



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:58 pm BST

PDB ID : 3FI0
Title : Crystal Structure Analysis of B. stearothermophilus Tryptophanyl-tRNA Synthetase Complexed with Tryptophan, AMP, and Inorganic Phosphate
Authors : Laowanapiban, P.; Kapustina, M.; Vonnrhein, C.; Delarue, M.; Koehl, P.; Carter Jr., C.W.
Deposited on : 2008-12-10
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

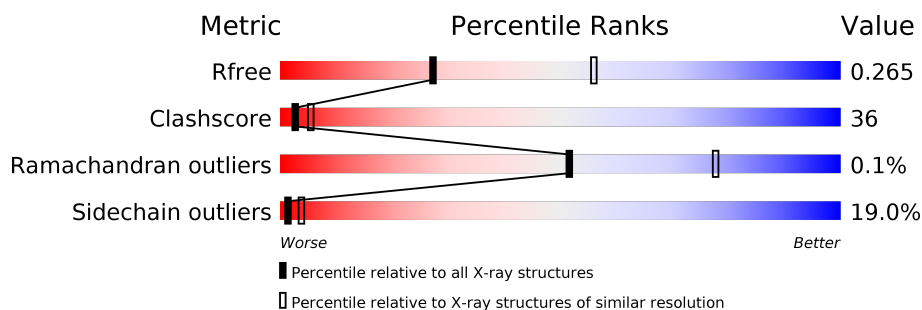
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	326	
1	B	326	
1	C	326	
1	D	326	
1	E	326	
1	F	326	
1	G	326	

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Mol	Chain	Length	Quality of chain
1	H	326	
1	I	326	
1	J	326	
1	K	326	
1	L	326	
1	M	326	
1	N	326	
1	O	326	
1	P	326	
1	Q	326	
1	R	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	E	1002	-	-	X	-
3	PO4	F	1002	-	-	X	-
3	PO4	H	1002	-	-	X	-
3	PO4	M	1002	-	-	X	-
3	PO4	N	1002	-	-	X	-
3	PO4	O	1002	-	-	X	-
3	PO4	P	1002	-	-	X	-
4	AMP	A	1003	-	-	X	-
4	AMP	B	1003	-	-	X	-
4	AMP	G	1003	-	-	X	-
4	AMP	I	1003	-	-	X	-
4	AMP	O	1003	-	-	X	-
4	AMP	P	1003	-	-	X	-
4	AMP	Q	1003	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43727 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	Se	0	0	0
			2383	1512	410	448	3	10			
1	B	295	Total	C	N	O	S	Se	0	0	0
			2370	1505	408	444	3	10			
1	C	297	Total	C	N	O	S	Se	0	0	0
			2383	1512	410	448	3	10			
1	D	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	E	293	Total	C	N	O	S	Se	0	0	0
			2342	1484	405	440	3	10			
1	F	296	Total	C	N	O	S	Se	0	0	0
			2368	1502	410	443	3	10			
1	G	302	Total	C	N	O	S	Se	0	0	0
			2416	1534	416	453	3	10			
1	H	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	I	298	Total	C	N	O	S	Se	0	0	0
			2377	1507	409	448	3	10			
1	J	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	K	296	Total	C	N	O	S	Se	0	0	0
			2367	1504	408	442	3	10			
1	L	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	M	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	N	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	O	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	P	295	Total	C	N	O	S	Se	0	0	0
			2361	1499	407	442	3	10			

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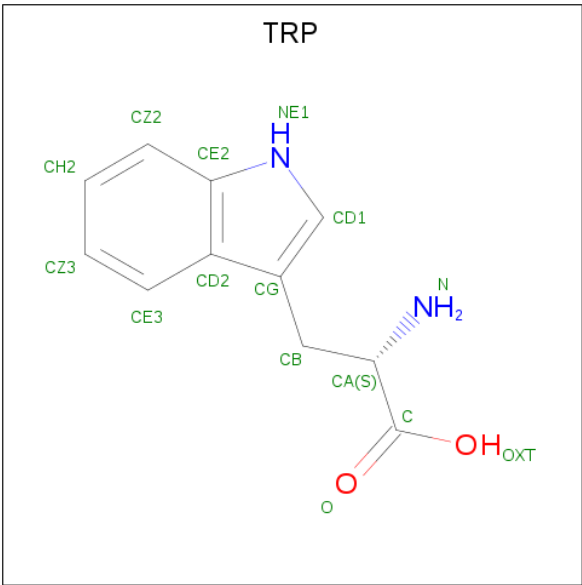
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	R	290	Total	C	N	O	S	Se	0	0	0
			2322	1473	399	437	3	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	LYS	CONFLICT	UNP P00953
D	64	LEU	LYS	CONFLICT	UNP P00953
B	64	LEU	LYS	CONFLICT	UNP P00953
C	64	LEU	LYS	CONFLICT	UNP P00953
E	64	LEU	LYS	CONFLICT	UNP P00953
F	64	LEU	LYS	CONFLICT	UNP P00953
G	64	LEU	LYS	CONFLICT	UNP P00953
H	64	LEU	LYS	CONFLICT	UNP P00953
I	64	LEU	LYS	CONFLICT	UNP P00953
J	64	LEU	LYS	CONFLICT	UNP P00953
K	64	LEU	LYS	CONFLICT	UNP P00953
L	64	LEU	LYS	CONFLICT	UNP P00953
M	64	LEU	LYS	CONFLICT	UNP P00953
N	64	LEU	LYS	CONFLICT	UNP P00953
O	64	LEU	LYS	CONFLICT	UNP P00953
P	64	LEU	LYS	CONFLICT	UNP P00953
Q	64	LEU	LYS	CONFLICT	UNP P00953
R	64	LEU	LYS	CONFLICT	UNP P00953

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂).



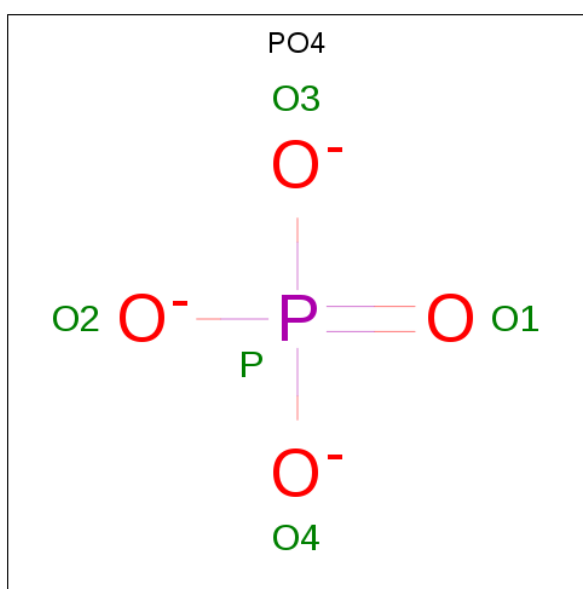
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	F	1	Total	C	N	O	0	0
			15	11	2	2		
2	G	1	Total	C	N	O	0	0
			15	11	2	2		
2	H	1	Total	C	N	O	0	0
			15	11	2	2		
2	I	1	Total	C	N	O	0	0
			15	11	2	2		
2	J	1	Total	C	N	O	0	0
			15	11	2	2		
2	K	1	Total	C	N	O	0	0
			15	11	2	2		
2	L	1	Total	C	N	O	0	0
			15	11	2	2		
2	M	1	Total	C	N	O	0	0
			15	11	2	2		
2	N	1	Total	C	N	O	0	0
			15	11	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	N	O	0	0
			15	11	2	2		
2	P	1	Total	C	N	O	0	0
			15	11	2	2		
2	Q	1	Total	C	N	O	0	0
			15	11	2	2		
2	R	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



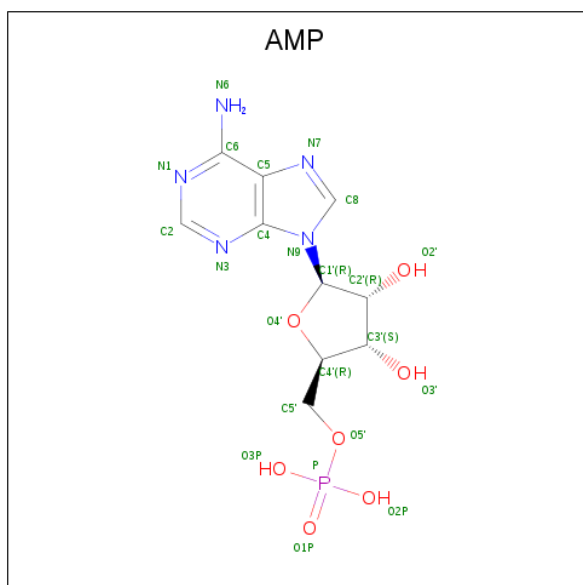
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		
3	N	1	Total	O	P	0	0
			5	4	1		
3	O	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	R	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

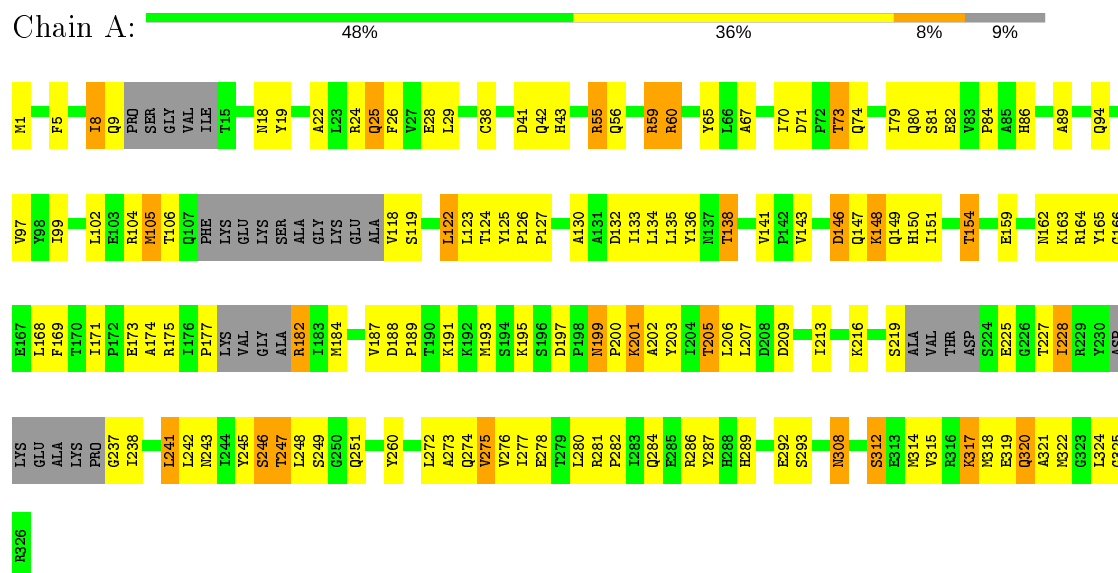


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	D	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	E	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	F	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	G	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	H	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	I	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	J	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	K	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	L	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	M	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	N	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	O	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	P	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	R	1	Total 23	C 10	N 5	O 7	P 1	0	0

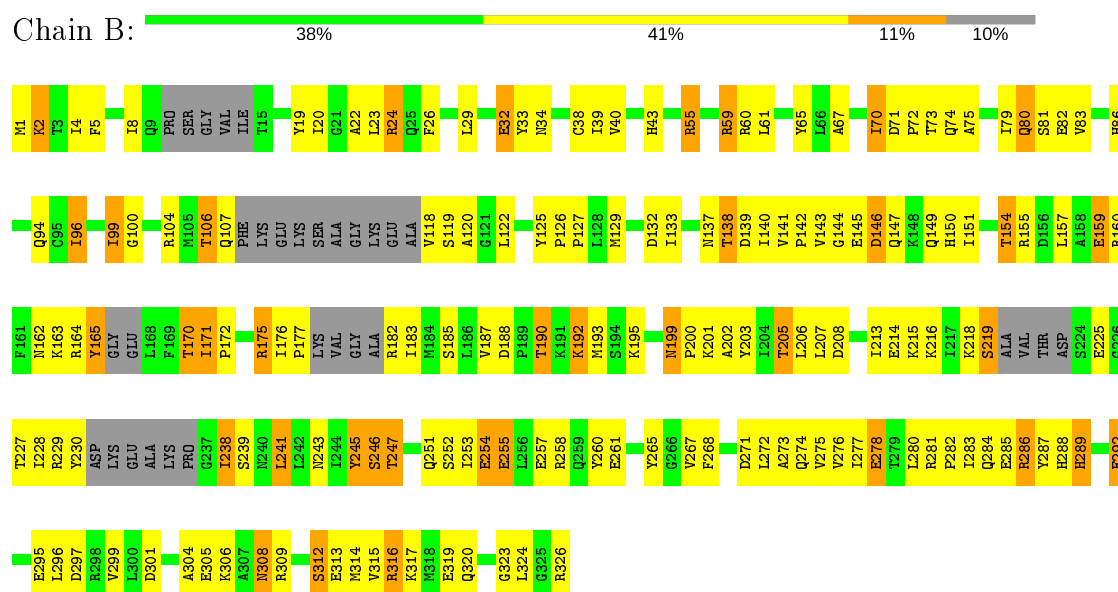
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Tryptophanyl-tRNA synthetase

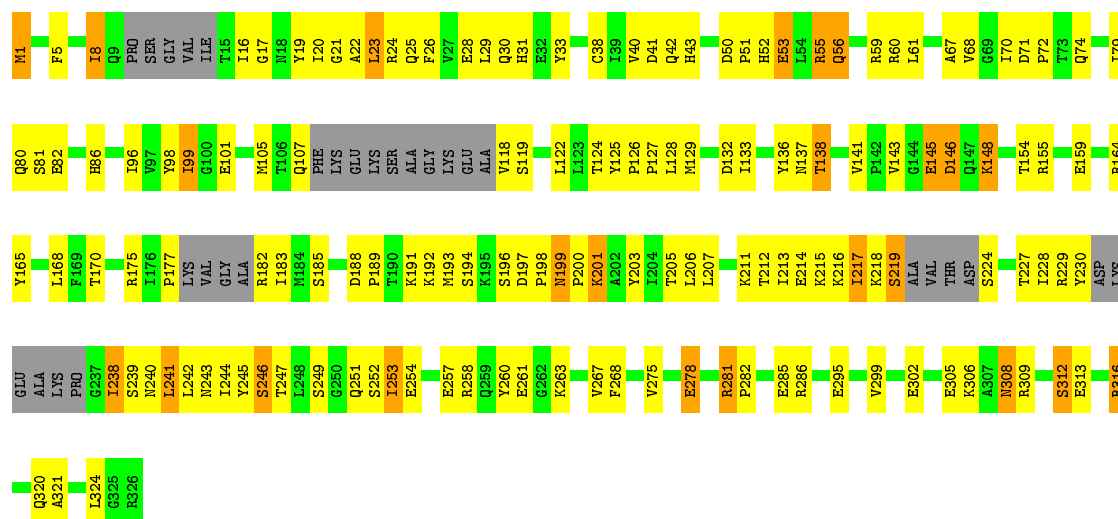


• Molecule 1: Tryptophanyl-tRNA synthetase



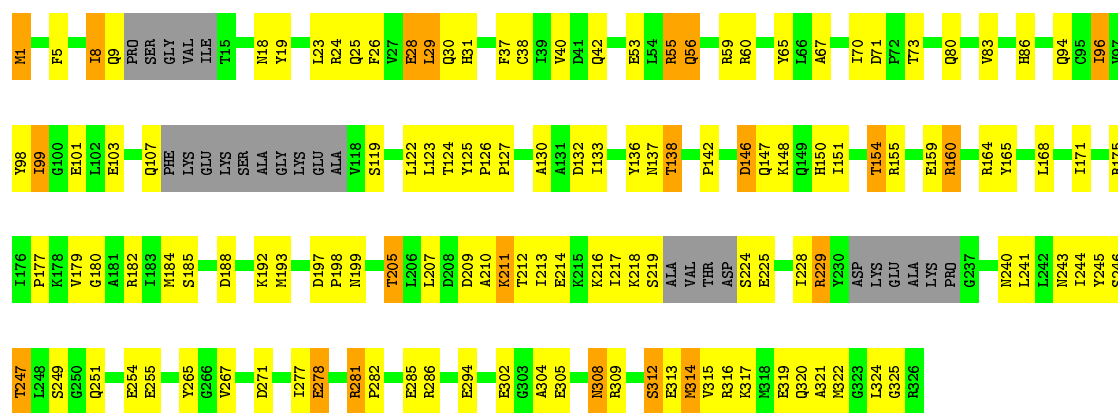
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain C: 



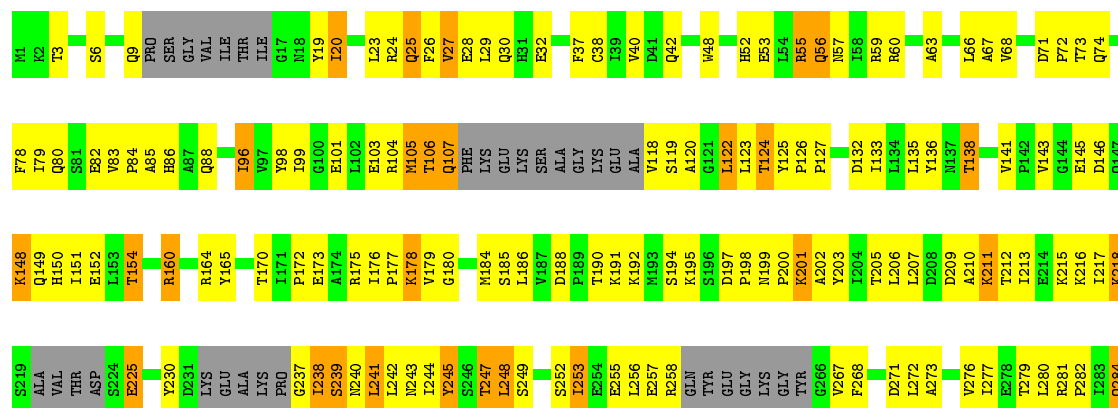
• Molecule 1: Tryptophanyl-tRNA synthetase

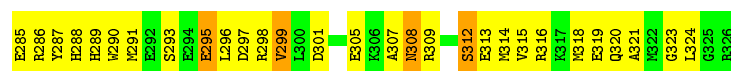
Chain D: 



• Molecule 1: Tryptophanyl-tRNA synthetase

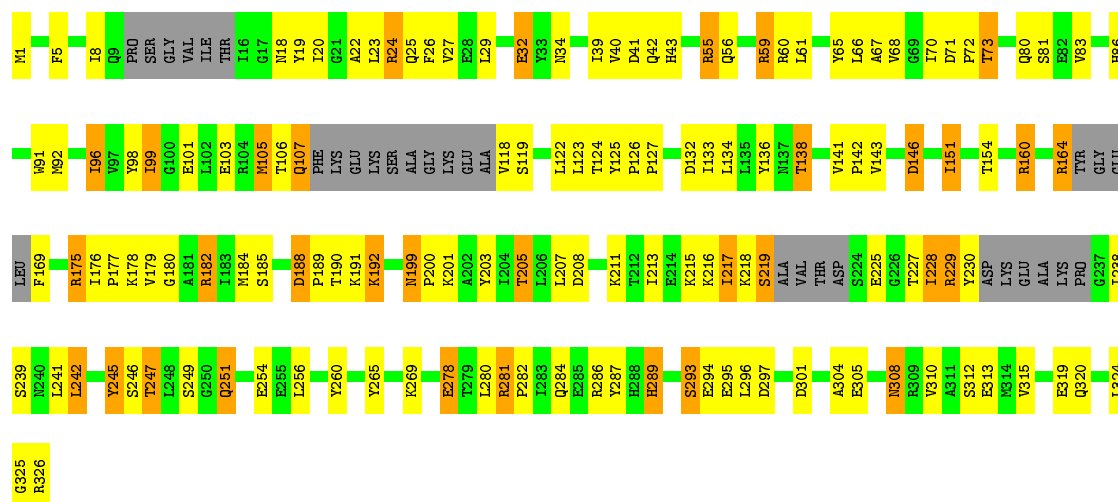
Chain E: 





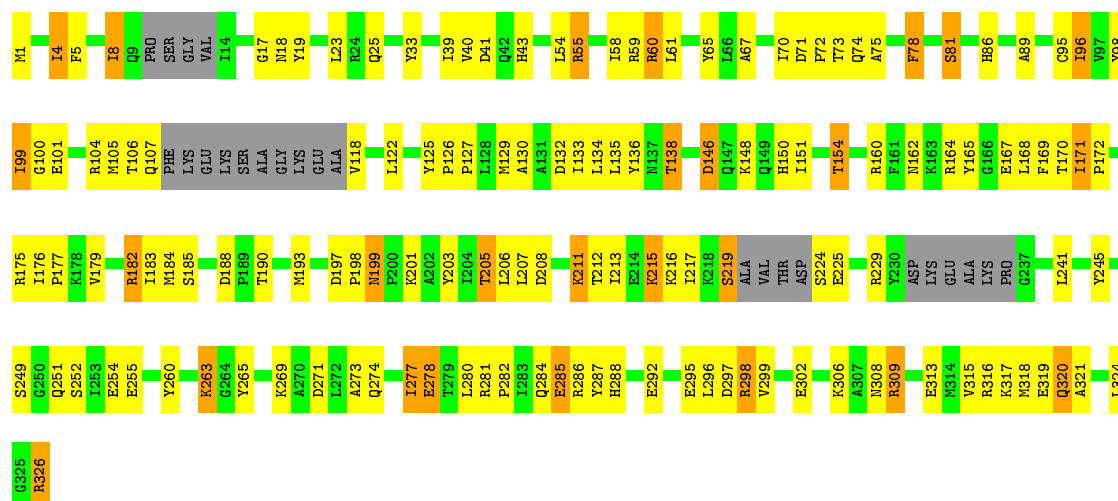
- Molecule 1: Tryptophanyl-tRNA synthetase

Chain F:  47% 33% 10% 9%



- Molecule 1: Tryptophanyl-tRNA synthetase

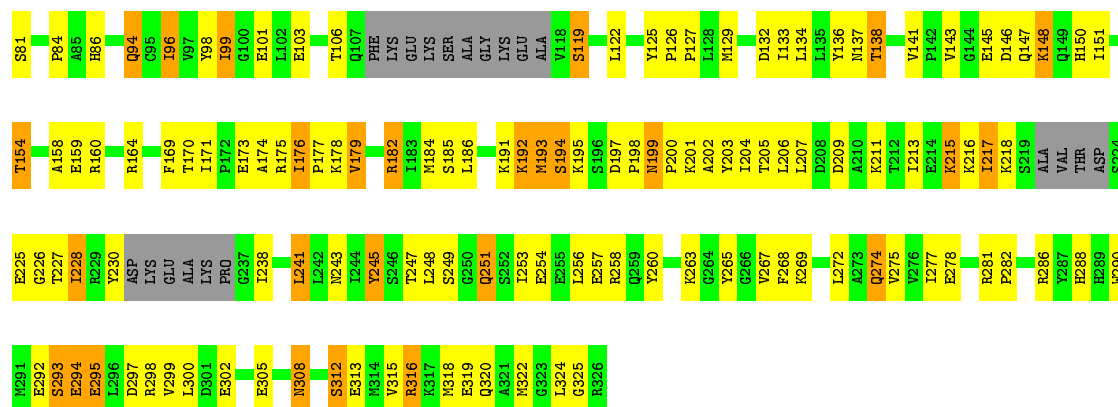
Chain G: 48% 36% 8% 7%



- Molecule 1: Tryptophanyl-tRNA synthetase

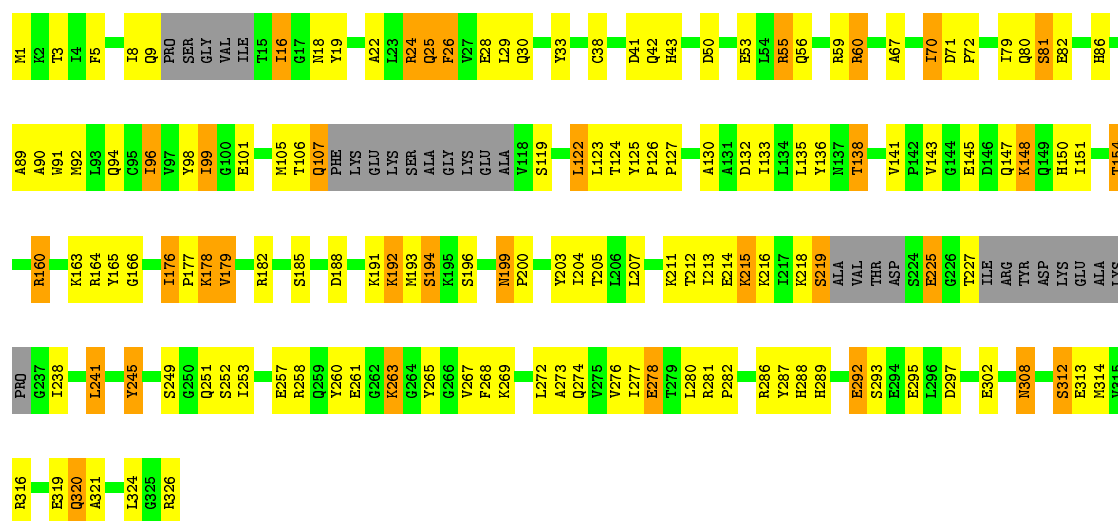
Chain H:  42% 41% 10% 8%





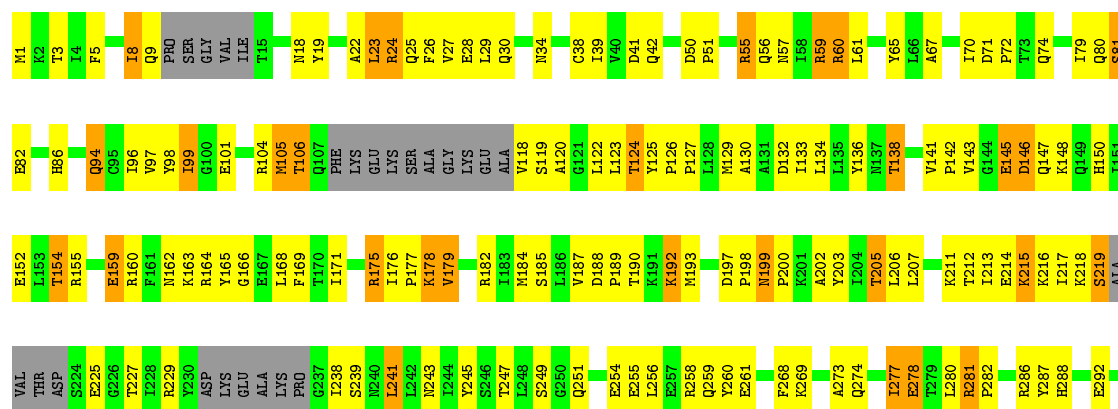
• Molecule 1: Tryptophanyl-tRNA synthetase

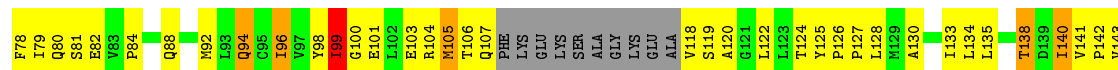
Chain I: 47% 34% 10% 9%

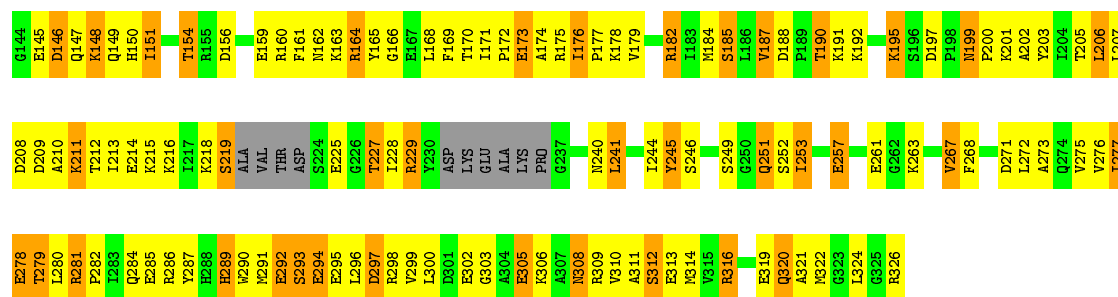


• Molecule 1: Tryptophanyl-tRNA synthetase

Chain J: 40% 42% 10% 8%

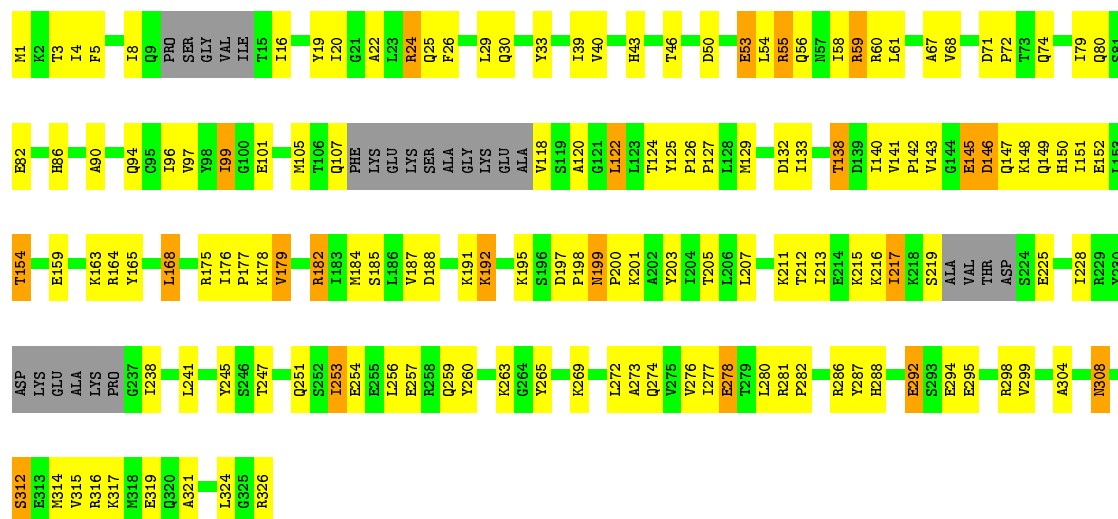






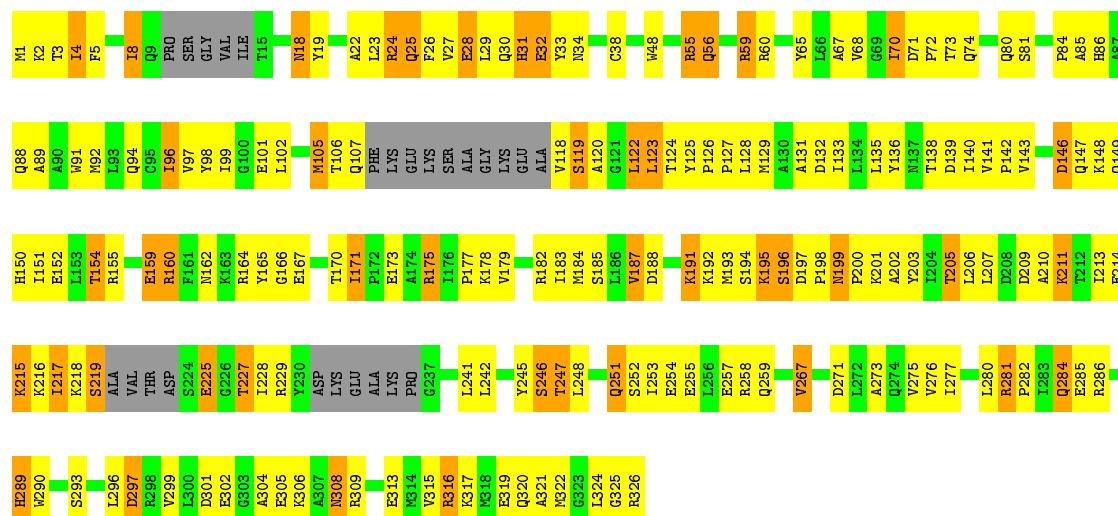
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain N: 48% 38% 6% 8%



