:177:ASP:HB2	2.03	0.41
1:O:226:GLU:O	1:O:226:GLU:CG	2.68	0.41
1:O:274:ILE:HG21	1:O:322:LEU:HD23	2.01	0.41
1:P:164:LEU:HD23	1:P:164:LEU:HA	1.91	0.41
1:H:289:LEU:HD12	1:H:318:ALA:HB2	2.03	0.41
1:K:64:CYS:SG	1:K:64:CYS:O	2.78	0.41
1:K:278:VAL:CG1	1:K:322:LEU:HD22	2.51	0.41
1:N:241:GLN:HA	1:N:241:GLN:OE1	2.21	0.41
1:N:343:VAL:HG23	1:N:375:TYR:CG	2.56	0.41
1:O:77:LEU:HD12	1:O:102:LEU:HD11	2.02	0.41
1:O:222:LEU:HD23	1:O:223:ILE:N	2.35	0.41
1:O:329:ALA:HA	1:O:330:PRO:HD3	1.90	0.41
1:A:142:LEU:HG	1:A:173:ALA:CB	2.50	0.41
1:B:250:THR:O	1:B:250:THR:HG23	2.21	0.41
1:E:107:SER:OG	1:F:285:ARG:HD2	2.21	0.41
1:E:135:THR:HG1	1:E:138:GLU:HG3	1.80	0.41
1:F:183:LEU:HD23	1:F:183:LEU:C	2.46	0.41
1:F:289:LEU:HD12	1:F:318:ALA:HB2	2.03	0.41
1:F:303:GLN:O	1:F:303:GLN:HG2	2.17	0.41
1:I:278:VAL:CG1	1:I:322:LEU:HD22	2.51	0.41
1:I:367:ASP:HA	1:I:368:PRO:HD2	1.90	0.41
1:L:145:LYS:HA	1:L:346:VAL:CG1	2.50	0.41
1:L:208:LEU:HD12	1:L:208:LEU:HA	1.91	0.41
1:L:347:LEU:HD11	1:L:375:TYR:CD2	2.56	0.41
1:A:194:GLN:O	1:A:194:GLN:HG2	2.21	0.41
1:A:214:ILE:O	1:A:214:ILE:HG23	2.20	0.41
1:B:226:GLU:O	1:B:226:GLU:HG2	2.21	0.41
1:C:33:VAL:HG22	1:C:44:ILE:HG23	2.02	0.41
1:D:212:LEU:CD2	1:D:219:LEU:HD11	2.51	0.41
1:E:133:GLN:HB2	1:E:189:SER:HB2	2.03	0.41
1:F:91:ASP:HB3	1:F:103:LYS:HB2	2.03	0.41
1:F:329:ALA:HA	1:F:330:PRO:HD3	1.89	0.41
1:G:21:VAL:CG1	1:G:31:SER:O	2.69	0.41
1:G:228:LEU:HB3	1:G:250:THR:HG22	2.03	0.41
1:I:3:LEU:N	1:I:3:LEU:CD2	2.83	0.41
1:J:301:PHE:O	1:J:330:PRO:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:130:THR:HG23	1:K:192:SER:HB2	2.02	0.41
1:L:135:THR:HG22	1:L:137:ARG:HB3	2.03	0.41
1:M:54:VAL:O	1:M:246:VAL:HA	2.21	0.41
1:M:69:GLU:HB3	1:M:116:ALA:CB	2.51	0.41
1:M:233:ASN:O	1:M:234:THR:HG22	2.21	0.41
1:N:230:VAL:CG1	1:N:248:PHE:HB3	2.50	0.41
1:N:305:SER:C	1:N:324:ILE:CG1	2.93	0.41
1:O:137:ARG:HG3	1:O:214:ILE:HG23	2.01	0.41
1:O:174:VAL:HG23	1:O:181:LEU:HD11	2.03	0.41
1:O:200:VAL:HA	1:O:201:PRO:HD3	1.87	0.41
1:O:248:PHE:CD1	1:O:248:PHE:O	2.73	0.41
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.89	0.41
1:F:104:SER:O	1:F:107:SER:HB2	2.21	0.41
1:F:300:ASN:ND2	1:F:332:GLU:HG3	2.36	0.41
1:G:162:THR:CG2	1:G:205:VAL:HG21	2.49	0.41
1:G:183:LEU:HB3	1:G:374:THR:HB	2.03	0.41
1:H:272:VAL:CG1	1:H:324:ILE:HD12	2.51	0.41
1:J:322:LEU:N	1:J:322:LEU:HD23	2.36	0.41
1:K:93:GLN:NE2	1:K:93:GLN:CA	2.82	0.41
1:K:106:ASN:ND2	1:L:321:ASP:O	2.49	0.41
1:N:164:LEU:HD23	1:N:164:LEU:HA	1.93	0.41
1:N:341:LEU:HD23	1:N:344:LEU:HD12	2.03	0.41
1:A:30:LEU:HD11	1:A:49:LEU:HG	2.02	0.40
1:D:214:ILE:HG12	1:E:216:ASP:HB3	2.03	0.40
1:G:59:LEU:HA	1:G:59:LEU:HD12	1.82	0.40
