



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 4, 2017 – 06:42 PM EST

PDB ID : 5JYG
EMDB ID: : EMD-8180
Title : Cryo-EM structure of the MamK filament at 6.5 Å
Authors : Bergeron, J.R.C.; Hutto, R.; Kollman, J.M.
Deposited on : 2016-05-13
Resolution : 6.50 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

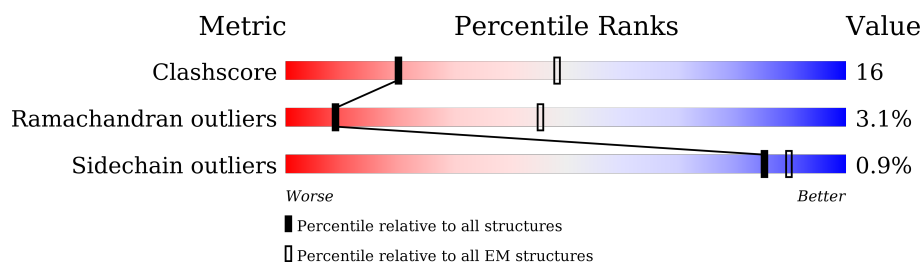
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	
1	D	347	
1	E	347	
1	F	347	
1	G	347	
1	H	347	
1	I	347	

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Mol	Chain	Length	Quality of chain
1	J	347	<div><div></div><div>79%</div><div>12%</div><div>• 5%</div></div>
1	K	347	<div><div></div><div>75%</div><div>15%</div><div>5% 5%</div></div>
1	L	347	<div><div></div><div>76%</div><div>14%</div><div>• 5%</div></div>
1	M	347	<div><div></div><div>74%</div><div>16%</div><div>5% 5%</div></div>
1	N	347	<div><div></div><div>80%</div><div>10%</div><div>• 5%</div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35462 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Actin-like ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	B	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	C	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	D	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	E	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	F	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	G	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	H	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	I	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	J	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	K	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	L	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	M	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		
1	N	328	Total	C	N	O	S	0	0
			2505	1592	430	471	12		

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

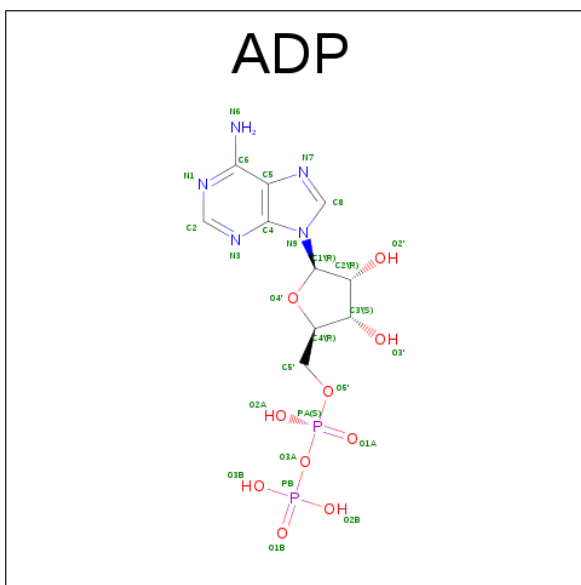
Mol	Chain	Residues	Atoms		AltConf
2	G	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
2	J	1	Total 1	Mg 1	0
2	D	1	Total 1	Mg 1	0
2	K	1	Total 1	Mg 1	0
2	E	1	Total 1	Mg 1	0
2	H	1	Total 1	Mg 1	0
2	B	1	Total 1	Mg 1	0
2	I	1	Total 1	Mg 1	0
2	C	1	Total 1	Mg 1	0
2	A	1	Total 1	Mg 1	0
2	N	1	Total 1	Mg 1	0
2	L	1	Total 1	Mg 1	0
2	F	1	Total 1	Mg 1	0
2	M	1	Total 1	Mg 1	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).




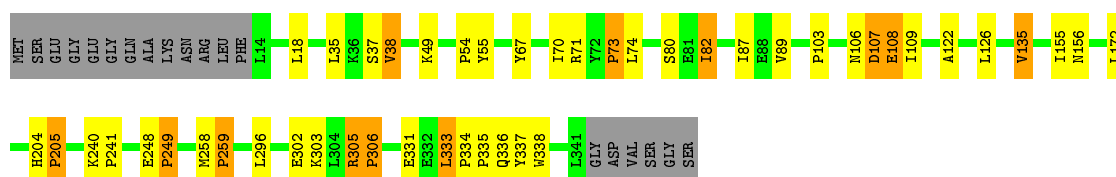
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0
3	K	1	Total 27	C 10	N 5	O 10	P 2	0
3	L	1	Total 27	C 10	N 5	O 10	P 2	0
3	M	1	Total 27	C 10	N 5	O 10	P 2	0
3	N	1	Total 27	C 10	N 5	O 10	P 2	0

3 Residue-property plots

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

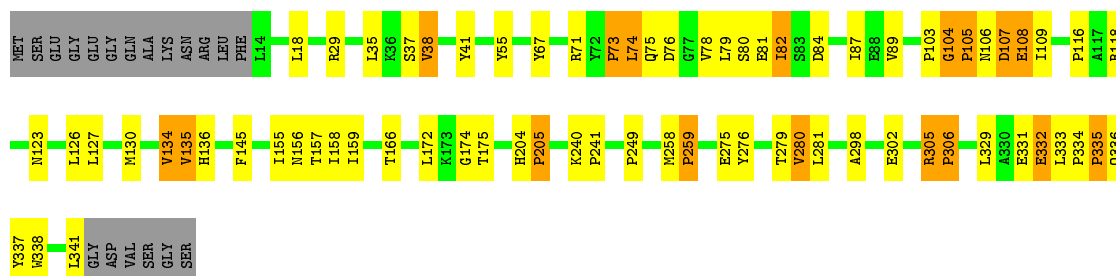
• Molecule 1: Actin-like ATPase

Chain A: 




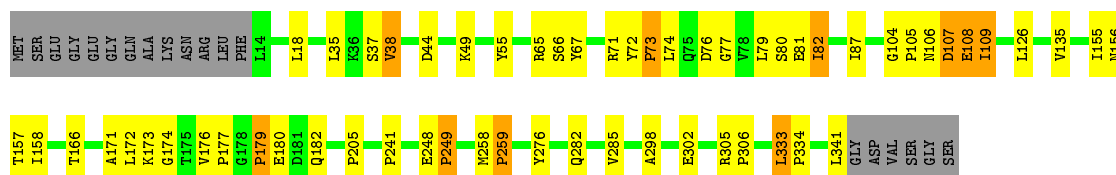
• Molecule 1: Actin-like ATPase

Chain B: 



• Molecule 1: Actin-like ATPase

Chain C: 

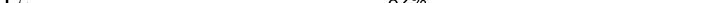


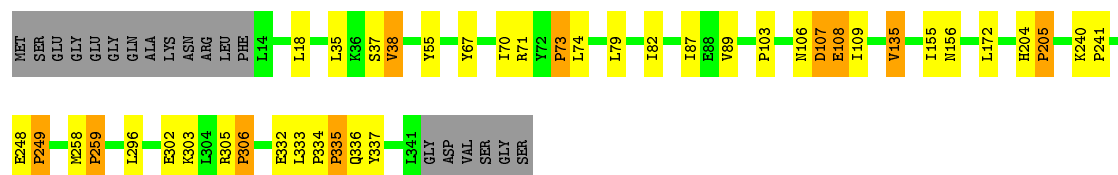
• Molecule 1: Actin-like ATPase

Chain D: 



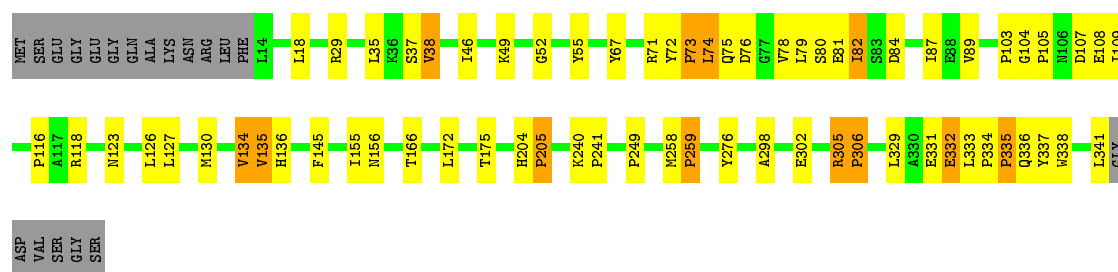
- Molecule 1: Actin-like ATPase

Chain E:  82% 9% • 5%

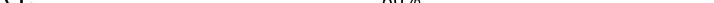


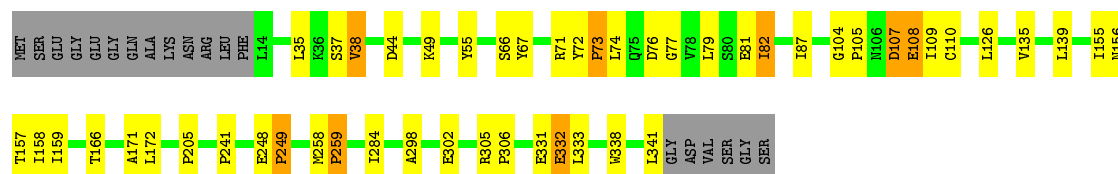
- Molecule 1: Actin-like ATPase

Chain F:  75% 16% 5%



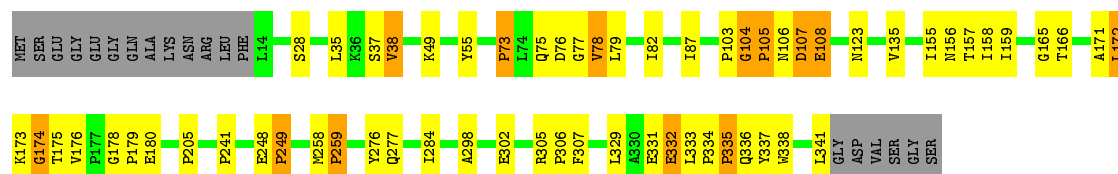
- Molecule 1: Actin-like ATPase

Chain G:  80% 12% • 5%



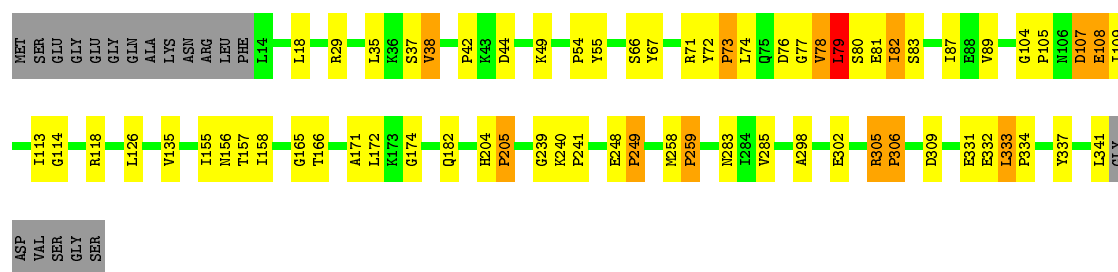
- Molecule 1: Actin-like ATPase

Chain H: 77% 14% 5%



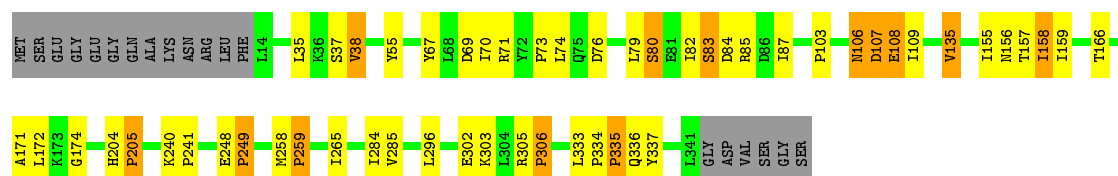
- Molecule 1: Actin-like ATPase

Chain I: 75% 16% 5%



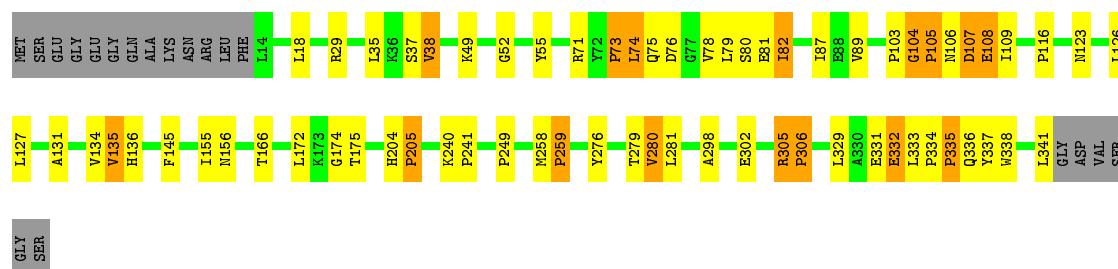
• Molecule 1: Actin-like ATPase

Chain J: 79% 12% 5%



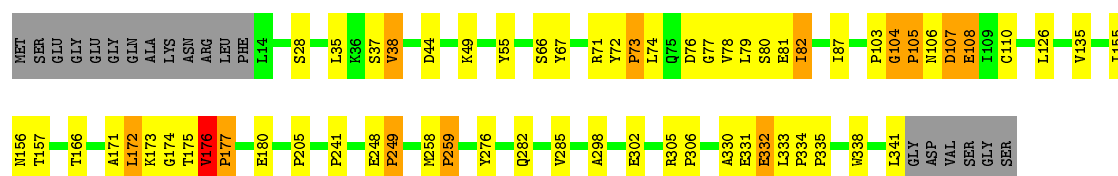
• Molecule 1: Actin-like ATPase

Chain K: 75% 15% 5% 5%



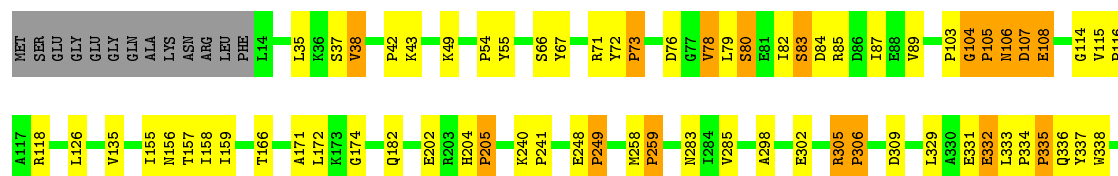
• Molecule 1: Actin-like ATPase

Chain L: 76% 14% 5%



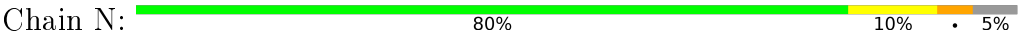
• Molecule 1: Actin-like ATPase

Chain M: 74% 16% 5% 5%



L341
GLY
ASP
VAL
SER
GLY
SER

● Molecule 1: Actin-like ATPase



MET	SER	GLU	GLY	GLY	GLY	GLN	ALA	LYS	ASN	ARG	LEU	PHE	L14	L35	K36	S37	V38	K49	P54	Y55	Y67	I70	R71	V72	P73	L79	I82	I87	F88	V89	P103	M106	D107	E108	I109	V134	V135	T155	N156	T157	I158	I159	A171	L172	K173	G174	
H204	P205	K240	P241	E248	P249	N258	P259	I284	V285	L296	E302	K303	L304	R305	P306	L333	P334	P335	Q336	Y337	L341	GLY	ASP	VAL	SER	GLY	SER																				

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	8129	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.76	4/2550 (0.2%)	0.68	1/3462 (0.0%)
1	B	0.78	4/2550 (0.2%)	0.73	2/3462 (0.1%)
1	C	0.77	4/2550 (0.2%)	0.70	2/3462 (0.1%)
1	D	0.76	4/2550 (0.2%)	0.75	2/3462 (0.1%)
1	E	0.76	4/2550 (0.2%)	0.68	1/3462 (0.0%)
1	F	0.77	4/2550 (0.2%)	0.69	2/3462 (0.1%)
1	G	0.77	4/2550 (0.2%)	0.71	2/3462 (0.1%)
1	H	0.77	4/2550 (0.2%)	0.78	3/3462 (0.1%)
1	I	0.77	4/2550 (0.2%)	0.73	2/3462 (0.1%)
1	J	0.76	4/2550 (0.2%)	0.68	1/3462 (0.0%)
1	K	0.78	4/2550 (0.2%)	0.73	2/3462 (0.1%)
1	L	0.77	4/2550 (0.2%)	0.78	4/3462 (0.1%)
1	M	0.77	4/2550 (0.2%)	0.74	3/3462 (0.1%)
1	N	0.77	4/2550 (0.2%)	0.69	1/3462 (0.0%)
All	All	0.77	56/35700 (0.2%)	0.72	28/48468 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
All	All	0	28