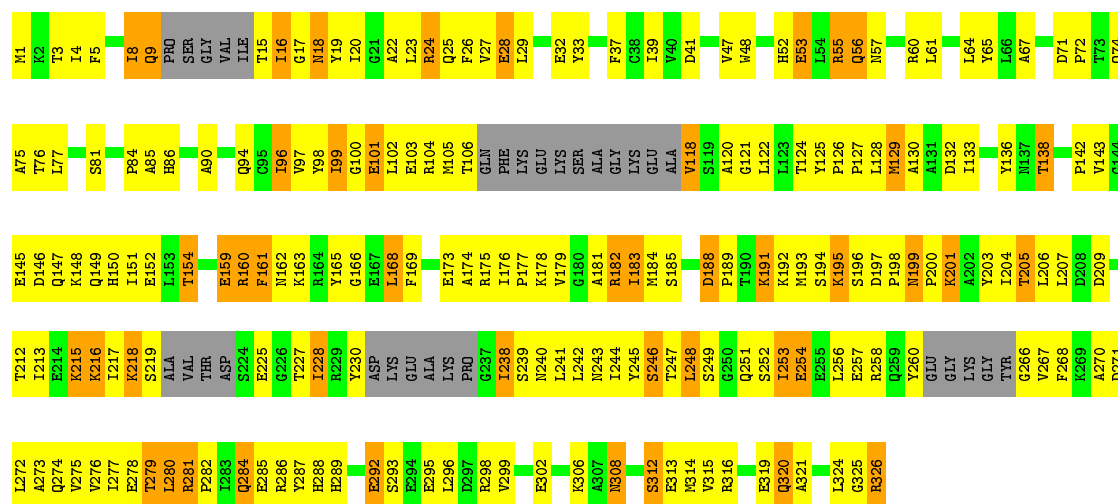
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain O: 36% 43% 14% 8%



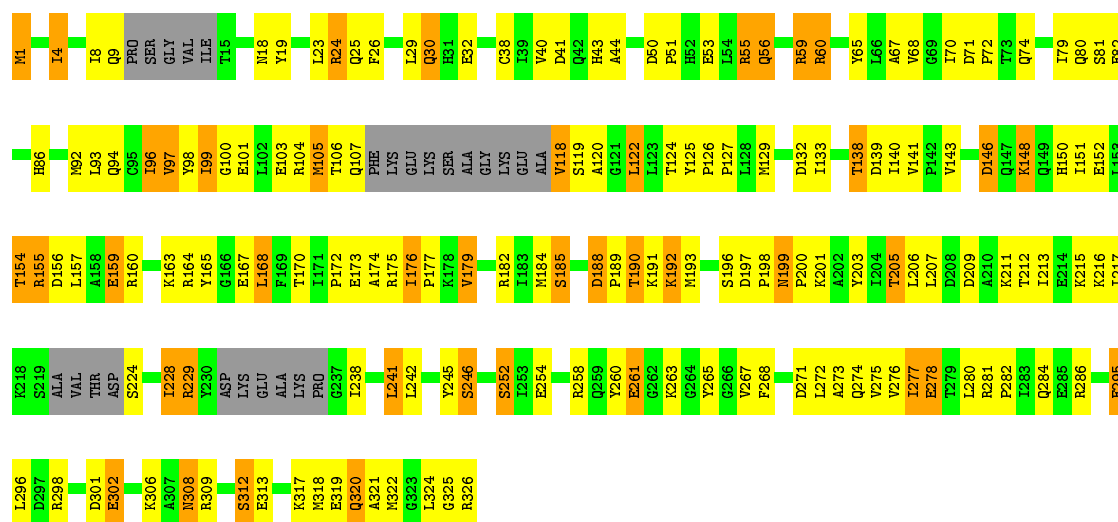
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain P: 



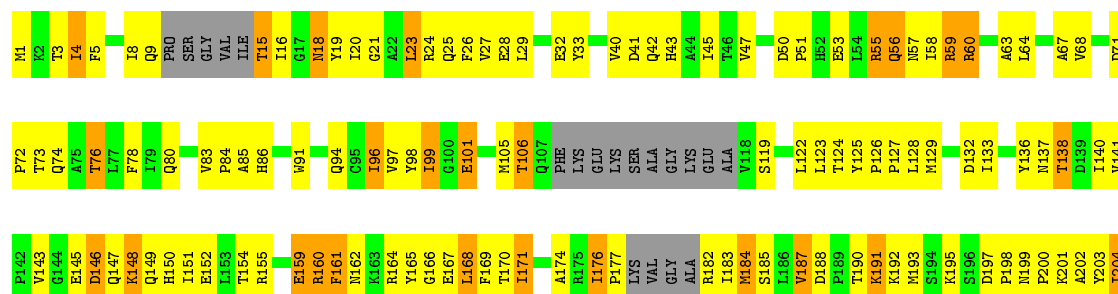
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain Q: 



• Molecule 1: Tryptophanyl-tRNA synthetase

Chain R: 



T206	T207	D208	D209	A210	K211	T212	I213	E214	K215	K216	I217	K218	S219	ALA	VAL	THR	ASP	S224	E225	G226	T227	I228	ARG	THR	ASP	LYS	GLU	ALA	LYS	PRO	G237	I238	S239	N240	I241	L242	N243	I244	Y245	S246	T247	L248		Q251	S252	I253	E254	E255	L256	E257		Y260	GLU	GLY	LYS	GLY	TYR	G266
V267	F268	K269	A270	L271	A272	A273	Q274	V275	V276	I277	E278	T279	L280	R281	P282	I283	Q284	E285	R286	Y287	H288	H289	W290	W291	E292	S293	E294	E295	L296	D297	R298	V299	L300	D301	E302		K306	A307	N308		S312	E313	K314	V315	R316		E319	Q320	A321		L324	G325	R326					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.03Å 122.40Å 122.34Å 79.90° 80.52° 79.81°	Depositor
Resolution (Å)	25.00 – 2.70 24.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (25.00-2.70) 99.0 (24.96-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.72Å)	Xtriage
Refinement program	REFMAC refmac _5.2.0019	Depositor
R, R_{free}	0.190 , 0.220 0.252 , 0.265	Depositor DCC
R_{free} test set	9262 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for l,h,k 0.048 for k,l,h 0.000 for -l,-k,-h 0.000 for -k,-h,-l 0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	43727	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.9719e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: AMP, PO4

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	0.38	0/2414	0.52	0/3242
1	B	0.30	0/2400	0.51	0/3222
1	C	0.31	0/2414	0.56	0/3242
1	D	0.32	0/2440	0.53	0/3278
1	E	0.29	0/2371	0.54	0/3184
1	F	0.29	0/2398	0.51	0/3219
1	G	0.30	0/2448	0.55	0/3289
1	H	0.29	0/2440	0.54	0/3278
1	I	0.31	0/2408	0.54	0/3235
1	J	0.30	0/2440	0.54	0/3278
1	K	0.28	0/2398	0.52	0/3220
1	L	0.31	0/2440	0.55	0/3278
1	M	0.28	0/2440	0.56	2/3278 (0.1%)
1	N	0.30	0/2440	0.56	0/3278
1	O	0.30	0/2440	0.56	0/3278
1	P	0.27	0/2391	0.57	1/3212 (0.0%)
1	Q	0.31	0/2440	0.57	1/3278 (0.0%)
1	R	0.29	0/2350	0.55	0/3156
All	All	0.30	0/43512	0.54	4/58445 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	44	ALA	CB-CA-C	-5.73	101.51	110.10
1	P	188	ASP	C-N-CD	-5.51	108.48	120.60
1	M	252	SER	N-CA-CB	-5.37	102.44	110.50
1	M	99	ILE	CB-CA-C	-5.31	100.98	111.60

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	2383	0	2390	141	0
1	B	2370	0	2380	197	0
1	C	2383	0	2390	129	0
1	D	2408	0	2421	130	0
1	E	2342	0	2355	219	0
1	F	2368	0	2384	141	0
1	G	2416	0	2432	139	0
1	H	2408	0	2421	158	0
1	I	2377	0	2388	138	0
1	J	2408	0	2421	137	0
1	K	2367	0	2382	207	0
1	L	2408	0	2421	123	0
1	M	2408	0	2421	264	0
1	N	2408	0	2421	143	0
1	O	2408	0	2421	198	0
1	P	2361	0	2378	355	0
1	Q	2408	0	2421	172	0
1	R	2322	0	2333	283	0
2	A	15	0	9	0	0
2	B	15	0	9	1	0
2	C	15	0	9	2	0
2	D	15	0	9	0	0
2	E	15	0	9	0	0
2	F	15	0	9	0	0
2	G	15	0	9	2	0
2	H	15	0	9	1	0
2	I	15	0	9	0	0
2	J	15	0	9	2	0
2	K	15	0	9	0	0
2	L	15	0	9	0	0
2	M	15	0	9	0	0
2	N	15	0	9	0	0
2	O	15	0	9	0	0
2	P	15	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	15	0	9	1	0
2	R	15	0	9	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	3	0
3	F	5	0	0	2	0
3	G	5	0	0	1	0
3	H	5	0	0	2	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	K	5	0	0	1	0
3	L	5	0	0	0	0
3	M	5	0	0	3	0
3	N	5	0	0	2	0
3	O	5	0	0	2	0
3	P	5	0	0	7	0
3	Q	5	0	0	0	0
3	R	5	0	0	1	0
4	A	23	0	12	10	0
4	B	23	0	12	8	0
4	C	23	0	12	3	0
4	D	23	0	12	5	0
4	E	23	0	12	4	0
4	F	23	0	12	2	0
4	G	23	0	12	9	0
4	H	23	0	12	1	0
4	I	23	0	12	7	0
4	J	23	0	12	3	0
4	K	23	0	12	4	0
4	L	23	0	12	1	0
4	M	23	0	12	5	0
4	N	23	0	12	6	0
4	O	23	0	12	17	0
4	P	23	0	12	12	0
4	Q	23	0	12	7	0
4	R	23	0	12	4	0
All	All	43727	0	43558	3147	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 36.