1:G:94:ILE:N	1:G:94:ILE:CD1	2.84	0.40
1:H:49:LEU:HD23	1:H:49:LEU:HA	1.73	0.40
1:L:243:ASP:C	1:L:243:ASP:OD1	2.63	0.40
1:M:136:GLN:HG2	1:M:219:LEU:HD11	2.02	0.40
1:O:320:GLU:CD	1:P:107:SER:OG	2.64	0.40
1:P:49:LEU:HD23	1:P:49:LEU:HA	1.79	0.40
1:B:17:VAL:HG21	1:B:46:GLY:N	2.36	0.40
1:F:152:VAL:O	1:F:152:VAL:CG1	2.70	0.40
1:I:1:MET:HE2	1:I:1:MET:HB3	1.89	0.40
1:J:289:LEU:HD12	1:J:318:ALA:HB2	2.02	0.40
1:J:293:LYS:HG3	1:K:24:ARG:NE	2.36	0.40
1:N:269:ASP:OD1	1:N:269:ASP:N	2.49	0.40
1:O:136:GLN:N	1:O:219:LEU:HD12	2.35	0.40
1:A:135:THR:CG2	1:A:216:ASP:HA	2.51	0.40
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.94	0.40
1:B:228:LEU:C	1:B:228:LEU:HD23	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:THR:HG23	1:C:192:SER:HB2	2.03	0.40
1:F:228:LEU:C	1:F:228:LEU:CD2	2.94	0.40
1:G:65:LEU:CD1	1:G:65:LEU:H	2.34	0.40
1:G:132:VAL:CG1	1:G:191:THR:CG2	2.89	0.40
1:H:2:ARG:NE	1:H:65:LEU:HD22	2.35	0.40
1:H:334:SER:O	1:H:380:MET:HG2	2.20	0.40
1:J:2:ARG:HG3	1:J:65:LEU:HD12	2.04	0.40
1:K:124:THR:C	1:K:126:ASN:N	2.80	0.40
1:M:286:VAL:HG12	1:M:310:ALA:CB	2.51	0.40
1:N:278:VAL:H	1:N:278:VAL:HG23	1.67	0.40
1:N:323:ALA:C	1:N:324:ILE:HG23	2.46	0.40
1:C:228:LEU:HB3	1:C:250:THR:HG22	2.02	0.40
1:D:11:LEU:HD13	1:D:81:CYS:CB	2.51	0.40
1:F:40:GLN:HB3	1:H:41:ALA:HB2	2.02	0.40
1:F:136:GLN:HG2	1:F:219:LEU:CD1	2.41	0.40
1:G:124:THR:O	1:G:124:THR:HG23	2.20	0.40
1:G:230:VAL:CG1	1:G:231:THR:N	2.83	0.40
1:L:92:LEU:CD2	1:L:102:LEU:HG	2.52	0.40
1:N:335:PHE:HZ	1:N:363:VAL:HG11	1.85	0.40
1:P:286:VAL:HG21	1:P:308:LEU:HB2	2.02	0.40
1:A:1:MET:HE2	1:A:1:MET:HB3	1.90	0.40
1:A:102:LEU:HD23	1:A:103:LYS:N	2.36	0.40
1:A:137:ARG:NH1	1:A:216:ASP:OD1	2.49	0.40
1:B:96:GLU:OE1	1:B:96:GLU:CA	2.70	0.40
1:E:70:THR:HG21	1:E:94:ILE:HG12	2.02	0.40
1:E:131:GLN:HG2	1:E:220:THR:HG23	2.03	0.40
1:F:92:LEU:CD2	1:F:102:LEU:HG	2.51	0.40
1:F:159:LEU:CD2	1:F:176:THR:HG23	2.51	0.40
1:H:340:LEU:HD12	1:H:340:LEU:N	2.37	0.40
1:L:145:LYS:HD2	1:L:346:VAL:CG1	2.51	0.40
1:L:240:GLU:OE2	1:L:240:GLU:HA	2.22	0.40
1:M:164:LEU:HD23	1:M:164:LEU:HA	1.96	0.40
1:N:137:ARG:HD3	1:N:214:ILE:HG12	2.03	0.40
1:N:270:LYS:H	1:N:270:LYS:HG2	1.58	0.40
1:O:54:VAL:HB	1:O:247:ARG:HB2	2.03	0.40
1:O:356:MET:HG3	1:O:363:VAL:HG13	2.02	0.40
1:P:195:LEU:HD22	1:P:196:VAL:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/388 (96%)	367 (98%)	6 (2%)	1 (0%)	36	59
1	B	380/388 (98%)	375 (99%)	5 (1%)	0	100	100
1	C	375/388 (97%)	365 (97%)	9 (2%)	1 (0%)	36	59
1	D	378/388 (97%)	370 (98%)	8 (2%)	0	100	100
1	E	380/388 (98%)	371 (98%)	9 (2%)	0	100	100
1	F	375/388 (97%)	369 (98%)	6 (2%)	0	100	100