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	249	PRO	N-CD	8.51	1.59	1.47
1	B	249	PRO	N-CD	8.51	1.59	1.47
1	F	249	PRO	N-CD	8.48	1.59	1.47
1	C	205	PRO	N-CD	8.29	1.59	1.47
1	L	205	PRO	N-CD	8.28	1.59	1.47
1	D	205	PRO	N-CD	8.28	1.59	1.47
1	G	205	PRO	N-CD	8.27	1.59	1.47
1	H	205	PRO	N-CD	8.27	1.59	1.47
1	M	205	PRO	N-CD	8.23	1.59	1.47
1	I	205	PRO	N-CD	8.21	1.59	1.47
1	B	205	PRO	N-CD	8.18	1.59	1.47
1	F	205	PRO	N-CD	8.16	1.59	1.47
1	K	205	PRO	N-CD	8.16	1.59	1.47
1	N	205	PRO	N-CD	7.95	1.58	1.47
1	A	205	PRO	N-CD	7.90	1.58	1.47
1	J	205	PRO	N-CD	7.89	1.58	1.47
1	E	205	PRO	N-CD	7.86	1.58	1.47
1	I	249	PRO	N-CD	7.34	1.58	1.47
1	M	249	PRO	N-CD	7.33	1.58	1.47
1	D	249	PRO	N-CD	7.30	1.58	1.47
1	N	249	PRO	N-CD	7.26	1.58	1.47
1	J	249	PRO	N-CD	7.24	1.57	1.47
1	C	249	PRO	N-CD	7.23	1.57	1.47
1	H	249	PRO	N-CD	7.21	1.57	1.47
1	A	249	PRO	N-CD	7.20	1.57	1.47
1	E	249	PRO	N-CD	7.20	1.57	1.47
1	G	249	PRO	N-CD	7.20	1.57	1.47
1	L	249	PRO	N-CD	7.17	1.57	1.47
1	B	259	PRO	N-CD	6.14	1.56	1.47
1	K	259	PRO	N-CD	6.13	1.56	1.47
1	A	259	PRO	N-CD	6.13	1.56	1.47
1	F	259	PRO	N-CD	6.13	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	259	PRO	N-CD	6.10	1.56	1.47
1	E	259	PRO	N-CD	6.10	1.56	1.47
1	D	259	PRO	N-CD	6.09	1.56	1.47
1	G	259	PRO	N-CD	6.09	1.56	1.47
1	H	259	PRO	N-CD	6.08	1.56	1.47
1	C	259	PRO	N-CD	6.06	1.56	1.47
1	N	259	PRO	N-CD	6.06	1.56	1.47
1	I	259	PRO	N-CD	6.04	1.56	1.47
1	L	259	PRO	N-CD	6.04	1.56	1.47
1	M	259	PRO	N-CD	6.03	1.56	1.47
1	G	241	PRO	N-CD	5.52	1.55	1.47
1	C	241	PRO	N-CD	5.52	1.55	1.47
1	H	241	PRO	N-CD	5.51	1.55	1.47
1	L	241	PRO	N-CD	5.51	1.55	1.47
1	D	306	PRO	N-CD	5.28	1.55	1.47
1	I	306	PRO	N-CD	5.23	1.55	1.47
1	M	306	PRO	N-CD	5.21	1.55	1.47
1	N	306	PRO	N-CD	5.12	1.55	1.47
1	J	306	PRO	N-CD	5.09	1.54	1.47
1	E	306	PRO	N-CD	5.09	1.54	1.47
1	K	306	PRO	N-CD	5.09	1.54	1.47
1	A	306	PRO	N-CD	5.08	1.54	1.47
1	F	306	PRO	N-CD	5.06	1.54	1.47
1	B	306	PRO	N-CD	5.05	1.54	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	72	TYR	C-N-CD	-17.57	81.95	120.60
1	H	178	GLY	C-N-CD	-17.54	82.02	120.60
1	L	176	VAL	C-N-CD	-16.55	84.20	120.60
1	K	104	GLY	C-N-CD	-15.82	85.80	120.60
1	B	104	GLY	C-N-CD	-15.59	86.31	120.60
1	H	104	GLY	C-N-CD	-12.89	92.24	120.60
1	I	72	TYR	C-N-CD	-12.76	92.52	120.60
1	L	104	GLY	C-N-CD	-12.75	92.54	120.60
1	M	104	GLY	C-N-CD	-12.24	93.67	120.60
1	G	72	TYR	C-N-CD	-10.47	97.56	120.60
1	M	72	TYR	C-N-CD	-9.86	98.91	120.60
1	C	72	TYR	C-N-CD	-8.94	100.94	120.60
1	L	72	TYR	C-N-CD	-8.86	101.11	120.60
1	D	306	PRO	CA-N-CD	-6.65	102.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	306	PRO	CA-N-CD	-6.65	102.19	111.50
1	M	306	PRO	CA-N-CD	-6.62	102.23	111.50
1	N	306	PRO	CA-N-CD	-6.60	102.26	111.50
1	J	306	PRO	CA-N-CD	-6.59	102.27	111.50
1	E	306	PRO	CA-N-CD	-6.59	102.27	111.50
1	F	306	PRO	CA-N-CD	-6.57	102.30	111.50
1	A	306	PRO	CA-N-CD	-6.57	102.30	111.50
1	K	306	PRO	CA-N-CD	-6.55	102.33	111.50
1	B	306	PRO	CA-N-CD	-6.53	102.36	111.50
1	G	306	PRO	CA-N-CD	-6.49	102.42	111.50
1	L	306	PRO	CA-N-CD	-6.47	102.44	111.50
1	C	306	PRO	CA-N-CD	-6.47	102.44	111.50
1	H	306	PRO	CA-N-CD	-6.46	102.45	111.50
1	F	72	TYR	C-N-CD	-6.26	106.83	120.60

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	ARG	Peptide
1	A	35	LEU	Mainchain
1	B	305	ARG	Peptide
1	B	35	LEU	Mainchain
1	C	305	ARG	Peptide
1	C	35	LEU	Mainchain
1	D	305	ARG	Peptide
1	D	35	LEU	Mainchain
1	E	305	ARG	Peptide
1	E	35	LEU	Mainchain
1	F	305	ARG	Peptide
1	F	35	LEU	Mainchain
1	G	305	ARG	Peptide
1	G	35	LEU	Mainchain
1	H	305	ARG	Peptide
1	H	35	LEU	Mainchain
1	I	305	ARG	Peptide
1	I	35	LEU	Mainchain
1	J	305	ARG	Peptide
1	J	35	LEU	Mainchain
1	K	305	ARG	Peptide
1	K	35	LEU	Mainchain
1	L	305	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	L	35	LEU	Mainchain
1	M	305	ARG	Peptide
1	M	35	LEU	Mainchain
1	N	305	ARG	Peptide
1	N	35	LEU	Mainchain

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	2505	0	2553	39	0
1	B	2505	0	2551	117	0
1	C	2505	0	2553	92	0
1	D	2505	0	2552	103	0
1	E	2505	0	2553	46	0
1	F	2505	0	2552	90	0
1	G	2505	0	2553	64	0
1	H	2505	0	2553	92	0
1	I	2505	0	2553	105	0
1	J	2505	0	2553	76	0
1	K	2505	0	2553	96	0
1	L	2505	0	2553	121	0
1	M	2505	0	2552	137	0
1	N	2505	0	2553	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	0	0
3	H	27	0	12	0	0
3	I	27	0	12	2	0
3	J	27	0	12	0	0
3	K	27	0	12	0	0
3	L	27	0	12	0	0
3	M	27	0	12	0	0
3	N	27	0	12	0	0
All	All	35462	0	35905	1148	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 16.