All (3147) 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:Q:140:ILE:CD1	1:Q:175:ARG:HG3	1.54	1.36
1:M:23:LEU:HD21	1:M:65:TYR:CE1	1.72	1.24
1:I:199:ASN:ND2	1:I:200:PRO:HD2	1.54	1.23
1:Q:140:ILE:HD11	1:Q:175:ARG:CG	1.69	1.22
1:B:94:GLN:NE2	1:E:124:THR:HG21	1.55	1.20
1:I:199:ASN:HD22	1:I:200:PRO:CD	1.54	1.19
1:P:176:ILE:HB	1:P:179:VAL:CG2	1.71	1.18
1:M:105:MSE:CE	1:M:150:HIS:CE1	2.27	1.17
1:P:245:TYR:CE1	1:P:275:VAL:HG21	1.77	1.17
1:M:23:LEU:CD2	1:M:65:TYR:HE1	1.55	1.17
1:I:199:ASN:HD22	1:I:200:PRO:HD2	1.01	1.17
1:P:244:ILE:O	1:P:248:LEU:HD13	1.44	1.16
1:R:24:ARG:O	1:R:27:VAL:HG22	1.43	1.16
1:R:252:SER:OG	1:R:255:GLU:HB2	1.46	1.15
1:M:210:ALA:HB1	1:M:277:ILE:HD13	1.18	1.14
1:P:142:PRO:HA	1:P:175:ARG:O	1.46	1.14
1:K:245:TYR:CE2	1:K:256:LEU:HD11	1.83	1.14
1:M:23:LEU:CD2	1:M:65:TYR:CE1	2.28	1.14
1:P:151:ILE:HD13	1:P:174:ALA:HB2	1.16	1.14
1:I:205:THR:HG22	1:I:207:LEU:H	1.13	1.13
1:P:271:ASP:O	1:P:275:VAL:HG23	1.45	1.13
1:R:228:ILE:HG21	1:R:260:TYR:CB	1.79	1.13
1:K:260:TYR:HA	1:K:263:LYS:HD3	1.25	1.12
1:M:156:ASP:O	1:M:160:ARG:HG3	1.48	1.12
1:P:273:ALA:O	1:P:277:ILE:HG12	1.49	1.12
1:R:276:VAL:O	1:R:280:LEU:HG	1.47	1.12
1:E:20:ILE:HD12	1:E:20:ILE:H	1.02	1.12
1:K:245:TYR:CE1	1:K:275:VAL:HG11	1.86	1.10
1:P:281:ARG:HG3	1:P:282:PRO:HD3	1.23	1.10
1:O:5:PHE:HB2	1:O:138:THR:HG21	1.34	1.10
1:E:252:SER:OG	1:E:255:GLU:HB2	1.51	1.10
1:P:176:ILE:O	1:P:179:VAL:HG23	1.52	1.09
1:M:25:GLN:HG3	1:M:29:LEU:CD1	1.82	1.08
1:A:18:ASN:HD21	4:A:1003:AMP:H5'1	1.15	1.08
1:K:241:LEU:H	1:K:241:LEU:HD12	1.09	1.08
1:P:253:ILE:HG22	1:P:254:GLU:OE2	1.53	1.08
1:P:245:TYR:HB2	1:P:272:LEU:HD13	1.12	1.07
1:P:228:ILE:HG22	1:P:238:ILE:HD11	1.33	1.07
1:K:245:TYR:CD2	1:K:256:LEU:HD12	1.88	1.07
1:M:205:THR:HG22	1:M:207:LEU:H	1.17	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:253:ILE:HG22	1:P:254:GLU:CD	1.75	1.06
1:P:245:TYR:CB	1:P:272:LEU:HD13	1.85	1.06
1:E:136:TYR:OH	1:E:307:ALA:HB1	1.55	1.06
1:B:29:LEU:CD1	1:B:177:PRO:HB2	1.86	1.05
1:K:191:LYS:HD3	1:K:192:LYS:H	1.19	1.05
1:R:187:VAL:HG22	1:R:202:ALA:HB2	1.35	1.05
1:P:126:PRO:HG2	1:P:127:PRO:HD3	1.38	1.05
1:B:29:LEU:HD11	1:B:177:PRO:HB2	1.39	1.04
1:E:211:LYS:HD3	1:E:211:LYS:H	1.19	1.04
1:B:94:GLN:HE21	1:E:124:THR:HG21	0.94	1.03
1:P:100:GLY:O	1:P:104:ARG:HG3	1.57	1.03
1:G:188:ASP:OD1	1:G:190:THR:HG22	1.57	1.02
1:N:19:TYR:O	1:N:24:ARG:HB3	1.59	1.02
1:O:26:PHE:HD2	1:O:29:LEU:HD12	1.24	1.02
1:R:133:ILE:O	1:R:138:THR:HG23	1.59	1.02
1:I:24:ARG:HG2	1:I:24:ARG:HH11	1.19	1.02
1:C:205:THR:HG22	1:C:207:LEU:H	1.19	1.02
1:E:20:ILE:HD12	1:E:20:ILE:N	1.75	1.02
1:B:19:TYR:O	1:B:24:ARG:HB3	1.58	1.01
1:M:175:ARG:NH1	1:M:177:PRO:HG3	1.74	1.01
1:P:181:ALA:HB1	1:P:243:ASN:HD22	1.23	1.01
1:B:319:GLU:HB3	1:B:324:LEU:HB2	1.38	1.01
1:P:151:ILE:CD1	1:P:174:ALA:HB2	1.91	1.01
1:Q:140:ILE:CD1	1:Q:175:ARG:CG	2.32	1.00
1:K:124:THR:O	1:K:127:PRO:HD2	1.57	1.00
1:M:25:GLN:HG3	1:M:29:LEU:HD11	1.43	1.00
1:I:176:ILE:HG13	1:I:179:VAL:HG13	1.43	1.00
1:K:134:LEU:HB3	1:K:169:PHE:CD1	1.96	1.00
1:R:228:ILE:HB	1:R:260:TYR:O	1.58	1.00
1:R:260:TYR:CD1	1:R:268:PHE:HD1	1.79	1.00
1:I:258:ARG:O	1:I:261:GLU:HG2	1.60	1.00
1:H:274:GLN:O	1:H:278:GLU:HG2	1.62	1.00
1:P:24:ARG:HH22	1:P:247:THR:HB	1.22	1.00
1:K:134:LEU:HB3	1:K:169:PHE:CE1	1.98	0.99
1:J:258:ARG:HA	1:J:261:GLU:OE2	1.61	0.99
1:M:176:ILE:HB	1:M:179:VAL:HG12	1.44	0.99
1:M:199:ASN:ND2	1:M:201:LYS:HG2	1.75	0.99
1:R:187:VAL:HG22	1:R:202:ALA:CB	1.92	0.99
1:P:151:ILE:HD13	1:P:174:ALA:CB	1.94	0.98
1:K:245:TYR:CD2	1:K:256:LEU:CD1	2.46	0.98
1:H:205:THR:HG22	1:H:207:LEU:H	1.24	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:18:ASN:O	1:P:18:ASN:ND2	1.96	0.98
1:R:228:ILE:HG21	1:R:260:TYR:HB2	1.42	0.98
1:C:1:MSE:HG2	1:D:211:LYS:HD2	1.42	0.98
1:K:245:TYR:CE2	1:K:256:LEU:CD1	2.47	0.98
1:K:60:ARG:HA	1:K:291:MSE:HE1	1.45	0.97
1:M:161:PHE:CD2	1:M:169:PHE:HE2	1.82	0.97
1:M:280:LEU:O	1:M:284:GLN:HG3	1.65	0.97
1:E:20:ILE:H	1:E:20:ILE:CD1	1.78	0.97
1:O:26:PHE:CD2	1:O:29:LEU:HD12	1.99	0.97
1:P:29:LEU:O	1:P:33:TYR:HB2	1.65	0.96
1:F:107:GLN:HE21	1:F:107:GLN:H	1.09	0.96
1:M:105:MSE:HE2	1:M:150:HIS:CE1	1.97	0.96
1:R:228:ILE:HG21	1:R:260:TYR:HB3	1.46	0.96
1:K:237:GLY:O	1:K:241:LEU:HD11	1.65	0.96
1:R:279:THR:O	1:R:282:PRO:HD2	1.64	0.96
1:F:182:ARG:NH1	1:F:192:LYS:HD3	1.80	0.95
1:M:210:ALA:CB	1:M:277:ILE:HD13	1.95	0.95
1:P:16:ILE:HD11	1:P:193:MSE:HE1	1.48	0.95
1:M:159:GLU:O	1:M:163:LYS:HG3	1.66	0.95
1:M:26:PHE:HA	1:M:29:LEU:HB2	1.49	0.95
1:P:24:ARG:NH2	1:P:247:THR:HB	1.81	0.95
1:K:191:LYS:CD	1:K:192:LYS:H	1.79	0.95
1:M:225:GLU:HG2	1:M:227:THR:HG23	1.46	0.94
1:C:55:ARG:HH22	1:F:320:GLN:NE2	1.64	0.94
1:M:105:MSE:CE	1:M:150:HIS:ND1	2.30	0.94
1:A:124:THR:HG21	1:D:94:GLN:NE2	1.82	0.94
1:I:24:ARG:CG	1:I:24:ARG:HH11	1.81	0.94
1:M:105:MSE:HE1	1:M:150:HIS:ND1	1.82	0.94
1:R:251:GLN:HG3	1:R:256:LEU:HD11	1.45	0.94
1:F:107:GLN:NE2	1:F:107:GLN:H	1.66	0.94
1:K:191:LYS:HD3	1:K:192:LYS:N	1.82	0.94
1:P:176:ILE:HB	1:P:179:VAL:HG22	1.45	0.94
1:R:187:VAL:CG2	1:R:202:ALA:HB2	1.98	0.94
1:C:26:PHE:HA	1:C:29:LEU:HB2	1.47	0.93
1:H:254:GLU:O	1:H:258:ARG:HG3	1.68	0.93
1:B:137:ASN:HD21	1:B:314:MSE:HE1	1.30	0.93
1:P:239:SER:O	1:P:242:LEU:HB2	1.68	0.93
1:P:126:PRO:CG	1:P:127:PRO:HD3	1.99	0.93
1:M:161:PHE:HE2	1:M:168:LEU:HD23	1.31	0.92
1:G:18:ASN:HD21	4:G:1003:AMP:H5'2	1.34	0.92
1:O:18:ASN:HA	4:O:1003:AMP:H1'	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:254:GLU:HA	1:P:257:GLU:HB3	1.51	0.92
1:N:126:PRO:HB2	1:N:127:PRO:HD3	1.50	0.92
1:P:274:GLN:O	1:P:278:GLU:HG2	1.70	0.92
1:K:161:PHE:CE2	1:K:168:LEU:HD12	2.04	0.92
1:M:199:ASN:HD21	1:M:201:LYS:HG2	1.32	0.92
1:E:27:VAL:HG12	1:E:28:GLU:HG2	1.51	0.92
1:Q:205:THR:HG22	1:Q:207:LEU:H	1.31	0.92
1:P:124:THR:C	1:P:126:PRO:HD2	1.90	0.91
1:I:260:TYR:C	1:I:263:LYS:HG2	1.91	0.91
1:M:294:GLU:HG3	1:M:298:ARG:HH21	1.35	0.91
1:P:125:TYR:N	1:P:126:PRO:CD	2.33	0.91
1:K:125:TYR:N	1:K:126:PRO:CD	2.34	0.91
1:B:137:ASN:HD21	1:B:314:MSE:CE	1.84	0.91
1:R:165:TYR:HB3	1:R:321:ALA:HB1	1.52	0.91
1:R:185:SER:OG	1:R:202:ALA:HB1	1.69	0.91
1:E:184:MSE:HE3	1:E:191:LYS:C	1.91	0.90
1:K:25:GLN:O	1:K:29:LEU:HG	1.71	0.90
3:M:1002:PO4:O2	4:M:1003:AMP:H8	1.54	0.90
1:M:140:ILE:HG12	1:M:175:ARG:HB3	1.51	0.90
1:Q:94:GLN:O	1:Q:97:VAL:HG12	1.72	0.90
1:K:56:GLN:HE21	1:K:56:GLN:HA	1.35	0.90
1:R:213:ILE:HD12	1:R:277:ILE:HG12	1.53	0.90
1:M:126:PRO:HB2	1:M:127:PRO:HD3	1.51	0.89
1:M:209:ASP:OD1	1:M:212:THR:HB	1.73	0.89
1:N:245:TYR:HE2	1:N:256:LEU:CD2	1.84	0.89
1:R:252:SER:HG	1:R:255:GLU:HB2	1.37	0.89
1:A:320:GLN:HE21	1:D:55:ARG:NH2	1.70	0.89
1:N:205:THR:HG22	1:N:207:LEU:H	1.32	0.89
1:A:205:THR:HG22	1:A:207:LEU:H	1.36	0.89
1:R:211:LYS:O	1:R:215:LYS:HB2	1.73	0.89
1:P:245:TYR:CD2	1:P:256:LEU:HD13	2.07	0.88
1:E:205:THR:HG22	1:E:207:LEU:H	1.35	0.88
1:K:106:THR:H	1:K:149:GLN:HE22	1.13	0.88
1:N:308:ASN:O	1:N:312:SER:HB2	1.71	0.88
1:B:288:HIS:O	1:B:292:GLU:HG2	1.73	0.88
1:H:182:ARG:HG3	1:H:182:ARG:HH11	1.36	0.88
1:D:126:PRO:HB2	1:D:127:PRO:HD3	1.56	0.88
1:O:199:ASN:HD22	1:O:200:PRO:HD2	1.37	0.88
1:P:245:TYR:HD2	1:P:256:LEU:HD13	1.39	0.88
1:I:24:ARG:HG2	1:I:24:ARG:NH1	1.78	0.88
1:M:302:GLU:O	1:M:306:LYS:HG3	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:176:ILE:O	1:N:179:VAL:HG22	1.72	0.88
1:H:308:ASN:O	1:H:312:SER:HB2	1.74	0.87
1:M:59:ARG:NH2	1:M:296:LEU:HD23	1.87	0.87
1:I:176:ILE:CG1	1:I:179:VAL:HG13	2.05	0.87
1:I:249:SER:OG	1:I:251:GLN:HG3	1.73	0.87
1:K:161:PHE:HE2	1:K:168:LEU:HD12	1.35	0.87
1:P:228:ILE:CG1	1:P:260:TYR:HB3	2.04	0.87
1:B:94:GLN:NE2	1:E:124:THR:CG2	2.37	0.87
1:E:211:LYS:HD3	1:E:211:LYS:N	1.88	0.87
1:E:98:TYR:HB2	1:E:101:GLU:HG3	1.57	0.87
1:H:56:GLN:HG2	1:H:60:ARG:CZ	2.04	0.87
1:M:161:PHE:CD2	1:M:169:PHE:CE2	2.61	0.87
1:R:225:GLU:OE2	1:R:227:THR:HG23	1.75	0.87
1:G:182:ARG:HG2	1:G:184:MSE:CE	2.05	0.86
1:M:282:PRO:HB2	1:M:286:ARG:HH21	1.40	0.86
1:E:30:GLN:HG3	1:E:74:GLN:HG2	1.57	0.86
1:N:50:ASP:HB3	1:N:53:GLU:HG2	1.58	0.86
1:D:19:TYR:O	1:D:24:ARG:HB2	1.75	0.86
1:E:241:LEU:HD22	1:E:241:LEU:N	1.89	0.86
1:K:159:GLU:OE2	1:K:163:LYS:HE3	1.76	0.86
1:P:245:TYR:HB2	1:P:272:LEU:CD1	2.03	0.86
1:R:105:MSE:HE1	1:R:150:HIS:HA	1.57	0.86
1:A:18:ASN:ND2	4:A:1003:AMP:H5'1	1.89	0.86
1:M:165:TYR:CE1	1:M:322:MSE:HA	2.09	0.86
1:R:308:ASN:O	1:R:312:SER:HB2	1.76	0.86
1:A:134:LEU:HB3	1:A:169:PHE:CD1	2.11	0.86
1:P:20:ILE:HD12	1:P:183:ILE:CD1	2.06	0.86
1:B:22:ALA:O	1:B:26:PHE:CD2	2.28	0.86
1:C:211:LYS:O	1:C:215:LYS:HG3	1.75	0.86
1:G:205:THR:HG22	1:G:207:LEU:H	1.41	0.86
1:E:19:TYR:HE1	1:E:68:VAL:HG13	1.41	0.86
1:F:25:GLN:O	1:F:29:LEU:HG	1.76	0.85
1:D:212:THR:HG22	1:D:216:LYS:HD2	1.58	0.85
1:P:181:ALA:HB1	1:P:243:ASN:ND2	1.90	0.85
1:H:199:ASN:ND2	1:H:201:LYS:H	1.74	0.85
1:N:24:ARG:HG2	1:N:24:ARG:HH11	1.42	0.85
1:P:228:ILE:CG2	1:P:238:ILE:HD11	2.06	0.85
1:K:141:VAL:HG12	1:K:143:VAL:HG13	1.59	0.85
1:E:280:LEU:O	1:E:284:GLN:HB2	1.76	0.85
1:A:320:GLN:NE2	1:D:55:ARG:NH2	2.24	0.85
1:P:121:GLY:O	1:P:125:TYR:HB3	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:28:GLU:HA	1:M:31:HIS:HD2	1.42	0.85
1:O:205:THR:HG22	1:O:207:LEU:H	1.41	0.85
1:B:2:LYS:H	1:B:2:LYS:HD2	1.41	0.85
1:G:171:ILE:HD13	1:G:171:ILE:N	1.92	0.85
1:F:22:ALA:O	1:F:26:PHE:CD2	2.30	0.85
1:O:205:THR:CG2	1:O:207:LEU:H	1.89	0.85
1:E:295:GLU:HG2	1:E:298:ARG:NH2	1.91	0.85
1:E:241:LEU:HD22	1:E:241:LEU:H	1.42	0.84
1:O:139:ASP:OD1	1:O:170:THR:HG21	1.77	0.84
1:R:29:LEU:O	1:R:33:TYR:HB2	1.75	0.84
1:E:30:GLN:HG3	1:E:74:GLN:CG	2.07	0.84
1:N:245:TYR:CE2	1:N:256:LEU:HD22	2.12	0.84
1:J:185:SER:HB3	1:J:188:ASP:O	1.78	0.84
1:M:182:ARG:HE	1:M:184:MSE:HE1	1.40	0.84
1:N:245:TYR:CE2	1:N:256:LEU:CD2	2.60	0.84
1:K:205:THR:HG22	1:K:207:LEU:H	1.43	0.84
1:P:125:TYR:N	1:P:126:PRO:HD2	1.90	0.84
1:I:99:ILE:HG12	1:L:118:VAL:O	1.75	0.84
1:R:213:ILE:CD1	1:R:277:ILE:HG12	2.08	0.84
1:R:282:PRO:O	1:R:286:ARG:HG3	1.77	0.84
1:R:16:ILE:O	1:R:20:ILE:HG12	1.76	0.84
1:M:165:TYR:CZ	1:M:322:MSE:HG2	2.12	0.84
1:B:126:PRO:HB2	1:B:127:PRO:HD3	1.57	0.84
1:C:316:ARG:HH21	1:C:316:ARG:HG3	1.42	0.83
1:I:99:ILE:CG1	1:L:118:VAL:O	2.26	0.83
1:H:176:ILE:O	1:H:179:VAL:HG22	1.78	0.83
1:I:199:ASN:HD22	1:I:200:PRO:N	1.76	0.83
1:M:143:VAL:HG21	1:M:151:ILE:HD11	1.60	0.83
1:M:164:ARG:NH1	1:P:48:TRP:CE2	2.46	0.83
1:G:171:ILE:H	1:G:171:ILE:HD13	1.42	0.83
1:M:23:LEU:HD22	1:M:65:TYR:CE1	2.11	0.83
1:B:320:GLN:NE2	1:E:55:ARG:NH2	2.27	0.83
1:N:22:ALA:O	1:N:26:PHE:CE2	2.31	0.83
1:P:272:LEU:O	1:P:276:VAL:HG23	1.79	0.83
1:Q:107:GLN:H	1:Q:107:GLN:NE2	1.76	0.83
1:K:124:THR:C	1:K:126:PRO:HD2	1.98	0.83
1:K:241:LEU:N	1:K:241:LEU:HD12	1.90	0.83
1:K:260:TYR:CA	1:K:263:LYS:HD3	2.07	0.83
1:L:281:ARG:HG3	1:L:281:ARG:HH11	1.41	0.83
1:M:94:GLN:O	1:P:120:ALA:HB3	1.79	0.83
1:O:118:VAL:HG12	1:R:99:ILE:HD11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:313:GLU:HG3	1:G:317:LYS:NZ	1.94	0.83
1:K:260:TYR:HA	1:K:263:LYS:CD	2.06	0.83
1:K:245:TYR:HE1	1:K:275:VAL:HG11	1.42	0.83
1:M:161:PHE:CE2	1:M:168:LEU:HD23	2.14	0.83
1:J:101:GLU:O	1:J:105:MSE:CE	2.26	0.83
1:R:217:ILE:HD12	1:R:273:ALA:HA	1.60	0.82
1:I:205:THR:HG22	1:I:207:LEU:N	1.94	0.82
1:N:24:ARG:HG2	1:N:24:ARG:NH1	1.93	0.82
1:C:199:ASN:HD21	1:C:201:LYS:HB2	1.43	0.82
1:K:258:ARG:O	1:K:261:GLU:HG3	1.80	0.82
1:M:294:GLU:HG3	1:M:298:ARG:NH2	1.93	0.82
1:K:26:PHE:HA	1:K:29:LEU:HB2	1.61	0.82
1:M:165:TYR:HD1	1:M:321:ALA:O	1.62	0.82
1:G:126:PRO:HB2	1:G:127:PRO:HD3	1.58	0.82
1:J:18:ASN:O	1:J:23:LEU:HB2	1.79	0.82
1:M:118:VAL:O	1:P:98:TYR:HA	1.80	0.82
1:P:281:ARG:HG3	1:P:282:PRO:CD	2.08	0.82
1:J:98:TYR:HB2	1:J:101:GLU:HG3	1.62	0.82
1:M:64:LEU:CD2	1:M:287:TYR:CD1	2.61	0.82
1:N:245:TYR:HE2	1:N:256:LEU:HD21	1.44	0.82
1:E:245:TYR:O	1:E:249:SER:HB3	1.79	0.82
1:J:19:TYR:O	1:J:24:ARG:HB3	1.80	0.82
3:M:1002:PO4:O2	4:M:1003:AMP:C8	2.32	0.82
1:E:136:TYR:HH	1:E:307:ALA:HB1	1.41	0.82
1:G:288:HIS:O	1:G:292:GLU:HG2	1.78	0.82
1:E:267:VAL:HB	1:G:309:ARG:HH11	1.44	0.82
1:N:26:PHE:HA	1:N:29:LEU:HB2	1.60	0.82
1:M:241:LEU:HB3	1:M:268:PHE:HE2	1.45	0.81
1:B:175:ARG:HG3	1:B:176:ILE:N	1.93	0.81
1:N:50:ASP:HB3	1:N:53:GLU:CG	2.09	0.81
1:M:295:GLU:O	1:M:299:VAL:HG23	1.80	0.81
1:P:148:LYS:O	1:P:152:GLU:HG2	1.81	0.81
1:P:253:ILE:HB	1:P:254:GLU:OE1	1.80	0.81
1:P:281:ARG:N	1:P:282:PRO:HD2	1.96	0.81
1:B:260:TYR:OH	1:B:271:ASP:CB	2.28	0.81
1:I:22:ALA:O	1:I:26:PHE:CE2	2.34	0.81
1:P:295:GLU:HA	1:P:295:GLU:OE1	1.81	0.81
1:Q:281:ARG:HH11	1:Q:281:ARG:HG3	1.45	0.81
1:H:23:LEU:O	1:H:26:PHE:HB2	1.81	0.81
1:M:175:ARG:HH12	1:M:177:PRO:HG3	1.45	0.81
1:P:101:GLU:O	1:P:105:MSE:HG2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:245:TYR:HD1	1:N:272:LEU:HD13	1.42	0.81
1:M:176:ILE:HB	1:M:179:VAL:CG1	2.10	0.81
1:E:199:ASN:OD1	1:E:201:LYS:HG3	1.81	0.81
1:G:182:ARG:HG2	1:G:184:MSE:HE1	1.61	0.81
1:P:238:ILE:HD12	1:P:238:ILE:O	1.80	0.81
1:P:25:GLN:HG2	1:P:178:LYS:CB	2.11	0.81
1:O:175:ARG:HH22	1:O:177:PRO:CB	1.93	0.81
1:P:245:TYR:CB	1:P:272:LEU:CD1	2.58	0.81
1:R:205:THR:HG22	1:R:207:LEU:H	1.44	0.81
1:R:281:ARG:O	1:R:285:GLU:HG3	1.81	0.81
1:E:184:MSE:CE	1:E:191:LYS:C	2.50	0.80
1:H:23:LEU:O	1:H:23:LEU:HD12	1.80	0.80
1:M:199:ASN:HD22	1:M:200:PRO:HD2	1.47	0.80
1:P:19:TYR:O	1:P:24:ARG:HB2	1.82	0.80
1:A:124:THR:HG21	1:D:124:THR:HG21	1.63	0.80
1:C:98:TYR:HB2	1:C:101:GLU:HG3	1.63	0.80
1:M:282:PRO:CB	1:M:286:ARG:HH21	1.95	0.80
1:P:245:TYR:CE1	1:P:275:VAL:CG2	2.63	0.80
1:B:72:PRO:HB3	1:B:299:VAL:HG13	1.63	0.80
1:P:126:PRO:CD	1:P:127:PRO:CD	2.60	0.80
1:P:20:ILE:CD1	1:P:183:ILE:HD11	2.11	0.80
1:H:126:PRO:HB2	1:H:127:PRO:HD3	1.63	0.80
1:K:191:LYS:CD	1:K:192:LYS:N	2.42	0.80
1:P:193:MSE:HB3	4:P:1003:AMP:N6	1.96	0.80
1:O:26:PHE:O	1:O:30:GLN:HG3	1.82	0.80
1:P:143:VAL:HG21	1:P:151:ILE:HD11	1.64	0.80
1:P:247:THR:OG1	1:P:248:LEU:HD12	1.81	0.80
1:K:124:THR:O	1:K:127:PRO:CD	2.30	0.80
1:R:260:TYR:CE1	1:R:268:PHE:HD1	1.99	0.80
1:R:288:HIS:O	1:R:292:GLU:HG2	1.81	0.80
1:K:126:PRO:N	1:K:127:PRO:HD2	1.97	0.80
1:M:25:GLN:HG3	1:M:29:LEU:HD12	1.63	0.80
1:P:25:GLN:HG2	1:P:178:LYS:HB2	1.64	0.80
1:R:176:ILE:HG13	1:R:176:ILE:O	1.80	0.80
1:R:260:TYR:CD1	1:R:268:PHE:CD1	2.69	0.80
1:R:84:PRO:HD2	1:R:308:ASN:HD21	1.46	0.80
1:E:213:ILE:HD13	1:E:276:VAL:HG12	1.64	0.80
4:G:1003:AMP:H5'1	4:G:1003:AMP:H8	1.46	0.80
4:B:1003:AMP:C8	4:B:1003:AMP:H5'1	2.17	0.79
1:C:55:ARG:NH2	1:F:320:GLN:NE2	2.28	0.79
1:K:106:THR:H	1:K:149:GLN:NE2	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:LEU:HB3	1:F:169:PHE:CE1	2.16	0.79
4:A:1003:AMP:H8	4:A:1003:AMP:H5'1	1.47	0.79
1:J:205:THR:HG22	1:J:207:LEU:H	1.46	0.79
1:P:24:ARG:HG2	1:P:24:ARG:HH11	1.47	0.79
1:A:308:ASN:O	1:A:312:SER:HB2	1.83	0.79
1:H:176:ILE:HB	1:H:179:VAL:HG13	1.64	0.79
1:H:22:ALA:O	1:H:26:PHE:CD2	2.36	0.79
1:P:150:HIS:O	1:P:154:THR:HG23	1.81	0.79
1:R:260:TYR:CE1	1:R:268:PHE:CD1	2.71	0.79
4:K:1003:AMP:H5'1	4:K:1003:AMP:H8	1.48	0.79
1:R:20:ILE:HG13	1:R:183:ILE:HD12	1.64	0.79
1:C:205:THR:HG22	1:C:207:LEU:N	1.97	0.79
1:R:200:PRO:O	1:R:216:LYS:HE2	1.82	0.79
1:M:23:LEU:HD21	1:M:65:TYR:CZ	2.18	0.79
1:M:64:LEU:HD23	1:M:287:TYR:CD1	2.18	0.79
1:P:150:HIS:O	1:P:154:THR:CG2	2.30	0.79
1:C:320:GLN:NE2	1:F:55:ARG:NH2	2.31	0.79
1:N:29:LEU:HD11	1:N:177:PRO:HB2	1.65	0.79
1:P:248:LEU:HD12	1:P:248:LEU:N	1.97	0.79
1:P:24:ARG:CG	1:P:24:ARG:HH11	1.96	0.79
1:P:253:ILE:HG22	1:P:254:GLU:OE1	1.83	0.79
1:B:142:PRO:HA	1:B:175:ARG:O	1.81	0.78
1:E:280:LEU:HB3	1:E:284:GLN:OE1	1.83	0.78
1:M:281:ARG:HH11	1:M:281:ARG:HG2	1.46	0.78
1:Q:141:VAL:HG12	1:Q:143:VAL:HG13	1.65	0.78
1:R:199:ASN:OD1	1:R:201:LYS:HG2	1.83	0.78
1:B:254:GLU:H	1:B:254:GLU:CD	1.84	0.78
1:C:308:ASN:O	1:C:312:SER:HB2	1.83	0.78
1:D:98:TYR:HB2	1:D:101:GLU:HG3	1.66	0.78
1:G:98:TYR:HB2	1:G:101:GLU:HG3	1.65	0.78
1:P:24:ARG:HG2	1:P:24:ARG:NH1	1.97	0.78
1:K:125:TYR:N	1:K:126:PRO:HD3	1.97	0.78
1:P:126:PRO:CD	1:P:127:PRO:HD3	2.14	0.78
1:P:84:PRO:HD2	1:P:308:ASN:HD21	1.49	0.78
1:A:94:GLN:HE22	1:D:94:GLN:HE22	1.31	0.78
1:E:241:LEU:H	1:E:241:LEU:CD2	1.96	0.78
1:I:98:TYR:HB2	1:I:101:GLU:HG3	1.64	0.78
1:J:288:HIS:O	1:J:292:GLU:HG2	1.84	0.78
1:E:209:ASP:O	1:E:213:ILE:HG13	1.84	0.78
1:K:148:LYS:O	1:K:152:GLU:HG2	1.82	0.78
1:I:253:ILE:O	1:I:257:GLU:HG3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:302:GLU:O	1:O:306:LYS:HG3	1.83	0.78
1:Q:205:THR:CG2	1:Q:207:LEU:H	1.95	0.78
1:J:185:SER:CB	1:J:188:ASP:O	2.32	0.77
1:P:228:ILE:CG2	1:P:238:ILE:CD1	2.62	0.77
1:P:253:ILE:CB	1:P:254:GLU:OE1	2.32	0.77
1:M:211:LYS:HD3	1:Q:1:MSE:HG2	1.66	0.77
1:P:151:ILE:CD1	1:P:174:ALA:CB	2.56	0.77
1:P:253:ILE:CG2	1:P:254:GLU:OE1	2.32	0.77
1:R:290:TRP:HZ3	1:R:295:GLU:HB3	1.47	0.77
1:A:105:MSE:HE2	1:A:105:MSE:CA	2.14	0.77
1:E:267:VAL:HB	1:G:309:ARG:NH1	1.99	0.77
1:C:205:THR:CG2	1:C:207:LEU:H	1.94	0.77
1:H:98:TYR:HB2	1:H:101:GLU:HG3	1.67	0.77
1:P:182:ARG:O	1:P:184:MSE:HE2	1.85	0.77
1:G:295:GLU:HG3	1:G:298:ARG:HD3	1.66	0.77
1:I:126:PRO:HB2	1:I:127:PRO:HD3	1.66	0.77
1:I:55:ARG:NH2	1:L:320:GLN:NE2	2.33	0.77
1:P:281:ARG:N	1:P:282:PRO:CD	2.46	0.77
1:F:98:TYR:HB2	1:F:101:GLU:HG3	1.66	0.77
1:K:261:GLU:O	1:K:263:LYS:HD2	1.85	0.77
1:M:156:ASP:O	1:M:160:ARG:CG	2.31	0.77
1:P:205:THR:HG22	1:P:207:LEU:H	1.48	0.77
1:C:212:THR:HG22	1:C:216:LYS:HE3	1.67	0.76
1:K:259:GLN:HG3	1:K:260:TYR:N	2.00	0.76
1:J:126:PRO:HB2	1:J:127:PRO:HD3	1.68	0.76
1:M:165:TYR:CD1	1:M:321:ALA:O	2.38	0.76
1:R:184:MSE:H	1:R:240:ASN:HD21	1.33	0.76
1:B:199:ASN:HD21	1:B:201:LYS:HB2	1.50	0.76
1:B:205:THR:CG2	1:B:207:LEU:H	1.99	0.76
1:E:198:PRO:O	1:E:200:PRO:HD3	1.84	0.76
1:G:295:GLU:O	1:G:299:VAL:HG23	1.86	0.76
1:A:168:LEU:HD11	1:A:317:LYS:HD2	1.66	0.76
1:A:124:THR:HG21	1:D:94:GLN:HE22	1.48	0.76
1:H:27:VAL:O	1:H:31:HIS:CE1	2.38	0.76
1:L:19:TYR:O	1:L:24:ARG:HB3	1.84	0.76
1:R:19:TYR:CE2	1:R:24:ARG:HD2	2.19	0.76
1:B:187:VAL:HG22	1:B:202:ALA:HB2	1.68	0.76
1:A:141:VAL:HG12	1:A:143:VAL:HG13	1.66	0.76
1:E:284:GLN:O	1:E:288:HIS:CD2	2.38	0.76
1:Q:94:GLN:HA	1:Q:97:VAL:CG1	2.16	0.76
1:R:251:GLN:CG	1:R:256:LEU:HD11	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:PHE:CD1	1:D:37:PHE:HE2	2.04	0.76
1:P:279:THR:O	1:P:282:PRO:HD2	1.85	0.76
1:E:238:ILE:HA	1:E:241:LEU:HD23	1.67	0.76
1:K:210:ALA:O	1:K:214:GLU:HG3	1.85	0.76
1:R:126:PRO:HB2	1:R:127:PRO:HD3	1.66	0.76
1:J:187:VAL:CG2	1:J:202:ALA:HB2	2.16	0.76
1:P:288:HIS:O	1:P:292:GLU:HG3	1.85	0.76
1:P:244:ILE:O	1:P:248:LEU:CD1	2.30	0.76