1	G	374/388 (96%)	366 (98%)	8 (2%)	0	100	100
1	H	381/388 (98%)	375 (98%)	6 (2%)	0	100	100
1	I	364/388 (94%)	352 (97%)	11 (3%)	1 (0%)	36	59
1	J	382/388 (98%)	372 (97%)	10 (3%)	0	100	100
1	K	358/388 (92%)	344 (96%)	12 (3%)	2 (1%)	21	45
1	L	344/388 (89%)	336 (98%)	7 (2%)	1 (0%)	36	59
1	M	374/388 (96%)	368 (98%)	5 (1%)	1 (0%)	36	59
1	N	364/388 (94%)	360 (99%)	3 (1%)	1 (0%)	36	59
1	O	345/388 (89%)	334 (97%)	11 (3%)	0	100	100
1	P	373/388 (96%)	359 (96%)	14 (4%)	0	100	100
All	All	5921/6208 (95%)	5783 (98%)	130 (2%)	8 (0%)	48	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	125	GLU
1	A	265	PRO
1	L	160	THR
1	N	265	PRO
1	K	115	PRO
1	C	265	PRO

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Mol	Chain	Res	Type
1	I	234	THR
1	M	73	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/341 (97%)	324 (98%)	6 (2%)	51	72
1	B	333/341 (98%)	322 (97%)	11 (3%)	33	58
1	C	329/341 (96%)	315 (96%)	14 (4%)	26	52
1	D	331/341 (97%)	320 (97%)	11 (3%)	33	58
1	E	333/341 (98%)	320 (96%)	13 (4%)	28	54
1	F	331/341 (97%)	320 (97%)	11 (3%)	33	58
1	G	329/341 (96%)	315 (96%)	14 (4%)	26	52
1	H	330/341 (97%)	317 (96%)	13 (4%)	28	54
1	I	321/341 (94%)	308 (96%)	13 (4%)	28	53
1	J	334/341 (98%)	330 (99%)	4 (1%)	63	79
1	K	314/341 (92%)	296 (94%)	18 (6%)	18	42
1	L	304/341 (89%)	290 (95%)	14 (5%)	24	50
1	M	328/341 (96%)	312 (95%)	16 (5%)	22	48
1	N	323/341 (95%)	311 (96%)	12 (4%)	30	55
1	O	309/341 (91%)	284 (92%)	25 (8%)	11	28
1	P	327/341 (96%)	311 (95%)	16 (5%)	22	48
All	All	5206/5456 (95%)	4995 (96%)	211 (4%)	27	53

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	128	GLN

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Mol	Chain	Res	Type
1	A	142	LEU
1	A	208	LEU
1	A	250	THR
1	A	364	LEU
1	B	13	VAL
1	B	42	LEU
1	B	44	ILE
1	B	97	ASP
1	B	124	THR
1	B	162	THR
1	B	240	GLU
1	B	243	ASP
1	B	341	LEU
1	B	357	THR
1	B	362	SER
1	C	37	THR
1	C	49	LEU
1	C	92	LEU
1	C	122	LEU
1	C	153	GLN
1	C	155	VAL
1	C	164	LEU
1	C	170	GLN
1	C	186	ILE
1	C	231	THR
1	C	263	VAL
1	C	273	LEU
1	C	303	GLN
1	C	322	LEU
1	D	3	LEU
1	D	24	ARG
1	D	65	LEU
1	D	102	LEU
1	D	135	THR
1	D	155	VAL
1	D	186	ILE
1	D	187	LEU
1	D	215	GLU
1	D	232	ILE
1	D	266	ARG
1	E	2	ARG
1	E	4	LYS

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Mol	Chain	Res	Type
1	E	71	THR
1	E	77	LEU
1	E	97	ASP
1	E	153	GLN
1	E	202	ARG
1	E	214	ILE
1	E	241	GLN
1	E	244	ILE
1	E	282	SER
1	E	322	LEU
1	E	356	MET
1	F	3	LEU
1	F	59	LEU
1	F	93	GLN
1	F	96	GLU
1	F	126	ASN
1	F	187	LEU
1	F	189	SER
1	F	195	LEU
1	F	246	VAL
1	F	293	LYS
1	F	303	GLN
1	G	5	ILE
1	G	8	GLU
1	G	11	LEU
1	G	59	LEU
1	G	61	GLU
1	G	155	VAL
1	G	191	THR
1	G	196	VAL