All (1148) 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:H:333:LEU:HD12	1:H:338:TRP:NE1	1.29	1.40
1:L:176:VAL:HG12	1:L:177:PRO:CD	1.50	1.40
1:L:176:VAL:CG1	1:L:177:PRO:HD2	1.51	1.40
1:L:155:ILE:CG2	1:M:67:TYR:OH	1.73	1.37
1:G:333:LEU:HD12	1:G:338:TRP:NE1	1.30	1.37
1:N:156:ASN:ND2	1:N:172:LEU:O	1.59	1.33
1:H:329:LEU:O	1:H:333:LEU:CD2	1.73	1.32
1:J:156:ASN:ND2	1:J:172:LEU:O	1.60	1.32
1:B:71:ARG:HD3	1:B:84:ASP:OD1	1.33	1.29
1:I:73:PRO:CG	1:I:89:VAL:HG11	1.63	1.28
1:J:107:ASP:O	1:J:109:ILE:HG12	1.34	1.28
1:K:134:VAL:O	1:K:135:VAL:HG12	1.31	1.27
1:L:155:ILE:CB	1:M:67:TYR:OH	1.81	1.27
1:E:107:ASP:O	1:E:109:ILE:HG12	1.35	1.27
1:L:110:CYS:SG	1:L:338:TRP:CZ3	2.27	1.26
1:H:276:TYR:OH	1:I:66:SER:HB3	1.24	1.26
1:C:176:VAL:HB	1:D:44:ASP:OD2	1.28	1.25
1:A:107:ASP:O	1:A:109:ILE:HG12	1.36	1.25
1:L:155:ILE:HG21	1:M:67:TYR:OH	1.20	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:107:ASP:O	1:N:109:ILE:HG12	1.33	1.25
1:H:333:LEU:CD1	1:H:338:TRP:HE1	1.49	1.24
1:M:82:ILE:O	1:M:84:ASP:N	1.70	1.22
1:C:156:ASN:ND2	1:C:172:LEU:O	1.72	1.22
1:B:175:THR:HG22	1:C:44:ASP:OD1	1.40	1.22
1:H:155:ILE:HB	1:I:67:TYR:OH	1.38	1.20
1:H:333:LEU:HB3	1:H:338:TRP:CZ2	1.78	1.19
1:M:80:SER:O	1:M:126:LEU:HD22	1.40	1.19
1:I:18:LEU:CD1	1:I:78:VAL:HA	1.73	1.19
1:L:333:LEU:HD12	1:L:333:LEU:O	1.41	1.19
1:L:276:TYR:OH	1:M:66:SER:HB2	1.39	1.19
1:D:43:LYS:HD2	1:D:69:ASP:HB2	1.23	1.18
1:G:110:CYS:SG	1:G:338:TRP:CZ3	2.37	1.17
1:C:177:PRO:HG3	1:C:180:GLU:OE1	1.45	1.17
1:F:333:LEU:HB3	1:F:338:TRP:NE1	1.59	1.17
1:H:76:ASP:HB3	1:H:165:GLY:HA2	1.17	1.17
1:M:82:ILE:HG23	1:M:89:VAL:HB	1.27	1.16
1:B:333:LEU:HB3	1:B:338:TRP:NE1	1.60	1.15
1:I:71:ARG:O	1:I:73:PRO:HD3	1.45	1.14
1:B:29:ARG:HH12	1:B:105:PRO:HG3	0.98	1.14
1:B:71:ARG:CD	1:B:84:ASP:OD1	1.96	1.14
1:D:73:PRO:HB3	1:D:89:VAL:HG11	1.30	1.14
1:H:174:GLY:HA2	1:I:44:ASP:OD2	1.45	1.13
1:B:130:MET:O	1:B:134:VAL:HG23	1.46	1.13
1:L:155:ILE:CG1	1:M:67:TYR:OH	1.96	1.13
1:L:173:LYS:HG2	1:L:180:GLU:CG	1.79	1.13
1:K:333:LEU:HB3	1:K:338:TRP:NE1	1.60	1.13
1:J:334:PRO:O	1:J:336:GLN:N	1.82	1.12
1:J:74:LEU:HD23	1:J:79:LEU:CA	1.78	1.12
1:F:130:MET:O	1:F:134:VAL:HG23	1.45	1.12
1:D:333:LEU:HB3	1:D:338:TRP:NE1	1.64	1.12
1:F:78:VAL:HB	1:F:116:PRO:HG3	1.16	1.12
1:L:155:ILE:HG12	1:M:67:TYR:OH	1.49	1.11
1:N:134:VAL:O	1:N:135:VAL:HG22	1.47	1.11
1:B:156:ASN:ND2	1:B:172:LEU:O	1.83	1.11
1:G:333:LEU:CD1	1:G:338:TRP:HE1	1.62	1.11
1:K:29:ARG:HH12	1:K:105:PRO:HG3	1.00	1.11
1:D:78:VAL:HG22	1:D:79:LEU:H	1.02	1.11
1:N:334:PRO:O	1:N:336:GLN:N	1.82	1.11
1:M:333:LEU:HB3	1:M:338:TRP:NE1	1.66	1.10
1:H:76:ASP:HB3	1:H:165:GLY:CA	1.80	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:173:LYS:HG2	1:H:174:GLY:H	1.07	1.10
1:C:177:PRO:HG2	1:C:180:GLU:HB2	1.17	1.09
1:B:29:ARG:NH1	1:B:105:PRO:HG3	1.67	1.09
1:L:173:LYS:HG3	1:L:174:GLY:H	0.97	1.09
1:C:276:TYR:OH	1:D:66:SER:HB2	1.53	1.08
1:I:78:VAL:CG1	1:I:113:ILE:HG22	1.81	1.08
1:K:78:VAL:HB	1:K:116:PRO:HG3	1.32	1.08
1:I:79:LEU:O	1:I:126:LEU:HD23	1.52	1.08
1:J:74:LEU:HD23	1:J:79:LEU:HA	1.15	1.08
1:K:104:GLY:N	1:K:105:PRO:CD	2.17	1.07
1:H:329:LEU:O	1:H:333:LEU:HD23	1.41	1.07
1:B:104:GLY:N	1:B:105:PRO:CD	2.17	1.07
1:M:78:VAL:HG12	1:M:79:LEU:N	1.65	1.07
1:B:78:VAL:HB	1:B:116:PRO:HG3	1.31	1.07
1:E:333:LEU:HG	1:E:337:TYR:CD1	1.89	1.06
1:M:79:LEU:O	1:M:126:LEU:HD23	1.54	1.06
1:H:79:LEU:CD1	1:H:123:ASN:OD1	2.03	1.06
1:G:156:ASN:ND2	1:G:172:LEU:O	1.88	1.05
1:F:175:THR:HG22	1:G:44:ASP:OD1	1.54	1.05
1:K:29:ARG:NH1	1:K:105:PRO:HG3	1.69	1.05
1:M:78:VAL:HG12	1:M:79:LEU:H	0.89	1.05
1:K:134:VAL:O	1:K:135:VAL:CG1	2.03	1.05
1:M:78:VAL:CG1	1:M:79:LEU:H	1.67	1.04
1:M:156:ASN:HD21	1:M:171:ALA:HB1	1.22	1.04
1:I:76:ASP:HB2	1:I:165:GLY:HA3	1.37	1.04
1:H:104:GLY:N	1:H:105:PRO:CD	2.21	1.03
1:H:329:LEU:O	1:H:333:LEU:HD21	1.53	1.02
1:B:79:LEU:HD11	1:B:127:LEU:HD21	1.41	1.02
1:I:78:VAL:CG1	1:I:113:ILE:CG2	2.36	1.02
1:B:104:GLY:N	1:B:105:PRO:HD2	1.73	1.02
1:M:104:GLY:N	1:M:105:PRO:CD	2.22	1.02
1:I:78:VAL:HG11	1:I:113:ILE:HG22	1.38	1.01
1:L:104:GLY:N	1:L:105:PRO:CD	2.22	1.01
1:I:156:ASN:HD21	1:I:171:ALA:HB1	1.22	1.01
1:K:79:LEU:HD11	1:K:127:LEU:HD21	1.43	1.01
1:G:74:LEU:HD23	1:G:74:LEU:O	1.60	1.01
1:H:333:LEU:HB3	1:H:338:TRP:CE2	1.93	1.01
1:I:79:LEU:O	1:I:126:LEU:CD2	2.09	1.00
1:M:82:ILE:HG23	1:M:89:VAL:CB	1.91	1.00
1:H:171:ALA:O	1:H:172:LEU:O	1.78	1.00
1:H:104:GLY:N	1:H:105:PRO:HD2	1.76	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:LEU:HB3	1:M:126:LEU:HD21	1.43	1.00
1:K:104:GLY:N	1:K:105:PRO:HD2	1.74	1.00
1:C:74:LEU:CD2	1:C:79:LEU:HD12	1.92	1.00
1:H:276:TYR:OH	1:I:66:SER:CB	2.10	0.99
1:K:333:LEU:HB3	1:K:338:TRP:HE1	1.24	0.99
1:B:276:TYR:OH	1:C:66:SER:CB	2.10	0.99
1:D:156:ASN:HD21	1:D:171:ALA:HB1	1.27	0.99
1:K:175:THR:HG22	1:L:44:ASP:OD1	1.63	0.99
1:H:155:ILE:CB	1:I:67:TYR:OH	2.11	0.98
1:I:18:LEU:HD13	1:I:78:VAL:HA	1.38	0.98
1:H:79:LEU:HD13	1:H:123:ASN:OD1	1.62	0.98
1:I:73:PRO:HG3	1:I:89:VAL:CG1	1.91	0.98
1:L:104:GLY:N	1:L:105:PRO:HD2	1.77	0.98
1:L:333:LEU:HD22	1:L:338:TRP:CZ2	1.98	0.98
1:L:155:ILE:HG21	1:M:67:TYR:HH	1.16	0.98
1:B:71:ARG:HD3	1:B:84:ASP:CG	1.84	0.97
1:G:333:LEU:CD1	1:G:338:TRP:NE1	2.23	0.97
1:M:104:GLY:N	1:M:105:PRO:HD2	1.77	0.97
1:L:110:CYS:HG	1:L:338:TRP:HZ3	0.99	0.97
1:H:174:GLY:O	1:I:44:ASP:OD1	1.81	0.97
1:C:176:VAL:CB	1:D:44:ASP:OD2	2.13	0.96
1:L:173:LYS:HG2	1:L:180:GLU:HG3	1.46	0.96
1:J:333:LEU:HG	1:J:337:TYR:CD1	1.99	0.96
1:B:333:LEU:HB3	1:B:338:TRP:HE1	1.24	0.96
1:I:73:PRO:HG3	1:I:89:VAL:HG11	0.98	0.96
1:C:177:PRO:CG	1:C:180:GLU:HB2	1.96	0.95
1:E:156:ASN:ND2	1:E:172:LEU:O	1.99	0.95
1:N:333:LEU:HG	1:N:337:TYR:CD1	1.99	0.95
1:A:156:ASN:ND2	1:A:172:LEU:O	2.00	0.95
1:G:74:LEU:HD21	1:G:77:GLY:HA2	1.47	0.95
1:M:157:THR:HG21	1:M:285:VAL:HG23	1.49	0.94
1:I:157:THR:HG21	1:I:285:VAL:HG23	1.49	0.94
1:M:333:LEU:HB3	1:M:338:TRP:CE2	2.02	0.94
1:B:276:TYR:OH	1:C:66:SER:HB2	1.67	0.94
1:L:176:VAL:CB	1:L:177:PRO:HD2	1.96	0.94
1:L:330:ALA:O	1:L:333:LEU:HD23	1.65	0.94
1:L:333:LEU:HD22	1:L:338:TRP:HZ2	1.30	0.94
1:C:18:LEU:HD21	1:C:74:LEU:HD11	1.46	0.94
1:L:173:LYS:HG3	1:L:174:GLY:N	1.80	0.94
1:D:78:VAL:HG22	1:D:79:LEU:N	1.82	0.94
1:M:79:LEU:C	1:M:126:LEU:CD2	2.36	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:82:ILE:O	1:J:84:ASP:N	2.00	0.93
1:L:176:VAL:CB	1:L:177:PRO:CD	2.43	0.93
1:H:333:LEU:CB	1:H:338:TRP:CZ2	2.50	0.93
1:I:18:LEU:CD1	1:I:78:VAL:HG12	1.97	0.93
1:L:333:LEU:HD13	1:L:338:TRP:CZ2	2.02	0.93
1:L:276:TYR:OH	1:M:66:SER:CB	2.17	0.93
1:I:78:VAL:HG11	1:I:113:ILE:CG2	1.97	0.92
1:D:157:THR:HG21	1:D:285:VAL:HG23	1.49	0.92
1:F:333:LEU:HB3	1:F:338:TRP:HE1	1.24	0.92
1:A:334:PRO:O	1:A:336:GLN:N	2.03	0.91
1:A:333:LEU:HG	1:A:337:TYR:CD1	2.05	0.91
1:E:333:LEU:HG	1:E:337:TYR:CE1	2.04	0.91
1:N:107:ASP:O	1:N:109:ILE:CG1	2.19	0.91
1:B:71:ARG:CD	1:B:84:ASP:CG	2.39	0.91
1:M:79:LEU:C	1:M:126:LEU:HD23	1.92	0.90
1:H:276:TYR:HH	1:I:66:SER:HB3	1.35	0.90
1:L:173:LYS:CG	1:L:174:GLY:H	1.80	0.90
1:D:333:LEU:HB3	1:D:338:TRP:CE2	2.07	0.90
1:D:73:PRO:CB	1:D:89:VAL:HG11	2.01	0.89
1:L:173:LYS:HG2	1:L:180:GLU:CB	2.01	0.89
1:L:176:VAL:CG1	1:L:177:PRO:CD	2.24	0.89
1:B:71:ARG:CZ	1:B:84:ASP:OD1	2.20	0.89
1:M:82:ILE:HG21	1:M:89:VAL:H	1.36	0.89
1:F:79:LEU:HD11	1:F:127:LEU:HD21	1.55	0.89
1:H:333:LEU:HD12	1:H:338:TRP:CD1	2.08	0.89
1:N:107:ASP:O	1:N:109:ILE:N	2.07	0.88
1:M:79:LEU:O	1:M:126:LEU:CD2	2.21	0.88
1:M:82:ILE:CG2	1:M:89:VAL:H	1.85	0.88
1:F:104:GLY:N	1:F:105:PRO:CD	2.36	0.88
1:I:18:LEU:HD11	1:I:78:VAL:HG12	1.51	0.88
1:L:176:VAL:HG12	1:L:177:PRO:HD2	0.88	0.88
1:M:329:LEU:O	1:M:333:LEU:CD2	2.22	0.88
1:J:107:ASP:O	1:J:109:ILE:N	2.07	0.88
1:K:175:THR:HG22	1:L:44:ASP:CG	1.94	0.87
1:E:107:ASP:O	1:E:109:ILE:N	2.08	0.87
1:J:70:ILE:O	1:J:70:ILE:HG22	1.70	0.87
1:H:173:LYS:HG2	1:H:174:GLY:N	1.89	0.87
1:M:79:LEU:HB3	1:M:126:LEU:CD2	2.05	0.87
1:B:29:ARG:HH12	1:B:105:PRO:CG	1.84	0.87
1:C:74:LEU:CD2	1:C:79:LEU:CD1	2.52	0.87
1:H:333:LEU:HD12	1:H:338:TRP:HE1	0.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:333:LEU:HD13	1:L:338:TRP:CH2	2.10	0.87
1:L:333:LEU:CD1	1:L:333:LEU:O	2.23	0.87
1:F:156:ASN:ND2	1:F:172:LEU:O	2.08	0.86
1:M:157:THR:CG2	1:M:285:VAL:HG23	2.06	0.86
1:J:107:ASP:O	1:J:109:ILE:CG1	2.21	0.86
1:N:71:ARG:O	1:N:73:PRO:HD3	1.75	0.86
1:D:79:LEU:HD21	1:D:130:MET:SD	2.15	0.86
1:F:78:VAL:HB	1:F:116:PRO:CG	2.02	0.86
1:C:177:PRO:HG2	1:C:180:GLU:CB	2.03	0.85
1:D:329:LEU:O	1:D:333:LEU:CD2	2.23	0.85
1:E:107:ASP:O	1:E:109:ILE:CG1	2.23	0.85
1:I:157:THR:CG2	1:I:285:VAL:HG23	2.06	0.85
1:J:74:LEU:CD2	1:J:79:LEU:CA	2.54	0.85
1:K:29:ARG:NH1	1:K:105:PRO:CG	2.39	0.85
1:I:78:VAL:HG12	1:I:113:ILE:CG2	2.04	0.85
1:B:71:ARG:NH1	1:B:84:ASP:OD1	2.10	0.85
1:F:104:GLY:N	1:F:105:PRO:HD2	1.91	0.85
1:L:155:ILE:HG21	1:M:67:TYR:CZ	2.11	0.85
1:A:107:ASP:O	1:A:109:ILE:N	2.08	0.85
1:B:71:ARG:NE	1:B:84:ASP:OD1	2.10	0.85
1:D:157:THR:CG2	1:D:285:VAL:HG23	2.06	0.85
1:K:29:ARG:HH12	1:K:105:PRO:CG	1.86	0.85
1:B:29:ARG:NH1	1:B:105:PRO:CG	2.38	0.85
1:L:173:LYS:HG2	1:L:180:GLU:HB3	1.59	0.85
1:E:71:ARG:O	1:E:73:PRO:HD3	1.77	0.84
1:F:333:LEU:CB	1:F:338:TRP:HE1	1.89	0.84
1:L:176:VAL:HG12	1:L:177:PRO:HD3	1.58	0.84
1:M:78:VAL:CG2	1:M:115:VAL:HA	2.07	0.84
1:B:329:LEU:O	1:B:333:LEU:CD2	2.25	0.84
1:K:329:LEU:O	1:K:333:LEU:CD2	2.25	0.84
1:H:28:SER:HB2	1:H:107:ASP:OD2	1.78	0.84
1:L:87:ILE:HG22	1:L:87:ILE:O	1.76	0.84
1:F:78:VAL:CB	1:F:116:PRO:HG3	2.06	0.84
1:C:74:LEU:HD22	1:C:79:LEU:HD12	1.59	0.84
1:I:18:LEU:HD12	1:I:78:VAL:CG1	2.06	0.84
1:C:155:ILE:HD11	1:C:172:LEU:HB2	1.60	0.84
1:F:49:LYS:O	1:F:52:GLY:O	1.96	0.84
1:G:87:ILE:O	1:G:87:ILE:HG22	1.76	0.84
1:I:104:GLY:N	1:I:105:PRO:HD2	1.93	0.84
1:D:104:GLY:N	1:D:105:PRO:HD2	1.93	0.84
1:K:79:LEU:CD1	1:K:127:LEU:HD21	2.06	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:GLY:N	1:G:105:PRO:HD2	1.93	0.83
1:K:49:LYS:O	1:K:52:GLY:O	1.96	0.83
1:B:79:LEU:CD1	1:B:127:LEU:HD21	2.07	0.83
1:B:333:LEU:CB	1:B:338:TRP:HE1	1.91	0.83
1:B:71:ARG:CD	1:B:84:ASP:OD2	2.26	0.83
1:K:333:LEU:CB	1:K:338:TRP:HE1	1.91	0.83
1:K:156:ASN:ND2	1:K:172:LEU:O	2.11	0.83
1:L:28:SER:HB2	1:L:107:ASP:OD2	1.78	0.83
1:H:87:ILE:HG22	1:H:87:ILE:O	1.76	0.83
1:B:71:ARG:HD2	1:B:84:ASP:OD2	1.79	0.83
1:C:87:ILE:HG22	1:C:87:ILE:O	1.76	0.83
1:J:71:ARG:O	1:J:73:PRO:HD3	1.79	0.83
1:I:104:GLY:N	1:I:105:PRO:CD	2.41	0.82
1:H:76:ASP:CB	1:H:165:GLY:HA2	2.04	0.82
1:J:157:THR:HG21	1:J:285:VAL:HG23	1.62	0.82
1:J:155:ILE:HG23	1:J:156:ASN:HB2	1.62	0.82
1:F:333:LEU:HB3	1:F:338:TRP:CE2	2.14	0.82
1:G:104:GLY:N	1:G:105:PRO:CD	2.43	0.82
1:M:79:LEU:CB	1:M:126:LEU:CD2	2.57	0.82
1:B:333:LEU:HB3	1:B:338:TRP:CE2	2.15	0.82
1:D:104:GLY:N	1:D:105:PRO:CD	2.41	0.81
1:H:333:LEU:CD1	1:H:338:TRP:NE1	2.19	0.81
1:C:18:LEU:CD2	1:C:74:LEU:HD11	2.10	0.81
1:J:69:ASP:OD1	1:J:71:ARG:HG3	1.80	0.81
1:A:107:ASP:O	1:A:109:ILE:CG1	2.25	0.81
1:B:175:THR:HG22	1:C:44:ASP:CG	2.01	0.81
1:N:155:ILE:HG23	1:N:156:ASN:HB2	1.63	0.81
1:D:334:PRO:O	1:D:336:GLN:N	2.15	0.80
1:F:329:LEU:O	1:F:333:LEU:CD2	2.28	0.80
1:J:156:ASN:OD1	1:J:172:LEU:N	2.15	0.80
1:B:155:ILE:HB	1:C:67:TYR:OH	1.82	0.80
1:H:28:SER:CB	1:H:107:ASP:OD2	2.30	0.80
1:L:28:SER:CB	1:L:107:ASP:OD2	2.30	0.80
1:K:333:LEU:HB3	1:K:338:TRP:CE2	2.16	0.79
1:M:329:LEU:O	1:M:333:LEU:HD23	1.79	0.79
1:L:155:ILE:CG2	1:M:67:TYR:HH	1.74	0.79
1:N:134:VAL:O	1:N:135:VAL:CG2	2.30	0.78
1:F:107:ASP:O	1:F:109:ILE:N	2.13	0.78
1:M:333:LEU:CG	1:M:338:TRP:HE1	1.97	0.78
1:M:42:PRO:HG2	1:M:49:LYS:HB2	1.65	0.78
1:E:333:LEU:HG	1:E:337:TYR:CG	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:VAL:HG23	1:B:116:PRO:HD2	1.66	0.78
1:E:87:ILE:O	1:E:87:ILE:HG22	1.84	0.78
1:N:73:PRO:HB3	1:N:89:VAL:HG11	1.64	0.78
1:N:156:ASN:OD1	1:N:172:LEU:N	2.16	0.78
1:E:73:PRO:HB3	1:E:89:VAL:HG11	1.65	0.78
1:M:87:ILE:O	1:M:87:ILE:HG22	1.84	0.77
1:I:18:LEU:CD1	1:I:78:VAL:CA	2.58	0.77
1:K:104:GLY:N	1:K:105:PRO:HD3	2.00	0.77
1:G:333:LEU:HD12	1:G:338:TRP:CD1	2.17	0.77
1:I:18:LEU:CD1	1:I:78:VAL:CG1	2.61	0.77
1:I:76:ASP:OD2	1:I:166:THR:N	2.14	0.77
1:D:71:ARG:O	1:D:72:TYR:O	2.01	0.77
1:B:104:GLY:N	1:B:105:PRO:HD3	2.00	0.77
1:H:155:ILE:CG2	1:I:67:TYR:OH	2.32	0.77
1:D:43:LYS:CD	1:D:69:ASP:HB2	2.12	0.76
1:D:333:LEU:HB3	1:D:338:TRP:HE1	1.46	0.76
1:M:333:LEU:HD12	1:M:338:TRP:CD1	2.20	0.76
1:M:333:LEU:HB3	1:M:338:TRP:HE1	1.49	0.76
1:M:333:LEU:CB	1:M:338:TRP:NE1	2.48	0.76
1:D:87:ILE:HG22	1:D:87:ILE:O	1.84	0.76
1:I:87:ILE:HG22	1:I:87:ILE:O	1.84	0.76
1:D:79:LEU:HD13	1:D:126:LEU:HB3	1.68	0.76
1:N:87:ILE:HG22	1:N:87:ILE:O	1.84	0.76
1:H:79:LEU:HD12	1:H:123:ASN:OD1	1.84	0.75
1:K:78:VAL:HG23	1:K:116:PRO:HD2	1.65	0.75
1:N:157:THR:HG21	1:N:285:VAL:HG23	1.68	0.75
1:J:74:LEU:CD2	1:J:79:LEU:HB2	2.15	0.75
1:A:87:ILE:O	1:A:87:ILE:HG22	1.84	0.75
1:F:79:LEU:CD1	1:F:127:LEU:HD21	2.16	0.75
1:F:175:THR:HG22	1:G:44:ASP:CG	2.06	0.75
1:B:78:VAL:CB	1:B:116:PRO:HG3	2.15	0.75
1:J:87:ILE:HG22	1:J:87:ILE:O	1.84	0.75
1:L:330:ALA:O	1:L:333:LEU:CD2	2.35	0.75
1:K:134:VAL:O	1:K:135:VAL:CB	2.35	0.74
1:M:82:ILE:C	1:M:84:ASP:H	1.89	0.74
1:G:333:LEU:HD12	1:G:338:TRP:HE1	0.93	0.74
1:M:334:PRO:O	1:M:336:GLN:N	2.20	0.74
1:L:155:ILE:HG12	1:M:67:TYR:HH	1.49	0.74
1:B:71:ARG:O	1:B:73:PRO:HD3	1.87	0.74
1:B:41:TYR:OH	1:B:71:ARG:NH2	2.20	0.74
1:H:76:ASP:CB	1:H:165:GLY:CA	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:71:ARG:O	1:K:73:PRO:HD3	1.88	0.74
1:C:276:TYR:OH	1:D:66:SER:CB	2.33	0.73
1:D:78:VAL:CG2	1:D:79:LEU:H	1.86	0.73
1:J:333:LEU:HG	1:J:337:TYR:CE1	2.22	0.73
1:I:76:ASP:CG	3:I:402:ADP:O2B	2.25	0.73
1:H:79:LEU:HD13	1:H:123:ASN:CG	2.08	0.73
1:D:156:ASN:ND2	1:D:171:ALA:HB1	2.01	0.73
1:H:173:LYS:CG	1:H:174:GLY:H	1.89	0.73
1:K:329:LEU:O	1:K:333:LEU:HD23	1.88	0.73
1:M:82:ILE:N	1:M:82:ILE:HD13	2.03	0.73
1:D:334:PRO:O	1:D:337:TYR:N	2.21	0.73
1:D:155:ILE:HG23	1:D:156:ASN:HB2	1.70	0.73
1:M:73:PRO:HB3	1:M:89:VAL:HG11	1.71	0.73
1:F:78:VAL:HG23	1:F:116:PRO:HD2	1.69	0.73
1:L:155:ILE:HB	1:M:67:TYR:OH	1.87	0.73
1:C:157:THR:OG1	1:C:282:GLN:HB3	1.89	0.72
1:K:131:ALA:HB1	1:K:136:HIS:O	1.88	0.72
1:M:334:PRO:O	1:M:337:TYR:N	2.21	0.72
1:L:155:ILE:CG1	1:M:67:TYR:HH	2.02	0.72
1:F:329:LEU:O	1:F:333:LEU:HD23	1.88	0.72
1:M:157:THR:HG21	1:M:285:VAL:CG2	2.20	0.72
1:D:333:LEU:CB	1:D:338:TRP:NE1	2.49	0.72
1:B:279:THR:O	1:B:281:LEU:N	2.23	0.72
1:N:333:LEU:HG	1:N:337:TYR:CE1	2.23	0.72
1:I:157:THR:HG21	1:I:285:VAL:CG2	2.20	0.72
1:J:74:LEU:CD2	1:J:79:LEU:CB	2.68	0.72
1:E:333:LEU:N	1:E:334:PRO:HD3	2.04	0.72
1:K:134:VAL:C	1:K:135:VAL:HG12	2.09	0.72
1:K:87:ILE:HG22	1:K:87:ILE:O	1.88	0.72
1:M:107:ASP:O	1:M:108:GLU:C	2.25	0.72
1:B:329:LEU:O	1:B:333:LEU:HD23	1.89	0.72
1:B:41:TYR:HE2	1:B:71:ARG:HE	1.35	0.72
1:F:87:ILE:O	1:F:87:ILE:HG22	1.88	0.72
1:H:107:ASP:O	1:H:108:GLU:O	2.08	0.71
1:M:333:LEU:HD12	1:M:338:TRP:NE1	2.05	0.71
1:B:87:ILE:O	1:B:87:ILE:HG22	1.88	0.71
1:G:110:CYS:HG	1:G:338:TRP:HZ3	1.25	0.71
1:L:175:THR:HG22	1:M:43:LYS:HE2	1.71	0.71
1:C:77:GLY:HA3	1:C:166:THR:HG23	1.72	0.71
1:D:329:LEU:O	1:D:333:LEU:HD23	1.89	0.71
1:J:82:ILE:O	1:J:85:ARG:N	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:78:VAL:CB	1:K:116:PRO:HG3	2.15	0.71
1:K:175:THR:HG22	1:L:44:ASP:OD2	1.90	0.71
1:E:333:LEU:CG	1:E:337:TYR:CD1	2.70	0.71
1:L:107:ASP:O	1:L:108:GLU:C	2.28	0.71
1:M:107:ASP:O	1:M:108:GLU:O	2.08	0.71
1:D:79:LEU:HD11	1:D:130:MET:SD	2.30	0.71
1:F:276:TYR:OH	1:G:66:SER:CB	2.38	0.71
1:L:107:ASP:O	1:L:108:GLU:O	2.08	0.71
1:M:333:LEU:CB	1:M:338:TRP:HE1	2.03	0.71
1:F:107:ASP:O	1:F:109:ILE:HG12	1.91	0.71
1:D:333:LEU:CB	1:D:338:TRP:HE1	2.04	0.71
1:F:71:ARG:O	1:F:73:PRO:HD3	1.89	0.71
1:I:78:VAL:CG1	1:I:113:ILE:HG21	2.19	0.71
1:K:279:THR:O	1:K:281:LEU:N	2.22	0.71
1:L:157:THR:OG1	1:L:282:GLN:HB3	1.90	0.71
1:L:175:THR:CG2	1:M:43:LYS:HE2	2.21	0.71
1:L:77:GLY:HA3	1:L:166:THR:HG23	1.72	0.70
1:A:334:PRO:C	1:A:336:GLN:H	1.93	0.70
1:B:41:TYR:HE2	1:B:71:ARG:NE	1.89	0.70
1:D:157:THR:HG21	1:D:285:VAL:CG2	2.20	0.70
1:L:332:GLU:O	1:L:333:LEU:HG	1.91	0.70
1:B:334:PRO:O	1:B:337:TYR:N	2.24	0.70
1:I:81:GLU:O	1:I:82:ILE:HB	1.91	0.70
1:I:76:ASP:CB	1:I:165:GLY:HA3	2.16	0.70
1:K:78:VAL:HB	1:K:116:PRO:CG	2.16	0.70
1:M:79:LEU:CB	1:M:126:LEU:HD21	2.18	0.70
1:K:175:THR:CG2	1:L:44:ASP:OD2	2.39	0.70
1:M:71:ARG:HG3	1:M:71:ARG:HH11	1.56	0.70
1:H:107:ASP:O	1:H:108:GLU:C	2.29	0.70
1:K:334:PRO:O	1:K:337:TYR:N	2.24	0.70
1:L:110:CYS:SG	1:L:338:TRP:HZ3	1.93	0.70
1:M:156:ASN:ND2	1:M:171:ALA:HB1	2.01	0.70
1:C:74:LEU:HD21	1:C:79:LEU:CD1	2.21	0.70
1:F:334:PRO:O	1:F:337:TYR:N	2.24	0.70
1:F:276:TYR:OH	1:G:66:SER:HB2	1.92	0.69
1:D:333:LEU:CG	1:D:338:TRP:HE1	2.05	0.69
1:H:104:GLY:H	1:H:105:PRO:CD	2.05	0.69
1:E:155:ILE:N	1:E:155:ILE:HD12	2.08	0.69