1:F:182:ARG:NH2	1:F:192:LYS:HG3	2.00	0.75
1:G:225:GLU:OE1	1:I:163:LYS:HD3	1.86	0.75
1:H:199:ASN:C	1:H:199:ASN:HD22	1.89	0.75
1:K:245:TYR:HD2	1:K:256:LEU:HD12	1.45	0.75
1:F:185:SER:HB3	1:F:188:ASP:O	1.86	0.75
1:K:238:ILE:HA	1:K:241:LEU:HD11	1.68	0.75
1:L:8:ILE:HD13	1:L:65:TYR:CZ	2.21	0.75
1:O:182:ARG:O	1:O:184:MSE:HE2	1.87	0.75
1:O:98:TYR:HB2	1:O:101:GLU:HG3	1.68	0.75
1:A:126:PRO:HB2	1:A:127:PRO:HD3	1.69	0.75
1:M:98:TYR:HB2	1:M:101:GLU:HG3	1.68	0.75
1:N:24:ARG:CG	1:N:24:ARG:HH11	1.99	0.75
1:P:245:TYR:HA	1:P:272:LEU:CD1	2.16	0.75
1:R:145:GLU:O	1:R:145:GLU:HG2	1.86	0.75
1:R:41:ASP:HB3	1:R:58:ILE:HD11	1.66	0.75
1:G:18:ASN:HD21	4:G:1003:AMP:C5'	1.98	0.75
1:M:141:VAL:O	1:M:174:ALA:HA	1.85	0.75
4:N:1003:AMP:H5'2	4:N:1003:AMP:C8	2.22	0.75
1:O:38:CYS:SG	1:O:80:GLN:HB2	2.26	0.75
1:P:16:ILE:HG23	1:P:204:ILE:HB	1.68	0.75
1:A:79:ILE:HB	1:A:82:GLU:HG3	1.68	0.75
1:K:56:GLN:HA	1:K:56:GLN:NE2	2.01	0.75
1:L:126:PRO:HB2	1:L:127:PRO:HD3	1.68	0.75
1:P:176:ILE:HB	1:P:179:VAL:HG23	1.65	0.75
1:P:245:TYR:CA	1:P:272:LEU:CD1	2.65	0.75
1:P:253:ILE:CG2	1:P:254:GLU:OE2	2.31	0.75
1:B:29:LEU:HD13	1:B:177:PRO:HB2	1.68	0.75
1:F:249:SER:OG	1:F:251:GLN:HG3	1.86	0.75
1:L:308:ASN:O	1:L:312:SER:HB2	1.87	0.75
1:B:187:VAL:CG2	1:B:202:ALA:HB2	2.16	0.75
1:G:171:ILE:CD1	1:G:171:ILE:N	2.50	0.75
1:L:16:ILE:O	1:L:20:ILE:HG13	1.87	0.75
1:M:140:ILE:HG12	1:M:175:ARG:CB	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:245:TYR:HD2	1:N:256:LEU:HD13	1.50	0.75
1:O:140:ILE:CD1	1:O:175:ARG:HD3	2.17	0.75
1:H:151:ILE:HG21	1:H:174:ALA:HB2	1.68	0.74
1:P:126:PRO:N	1:P:127:PRO:HD2	2.02	0.74
1:R:184:MSE:H	1:R:240:ASN:ND2	1.85	0.74
1:A:243:ASN:O	1:A:247:THR:HG23	1.86	0.74
1:J:187:VAL:HG22	1:J:202:ALA:HB2	1.69	0.74
1:J:249:SER:OG	1:J:251:GLN:HG3	1.88	0.74
1:B:79:ILE:HB	1:B:82:GLU:HG3	1.68	0.74
1:F:205:THR:CG2	1:F:207:LEU:H	1.98	0.74
1:H:290:TRP:HZ3	1:H:295:GLU:HB3	1.53	0.74
1:A:124:THR:O	1:A:127:PRO:HD2	1.86	0.74
1:O:214:GLU:O	1:O:218:LYS:HG3	1.88	0.74
1:A:319:GLU:HB3	1:A:324:LEU:HB2	1.68	0.74
1:F:228:ILE:O	1:F:229:ARG:HG2	1.87	0.74
1:P:16:ILE:CG2	1:P:204:ILE:HB	2.17	0.74
1:M:165:TYR:HB3	1:M:321:ALA:HB1	1.69	0.74
1:Q:140:ILE:HD11	1:Q:175:ARG:O	1.87	0.74
1:R:225:GLU:CD	1:R:227:THR:HG23	2.08	0.74
1:I:124:THR:OG1	1:L:94:GLN:NE2	2.21	0.74
1:K:124:THR:C	1:K:126:PRO:CD	2.56	0.74
1:O:143:VAL:HG21	1:O:151:ILE:HD11	1.70	0.74
1:P:238:ILE:CD1	1:P:238:ILE:O	2.35	0.74
1:A:105:MSE:HE2	1:A:105:MSE:HA	1.68	0.74
1:K:15:THR:HA	1:K:204:ILE:O	1.88	0.74
1:D:246:SER:HB2	1:D:251:GLN:O	1.87	0.73
1:B:99:ILE:HD13	1:E:120:ALA:HA	1.69	0.73
1:P:126:PRO:N	1:P:127:PRO:CD	2.51	0.73
1:A:67:ALA:O	1:A:286:ARG:NH1	2.21	0.73
1:B:22:ALA:O	1:B:26:PHE:HD2	1.67	0.73
1:G:134:LEU:HB3	1:G:169:PHE:CD1	2.22	0.73
1:I:205:THR:CG2	1:I:207:LEU:H	1.98	0.73
1:I:308:ASN:O	1:I:312:SER:HB2	1.88	0.73
1:P:213:ILE:HD13	1:P:277:ILE:HD13	1.69	0.73
1:Q:211:LYS:O	1:Q:215:LYS:HG3	1.87	0.73
1:O:118:VAL:O	1:R:99:ILE:HG12	1.88	0.73
1:R:15:THR:HA	1:R:204:ILE:O	1.88	0.73
1:E:148:LYS:O	1:E:152:GLU:HG2	1.87	0.73
1:K:106:THR:N	1:K:149:GLN:HE22	1.84	0.73
1:M:105:MSE:HE3	1:M:150:HIS:CE1	2.23	0.73
1:Q:148:LYS:HD2	1:Q:152:GLU:OE1	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:GLU:HA	1:C:31:HIS:HD2	1.54	0.73
1:F:107:GLN:N	1:F:107:GLN:HE21	1.85	0.73
1:B:8:ILE:HG22	1:B:61:LEU:HD21	1.70	0.73
1:G:205:THR:CG2	1:G:207:LEU:H	2.00	0.73
1:G:249:SER:OG	1:G:251:GLN:HG3	1.87	0.73
1:L:249:SER:OG	1:L:251:GLN:HG3	1.89	0.73
1:M:210:ALA:HB1	1:M:277:ILE:CD1	2.11	0.73
1:O:19:TYR:HE1	1:O:68:VAL:HG13	1.53	0.73
4:K:1003:AMP:H5'1	4:K:1003:AMP:C8	2.23	0.73
1:K:237:GLY:O	1:K:241:LEU:CD1	2.37	0.73
1:Q:209:ASP:O	1:Q:213:ILE:HG13	1.88	0.73
1:R:59:ARG:HD3	1:R:291:MSE:HE1	1.70	0.73
1:A:205:THR:HG22	1:A:207:LEU:N	2.04	0.73
1:B:137:ASN:ND2	1:B:314:MSE:CE	2.51	0.73
1:E:120:ALA:O	1:E:124:THR:HG23	1.88	0.73
1:J:101:GLU:O	1:J:105:MSE:HE1	1.88	0.73
1:J:146:ASP:OD1	1:J:146:ASP:N	2.22	0.73
1:N:212:THR:HG22	1:N:216:LYS:HD2	1.70	0.73
1:H:134:LEU:HB3	1:H:169:PHE:CD1	2.24	0.72
1:D:249:SER:OG	1:D:251:GLN:HG3	1.89	0.72
1:A:22:ALA:O	1:A:25:GLN:HG2	1.89	0.72
1:G:41:ASP:OD2	1:G:81:SER:HB3	1.88	0.72
1:I:249:SER:CB	1:I:251:GLN:HG3	2.19	0.72
1:I:260:TYR:CA	1:I:263:LYS:HG2	2.18	0.72
1:K:188:ASP:OD1	1:K:190:THR:HB	1.88	0.72
1:R:272:LEU:HD12	1:R:272:LEU:O	1.89	0.72
1:D:25:GLN:O	1:D:29:LEU:HG	1.88	0.72
1:E:56:GLN:HB3	1:E:60:ARG:NH2	2.04	0.72
1:C:55:ARG:NH2	1:F:320:GLN:HE22	1.87	0.72
1:P:100:GLY:O	1:P:104:ARG:CG	2.37	0.72
1:P:228:ILE:HG23	1:P:238:ILE:HD13	1.70	0.72
1:B:187:VAL:HG22	1:B:202:ALA:CB	2.18	0.72
1:C:199:ASN:ND2	1:C:201:LYS:H	1.87	0.72
1:D:205:THR:HG22	1:D:207:LEU:H	1.54	0.72
1:J:256:LEU:HD23	1:J:259:GLN:NE2	2.04	0.72
1:P:289:HIS:O	1:P:293:SER:CB	2.37	0.72
1:M:54:LEU:O	1:M:58:ILE:HG13	1.88	0.72
1:H:205:THR:HG22	1:H:207:LEU:N	2.02	0.72
1:M:185:SER:OG	1:M:187:VAL:HG23	1.90	0.72
1:A:281:ARG:HG3	1:A:281:ARG:HH11	1.54	0.72
1:G:309:ARG:HB3	1:G:309:ARG:CZ	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:GLN:HG2	1:H:60:ARG:NH2	2.05	0.72
1:P:289:HIS:O	1:P:293:SER:HB3	1.90	0.72
1:Q:157:LEU:CD2	1:Q:160:ARG:NH2	2.52	0.72
1:J:184:MSE:HB3	1:J:189:PRO:O	1.88	0.72
1:A:205:THR:CG2	1:A:207:LEU:H	2.01	0.72
1:L:162:ASN:HA	1:L:166:GLY:O	1.90	0.72
1:P:118:VAL:HG12	1:P:122:LEU:CD1	2.20	0.72
1:H:243:ASN:O	1:H:247:THR:HG23	1.90	0.71
1:I:258:ARG:HA	1:I:261:GLU:OE2	1.90	0.71
1:J:308:ASN:O	1:J:312:SER:HB2	1.90	0.71
1:J:8:ILE:HD12	1:J:65:TYR:OH	1.90	0.71
1:D:67:ALA:O	1:D:286:ARG:NH1	2.24	0.71
1:J:205:THR:CG2	1:J:207:LEU:H	2.02	0.71
1:M:134:LEU:HB3	1:M:169:PHE:CE1	2.25	0.71
1:N:120:ALA:HB3	1:Q:97:VAL:CG1	2.20	0.71
1:M:195:LYS:HG2	3:M:1002:PO4:O3	1.90	0.71
1:O:3:THR:HG22	1:O:138:THR:HG22	1.71	0.71
1:E:105:MSE:HA	1:E:105:MSE:HE2	1.72	0.71
1:F:182:ARG:CZ	1:F:192:LYS:HG3	2.21	0.71
1:Q:100:GLY:O	1:Q:104:ARG:HG3	1.90	0.71
1:E:211:LYS:H	1:E:211:LYS:CD	2.02	0.71
1:P:238:ILE:O	1:P:238:ILE:CG1	2.37	0.71
1:C:126:PRO:HB2	1:C:127:PRO:HD3	1.72	0.71
1:L:5:PHE:HB2	1:L:138:THR:HG21	1.73	0.71
1:P:16:ILE:HG12	1:P:17:GLY:N	2.04	0.71
1:Q:126:PRO:HB2	1:Q:127:PRO:HD3	1.72	0.71
1:E:211:LYS:N	1:E:211:LYS:CD	2.52	0.71
1:F:141:VAL:HG12	1:F:143:VAL:HG13	1.71	0.71
1:K:241:LEU:H	1:K:241:LEU:CD1	1.87	0.71
1:L:243:ASN:O	1:L:247:THR:HG23	1.90	0.71
1:M:281:ARG:O	1:M:285:GLU:HB2	1.91	0.71
1:A:249:SER:OG	1:A:251:GLN:HG3	1.90	0.71
1:G:175:ARG:O	1:G:177:PRO:HD3	1.91	0.71
1:G:19:TYR:HA	1:G:23:LEU:HB3	1.72	0.71
1:O:8:ILE:HD12	1:O:65:TYR:OH	1.90	0.71
1:R:86:HIS:HD2	1:R:132:ASP:OD1	1.74	0.71
1:G:133:ILE:O	1:G:138:THR:HG23	1.90	0.71
1:G:271:ASP:OD1	1:K:309:ARG:NH1	2.23	0.71
1:M:120:ALA:HB2	1:P:102:LEU:HD12	1.73	0.71
1:B:199:ASN:ND2	1:B:201:LYS:HB2	2.05	0.71
1:B:230:TYR:CE1	1:B:239:SER:HB3	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:LYS:HG3	1:E:149:GLN:H	1.56	0.71
1:G:96:ILE:O	1:G:160:ARG:NH1	2.24	0.71
1:Q:151:ILE:O	1:Q:155:ARG:HG3	1.91	0.71
1:Q:157:LEU:HD23	1:Q:160:ARG:NH2	2.06	0.71
1:A:71:ASP:OD1	1:A:73:THR:HG23	1.91	0.70
1:M:25:GLN:CG	1:M:29:LEU:HD11	2.20	0.70
1:A:94:GLN:NE2	1:D:94:GLN:HE22	1.89	0.70
1:H:15:THR:HB	1:H:204:ILE:O	1.91	0.70
1:C:243:ASN:O	1:C:247:THR:HG23	1.91	0.70
1:F:19:TYR:CE2	1:F:24:ARG:HD2	2.26	0.70
1:Q:140:ILE:HD12	1:Q:175:ARG:CG	2.19	0.70
1:E:126:PRO:HB2	1:E:127:PRO:HD3	1.71	0.70
1:F:315:VAL:O	1:F:319:GLU:HG3	1.90	0.70
1:H:182:ARG:HH11	1:H:182:ARG:CG	2.03	0.70
1:H:67:ALA:O	1:H:286:ARG:NH1	2.24	0.70
1:M:5:PHE:HB2	1:M:138:THR:HG21	1.72	0.70
1:B:96:ILE:O	1:B:160:ARG:NH1	2.24	0.70
1:I:18:ASN:HD21	4:I:1003:AMP:H5'2	1.56	0.70
1:B:150:HIS:O	1:B:154:THR:HG22	1.92	0.70
1:J:273:ALA:O	1:J:277:ILE:HD12	1.92	0.70
1:M:319:GLU:HG2	1:M:324:LEU:HD12	1.72	0.70
1:D:133:ILE:O	1:D:138:THR:HG23	1.92	0.70
1:C:320:GLN:NE2	1:F:55:ARG:HH22	1.90	0.70
1:K:238:ILE:O	1:K:241:LEU:CD1	2.39	0.70
1:K:98:TYR:HB2	1:K:101:GLU:HG3	1.73	0.70
1:O:326:ARG:HH12	1:R:300:LEU:HB2	1.57	0.70
1:Q:205:THR:HG22	1:Q:207:LEU:N	2.06	0.70
1:H:99:ILE:O	1:H:103:GLU:HG3	1.92	0.70
1:H:199:ASN:HD22	1:H:201:LYS:H	1.39	0.70
1:M:199:ASN:HD22	1:M:200:PRO:CD	2.04	0.70
1:P:228:ILE:HG13	1:P:260:TYR:HB3	1.73	0.70
1:P:241:LEU:HD23	1:P:244:ILE:HD12	1.72	0.70
1:E:184:MSE:HE3	1:E:191:LYS:N	2.06	0.70
1:E:184:MSE:HE3	1:E:191:LYS:O	1.91	0.70
1:M:214:GLU:O	1:M:218:LYS:HG3	1.91	0.70
1:M:282:PRO:HB2	1:M:286:ARG:NH2	2.06	0.70
1:N:245:TYR:CD1	1:N:272:LEU:HD13	2.25	0.70
1:P:15:THR:HA	1:P:204:ILE:O	1.92	0.70
1:R:129:MSE:O	1:R:132:ASP:HB2	1.91	0.70
1:M:94:GLN:OE1	1:M:124:THR:HB	1.92	0.70
1:P:213:ILE:CD1	1:P:277:ILE:HD13	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:308:ASN:O	1:M:312:SER:HB2	1.91	0.69
4:N:1003:AMP:H5'2	4:N:1003:AMP:H8	1.56	0.69
1:P:20:ILE:HD13	1:P:183:ILE:HD11	1.73	0.69
1:R:290:TRP:CZ3	1:R:295:GLU:HB3	2.26	0.69
1:E:184:MSE:SE	1:E:192:LYS:HA	2.43	0.69
1:G:273:ALA:O	1:G:277:ILE:HD12	1.92	0.69
1:H:29:LEU:CD1	1:H:177:PRO:HB2	2.22	0.69
1:P:67:ALA:O	1:P:286:ARG:NH1	2.25	0.69
1:E:245:TYR:CA	1:E:272:LEU:HD13	2.22	0.69
1:J:120:ALA:O	1:J:124:THR:CG2	2.40	0.69
1:B:199:ASN:HD22	1:B:200:PRO:HD2	1.57	0.69
1:M:214:GLU:OE1	1:Q:1:MSE:HE2	1.92	0.69
1:O:105:MSE:HA	1:O:105:MSE:HE2	1.73	0.69
1:P:122:LEU:O	1:P:125:TYR:CD1	2.46	0.69
1:C:22:ALA:O	1:C:26:PHE:CE2	2.45	0.69
1:G:165:TYR:HB3	1:G:321:ALA:HB1	1.73	0.69
1:K:3:THR:HB	1:K:138:THR:HA	1.73	0.69
1:M:205:THR:HG22	1:M:207:LEU:N	1.99	0.69
1:R:19:TYR:HE1	1:R:68:VAL:HG13	1.57	0.69
1:A:280:LEU:O	1:A:284:GLN:HG3	1.93	0.69
1:C:55:ARG:HH22	1:F:320:GLN:HE22	1.40	0.69
1:E:27:VAL:CG1	1:E:28:GLU:HG2	2.21	0.69
1:B:137:ASN:HA	1:B:170:THR:HG23	1.74	0.69
1:B:205:THR:HG23	1:B:207:LEU:H	1.58	0.69
1:K:25:GLN:O	1:K:29:LEU:CG	2.40	0.69
1:K:79:ILE:HB	1:K:82:GLU:HG3	1.74	0.69
1:L:273:ALA:O	1:L:277:ILE:HG13	1.93	0.69
1:P:241:LEU:HD22	1:P:272:LEU:CD2	2.23	0.69
1:O:120:ALA:HA	1:R:99:ILE:HD13	1.74	0.69
1:I:150:HIS:O	1:I:154:THR:HG23	1.93	0.69
1:K:281:ARG:N	1:K:282:PRO:HD2	2.08	0.69
1:M:199:ASN:ND2	1:M:200:PRO:HD2	2.07	0.69
1:O:27:VAL:O	1:O:30:GLN:NE2	2.24	0.69
1:O:315:VAL:O	1:O:319:GLU:HG3	1.92	0.69
1:R:253:ILE:O	1:R:257:GLU:HB2	1.92	0.69
1:E:225:GLU:HG2	1:E:225:GLU:O	1.91	0.69
1:H:99:ILE:HG13	1:K:118:VAL:HB	1.74	0.69
1:I:133:ILE:O	1:I:138:THR:HG23	1.92	0.69
1:K:295:GLU:HG2	1:K:298:ARG:NH1	2.07	0.69
1:G:224:SER:HB3	1:I:166:GLY:HA2	1.74	0.69
1:R:228:ILE:CB	1:R:260:TYR:O	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ARG:HH11	1:B:281:ARG:HG3	1.58	0.69
1:B:72:PRO:HB3	1:B:299:VAL:CG1	2.22	0.69
1:P:145:GLU:CD	1:P:145:GLU:H	1.96	0.69
1:P:56:GLN:OE1	1:P:60:ARG:NH2	2.26	0.69
1:Q:260:TYR:O	1:Q:263:LYS:HB2	1.93	0.69
1:R:273:ALA:O	1:R:277:ILE:HG13	1.93	0.69
1:R:291:MSE:HE3	1:R:291:MSE:O	1.93	0.69
1:H:150:HIS:O	1:H:154:THR:HG22	1.93	0.68
1:K:238:ILE:O	1:K:241:LEU:HD13	1.93	0.68
1:O:175:ARG:HH22	1:O:177:PRO:CA	2.06	0.68
1:M:281:ARG:CG	1:M:281:ARG:HH11	2.05	0.68
1:R:165:TYR:CD2	1:R:321:ALA:O	2.46	0.68
1:R:252:SER:OG	1:R:255:GLU:CB	2.36	0.68
1:D:315:VAL:O	1:D:319:GLU:HG3	1.93	0.68
1:K:287:TYR:OH	1:K:291:MSE:HE3	1.93	0.68
1:M:23:LEU:HD21	1:M:65:TYR:HE1	1.16	0.68
1:R:208:ASP:OD2	1:R:216:LYS:NZ	2.25	0.68
1:F:175:ARG:O	1:F:175:ARG:HG3	1.94	0.68
1:J:120:ALA:O	1:J:124:THR:HG23	1.94	0.68
1:O:147:GLN:O	1:O:151:ILE:HG12	1.94	0.68
1:E:125:TYR:CD2	1:E:126:PRO:HD3	2.28	0.68
1:I:185:SER:HB3	1:I:188:ASP:O	1.93	0.68
1:K:280:LEU:O	1:K:284:GLN:HG3	1.93	0.68
1:H:260:TYR:HD1	1:H:263:LYS:HG3	1.59	0.68
1:H:290:TRP:CZ3	1:H:295:GLU:HB3	2.28	0.68
1:R:98:TYR:HB2	1:R:101:GLU:HG3	1.73	0.68
1:K:20:ILE:HD12	1:K:183:ILE:HG13	1.76	0.68
1:M:185:SER:HG	1:M:187:VAL:HG23	1.59	0.68
1:A:124:THR:CG2	1:D:94:GLN:NE2	2.57	0.68
1:B:151:ILE:HA	1:B:154:THR:HG23	1.76	0.68
1:B:71:ASP:HB3	1:B:74:GLN:HB3	1.75	0.68
1:E:252:SER:OG	1:E:255:GLU:CB	2.35	0.68
1:M:200:PRO:HA	1:M:203:TYR:CE2	2.28	0.68
1:P:122:LEU:O	1:P:125:TYR:HD1	1.77	0.68
1:R:272:LEU:HA	1:R:275:VAL:CG1	2.24	0.68
1:B:155:ARG:NH1	1:B:172:PRO:O	2.27	0.68
1:F:134:LEU:HB3	1:F:169:PHE:CD1	2.29	0.68
1:G:193:MSE:HB3	4:G:1003:AMP:HN62	1.59	0.68
1:K:125:TYR:CD1	1:K:126:PRO:HD3	2.29	0.68
1:K:318:MSE:O	1:K:322:MSE:HG3	1.93	0.68
1:N:67:ALA:O	1:N:286:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:71:ASP:OD2	1:O:74:GLN:N	2.27	0.68
1:E:205:THR:HG22	1:E:207:LEU:N	2.09	0.68
1:R:43:HIS:CE1	1:R:80:GLN:HE22	2.11	0.68
1:H:137:ASN:HD22	1:H:170:THR:HG23	1.59	0.67
1:K:105:MSE:CE	1:K:150:HIS:ND1	2.57	0.67
1:B:304:ALA:O	1:B:308:ASN:HB2	1.95	0.67
1:C:22:ALA:O	1:C:26:PHE:CD2	2.48	0.67
1:C:29:LEU:HD22	1:C:33:TYR:CE1	2.29	0.67
1:D:23:LEU:HD13	1:D:65:TYR:CZ	2.30	0.67
1:H:27:VAL:O	1:H:31:HIS:HE1	1.77	0.67
1:J:67:ALA:O	1:J:286:ARG:NH1	2.27	0.67
1:M:261:GLU:O	1:M:263:LYS:HG2	1.94	0.67
1:E:188:ASP:OD1	1:E:190:THR:HG23	1.94	0.67
1:H:29:LEU:HD13	1:H:177:PRO:HB2	1.76	0.67
1:M:165:TYR:HE1	1:M:322:MSE:HA	1.54	0.67
1:N:217:ILE:O	1:N:269:LYS:HE2	1.94	0.67
1:R:218:LYS:HG2	1:R:219:SER:N	2.10	0.67
1:E:245:TYR:CB	1:E:272:LEU:HD13	2.24	0.67
1:M:207:LEU:HD11	1:M:287:TYR:CZ	2.29	0.67
1:N:245:TYR:HD2	1:N:256:LEU:CD1	2.07	0.67
1:P:267:VAL:O	1:P:271:ASP:N	2.27	0.67
1:B:305:GLU:O	1:B:309:ARG:HG3	1.95	0.67
1:D:8:ILE:HD12	1:D:65:TYR:OH	1.94	0.67
1:E:148:LYS:HG3	1:E:149:GLN:N	2.10	0.67
1:N:16:ILE:O	1:N:20:ILE:HG13	1.95	0.67
4:P:1003:AMP:H5'2	4:P:1003:AMP:C4	2.28	0.67
1:Q:176:ILE:O	1:Q:176:ILE:HG13	1.91	0.67
1:R:214:GLU:HB3	1:R:273:ALA:HB1	1.76	0.67
1:F:151:ILE:HD13	1:F:151:ILE:N	2.10	0.67
1:J:41:ASP:OD2	1:J:81:SER:HB3	1.94	0.67
1:M:134:LEU:HB3	1:M:169:PHE:CD1	2.30	0.67
1:M:278:GLU:OE1	1:M:281:ARG:NH2	2.26	0.67
1:O:193:MSE:HB3	4:O:1003:AMP:N6	2.10	0.67
1:R:147:GLN:O	1:R:150:HIS:HB2	1.94	0.67
1:A:125:TYR:CD2	1:A:126:PRO:HD3	2.30	0.67
1:A:320:GLN:NE2	1:D:55:ARG:HH22	1.90	0.67
1:D:19:TYR:HA	1:D:23:LEU:HB3	1.76	0.67
1:N:273:ALA:O	1:N:277:ILE:HD12	1.95	0.67
1:P:245:TYR:HD2	1:P:256:LEU:CD1	2.08	0.67
1:R:199:ASN:OD1	1:R:201:LYS:CG	2.43	0.67
1:B:8:ILE:CG2	1:B:61:LEU:HD21	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:LEU:HD21	1:D:314:MSE:SE	2.45	0.67
1:E:133:ILE:HD13	1:E:141:VAL:HG21	1.77	0.67
1:N:245:TYR:CE2	1:N:256:LEU:HD21	2.26	0.67
1:J:193:MSE:HB3	4:J:1003:AMP:HN62	1.60	0.67
1:L:313:GLU:HG3	1:L:317:LYS:NZ	2.09	0.67
1:R:206:LEU:O	1:R:207:LEU:HD23	1.95	0.67
1:B:320:GLN:NE2	1:E:55:ARG:HH22	1.91	0.67
1:L:319:GLU:HB3	1:L:324:LEU:HB2	1.77	0.67
1:M:188:ASP:OD2	1:M:190:THR:HB	1.95	0.67
1:R:25:GLN:H	1:R:25:GLN:CD	1.97	0.67
1:E:185:SER:HB3	1:E:188:ASP:O	1.95	0.66
1:H:313:GLU:OE2	1:H:316:ARG:NH1	2.28	0.66
1:I:214:GLU:O	1:I:218:LYS:HG3	1.96	0.66
1:M:84:PRO:O	1:M:88:GLN:HG3	1.96	0.66
1:N:22:ALA:O	1:N:26:PHE:HE2	1.77	0.66
1:Q:308:ASN:O	1:Q:312:SER:HB2	1.94	0.66
1:C:199:ASN:HD22	1:C:201:LYS:H	1.44	0.66
1:L:199:ASN:HD22	1:L:200:PRO:HD2	1.60	0.66
1:M:28:GLU:HA	1:M:31:HIS:CD2	2.27	0.66
1:P:20:ILE:HD12	1:P:183:ILE:HD12	1.75	0.66
1:P:90:ALA:HB2	1:P:128:LEU:HD12	1.76	0.66
1:R:19:TYR:CD2	1:R:24:ARG:HD2	2.31	0.66
1:R:272:LEU:HA	1:R:275:VAL:HG12	1.76	0.66
1:B:255:GLU:HA	1:B:258:ARG:HH21	1.60	0.66
1:P:209:ASP:OD1	1:P:212:THR:HB	1.95	0.66
1:P:238:ILE:O	1:P:238:ILE:HG13	1.95	0.66
1:M:188:ASP:OD1	1:M:190:THR:HB	1.95	0.66
1:B:188:ASP:OD1	1:B:190:THR:HB	1.94	0.66
1:E:314:MSE:O	1:E:318:MSE:HG3	1.95	0.66
1:F:67:ALA:O	1:F:286:ARG:NH1	2.28	0.66
1:J:193:MSE:O	4:J:1003:AMP:N6	2.28	0.66
1:M:188:ASP:CG	1:M:190:THR:HB	2.16	0.66
1:P:245:TYR:HD1	1:P:272:LEU:HD12	1.60	0.66
1:R:199:ASN:OD1	1:R:201:LYS:N	2.26	0.66
1:R:23:LEU:O	1:R:26:PHE:HB2	1.95	0.66
1:A:193:MSE:HB3	4:A:1003:AMP:HN62	1.61	0.66
1:B:272:LEU:HA	1:B:275:VAL:HG13	1.77	0.66
1:C:199:ASN:ND2	1:C:201:LYS:HB2	2.09	0.66
1:E:79:ILE:HB	1:E:82:GLU:HG3	1.76	0.66
1:G:71:ASP:O	1:G:75:ALA:N	2.27	0.66
1:J:141:VAL:HG12	1:J:143:VAL:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:94:GLN:HA	1:Q:97:VAL:HG12	1.77	0.66
1:R:72:PRO:HB3	1:R:299:VAL:HG13	1.78	0.66
1:B:288:HIS:O	1:B:292:GLU:CG	2.44	0.66
1:G:260:TYR:HA	1:G:263:LYS:HG3	1.77	0.66
1:J:57:ASN:OD1	1:J:60:ARG:NH2	2.28	0.66
1:M:32:GLU:O	1:M:32:GLU:HG3	1.93	0.66
1:Q:302:GLU:O	1:Q:306:LYS:HG3	1.95	0.66
1:R:5:PHE:HB2	1:R:138:THR:HG21	1.78	0.66
1:R:270:ALA:O	1:R:273:ALA:HB3	1.96	0.66
1:E:281:ARG:HB3	1:E:282:PRO:HD3	1.78	0.66
1:F:29:LEU:CD1	1:F:177:PRO:HB2	2.25	0.66
1:G:324:LEU:O	1:J:55:ARG:NH1	2.28	0.66
1:I:67:ALA:O	1:I:286:ARG:NH1	2.28	0.66
1:M:98:TYR:CE2	1:M:160:ARG:NH2	2.64	0.66
1:N:94:GLN:O	1:N:97:VAL:HG12	1.95	0.66
1:O:140:ILE:HD13	1:O:175:ARG:HD3	1.77	0.66
1:O:199:ASN:HD22	1:O:200:PRO:CD	2.07	0.66
1:P:37:PHE:HB2	1:P:77:LEU:HD12	1.76	0.66
1:A:281:ARG:HG3	1:A:281:ARG:NH1	2.11	0.66
1:E:184:MSE:HE3	1:E:191:LYS:CA	2.26	0.66
1:B:260:TYR:OH	1:B:271:ASP:HB3	1.96	0.66
1:E:241:LEU:CD2	1:E:241:LEU:N	2.56	0.66
1:J:184:MSE:CB	1:J:189:PRO:O	2.44	0.66
1:L:199:ASN:HD22	1:L:200:PRO:CD	2.08	0.66
1:M:176:ILE:CB	1:M:179:VAL:HG12	2.24	0.66
1:P:143:VAL:CG2	1:P:151:ILE:HD11	2.25	0.66
1:R:198:PRO:O	1:R:200:PRO:HD3	1.96	0.66
1:R:206:LEU:C	1:R:207:LEU:HD23	2.16	0.66
1:B:281:ARG:HG3	1:B:281:ARG:NH1	2.10	0.65
1:K:205:THR:CG2	1:K:207:LEU:H	2.09	0.65
1:L:23:LEU:O	1:L:26:PHE:HB2	1.95	0.65
1:I:324:LEU:O	1:L:55:ARG:NH1	2.29	0.65
1:M:175:ARG:HH11	1:M:177:PRO:HG3	1.58	0.65
1:O:126:PRO:HB2	1:O:127:PRO:HD3	1.77	0.65
1:A:125:TYR:CG	1:A:126:PRO:HD3	2.31	0.65
1:K:301:ASP:O	1:K:305:GLU:HB2	1.95	0.65
1:K:308:ASN:O	1:K:312:SER:HB2	1.96	0.65
1:P:254:GLU:N	1:P:254:GLU:CD	2.49	0.65
1:P:284:GLN:O	1:P:288:HIS:ND1	2.28	0.65
1:P:71:ASP:HB3	1:P:74:GLN:HB3	1.78	0.65
1:R:98:TYR:HB2	1:R:101:GLU:CG	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LEU:CD1	1:D:65:TYR:CZ	2.79	0.65
1:I:55:ARG:NH1	1:L:324:LEU:O	2.30	0.65
1:K:151:ILE:HA	1:K:154:THR:HG23	1.77	0.65
1:P:136:TYR:HB2	1:P:138:THR:HG22	1.79	0.65
1:B:60:ARG:HG2	1:B:287:TYR:OH	1.94	0.65
1:G:67:ALA:O	1:G:286:ARG:NH1	2.29	0.65
1:H:199:ASN:HD22	1:H:200:PRO:N	1.95	0.65
1:I:260:TYR:HA	1:I:263:LYS:HG2	1.79	0.65
1:I:288:HIS:O	1:I:292:GLU:HG2	1.95	0.65
1:P:64:LEU:HD21	1:P:207:LEU:HD21	1.78	0.65
1:N:99:ILE:HG12	1:Q:118:VAL:O	1.96	0.65
1:B:254:GLU:O	1:B:258:ARG:HG3	1.97	0.65
1:P:169:PHE:CE1	1:P:314:MSE:HE3	2.31	0.65
1:P:228:ILE:HG12	1:P:260:TYR:HB3	1.77	0.65
1:R:228:ILE:HG13	1:R:260:TYR:HB3	1.77	0.65
1:G:205:THR:HG22	1:G:207:LEU:N	2.08	0.65
1:M:324:LEU:O	1:P:55:ARG:NH1	2.30	0.65
1:R:279:THR:O	1:R:282:PRO:CD	2.43	0.65
1:G:101:GLU:CD	1:G:160:ARG:HH22	2.00	0.65