1	G	240	GLU
1	G	243	ASP
1	G	273	LEU
1	G	274	ILE
1	G	278	VAL
1	G	303	GLN
1	H	0	HIS
1	H	59	LEU
1	H	124	THR
1	H	126	ASN
1	H	158	TYR
1	H	162	THR

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Mol	Chain	Res	Type
1	H	166	ILE
1	H	167	ASP
1	H	172	ARG
1	H	175	THR
1	H	191	THR
1	H	322	LEU
1	H	356	MET
1	I	21	VAL
1	I	33	VAL
1	I	35	ILE
1	I	59	LEU
1	I	111	LEU
1	I	167	ASP
1	I	195	LEU
1	I	208	LEU
1	I	250	THR
1	I	264	ILE
1	I	295	ARG
1	I	353	ASN
1	I	356	MET
1	J	-2	HIS
1	J	191	THR
1	J	195	LEU
1	J	269	ASP
1	K	1	MET
1	K	14	LEU
1	K	17	VAL
1	K	37	THR
1	K	42	LEU
1	K	45	THR
1	K	59	LEU
1	K	65	LEU
1	K	93	GLN
1	K	113	THR
1	K	131	GLN
1	K	137	ARG
1	K	194	GLN
1	K	195	LEU
1	K	220	THR
1	K	246	VAL
1	K	282	SER
1	K	372	ASP

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Mol	Chain	Res	Type
1	L	3	LEU
1	L	8	GLU
1	L	138	GLU
1	L	155	VAL
1	L	170	GLN
1	L	183	LEU
1	L	195	LEU
1	L	215	GLU
1	L	216	ASP
1	L	218	GLN
1	L	220	THR
1	L	286	VAL
1	L	347	LEU
1	L	357	THR
1	M	71	THR
1	M	78	MET
1	M	95	THR
1	M	101	ILE
1	M	107	SER
1	M	117	GLU
1	M	128	GLN
1	M	155	VAL
1	M	156	ARG
1	M	176	THR
1	M	186	ILE
1	M	195	LEU
1	M	214	ILE
1	M	262	ARG
1	M	361	GLN
1	M	378	MET
1	N	5	ILE
1	N	44	ILE
1	N	187	LEU
1	N	214	ILE
1	N	216	ASP
1	N	259	ASP
1	N	270	LYS
1	N	273	LEU
1	N	278	VAL
1	N	319	ILE
1	N	346	VAL
1	N	363	VAL

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Mol	Chain	Res	Type
1	O	12	ASN
1	O	51	VAL
1	O	65	LEU
1	O	92	LEU
1	O	94	ILE
1	O	96	GLU
1	O	98	GLN
1	O	100	CYS
1	O	152	VAL
1	O	156	ARG
1	O	159	LEU
1	O	160	THR
1	O	162	THR
1	O	174	VAL
1	O	185	GLU
1	O	220	THR
1	O	222	LEU
1	O	230	VAL
1	O	245	THR
1	O	246	VAL
1	O	274	ILE
1	O	299	LEU
1	O	322	LEU
1	O	346	VAL
1	O	348	ASP
1	P	5	ILE
1	P	11	LEU
1	P	71	THR
1	P	124	THR
1	P	127	SER
1	P	155	VAL
1	P	186	ILE
1	P	195	LEU
1	P	228	LEU
1	P	246	VAL
1	P	269	ASP
1	P	272	VAL
1	P	274	ILE
1	P	282	SER
1	P	322	LEU
1	P	325	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	131	GLN
1	A	169	ASN
1	A	271	HIS
1	A	302	ASN
1	B	12	ASN
1	B	126	ASN
1	B	271	HIS
1	B	302	ASN
1	B	311	ASN
1	C	128	GLN
1	C	133	GLN
1	C	197	GLN
1	C	209	GLN
1	C	303	GLN
1	C	373	GLN
1	D	12	ASN
1	D	16	HIS
1	D	98	GLN
1	D	284	GLN
1	D	291	ASN
1	D	302	ASN
1	E	0	HIS
1	E	136	GLN
1	E	169	ASN
1	E	194	GLN
1	E	218	GLN
1	E	302	ASN
1	E	325	GLN
1	E	361	GLN
1	F	32	ASN
1	F	36	GLN
1	F	126	ASN
1	F	131	GLN
1	F	133	GLN
1	F	153	GLN
1	F	218	GLN
1	F	233	ASN
1	F	302	ASN
1	F	373	GLN
1	G	0	HIS
1	G	233	ASN

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Mol	Chain	Res	Type
1	G	307	GLN
1	G	361	GLN
1	G	373	GLN
1	H	36	GLN
1	H	93	GLN
1	H	126	ASN
1	H	133	GLN
1	H	218	GLN
1	H	229	ASN
1	H	325	GLN