1:K:78:VAL:HG23	1:K:116:PRO:CD	2.23	0.69
1:M:78:VAL:HG21	1:M:115:VAL:HA	1.74	0.69
1:F:334:PRO:O	1:F:336:GLN:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:74:LEU:CD2	1:G:77:GLY:HA2	2.21	0.69
1:B:334:PRO:O	1:B:336:GLN:N	2.26	0.69
1:M:79:LEU:CB	1:M:126:LEU:HD23	2.21	0.69
1:M:82:ILE:HG23	1:M:89:VAL:CG2	2.22	0.69
1:A:155:ILE:HD12	1:A:155:ILE:N	2.08	0.68
1:B:78:VAL:HB	1:B:116:PRO:CG	2.15	0.68
1:G:110:CYS:SG	1:G:338:TRP:CH2	2.86	0.68
1:H:155:ILE:HB	1:I:67:TYR:HH	1.54	0.68
1:M:104:GLY:H	1:M:105:PRO:CD	2.05	0.68
1:G:77:GLY:HA3	1:G:166:THR:HG23	1.76	0.68
1:J:156:ASN:CG	1:J:172:LEU:O	2.31	0.68
1:L:176:VAL:CG1	1:L:177:PRO:HD3	2.20	0.68
1:G:79:LEU:HB3	1:G:126:LEU:CD1	2.22	0.68
1:L:276:TYR:HH	1:M:66:SER:CB	2.05	0.68
1:F:109:ILE:CG2	1:F:136:HIS:CE1	2.77	0.68
1:F:333:LEU:CG	1:F:338:TRP:HE1	2.06	0.68
1:I:156:ASN:ND2	1:I:171:ALA:HB1	2.02	0.68
1:N:156:ASN:CG	1:N:172:LEU:O	2.32	0.68
1:B:279:THR:C	1:B:281:LEU:H	1.97	0.68
1:B:109:ILE:CG2	1:B:136:HIS:CE1	2.77	0.68
1:I:73:PRO:HG2	1:I:89:VAL:HG11	1.67	0.68
1:B:109:ILE:HG22	1:B:136:HIS:CE1	2.29	0.68
1:C:276:TYR:HH	1:D:66:SER:HB2	1.59	0.68
1:J:334:PRO:O	1:J:337:TYR:N	2.26	0.68
1:L:173:LYS:CG	1:L:180:GLU:HG3	2.22	0.68
1:L:110:CYS:SG	1:L:338:TRP:CH2	2.84	0.68
1:I:155:ILE:HG23	1:I:156:ASN:HB2	1.76	0.67
1:K:334:PRO:O	1:K:336:GLN:N	2.28	0.67
1:K:279:THR:C	1:K:281:LEU:H	1.97	0.67
1:M:155:ILE:HG23	1:M:156:ASN:HB2	1.75	0.67
1:C:156:ASN:HD21	1:C:172:LEU:N	1.93	0.67
1:A:73:PRO:HB3	1:A:89:VAL:HG11	1.76	0.67
1:I:18:LEU:HD12	1:I:78:VAL:HA	1.75	0.67
1:N:134:VAL:C	1:N:135:VAL:HG13	2.14	0.67
1:G:77:GLY:HA3	1:G:166:THR:CG2	2.25	0.67
1:I:78:VAL:HG12	1:I:113:ILE:HG21	1.77	0.67
1:D:156:ASN:CG	1:D:172:LEU:H	1.98	0.67
1:I:71:ARG:HH11	1:I:71:ARG:HG3	1.60	0.67
1:B:104:GLY:H	1:B:105:PRO:CD	2.08	0.67
1:C:108:GLU:HG2	1:C:108:GLU:O	1.95	0.67
1:M:71:ARG:HG3	1:M:71:ARG:NH1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:331:GLU:HG2	1:L:332:GLU:HA	1.77	0.66
1:B:78:VAL:HG23	1:B:116:PRO:CD	2.24	0.66
1:C:176:VAL:HB	1:D:44:ASP:CG	2.13	0.66
1:F:109:ILE:HG22	1:F:136:HIS:CE1	2.29	0.66
1:H:104:GLY:H	1:H:105:PRO:HD2	1.60	0.66
1:N:157:THR:CG2	1:N:285:VAL:HG23	2.26	0.66
1:N:334:PRO:O	1:N:337:TYR:N	2.27	0.66
1:M:82:ILE:H	1:M:82:ILE:HD13	1.58	0.66
1:J:157:THR:CG2	1:J:285:VAL:HG23	2.25	0.65
1:L:333:LEU:CD2	1:L:338:TRP:CZ2	2.79	0.65
1:J:74:LEU:HD21	1:J:79:LEU:HB2	1.77	0.65
1:K:104:GLY:H	1:K:105:PRO:CD	2.08	0.65
1:F:333:LEU:HD12	1:F:338:TRP:CD1	2.32	0.65
1:L:104:GLY:H	1:L:105:PRO:CD	2.06	0.65
1:L:106:ASN:O	1:L:108:GLU:N	2.27	0.65
1:B:333:LEU:CG	1:B:338:TRP:HE1	2.09	0.65
1:I:81:GLU:O	1:I:82:ILE:CB	2.44	0.65
1:K:18:LEU:HD21	1:K:74:LEU:HD11	1.77	0.65
1:B:18:LEU:HD21	1:B:74:LEU:HD11	1.79	0.65
1:C:107:ASP:C	1:C:109:ILE:H	1.99	0.65
1:J:74:LEU:HD23	1:J:79:LEU:CB	2.27	0.65
1:K:333:LEU:CG	1:K:338:TRP:HE1	2.09	0.65
1:G:331:GLU:HG2	1:G:332:GLU:HA	1.77	0.65
1:A:71:ARG:O	1:A:73:PRO:HD3	1.97	0.65
1:G:81:GLU:O	1:G:82:ILE:O	2.15	0.64
1:G:107:ASP:O	1:G:109:ILE:N	2.30	0.64
1:J:156:ASN:ND2	1:J:172:LEU:C	2.49	0.64
1:H:307:PHE:CE1	1:I:240:LYS:NZ	2.66	0.64
1:L:173:LYS:HE2	1:L:180:GLU:HG3	1.79	0.64
1:C:74:LEU:HD23	1:C:79:LEU:HA	1.79	0.64
1:M:82:ILE:HG22	1:M:84:ASP:HB2	1.79	0.64
1:M:73:PRO:CB	1:M:89:VAL:HG11	2.28	0.64
1:G:74:LEU:CD2	1:G:74:LEU:O	2.43	0.64
1:J:333:LEU:HG	1:J:337:TYR:CG	2.32	0.64
1:H:106:ASN:O	1:H:108:GLU:N	2.28	0.64
1:J:76:ASP:HB3	1:J:166:THR:HG23	1.80	0.64
1:B:79:LEU:CD1	1:B:127:LEU:CD2	2.76	0.63
1:B:75:GLN:O	1:B:78:VAL:HG12	1.99	0.63
1:C:156:ASN:HD21	1:C:171:ALA:C	2.02	0.63
1:J:333:LEU:CG	1:J:337:TYR:CD1	2.81	0.63
1:C:276:TYR:HH	1:D:66:SER:CB	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:LEU:CG	1:E:337:TYR:CE1	2.80	0.63
1:K:79:LEU:CD1	1:K:127:LEU:CD2	2.76	0.63
1:D:329:LEU:O	1:D:333:LEU:HD21	1.99	0.63
1:M:82:ILE:HG21	1:M:89:VAL:N	2.11	0.63
1:N:333:LEU:HG	1:N:337:TYR:CG	2.33	0.63
1:I:107:ASP:O	1:I:109:ILE:N	2.32	0.63
1:L:77:GLY:HA3	1:L:166:THR:CG2	2.29	0.63
1:C:77:GLY:HA3	1:C:166:THR:CG2	2.29	0.62
1:L:333:LEU:CD1	1:L:338:TRP:CZ2	2.81	0.62
1:M:78:VAL:HG21	1:M:115:VAL:HG12	1.81	0.62
1:M:42:PRO:HG2	1:M:49:LYS:CB	2.27	0.62
1:D:107:ASP:O	1:D:109:ILE:N	2.32	0.62
1:I:71:ARG:NH1	1:I:71:ARG:HG3	2.13	0.62
1:K:103:PRO:C	1:K:105:PRO:HD2	2.20	0.62
1:N:333:LEU:CG	1:N:337:TYR:CD1	2.81	0.62
1:K:81:GLU:O	1:K:82:ILE:HB	1.99	0.62
1:M:156:ASN:CG	1:M:172:LEU:H	2.02	0.62
1:B:103:PRO:C	1:B:105:PRO:HD2	2.19	0.62
1:B:79:LEU:HB3	1:B:126:LEU:HD23	1.82	0.62
1:C:174:GLY:HA3	1:D:66:SER:O	1.99	0.62
1:D:43:LYS:HD2	1:D:69:ASP:CB	2.14	0.62
1:D:45:VAL:O	1:D:45:VAL:HG12	2.00	0.62
1:H:331:GLU:HG2	1:H:332:GLU:HA	1.81	0.62
1:B:81:GLU:O	1:B:82:ILE:HB	2.00	0.62
1:H:104:GLY:N	1:H:105:PRO:HD3	2.13	0.62
1:B:329:LEU:O	1:B:333:LEU:HD21	2.00	0.61
1:J:135:VAL:O	1:J:135:VAL:HG23	2.00	0.61
1:K:75:GLN:O	1:K:78:VAL:HG12	1.99	0.61
1:L:28:SER:OG	1:L:107:ASP:OD2	2.18	0.61
1:H:329:LEU:C	1:H:333:LEU:CD2	2.65	0.61
1:M:333:LEU:HD12	1:M:338:TRP:HE1	1.64	0.61
1:H:78:VAL:O	1:H:78:VAL:HG13	2.00	0.61
1:B:118:ARG:NH1	1:I:118:ARG:HH12	1.98	0.61
1:I:156:ASN:CG	1:I:172:LEU:H	2.03	0.61
1:N:107:ASP:O	1:N:108:GLU:C	2.39	0.61
1:C:156:ASN:ND2	1:C:172:LEU:C	2.54	0.61
1:H:333:LEU:CG	1:H:338:TRP:HE1	2.11	0.61
1:A:333:LEU:N	1:A:334:PRO:HD3	2.14	0.61
1:D:104:GLY:H	1:D:105:PRO:CD	2.13	0.61
1:D:49:LYS:O	1:D:54:PRO:CA	2.49	0.61
1:J:334:PRO:O	1:J:335:PRO:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:GLU:O	1:F:82:ILE:HB	2.00	0.61
1:I:49:LYS:O	1:I:54:PRO:CA	2.49	0.61
1:M:49:LYS:O	1:M:54:PRO:CA	2.49	0.61
1:F:78:VAL:HG23	1:F:116:PRO:CD	2.31	0.61
1:F:75:GLN:O	1:F:78:VAL:HG12	2.00	0.61
1:E:155:ILE:HB	1:F:67:TYR:OH	2.01	0.60
1:G:108:GLU:O	1:G:108:GLU:HG2	2.01	0.60
1:G:110:CYS:SG	1:G:338:TRP:HZ3	2.12	0.60
1:N:156:ASN:ND2	1:N:172:LEU:C	2.50	0.60
1:A:155:ILE:HB	1:B:67:TYR:OH	2.02	0.60
1:C:174:GLY:HA2	1:D:67:TYR:CD1	2.35	0.60
1:M:333:LEU:CD1	1:M:338:TRP:HE1	2.14	0.60
1:E:135:VAL:O	1:E:135:VAL:HG23	2.00	0.60
1:F:155:ILE:CG1	1:G:67:TYR:OH	2.49	0.60
1:I:104:GLY:H	1:I:105:PRO:CD	2.13	0.60
1:A:135:VAL:HG23	1:A:135:VAL:O	2.00	0.60
1:M:78:VAL:HG23	1:M:115:VAL:HA	1.83	0.60
1:N:334:PRO:O	1:N:335:PRO:C	2.39	0.60
1:F:155:ILE:HG12	1:G:67:TYR:OH	2.01	0.60
1:M:73:PRO:HG3	1:M:89:VAL:HG11	1.84	0.60
1:C:155:ILE:HD11	1:C:172:LEU:CB	2.30	0.60
1:C:157:THR:O	1:C:157:THR:HG22	2.00	0.60
1:G:104:GLY:H	1:G:105:PRO:CD	2.13	0.60
1:K:107:ASP:O	1:K:108:GLU:C	2.40	0.60
1:L:74:LEU:O	1:L:74:LEU:HG	2.01	0.60
1:G:107:ASP:O	1:G:109:ILE:HG12	2.01	0.60
1:K:79:LEU:HB3	1:K:126:LEU:HD23	1.83	0.60
1:I:78:VAL:HG13	1:I:114:GLY:O	2.00	0.59
1:C:81:GLU:O	1:C:82:ILE:O	2.20	0.59
1:F:333:LEU:HD12	1:F:338:TRP:NE1	2.16	0.59
1:J:82:ILE:N	1:J:82:ILE:HD13	2.16	0.59
1:L:79:LEU:HB3	1:L:126:LEU:HD13	1.84	0.59
1:M:104:GLY:N	1:M:105:PRO:HD3	2.12	0.59
1:N:334:PRO:C	1:N:336:GLN:N	2.55	0.59
1:H:155:ILE:HG21	1:I:67:TYR:CE1	2.38	0.59
1:C:79:LEU:HB3	1:C:126:LEU:HD13	1.85	0.59
1:M:82:ILE:CG2	1:M:89:VAL:HB	2.18	0.59
1:B:155:ILE:HG12	1:C:67:TYR:OH	2.02	0.59
1:D:108:GLU:O	1:D:108:GLU:HG2	2.03	0.59
1:M:80:SER:O	1:M:126:LEU:CD2	2.33	0.59
1:F:78:VAL:HG22	1:F:123:ASN:ND2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:ASP:HB3	1:H:165:GLY:HA3	1.79	0.59
1:B:333:LEU:HD12	1:B:338:TRP:CD1	2.38	0.59
1:D:333:LEU:HD12	1:D:338:TRP:CD1	2.37	0.59
1:N:135:VAL:O	1:N:135:VAL:HG23	2.02	0.59
1:F:104:GLY:H	1:F:105:PRO:CD	2.14	0.58
1:I:79:LEU:O	1:I:126:LEU:HD22	2.02	0.58
1:K:333:LEU:HD12	1:K:338:TRP:CD1	2.38	0.58
1:B:157:THR:O	1:B:159:ILE:HG13	2.03	0.58
1:K:81:GLU:O	1:K:82:ILE:CB	2.50	0.58
1:A:18:LEU:CD2	1:A:74:LEU:HD11	2.33	0.58
1:E:333:LEU:CD2	1:E:337:TYR:CE1	2.86	0.58
1:I:18:LEU:HD12	1:I:78:VAL:HG13	1.84	0.58
1:F:81:GLU:O	1:F:82:ILE:CB	2.52	0.58
1:J:82:ILE:C	1:J:84:ASP:N	2.56	0.58
1:B:155:ILE:CB	1:C:67:TYR:OH	2.52	0.58
1:D:71:ARG:HG3	1:D:71:ARG:HH11	1.68	0.58
1:C:176:VAL:HG12	1:C:176:VAL:O	2.02	0.58
1:H:307:PHE:CZ	1:I:240:LYS:NZ	2.70	0.58
1:J:82:ILE:C	1:J:84:ASP:H	2.06	0.58
1:B:73:PRO:HB3	1:B:89:VAL:HG11	1.85	0.58
1:E:332:GLU:O	1:E:333:LEU:C	2.40	0.58
1:G:87:ILE:CG2	1:G:87:ILE:O	2.49	0.58
1:L:333:LEU:CD1	1:L:338:TRP:CH2	2.86	0.58
1:D:76:ASP:OD1	1:D:164:ALA:C	2.34	0.58
1:I:18:LEU:HD12	1:I:78:VAL:CA	2.32	0.58
1:K:329:LEU:O	1:K:333:LEU:HD21	2.01	0.58
1:L:104:GLY:N	1:L:105:PRO:HD3	2.13	0.58
1:D:333:LEU:HD12	1:D:338:TRP:NE1	2.19	0.57
1:H:28:SER:OG	1:H:107:ASP:OD2	2.21	0.57
1:B:106:ASN:C	1:B:108:GLU:H	2.07	0.57
1:B:81:GLU:O	1:B:82:ILE:CB	2.52	0.57
1:D:182:GLN:N	1:D:182:GLN:OE1	2.38	0.57
1:L:81:GLU:O	1:L:82:ILE:O	2.21	0.57
1:F:333:LEU:HD12	1:F:338:TRP:HE1	1.70	0.57
1:I:107:ASP:O	1:I:109:ILE:HG12	2.04	0.57
1:J:107:ASP:O	1:J:108:GLU:C	2.41	0.57
1:M:82:ILE:O	1:M:85:ARG:N	2.35	0.57
1:N:334:PRO:C	1:N:336:GLN:H	2.08	0.57
1:C:104:GLY:N	1:C:105:PRO:HD2	2.20	0.57
1:L:173:LYS:CG	1:L:180:GLU:HB3	2.31	0.57
1:N:103:PRO:HA	1:N:107:ASP:OD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:PRO:HB3	1:K:89:VAL:HG11	1.87	0.57
1:M:182:GLN:OE1	1:M:182:GLN:N	2.38	0.57
1:M:329:LEU:O	1:M:333:LEU:HD21	2.04	0.57
1:C:107:ASP:HB3	1:C:109:ILE:HG12	1.85	0.57
1:H:76:ASP:CA	1:H:165:GLY:HA3	2.35	0.57
1:L:79:LEU:HB3	1:L:126:LEU:CD1	2.35	0.57
1:B:175:THR:CG2	1:C:44:ASP:OD2	2.52	0.57
1:K:135:VAL:HG13	1:K:135:VAL:O	2.04	0.57
1:D:107:ASP:O	1:D:109:ILE:HG12	2.05	0.56
1:I:182:GLN:N	1:I:182:GLN:OE1	2.38	0.56
1:K:333:LEU:HD12	1:K:338:TRP:NE1	2.20	0.56
1:B:280:VAL:O	1:B:281:LEU:HD23	2.05	0.56
1:B:155:ILE:CG1	1:C:67:TYR:OH	2.53	0.56
1:F:109:ILE:CG2	1:F:136:HIS:HE1	2.17	0.56
1:H:329:LEU:C	1:H:333:LEU:HD21	2.23	0.56
1:K:280:VAL:O	1:K:281:LEU:HD23	2.04	0.56
1:H:334:PRO:O	1:H:337:TYR:N	2.38	0.56
1:M:79:LEU:HB2	1:M:126:LEU:HD23	1.87	0.56
1:B:109:ILE:CG2	1:B:136:HIS:HE1	2.17	0.56
1:C:79:LEU:HB3	1:C:126:LEU:CD1	2.35	0.56
1:G:104:GLY:H	1:G:105:PRO:HD2	1.68	0.56
1:J:333:LEU:N	1:J:334:PRO:HD3	2.21	0.56
1:M:82:ILE:CG2	1:M:89:VAL:N	2.65	0.56
1:J:334:PRO:C	1:J:336:GLN:H	2.08	0.56
1:A:103:PRO:HA	1:A:107:ASP:OD2	2.06	0.56
1:B:333:LEU:HD12	1:B:338:TRP:NE1	2.20	0.56
1:C:107:ASP:O	1:C:109:ILE:N	2.38	0.56
1:G:156:ASN:HD21	1:G:172:LEU:N	2.03	0.56
1:H:75:GLN:HB3	1:H:78:VAL:HG12	1.87	0.56
1:J:103:PRO:HA	1:J:107:ASP:OD2	2.05	0.56
1:K:106:ASN:O	1:K:108:GLU:N	2.31	0.56
1:N:333:LEU:N	1:N:334:PRO:HD3	2.21	0.56
1:F:79:LEU:HB3	1:F:126:LEU:HD23	1.88	0.56
1:M:106:ASN:O	1:M:108:GLU:N	2.32	0.56
1:L:157:THR:HG22	1:L:157:THR:O	2.05	0.56
1:I:49:LYS:O	1:I:54:PRO:HA	2.06	0.56
1:K:106:ASN:C	1:K:108:GLU:H	2.09	0.56
1:L:155:ILE:HG12	1:M:67:TYR:CZ	2.38	0.56
1:L:74:LEU:HD12	1:L:78:VAL:N	2.20	0.56
1:B:106:ASN:O	1:B:108:GLU:N	2.38	0.56
1:E:107:ASP:O	1:E:108:GLU:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:THR:CG2	1:C:285:VAL:HG23	2.36	0.55
1:D:156:ASN:ND2	1:D:172:LEU:H	2.03	0.55
1:M:78:VAL:CG2	1:M:114:GLY:O	2.54	0.55
1:M:78:VAL:HG22	1:M:114:GLY:O	2.06	0.55
1:M:78:VAL:HG23	1:M:116:PRO:HD3	1.88	0.55
1:D:71:ARG:HG3	1:D:71:ARG:NH1	2.19	0.55
1:E:103:PRO:HA	1:E:107:ASP:OD2	2.06	0.55
1:L:156:ASN:HD21	1:L:172:LEU:N	2.03	0.55
1:H:175:THR:HG22	1:H:176:VAL:HG23	1.87	0.55
1:H:333:LEU:CB	1:H:338:TRP:CE2	2.82	0.55
1:L:171:ALA:O	1:L:172:LEU:C	2.44	0.55
1:B:41:TYR:CE2	1:B:71:ARG:NE	2.62	0.55
1:F:329:LEU:O	1:F:333:LEU:HD21	2.07	0.55
1:H:333:LEU:CB	1:H:338:TRP:HZ2	2.14	0.55
1:G:79:LEU:HB3	1:G:126:LEU:HD13	1.88	0.55
1:D:80:SER:O	1:D:81:GLU:HG3	2.07	0.55
1:F:29:ARG:HD3	1:F:107:ASP:OD2	2.07	0.55
1:J:70:ILE:CG2	1:J:70:ILE:O	2.44	0.55
1:L:74:LEU:HD13	1:L:79:LEU:HD12	1.89	0.55
1:G:333:LEU:HD12	1:G:338:TRP:CE2	2.32	0.54
1:L:176:VAL:HB	1:L:177:PRO:HD2	1.89	0.54
1:L:104:GLY:H	1:L:105:PRO:HD2	1.61	0.54
1:D:156:ASN:HD21	1:D:171:ALA:CB	2.12	0.54
1:H:135:VAL:O	1:H:135:VAL:HG12	2.07	0.54
1:I:80:SER:O	1:I:81:GLU:HG3	2.08	0.54
1:K:333:LEU:HD12	1:K:338:TRP:HE1	1.72	0.54
1:D:49:LYS:O	1:D:54:PRO:HA	2.06	0.54
1:H:171:ALA:O	1:H:172:LEU:C	2.46	0.54
1:C:135:VAL:O	1:C:135:VAL:HG12	2.07	0.54
1:E:332:GLU:C	1:E:334:PRO:HD3	2.27	0.54
1:H:174:GLY:CA	1:I:44:ASP:OD2	2.38	0.54
1:A:107:ASP:O	1:A:108:GLU:C	2.45	0.54
1:D:135:VAL:O	1:D:135:VAL:HG12	2.08	0.54
1:J:82:ILE:H	1:J:82:ILE:HD13	1.71	0.54
1:F:135:VAL:HG12	1:F:135:VAL:O	2.07	0.54
1:G:135:VAL:O	1:G:135:VAL:HG12	2.07	0.54
1:E:303:LYS:HA	1:E:306:PRO:HB3	1.90	0.54
1:I:73:PRO:CG	1:I:89:VAL:CG1	2.59	0.54
1:M:49:LYS:O	1:M:54:PRO:HA	2.07	0.54
1:H:277:GLN:HE22	1:I:239:GLY:HA3	1.73	0.54
1:H:329:LEU:C	1:H:333:LEU:HD23	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:156:ASN:HD21	1:J:172:LEU:N	2.05	0.54
1:L:156:ASN:HD21	1:L:171:ALA:C	2.12	0.54
1:C:104:GLY:N	1:C:105:PRO:CD	2.71	0.54
1:L:135:VAL:O	1:L:135:VAL:HG12	2.07	0.54
1:I:135:VAL:O	1:I:135:VAL:HG12	2.07	0.53
1:M:76:ASP:HB3	1:M:166:THR:HG23	1.89	0.53
1:G:79:LEU:HB3	1:G:126:LEU:HD12	1.90	0.53
1:B:333:LEU:HD12	1:B:338:TRP:HE1	1.72	0.53
1:C:179:PRO:HA	1:C:182:GLN:HG2	1.90	0.53
1:F:333:LEU:CD1	1:F:338:TRP:HE1	2.21	0.53
1:M:333:LEU:HB3	1:M:338:TRP:CZ2	2.43	0.53
1:F:175:THR:CG2	1:G:44:ASP:OD2	2.57	0.53
1:I:76:ASP:OD1	3:I:402:ADP:O2B	2.25	0.53
1:A:303:LYS:HA	1:A:306:PRO:HB3	1.90	0.53
1:B:135:VAL:HG12	1:B:135:VAL:O	2.07	0.53
1:M:135:VAL:HG12	1:M:135:VAL:O	2.07	0.53
1:B:41:TYR:HE2	1:B:71:ARG:CD	2.22	0.53
1:K:104:GLY:H	1:K:105:PRO:HD3	1.69	0.53
1:K:107:ASP:HB2	1:K:109:ILE:HD11	1.91	0.53
1:D:333:LEU:HD12	1:D:338:TRP:HE1	1.73	0.53
1:D:81:GLU:O	1:D:82:ILE:HB	2.08	0.53
1:L:333:LEU:HD13	1:L:338:TRP:CE2	2.41	0.53
1:D:73:PRO:CB	1:D:89:VAL:CG1	2.83	0.52
1:E:333:LEU:HG	1:E:337:TYR:CZ	2.44	0.52
1:F:79:LEU:CD1	1:F:127:LEU:CD2	2.86	0.52
1:F:118:ARG:NH1	1:M:118:ARG:HH12	2.07	0.52
1:B:73:PRO:HB3	1:B:89:VAL:CG1	2.39	0.52
1:K:73:PRO:HB3	1:K:89:VAL:CG1	2.39	0.52
1:I:76:ASP:HB2	1:I:165:GLY:CA	2.24	0.52
1:M:87:ILE:O	1:M:87:ILE:CG2	2.57	0.52
1:B:175:THR:CG2	1:C:44:ASP:CG	2.75	0.52
1:L:155:ILE:HG23	1:L:156:ASN:HB2	1.91	0.52
1:B:175:THR:HG23	1:C:44:ASP:OD2	2.10	0.52
1:N:333:LEU:N	1:N:333:LEU:CD1	2.73	0.52
1:J:74:LEU:CD2	1:J:79:LEU:N	2.72	0.52
1:C:155:ILE:CD1	1:C:172:LEU:HB2	2.37	0.52
1:C:71:ARG:O	1:C:73:PRO:HD3	2.10	0.52
1:D:155:ILE:HB	1:E:67:TYR:OH	2.10	0.52
1:F:103:PRO:C	1:F:105:PRO:HD2	2.30	0.52
1:L:87:ILE:CG2	1:L:87:ILE:O	2.49	0.52
1:M:155:ILE:HB	1:N:67:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:303:LYS:HA	1:J:306:PRO:HB3	1.91	0.51
1:I:155:ILE:HB	1:J:67:TYR:OH	2.10	0.51
1:K:276:TYR:OH	1:L:66:SER:CB	2.58	0.51
1:L:71:ARG:O	1:L:73:PRO:HD3	2.10	0.51
1:A:334:PRO:C	1:A:336:GLN:N	2.58	0.51
1:B:279:THR:C	1:B:281:LEU:N	2.63	0.51
1:D:71:ARG:O	1:D:72:TYR:C	2.47	0.51
1:E:87:ILE:O	1:E:87:ILE:CG2	2.57	0.51
1:N:303:LYS:HA	1:N:306:PRO:HB3	1.92	0.51
1:D:334:PRO:O	1:D:335:PRO:C	2.48	0.51
1:F:76:ASP:HB3	1:F:166:THR:CG2	2.40	0.51
1:F:155:ILE:HB	1:G:67:TYR:OH	2.10	0.51
1:J:157:THR:O	1:J:159:ILE:N	2.43	0.51
1:E:155:ILE:N	1:E:155:ILE:CD1	2.73	0.51
1:M:73:PRO:CG	1:M:89:VAL:HG11	2.40	0.51
1:B:333:LEU:CD1	1:B:338:TRP:HE1	2.24	0.51
1:C:156:ASN:CG	1:C:172:LEU:O	2.43	0.51
1:I:108:GLU:HG2	1:I:108:GLU:O	2.09	0.51
1:K:155:ILE:HG22	1:K:276:TYR:CE1	2.45	0.51
1:N:73:PRO:O	1:N:79:LEU:HD23	2.11	0.51
1:J:333:LEU:HA	1:J:337:TYR:CB	2.40	0.51
1:A:122:ALA:O	1:A:126:LEU:HG	2.10	0.51
1:A:155:ILE:CD1	1:A:155:ILE:N	2.73	0.51
1:B:104:GLY:H	1:B:105:PRO:HD3	1.69	0.51
1:D:79:LEU:CD2	1:D:130:MET:SD	2.95	0.50
1:J:156:ASN:ND2	1:J:172:LEU:N	2.59	0.50
1:J:333:LEU:N	1:J:333:LEU:CD1	2.73	0.50
1:K:175:THR:HG23	1:L:44:ASP:OD2	2.10	0.50
1:L:173:LYS:CE	1:L:180:GLU:HG3	2.41	0.50
1:N:333:LEU:HA	1:N:337:TYR:CB	2.40	0.50
1:K:107:ASP:O	1:K:108:GLU:O	2.30	0.50
1:G:73:PRO:HB3	1:G:82:ILE:HD11	1.94	0.50
1:J:82:ILE:HG22	1:J:84:ASP:HB2	1.94	0.50
1:N:107:ASP:HB3	1:N:109:ILE:HD11	1.94	0.50
1:D:333:LEU:CD1	1:D:338:TRP:HE1	2.24	0.50
1:F:258:MET:N	1:F:259:PRO:CD	2.75	0.50
1:L:173:LYS:CG	1:L:180:GLU:CG	2.71	0.50
1:C:157:THR:HG21	1:C:285:VAL:HG23	1.94	0.50
1:D:122:ALA:O	1:D:126:LEU:HG	2.11	0.50
1:K:258:MET:N	1:K:259:PRO:CD	2.74	0.50
1:B:258:MET:N	1:B:259:PRO:CD	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:ILE:HG22	1:F:276:TYR:CE1	2.46	0.50
1:I:71:ARG:C	1:I:73:PRO:HD3	2.26	0.50
1:J:74:LEU:HD21	1:J:79:LEU:HD13	1.92	0.50
1:H:79:LEU:HG	1:H:79:LEU:O	2.12	0.49
1:N:158:ILE:O	1:N:284:ILE:HG23	2.12	0.49
1:H:87:ILE:CG2	1:H:87:ILE:O	2.49	0.49
1:M:82:ILE:O	1:M:84:ASP:CA	2.57	0.49
1:N:134:VAL:O	1:N:135:VAL:HG13	2.12	0.49
1:C:107:ASP:C	1:C:109:ILE:N	2.66	0.49
1:D:104:GLY:H	1:D:105:PRO:HD2	1.71	0.49
1:J:156:ASN:HD21	1:J:171:ALA:C	2.16	0.49
1:K:333:LEU:CD1	1:K:338:TRP:HE1	2.24	0.49
1:L:276:TYR:CZ	1:M:66:SER:HB2	2.42	0.49
1:M:73:PRO:HG3	1:M:89:VAL:CG1	2.43	0.49
1:H:76:ASP:CB	1:H:165:GLY:HA3	2.40	0.49
1:K:279:THR:C	1:K:281:LEU:N	2.64	0.49
1:C:176:VAL:N	1:C:177:PRO:HD3	2.28	0.49
1:H:171:ALA:C	1:H:172:LEU:O	2.44	0.49