1:K:239:SER:O	1:K:242:LEU:HB2	1.96	0.65
1:L:313:GLU:HG3	1:L:317:LYS:HZ3	1.60	0.65
1:N:205:THR:CG2	1:N:207:LEU:H	2.08	0.65
1:B:199:ASN:HD22	1:B:201:LYS:H	1.45	0.65
1:C:86:HIS:HD2	1:C:132:ASP:OD1	1.80	0.65
1:E:57:ASN:OD1	1:E:60:ARG:NH1	2.30	0.65
1:G:252:SER:OG	1:G:255:GLU:HB2	1.96	0.65
1:P:254:GLU:O	1:P:257:GLU:N	2.30	0.65
1:C:188:ASP:HB3	1:C:191:LYS:HB2	1.78	0.65
1:E:210:ALA:HA	1:E:277:ILE:HG12	1.78	0.65
1:P:126:PRO:O	1:P:129:MSE:HB3	1.95	0.65
1:Q:67:ALA:O	1:Q:286:ARG:NH1	2.29	0.65
1:C:240:ASN:O	1:C:244:ILE:HG13	1.97	0.65
4:E:1003:AMP:H4'	4:E:1003:AMP:O3P	1.97	0.65
1:H:205:THR:CG2	1:H:207:LEU:H	2.03	0.65
1:L:23:LEU:HD13	1:L:65:TYR:CZ	2.33	0.65
1:O:199:ASN:ND2	1:O:200:PRO:HD2	2.12	0.65
1:B:8:ILE:HD13	1:B:65:TYR:CZ	2.32	0.64
1:D:18:ASN:ND2	4:D:1003:AMP:H5'1	2.12	0.64
1:E:67:ALA:O	1:E:286:ARG:NH1	2.30	0.64
1:I:260:TYR:HA	1:I:263:LYS:CG	2.27	0.64
1:J:72:PRO:HB3	1:J:299:VAL:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:THR:CB	1:K:149:GLN:HE22	2.09	0.64
1:I:99:ILE:HG13	1:L:118:VAL:HB	1.79	0.64
1:L:146:ASP:OD1	1:L:146:ASP:N	2.30	0.64
1:N:324:LEU:O	1:Q:55:ARG:NH1	2.31	0.64
1:R:50:ASP:HB3	1:R:53:GLU:HB2	1.79	0.64
1:A:199:ASN:HD22	1:A:200:PRO:HD2	1.62	0.64
1:B:252:SER:O	1:B:255:GLU:CB	2.46	0.64
1:B:67:ALA:O	1:B:286:ARG:NH1	2.30	0.64
1:E:245:TYR:O	1:E:249:SER:CB	2.44	0.64
1:F:43:HIS:HE1	1:F:132:ASP:OD2	1.78	0.64
1:M:187:VAL:HG22	1:M:202:ALA:HA	1.78	0.64
1:N:281:ARG:HB3	1:N:282:PRO:HD3	1.77	0.64
1:M:211:LYS:CD	1:Q:1:MSE:HG2	2.27	0.64
1:R:272:LEU:HD12	1:R:272:LEU:C	2.18	0.64
3:O:1002:PO4:O3	4:O:1003:AMP:H5'2	1.96	0.64
1:P:143:VAL:O	1:P:176:ILE:HD11	1.97	0.64
1:A:55:ARG:NH1	1:D:324:LEU:O	2.31	0.64
1:A:55:ARG:NH2	1:D:320:GLN:NE2	2.46	0.64
1:B:32:GLU:HG3	1:B:33:TYR:CD1	2.33	0.64
1:D:205:THR:CG2	1:D:207:LEU:H	2.10	0.64
1:D:56:GLN:O	1:D:60:ARG:HG3	1.97	0.64
4:E:1003:AMP:H5'2	4:E:1003:AMP:C8	2.33	0.64
1:E:238:ILE:CA	1:E:241:LEU:HD23	2.27	0.64
1:E:313:GLU:OE2	1:E:316:ARG:NH2	2.30	0.64
1:L:281:ARG:HG3	1:L:281:ARG:NH1	2.13	0.64
1:P:96:ILE:O	1:P:160:ARG:NH1	2.31	0.64
1:Q:176:ILE:HG12	1:Q:179:VAL:HB	1.79	0.64
1:Q:199:ASN:HD21	1:Q:201:LYS:HB2	1.63	0.64
1:P:228:ILE:HG23	1:P:238:ILE:CD1	2.28	0.64
1:P:71:ASP:HB3	1:P:74:GLN:CB	2.27	0.64
1:P:94:GLN:HA	1:P:97:VAL:HG12	1.80	0.64
1:I:19:TYR:CE2	1:I:24:ARG:HD3	2.33	0.64
1:I:281:ARG:HB3	1:I:282:PRO:HD3	1.80	0.64
1:K:22:ALA:O	1:K:26:PHE:CD2	2.51	0.64
1:N:278:GLU:OE1	1:N:281:ARG:NH2	2.30	0.64
1:O:146:ASP:N	1:O:146:ASP:OD1	2.29	0.64
1:O:162:ASN:HA	1:O:166:GLY:O	1.98	0.64
1:P:245:TYR:HE1	1:P:275:VAL:HG21	1.58	0.64
1:O:118:VAL:HG12	1:R:99:ILE:CD1	2.26	0.64
4:A:1003:AMP:H8	4:A:1003:AMP:C5'	2.11	0.64
1:E:184:MSE:CE	1:E:191:LYS:CA	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:GLU:OE2	1:G:298:ARG:NH1	2.30	0.64
1:J:134:LEU:HB3	1:J:169:PHE:CD1	2.32	0.64
1:N:145:GLU:HA	1:N:148:LYS:HG2	1.79	0.64
1:O:101:GLU:O	1:O:105:MSE:HE3	1.98	0.64
1:O:313:GLU:OE2	1:O:316:ARG:NH1	2.28	0.64
1:O:28:GLU:HA	1:O:31:HIS:HE1	1.62	0.64
1:Q:280:LEU:O	1:Q:284:GLN:HG3	1.98	0.64
1:B:24:ARG:HG2	1:B:24:ARG:O	1.96	0.64
1:E:84:PRO:O	1:E:88:GLN:HG3	1.97	0.64
1:G:5:PHE:HB2	1:G:138:THR:HG21	1.80	0.64
1:H:182:ARG:HG3	1:H:182:ARG:NH1	2.12	0.64
1:H:19:TYR:O	1:H:24:ARG:HB2	1.97	0.64
1:P:209:ASP:OD1	1:P:212:THR:CB	2.45	0.64
1:P:313:GLU:OE2	1:P:316:ARG:NH2	2.27	0.64
1:C:165:TYR:HB3	1:C:321:ALA:HB1	1.80	0.64
1:C:249:SER:OG	1:C:251:GLN:HG3	1.98	0.64
1:E:195:LYS:HG2	3:E:1002:PO4:O1	1.98	0.64
1:I:99:ILE:HG13	1:L:118:VAL:O	1.98	0.64
1:J:255:GLU:O	1:J:259:GLN:HB2	1.98	0.64
1:A:171:ILE:N	1:A:171:ILE:HD13	2.13	0.64
1:E:240:ASN:O	1:E:243:ASN:HB2	1.97	0.64
1:G:182:ARG:HG2	1:G:184:MSE:HE2	1.79	0.64
1:K:134:LEU:HB3	1:K:169:PHE:HD1	1.60	0.64
1:N:55:ARG:NH1	1:Q:324:LEU:O	2.29	0.64
1:Q:93:LEU:O	1:Q:97:VAL:HB	1.98	0.64
1:E:295:GLU:HG2	1:E:298:ARG:HH21	1.62	0.63
1:F:105:MSE:CA	1:F:105:MSE:HE2	2.27	0.63
1:P:195:LYS:NZ	3:P:1002:PO4:O1	2.30	0.63
3:P:1002:PO4:O3	4:P:1003:AMP:N7	2.31	0.63
1:Q:140:ILE:HD11	1:Q:175:ARG:HG3	0.73	0.63
1:E:237:GLY:O	1:E:241:LEU:HD21	1.97	0.63
1:F:99:ILE:O	1:F:103:GLU:HG3	1.98	0.63
1:G:280:LEU:O	1:G:284:GLN:HG3	1.96	0.63
1:L:141:VAL:HG12	1:L:143:VAL:HG13	1.79	0.63
1:O:67:ALA:O	1:O:286:ARG:NH1	2.30	0.63
1:P:215:LYS:O	1:P:215:LYS:HE2	1.97	0.63
1:P:245:TYR:CD1	1:P:272:LEU:HA	2.33	0.63
1:B:199:ASN:ND2	1:B:200:PRO:HD2	2.12	0.63
1:B:324:LEU:O	1:E:55:ARG:NH1	2.32	0.63
1:D:1:MSE:SE	1:O:211:LYS:HD2	2.49	0.63
1:G:326:ARG:NH2	1:J:301:ASP:OD1	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:274:GLN:O	1:L:278:GLU:HG2	1.99	0.63
1:M:140:ILE:HD11	1:M:175:ARG:HD3	1.79	0.63
1:M:59:ARG:CZ	1:M:296:LEU:HD23	2.28	0.63
1:A:209:ASP:O	1:A:213:ILE:HG13	1.97	0.63
1:D:99:ILE:O	1:D:103:GLU:HG3	1.97	0.63
1:F:105:MSE:HE2	1:F:105:MSE:HA	1.80	0.63
1:F:205:THR:HG22	1:F:207:LEU:N	2.13	0.63
1:G:118:VAL:HB	1:J:99:ILE:HG13	1.79	0.63
1:K:22:ALA:O	1:K:26:PHE:CE2	2.50	0.63
1:I:55:ARG:HH22	1:L:320:GLN:NE2	1.93	0.63
1:O:205:THR:HG22	1:O:207:LEU:N	2.11	0.63
1:P:195:LYS:H	3:P:1002:PO4:P	2.21	0.63
1:R:274:GLN:HA	1:R:277:ILE:HD12	1.79	0.63
1:E:71:ASP:OD1	1:E:73:THR:HG23	1.99	0.63
1:R:218:LYS:HG2	1:R:219:SER:H	1.63	0.63
1:B:2:LYS:N	1:B:2:LYS:HD2	2.13	0.63
1:C:193:MSE:HB3	4:C:1003:AMP:N6	2.14	0.63
1:E:107:GLN:CD	1:E:150:HIS:HE2	2.02	0.63
1:C:324:LEU:O	1:F:55:ARG:NH1	2.31	0.63
1:N:245:TYR:HD1	1:N:272:LEU:CD1	2.12	0.63
1:E:245:TYR:HA	1:E:272:LEU:HD13	1.78	0.63
1:B:320:GLN:HE22	1:E:55:ARG:NH2	1.96	0.63
1:K:16:ILE:HD13	1:K:204:ILE:HB	1.79	0.63
1:M:184:MSE:SE	1:M:191:LYS:O	2.67	0.63
1:P:245:TYR:HD1	1:P:272:LEU:CD1	2.12	0.63
1:D:214:GLU:O	1:D:218:LYS:HG3	1.98	0.63
1:E:217:ILE:HD12	1:E:273:ALA:HA	1.80	0.63
1:H:56:GLN:O	1:H:60:ARG:HG3	1.99	0.63
1:P:271:ASP:O	1:P:275:VAL:CG2	2.35	0.63
1:B:246:SER:HB2	1:B:251:GLN:O	1.99	0.63
1:K:238:ILE:HA	1:K:241:LEU:CD1	2.28	0.63
1:K:256:LEU:CD2	1:K:259:GLN:HG2	2.29	0.63
1:H:324:LEU:O	1:K:55:ARG:NH1	2.32	0.63
1:L:41:ASP:OD2	1:L:81:SER:HB3	1.98	0.63
1:O:324:LEU:O	1:R:55:ARG:NH1	2.32	0.63
1:D:182:ARG:HE	1:D:192:LYS:HG3	1.64	0.62
1:E:101:GLU:O	1:E:105:MSE:HE3	1.99	0.62
1:E:267:VAL:HG13	1:E:268:PHE:H	1.63	0.62
1:E:276:VAL:O	1:E:280:LEU:HG	1.99	0.62
1:H:55:ARG:NH1	1:K:324:LEU:O	2.32	0.62
1:M:165:TYR:CE1	1:M:322:MSE:HG2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:ILE:HB	1:M:82:GLU:HG3	1.81	0.62
1:P:15:THR:HG22	1:P:203:TYR:HB2	1.80	0.62
1:A:18:ASN:HD21	4:A:1003:AMP:C5'	2.04	0.62
1:G:302:GLU:O	1:G:306:LYS:HG3	1.99	0.62
1:O:25:GLN:HG3	1:O:29:LEU:HD11	1.80	0.62
1:E:106:THR:HB	1:E:149:GLN:OE1	1.98	0.62
1:G:129:MSE:HE3	2:G:1001:TRP:CE3	2.34	0.62
1:G:313:GLU:OE2	1:G:316:ARG:NH2	2.33	0.62
1:H:133:ILE:O	1:H:138:THR:HG23	1.99	0.62
1:O:19:TYR:CE2	1:O:24:ARG:HD3	2.34	0.62
1:P:126:PRO:CD	1:P:127:PRO:HD2	2.27	0.62
1:E:3:THR:HB	1:E:138:THR:HA	1.81	0.62
1:I:19:TYR:O	1:I:24:ARG:CB	2.46	0.62
1:K:122:LEU:O	1:K:125:TYR:HE1	1.83	0.62
1:M:147:GLN:O	1:M:151:ILE:HG12	2.00	0.62
1:Q:200:PRO:HA	1:Q:203:TYR:CE2	2.34	0.62
1:D:142:PRO:HA	1:D:175:ARG:O	1.99	0.62
1:E:240:ASN:O	1:E:244:ILE:HG13	2.00	0.62
1:F:71:ASP:OD1	1:F:73:THR:HG23	2.00	0.62
1:K:238:ILE:CA	1:K:241:LEU:HD11	2.30	0.62
4:M:1003:AMP:C3'	4:M:1003:AMP:O1P	2.46	0.62
1:N:265:TYR:O	1:N:269:LYS:HG3	1.99	0.62
1:P:205:THR:CG2	1:P:207:LEU:H	2.13	0.62
1:Q:107:GLN:H	1:Q:107:GLN:CD	2.01	0.62
1:K:126:PRO:N	1:K:127:PRO:CD	2.63	0.62
1:P:245:TYR:CD2	1:P:256:LEU:CD1	2.81	0.62
1:B:200:PRO:HA	1:B:203:TYR:CE2	2.35	0.62
1:G:193:MSE:O	4:G:1003:AMP:N6	2.32	0.62
1:I:5:PHE:HB2	1:I:138:THR:HG21	1.79	0.62
1:J:254:GLU:OE1	1:J:254:GLU:N	2.32	0.62
1:K:134:LEU:CB	1:K:169:PHE:CE1	2.80	0.62
1:R:228:ILE:CG2	1:R:260:TYR:HB3	2.25	0.62
1:A:102:LEU:O	1:A:105:MSE:HB2	1.99	0.62
1:E:125:TYR:CG	1:E:126:PRO:HD3	2.35	0.62
1:E:253:ILE:O	1:E:257:GLU:HB2	2.00	0.62
1:N:272:LEU:O	1:N:276:VAL:HG23	2.00	0.62
1:N:288:HIS:O	1:N:292:GLU:HG2	2.00	0.62
1:Q:182:ARG:HE	1:Q:184:MSE:HE1	1.64	0.62
1:M:271:ASP:OD1	1:Q:309:ARG:NE	2.32	0.62
1:R:106:THR:H	1:R:149:GLN:HE22	1.48	0.62
1:R:19:TYR:CE2	1:R:24:ARG:CG	2.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:VAL:HG12	1:E:180:GLY:O	2.00	0.62
1:J:187:VAL:HG22	1:J:202:ALA:CB	2.29	0.62
1:J:86:HIS:HD2	1:J:132:ASP:OD1	1.82	0.62
1:N:205:THR:HG22	1:N:207:LEU:N	2.09	0.62
1:O:105:MSE:CA	1:O:105:MSE:HE2	2.28	0.62
1:O:30:GLN:OE1	1:O:71:ASP:N	2.31	0.62
1:P:206:LEU:N	1:P:206:LEU:HD23	2.14	0.62
1:R:185:SER:HB3	1:R:188:ASP:O	1.98	0.62
1:B:254:GLU:OE1	1:B:254:GLU:N	2.32	0.62
1:C:309:ARG:NH1	1:D:271:ASP:OD1	2.33	0.62
1:J:193:MSE:HB3	4:J:1003:AMP:N6	2.15	0.62
1:M:240:ASN:O	1:M:244:ILE:HG13	2.00	0.62
1:M:280:LEU:O	1:M:284:GLN:CG	2.45	0.62
1:P:118:VAL:CG1	1:P:122:LEU:CD1	2.78	0.62
1:P:213:ILE:HG22	1:P:217:ILE:HD12	1.82	0.62
1:B:205:THR:HG22	1:B:208:ASP:N	2.14	0.61
1:K:106:THR:OG1	1:K:149:GLN:NE2	2.33	0.61
1:K:185:SER:HB3	1:K:188:ASP:O	1.99	0.61
1:O:253:ILE:HG22	1:O:257:GLU:OE2	2.00	0.61
1:O:280:LEU:HB3	1:O:284:GLN:OE1	2.00	0.61
1:P:126:PRO:HD2	1:P:127:PRO:CD	2.30	0.61
1:P:16:ILE:CD1	1:P:193:MSE:HE1	2.26	0.61
1:P:308:ASN:O	1:P:312:SER:HB2	1.99	0.61
1:R:106:THR:H	1:R:149:GLN:NE2	1.98	0.61
1:R:29:LEU:CD1	1:R:177:PRO:HG2	2.29	0.61
1:A:274:GLN:O	1:A:278:GLU:HG2	2.00	0.61
1:K:176:ILE:O	1:K:179:VAL:HG22	2.01	0.61
1:P:25:GLN:HG2	1:P:178:LYS:HB3	1.81	0.61
1:C:29:LEU:HD22	1:C:33:TYR:CD1	2.35	0.61
1:F:280:LEU:O	1:F:284:GLN:HG3	2.01	0.61
1:P:193:MSE:HB3	4:P:1003:AMP:HN61	1.64	0.61
1:P:251:GLN:HG3	1:P:256:LEU:HD11	1.82	0.61
1:P:245:TYR:HD1	1:P:272:LEU:HA	1.65	0.61
1:P:319:GLU:HB3	1:P:324:LEU:HB2	1.80	0.61
1:B:29:LEU:HD22	1:B:33:TYR:HE1	1.65	0.61
1:P:266:GLY:O	1:P:270:ALA:HB2	2.00	0.61
1:M:55:ARG:HD2	1:P:325:GLY:O	2.01	0.61
1:R:162:ASN:HA	1:R:166:GLY:O	2.00	0.61
1:P:253:ILE:CG2	1:P:254:GLU:CD	2.59	0.61
1:R:133:ILE:O	1:R:138:THR:CG2	2.45	0.61
1:F:228:ILE:O	1:F:229:ARG:CG	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:241:LEU:HB3	1:J:268:PHE:HE2	1.64	0.61
1:M:133:ILE:O	1:M:138:THR:HG23	2.00	0.61
1:P:175:ARG:HG2	1:P:176:ILE:N	2.14	0.61
1:R:284:GLN:O	1:R:288:HIS:ND1	2.31	0.61
1:B:214:GLU:O	1:B:218:LYS:HG3	2.01	0.61
1:B:253:ILE:HG22	1:B:257:GLU:OE1	2.01	0.61
1:G:212:THR:CG2	1:G:216:LYS:HE3	2.31	0.61
1:M:305:GLU:O	1:M:309:ARG:HG3	2.01	0.61
1:O:31:HIS:N	1:O:31:HIS:ND1	2.48	0.61
1:P:60:ARG:HD2	1:P:287:TYR:OH	2.00	0.61
1:R:19:TYR:O	1:R:24:ARG:HG3	2.00	0.61
1:E:267:VAL:HG13	1:E:268:PHE:N	2.15	0.61
1:L:60:ARG:HG2	1:L:287:TYR:OH	2.00	0.61
1:O:185:SER:HB2	1:O:202:ALA:HB1	1.83	0.61
1:P:176:ILE:CB	1:P:179:VAL:HG22	2.26	0.61
1:C:306:LYS:HA	1:D:267:VAL:HG12	1.82	0.61
3:F:1002:PO4:O1	4:F:1003:AMP:H5'2	2.01	0.61
1:H:86:HIS:HD2	1:H:132:ASP:OD1	1.83	0.61
1:M:297:ASP:OD2	1:P:326:ARG:NH1	2.33	0.61
1:P:161:PHE:C	1:P:161:PHE:CD2	2.73	0.61
1:B:260:TYR:OH	1:B:271:ASP:CG	2.39	0.60
1:D:5:PHE:HB2	1:D:138:THR:HG21	1.82	0.60
1:E:19:TYR:HE1	1:E:68:VAL:CG1	2.13	0.60
1:H:249:SER:OG	1:H:251:GLN:HG3	2.01	0.60
1:J:213:ILE:O	1:J:217:ILE:HG13	2.00	0.60
1:P:118:VAL:HG12	1:P:122:LEU:HD12	1.83	0.60
1:J:205:THR:HG22	1:J:207:LEU:N	2.14	0.60
1:K:125:TYR:CG	1:K:126:PRO:HD3	2.36	0.60
1:O:65:TYR:O	1:O:70:ILE:HB	2.01	0.60
1:E:284:GLN:O	1:E:288:HIS:HD2	1.83	0.60
1:F:205:THR:HG23	1:F:207:LEU:H	1.65	0.60
1:I:245:TYR:O	1:I:245:TYR:HD1	1.83	0.60
1:O:183:ILE:O	4:O:1003:AMP:N6	2.27	0.60
1:R:184:MSE:HE3	1:R:192:LYS:HA	1.82	0.60
1:C:67:ALA:O	1:C:286:ARG:NH1	2.34	0.60
1:D:278:GLU:OE2	1:D:281:ARG:NH2	2.35	0.60
1:G:224:SER:HB2	1:I:166:GLY:N	2.16	0.60
1:K:208:ASP:O	1:K:284:GLN:NE2	2.34	0.60
1:L:105:MSE:HE2	1:L:150:HIS:CE1	2.35	0.60
1:M:241:LEU:HB3	1:M:268:PHE:CE2	2.33	0.60
1:M:120:ALA:HB2	1:P:102:LEU:CD1	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ARG:HB3	1:B:282:PRO:CD	2.32	0.60
1:D:308:ASN:O	1:D:312:SER:HB2	2.01	0.60
1:G:55:ARG:NH1	1:J:324:LEU:O	2.34	0.60
1:R:218:LYS:CG	1:R:219:SER:N	2.63	0.60
1:I:147:GLN:O	1:I:151:ILE:HG12	2.01	0.60
1:R:43:HIS:HE1	1:R:132:ASP:OD2	1.84	0.60
1:R:27:VAL:HG23	1:R:28:GLU:HG2	1.83	0.60
1:B:4:ILE:HG12	1:B:140:ILE:HB	1.82	0.60
1:E:184:MSE:CE	1:E:191:LYS:N	2.64	0.60
1:F:19:TYR:CZ	1:F:24:ARG:HG3	2.37	0.60
1:K:228:ILE:HG22	1:K:228:ILE:O	2.02	0.60
1:M:229:ARG:HG3	1:M:257:GLU:HG2	1.83	0.60
1:O:26:PHE:CD2	1:O:29:LEU:CD1	2.82	0.60
1:B:125:TYR:N	1:B:126:PRO:CD	2.65	0.60
1:H:43:HIS:HE1	1:H:132:ASP:OD2	1.84	0.60
1:P:244:ILE:HG22	1:P:272:LEU:HD11	1.84	0.60
1:R:147:GLN:HA	1:R:150:HIS:HD2	1.65	0.60
1:A:84:PRO:HD2	1:A:308:ASN:HD21	1.67	0.60
1:B:100:GLY:O	1:B:104:ARG:HG2	2.02	0.60
1:D:86:HIS:HD2	1:D:132:ASP:OD1	1.85	0.60
1:G:99:ILE:HG13	1:J:118:VAL:HB	1.83	0.60
1:K:185:SER:N	1:K:191:LYS:O	2.33	0.60
1:P:118:VAL:CG1	1:P:122:LEU:HD12	2.32	0.60
1:Q:125:TYR:CD2	1:Q:126:PRO:HD3	2.36	0.60
1:A:151:ILE:HG21	1:A:174:ALA:HB2	1.83	0.60
1:B:255:GLU:CA	1:B:258:ARG:HH21	2.14	0.60
1:E:253:ILE:CG1	1:E:253:ILE:O	2.49	0.60
1:E:315:VAL:O	1:E:319:GLU:HG3	2.02	0.60
1:G:105:MSE:HE2	1:G:105:MSE:HA	1.83	0.60
1:G:313:GLU:HG3	1:G:317:LYS:HZ3	1.66	0.60
1:K:86:HIS:HD2	1:K:132:ASP:OD1	1.85	0.60
4:P:1003:AMP:H2'	4:P:1003:AMP:N3	2.16	0.60
1:P:124:THR:CA	1:P:126:PRO:HD2	2.32	0.60
1:E:29:LEU:HD11	1:E:177:PRO:HB2	1.83	0.59
1:E:71:ASP:HB3	1:E:74:GLN:HB2	1.84	0.59
1:G:193:MSE:HE2	1:G:203:TYR:HA	1.83	0.59
1:H:22:ALA:O	1:H:26:PHE:CE2	2.54	0.59
1:I:16:ILE:HG12	1:I:204:ILE:HB	1.83	0.59
1:A:124:THR:HG21	1:D:94:GLN:HE21	1.67	0.59
1:C:316:ARG:CG	1:C:316:ARG:HH21	2.13	0.59
1:K:287:TYR:CZ	1:K:291:MSE:CE	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:282:PRO:O	1:L:286:ARG:HG3	2.02	0.59
1:M:64:LEU:HD23	1:M:287:TYR:HD1	1.64	0.59
1:P:245:TYR:CD1	1:P:272:LEU:HD12	2.36	0.59
1:Q:29:LEU:HD11	1:Q:177:PRO:HB2	1.84	0.59
1:A:184:MSE:HB3	1:A:191:LYS:O	2.03	0.59
1:J:155:ARG:HG2	1:J:171:ILE:HG23	1.83	0.59
1:K:245:TYR:HE1	1:K:275:VAL:CG1	2.13	0.59
1:L:23:LEU:CD1	1:L:65:TYR:CE2	2.85	0.59
1:N:126:PRO:CB	1:N:127:PRO:HD3	2.29	0.59
1:Q:199:ASN:ND2	1:Q:201:LYS:H	1.99	0.59
1:R:105:MSE:HA	1:R:149:GLN:OE1	2.02	0.59
1:E:197:ASP:OD1	1:E:198:PRO:HD2	2.03	0.59
4:I:1003:AMP:C8	4:I:1003:AMP:H5'1	2.37	0.59
1:I:90:ALA:O	1:I:94:GLN:HG3	2.01	0.59
1:J:39:ILE:HG23	1:J:61:LEU:HD23	1.83	0.59
1:H:48:TRP:CZ2	1:K:164:ARG:NH1	2.70	0.59
1:K:314:MSE:O	1:K:318:MSE:HG3	2.02	0.59
1:L:171:ILE:O	1:L:171:ILE:HG22	2.02	0.59
1:M:164:ARG:NH1	1:P:48:TRP:CZ2	2.69	0.59
1:P:254:GLU:O	1:P:258:ARG:N	2.30	0.59
1:A:318:MSE:O	1:A:322:MSE:HG3	2.02	0.59
1:D:18:ASN:HD21	4:D:1003:AMP:H5'1	1.67	0.59
1:H:134:LEU:HB3	1:H:169:PHE:CE1	2.38	0.59
1:I:3:THR:HB	1:I:138:THR:HA	1.83	0.59
1:N:56:GLN:OE1	1:N:60:ARG:NH2	2.35	0.59
1:O:326:ARG:NH1	1:R:300:LEU:HB2	2.17	0.59
1:R:253:ILE:O	1:R:257:GLU:CB	2.50	0.59
1:B:38:CYS:SG	1:B:80:GLN:HB2	2.42	0.59
1:F:278:GLU:OE1	1:F:278:GLU:HA	2.03	0.59
1:G:193:MSE:HB3	4:G:1003:AMP:N6	2.18	0.59
1:H:206:LEU:HD23	1:H:206:LEU:N	2.17	0.59
1:I:26:PHE:O	1:I:30:GLN:HG2	2.02	0.59
1:J:125:TYR:N	1:J:126:PRO:CD	2.65	0.59
1:J:295:GLU:OE2	1:J:298:ARG:NH2	2.27	0.59
1:M:146:ASP:OD1	1:M:146:ASP:N	2.30	0.59
1:O:18:ASN:HA	4:O:1003:AMP:C1'	2.30	0.59
1:E:125:TYR:N	1:E:126:PRO:HD2	2.17	0.59
1:E:26:PHE:CD1	1:E:37:PHE:HE2	2.20	0.59
1:K:259:GLN:O	1:K:263:LYS:HE2	2.02	0.59
1:N:213:ILE:HD11	1:N:280:LEU:HD12	1.84	0.59
1:A:133:ILE:O	1:A:138:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:142:PRO:HA	1:N:175:ARG:O	2.03	0.59
1:P:267:VAL:HG23	1:P:268:PHE:N	2.17	0.59
1:R:272:LEU:O	1:R:275:VAL:HG13	2.02	0.59
1:B:313:GLU:OE2	1:B:316:ARG:NH2	2.32	0.59
1:E:30:GLN:CG	1:E:74:GLN:HG2	2.31	0.59
1:K:59:ARG:NH2	1:K:296:LEU:HD23	2.17	0.59
1:N:295:GLU:OE2	1:N:298:ARG:NH2	2.32	0.59
1:Q:185:SER:O	1:Q:188:ASP:O	2.20	0.59
1:Q:199:ASN:ND2	1:Q:201:LYS:HB2	2.18	0.59
1:R:187:VAL:HG13	1:R:201:LYS:HB2	1.85	0.59
1:R:291:MSE:HE3	1:R:291:MSE:CA	2.32	0.59
1:E:245:TYR:HA	1:E:272:LEU:CD1	2.33	0.59
1:F:83:VAL:HG13	1:F:308:ASN:HA	1.83	0.59
1:H:125:TYR:N	1:H:126:PRO:CD	2.66	0.59
1:M:105:MSE:HE2	1:M:150:HIS:ND1	2.09	0.59
1:M:253:ILE:O	1:M:257:GLU:HB2	2.03	0.59
4:B:1003:AMP:H8	4:B:1003:AMP:H5'1	1.66	0.58
1:E:52:HIS:O	1:E:56:GLN:HB2	2.02	0.58
1:G:125:TYR:N	1:G:126:PRO:CD	2.66	0.58
1:K:238:ILE:C	1:K:241:LEU:CD1	2.71	0.58
1:M:209:ASP:OD1	1:M:212:THR:CB	2.50	0.58
1:M:42:GLN:HB2	1:M:80:GLN:OE1	2.03	0.58
1:Q:38:CYS:SG	1:Q:80:GLN:HB2	2.43	0.58
1:A:105:MSE:CE	1:A:105:MSE:HA	2.32	0.58
1:J:129:MSE:HE3	2:J:1001:TRP:CE3	2.38	0.58
1:J:217:ILE:O	1:J:269:LYS:HD3	2.03	0.58
1:M:99:ILE:O	1:M:103:GLU:HG3	2.03	0.58
1:N:203:TYR:O	1:N:216:LYS:NZ	2.33	0.58
1:Q:19:TYR:CE2	1:Q:24:ARG:HD3	2.38	0.58
1:B:241:LEU:HB3	1:B:268:PHE:HE2	1.68	0.58
1:C:41:ASP:OD2	1:C:81:SER:HB3	2.03	0.58
1:D:240:ASN:O	1:D:244:ILE:HG13	2.03	0.58
1:G:105:MSE:CA	1:G:105:MSE:HE2	2.33	0.58
1:H:141:VAL:HG12	1:H:143:VAL:HG13	1.83	0.58
1:I:281:ARG:HB3	1:I:282:PRO:CD	2.33	0.58
1:J:101:GLU:O	1:J:105:MSE:HE2	2.00	0.58
1:K:183:ILE:N	1:K:183:ILE:HD13	2.17	0.58
1:O:281:ARG:N	1:O:282:PRO:HD2	2.18	0.58
1:Q:272:LEU:HA	1:Q:275:VAL:HG13	1.83	0.58
1:R:199:ASN:OD1	1:R:201:LYS:CB	2.51	0.58
1:B:55:ARG:NH1	1:E:324:LEU:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:ALA:O	1:F:26:PHE:CE2	2.55	0.58
1:I:86:HIS:HD2	1:I:132:ASP:OD1	1.87	0.58
1:J:60:ARG:HG2	1:J:287:TYR:OH	2.03	0.58
1:M:16:ILE:O	1:M:20:ILE:HG13	2.03	0.58
1:N:90:ALA:O	1:N:94:GLN:HG3	2.03	0.58
1:R:125:TYR:N	1:R:126:PRO:CD	2.67	0.58
1:C:215:LYS:O	1:C:219:SER:OG	2.20	0.58
1:G:126:PRO:CB	1:G:127:PRO:HD3	2.33	0.58
1:H:126:PRO:HB2	1:H:127:PRO:CD	2.33	0.58
1:I:199:ASN:ND2	1:I:200:PRO:CD	2.31	0.58
1:O:89:ALA:HB2	1:O:135:LEU:HD21	1.84	0.58
1:P:118:VAL:HG12	1:P:122:LEU:HD11	1.85	0.58
1:A:105:MSE:HE2	1:A:105:MSE:N	2.17	0.58
1:I:313:GLU:OE2	1:I:316:ARG:NH2	2.30	0.58
1:K:205:THR:HG22	1:K:207:LEU:N	2.16	0.58
1:P:241:LEU:HB3	1:P:272:LEU:HD22	1.86	0.58
1:A:86:HIS:HD2	1:A:132:ASP:OD1	1.86	0.58
1:B:118:VAL:CG1	1:E:99:ILE:HD12	2.34	0.58
1:C:129:MSE:HE3	2:C:1001:TRP:CE3	2.39	0.58
1:D:31:HIS:O	1:O:215:LYS:HE2	2.03	0.58
1:O:56:GLN:O	1:O:60:ARG:HB2	2.04	0.58
1:P:126:PRO:CG	1:P:127:PRO:CD	2.76	0.58
1:P:71:ASP:O	1:P:75:ALA:N	2.36	0.58
1:R:16:ILE:O	1:R:20:ILE:CG1	2.49	0.58
1:B:295:GLU:O	1:B:299:VAL:HG23	2.03	0.58
1:F:23:LEU:CD2	1:F:68:VAL:HG11	2.33	0.58
1:G:320:GLN:NE2	1:J:55:ARG:NH2	2.52	0.58
1:M:200:PRO:O	1:M:216:LYS:NZ	2.32	0.58
1:M:281:ARG:N	1:M:282:PRO:HD2	2.18	0.58
1:M:56:GLN:NE2	1:M:60:ARG:NH2	2.52	0.58
1:O:142:PRO:HA	1:O:175:ARG:O	2.04	0.58
1:B:319:GLU:O	1:B:323:GLY:N	2.32	0.58