1	H	338	GLN
1	H	353	ASN
1	H	361	GLN
1	I	40	GLN
1	I	98	GLN
1	I	153	GLN
1	I	170	GLN
1	I	229	ASN
1	I	281	GLN
1	I	311	ASN
1	I	353	ASN
1	J	0	HIS
1	J	128	GLN
1	J	133	GLN
1	J	153	GLN
1	J	194	GLN
1	J	291	ASN
1	J	302	ASN
1	J	315	GLN
1	J	366	GLN
1	J	370	HIS
1	K	126	ASN
1	K	131	GLN
1	K	133	GLN
1	K	197	GLN
1	K	218	GLN
1	K	291	ASN
1	L	-1	HIS
1	L	128	GLN
1	L	136	GLN
1	L	281	GLN
1	L	284	GLN

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Mol	Chain	Res	Type
1	L	302	ASN
1	L	303	GLN
1	M	12	ASN
1	M	136	GLN
1	M	170	GLN
1	M	302	ASN
1	M	315	GLN
1	M	325	GLN
1	M	327	GLN
1	M	353	ASN
1	M	366	GLN
1	N	0	HIS
1	N	36	GLN
1	N	98	GLN
1	N	128	GLN
1	N	131	GLN
1	N	133	GLN
1	N	302	ASN
1	O	40	GLN
1	O	98	GLN
1	O	153	GLN
1	O	179	HIS
1	O	209	GLN
1	O	218	GLN
1	O	291	ASN
1	O	311	ASN
1	O	327	GLN
1	P	36	GLN
1	P	302	ASN
1	P	307	GLN
1	P	327	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	378/388 (97%)	0.57	24 (6%)	26	22	27, 56, 94, 134	0
1	B	382/388 (98%)	0.40	13 (3%)	48	41	18, 44, 86, 118	0
1	C	379/388 (97%)	0.63	27 (7%)	22	19	30, 54, 92, 114	1 (0%)
1	D	382/388 (98%)	0.36	21 (5%)	30	25	15, 39, 72, 101	1 (0%)
1	E	382/388 (98%)	0.12	9 (2%)	59	51	12, 32, 63, 132	0
1	F	379/388 (97%)	0.37	11 (2%)	53	46	26, 46, 76, 121	1 (0%)
1	G	378/388 (97%)	0.58	22 (5%)	29	24	21, 50, 89, 128	2 (0%)
1	H	383/388 (98%)	0.69	27 (7%)	22	19	30, 59, 95, 128	0
1	I	370/388 (95%)	0.80	34 (9%)	14	13	28, 65, 98, 148	3 (0%)
1	J	384/388 (98%)	0.53	21 (5%)	30	25	22, 52, 85, 108	1 (0%)
1	K	365/388 (94%)	0.93	69 (18%)	3	3	20, 51, 110, 134	4 (1%)
1	L	356/388 (91%)	1.13	67 (18%)	3	3	29, 78, 116, 149	1 (0%)
1	M	378/388 (97%)	0.58	20 (5%)	32	27	20, 53, 96, 118	0
1	N	372/388 (95%)	0.75	22 (5%)	28	23	22, 64, 98, 120	2 (0%)
1	O	357/388 (92%)	1.39	70 (19%)	3	3	39, 81, 108, 136	0
1	P	377/388 (97%)	0.80	27 (7%)	21	19	30, 63, 105, 132	0
All	All	6002/6208 (96%)	0.66	484 (8%)	18	16	12, 55, 101, 149	16 (0%)

All (484) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	102	LEU	5.6
1	D	235	PRO	5.6
1	K	5	ILE	5.6
1	G	195	LEU	5.6
1	G	188	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	187	LEU	5.5
1	K	63	ALA	5.4
1	J	289	LEU	5.0
1	K	46	GLY	5.0
1	D	188	ALA	5.0
1	G	37	THR	5.0
1	M	37	THR	4.9
1	K	3	LEU	4.7
1	K	33	VAL	4.7
1	B	191	THR	4.7
1	H	-2	HIS	4.7
1	K	64	CYS	4.6
1	G	64	CYS	4.6
1	K	42	LEU	4.5
1	N	60	SER	4.5
1	L	243	ASP	4.4
1	L	283	LEU	4.4
1	C	266	ARG	4.2
1	L	214	ILE	4.2
1	H	127	SER	4.2
1	F	155	VAL	4.1
1	G	304	ASP	4.1
1	B	190	SER	4.1
1	K	95	THR	4.0
1	O	153	GLN	4.0
1	J	381	ARG	4.0
1	B	155	VAL	4.0
1	K	62	GLY	3.9
1	D	356	MET	3.9
1	I	369	ALA	3.9
1	O	66	GLU	3.8
1	O	59	LEU	3.8
1	M	78	MET	3.8