1:I:258:MET:N	1:I:259:PRO:CD	2.76	0.49
1:B:107:ASP:O	1:B:108:GLU:C	2.51	0.49
1:C:176:VAL:CG2	1:D:44:ASP:OD2	2.59	0.49
1:L:157:THR:CG2	1:L:285:VAL:HG23	2.43	0.49
1:M:334:PRO:O	1:M:335:PRO:C	2.50	0.49
1:E:107:ASP:HB3	1:E:109:ILE:HD11	1.94	0.49
1:C:155:ILE:HG13	1:C:156:ASN:CB	2.43	0.48
1:C:87:ILE:CG2	1:C:87:ILE:O	2.49	0.48
1:M:155:ILE:HA	1:M:156:ASN:HA	1.51	0.48
1:I:78:VAL:HG11	1:I:113:ILE:HG21	1.87	0.48
1:J:107:ASP:HB3	1:J:109:ILE:HD11	1.94	0.48
1:K:81:GLU:C	1:K:82:ILE:HG12	2.34	0.48
1:N:87:ILE:CG2	1:N:87:ILE:O	2.57	0.48
1:D:258:MET:N	1:D:259:PRO:CD	2.76	0.48
1:J:71:ARG:O	1:J:73:PRO:CD	2.57	0.48
1:M:258:MET:N	1:M:259:PRO:CD	2.76	0.48
1:A:107:ASP:HB3	1:A:109:ILE:HD11	1.94	0.48
1:H:103:PRO:C	1:H:105:PRO:HD2	2.32	0.48
1:I:81:GLU:O	1:I:82:ILE:HG12	2.13	0.48
1:L:176:VAL:HB	1:L:177:PRO:CD	2.37	0.48
1:D:331:GLU:HA	1:D:332:GLU:HA	1.60	0.48
1:M:103:PRO:C	1:M:105:PRO:HD2	2.30	0.48
1:N:155:ILE:HG12	1:N:174:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:156:ASN:HD21	1:N:172:LEU:N	2.11	0.48
1:I:87:ILE:CG2	1:I:87:ILE:O	2.57	0.48
1:J:155:ILE:HG12	1:J:174:GLY:HA2	1.96	0.48
1:K:78:VAL:CG2	1:K:116:PRO:CD	2.91	0.48
1:H:334:PRO:O	1:H:336:GLN:N	2.47	0.48
1:H:77:GLY:HA3	1:H:166:THR:HG23	1.94	0.48
1:L:175:THR:HG21	1:M:43:LYS:NZ	2.28	0.48
1:B:135:VAL:O	1:B:136:HIS:CG	2.67	0.47
1:B:156:ASN:HD21	1:B:172:LEU:N	2.12	0.47
1:G:73:PRO:HB3	1:G:82:ILE:CD1	2.44	0.47
1:N:157:THR:O	1:N:159:ILE:N	2.47	0.47
1:B:78:VAL:CG2	1:B:116:PRO:CD	2.92	0.47
1:B:76:ASP:HB3	1:B:166:THR:HG23	1.94	0.47
1:G:71:ARG:O	1:G:73:PRO:HD3	2.15	0.47
1:J:74:LEU:HD22	1:J:79:LEU:N	2.29	0.47
1:L:332:GLU:C	1:L:333:LEU:HG	2.35	0.47
1:K:155:ILE:CG1	1:L:67:TYR:OH	2.61	0.47
1:M:104:GLY:H	1:M:105:PRO:HD2	1.63	0.47
1:H:333:LEU:CG	1:H:338:TRP:NE1	2.74	0.47
1:I:155:ILE:HG12	1:I:174:GLY:HA2	1.97	0.47
1:I:81:GLU:C	1:I:82:ILE:HG12	2.34	0.47
1:J:204:HIS:N	1:J:205:PRO:CD	2.78	0.47
1:D:334:PRO:C	1:D:336:GLN:N	2.68	0.47
1:H:329:LEU:O	1:H:333:LEU:CG	2.53	0.47
1:A:334:PRO:O	1:A:337:TYR:N	2.47	0.47
1:E:204:HIS:N	1:E:205:PRO:CD	2.78	0.47
1:E:334:PRO:HB3	1:E:335:PRO:HD2	1.96	0.47
1:F:135:VAL:O	1:F:136:HIS:CG	2.67	0.47
1:F:331:GLU:HA	1:F:332:GLU:HA	1.59	0.47
1:L:173:LYS:HE2	1:L:180:GLU:CG	2.44	0.47
1:M:42:PRO:HG2	1:M:49:LYS:CG	2.44	0.47
1:A:204:HIS:N	1:A:205:PRO:CD	2.78	0.47
1:H:155:ILE:HA	1:H:156:ASN:HA	1.47	0.47
1:M:104:GLY:H	1:M:105:PRO:HD3	1.75	0.47
1:B:334:PRO:O	1:B:335:PRO:C	2.53	0.47
1:F:155:ILE:HA	1:F:156:ASN:HA	1.49	0.47
1:I:155:ILE:HA	1:I:156:ASN:HA	1.51	0.47
1:J:156:ASN:CG	1:J:172:LEU:N	2.67	0.47
1:K:134:VAL:O	1:K:135:VAL:HB	2.12	0.47
1:N:157:THR:HG21	1:N:285:VAL:CG2	2.42	0.47
1:B:78:VAL:HG22	1:B:123:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:LEU:HA	1:E:337:TYR:CB	2.44	0.47
1:F:334:PRO:O	1:F:335:PRO:C	2.53	0.47
1:L:333:LEU:HB2	1:L:338:TRP:CE2	2.49	0.47
1:B:331:GLU:HA	1:B:332:GLU:HA	1.61	0.47
1:I:71:ARG:HH11	1:I:71:ARG:CG	2.27	0.47
1:N:204:HIS:N	1:N:205:PRO:CD	2.78	0.47
1:C:37:SER:O	1:C:38:VAL:HB	2.15	0.47
1:F:78:VAL:CG2	1:F:123:ASN:ND2	2.78	0.47
1:F:81:GLU:C	1:F:82:ILE:HG12	2.35	0.47
1:H:173:LYS:CG	1:H:174:GLY:N	2.59	0.47
1:H:37:SER:O	1:H:38:VAL:HB	2.15	0.47
1:K:331:GLU:HA	1:K:332:GLU:HA	1.61	0.47
1:G:76:ASP:O	1:G:166:THR:CG2	2.63	0.46
1:G:37:SER:O	1:G:38:VAL:HB	2.15	0.46
1:K:334:PRO:O	1:K:335:PRO:C	2.53	0.46
1:L:104:GLY:H	1:L:105:PRO:HD3	1.78	0.46
1:A:87:ILE:O	1:A:87:ILE:CG2	2.57	0.46
1:D:29:ARG:HH22	1:D:105:PRO:HD3	1.80	0.46
1:F:84:ASP:O	1:M:202:GLU:OE2	2.32	0.46
1:K:145:PHE:CD1	1:K:145:PHE:N	2.84	0.46
1:K:37:SER:O	1:K:38:VAL:HB	2.16	0.46
1:L:175:THR:CG2	1:M:43:LYS:CE	2.92	0.46
1:L:110:CYS:HB2	1:L:338:TRP:CH2	2.51	0.46
1:K:155:ILE:HG12	1:L:67:TYR:OH	2.16	0.46
1:A:258:MET:N	1:A:259:PRO:CD	2.79	0.46
1:B:81:GLU:C	1:B:82:ILE:HG12	2.36	0.46
1:F:37:SER:O	1:F:38:VAL:HB	2.16	0.46
1:J:87:ILE:CG2	1:J:87:ILE:O	2.57	0.46
1:K:155:ILE:HA	1:K:156:ASN:HA	1.48	0.46
1:C:74:LEU:HD21	1:C:79:LEU:HG	1.97	0.46
1:H:156:ASN:HD21	1:H:171:ALA:C	2.18	0.46
1:L:37:SER:O	1:L:38:VAL:HB	2.15	0.46
1:M:155:ILE:HG12	1:M:174:GLY:HA2	1.97	0.46
1:M:79:LEU:C	1:M:126:LEU:HD21	2.31	0.46
1:N:258:MET:N	1:N:259:PRO:CD	2.79	0.46
1:F:109:ILE:HB	1:F:136:HIS:HE1	1.81	0.46
1:I:29:ARG:HH22	1:I:105:PRO:HD3	1.81	0.46
1:J:157:THR:HG21	1:J:285:VAL:CG2	2.39	0.46
1:K:78:VAL:HG22	1:K:123:ASN:ND2	2.30	0.46
1:M:71:ARG:HB3	1:M:83:SER:OG	2.16	0.46
1:C:74:LEU:CD2	1:C:79:LEU:CG	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ILE:HA	1:D:156:ASN:HA	1.51	0.46
1:B:37:SER:O	1:B:38:VAL:HB	2.16	0.46
1:I:331:GLU:HA	1:I:332:GLU:HA	1.69	0.46
1:D:37:SER:O	1:D:38:VAL:HB	2.17	0.45
1:I:37:SER:O	1:I:38:VAL:HB	2.17	0.45
1:K:76:ASP:HB3	1:K:166:THR:HG23	1.98	0.45
1:B:78:VAL:CG2	1:B:116:PRO:CG	2.95	0.45
1:G:156:ASN:HD21	1:G:171:ALA:C	2.19	0.45
1:J:333:LEU:N	1:J:333:LEU:HD12	2.32	0.45
1:N:106:ASN:O	1:N:108:GLU:N	2.49	0.45
1:B:174:GLY:HA3	1:C:67:TYR:HE1	1.81	0.45
1:C:177:PRO:CG	1:C:180:GLU:CB	2.79	0.45
1:G:155:ILE:HA	1:G:156:ASN:HA	1.47	0.45
1:H:155:ILE:HG21	1:I:67:TYR:HE1	1.80	0.45
1:J:258:MET:N	1:J:259:PRO:CD	2.79	0.45
1:L:155:ILE:N	1:L:155:ILE:HD12	2.31	0.45
1:M:333:LEU:CD1	1:M:338:TRP:NE1	2.75	0.45
1:B:145:PHE:N	1:B:145:PHE:CD1	2.84	0.45
1:D:87:ILE:O	1:D:87:ILE:CG2	2.57	0.45
1:L:103:PRO:C	1:L:105:PRO:HD2	2.33	0.45
1:L:173:LYS:CD	1:L:180:GLU:HG3	2.46	0.45
1:N:156:ASN:ND2	1:N:172:LEU:N	2.65	0.45
1:D:155:ILE:HG12	1:D:174:GLY:HA2	1.98	0.45
1:F:175:THR:HG22	1:G:44:ASP:OD2	2.17	0.45
1:M:49:LYS:O	1:M:54:PRO:N	2.49	0.45
1:B:104:GLY:H	1:B:105:PRO:HD2	1.71	0.45
1:D:79:LEU:HB3	1:D:126:LEU:HD13	1.98	0.45
1:F:175:THR:HG23	1:G:44:ASP:OD2	2.17	0.45
1:E:258:MET:N	1:E:259:PRO:CD	2.79	0.45
1:E:296:LEU:HD23	1:E:296:LEU:C	2.37	0.45
1:E:334:PRO:C	1:E:336:GLN:H	2.20	0.45
1:E:73:PRO:O	1:E:79:LEU:HD23	2.17	0.45
1:I:49:LYS:O	1:I:54:PRO:N	2.50	0.45
1:K:78:VAL:CG2	1:K:116:PRO:CG	2.94	0.45
1:M:248:GLU:N	1:M:249:PRO:CD	2.80	0.45
1:N:296:LEU:HD23	1:N:296:LEU:C	2.37	0.45
1:D:42:PRO:HG2	1:D:49:LYS:HB2	1.99	0.45
1:F:145:PHE:CD1	1:F:145:PHE:N	2.84	0.45
1:L:157:THR:HG21	1:L:285:VAL:HG23	1.98	0.45
1:L:80:SER:O	1:L:126:LEU:HD11	2.17	0.45
1:M:334:PRO:C	1:M:336:GLN:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD23	1:A:296:LEU:C	2.37	0.44
1:H:258:MET:N	1:H:259:PRO:CD	2.80	0.44
1:M:298:ALA:O	1:M:302:GLU:HB2	2.17	0.44
1:N:157:THR:O	1:N:159:ILE:HG13	2.17	0.44
1:D:298:ALA:O	1:D:302:GLU:HB2	2.16	0.44
1:D:333:LEU:HB3	1:D:338:TRP:CZ2	2.52	0.44
1:I:204:HIS:N	1:I:205:PRO:CD	2.80	0.44
1:K:298:ALA:O	1:K:302:GLU:HB2	2.17	0.44
1:M:78:VAL:CG1	1:M:79:LEU:N	2.38	0.44
1:M:82:ILE:HG23	1:M:89:VAL:HG23	1.96	0.44
1:C:74:LEU:CD2	1:C:79:LEU:HG	2.48	0.44
1:D:204:HIS:N	1:D:205:PRO:CD	2.80	0.44
1:D:49:LYS:O	1:D:54:PRO:N	2.50	0.44
1:I:248:GLU:N	1:I:249:PRO:CD	2.80	0.44
1:J:258:MET:HB2	1:J:259:PRO:HD3	2.00	0.44
1:J:296:LEU:C	1:J:296:LEU:HD23	2.37	0.44
1:M:37:SER:O	1:M:38:VAL:HB	2.17	0.44
1:B:107:ASP:O	1:B:108:GLU:O	2.35	0.44
1:B:76:ASP:HB3	1:B:166:THR:CG2	2.48	0.44
1:D:248:GLU:N	1:D:249:PRO:CD	2.80	0.44
1:D:258:MET:HB2	1:D:259:PRO:HD3	1.99	0.44
1:I:258:MET:HB2	1:I:259:PRO:HD3	1.99	0.44
1:I:42:PRO:HG2	1:I:49:LYS:HB2	1.99	0.44
1:I:71:ARG:HB3	1:I:83:SER:OG	2.18	0.44
1:B:155:ILE:HA	1:B:156:ASN:HA	1.47	0.44
1:C:18:LEU:CD2	1:C:74:LEU:CD1	2.88	0.44
1:E:258:MET:HB2	1:E:259:PRO:HD3	2.00	0.44
1:E:37:SER:O	1:E:38:VAL:HB	2.18	0.44
1:C:80:SER:O	1:C:126:LEU:HD11	2.17	0.44
1:J:158:ILE:O	1:J:284:ILE:HG23	2.17	0.44
1:L:258:MET:N	1:L:259:PRO:CD	2.80	0.44
1:A:258:MET:HB2	1:A:259:PRO:HD3	2.00	0.44
1:D:71:ARG:C	1:D:72:TYR:O	2.56	0.44
1:G:258:MET:N	1:G:259:PRO:CD	2.80	0.44
1:I:333:LEU:CD1	1:I:337:TYR:CD1	3.01	0.44
1:C:258:MET:N	1:C:259:PRO:CD	2.80	0.44
1:I:298:ALA:O	1:I:302:GLU:HB2	2.17	0.44
1:J:157:THR:O	1:J:159:ILE:HG13	2.18	0.44
1:M:204:HIS:N	1:M:205:PRO:CD	2.80	0.44
1:N:134:VAL:O	1:N:135:VAL:CB	2.66	0.44
1:N:333:LEU:N	1:N:333:LEU:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:333:LEU:CA	1:N:337:TYR:HB3	2.48	0.44
1:N:37:SER:O	1:N:38:VAL:HB	2.18	0.44
1:A:37:SER:O	1:A:38:VAL:HB	2.18	0.44
1:C:155:ILE:HA	1:C:156:ASN:HA	1.50	0.44
1:C:76:ASP:O	1:C:166:THR:CG2	2.66	0.44
1:E:334:PRO:O	1:E:336:GLN:N	2.51	0.44
1:L:334:PRO:HA	1:L:335:PRO:HD3	1.94	0.44
1:N:156:ASN:HD21	1:N:171:ALA:C	2.22	0.44
1:N:156:ASN:CG	1:N:172:LEU:N	2.71	0.44
1:N:258:MET:HB2	1:N:259:PRO:HD3	2.00	0.44
1:A:80:SER:OG	1:A:82:ILE:HD13	2.18	0.43
1:E:155:ILE:HA	1:E:156:ASN:HA	1.49	0.43
1:J:37:SER:O	1:J:38:VAL:HB	2.18	0.43
1:L:258:MET:HB2	1:L:259:PRO:HD3	2.00	0.43
1:F:298:ALA:O	1:F:302:GLU:HB2	2.17	0.43
1:M:258:MET:HB2	1:M:259:PRO:HD3	1.99	0.43
1:C:157:THR:O	1:C:158:ILE:C	2.56	0.43
1:D:240:LYS:N	1:D:241:PRO:CD	2.81	0.43
1:A:18:LEU:HD21	1:A:74:LEU:HD11	2.01	0.43
1:B:240:LYS:N	1:B:241:PRO:CD	2.82	0.43
1:B:298:ALA:O	1:B:302:GLU:HB2	2.17	0.43
1:H:104:GLY:H	1:H:105:PRO:HD3	1.77	0.43
1:M:331:GLU:HA	1:M:332:GLU:HA	1.60	0.43
1:B:109:ILE:HB	1:B:136:HIS:HE1	1.82	0.43
1:C:105:PRO:O	1:C:106:ASN:C	2.56	0.43
1:C:258:MET:HB2	1:C:259:PRO:HD3	2.00	0.43
1:H:331:GLU:CG	1:H:332:GLU:HA	2.48	0.43
1:I:240:LYS:N	1:I:241:PRO:CD	2.81	0.43
1:M:79:LEU:CA	1:M:126:LEU:HD23	2.48	0.43
1:C:179:PRO:HA	1:C:182:GLN:CD	2.39	0.43
1:D:71:ARG:O	1:D:73:PRO:HD3	2.19	0.43
1:F:276:TYR:OH	1:G:66:SER:OG	2.35	0.43
1:H:276:TYR:CZ	1:I:66:SER:CB	3.00	0.43
1:K:135:VAL:O	1:K:135:VAL:HG22	2.18	0.43
1:K:258:MET:HB2	1:K:259:PRO:HD3	2.01	0.43
1:K:155:ILE:CG2	1:K:276:TYR:CE1	3.01	0.43
1:M:333:LEU:HG	1:M:338:TRP:HE1	1.81	0.43
1:E:240:LYS:N	1:E:241:PRO:CD	2.82	0.43
1:F:155:ILE:CG2	1:F:276:TYR:CE1	3.01	0.43
1:G:81:GLU:O	1:G:82:ILE:C	2.57	0.43
1:J:248:GLU:N	1:J:249:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:333:LEU:CA	1:J:337:TYR:HB3	2.47	0.43
1:M:240:LYS:N	1:M:241:PRO:CD	2.81	0.43
1:N:240:LYS:N	1:N:241:PRO:CD	2.82	0.43
1:A:248:GLU:N	1:A:249:PRO:CD	2.82	0.43
1:E:248:GLU:N	1:E:249:PRO:CD	2.82	0.43
1:H:258:MET:HB2	1:H:259:PRO:HD3	2.00	0.43
1:H:341:LEU:HG	1:H:341:LEU:O	2.19	0.43
1:J:240:LYS:N	1:J:241:PRO:CD	2.82	0.43
1:C:341:LEU:HG	1:C:341:LEU:O	2.19	0.43
1:D:79:LEU:CD1	1:D:126:LEU:HB3	2.42	0.43
1:G:341:LEU:O	1:G:341:LEU:HG	2.19	0.43
1:K:334:PRO:C	1:K:336:GLN:N	2.72	0.43
1:K:81:GLU:O	1:K:82:ILE:HG12	2.17	0.43
1:N:248:GLU:N	1:N:249:PRO:CD	2.82	0.43
1:A:240:LYS:N	1:A:241:PRO:CD	2.82	0.43
1:B:258:MET:HB2	1:B:259:PRO:HD3	2.01	0.43
1:B:305:ARG:N	1:B:306:PRO:HA	2.34	0.43
1:G:258:MET:HB2	1:G:259:PRO:HD3	2.00	0.43
1:H:77:GLY:HA3	1:H:166:THR:CG2	2.49	0.43
1:F:78:VAL:CB	1:F:116:PRO:CG	2.82	0.42
1:I:333:LEU:CD1	1:I:337:TYR:CE1	3.02	0.42
1:N:155:ILE:HA	1:N:156:ASN:HA	1.49	0.42
1:E:334:PRO:CB	1:E:335:PRO:CD	2.97	0.42
1:F:240:LYS:N	1:F:241:PRO:CD	2.82	0.42
1:G:110:CYS:HB2	1:G:338:TRP:CH2	2.53	0.42
1:I:18:LEU:HD13	1:I:77:GLY:O	2.19	0.42
1:L:341:LEU:HG	1:L:341:LEU:O	2.19	0.42
1:M:71:ARG:O	1:M:73:PRO:HD3	2.19	0.42
1:F:334:PRO:C	1:F:336:GLN:N	2.72	0.42
1:K:240:LYS:N	1:K:241:PRO:CD	2.82	0.42
1:B:341:LEU:HG	1:B:341:LEU:O	2.20	0.42
1:J:106:ASN:O	1:J:108:GLU:N	2.52	0.42
1:C:179:PRO:HA	1:C:182:GLN:CG	2.49	0.42
1:D:71:ARG:HB3	1:D:83:SER:OG	2.20	0.42
1:I:305:ARG:N	1:I:306:PRO:HA	2.35	0.42
1:I:341:LEU:O	1:I:341:LEU:HG	2.20	0.42
1:K:106:ASN:C	1:K:108:GLU:N	2.72	0.42
1:K:109:ILE:CG2	1:K:136:HIS:CE1	3.02	0.42
1:K:204:HIS:N	1:K:205:PRO:CD	2.83	0.42
1:M:305:ARG:N	1:M:306:PRO:HA	2.35	0.42
1:F:76:ASP:HB3	1:F:166:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:GLU:N	1:G:249:PRO:CD	2.83	0.42
1:H:248:GLU:N	1:H:249:PRO:CD	2.83	0.42
1:C:248:GLU:N	1:C:249:PRO:CD	2.83	0.42
1:D:29:ARG:HH22	1:D:105:PRO:CD	2.33	0.42
1:D:305:ARG:N	1:D:306:PRO:HA	2.35	0.42
1:F:78:VAL:CG2	1:F:116:PRO:CG	2.98	0.42
1:F:204:HIS:N	1:F:205:PRO:CD	2.83	0.42
1:G:157:THR:O	1:G:159:ILE:HG13	2.19	0.42
1:H:73:PRO:HB3	1:H:82:ILE:HD11	2.02	0.42
1:J:79:LEU:O	1:J:80:SER:O	2.38	0.42
1:K:109:ILE:HG22	1:K:136:HIS:CE1	2.54	0.42
1:L:173:LYS:CB	1:L:180:GLU:HB3	2.49	0.42
1:A:333:LEU:HG	1:A:337:TYR:CE1	2.52	0.42
1:C:157:THR:HG1	1:C:282:GLN:HB3	1.80	0.42
1:F:109:ILE:O	1:F:136:HIS:ND1	2.33	0.42
1:F:258:MET:HB2	1:F:259:PRO:HD3	2.00	0.42
1:F:18:LEU:CD2	1:F:74:LEU:HD21	2.49	0.42
1:I:81:GLU:O	1:I:82:ILE:CG1	2.67	0.42
1:L:333:LEU:CG	1:L:338:TRP:CZ2	3.03	0.42
1:M:156:ASN:ND2	1:M:172:LEU:H	2.17	0.42
1:A:333:LEU:HA	1:A:337:TYR:HB3	2.02	0.42
1:B:204:HIS:N	1:B:205:PRO:CD	2.83	0.42
1:B:334:PRO:C	1:B:336:GLN:N	2.72	0.42
1:E:333:LEU:N	1:E:334:PRO:CD	2.78	0.42
1:E:18:LEU:CD2	1:E:74:LEU:HD11	2.49	0.42
1:H:157:THR:O	1:H:159:ILE:HG13	2.19	0.42
1:I:29:ARG:HH22	1:I:105:PRO:CD	2.33	0.42
1:F:109:ILE:HB	1:F:136:HIS:CE1	2.55	0.42
1:F:81:GLU:O	1:F:82:ILE:HG12	2.20	0.42
1:K:305:ARG:N	1:K:306:PRO:HA	2.34	0.42
1:B:106:ASN:C	1:B:108:GLU:N	2.72	0.41
1:B:107:ASP:HB2	1:B:109:ILE:HD11	2.01	0.41
1:F:305:ARG:N	1:F:306:PRO:HA	2.34	0.41
1:L:298:ALA:O	1:L:302:GLU:HB2	2.20	0.41
1:C:333:LEU:N	1:C:333:LEU:CD2	2.83	0.41
1:F:333:LEU:HB3	1:F:338:TRP:CZ2	2.55	0.41
1:F:341:LEU:HG	1:F:341:LEU:O	2.19	0.41
1:G:77:GLY:HA3	1:G:166:THR:HG21	1.98	0.41
1:I:157:THR:HG23	1:I:283:ASN:O	2.20	0.41
1:L:248:GLU:N	1:L:249:PRO:CD	2.83	0.41
1:L:73:PRO:HB3	1:L:82:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HB2	1:A:54:PRO:HA	2.02	0.41
1:E:334:PRO:O	1:E:337:TYR:N	2.53	0.41
1:F:104:GLY:H	1:F:105:PRO:HD3	1.83	0.41
1:H:156:ASN:HD21	1:H:172:LEU:N	2.17	0.41
1:K:334:PRO:HA	1:K:335:PRO:HD3	1.91	0.41
1:K:76:ASP:HB3	1:K:166:THR:CG2	2.51	0.41
1:L:76:ASP:O	1:L:166:THR:CG2	2.68	0.41
1:M:341:LEU:HG	1:M:341:LEU:O	2.20	0.41
1:B:41:TYR:OH	1:B:71:ARG:NE	2.54	0.41
1:D:94:LEU:HD21	1:D:130:MET:HE2	2.01	0.41
1:I:78:VAL:HB	1:I:79:LEU:H	1.68	0.41
1:K:341:LEU:HG	1:K:341:LEU:O	2.20	0.41
1:G:158:ILE:O	1:G:284:ILE:HG23	2.20	0.41
1:J:82:ILE:O	1:J:83:SER:C	2.55	0.41
1:N:67:TYR:N	1:N:67:TYR:CD1	2.89	0.41
1:A:333:LEU:HB3	1:A:338:TRP:NE1	2.35	0.41
1:B:155:ILE:HG23	1:B:156:ASN:HB2	2.03	0.41
1:B:81:GLU:O	1:B:82:ILE:HG12	2.21	0.41
1:C:173:LYS:O	1:D:67:TYR:CE1	2.74	0.41
1:D:157:THR:HG23	1:D:283:ASN:O	2.20	0.41
1:D:341:LEU:O	1:D:341:LEU:HG	2.20	0.41
1:C:173:LYS:O	1:D:67:TYR:HE1	2.03	0.41
1:H:298:ALA:O	1:H:302:GLU:HB2	2.20	0.41
1:N:302:GLU:HB3	1:N:303:LYS:H	1.71	0.41
1:E:334:PRO:C	1:E:336:GLN:N	2.74	0.41
1:H:334:PRO:O	1:H:335:PRO:C	2.59	0.41
1:B:118:ARG:HH12	1:I:118:ARG:NH1	2.18	0.41
1:J:156:ASN:OD1	1:J:172:LEU:HB2	2.21	0.41
1:N:49:LYS:HB2	1:N:54:PRO:HA	2.03	0.41
1:B:87:ILE:O	1:B:87:ILE:CG2	2.61	0.41
1:M:157:THR:HG23	1:M:283:ASN:O	2.21	0.41
1:B:332:GLU:HG2	1:B:332:GLU:O	2.20	0.41
1:D:79:LEU:CD1	1:D:130:MET:SD	3.06	0.41
1:G:77:GLY:CA	1:G:166:THR:HG23	2.48	0.41
1:G:298:ALA:O	1:G:302:GLU:HB2	2.21	0.41
1:H:158:ILE:O	1:H:284:ILE:HG23	2.20	0.41
1:K:174:GLY:HA3	1:L:67:TYR:HE1	1.86	0.41
1:B:109:ILE:HB	1:B:136:HIS:CE1	2.56	0.41
1:C:74:LEU:HD21	1:C:79:LEU:CG	2.50	0.41
1:D:29:ARG:NH2	1:D:105:PRO:CD	2.84	0.41
1:F:46:ILE:HG23	1:F:46:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:PRO:HB3	1:F:89:VAL:HG11	2.03	0.41
1:G:331:GLU:CG	1:G:332:GLU:HA	2.49	0.41
1:C:156:ASN:HD21	1:C:172:LEU:C	2.23	0.41
1:G:139:LEU:HD11	1:G:338:TRP:CE2	2.56	0.41
1:J:158:ILE:HD13	1:J:265:ILE:HG23	2.03	0.41
1:A:67:TYR:CD1	1:A:67:TYR:N	2.89	0.40
1:D:329:LEU:HA	1:D:333:LEU:HD21	2.03	0.40
1:C:174:GLY:HA2	1:D:67:TYR:CE1	2.55	0.40
1:F:334:PRO:HA	1:F:335:PRO:HD3	1.91	0.40
1:I:156:ASN:ND2	1:I:172:LEU:H	2.19	0.40
1:M:157:THR:O	1:M:159:ILE:HG13	2.21	0.40
1:C:176:VAL:N	1:C:177:PRO:CD	2.84	0.40
1:B:275:GLU:HB3	1:C:65:ARG:NH2	2.36	0.40
1:D:80:SER:O	1:D:81:GLU:CG	2.70	0.40
1:E:67:TYR:N	1:E:67:TYR:CD1	2.89	0.40
1:A:305:ARG:N	1:A:306:PRO:HA	2.37	0.40
1:C:298:ALA:O	1:C:302:GLU:HB2	2.21	0.40
1:K:276:TYR:OH	1:L:66:SER:HB2	2.22	0.40
1:N:305:ARG:N	1:N:306:PRO:HA	2.37	0.40
1:F:107:ASP:C	1:F:109:ILE:N	2.74	0.40
1:J:67:TYR:N	1:J:67:TYR:CD1	2.89	0.40
1:M:71:ARG:CG	1:M:71:ARG:HH11	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	326/347 (94%)	287 (88%)	29 (9%)	10 (3%)	5	42
1	B	326/347 (94%)	285 (87%)	28 (9%)	13 (4%)	4	35
1	C	326/347 (94%)	282 (86%)	35 (11%)	9 (3%)	6	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	326/347 (94%)	281 (86%)	35 (11%)	10 (3%)	5	42
1	E	326/347 (94%)	287 (88%)	30 (9%)	9 (3%)	6	44
1	F	326/347 (94%)	288 (88%)	29 (9%)	9 (3%)	6	44
1	G	326/347 (94%)	289 (89%)	31 (10%)	6 (2%)	11	53
1	H	326/347 (94%)	279 (86%)	36 (11%)	11 (3%)	5	40
1	I	326/347 (94%)	285 (87%)	31 (10%)	10 (3%)	5	42
1	J	326/347 (94%)	287 (88%)	29 (9%)	10 (3%)	5	42
1	K	326/347 (94%)	287 (88%)	28 (9%)	11 (3%)	5	40
1	L	326/347 (94%)	282 (86%)	33 (10%)	11 (3%)	5	40
1	M	326/347 (94%)	283 (87%)	31 (10%)	12 (4%)	4	37
1	N	326/347 (94%)	289 (89%)	27 (8%)	10 (3%)	5	42
All	All	4564/4858 (94%)	3991 (87%)	432 (10%)	141 (3%)	9	42