1:D:147:GLN:O	1:D:151:ILE:HG12	2.03	0.58
1:H:199:ASN:HD21	1:H:201:LYS:HB2	1.68	0.58
1:J:168:LEU:HD11	1:J:317:LYS:HD3	1.85	0.58
1:O:273:ALA:O	1:O:277:ILE:HG13	2.03	0.58
1:O:72:PRO:HB3	1:O:299:VAL:HG13	1.85	0.58
1:P:245:TYR:CD1	1:P:272:LEU:CD1	2.86	0.58
1:Q:157:LEU:CD2	1:Q:160:ARG:HH21	2.17	0.58
1:Q:190:THR:HG23	1:Q:190:THR:O	2.03	0.58
1:A:315:VAL:O	1:A:319:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:TYR:CG	1:D:126:PRO:HD3	2.39	0.57
1:D:175:ARG:O	1:D:177:PRO:HD3	2.04	0.57
1:H:277:ILE:O	1:H:281:ARG:HB2	2.04	0.57
1:H:59:ARG:NH2	1:H:297:ASP:OD1	2.27	0.57
1:H:5:PHE:HB2	1:H:138:THR:HG21	1.86	0.57
1:M:64:LEU:HD21	1:M:287:TYR:CD1	2.36	0.57
1:O:297:ASP:OD2	1:R:326:ARG:NH1	2.37	0.57
1:Q:24:ARG:HH11	1:Q:24:ARG:CG	2.17	0.57
1:Q:281:ARG:NH1	1:Q:281:ARG:HG3	2.14	0.57
1:B:205:THR:HG22	1:B:207:LEU:H	1.69	0.57
1:E:176:ILE:HB	1:E:179:VAL:HG22	1.85	0.57
1:E:96:ILE:O	1:E:160:ARG:NH1	2.37	0.57
1:F:200:PRO:O	1:F:216:LYS:NZ	2.37	0.57
1:K:124:THR:O	1:K:127:PRO:CG	2.52	0.57
1:M:295:GLU:HG3	1:M:295:GLU:O	2.04	0.57
1:O:254:GLU:O	1:O:258:ARG:HB2	2.04	0.57
1:P:16:ILE:HD13	1:P:204:ILE:HB	1.86	0.57
1:Q:272:LEU:O	1:Q:276:VAL:HG23	2.04	0.57
1:R:281:ARG:N	1:R:282:PRO:HD2	2.18	0.57
1:B:72:PRO:O	1:B:306:LYS:NZ	2.33	0.57
1:C:141:VAL:HG12	1:C:143:VAL:HG13	1.86	0.57
1:E:99:ILE:O	1:E:103:GLU:HG3	2.04	0.57
1:H:241:LEU:HB3	1:H:268:PHE:HE2	1.69	0.57
1:K:124:THR:C	1:K:127:PRO:HD2	2.24	0.57
1:O:175:ARG:HH22	1:O:177:PRO:HB3	1.66	0.57
1:P:9:GLN:HE21	1:P:9:GLN:HA	1.68	0.57
1:R:141:VAL:HG12	1:R:143:VAL:HG13	1.86	0.57
1:C:126:PRO:HB2	1:C:127:PRO:CD	2.33	0.57
1:D:278:GLU:HA	1:D:278:GLU:OE1	2.04	0.57
1:L:165:TYR:HB3	1:L:321:ALA:HB1	1.85	0.57
1:O:84:PRO:O	1:O:88:GLN:HG3	2.03	0.57
1:R:282:PRO:O	1:R:286:ARG:CG	2.50	0.57
1:A:193:MSE:HB3	4:A:1003:AMP:N6	2.20	0.57
1:B:199:ASN:ND2	1:B:201:LYS:H	2.03	0.57
1:B:245:TYR:CD2	1:B:272:LEU:HB2	2.40	0.57
1:H:260:TYR:CD1	1:H:263:LYS:HG3	2.39	0.57
1:J:185:SER:O	1:J:189:PRO:HA	2.04	0.57
1:J:79:ILE:HB	1:J:82:GLU:HG3	1.87	0.57
1:M:98:TYR:N	1:M:101:GLU:OE1	2.22	0.57
1:M:22:ALA:O	1:M:26:PHE:CD2	2.57	0.57
1:O:254:GLU:CD	1:O:254:GLU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:145:GLU:N	1:P:145:GLU:OE1	2.33	0.57
4:Q:1003:AMP:H8	4:Q:1003:AMP:C5'	2.17	0.57
1:H:30:GLN:O	1:H:74:GLN:NE2	2.38	0.57
1:I:38:CYS:SG	1:I:80:GLN:HB2	2.45	0.57
1:L:8:ILE:HD13	1:L:65:TYR:OH	2.04	0.57
1:P:241:LEU:HD22	1:P:272:LEU:HD21	1.86	0.57
1:P:246:SER:HA	1:P:249:SER:HG	1.68	0.57
1:A:146:ASP:N	1:A:146:ASP:OD1	2.37	0.57
1:C:19:TYR:HB2	1:C:206:LEU:HD21	1.86	0.57
1:C:56:GLN:O	1:C:60:ARG:HG3	2.05	0.57
1:E:240:ASN:HB3	1:E:241:LEU:HD22	1.87	0.57
1:P:106:THR:O	1:P:106:THR:HG22	2.04	0.57
1:R:203:TYR:O	1:R:216:LYS:HD3	2.04	0.57
1:R:291:MSE:HA	1:R:291:MSE:HE3	1.86	0.57
3:F:1002:PO4:O1	4:F:1003:AMP:H8	1.87	0.57
1:G:136:TYR:HB2	1:G:138:THR:HG22	1.87	0.57
1:G:146:ASP:N	1:G:146:ASP:OD1	2.29	0.57
1:H:230:TYR:C	1:H:230:TYR:CD1	2.78	0.57
1:K:258:ARG:HA	1:K:261:GLU:HG3	1.86	0.57
1:L:125:TYR:N	1:L:126:PRO:CD	2.68	0.57
1:O:325:GLY:C	1:O:326:ARG:HG3	2.24	0.57
1:P:20:ILE:CD1	1:P:183:ILE:CD1	2.74	0.57
1:Q:133:ILE:O	1:Q:138:THR:CG2	2.53	0.57
1:C:214:GLU:O	1:C:218:LYS:HG3	2.04	0.57
1:E:146:ASP:N	1:E:146:ASP:OD1	2.36	0.57
1:K:7:GLY:C	1:K:8:ILE:HD13	2.25	0.57
1:L:133:ILE:O	1:L:138:THR:HG23	2.04	0.57
1:I:326:ARG:NH1	1:L:297:ASP:OD2	2.35	0.57
1:M:311:ALA:O	1:M:314:MSE:N	2.38	0.57
1:M:8:ILE:HD12	1:M:65:TYR:CZ	2.40	0.57
1:P:247:THR:OG1	1:P:248:LEU:CD1	2.51	0.57
1:R:184:MSE:HE3	1:R:192:LYS:CA	2.35	0.57
1:R:19:TYR:CE2	1:R:24:ARG:HG2	2.40	0.57
1:E:197:ASP:HB3	1:E:202:ALA:HB3	1.86	0.57
1:L:313:GLU:OE2	1:L:317:LYS:NZ	2.37	0.57
1:B:255:GLU:HA	1:B:258:ARG:NH2	2.20	0.56
1:M:118:VAL:HB	1:P:99:ILE:HG13	1.87	0.56
1:N:55:ARG:NH2	1:Q:320:GLN:HE21	2.03	0.56
1:R:136:TYR:HB2	1:R:138:THR:HG22	1.86	0.56
1:D:96:ILE:HD12	1:D:160:ARG:HG2	1.86	0.56
1:J:256:LEU:O	1:J:260:TYR:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:ILE:HG22	1:L:61:LEU:HD21	1.86	0.56
1:Q:212:THR:HG22	1:Q:216:LYS:HE3	1.86	0.56
1:A:18:ASN:ND2	4:A:1003:AMP:C8	2.73	0.56
1:A:168:LEU:O	1:A:314:MSE:HE1	2.06	0.56
1:A:71:ASP:HB3	1:A:74:GLN:HB2	1.87	0.56
1:B:315:VAL:O	1:B:319:GLU:HG3	2.05	0.56
1:B:94:GLN:NE2	1:E:124:THR:CB	2.68	0.56
1:N:176:ILE:HB	1:N:179:VAL:HG13	1.86	0.56
1:P:16:ILE:HG12	1:P:17:GLY:H	1.69	0.56
1:Q:139:ASP:OD1	1:Q:170:THR:HG21	2.04	0.56
1:F:184:MSE:HE2	1:F:189:PRO:O	2.05	0.56
1:F:86:HIS:HD2	1:F:132:ASP:OD1	1.88	0.56
1:P:3:THR:HB	1:P:138:THR:HA	1.87	0.56
1:R:171:ILE:N	1:R:171:ILE:HD13	2.19	0.56
1:R:91:TRP:HE3	1:R:94:GLN:OE1	1.88	0.56
1:R:94:GLN:HA	1:R:97:VAL:HG12	1.87	0.56
1:B:230:TYR:CD1	1:B:239:SER:HB3	2.41	0.56
1:B:286:ARG:HA	1:B:289:HIS:HB3	1.87	0.56
1:C:125:TYR:CD2	1:C:126:PRO:HD3	2.41	0.56
1:O:24:ARG:CG	1:O:24:ARG:HH11	2.19	0.56
1:P:248:LEU:CD1	1:P:248:LEU:N	2.67	0.56
1:R:19:TYR:CE2	1:R:24:ARG:CD	2.88	0.56
1:E:243:ASN:O	1:E:247:THR:CG2	2.53	0.56
1:L:86:HIS:HD2	1:L:132:ASP:OD1	1.88	0.56
1:P:195:LYS:N	3:P:1002:PO4:O2	2.37	0.56
1:B:29:LEU:HD22	1:B:33:TYR:CE1	2.40	0.56
1:C:38:CYS:SG	1:C:80:GLN:HB2	2.46	0.56
1:H:145:GLU:O	1:H:148:LYS:HG2	2.05	0.56
1:I:273:ALA:O	1:I:277:ILE:HD12	2.05	0.56
1:N:125:TYR:N	1:N:126:PRO:CD	2.69	0.56
1:P:245:TYR:HE1	1:P:275:VAL:CG2	2.17	0.56
1:Q:59:ARG:NH2	1:Q:296:LEU:HD23	2.20	0.56
1:Q:79:ILE:HB	1:Q:82:GLU:HG3	1.86	0.56
1:R:195:LYS:HG2	3:R:1002:PO4:O1	2.05	0.56
1:R:29:LEU:HD11	1:R:177:PRO:HG2	1.87	0.56
1:H:293:SER:OG	1:H:295:GLU:HB2	2.05	0.56
1:K:147:GLN:OE1	1:K:150:HIS:HD2	1.89	0.56
1:Q:151:ILE:HG13	1:Q:174:ALA:HB2	1.88	0.56
1:R:126:PRO:CB	1:R:127:PRO:HD3	2.36	0.56
1:R:145:GLU:CG	1:R:145:GLU:O	2.53	0.56
1:B:137:ASN:HB3	1:B:170:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:GLU:H	1:D:254:GLU:CD	2.08	0.56
1:G:319:GLU:HB3	1:G:324:LEU:HB2	1.86	0.56
1:H:56:GLN:HG2	1:H:60:ARG:NH1	2.20	0.56
1:L:258:ARG:O	1:L:261:GLU:HB2	2.06	0.56
1:L:24:ARG:HG3	1:L:25:GLN:N	2.19	0.56
1:P:246:SER:HA	1:P:249:SER:OG	2.05	0.56
1:R:248:LEU:HD12	1:R:275:VAL:HG22	1.88	0.56
1:B:99:ILE:CD1	1:E:120:ALA:HA	2.36	0.56
1:H:281:ARG:HH11	1:H:281:ARG:HG3	1.70	0.56
1:L:205:THR:CG2	1:L:207:LEU:H	2.18	0.56
1:M:200:PRO:HA	1:M:203:TYR:CZ	2.41	0.56
1:M:45:ILE:C	1:M:47:VAL:H	2.10	0.56
1:R:165:TYR:CB	1:R:321:ALA:HB1	2.32	0.56
4:G:1003:AMP:H5'1	4:G:1003:AMP:C8	2.35	0.56
1:I:19:TYR:O	1:I:24:ARG:HB3	2.06	0.56
1:K:281:ARG:N	1:K:282:PRO:CD	2.69	0.56
1:P:26:PHE:HA	1:P:29:LEU:HB2	1.88	0.56
1:R:184:MSE:HE3	1:R:192:LYS:HB3	1.88	0.56
1:E:245:TYR:HB2	1:E:272:LEU:HD13	1.89	0.55
1:M:125:TYR:N	1:M:126:PRO:CD	2.69	0.55
1:M:105:MSE:HA	1:M:149:GLN:NE2	2.22	0.55
1:M:161:PHE:CE2	1:M:169:PHE:HE2	2.24	0.55
1:P:133:ILE:O	1:P:138:THR:HG23	2.05	0.55
1:B:137:ASN:HA	1:B:170:THR:CG2	2.35	0.55
1:B:252:SER:O	1:B:255:GLU:HB2	2.05	0.55
1:J:26:PHE:CD2	1:J:29:LEU:HD12	2.41	0.55
1:K:238:ILE:CD1	1:K:268:PHE:CE2	2.89	0.55
1:Q:24:ARG:NH1	1:Q:24:ARG:HG2	2.21	0.55
1:B:281:ARG:HB3	1:B:282:PRO:HD3	1.87	0.55
1:G:278:GLU:HA	1:G:278:GLU:OE1	2.05	0.55
1:H:295:GLU:OE2	1:H:295:GLU:HA	2.05	0.55
1:I:101:GLU:O	1:I:105:MSE:HE2	2.06	0.55
1:M:228:ILE:HG22	1:M:228:ILE:O	2.05	0.55
1:E:133:ILE:O	1:E:138:THR:HG23	2.06	0.55
1:F:27:VAL:HG12	1:F:27:VAL:O	2.05	0.55
1:K:245:TYR:CD1	1:K:275:VAL:HG11	2.38	0.55
1:K:293:SER:OG	1:K:295:GLU:HB2	2.05	0.55
1:L:205:THR:HG22	1:L:207:LEU:H	1.72	0.55
1:M:40:VAL:O	1:M:40:VAL:HG23	2.07	0.55
1:N:141:VAL:HG12	1:N:143:VAL:HG13	1.88	0.55
1:Q:94:GLN:C	1:Q:97:VAL:HG12	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:105:MSE:HE1	1:R:150:HIS:CA	2.34	0.55
1:O:55:ARG:NH1	1:R:324:LEU:O	2.39	0.55
1:G:170:THR:O	1:G:172:PRO:HD3	2.06	0.55
1:K:150:HIS:O	1:K:154:THR:HG22	2.07	0.55
1:M:300:LEU:O	1:M:303:GLY:N	2.38	0.55
1:N:199:ASN:ND2	1:N:201:LYS:HB2	2.21	0.55
1:N:79:ILE:HB	1:N:82:GLU:HG3	1.87	0.55
1:O:175:ARG:HH21	1:O:175:ARG:CG	2.20	0.55
1:P:266:GLY:O	1:P:270:ALA:CB	2.54	0.55
1:R:241:LEU:HA	1:R:244:ILE:HD12	1.89	0.55
1:R:272:LEU:O	1:R:275:VAL:CG1	2.53	0.55
1:B:147:GLN:O	1:B:151:ILE:HG12	2.07	0.55
1:D:243:ASN:O	1:D:247:THR:OG1	2.25	0.55
1:H:288:HIS:O	1:H:292:GLU:HG2	2.06	0.55
1:I:26:PHE:HD2	1:I:26:PHE:N	2.04	0.55
1:L:164:ARG:HB3	1:L:165:TYR:CD2	2.42	0.55
1:M:126:PRO:CB	1:M:127:PRO:HD3	2.32	0.55
1:N:50:ASP:HB3	1:N:53:GLU:HG3	1.87	0.55
1:P:52:HIS:O	1:P:56:GLN:HG3	2.05	0.55
1:D:228:ILE:HD13	1:D:265:TYR:CE1	2.42	0.55
1:B:326:ARG:NH2	1:E:301:ASP:OD1	2.29	0.55
1:H:96:ILE:O	1:H:160:ARG:NH1	2.39	0.55
1:J:19:TYR:HB2	1:J:206:LEU:HD21	1.89	0.55
1:K:287:TYR:OH	1:K:291:MSE:CE	2.55	0.55
1:P:90:ALA:O	1:P:94:GLN:HG3	2.07	0.55
1:Q:176:ILE:CG1	1:Q:179:VAL:HB	2.36	0.55
1:R:29:LEU:HD22	1:R:33:TYR:CE1	2.42	0.55
1:B:260:TYR:CE1	1:B:271:ASP:OD2	2.59	0.55
1:E:145:GLU:O	1:E:145:GLU:HG3	2.06	0.55
1:M:64:LEU:HD21	1:M:207:LEU:HD21	1.88	0.55
1:M:213:ILE:HD11	1:M:280:LEU:HD12	1.89	0.55
1:N:101:GLU:O	1:N:105:MSE:HE2	2.07	0.55
1:P:241:LEU:HD22	1:P:272:LEU:HD23	1.89	0.55
1:P:169:PHE:CD1	1:P:314:MSE:HE3	2.42	0.55
1:P:86:HIS:HD2	1:P:132:ASP:OD1	1.90	0.55
1:R:18:ASN:ND2	4:R:1003:AMP:O4'	2.40	0.55
1:B:192:LYS:HE3	1:B:193:MSE:O	2.06	0.55
1:E:244:ILE:O	1:E:248:LEU:HB2	2.06	0.55
1:F:146:ASP:OD1	1:F:146:ASP:N	2.31	0.55
1:F:65:TYR:O	1:F:70:ILE:HB	2.06	0.55
1:G:129:MSE:O	1:G:132:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:LYS:N	3:H:1002:PO4:O2	2.29	0.55
1:H:175:ARG:O	1:H:177:PRO:HD3	2.07	0.55
1:K:191:LYS:HD2	1:K:192:LYS:N	2.21	0.55
1:K:238:ILE:CA	1:K:241:LEU:CD1	2.84	0.55
1:M:275:VAL:O	1:M:279:THR:OG1	2.24	0.55
1:Q:99:ILE:O	1:Q:103:GLU:HG3	2.07	0.55
1:B:106:THR:HB	1:B:149:GLN:OE1	2.07	0.55
1:C:43:HIS:HE1	1:C:132:ASP:OD2	1.90	0.55
1:A:55:ARG:HH22	1:D:320:GLN:NE2	2.05	0.55
1:F:304:ALA:O	1:F:308:ASN:HB2	2.07	0.55
1:I:145:GLU:O	1:I:148:LYS:HG2	2.06	0.55
1:Q:125:TYR:N	1:Q:126:PRO:CD	2.70	0.55
1:R:187:VAL:HG11	1:R:199:ASN:ND2	2.22	0.55
1:R:281:ARG:HB3	1:R:282:PRO:HD3	1.89	0.55
1:E:105:MSE:CA	1:E:105:MSE:HE2	2.36	0.54
1:M:313:GLU:OE2	1:M:316:ARG:NH2	2.40	0.54
1:M:41:ASP:OD1	1:M:80:GLN:HB3	2.08	0.54
1:P:289:HIS:O	1:P:293:SER:HB2	2.06	0.54
1:Q:182:ARG:HA	4:Q:1003:AMP:H2	1.72	0.54
1:Q:125:TYR:CG	1:Q:126:PRO:HD3	2.42	0.54
1:E:19:TYR:O	1:E:24:ARG:CB	2.55	0.54
1:I:249:SER:HB2	1:I:251:GLN:HG3	1.90	0.54
1:K:199:ASN:ND2	1:K:201:LYS:HB2	2.22	0.54
1:M:190:THR:HG22	1:M:191:LYS:N	2.22	0.54
1:M:19:TYR:HA	1:M:23:LEU:HB2	1.88	0.54
1:M:22:ALA:O	1:M:25:GLN:HG2	2.07	0.54
1:O:24:ARG:NH2	1:O:247:THR:O	2.40	0.54
1:N:120:ALA:HB3	1:Q:97:VAL:HG12	1.88	0.54
1:R:5:PHE:HE2	1:R:136:TYR:CE2	2.25	0.54
1:B:238:ILE:HG13	1:B:265:TYR:CE1	2.43	0.54
1:E:243:ASN:O	1:E:247:THR:HG23	2.07	0.54
1:H:253:ILE:O	1:H:253:ILE:CG2	2.56	0.54
1:J:213:ILE:HD11	1:J:280:LEU:HD12	1.90	0.54
1:O:118:VAL:HG12	1:R:99:ILE:CG1	2.37	0.54
1:P:182:ARG:NH1	1:P:192:LYS:HD2	2.22	0.54
1:P:241:LEU:HD23	1:P:244:ILE:CD1	2.36	0.54
1:P:280:LEU:C	1:P:282:PRO:HD2	2.28	0.54
1:A:199:ASN:HD22	1:A:200:PRO:CD	2.19	0.54
1:B:260:TYR:HE1	1:B:271:ASP:OD2	1.91	0.54
1:B:29:LEU:HD11	1:B:177:PRO:CB	2.27	0.54
1:C:129:MSE:HE3	2:C:1001:TRP:CZ3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1003:AMP:O1P	4:D:1003:AMP:H8	1.90	0.54
1:D:179:VAL:HG22	1:D:180:GLY:N	2.23	0.54
1:E:281:ARG:HB3	1:E:282:PRO:CD	2.37	0.54
1:F:294:GLU:HG3	1:F:294:GLU:O	2.07	0.54
1:I:141:VAL:HG12	1:I:143:VAL:HG13	1.89	0.54
1:K:199:ASN:HD22	1:K:201:LYS:H	1.54	0.54
1:M:5:PHE:CB	1:M:138:THR:HG21	2.37	0.54
4:N:1003:AMP:C5'	4:N:1003:AMP:C8	2.91	0.54
4:Q:1003:AMP:H5'1	4:Q:1003:AMP:H8	1.72	0.54
1:Q:94:GLN:CA	1:Q:97:VAL:HG12	2.36	0.54
1:R:244:ILE:O	1:R:248:LEU:HB2	2.08	0.54
1:D:126:PRO:HB2	1:D:127:PRO:CD	2.35	0.54
1:F:125:TYR:N	1:F:126:PRO:CD	2.70	0.54
1:L:98:TYR:HB2	1:L:101:GLU:HG3	1.89	0.54
1:N:71:ASP:HB3	1:N:74:GLN:HB2	1.89	0.54
1:P:15:THR:CG2	1:P:203:TYR:HB2	2.37	0.54
1:C:278:GLU:OE1	1:C:278:GLU:HA	2.07	0.54
1:F:59:ARG:HH11	1:F:59:ARG:CG	2.21	0.54
1:I:43:HIS:HE1	1:I:132:ASP:OD2	1.90	0.54
1:I:320:GLN:O	1:I:320:GLN:HG3	2.08	0.54
1:R:237:GLY:O	1:R:241:LEU:HD12	2.07	0.54
1:D:26:PHE:CD1	1:D:37:PHE:CE2	2.92	0.54
1:M:145:GLU:OE2	1:M:148:LYS:NZ	2.36	0.54
1:M:282:PRO:CB	1:M:286:ARG:NH2	2.67	0.54
1:N:29:LEU:HD22	1:N:33:TYR:CE1	2.42	0.54
1:O:72:PRO:HB3	1:O:299:VAL:CG1	2.37	0.54
1:Q:71:ASP:OD1	1:Q:72:PRO:HD2	2.08	0.54
1:A:278:GLU:HA	1:A:278:GLU:OE1	2.07	0.54
1:C:5:PHE:HB2	1:C:138:THR:HG21	1.89	0.54
1:J:162:ASN:O	1:J:166:GLY:CA	2.55	0.54
1:K:239:SER:O	1:K:242:LEU:N	2.34	0.54
1:O:24:ARG:HG2	1:O:24:ARG:NH1	2.22	0.54
1:O:26:PHE:HD2	1:O:29:LEU:CD1	2.08	0.54
1:N:124:THR:HG21	1:Q:124:THR:HG21	1.90	0.54
1:E:119:SER:O	1:E:122:LEU:HB2	2.08	0.54
1:K:295:GLU:HG2	1:K:298:ARG:CZ	2.38	0.54
1:M:150:HIS:O	1:M:154:THR:HG23	2.08	0.54
1:M:199:ASN:ND2	1:M:201:LYS:H	2.05	0.54
1:M:289:HIS:HA	1:M:292:GLU:HG2	1.89	0.54
1:A:200:PRO:HA	1:A:203:TYR:CZ	2.43	0.54
1:B:133:ILE:O	1:B:138:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ILE:HG12	1:E:118:VAL:O	2.07	0.54
1:E:125:TYR:N	1:E:126:PRO:CD	2.71	0.54
1:E:152:GLU:HA	1:E:152:GLU:OE1	2.08	0.54
1:E:237:GLY:O	1:E:241:LEU:CD2	2.56	0.54
1:K:134:LEU:HB3	1:K:169:PHE:HE1	1.63	0.54
1:M:105:MSE:HE2	1:M:150:HIS:HE1	1.69	0.54
1:M:164:ARG:NH2	1:P:48:TRP:CE3	2.76	0.54
1:O:200:PRO:HA	1:O:203:TYR:CE2	2.43	0.54
1:Q:50:ASP:OD1	1:Q:51:PRO:HD2	2.08	0.54
1:B:190:THR:O	1:B:190:THR:CG2	2.56	0.53
1:F:5:PHE:HB2	1:F:138:THR:HG21	1.89	0.53
1:F:25:GLN:HG2	1:F:178:LYS:O	2.09	0.53
1:G:281:ARG:N	1:G:282:PRO:HD2	2.23	0.53
1:H:281:ARG:HB3	1:H:282:PRO:CD	2.38	0.53
4:P:1003:AMP:O3P	4:P:1003:AMP:H4'	2.06	0.53
1:P:143:VAL:HG21	1:P:151:ILE:CD1	2.34	0.53
1:E:126:PRO:N	1:E:127:PRO:HD2	2.23	0.53
1:E:281:ARG:N	1:E:282:PRO:HD2	2.23	0.53
1:G:129:MSE:HE3	2:G:1001:TRP:CD2	2.43	0.53
1:H:19:TYR:CE2	1:H:24:ARG:HD3	2.43	0.53
1:M:4:ILE:HG23	1:M:140:ILE:HG22	1.90	0.53
1:P:192:LYS:HE3	4:P:1003:AMP:C2	2.43	0.53
1:P:253:ILE:CG2	1:P:257:GLU:OE1	2.56	0.53
1:P:8:ILE:HD12	1:P:65:TYR:OH	2.07	0.53
1:Q:193:MSE:HB3	4:Q:1003:AMP:N6	2.22	0.53
1:R:288:HIS:O	1:R:292:GLU:CG	2.54	0.53
1:A:148:LYS:HG2	1:A:148:LYS:O	2.08	0.53
1:A:41:ASP:OD2	1:A:81:SER:HB3	2.08	0.53
1:B:175:ARG:CG	1:B:176:ILE:N	2.66	0.53
4:C:1003:AMP:H8	4:C:1003:AMP:H5'2	1.73	0.53
1:C:199:ASN:C	1:C:199:ASN:HD22	2.11	0.53
1:H:20:ILE:HD11	1:H:248:LEU:HG	1.90	0.53
1:I:272:LEU:O	1:I:276:VAL:HG23	2.09	0.53
1:L:25:GLN:O	1:L:29:LEU:HG	2.08	0.53
1:M:175:ARG:NH1	1:M:177:PRO:CG	2.61	0.53
1:N:4:ILE:HG21	1:N:26:PHE:HE1	1.73	0.53
1:Q:133:ILE:O	1:Q:138:THR:HG23	2.08	0.53
1:Q:159:GLU:O	1:Q:163:LYS:HG3	2.09	0.53
1:D:319:GLU:HB3	1:D:324:LEU:HB2	1.89	0.53
1:I:26:PHE:CD2	1:I:26:PHE:N	2.75	0.53
1:K:126:PRO:CD	1:K:127:PRO:HD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:228:ILE:HD11	1:K:264:GLY:O	2.07	0.53
1:L:106:THR:OG1	1:L:107:GLN:NE2	2.41	0.53
1:R:214:GLU:HB3	1:R:273:ALA:CB	2.38	0.53
1:B:274:GLN:O	1:B:278:GLU:HB2	2.09	0.53
1:F:289:HIS:O	1:F:293:SER:HB3	2.08	0.53
1:M:22:ALA:O	1:M:26:PHE:HD2	1.91	0.53
1:N:22:ALA:O	1:N:26:PHE:CD2	2.61	0.53
1:N:274:GLN:O	1:N:278:GLU:HB2	2.09	0.53
1:N:281:ARG:HB3	1:N:282:PRO:CD	2.38	0.53
1:C:17:GLY:HA2	1:C:183:ILE:HG13	1.91	0.53
1:E:150:HIS:O	1:E:154:THR:CG2	2.57	0.53
1:E:308:ASN:O	1:E:312:SER:HB3	2.08	0.53
1:F:256:LEU:HD22	1:F:260:TYR:HE2	1.74	0.53
1:H:129:MSE:HG3	2:H:1001:TRP:CE2	2.44	0.53
1:O:195:LYS:CG	1:O:196:SER:N	2.72	0.53
1:O:19:TYR:CE2	1:O:24:ARG:CD	2.92	0.53
1:R:187:VAL:CG1	1:R:201:LYS:HB2	2.39	0.53
1:A:8:ILE:HD12	1:A:65:TYR:OH	2.08	0.53
1:C:125:TYR:CG	1:C:126:PRO:HD3	2.44	0.53
1:C:72:PRO:HB3	1:C:299:VAL:HG13	1.91	0.53
1:E:40:VAL:O	1:E:40:VAL:HG23	2.08	0.53
1:G:8:ILE:HD12	1:G:65:TYR:OH	2.08	0.53
1:N:43:HIS:HE1	1:N:132:ASP:OD2	1.91	0.53
1:N:165:TYR:HB3	1:N:321:ALA:HB1	1.91	0.53
1:O:125:TYR:N	1:O:126:PRO:CD	2.70	0.53
1:O:86:HIS:HE1	1:O:136:TYR:OH	1.91	0.53
1:P:248:LEU:HD12	1:P:248:LEU:H	1.70	0.53
1:R:40:VAL:HG23	1:R:40:VAL:O	2.09	0.53
1:O:118:VAL:CG1	1:R:99:ILE:HD11	2.35	0.53
1:B:118:VAL:HG12	1:E:99:ILE:HD12	1.90	0.53
1:G:39:ILE:HG23	1:G:61:LEU:HD23	1.91	0.53
1:Q:26:PHE:O	1:Q:30:GLN:HB3	2.09	0.53
1:R:19:TYR:CZ	1:R:24:ARG:HG2	2.43	0.53
1:E:73:THR:OG1	1:E:74:GLN:N	2.41	0.53
1:F:199:ASN:ND2	1:F:201:LYS:H	2.06	0.53
1:H:199:ASN:C	1:H:199:ASN:ND2	2.62	0.53
1:M:48:TRP:C	1:M:49:GLN:HG2	2.28	0.53
1:M:71:ASP:O	1:M:75:ALA:N	2.34	0.53
1:N:182:ARG:O	1:N:184:MSE:HE2	2.08	0.53
1:B:199:ASN:HD22	1:B:199:ASN:C	2.11	0.53
1:G:176:ILE:O	1:G:179:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:PRO:HB3	1:H:299:VAL:HG13	1.90	0.53
1:K:287:TYR:CE1	1:K:291:MSE:HE2	2.43	0.53
1:K:8:ILE:N	1:K:8:ILE:HD13	2.23	0.53
1:L:128:LEU:O	1:L:128:LEU:HD12	2.09	0.53
1:M:205:THR:CG2	1:M:207:LEU:H	2.07	0.53
1:N:254:GLU:H	1:N:254:GLU:CD	2.12	0.53
1:P:126:PRO:HD2	1:P:127:PRO:HD2	1.90	0.53
1:R:205:THR:HG22	1:R:207:LEU:N	2.21	0.53
1:R:85:ALA:HB1	1:R:315:VAL:HG21	1.91	0.53
1:A:43:HIS:HE1	1:A:132:ASP:OD2	1.91	0.52
1:B:243:ASN:O	1:B:247:THR:OG1	2.25	0.52
1:B:40:VAL:O	1:B:40:VAL:HG23	2.09	0.52
1:C:8:ILE:HB	1:C:61:LEU:HD21	1.91	0.52
1:D:71:ASP:OD2	1:D:73:THR:OG1	2.26	0.52
1:G:40:VAL:O	1:G:40:VAL:HG23	2.08	0.52
1:G:78:PHE:CD1	1:G:78:PHE:N	2.77	0.52
1:G:224:SER:HB3	1:I:166:GLY:CA	2.37	0.52
1:J:182:ARG:O	1:J:184:MSE:HE2	2.09	0.52
1:L:26:PHE:CD1	1:L:37:PHE:HE2	2.27	0.52
1:O:131:ALA:O	1:O:135:LEU:HG	2.09	0.52
1:O:301:ASP:OD1	1:R:326:ARG:NH2	2.40	0.52
1:O:304:ALA:O	1:O:308:ASN:HB2	2.09	0.52
1:P:195:LYS:HB3	1:P:195:LYS:HZ2	1.74	0.52
1:A:147:GLN:O	1:A:151:ILE:HG12	2.09	0.52
1:B:39:ILE:HG23	1:B:61:LEU:HD23	1.91	0.52
1:C:30:GLN:O	1:C:74:GLN:HG3	2.09	0.52
1:E:107:GLN:OE1	1:E:150:HIS:NE2	2.42	0.52
1:F:42:GLN:HB2	1:F:80:GLN:OE1	2.08	0.52
1:H:31:HIS:HA	1:H:74:GLN:NE2	2.24	0.52
1:G:224:SER:CB	1:I:166:GLY:CA	2.87	0.52
1:G:320:GLN:NE2	1:J:55:ARG:HH22	2.08	0.52
1:M:182:ARG:NE	1:M:184:MSE:HE1	2.18	0.52
1:N:120:ALA:CB	1:Q:97:VAL:HG13	2.39	0.52
1:R:71:ASP:OD2	1:R:73:THR:OG1	2.27	0.52
1:B:255:GLU:HG3	1:B:258:ARG:NH2	2.24	0.52
1:C:125:TYR:N	1:C:126:PRO:CD	2.72	0.52
1:G:59:ARG:NH2	1:G:296:LEU:HD23	2.24	0.52
1:L:105:MSE:CE	1:L:150:HIS:CE1	2.91	0.52
1:O:175:ARG:NH2	1:O:177:PRO:CA	2.72	0.52
1:O:22:ALA:O	1:O:26:PHE:CE1	2.63	0.52
1:O:2:LYS:O	1:O:33:TYR:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:126:PRO:HD2	1:P:127:PRO:HD3	1.88	0.52
1:P:147:GLN:HA	1:P:150:HIS:HD2	1.75	0.52
1:R:252:SER:OG	1:R:255:GLU:N	2.43	0.52
1:B:59:ARG:NH2	1:B:296:LEU:HD23	2.24	0.52
1:D:150:HIS:O	1:D:154:THR:HG22	2.09	0.52