1	L	139	LEU	3.8
1	M	195	LEU	3.8
1	C	359	ALA	3.7
1	L	354	MET	3.7
1	P	5	ILE	3.7
1	G	189	SER	3.7
1	N	279	PHE	3.7
1	E	37	THR	3.7
1	A	268	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	O	244	ILE	3.6
1	C	37	THR	3.6
1	G	187	LEU	3.6
1	D	236	SER	3.6
1	O	223	ILE	3.6
1	H	37	THR	3.6
1	M	269	ASP	3.6
1	N	37	THR	3.6
1	O	357	THR	3.6
1	K	53	LEU	3.6
1	G	193	SER	3.5
1	K	37	THR	3.5
1	K	17	VAL	3.5
1	O	363	VAL	3.5
1	F	356	MET	3.5
1	L	265	PRO	3.5
1	L	187	LEU	3.5
1	L	190	SER	3.4
1	O	376	VAL	3.4
1	B	154	ASP	3.4
1	D	243	ASP	3.4
1	O	221	LEU	3.4
1	K	78	MET	3.4
1	H	61	GLU	3.3
1	H	-1	HIS	3.3
1	K	127	SER	3.3
1	O	303	GLN	3.3
1	O	228	LEU	3.3
1	K	86	THR	3.3
1	K	96	GLU	3.3
1	L	168	GLU	3.3
1	O	199	ILE	3.3
1	K	55	ALA	3.3
1	P	156	ARG	3.3
1	K	11	LEU	3.2
1	O	369	ALA	3.2
1	J	155	VAL	3.2
1	K	54	VAL	3.2
1	O	368	PRO	3.2
1	O	154	ASP	3.2
1	L	183	LEU	3.2
1	I	25	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	N	322	LEU	3.1
1	C	-2	HIS	3.1
1	G	303	GLN	3.1
1	O	314	GLU	3.1
1	J	266	ARG	3.1
1	K	195	LEU	3.1
1	I	203	LYS	3.1
1	E	242	GLY	3.1
1	L	285	ARG	3.1
1	J	348	ASP	3.1
1	O	155	VAL	3.1
1	P	243	ASP	3.1
1	L	347	LEU	3.1
1	F	351	ASP	3.1
1	O	362	SER	3.1
1	I	29	ILE	3.1
1	M	191	THR	3.1
1	L	279	PHE	3.0
1	A	129	GLY	3.0
1	G	194	GLN	3.0
1	D	262	ARG	3.0
1	O	1	MET	3.0
1	K	35	ILE	3.0
1	A	353	ASN	3.0
1	O	273	LEU	3.0
1	J	78	MET	3.0
1	K	44	ILE	3.0
1	L	223	ILE	3.0
1	L	355	SER	3.0
1	M	189	SER	3.0
1	A	41	ALA	3.0
1	I	187	LEU	2.9
1	K	47	SER	2.9
1	P	236	SER	2.9
1	L	356	MET	2.9
1	O	377	VAL	2.9
1	O	274	ILE	2.9
1	K	65	LEU	2.9
1	D	126	ASN	2.9
1	K	191	THR	2.9
1	L	258	PRO	2.9
1	C	78	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	192	SER	2.9
1	K	57	THR	2.9
1	C	331	LEU	2.9
1	I	28	ASN	2.9
1	K	116	ALA	2.9
1	O	51	VAL	2.9
1	O	259	ASP	2.9
1	O	367	ASP	2.9
1	F	225	ARG	2.9
1	I	192	SER	2.9
1	O	60	SER	2.9
1	I	49	LEU	2.9
1	L	289	LEU	2.9
1	P	214	ILE	2.9
1	M	242	GLY	2.8
1	A	356	MET	2.8
1	B	78	MET	2.8
1	C	128	GLN	2.8
1	N	369	ALA	2.8
1	O	304	ASP	2.8
1	C	190	SER	2.8
1	M	356	MET	2.8
1	C	153	GLN	2.8
1	D	258	PRO	2.8
1	D	186	ILE	2.8
1	L	264	ILE	2.8
1	L	364	LEU	2.8
1	L	220	THR	2.8
1	J	243	ASP	2.8
1	H	355	SER	2.8
1	K	104	SER	2.8
1	O	234	THR	2.8
1	I	55	ALA	2.8
1	L	323	ALA	2.8
1	L	353	ASN	2.8
1	K	71	THR	2.8
1	I	46	GLY	2.8
1	L	181	LEU	2.7
1	L	-1	HIS	2.7
1	F	242	GLY	2.7
1	N	168	GLU	2.7
1	K	6	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	171	LEU	2.7
1	O	42	LEU	2.7
1	D	-2	HIS	2.7
1	E	78	MET	2.7
1	H	78	MET	2.7
1	B	37	THR	2.7
1	E	243	ASP	2.7
1	O	355	SER	2.7
1	P	60	SER	2.7
1	H	128	GLN	2.7
1	C	323	ALA	2.7
1	I	42	LEU	2.7
1	L	195	LEU	2.7
1	G	100	CYS	2.7
1	G	356	MET	2.7
1	I	235	PRO	2.7