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	TYR
1	A	108	GLU
1	B	55	TYR
1	B	105	PRO
1	B	134	VAL
1	B	280	VAL
1	C	55	TYR
1	C	73	PRO
1	D	55	TYR
1	D	72	TYR
1	D	73	PRO
1	D	108	GLU
1	D	335	PRO
1	E	55	TYR
1	E	108	GLU
1	F	55	TYR
1	F	73	PRO
1	F	108	GLU
1	F	134	VAL
1	G	55	TYR
1	G	73	PRO
1	G	82	ILE

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Mol	Chain	Res	Type
1	G	108	GLU
1	H	55	TYR
1	H	105	PRO
1	H	108	GLU
1	H	172	LEU
1	H	179	PRO
1	I	73	PRO
1	I	82	ILE
1	I	108	GLU
1	J	55	TYR
1	J	80	SER
1	J	83	SER
1	J	107	ASP
1	J	108	GLU
1	J	158	ILE
1	J	335	PRO
1	K	55	TYR
1	K	105	PRO
1	K	135	VAL
1	K	280	VAL
1	L	55	TYR
1	L	73	PRO
1	L	105	PRO
1	L	108	GLU
1	L	176	VAL
1	L	177	PRO
1	M	73	PRO
1	M	83	SER
1	M	105	PRO
1	M	108	GLU
1	M	335	PRO
1	N	55	TYR
1	N	107	ASP
1	N	108	GLU
1	N	158	ILE
1	N	335	PRO
1	A	38	VAL
1	A	107	ASP
1	B	38	VAL
1	B	82	ILE
1	B	107	ASP
1	B	158	ILE