1:E:253:ILE:HG13	1:E:253:ILE:O	2.10	0.52
1:H:19:TYR:HA	1:H:23:LEU:HB3	1.90	0.52
1:N:72:PRO:HB3	1:N:299:VAL:HG13	1.91	0.52
1:B:141:VAL:HG12	1:B:143:VAL:HG13	1.92	0.52
1:D:281:ARG:HG3	1:D:281:ARG:NH1	2.25	0.52
1:F:106:THR:HG22	1:F:107:GLN:N	2.25	0.52
1:M:65:TYR:O	1:M:70:ILE:HG12	2.10	0.52
1:N:253:ILE:O	1:N:257:GLU:HG3	2.10	0.52
1:N:259:GLN:O	1:N:263:LYS:HE3	2.10	0.52
1:P:106:THR:O	1:P:106:THR:CG2	2.56	0.52
1:P:176:ILE:CB	1:P:179:VAL:CG2	2.65	0.52
1:A:125:TYR:N	1:A:126:PRO:CD	2.73	0.52
1:C:29:LEU:HD11	1:C:177:PRO:HB2	1.90	0.52
1:D:125:TYR:N	1:D:126:PRO:CD	2.72	0.52
1:O:25:GLN:HE21	1:O:25:GLN:H	1.56	0.52
1:P:161:PHE:O	1:P:161:PHE:CD2	2.63	0.52
1:P:295:GLU:OE1	1:P:298:ARG:NH2	2.43	0.52
1:F:133:ILE:O	1:F:138:THR:HG23	2.09	0.52
1:F:200:PRO:HA	1:F:203:TYR:CE2	2.45	0.52
1:H:72:PRO:CB	1:H:299:VAL:HG13	2.40	0.52
1:I:212:THR:HG22	1:I:216:LYS:HE3	1.92	0.52
1:J:313:GLU:HA	1:J:313:GLU:OE1	2.10	0.52
1:L:23:LEU:HD11	1:L:65:TYR:CE2	2.45	0.52
1:P:127:PRO:O	1:P:130:ALA:HB3	2.09	0.52
1:N:326:ARG:NH2	1:Q:301:ASP:OD1	2.43	0.52
3:E:1002:PO4:O2	4:E:1003:AMP:O5'	2.28	0.52
1:H:313:GLU:HA	1:H:313:GLU:OE1	2.10	0.52
1:I:125:TYR:N	1:I:126:PRO:CD	2.72	0.52
1:O:126:PRO:HB2	1:O:127:PRO:CD	2.40	0.52
1:Q:199:ASN:HD22	1:Q:200:PRO:HD2	1.75	0.52
1:D:26:PHE:O	1:D:30:GLN:HB3	2.10	0.52
1:E:290:TRP:CH2	1:E:299:VAL:HG21	2.44	0.52
1:N:59:ARG:CG	1:N:59:ARG:HH11	2.23	0.52
1:P:175:ARG:CG	1:P:176:ILE:N	2.73	0.52
1:P:18:ASN:C	1:P:18:ASN:ND2	2.56	0.52
1:P:295:GLU:O	1:P:299:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLN:NE2	1:A:25:GLN:H	2.07	0.52
1:C:242:LEU:HB3	1:C:253:ILE:HD13	1.91	0.52
1:E:238:ILE:O	1:E:241:LEU:N	2.43	0.52
1:G:60:ARG:HG2	1:G:287:TYR:OH	2.09	0.52
1:H:25:GLN:HG2	1:H:178:LYS:O	2.10	0.52
1:H:99:ILE:HG12	1:K:118:VAL:O	2.10	0.52
1:K:297:ASP:O	1:K:301:ASP:OD1	2.27	0.52
1:O:126:PRO:CD	1:O:127:PRO:HD2	2.39	0.52
1:P:125:TYR:C	1:P:127:PRO:HD2	2.30	0.52
1:P:253:ILE:O	1:P:257:GLU:N	2.43	0.52
1:P:295:GLU:OE1	1:P:298:ARG:NE	2.43	0.52
1:B:125:TYR:CD2	1:B:126:PRO:HD3	2.45	0.51
1:F:19:TYR:CE2	1:F:24:ARG:HG3	2.45	0.51
1:H:228:ILE:CD1	1:H:228:ILE:N	2.74	0.51
1:I:213:ILE:HD11	1:I:280:LEU:HD12	1.92	0.51
1:O:177:PRO:O	1:O:178:LYS:HB2	2.09	0.51
1:P:5:PHE:HB2	1:P:138:THR:HG21	1.91	0.51
1:R:241:LEU:HD12	1:R:241:LEU:H	1.74	0.51
1:E:301:ASP:O	1:E:305:GLU:HB2	2.11	0.51
1:F:59:ARG:HG3	1:F:59:ARG:HH11	1.76	0.51
1:G:18:ASN:ND2	4:G:1003:AMP:C5'	2.69	0.51
1:G:182:ARG:O	1:G:184:MSE:HE2	2.10	0.51
1:H:129:MSE:HE1	1:H:147:GLN:OE1	2.10	0.51
1:K:190:THR:CG2	1:K:190:THR:O	2.58	0.51
1:K:200:PRO:O	1:K:216:LYS:HE2	2.10	0.51
1:L:205:THR:HG22	1:L:207:LEU:N	2.25	0.51
1:N:151:ILE:HA	1:N:154:THR:HG23	1.91	0.51
1:O:183:ILE:N	4:O:1003:AMP:N1	2.56	0.51
1:Q:41:ASP:OD2	1:Q:81:SER:HB3	2.09	0.51
1:R:274:GLN:O	1:R:277:ILE:HB	2.10	0.51
1:R:280:LEU:HD23	1:R:280:LEU:N	2.24	0.51
1:C:146:ASP:OD1	1:C:146:ASP:N	2.39	0.51
1:C:53:GLU:OE2	1:C:53:GLU:HA	2.09	0.51
1:E:59:ARG:NH2	1:E:296:LEU:HD23	2.25	0.51
1:F:66:LEU:HD12	1:F:296:LEU:CD1	2.40	0.51
1:G:199:ASN:C	1:G:199:ASN:HD22	2.14	0.51
1:H:29:LEU:HD22	1:H:33:TYR:HE1	1.74	0.51
1:J:152:GLU:HA	1:J:152:GLU:OE1	2.10	0.51
1:L:151:ILE:HG13	1:L:174:ALA:HB2	1.91	0.51
1:O:91:TRP:HE1	1:R:42:GLN:HB3	1.76	0.51
1:P:238:ILE:HD13	1:P:268:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:HB3	1:A:169:PHE:CE1	2.45	0.51
1:C:295:GLU:OE2	1:C:295:GLU:HA	2.10	0.51
1:E:38:CYS:SG	1:E:80:GLN:HB2	2.50	0.51
1:I:193:MSE:HE2	1:I:203:TYR:HA	1.93	0.51
1:I:24:ARG:CB	1:I:24:ARG:HH11	2.23	0.51
1:M:245:TYR:HB2	1:M:272:LEU:HD13	1.91	0.51
1:M:73:THR:OG1	1:M:74:GLN:N	2.44	0.51
1:O:297:ASP:O	1:O:301:ASP:OD1	2.29	0.51
1:P:184:MSE:H	1:P:240:ASN:ND2	2.08	0.51
1:R:187:VAL:HG22	1:R:202:ALA:HB1	1.84	0.51
1:R:19:TYR:CD2	1:R:24:ARG:CG	2.94	0.51
1:R:287:TYR:CE2	1:R:291:MSE:CG	2.94	0.51
1:R:287:TYR:CE2	1:R:291:MSE:HG2	2.45	0.51
1:E:164:ARG:HD3	1:E:165:TYR:CE2	2.46	0.51
1:E:9:GLN:NE2	1:E:9:GLN:HA	2.26	0.51
1:G:199:ASN:HD22	1:G:201:LYS:H	1.58	0.51
1:J:5:PHE:O	1:J:142:PRO:HD2	2.11	0.51
1:L:43:HIS:HE1	1:L:132:ASP:OD2	1.94	0.51
1:M:170:THR:O	1:M:172:PRO:HD3	2.11	0.51
1:Q:252:SER:OG	1:Q:254:GLU:HG2	2.09	0.51
1:Q:213:ILE:HD12	1:Q:277:ILE:HG13	1.92	0.51
1:H:23:LEU:HG	1:H:68:VAL:HG11	1.92	0.51
1:I:55:ARG:NH2	1:L:320:GLN:HE22	2.05	0.51
1:J:145:GLU:C	1:J:147:GLN:H	2.14	0.51
1:J:134:LEU:HB3	1:J:169:PHE:HD1	1.76	0.51
1:J:71:ASP:OD1	1:J:72:PRO:HD2	2.10	0.51
1:M:273:ALA:O	1:M:277:ILE:HG13	2.10	0.51
1:N:60:ARG:HG2	1:N:287:TYR:OH	2.09	0.51
1:O:213:ILE:HD12	1:O:277:ILE:HG12	1.92	0.51
3:P:1002:PO4:O1	4:P:1003:AMP:O1P	2.28	0.51
1:P:159:GLU:OE2	1:P:163:LYS:HE3	2.09	0.51
1:A:124:THR:CB	1:D:94:GLN:NE2	2.74	0.51
1:A:187:VAL:HG13	1:A:202:ALA:HA	1.92	0.51
1:B:171:ILE:N	1:B:171:ILE:HD13	2.26	0.51
1:C:105:MSE:HE2	1:C:105:MSE:CA	2.41	0.51
1:E:286:ARG:O	1:E:289:HIS:HB3	2.11	0.51
1:G:162:ASN:OD1	1:G:168:LEU:N	2.31	0.51
1:H:217:ILE:O	1:H:269:LYS:HE2	2.11	0.51
1:J:145:GLU:C	1:J:147:GLN:N	2.62	0.51
1:O:126:PRO:N	1:O:127:PRO:HD2	2.26	0.51
1:P:228:ILE:HD13	1:P:228:ILE:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:VAL:HG21	1:B:202:ALA:HB2	1.93	0.51
1:E:176:ILE:O	1:E:179:VAL:HG23	2.10	0.51
1:E:268:PHE:O	1:E:271:ASP:HB2	2.10	0.51
1:G:130:ALA:CB	1:G:154:THR:HB	2.40	0.51
1:G:43:HIS:HE1	1:G:132:ASP:OD2	1.93	0.51
1:G:313:GLU:HG3	1:G:317:LYS:HZ2	1.73	0.51
1:H:52:HIS:CE1	1:H:56:GLN:HE22	2.29	0.51
1:I:265:TYR:O	1:I:269:LYS:HG3	2.10	0.51
1:K:261:GLU:N	1:K:263:LYS:HD2	2.26	0.51
1:M:8:ILE:HD12	1:M:65:TYR:OH	2.10	0.51
1:P:151:ILE:HD12	1:P:174:ALA:CB	2.40	0.51
1:R:148:LYS:O	1:R:152:GLU:HG2	2.11	0.51
1:I:79:ILE:HB	1:I:82:GLU:HG3	1.93	0.51
1:K:165:TYR:CE1	1:K:322:MSE:HA	2.45	0.51
1:K:155:ARG:NH1	1:K:171:ILE:CG2	2.74	0.51
1:L:298:ARG:O	1:L:302:GLU:HB2	2.11	0.51
1:M:215:LYS:O	1:M:219:SER:OG	2.29	0.51
1:P:238:ILE:CD1	1:P:268:PHE:CE2	2.94	0.51
1:P:27:VAL:HG13	1:P:28:GLU:OE1	2.10	0.51
1:R:279:THR:C	1:R:282:PRO:HD2	2.30	0.51
1:R:295:GLU:HA	1:R:295:GLU:OE2	2.10	0.51
1:D:175:ARG:C	1:D:177:PRO:HD3	2.32	0.51
1:D:210:ALA:HA	1:D:277:ILE:HG12	1.92	0.51
1:J:106:THR:HG23	1:J:106:THR:O	2.10	0.51
1:K:271:ASP:O	1:K:275:VAL:CG1	2.59	0.51
1:O:215:LYS:O	1:O:219:SER:OG	2.29	0.51
1:P:17:GLY:HA2	1:P:183:ILE:HD12	1.93	0.51
1:R:162:ASN:HD21	1:R:169:PHE:H	1.59	0.51
1:R:43:HIS:CE1	1:R:132:ASP:OD2	2.64	0.51
1:G:199:ASN:ND2	1:G:201:LYS:H	2.08	0.50
1:H:86:HIS:HE1	1:H:136:TYR:OH	1.94	0.50
1:M:184:MSE:SE	1:M:192:LYS:HA	2.61	0.50
1:P:245:TYR:HA	1:P:272:LEU:HD12	1.93	0.50
1:Q:318:MSE:O	1:Q:322:MSE:HG3	2.11	0.50
1:A:182:ARG:O	1:A:184:MSE:HE2	2.12	0.50
1:I:5:PHE:CB	1:I:138:THR:HG21	2.41	0.50
1:H:45:ILE:HG21	1:K:322:MSE:HE2	1.93	0.50
1:M:141:VAL:N	1:M:173:GLU:O	2.43	0.50
1:N:3:THR:HB	1:N:138:THR:HA	1.92	0.50
1:O:187:VAL:HG13	1:O:202:ALA:HA	1.93	0.50
1:Q:319:GLU:HG2	1:Q:324:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:187:VAL:CG1	1:R:199:ASN:ND2	2.75	0.50
1:B:238:ILE:CG1	1:B:265:TYR:CE1	2.95	0.50
1:B:23:LEU:HD12	1:B:23:LEU:O	2.12	0.50
1:B:252:SER:O	1:B:255:GLU:HB3	2.11	0.50
1:B:29:LEU:CD1	1:B:177:PRO:CB	2.75	0.50
1:B:313:GLU:O	1:B:317:LYS:HG3	2.10	0.50
1:B:59:ARG:HH11	1:B:59:ARG:CG	2.24	0.50
1:D:151:ILE:O	1:D:155:ARG:HG3	2.12	0.50
1:F:182:ARG:NH1	1:F:192:LYS:CD	2.65	0.50
1:H:203:TYR:O	1:H:216:LYS:HD3	2.11	0.50
1:K:238:ILE:HD12	1:K:268:PHE:HE2	1.75	0.50
1:L:147:GLN:O	1:L:150:HIS:HB2	2.12	0.50
1:L:182:ARG:HG2	1:L:184:MSE:CE	2.42	0.50
1:O:193:MSE:CB	4:O:1003:AMP:N6	2.74	0.50
1:O:210:ALA:HB1	1:O:277:ILE:HD13	1.93	0.50
1:Q:19:TYR:HA	1:Q:23:LEU:HB3	1.93	0.50
1:R:86:HIS:CD2	1:R:132:ASP:OD1	2.60	0.50
1:C:86:HIS:HE1	1:C:136:TYR:OH	1.95	0.50
1:D:193:MSE:HB3	4:D:1003:AMP:N6	2.25	0.50
1:D:86:HIS:HE1	1:D:136:TYR:OH	1.94	0.50
4:I:1003:AMP:H8	4:I:1003:AMP:H5'1	1.77	0.50
1:L:125:TYR:CD2	1:L:126:PRO:HD3	2.46	0.50
1:L:185:SER:OG	1:L:187:VAL:HG22	2.11	0.50
1:M:94:GLN:HG3	1:M:127:PRO:HG2	1.93	0.50
1:P:254:GLU:OE1	1:P:254:GLU:N	2.44	0.50
1:B:159:GLU:O	1:B:163:LYS:HG3	2.11	0.50
1:D:281:ARG:HH11	1:D:281:ARG:HG3	1.76	0.50
1:E:194:SER:O	1:E:203:TYR:CD2	2.65	0.50
1:F:185:SER:CB	1:F:188:ASP:O	2.58	0.50
1:J:133:ILE:O	1:J:138:THR:HG23	2.11	0.50
1:J:22:ALA:O	1:J:25:GLN:HG2	2.10	0.50
1:K:122:LEU:O	1:K:125:TYR:CE1	2.63	0.50
1:M:100:GLY:O	1:M:104:ARG:HG3	2.11	0.50
1:M:43:HIS:CE1	1:M:128:LEU:HG	2.46	0.50
1:N:200:PRO:O	1:N:216:LYS:NZ	2.35	0.50
1:P:24:ARG:CB	1:P:24:ARG:HH11	2.24	0.50
1:A:130:ALA:CB	1:A:154:THR:HB	2.42	0.50
1:A:19:TYR:CZ	1:A:24:ARG:HD2	2.46	0.50
1:C:242:LEU:O	1:C:246:SER:HB3	2.11	0.50
1:H:253:ILE:O	1:H:253:ILE:HG22	2.11	0.50
1:I:91:TRP:HE1	1:L:42:GLN:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:159:GLU:O	1:J:163:LYS:HG3	2.12	0.50
1:K:46:THR:O	1:K:122:LEU:HD22	2.12	0.50
1:K:256:LEU:HD23	1:K:259:GLN:HG2	1.93	0.50
1:K:256:LEU:HD22	1:K:260:TYR:CE1	2.46	0.50
1:K:293:SER:HG	1:K:295:GLU:H	1.59	0.50
1:L:230:TYR:CD1	1:L:230:TYR:C	2.85	0.50
3:N:1002:PO4:O1	4:N:1003:AMP:O1P	2.30	0.50
1:P:254:GLU:OE2	1:P:257:GLU:OE1	2.30	0.50
1:A:124:THR:OG1	1:D:94:GLN:NE2	2.45	0.50
1:C:21:GLY:O	1:C:25:GLN:NE2	2.45	0.50
1:E:184:MSE:HE1	1:E:191:LYS:CA	2.41	0.50
1:F:23:LEU:HA	1:F:26:PHE:HD2	1.77	0.50
1:L:315:VAL:O	1:L:319:GLU:HG3	2.11	0.50
1:M:281:ARG:CG	1:M:281:ARG:NH1	2.70	0.50
1:P:199:ASN:ND2	1:P:201:LYS:HB2	2.26	0.50
1:P:184:MSE:H	1:P:240:ASN:HD21	1.59	0.50
1:Q:92:MSE:O	1:Q:96:ILE:HG23	2.12	0.50
1:R:313:GLU:OE2	1:R:316:ARG:NE	2.45	0.50
1:B:126:PRO:HB2	1:B:127:PRO:CD	2.36	0.50
1:E:126:PRO:HB2	1:E:127:PRO:CD	2.42	0.50
1:E:86:HIS:HD2	1:E:132:ASP:OD1	1.95	0.50
1:G:101:GLU:OE2	1:G:160:ARG:NH2	2.44	0.50
1:K:164:ARG:HG2	1:K:165:TYR:CE2	2.46	0.50
1:L:92:MSE:O	1:L:96:ILE:HG23	2.12	0.50
1:M:281:ARG:H	1:M:282:PRO:HD2	1.77	0.50
1:N:29:LEU:CD1	1:N:177:PRO:HB2	2.37	0.50
1:O:253:ILE:CG2	1:O:257:GLU:OE2	2.60	0.50
1:P:198:PRO:O	1:P:200:PRO:HD3	2.12	0.50
1:A:94:GLN:HE22	1:D:94:GLN:NE2	2.04	0.50
1:B:326:ARG:NH1	1:E:297:ASP:HA	2.27	0.50
1:C:8:ILE:O	1:C:40:VAL:HG22	2.12	0.50
1:D:165:TYR:CZ	1:D:322:MSE:HG2	2.47	0.50
1:F:124:THR:O	1:F:127:PRO:HD2	2.12	0.50
1:F:185:SER:O	1:F:188:ASP:O	2.30	0.50
1:G:100:GLY:O	1:G:104:ARG:HG3	2.11	0.50
1:J:150:HIS:O	1:J:154:THR:HG23	2.12	0.50
1:K:213:ILE:O	1:K:217:ILE:HG12	2.12	0.50
1:K:287:TYR:CZ	1:K:291:MSE:HE2	2.46	0.50
1:O:124:THR:HG21	1:R:124:THR:HG21	1.93	0.50
1:O:26:PHE:HA	1:O:29:LEU:HD12	1.93	0.50
1:P:213:ILE:CG2	1:P:217:ILE:HD12	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:9:GLN:HA	1:P:9:GLN:NE2	2.26	0.50
1:Q:182:ARG:NE	1:Q:184:MSE:HE1	2.27	0.50
1:B:137:ASN:CA	1:B:170:THR:CG2	2.90	0.49
1:B:199:ASN:HD22	1:B:200:PRO:CD	2.23	0.49
1:B:260:TYR:OH	1:B:271:ASP:OD2	2.30	0.49
1:H:272:LEU:HA	1:H:275:VAL:HG13	1.94	0.49
1:I:41:ASP:OD2	1:I:81:SER:HB3	2.12	0.49
1:K:238:ILE:HD11	1:K:268:PHE:CE2	2.47	0.49
1:L:213:ILE:HD11	1:L:280:LEU:HD12	1.93	0.49
1:O:193:MSE:H	4:O:1003:AMP:N6	2.10	0.49
1:O:193:MSE:N	4:O:1003:AMP:N6	2.60	0.49
1:P:213:ILE:HG23	1:P:276:VAL:HG11	1.94	0.49
1:Q:146:ASP:N	1:Q:146:ASP:OD1	2.32	0.49
1:R:267:VAL:O	1:R:267:VAL:HG12	2.12	0.49
1:A:200:PRO:HA	1:A:203:TYR:CE2	2.48	0.49
1:F:182:ARG:CZ	1:F:192:LYS:CG	2.89	0.49
1:H:295:GLU:O	1:H:298:ARG:N	2.42	0.49
4:K:1003:AMP:H8	4:K:1003:AMP:C5'	2.21	0.49
1:N:86:HIS:CD2	1:N:132:ASP:HA	2.46	0.49
1:O:141:VAL:HG12	1:O:143:VAL:HG13	1.93	0.49
1:B:139:ASP:HB2	1:B:140:ILE:HD12	1.95	0.49
1:B:175:ARG:HG3	1:B:176:ILE:H	1.72	0.49
1:B:22:ALA:HB1	1:B:26:PHE:HE2	1.77	0.49
1:C:133:ILE:O	1:C:138:THR:HG23	2.12	0.49
1:C:258:ARG:O	1:C:261:GLU:HG3	2.11	0.49
1:F:185:SER:HB3	1:F:188:ASP:HB3	1.92	0.49
3:G:1002:PO4:O2	4:G:1003:AMP:O2P	2.29	0.49
1:K:146:ASP:N	1:K:146:ASP:OD1	2.29	0.49
1:K:191:LYS:HD2	1:K:192:LYS:H	1.71	0.49
1:P:29:LEU:CD1	1:P:177:PRO:HB2	2.42	0.49
1:Q:199:ASN:C	1:Q:199:ASN:HD22	2.15	0.49
1:A:118:VAL:O	1:D:98:TYR:HA	2.13	0.49
1:B:162:ASN:O	1:B:165:TYR:O	2.30	0.49
1:C:227:THR:HG22	1:C:229:ARG:HG3	1.94	0.49
1:G:126:PRO:HB2	1:G:127:PRO:CD	2.37	0.49
1:J:129:MSE:HE3	2:J:1001:TRP:CZ3	2.47	0.49
1:J:211:LYS:O	1:J:215:LYS:HG2	2.13	0.49
1:J:26:PHE:CE2	1:J:29:LEU:HD12	2.48	0.49
1:N:126:PRO:HB2	1:N:127:PRO:CD	2.32	0.49
1:R:184:MSE:HE2	1:R:191:LYS:O	2.13	0.49
1:B:29:LEU:HD13	1:B:177:PRO:CB	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ALA:O	1:C:26:PHE:HE2	1.92	0.49
1:F:101:GLU:O	1:F:105:MSE:HE3	2.12	0.49
1:K:105:MSE:HE1	1:K:150:HIS:ND1	2.27	0.49
1:P:215:LYS:CE	1:P:215:LYS:O	2.61	0.49
1:P:41:ASP:OD2	1:P:81:SER:HB3	2.12	0.49
1:R:59:ARG:CG	1:R:59:ARG:HH11	2.26	0.49
1:B:238:ILE:HD11	1:B:265:TYR:CD1	2.48	0.49
1:B:281:ARG:CG	1:B:281:ARG:HH11	2.25	0.49
1:D:125:TYR:N	1:D:126:PRO:HD2	2.27	0.49
1:D:125:TYR:CD2	1:D:126:PRO:HD3	2.47	0.49
1:E:150:HIS:O	1:E:154:THR:HG23	2.12	0.49
1:F:96:ILE:O	1:F:160:ARG:NH1	2.44	0.49
1:J:59:ARG:CG	1:J:59:ARG:HH11	2.25	0.49
1:L:59:ARG:HH11	1:L:59:ARG:CG	2.25	0.49
1:L:9:GLN:HG2	1:L:40:VAL:CG2	2.42	0.49
1:M:267:VAL:HG13	1:Q:306:LYS:HA	1.93	0.49
1:N:39:ILE:HG23	1:N:61:LEU:HD23	1.95	0.49
1:N:55:ARG:NH2	1:Q:320:GLN:NE2	2.60	0.49
1:O:128:LEU:O	1:O:132:ASP:OD1	2.31	0.49
1:P:16:ILE:HG21	1:P:204:ILE:HB	1.91	0.49
1:B:205:THR:HG22	1:B:208:ASP:H	1.75	0.49
1:B:71:ASP:O	1:B:75:ALA:N	2.40	0.49
1:E:170:THR:O	1:E:172:PRO:HD3	2.12	0.49
1:E:48:TRP:HB2	1:O:188:ASP:OD1	2.13	0.49
1:F:92:MSE:O	1:F:96:ILE:HG23	2.13	0.49
1:G:212:THR:HG22	1:G:216:LYS:HE3	1.94	0.49
1:I:18:ASN:ND2	4:I:1003:AMP:O4'	2.45	0.49
1:M:292:GLU:HG3	1:M:293:SER:N	2.28	0.49
1:N:54:LEU:O	1:N:58:ILE:HG13	2.12	0.49
1:R:18:ASN:HD21	4:R:1003:AMP:H5'1	1.77	0.49
1:A:199:ASN:HD21	1:A:201:LYS:HG3	1.78	0.49
1:A:59:ARG:HH11	1:A:59:ARG:CG	2.26	0.49
1:J:27:VAL:HG12	1:J:27:VAL:O	2.13	0.49
1:K:19:TYR:O	1:K:24:ARG:HB3	2.13	0.49
1:N:228:ILE:CD1	1:N:265:TYR:HD1	2.26	0.49
1:O:171:ILE:CD1	1:O:171:ILE:N	2.76	0.49
1:Q:26:PHE:HA	1:Q:29:LEU:HB2	1.95	0.49
1:R:162:ASN:O	1:R:166:GLY:O	2.31	0.49
1:R:41:ASP:CB	1:R:58:ILE:HD11	2.39	0.49
1:C:5:PHE:CB	1:C:138:THR:HG21	2.43	0.49
1:D:228:ILE:HD11	1:D:265:TYR:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:MSE:HE2	1:F:105:MSE:N	2.28	0.49
1:C:99:ILE:HG12	1:F:118:VAL:O	2.13	0.49
1:C:118:VAL:HB	1:F:99:ILE:HG13	1.93	0.49
1:H:72:PRO:HB3	1:H:299:VAL:CG1	2.42	0.49
1:I:176:ILE:HG12	1:I:179:VAL:HG13	1.91	0.49
1:L:80:GLN:NE2	1:L:132:ASP:OD1	2.43	0.49
1:M:175:ARG:HH12	1:M:177:PRO:CG	2.22	0.49
1:M:281:ARG:NH1	1:M:281:ARG:HB3	2.28	0.49
1:N:99:ILE:HD13	1:Q:120:ALA:HA	1.93	0.49
1:O:4:ILE:CG2	1:O:142:PRO:HD3	2.42	0.49
1:P:124:THR:O	1:P:127:PRO:HD2	2.13	0.49
1:N:99:ILE:CD1	1:Q:120:ALA:HA	2.42	0.49
1:R:56:GLN:OE1	1:R:57:ASN:ND2	2.46	0.49
1:A:195:LYS:HE2	3:A:1002:PO4:P	2.53	0.49
1:B:215:LYS:O	1:B:219:SER:OG	2.30	0.49
1:E:238:ILE:C	1:E:241:LEU:HD23	2.34	0.49
1:G:274:GLN:O	1:G:278:GLU:HB2	2.13	0.49
1:J:193:MSE:HE2	1:J:203:TYR:HA	1.94	0.49
1:J:320:GLN:O	1:J:320:GLN:HG3	2.13	0.49
1:K:155:ARG:HG2	1:K:171:ILE:HG23	1.95	0.49
1:O:193:MSE:CA	4:O:1003:AMP:HN61	2.25	0.49
1:O:5:PHE:CZ	1:O:38:CYS:HB2	2.48	0.49
1:P:245:TYR:CE2	1:P:256:LEU:HD13	2.46	0.49
1:A:159:GLU:HG3	1:A:163:LYS:HE2	1.95	0.48
1:B:245:TYR:O	1:B:245:TYR:HD1	1.95	0.48
1:C:212:THR:O	1:C:216:LYS:HB2	2.13	0.48
1:F:22:ALA:O	1:F:26:PHE:HD2	1.92	0.48
1:F:228:ILE:HD13	1:F:265:TYR:CE1	2.47	0.48
1:H:199:ASN:ND2	1:H:201:LYS:HB2	2.27	0.48
4:N:1003:AMP:H4'	4:N:1003:AMP:O3P	2.13	0.48
1:O:92:MSE:HB3	1:O:322:MSE:SE	2.63	0.48
1:Q:165:TYR:HB3	1:Q:321:ALA:HB1	1.95	0.48
1:R:53:GLU:OE2	1:R:56:GLN:NE2	2.45	0.48
1:C:295:GLU:O	1:C:299:VAL:HG23	2.13	0.48
1:J:197:ASP:OD1	1:J:198:PRO:HD2	2.13	0.48
1:J:315:VAL:HG12	1:J:316:ARG:N	2.27	0.48
1:M:209:ASP:O	1:M:213:ILE:HG13	2.14	0.48
1:M:278:GLU:OE1	1:M:278:GLU:HA	2.12	0.48
1:P:215:LYS:HE2	1:P:215:LYS:C	2.34	0.48
1:Q:150:HIS:O	1:Q:154:THR:HG22	2.13	0.48
1:Q:156:ASP:O	1:Q:160:ARG:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:238:ILE:CD1	1:Q:265:TYR:CE1	2.96	0.48
1:R:20:ILE:HG13	1:R:183:ILE:CD1	2.40	0.48
1:R:238:ILE:HA	1:R:241:LEU:CD1	2.43	0.48
1:A:289:HIS:O	1:A:293:SER:HB2	2.13	0.48
1:B:29:LEU:HD11	1:B:177:PRO:O	2.13	0.48
1:D:228:ILE:HD13	1:D:265:TYR:HE1	1.78	0.48
1:F:185:SER:C	1:F:188:ASP:O	2.52	0.48
1:H:22:ALA:O	1:H:26:PHE:HD2	1.94	0.48
1:I:91:TRP:NE1	1:L:42:GLN:HB3	2.29	0.48
1:M:195:LYS:C	1:M:197:ASP:H	2.16	0.48
1:N:304:ALA:O	1:N:308:ASN:HB2	2.13	0.48
1:P:298:ARG:NH1	1:P:298:ARG:HG3	2.28	0.48
1:Q:65:TYR:O	1:Q:70:ILE:HB	2.13	0.48
1:B:1:MSE:HE3	1:B:34:ASN:HB2	1.94	0.48
1:B:83:VAL:HG13	1:B:308:ASN:ND2	2.28	0.48
1:E:267:VAL:CG1	1:E:268:PHE:H	2.26	0.48
1:H:185:SER:HB2	1:H:202:ALA:HB1	1.95	0.48
1:M:71:ASP:OD1	1:M:73:THR:HG23	2.12	0.48
1:O:289:HIS:CG	1:O:290:TRP:N	2.81	0.48
1:Q:24:ARG:CG	1:Q:24:ARG:NH1	2.75	0.48
1:R:123:LEU:O	1:R:123:LEU:HG	2.11	0.48
1:D:146:ASP:N	1:D:146:ASP:OD1	2.30	0.48
1:D:205:THR:HG22	1:D:207:LEU:N	2.24	0.48
1:F:308:ASN:O	1:F:312:SER:HB2	2.14	0.48
1:G:260:TYR:OH	1:G:271:ASP:OD2	2.27	0.48
1:L:30:GLN:O	1:L:74:GLN:HG3	2.14	0.48
1:N:124:THR:O	1:N:127:PRO:HD2	2.12	0.48
1:O:193:MSE:O	4:O:1003:AMP:N7	2.47	0.48
1:R:240:ASN:O	1:R:243:ASN:HB2	2.11	0.48
1:R:3:THR:HB	1:R:138:THR:HA	1.95	0.48
1:E:42:GLN:HB2	1:E:80:GLN:OE1	2.13	0.48
1:F:126:PRO:N	1:F:127:PRO:CD	2.77	0.48
1:C:320:GLN:HE22	1:F:55:ARG:NH2	2.07	0.48
1:H:19:TYR:HB2	1:H:206:LEU:HD11	1.94	0.48
1:H:84:PRO:HD2	1:H:308:ASN:HD21	1.78	0.48
1:I:136:TYR:HB2	1:I:138:THR:HG22	1.95	0.48
1:L:23:LEU:HD13	1:L:65:TYR:CE2	2.46	0.48
1:P:16:ILE:CG1	1:P:17:GLY:N	2.76	0.48
1:P:72:PRO:HB3	1:P:299:VAL:HG13	1.95	0.48
1:Q:188:ASP:HB3	1:Q:191:LYS:HB3	1.95	0.48
1:R:71:ASP:OD2	1:R:74:GLN:OE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ILE:HA	1:D:154:THR:HG23	1.95	0.48
1:A:325:GLY:O	1:D:55:ARG:HD2	2.12	0.48
1:G:150:HIS:O	1:G:154:THR:CG2	2.61	0.48
1:H:27:VAL:O	1:H:30:GLN:HG2	2.14	0.48
1:J:199:ASN:HD22	1:J:200:PRO:HD2	1.78	0.48
1:H:119:SER:HA	1:K:97:VAL:O	2.14	0.48
1:O:254:GLU:N	1:O:254:GLU:OE1	2.47	0.48
1:O:29:LEU:O	1:O:32:GLU:N	2.41	0.48
1:Q:140:ILE:CD1	1:Q:175:ARG:O	2.61	0.48
1:N:120:ALA:CB	1:Q:97:VAL:CG1	2.91	0.48
1:R:19:TYR:CD2	1:R:24:ARG:CD	2.96	0.48
1:R:237:GLY:O	1:R:241:LEU:CD1	2.62	0.48
1:A:273:ALA:O	1:A:277:ILE:HG13	2.14	0.48
1:D:130:ALA:CB	1:D:154:THR:HB	2.44	0.48
1:D:282:PRO:O	1:D:286:ARG:HG3	2.14	0.48
1:E:245:TYR:O	1:E:245:TYR:HD1	1.97	0.48
1:L:185:SER:OG	1:L:187:VAL:CG2	2.62	0.48
1:P:212:THR:O	1:P:216:LYS:HB3	2.13	0.48
1:P:22:ALA:O	1:P:26:PHE:HD2	1.95	0.48