1	L	362	SER	2.7
1	L	132	VAL	2.7
1	L	322	LEU	2.7
1	K	88	ALA	2.7
1	O	156	ARG	2.7
1	A	242	GLY	2.7
1	O	220	THR	2.7
1	O	267	GLY	2.7
1	P	191	THR	2.7
1	L	342	ASP	2.7
1	D	92	LEU	2.7
1	O	306	LEU	2.7
1	N	354	MET	2.6
1	F	37	THR	2.6
1	L	340	LEU	2.6
1	L	186	ILE	2.6
1	M	190	SER	2.6
1	O	179	HIS	2.6
1	L	345	GLY	2.6
1	G	169	ASN	2.6
1	G	325	GLN	2.6
1	K	18	VAL	2.6
1	M	92	LEU	2.6
1	K	109	PHE	2.6
1	K	100	CYS	2.6
1	A	191	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	162	THR	2.6
1	C	154	ASP	2.6
1	C	243	ASP	2.6
1	P	58	ALA	2.6
1	A	127	SER	2.6
1	C	189	SER	2.6
1	D	195	LEU	2.6
1	H	155	VAL	2.6
1	L	166	ILE	2.6
1	O	90	ILE	2.6
1	B	157	PHE	2.6
1	F	126	ASN	2.6
1	K	87	ALA	2.6
1	M	126	ASN	2.6
1	O	55	ALA	2.6
1	O	67	ALA	2.6
1	M	-1	HIS	2.5
1	J	334	SER	2.5
1	A	273	LEU	2.5
1	L	339	TYR	2.5
1	O	65	LEU	2.5
1	L	286	VAL	2.5
1	L	335	PHE	2.5
1	O	248	PHE	2.5
1	N	360	ASN	2.5
1	H	267	GLY	2.5
1	K	10	LEU	2.5
1	K	111	LEU	2.5
1	L	341	LEU	2.5
1	M	268	GLY	2.5
1	N	299	LEU	2.5
1	O	102	LEU	2.5
1	K	1	MET	2.5
1	K	72	VAL	2.5
1	P	109	PHE	2.5
1	N	353	ASN	2.5
1	C	127	SER	2.5
1	H	129	GLY	2.5
1	E	67	ALA	2.5
1	O	250	THR	2.5
1	A	271	HIS	2.5
1	O	78	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	164	LEU	2.5
1	O	349	GLY	2.5
1	B	156	ARG	2.5
1	K	43	THR	2.5
1	K	45	THR	2.5
1	C	302	ASN	2.5
1	I	81	CYS	2.5
1	K	126	ASN	2.5
1	C	187	LEU	2.4
1	F	304	ASP	2.4
1	K	14	LEU	2.4
1	H	235	PRO	2.4
1	K	90	ILE	2.4
1	L	141	ARG	2.4
1	A	40	GLN	2.4
1	G	58	ALA	2.4
1	H	63	ALA	2.4
1	O	270	LYS	2.4
1	E	57	THR	2.4
1	F	357	THR	2.4
1	I	378	MET	2.4
1	L	184	CYS	2.4
1	L	304	ASP	2.4
1	P	155	VAL	2.4
1	K	4	LYS	2.4
1	L	257	PHE	2.4
1	O	165	GLU	2.4
1	P	157	PHE	2.4
1	I	303	GLN	2.4
1	N	42	LEU	2.4
1	O	252	LEU	2.4
1	N	167	ASP	2.4
1	O	268	GLY	2.4
1	L	237	ARG	2.4
1	K	66	GLU	2.4
1	D	37	THR	2.4
1	I	26	THR	2.4
1	B	-1	HIS	2.4
1	J	187	LEU	2.4
1	J	322	LEU	2.4
1	O	253	ILE	2.4
1	A	277	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	254	ASP	2.4
1	I	87	ALA	2.4
1	I	193	SER	2.4
1	A	130	THR	2.4
1	L	158	TYR	2.4
1	K	59	LEU	2.4
1	I	258	PRO	2.4
1	K	360	ASN	2.3
1	H	269	ASP	2.3
1	M	243	ASP	2.3
1	P	91	ASP	2.3
1	K	36	GLN	2.3
1	L	236	SER	2.3
1	I	11	LEU	2.3
1	O	260	TYR	2.3
1	L	235	PRO	2.3
1	L	278	VAL	2.3
1	G	62	GLY	2.3
1	J	242	GLY	2.3
1	K	97	ASP	2.3
1	J	303	GLN	2.3
1	N	327	GLN	2.3
1	P	283	LEU	2.3
1	N	-1	HIS	2.3
1	B	5	ILE	2.3
1	K	101	ILE	2.3
1	A	13	VAL	2.3
1	L	318	ALA	2.3
1	O	310	ALA	2.3
1	J	49	LEU	2.3
1	N	171	LEU	2.3
1	O	222	LEU	2.3
1	I	223	ILE	2.3
1	L	260	TYR	2.3
1	H	62	GLY	2.3
1	H	242	GLY	2.3
1	A	128	GLN	2.3
1	C	166	ILE	2.3
1	G	81	CYS	2.3
1	J	-1	HIS	2.3
1	C	191	THR	2.3
1	D	189	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	374	THR	2.3