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Mol	Chain	Res	Type
1	B	335	PRO
1	C	38	VAL
1	C	82	ILE
1	C	108	GLU
1	D	38	VAL
1	D	309	ASP
1	E	38	VAL
1	E	107	ASP
1	F	38	VAL
1	F	82	ILE
1	F	335	PRO
1	G	38	VAL
1	H	38	VAL
1	H	107	ASP
1	I	38	VAL
1	I	55	TYR
1	I	79	LEU
1	I	309	ASP
1	J	38	VAL
1	K	38	VAL
1	K	82	ILE
1	K	107	ASP
1	K	108	GLU
1	K	335	PRO
1	L	38	VAL
1	L	49	LYS
1	L	82	ILE
1	L	107	ASP
1	M	38	VAL
1	M	55	TYR
1	M	107	ASP
1	M	309	ASP
1	N	38	VAL
1	N	135	VAL
1	A	331	GLU
1	A	335	PRO
1	B	108	GLU
1	C	49	LYS
1	C	179	PRO
1	G	49	LYS
1	H	49	LYS
1	M	158	ILE

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Mol	Chain	Res	Type
1	A	135	VAL
1	A	302	GLU
1	B	73	PRO
1	B	80	SER
1	C	334	PRO
1	D	78	VAL
1	D	158	ILE
1	E	135	VAL
1	E	302	GLU
1	F	80	SER
1	I	158	ILE
1	J	135	VAL
1	J	302	GLU
1	K	80	SER
1	M	80	SER
1	N	302	GLU
1	A	73	PRO
1	A	82	ILE
1	D	82	ILE
1	E	82	ILE
1	H	335	PRO
1	I	78	VAL
1	I	334	PRO
1	K	73	PRO
1	L	172	LEU
1	N	82	ILE
1	B	135	VAL
1	E	73	PRO
1	F	135	VAL
1	H	174	GLY
1	N	73	PRO
1	E	335	PRO
1	H	73	PRO
1	M	78	VAL
1	C	109	ILE