1	L	263	VAL	2.3
1	N	196	VAL	2.3
1	K	378[A]	MET	2.2
1	C	369	ALA	2.2
1	I	27	LEU	2.2
1	P	53	LEU	2.2
1	O	366	GLN	2.2
1	O	44	ILE	2.2
1	K	99	ARG	2.2
1	L	176	THR	2.2
1	C	326	TYR	2.2
1	G	190	SER	2.2
1	L	305	SER	2.2
1	L	368	PRO	2.2
1	H	158	TYR	2.2
1	P	380	MET	2.2
1	I	228	LEU	2.2
1	K	61	GLU	2.2
1	K	7	LYS	2.2
1	P	82	LYS	2.2
1	H	223	ILE	2.2
1	K	98	GLN	2.2
1	E	277	ASP	2.2
1	A	17	VAL	2.2
1	D	234	THR	2.2
1	L	37	THR	2.2
1	D	267	GLY	2.2
1	L	28	ASN	2.2
1	H	330	PRO	2.2
1	M	124	THR	2.2
1	H	178	GLY	2.2
1	O	193	SER	2.2
1	O	171	LEU	2.2
1	A	217	GLU	2.2
1	H	58	ALA	2.2
1	N	359	ALA	2.2
1	L	29	ILE	2.2
1	I	32	ASN	2.2
1	O	229	ASN	2.2
1	E	-1	HIS	2.2
1	C	167	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	330	PRO	2.2
1	C	376	VAL	2.2
1	K	91	ASP	2.2
1	K	110	VAL	2.2
1	A	37	THR	2.2
1	O	175	THR	2.2
1	L	301	PHE	2.2
1	O	257	PHE	2.2
1	B	195	LEU	2.2
1	K	211	LEU	2.2
1	P	59	LEU	2.2
1	P	102	LEU	2.2
1	F	58	ALA	2.2
1	J	359	ALA	2.2
1	K	58	ALA	2.2
1	K	244	ILE	2.1
1	L	284	GLN	2.1
1	O	325	GLN	2.1
1	N	28	ASN	2.1
1	P	0	HIS	2.1
1	O	230	VAL	2.1
1	H	380	MET	2.1
1	D	239	LYS	2.1
1	K	112	GLY	2.1
1	I	102	LEU	2.1
1	I	109	PHE	2.1
1	K	248	PHE	2.1
1	O	299	LEU	2.1
1	A	369	ALA	2.1
1	G	63	ALA	2.1
1	I	190	SER	2.1
1	M	193	SER	2.1
1	P	190	SER	2.1
1	I	311	ASN	2.1
1	K	28	ASN	2.1
1	J	272	VAL	2.1
1	N	273	LEU	2.1
1	A	193	SER	2.1
1	I	186	ILE	2.1
1	J	332	GLU	2.1
1	P	107	SER	2.1
1	D	194	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	134	VAL	2.1
1	L	280	LYS	2.1
1	N	78	MET	2.1
1	O	205	VAL	2.1
1	J	368	PRO	2.1
1	D	269	ASP	2.1
1	I	65	LEU	2.1
1	L	349	GLY	2.1
1	N	283	LEU	2.1
1	O	341	LEU	2.1
1	P	65	LEU	2.1
1	K	220	THR	2.1
1	P	269	ASP	2.1
1	H	261	ARG	2.1
1	K	325	GLN	2.1
1	I	201	PRO	2.1
1	G	353	ASN	2.1
1	J	126	ASN	2.1
1	H	65	LEU	2.1
1	A	267	GLY	2.1
1	D	-1	HIS	2.0
1	E	325	GLN	2.0
1	H	271	HIS	2.0
1	J	271	HIS	2.0
1	B	330	PRO	2.0
1	A	187	LEU	2.0
1	B	126	ASN	2.0
1	G	92	LEU	2.0
1	P	2	ARG	2.0
1	A	220	THR	2.0
1	C	367	ASP	2.0
1	G	186	ILE	2.0
1	K	113	THR	2.0
1	I	198	ALA	2.0
1	L	367	ASP	2.0
1	M	215	GLU	2.0
1	K	34	LYS	2.0
1	A	78	MET	2.0
1	H	378	MET	2.0
1	C	60	SER	2.0
1	I	9	SER	2.0
1	P	192	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	59	LEU	2.0
1	L	49	LEU	2.0
1	C	28	ASN	2.0
1	C	126	ASN	2.0
1	H	130	THR	2.0
1	M	58	ALA	2.0
1	O	37	THR	2.0
1	O	130	THR	2.0
1	O	374	THR	2.0
1	J	217	GLU	2.0
1	L	348	ASP	2.0
1	M	48	ASP	2.0
1	P	117	GLU	2.0
1	P	348	ASP	2.0
1	F	78	MET	2.0
1	O	378	MET	2.0
1	L	174	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	C	401	1/1	0.83	0.09	30,30,30,30	0
2	MG	J	401	1/1	0.95	0.08	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.