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 PDB entries followed by that with respect to all EM entries.

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	271/285 (95%)	268 (99%)	3 (1%)	80	91
1	B	271/285 (95%)	269 (99%)	2 (1%)	88	94
1	C	271/285 (95%)	269 (99%)	2 (1%)	88	94
1	D	271/285 (95%)	266 (98%)	5 (2%)	66	87
1	E	271/285 (95%)	269 (99%)	2 (1%)	88	94
1	F	271/285 (95%)	269 (99%)	2 (1%)	88	94
1	G	271/285 (95%)	269 (99%)	2 (1%)	88	94
1	H	271/285 (95%)	268 (99%)	3 (1%)	80	91
1	I	271/285 (95%)	267 (98%)	4 (2%)	72	88
1	J	271/285 (95%)	270 (100%)	1 (0%)	93	96
1	K	271/285 (95%)	269 (99%)	2 (1%)	88	94
1	L	271/285 (95%)	270 (100%)	1 (0%)	93	96
1	M	271/285 (95%)	269 (99%)	2 (1%)	88	94
1	N	271/285 (95%)	269 (99%)	2 (1%)	88	94
All	All	3794/3990 (95%)	3761 (99%)	33 (1%)	85	93

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ILE
1	A	106	ASN
1	A	333	LEU
1	B	74	LEU
1	B	332	GLU
1	C	107	ASP
1	C	333	LEU
1	D	43	LYS
1	D	70	ILE
1	D	74	LEU
1	D	107	ASP
1	D	332	GLU
1	E	70	ILE
1	E	106	ASN
1	F	74	LEU
1	F	332	GLU
1	G	107	ASP

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Mol	Chain	Res	Type
1	G	332	GLU
1	H	78	VAL
1	H	180	GLU
1	H	332	GLU
1	I	74	LEU
1	I	79	LEU
1	I	107	ASP
1	I	333	LEU
1	J	106	ASN
1	K	74	LEU
1	K	332	GLU
1	L	332	GLU
1	M	106	ASN
1	M	332	GLU
1	N	70	ILE
1	N	106	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	123	ASN
1	C	156	ASN
1	F	123	ASN
1	H	277	GLN
1	K	123	ASN
1	K	282	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ADP	A	402	-	24,29,29	0.90	1 (4%)	23,45,45	2.36	5 (21%)
3	ADP	B	402	-	24,29,29	0.90	1 (4%)	23,45,45	2.37	5 (21%)
3	ADP	C	402	-	24,29,29	0.89	1 (4%)	23,45,45	2.36	5 (21%)
3	ADP	D	402	-	24,29,29	0.91	1 (4%)	23,45,45	2.37	5 (21%)
3	ADP	E	402	-	24,29,29	0.89	1 (4%)	23,45,45	2.35	5 (21%)
3	ADP	F	402	-	24,29,29	0.90	1 (4%)	23,45,45	2.36	5 (21%)
3	ADP	G	402	-	24,29,29	0.88	1 (4%)	23,45,45	2.35	5 (21%)
3	ADP	H	402	-	24,29,29	0.89	1 (4%)	23,45,45	2.35	5 (21%)
3	ADP	I	402	-	24,29,29	0.90	1 (4%)	23,45,45	2.36	5 (21%)
3	ADP	J	402	-	24,29,29	0.89	1 (4%)	23,45,45	2.35	5 (21%)
3	ADP	K	402	-	24,29,29	0.90	1 (4%)	23,45,45	2.36	5 (21%)
3	ADP	L	402	-	24,29,29	0.89	1 (4%)	23,45,45	2.36	5 (21%)
3	ADP	M	402	-	24,29,29	0.90	1 (4%)	23,45,45	2.36	5 (21%)
3	ADP	N	402	-	24,29,29	0.89	1 (4%)	23,45,45	2.35	5 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	402	-	-	0/12/32/32	0/3/3/3
3	ADP	B	402	-	-	0/12/32/32	0/3/3/3
3	ADP	C	402	-	-	0/12/32/32	0/3/3/3
3	ADP	D	402	-	-	0/12/32/32	0/3/3/3
3	ADP	E	402	-	-	0/12/32/32	0/3/3/3
3	ADP	F	402	-	-	0/12/32/32	0/3/3/3
3	ADP	G	402	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	H	402	-	-	0/12/32/32	0/3/3/3
3	ADP	I	402	-	-	0/12/32/32	0/3/3/3
3	ADP	J	402	-	-	0/12/32/32	0/3/3/3
3	ADP	K	402	-	-	0/12/32/32	0/3/3/3
3	ADP	L	402	-	-	0/12/32/32	0/3/3/3
3	ADP	M	402	-	-	0/12/32/32	0/3/3/3
3	ADP	N	402	-	-	0/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	402	ADP	C5-C4	2.55	1.46	1.40
3	B	402	ADP	C5-C4	2.55	1.46	1.40
3	G	402	ADP	C5-C4	2.55	1.46	1.40
3	E	402	ADP	C5-C4	2.56	1.46	1.40
3	J	402	ADP	C5-C4	2.57	1.46	1.40
3	H	402	ADP	C5-C4	2.58	1.46	1.40
3	L	402	ADP	C5-C4	2.58	1.46	1.40
3	C	402	ADP	C5-C4	2.59	1.46	1.40
3	K	402	ADP	C5-C4	2.59	1.46	1.40
3	F	402	ADP	C5-C4	2.60	1.46	1.40
3	A	402	ADP	C5-C4	2.61	1.46	1.40
3	I	402	ADP	C5-C4	2.62	1.46	1.40
3	D	402	ADP	C5-C4	2.63	1.46	1.40
3	M	402	ADP	C5-C4	2.63	1.46	1.40

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	ADP	N3-C2-N1	-8.19	122.43	128.87
3	B	402	ADP	N3-C2-N1	-8.17	122.45	128.87
3	I	402	ADP	N3-C2-N1	-8.12	122.49	128.87
3	C	402	ADP	N3-C2-N1	-8.12	122.50	128.87
3	K	402	ADP	N3-C2-N1	-8.11	122.50	128.87
3	F	402	ADP	N3-C2-N1	-8.11	122.50	128.87
3	M	402	ADP	N3-C2-N1	-8.10	122.51	128.87
3	A	402	ADP	N3-C2-N1	-8.10	122.51	128.87
3	J	402	ADP	N3-C2-N1	-8.10	122.51	128.87
3	L	402	ADP	N3-C2-N1	-8.09	122.51	128.87
3	G	402	ADP	N3-C2-N1	-8.09	122.52	128.87
3	N	402	ADP	N3-C2-N1	-8.08	122.52	128.87
3	E	402	ADP	N3-C2-N1	-8.08	122.53	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	402	ADP	N3-C2-N1	-8.06	122.54	128.87
3	L	402	ADP	C1'-N9-C4	-4.30	122.00	126.81
3	D	402	ADP	C1'-N9-C4	-4.29	122.01	126.81
3	H	402	ADP	C1'-N9-C4	-4.29	122.02	126.81
3	I	402	ADP	C1'-N9-C4	-4.28	122.03	126.81
3	M	402	ADP	C1'-N9-C4	-4.27	122.04	126.81
3	C	402	ADP	C1'-N9-C4	-4.27	122.04	126.81
3	G	402	ADP	C1'-N9-C4	-4.26	122.05	126.81
3	B	402	ADP	C1'-N9-C4	-4.25	122.07	126.81
3	F	402	ADP	C1'-N9-C4	-4.25	122.07	126.81
3	E	402	ADP	C1'-N9-C4	-4.24	122.08	126.81
3	J	402	ADP	C1'-N9-C4	-4.24	122.08	126.81
3	A	402	ADP	C1'-N9-C4	-4.23	122.08	126.81
3	N	402	ADP	C1'-N9-C4	-4.23	122.08	126.81
3	K	402	ADP	C1'-N9-C4	-4.23	122.09	126.81
3	A	402	ADP	C4'-O4'-C1'	-3.89	105.52	109.64
3	M	402	ADP	C4'-O4'-C1'	-3.88	105.53	109.64
3	E	402	ADP	C4'-O4'-C1'	-3.87	105.54	109.64
3	I	402	ADP	C4'-O4'-C1'	-3.87	105.55	109.64
3	B	402	ADP	C4'-O4'-C1'	-3.86	105.55	109.64
3	J	402	ADP	C4'-O4'-C1'	-3.86	105.56	109.64
3	F	402	ADP	C4'-O4'-C1'	-3.85	105.56	109.64
3	K	402	ADP	C4'-O4'-C1'	-3.85	105.56	109.64
3	N	402	ADP	C4'-O4'-C1'	-3.84	105.57	109.64
3	D	402	ADP	C4'-O4'-C1'	-3.84	105.57	109.64
3	G	402	ADP	C4'-O4'-C1'	-3.82	105.59	109.64
3	C	402	ADP	C4'-O4'-C1'	-3.82	105.59	109.64
3	H	402	ADP	C4'-O4'-C1'	-3.79	105.62	109.64
3	L	402	ADP	C4'-O4'-C1'	-3.79	105.62	109.64
3	N	402	ADP	C2-N1-C6	2.15	122.60	118.77
3	E	402	ADP	C2-N1-C6	2.15	122.61	118.77
3	J	402	ADP	C2-N1-C6	2.17	122.63	118.77
3	G	402	ADP	C2-N1-C6	2.17	122.64	118.77
3	D	402	ADP	C2-N1-C6	2.17	122.64	118.77
3	A	402	ADP	C2-N1-C6	2.17	122.64	118.77
3	M	402	ADP	C2-N1-C6	2.17	122.65	118.77
3	I	402	ADP	C2-N1-C6	2.18	122.65	118.77
3	K	402	ADP	C2-N1-C6	2.18	122.65	118.77
3	F	402	ADP	C2-N1-C6	2.18	122.65	118.77
3	B	402	ADP	C2-N1-C6	2.19	122.67	118.77
3	H	402	ADP	C2-N1-C6	2.19	122.67	118.77
3	C	402	ADP	C2-N1-C6	2.20	122.69	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	402	ADP	C2-N1-C6	2.22	122.72	118.77
3	M	402	ADP	O4'-C1'-N9	2.67	113.14	108.11
3	I	402	ADP	O4'-C1'-N9	2.67	113.16	108.11
3	A	402	ADP	O4'-C1'-N9	2.68	113.17	108.11
3	D	402	ADP	O4'-C1'-N9	2.68	113.17	108.11
3	F	402	ADP	O4'-C1'-N9	2.68	113.17	108.11
3	B	402	ADP	O4'-C1'-N9	2.68	113.18	108.11
3	J	402	ADP	O4'-C1'-N9	2.69	113.18	108.11
3	E	402	ADP	O4'-C1'-N9	2.69	113.19	108.11
3	K	402	ADP	O4'-C1'-N9	2.69	113.20	108.11
3	L	402	ADP	O4'-C1'-N9	2.70	113.20	108.11
3	G	402	ADP	O4'-C1'-N9	2.70	113.20	108.11
3	C	402	ADP	O4'-C1'-N9	2.70	113.21	108.11
3	H	402	ADP	O4'-C1'-N9	2.71	113.22	108.11
3	N	402	ADP	O4'-C1'-N9	2.71	113.23	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	402	ADP	2	0

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.