1:P:238:ILE:CD1	1:P:268:PHE:HE2	2.26	0.48
1:P:295:GLU:OE1	1:P:298:ARG:CZ	2.62	0.48
1:Q:199:ASN:HD22	1:Q:200:PRO:CD	2.27	0.48
1:R:124:THR:O	1:R:127:PRO:HD2	2.13	0.48
1:A:18:ASN:ND2	4:A:1003:AMP:H8	2.12	0.48
1:A:56:GLN:HG2	1:A:60:ARG:NH2	2.28	0.48
1:A:97:VAL:O	1:D:119:SER:HA	2.14	0.48
1:E:205:THR:CG2	1:E:207:LEU:H	2.15	0.48
1:E:84:PRO:HD2	1:E:308:ASN:HD21	1.78	0.48
1:F:213:ILE:HD11	1:F:280:LEU:HD12	1.95	0.48
1:J:120:ALA:O	1:J:124:THR:HG22	2.14	0.48
1:O:126:PRO:HD2	1:O:127:PRO:HD2	1.94	0.48
1:A:56:GLN:CG	1:A:60:ARG:NH2	2.76	0.48
1:B:143:VAL:HB	1:B:147:GLN:HB2	1.95	0.48
1:C:211:LYS:HE3	1:C:215:LYS:HD2	1.95	0.48
1:D:147:GLN:OE1	1:D:150:HIS:HD2	1.96	0.48
1:G:215:LYS:O	1:G:219:SER:OG	2.28	0.48
1:G:224:SER:CB	1:I:166:GLY:HA2	2.42	0.48
1:M:27:VAL:HB	1:M:28:GLU:OE1	2.14	0.48
1:M:84:PRO:HD2	1:M:308:ASN:HD21	1.79	0.48
1:P:151:ILE:CD1	1:P:174:ALA:HB1	2.42	0.48
1:A:162:ASN:HA	1:A:166:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:HIS:CD2	1:B:132:ASP:HA	2.49	0.47
1:G:224:SER:CB	1:I:166:GLY:N	2.77	0.47
1:G:54:LEU:O	1:G:58:ILE:HG13	2.13	0.47
1:J:215:LYS:O	1:J:219:SER:OG	2.32	0.47
1:M:41:ASP:OD2	1:M:81:SER:HB3	2.13	0.47
1:O:133:ILE:HG23	1:O:138:THR:OG1	2.14	0.47
1:O:175:ARG:HH22	1:O:177:PRO:CG	2.26	0.47
1:O:184:MSE:HB3	1:O:191:LYS:O	2.14	0.47
1:Q:86:HIS:HD2	1:Q:132:ASP:OD1	1.97	0.47
1:R:272:LEU:CA	1:R:275:VAL:HG12	2.43	0.47
1:B:182:ARG:HA	4:B:1003:AMP:H2	1.78	0.47
1:C:42:GLN:HB3	1:F:91:TRP:HE1	1.79	0.47
1:E:293:SER:OG	1:E:295:GLU:HB2	2.14	0.47
1:E:313:GLU:CD	1:E:316:ARG:HE	2.18	0.47
1:E:71:ASP:OD1	1:E:72:PRO:HD2	2.15	0.47
1:F:313:GLU:OE1	1:F:313:GLU:HA	2.15	0.47
1:F:41:ASP:OD2	1:F:81:SER:HB3	2.13	0.47
1:M:140:ILE:CD1	1:M:175:ARG:HD3	2.44	0.47
1:M:199:ASN:HD22	1:M:201:LYS:H	1.62	0.47
1:P:182:ARG:HH11	1:P:192:LYS:HD2	1.79	0.47
1:P:225:GLU:CD	1:P:227:THR:OG1	2.52	0.47
1:P:245:TYR:HE1	1:P:271:ASP:O	1.97	0.47
1:R:5:PHE:CE2	1:R:136:TYR:CE2	3.02	0.47
1:R:187:VAL:HG23	1:R:188:ASP:N	2.29	0.47
1:B:273:ALA:O	1:B:277:ILE:HG13	2.15	0.47
1:D:304:ALA:O	1:D:308:ASN:HB2	2.14	0.47
1:D:83:VAL:HG13	1:D:308:ASN:HA	1.97	0.47
1:E:185:SER:N	1:E:191:LYS:O	2.36	0.47
1:G:213:ILE:O	1:G:217:ILE:HG12	2.13	0.47
1:J:168:LEU:HD11	1:J:317:LYS:HB3	1.95	0.47
1:J:318:MSE:O	1:J:322:MSE:HG3	2.14	0.47
1:K:167:GLU:HG2	1:K:167:GLU:O	2.13	0.47
1:L:258:ARG:O	1:L:259:GLN:C	2.51	0.47
1:L:23:LEU:CD1	1:L:65:TYR:CZ	2.97	0.47
1:M:214:GLU:OE1	1:Q:1:MSE:CE	2.62	0.47
1:O:59:ARG:NH2	1:O:296:LEU:HD23	2.28	0.47
1:R:151:ILE:HG13	1:R:174:ALA:HB2	1.95	0.47
1:R:313:GLU:OE2	1:R:316:ARG:NH2	2.47	0.47
1:A:89:ALA:HB2	1:A:135:LEU:HD21	1.96	0.47
1:E:165:TYR:HB3	1:E:321:ALA:HB1	1.97	0.47
1:M:185:SER:HG	1:M:188:ASP:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:281:ARG:N	1:M:282:PRO:CD	2.77	0.47
1:N:133:ILE:O	1:N:138:THR:HG23	2.14	0.47
1:O:25:GLN:O	1:O:29:LEU:HG	2.13	0.47
1:O:4:ILE:HD11	1:O:33:TYR:CG	2.48	0.47
1:A:5:PHE:HB2	1:A:138:THR:HG21	1.97	0.47
1:B:213:ILE:HD12	1:B:277:ILE:HG12	1.95	0.47
1:F:179:VAL:HG12	1:F:180:GLY:O	2.14	0.47
1:F:215:LYS:O	1:F:219:SER:OG	2.29	0.47
4:I:1003:AMP:H8	4:I:1003:AMP:C5'	2.27	0.47
1:I:241:LEU:HB3	1:I:268:PHE:HE2	1.80	0.47
1:K:165:TYR:CD1	1:K:321:ALA:HB1	2.48	0.47
1:P:124:THR:C	1:P:127:PRO:HD2	2.35	0.47
1:Q:101:GLU:O	1:Q:105:MSE:HE3	2.15	0.47
1:Q:175:ARG:O	1:Q:175:ARG:HG3	2.14	0.47
1:Q:260:TYR:OH	1:Q:271:ASP:OD2	2.27	0.47
1:R:105:MSE:CE	1:R:150:HIS:ND1	2.78	0.47
4:A:1003:AMP:C8	4:A:1003:AMP:C5'	2.97	0.47
1:A:22:ALA:C	1:A:25:GLN:HE21	2.18	0.47
1:A:248:LEU:HD12	1:A:276:VAL:HG22	1.96	0.47
1:A:281:ARG:N	1:A:282:PRO:HD2	2.29	0.47
1:B:297:ASP:O	1:B:301:ASP:OD1	2.32	0.47
1:E:133:ILE:O	1:E:138:THR:CG2	2.62	0.47
1:F:59:ARG:CG	1:F:59:ARG:NH1	2.77	0.47
1:H:281:ARG:HB3	1:H:282:PRO:HD3	1.96	0.47
1:I:263:LYS:HD2	1:I:263:LYS:N	2.29	0.47
1:J:125:TYR:CD2	1:J:126:PRO:HD3	2.49	0.47
1:J:24:ARG:O	1:J:24:ARG:HG3	2.14	0.47
1:K:248:LEU:HD22	1:K:279:THR:HG21	1.96	0.47
1:O:19:TYR:CE1	1:O:68:VAL:HG13	2.40	0.47
1:A:105:MSE:CA	1:A:105:MSE:CE	2.86	0.47
1:B:107:GLN:NE2	1:B:107:GLN:H	2.13	0.47
1:C:194:SER:O	1:C:197:ASP:HB2	2.15	0.47
1:F:199:ASN:HD22	1:F:199:ASN:C	2.18	0.47
1:C:55:ARG:HD2	1:F:325:GLY:O	2.15	0.47
1:G:89:ALA:HB2	1:G:135:LEU:HD21	1.96	0.47
1:O:193:MSE:H	4:O:1003:AMP:HN62	1.61	0.47
1:O:217:ILE:HD11	1:O:276:VAL:HG21	1.96	0.47
1:P:185:SER:HB3	1:P:188:ASP:O	2.14	0.47
4:Q:1003:AMP:C8	4:Q:1003:AMP:H5'1	2.49	0.47
1:Q:56:GLN:O	1:Q:60:ARG:HB2	2.15	0.47
1:A:38:CYS:SG	1:A:80:GLN:HB2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:O	1:B:276:VAL:HG23	2.14	0.47
1:C:137:ASN:ND2	1:C:170:THR:OG1	2.37	0.47
1:C:200:PRO:HA	1:C:203:TYR:CE2	2.50	0.47
1:E:248:LEU:HD13	1:E:279:THR:OG1	2.14	0.47
1:G:211:LYS:HG3	1:G:211:LYS:O	2.14	0.47
1:H:256:LEU:O	1:H:260:TYR:HD2	1.97	0.47
1:I:319:GLU:HG2	1:I:324:LEU:HD12	1.97	0.47
1:J:214:GLU:O	1:J:218:LYS:HG3	2.15	0.47
1:N:168:LEU:HD21	1:N:317:LYS:HD3	1.97	0.47
1:P:195:LYS:HB3	3:P:1002:PO4:O2	2.15	0.47
1:P:194:SER:HA	3:P:1002:PO4:O4	2.15	0.47
1:P:71:ASP:HB3	1:P:74:GLN:HB2	1.96	0.47
1:P:97:VAL:CG1	1:P:102:LEU:HD11	2.45	0.47
1:Q:107:GLN:NE2	1:Q:107:GLN:N	2.53	0.47
1:Q:203:TYR:O	1:Q:216:LYS:HD3	2.15	0.47
1:C:128:LEU:HD22	1:F:91:TRP:CE2	2.50	0.47
1:A:124:THR:CG2	1:D:124:THR:HG21	2.41	0.47
1:E:194:SER:HA	3:E:1002:PO4:O4	2.15	0.47
1:F:205:THR:CG2	1:F:207:LEU:N	2.70	0.47
1:H:158:ALA:HB3	1:H:171:ILE:HD12	1.95	0.47
1:H:137:ASN:ND2	1:H:170:THR:HG23	2.27	0.47
1:K:43:HIS:HE1	1:K:132:ASP:OD2	1.96	0.47
1:K:56:GLN:O	1:K:60:ARG:HG3	2.14	0.47
1:L:152:GLU:HA	1:L:152:GLU:OE1	2.14	0.47
1:M:96:ILE:O	1:M:160:ARG:NH2	2.48	0.47
1:N:192:LYS:NZ	3:N:1002:PO4:O3	2.48	0.47
1:Q:4:ILE:HG23	1:Q:140:ILE:HG23	1.97	0.47
1:A:86:HIS:HE1	1:A:136:TYR:OH	1.98	0.47
1:C:257:GLU:O	1:C:261:GLU:HG2	2.14	0.47
1:J:123:LEU:HG	1:J:123:LEU:O	2.15	0.47
1:J:3:THR:HB	1:J:138:THR:HA	1.97	0.47
1:K:184:MSE:HB2	1:K:240:ASN:OD1	2.14	0.47
1:K:228:ILE:CD1	1:K:260:TYR:HB3	2.45	0.47
1:M:25:GLN:O	1:M:29:LEU:HG	2.15	0.47
1:O:102:LEU:O	1:O:105:MSE:HB2	2.15	0.47
1:O:105:MSE:CE	1:O:105:MSE:CA	2.92	0.47
1:O:197:ASP:HA	1:O:198:PRO:HD3	1.75	0.47
1:P:228:ILE:CG2	1:P:268:PHE:CE2	2.98	0.47
1:R:56:GLN:HG2	1:R:60:ARG:HH21	1.80	0.47
1:A:320:GLN:NE2	1:D:55:ARG:HH21	2.06	0.47
1:C:212:THR:CG2	1:C:216:LYS:HE3	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:CYS:O	1:J:119:SER:OG	2.29	0.47
1:H:315:VAL:O	1:H:319:GLU:HG3	2.15	0.47
1:H:42:GLN:HB2	1:H:80:GLN:OE1	2.14	0.47
1:I:25:GLN:OE1	1:I:178:LYS:O	2.33	0.47
1:J:124:THR:OG1	1:J:124:THR:O	2.32	0.47
4:M:1003:AMP:O3'	4:M:1003:AMP:O1P	2.29	0.47
4:M:1003:AMP:H3'	4:M:1003:AMP:P	2.55	0.47
4:N:1003:AMP:H2'	4:N:1003:AMP:H5'1	1.72	0.47
1:O:105:MSE:SE	1:O:149:GLN:HG2	2.65	0.47
1:O:213:ILE:HG21	1:O:276:VAL:CG1	2.45	0.47
1:O:228:ILE:O	1:O:228:ILE:HG22	2.13	0.47
1:R:5:PHE:CB	1:R:138:THR:HG21	2.44	0.47
1:R:56:GLN:CG	1:R:60:ARG:NH2	2.78	0.47
1:B:43:HIS:HE1	1:B:132:ASP:OD2	1.97	0.46
1:F:217:ILE:O	1:F:269:LYS:HE2	2.14	0.46
1:G:309:ARG:HB3	1:G:309:ARG:NH1	2.30	0.46
1:H:228:ILE:HD12	1:H:228:ILE:N	2.31	0.46
1:H:281:ARG:HG3	1:H:281:ARG:NH1	2.30	0.46
1:J:30:GLN:O	1:J:74:GLN:HG3	2.15	0.46
1:L:8:ILE:HD13	1:L:65:TYR:CE2	2.49	0.46
1:P:165:TYR:HB3	1:P:321:ALA:HB1	1.97	0.46
1:R:4:ILE:HG13	1:R:140:ILE:HB	1.97	0.46
1:R:205:THR:C	1:R:207:LEU:H	2.17	0.46
1:D:228:ILE:CD1	1:D:265:TYR:CD1	2.98	0.46
1:F:107:GLN:N	1:F:107:GLN:NE2	2.46	0.46
1:G:86:HIS:HD2	1:G:132:ASP:OD1	1.98	0.46
1:I:70:ILE:HD12	1:I:70:ILE:HA	1.70	0.46
1:K:124:THR:CA	1:K:126:PRO:HD2	2.45	0.46
1:M:126:PRO:HB2	1:M:127:PRO:CD	2.33	0.46
1:N:120:ALA:HB3	1:Q:97:VAL:HG13	1.97	0.46
1:N:253:ILE:HG22	1:N:254:GLU:N	2.31	0.46
1:O:319:GLU:HB3	1:O:324:LEU:HB2	1.96	0.46
1:O:85:ALA:HA	1:O:88:GLN:HG3	1.96	0.46
1:P:9:GLN:HE21	1:P:9:GLN:CA	2.23	0.46
1:R:205:THR:C	1:R:207:LEU:N	2.69	0.46
1:R:63:ALA:O	1:R:67:ALA:HB2	2.15	0.46
1:B:71:ASP:HB3	1:B:74:GLN:CB	2.44	0.46
1:D:5:PHE:O	1:D:142:PRO:HD2	2.16	0.46
1:I:278:GLU:OE1	1:I:281:ARG:NH2	2.49	0.46
1:J:274:GLN:O	1:J:278:GLU:HB2	2.16	0.46
1:K:295:GLU:CG	1:K:298:ARG:NH1	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:5:PHE:HB2	1:N:138:THR:HG21	1.97	0.46
1:P:238:ILE:HD13	1:P:268:PHE:HE2	1.80	0.46
1:R:213:ILE:HD13	1:R:277:ILE:HG12	1.92	0.46
1:B:205:THR:HG22	1:B:207:LEU:N	2.29	0.46
1:B:281:ARG:N	1:B:282:PRO:HD2	2.31	0.46
1:B:65:TYR:O	1:B:70:ILE:HB	2.15	0.46
1:D:228:ILE:CD1	1:D:265:TYR:HD1	2.27	0.46
1:G:125:TYR:CD2	1:G:126:PRO:HD3	2.51	0.46
1:G:199:ASN:HD21	1:G:201:LYS:HG3	1.80	0.46
1:J:130:ALA:CB	1:J:154:THR:HB	2.45	0.46
1:K:106:THR:CB	1:K:149:GLN:NE2	2.78	0.46
1:M:74:GLN:HE21	1:M:74:GLN:HA	1.81	0.46
1:O:175:ARG:NH2	1:O:175:ARG:CG	2.78	0.46
1:O:29:LEU:O	1:O:30:GLN:C	2.54	0.46
1:P:209:ASP:OD1	1:P:212:THR:OG1	2.30	0.46
1:C:227:THR:HG21	1:C:229:ARG:CZ	2.46	0.46
1:C:1:MSE:CG	1:D:211:LYS:HD2	2.29	0.46
1:F:297:ASP:O	1:F:301:ASP:OD1	2.33	0.46
1:H:158:ALA:HB3	1:H:171:ILE:CD1	2.45	0.46
1:J:5:PHE:HB2	1:J:138:THR:HG21	1.97	0.46
1:K:245:TYR:CE1	1:K:275:VAL:CG1	2.77	0.46
1:K:256:LEU:HD23	1:K:256:LEU:HA	1.79	0.46
1:K:272:LEU:HA	1:K:275:VAL:HG13	1.98	0.46
1:I:225:GLU:HG3	1:N:163:LYS:HD3	1.98	0.46
1:M:55:ARG:HH22	1:P:320:GLN:CD	2.18	0.46
1:Q:273:ALA:O	1:Q:277:ILE:HD12	2.16	0.46
1:A:241:LEU:HD12	1:A:241:LEU:HA	1.73	0.46
1:C:155:ARG:O	1:C:159:GLU:HB2	2.16	0.46
1:D:254:GLU:CD	1:D:254:GLU:N	2.69	0.46
1:G:211:LYS:HD2	1:K:1:MSE:CG	2.45	0.46
1:K:40:VAL:O	1:K:40:VAL:HG23	2.15	0.46
1:L:289:HIS:O	1:L:293:SER:HB3	2.15	0.46
1:L:40:VAL:O	1:L:40:VAL:HG23	2.16	0.46
1:M:290:TRP:O	1:M:292:GLU:N	2.48	0.46
1:O:102:LEU:HD22	1:O:123:LEU:O	2.15	0.46
1:O:213:ILE:CG2	1:O:276:VAL:HG11	2.45	0.46
1:P:29:LEU:HD11	1:P:177:PRO:HB2	1.97	0.46
1:A:320:GLN:HE21	1:D:55:ARG:HH22	1.45	0.46
1:K:105:MSE:CE	1:K:150:HIS:CE1	2.99	0.46
1:M:161:PHE:CE2	1:M:169:PHE:CE2	3.02	0.46
1:N:159:GLU:O	1:N:163:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:228:ILE:HD11	1:N:265:TYR:HD1	1.81	0.46
1:O:165:TYR:HB3	1:O:321:ALA:HB1	1.98	0.46
1:P:245:TYR:CZ	1:P:275:VAL:HG21	2.42	0.46
4:Q:1003:AMP:C8	4:Q:1003:AMP:C5'	2.98	0.46
1:C:254:GLU:OE1	1:C:254:GLU:N	2.42	0.46
1:D:65:TYR:O	1:D:70:ILE:HB	2.16	0.46
4:E:1003:AMP:C5'	4:E:1003:AMP:C8	2.98	0.46
1:I:215:LYS:O	1:I:219:SER:OG	2.33	0.46
1:K:192:LYS:HB3	1:K:192:LYS:HE2	1.52	0.46
1:K:259:GLN:HG3	1:K:260:TYR:H	1.78	0.46
1:O:326:ARG:NH1	1:R:300:LEU:CB	2.79	0.46
1:O:33:TYR:N	1:O:33:TYR:CD1	2.84	0.46
1:P:193:MSE:HB3	4:P:1003:AMP:HN62	1.77	0.46
1:P:64:LEU:HG	1:P:287:TYR:CD1	2.51	0.46
1:Q:228:ILE:HG13	1:Q:260:TYR:HB3	1.98	0.46
1:R:184:MSE:CE	1:R:191:LYS:O	2.64	0.46
1:B:238:ILE:HD11	1:B:265:TYR:CE1	2.50	0.46
1:B:32:GLU:CG	1:B:33:TYR:CE1	2.99	0.46
1:E:9:GLN:HE21	1:E:9:GLN:HA	1.81	0.46
1:F:25:GLN:HB3	1:F:178:LYS:HB2	1.98	0.46
1:G:295:GLU:HG2	1:G:295:GLU:O	2.16	0.46
1:J:175:ARG:O	1:J:177:PRO:HD3	2.15	0.46
1:K:124:THR:O	1:K:127:PRO:HG2	2.14	0.46
1:M:161:PHE:HD2	1:M:169:PHE:CD2	2.34	0.46
1:O:3:THR:CG2	1:O:138:THR:HG22	2.43	0.46
1:O:71:ASP:OD2	1:O:73:THR:N	2.49	0.46
1:P:26:PHE:HZ	1:P:142:PRO:CB	2.29	0.46
1:P:4:ILE:HD12	1:P:33:TYR:CD2	2.51	0.46
4:R:1003:AMP:H8	4:R:1003:AMP:C5'	2.29	0.46
1:R:51:PRO:O	1:R:55:ARG:HB2	2.15	0.46
1:A:281:ARG:HH11	1:A:281:ARG:CG	2.26	0.46
1:A:26:PHE:HA	1:A:29:LEU:HB2	1.98	0.46
1:C:29:LEU:HA	1:C:29:LEU:HD23	1.84	0.46
1:D:38:CYS:SG	1:D:80:GLN:HB2	2.57	0.46
1:F:106:THR:O	1:F:107:GLN:C	2.53	0.46
1:G:197:ASP:C	1:G:199:ASN:N	2.69	0.46
1:G:197:ASP:C	1:G:199:ASN:H	2.20	0.46
1:H:101:GLU:CD	1:H:160:ARG:HH22	2.18	0.46
1:M:210:ALA:CB	1:M:277:ILE:CD1	2.80	0.46
1:N:20:ILE:HD13	1:N:247:THR:OG1	2.16	0.46
1:N:26:PHE:O	1:N:30:GLN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:230:TYR:CD2	1:P:253:ILE:CD1	2.99	0.46
1:R:184:MSE:HE3	1:R:192:LYS:CB	2.46	0.46
1:R:257:GLU:O	1:R:260:TYR:C	2.54	0.46
1:A:242:LEU:O	1:A:246:SER:HB3	2.16	0.45
1:B:59:ARG:NH1	1:B:59:ARG:CG	2.79	0.45
1:N:185:SER:HB3	1:N:188:ASP:O	2.16	0.45
1:O:306:LYS:HG2	1:O:309:ARG:NH2	2.31	0.45
1:R:319:GLU:HB3	1:R:324:LEU:HB2	1.97	0.45
1:C:79:ILE:HB	1:C:82:GLU:HG3	1.97	0.45
1:E:126:PRO:N	1:E:127:PRO:CD	2.79	0.45
1:E:63:ALA:CB	1:E:291:MSE:SE	3.14	0.45
1:F:205:THR:HG22	1:F:207:LEU:H	1.66	0.45
1:F:245:TYR:CE1	1:F:256:LEU:HD21	2.51	0.45
1:F:245:TYR:CD1	1:F:256:LEU:HD11	2.51	0.45
1:G:169:PHE:HZ	1:G:318:MSE:HE3	1.82	0.45
1:O:18:ASN:OD1	4:O:1003:AMP:O4'	2.34	0.45
1:O:4:ILE:HG22	1:O:142:PRO:HD3	1.98	0.45
1:P:143:VAL:CG2	1:P:151:ILE:CD1	2.94	0.45
1:P:251:GLN:HG3	1:P:256:LEU:HD21	1.99	0.45
1:Q:295:GLU:HG2	1:Q:298:ARG:NH1	2.32	0.45
1:A:213:ILE:HD11	1:A:280:LEU:HD12	1.98	0.45
1:A:42:GLN:HB2	1:A:80:GLN:OE1	2.16	0.45
3:B:1002:PO4:O4	4:B:1003:AMP:O1P	2.35	0.45
1:E:19:TYR:O	1:E:24:ARG:HB2	2.15	0.45
1:H:199:ASN:ND2	1:H:201:LYS:N	2.54	0.45
1:M:208:ASP:O	1:M:284:GLN:NE2	2.48	0.45
1:N:197:ASP:HA	1:N:198:PRO:HD3	1.79	0.45
1:O:205:THR:HG23	1:O:207:LEU:H	1.73	0.45
1:P:101:GLU:O	1:P:105:MSE:CG	2.60	0.45
1:P:5:PHE:CE1	1:P:132:ASP:HB3	2.52	0.45
1:P:249:SER:CB	1:P:251:GLN:HG2	2.46	0.45
1:Q:238:ILE:HD11	1:Q:265:TYR:CD1	2.52	0.45
1:R:281:ARG:N	1:R:282:PRO:CD	2.79	0.45
1:B:280:LEU:HA	1:B:283:ILE:HD12	1.97	0.45
1:C:192:LYS:HE3	4:C:1003:AMP:C5	2.51	0.45
1:C:213:ILE:O	1:C:217:ILE:HG13	2.16	0.45
1:B:120:ALA:HA	1:E:99:ILE:CG1	2.47	0.45
1:F:191:LYS:HB3	1:F:191:LYS:HE2	1.62	0.45
1:F:281:ARG:N	1:F:282:PRO:HD2	2.31	0.45
1:I:165:TYR:HB3	1:I:321:ALA:HB1	1.98	0.45
1:K:86:HIS:HE1	1:K:136:TYR:OH	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:57:ASN:OD1	1:L:60:ARG:NH2	2.50	0.45
1:Q:140:ILE:CD1	1:Q:175:ARG:CZ	2.95	0.45
1:Q:155:ARG:HD2	1:Q:172:PRO:O	2.15	0.45
1:R:126:PRO:N	1:R:127:PRO:CD	2.80	0.45
1:R:210:ALA:O	1:R:214:GLU:HG3	2.17	0.45
1:A:59:ARG:HH11	1:A:59:ARG:HG3	1.82	0.45
1:F:136:TYR:HB2	1:F:138:THR:HG22	1.97	0.45
1:F:179:VAL:CG1	1:F:180:GLY:O	2.64	0.45
1:G:208:ASP:O	1:G:284:GLN:NE2	2.46	0.45
1:M:290:TRP:C	1:M:292:GLU:N	2.69	0.45
1:O:125:TYR:CD2	1:O:126:PRO:HD3	2.51	0.45
1:O:150:HIS:O	1:O:154:THR:HG23	2.16	0.45
1:O:271:ASP:O	1:O:275:VAL:HG13	2.17	0.45
1:R:193:MSE:HE2	1:R:203:TYR:HA	1.98	0.45
1:R:246:SER:HA	1:R:251:GLN:HB2	1.98	0.45
1:B:241:LEU:HD12	1:B:241:LEU:HA	1.73	0.45
1:B:8:ILE:HD13	1:B:65:TYR:OH	2.16	0.45
1:D:136:TYR:HB2	1:D:138:THR:HG22	1.98	0.45
1:E:123:LEU:HG	1:E:123:LEU:O	2.17	0.45
1:I:105:MSE:HB2	1:I:105:MSE:HE2	1.78	0.45
1:M:164:ARG:NH2	1:P:48:TRP:CD2	2.84	0.45
1:O:74:GLN:HG3	1:O:74:GLN:O	2.17	0.45
1:P:238:ILE:O	1:P:242:LEU:HG	2.16	0.45
1:P:25:GLN:O	1:P:29:LEU:HG	2.17	0.45
1:Q:96:ILE:O	1:Q:160:ARG:NH2	2.49	0.45
1:R:24:ARG:NH1	1:R:247:THR:O	2.49	0.45
1:R:278:GLU:O	1:R:282:PRO:HD3	2.17	0.45
1:R:45:ILE:C	1:R:47:VAL:H	2.19	0.45
1:A:19:TYR:CE2	1:A:24:ARG:HD2	2.52	0.45
1:C:313:GLU:OE2	1:C:316:ARG:NH2	2.50	0.45
1:D:182:ARG:HD3	1:D:184:MSE:HE1	1.99	0.45
1:D:40:VAL:O	1:D:40:VAL:HG23	2.17	0.45
1:G:315:VAL:O	1:G:319:GLU:HG3	2.17	0.45
1:I:71:ASP:HA	1:I:72:PRO:HD2	1.84	0.45
1:L:122:LEU:HA	1:L:122:LEU:HD12	1.84	0.45
1:M:99:ILE:O	1:M:99:ILE:HG23	2.16	0.45
1:N:80:GLN:NE2	1:N:132:ASP:OD1	2.49	0.45
1:N:213:ILE:O	1:N:217:ILE:HG13	2.16	0.45
1:O:209:ASP:O	1:O:213:ILE:HG13	2.16	0.45
1:P:315:VAL:O	1:P:319:GLU:HG3	2.16	0.45
1:N:99:ILE:CG1	1:Q:118:VAL:O	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:192:LYS:HB3	1:Q:192:LYS:HE2	1.55	0.45
1:Q:24:ARG:HH11	1:Q:24:ARG:HG2	1.78	0.45
1:Q:278:GLU:OE1	1:Q:281:ARG:NH2	2.47	0.45
1:R:105:MSE:CE	1:R:150:HIS:HA	2.40	0.45
1:B:182:ARG:HA	4:B:1003:AMP:C2	2.52	0.45
1:D:19:TYR:O	1:D:24:ARG:CB	2.56	0.45
1:H:226:GLY:HA2	1:H:265:TYR:CZ	2.52	0.45
1:H:254:GLU:O	1:H:258:ARG:CG	2.52	0.45
1:H:49:GLN:O	1:K:164:ARG:NH2	2.45	0.45
1:I:123:LEU:O	1:I:123:LEU:HG	2.16	0.45
1:I:249:SER:HB2	1:I:251:GLN:CG	2.46	0.45
1:J:241:LEU:HA	1:J:241:LEU:HD12	1.71	0.45
1:M:78:PHE:N	1:M:78:PHE:CD1	2.85	0.45
1:R:275:VAL:HG13	1:R:276:VAL:H	1.82	0.45
1:E:151:ILE:HA	1:E:154:THR:HG23	1.98	0.45
1:I:260:TYR:HA	1:I:263:LYS:HG3	1.95	0.45
1:J:168:LEU:CD1	1:J:317:LYS:HD3	2.47	0.45
1:K:256:LEU:HD22	1:K:260:TYR:CD1	2.52	0.45
1:K:71:ASP:O	1:K:75:ALA:N	2.31	0.45
1:L:281:ARG:HB3	1:L:282:PRO:CD	2.46	0.45
1:M:120:ALA:HA	1:P:99:ILE:HD13	1.98	0.45
1:M:162:ASN:HA	1:M:166:GLY:O	2.17	0.45
1:P:181:ALA:CB	1:P:243:ASN:ND2	2.73	0.45
1:P:8:ILE:HB	1:P:61:LEU:HD21	1.98	0.45
1:P:99:ILE:H	1:P:99:ILE:HG12	1.29	0.45
1:R:155:ARG:O	1:R:159:GLU:HB2	2.17	0.45
1:R:225:GLU:CD	1:R:227:THR:CG2	2.81	0.45
1:R:302:GLU:O	1:R:306:LYS:HG3	2.17	0.45
1:A:200:PRO:O	1:A:216:LYS:NZ	2.50	0.45
1:A:25:GLN:CD	1:A:25:GLN:H	2.21	0.45
1:C:118:VAL:O	1:F:99:ILE:HG13	2.17	0.45
1:D:171:ILE:N	1:D:171:ILE:HD12	2.32	0.45
1:E:25:GLN:NE2	1:E:178:LYS:O	2.45	0.45
1:E:230:TYR:HB2	1:E:242:LEU:HD13	1.99	0.45
1:G:134:LEU:HB3	1:G:169:PHE:CE1	2.52	0.45
1:H:209:ASP:O	1:H:213:ILE:HG13	2.17	0.45
1:I:199:ASN:C	1:I:199:ASN:HD22	2.14	0.45
1:I:60:ARG:HG2	1:I:287:TYR:OH	2.17	0.45
1:J:162:ASN:O	1:J:166:GLY:N	2.50	0.45
1:L:59:ARG:NH1	1:L:59:ARG:CG	2.79	0.45
1:M:253:ILE:O	1:M:257:GLU:OE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:72:PRO:HG3	1:M:299:VAL:HG11	1.99	0.45
1:N:86:HIS:HD2	1:N:132:ASP:OD1	2.00	0.45
1:P:162:ASN:O	1:P:166:GLY:N	2.50	0.45
1:P:241:LEU:HB3	1:P:272:LEU:CD2	2.46	0.45
1:R:171:ILE:CD1	1:R:171:ILE:N	2.80	0.45
1:B:183:ILE:N	4:B:1003:AMP:N1	2.55	0.44
1:B:129:MSE:O	1:B:132:ASP:HB2	2.16	0.44
1:D:192:LYS:HB3	1:D:192:LYS:HE2	1.82	0.44
1:K:271:ASP:O	1:K:275:VAL:HG12	2.16	0.44
1:M:161:PHE:CD2	1:M:169:PHE:CD2	3.05	0.44
1:N:228:ILE:CD1	1:N:265:TYR:CD1	2.99	0.44
1:N:245:TYR:CD2	1:N:256:LEU:CD1	2.96	0.44
1:P:162:ASN:O	1:P:166:GLY:CA	2.65	0.44
1:P:245:TYR:CA	1:P:272:LEU:HD11	2.45	0.44
1:P:24:ARG:O	1:P:27:VAL:HG12	2.17	0.44
1:Q:26:PHE:HD2	1:Q:29:LEU:HD12	1.82	0.44
1:A:188:ASP:OD2	1:A:191:LYS:HB2	2.17	0.44
1:H:25:GLN:HG2	1:H:178:LYS:HB2	1.98	0.44
1:G:55:ARG:HD2	1:J:325:GLY:O	2.17	0.44
3:K:1002:PO4:O2	4:K:1003:AMP:O1P	2.36	0.44
1:M:124:THR:HG21	1:P:124:THR:HG21	1.98	0.44
1:O:119:SER:O	1:O:122:LEU:HB2	2.16	0.44
1:P:151:ILE:HG21	1:P:174:ALA:HB2	1.97	0.44
1:R:183:ILE:C	1:R:184:MSE:HG2	2.33	0.44
1:R:199:ASN:OD1	1:R:201:LYS:HB2	2.18	0.44
1:R:254:GLU:OE1	1:R:254:GLU:N	2.51	0.44
1:R:59:ARG:CG	1:R:59:ARG:NH1	2.81	0.44
1:R:83:VAL:HG13	1:R:308:ASN:ND2	2.32	0.44
1:B:8:ILE:CD1	1:B:65:TYR:CZ	3.00	0.44
1:C:228:ILE:O	1:C:229:ARG:HG2	2.18	0.44
1:G:211:LYS:HD2	1:K:1:MSE:HG3	2.00	0.44
1:H:197:ASP:HA	1:H:198:PRO:HD3	1.52	0.44
1:H:41:ASP:N	1:H:41:ASP:OD1	2.49	0.44
1:I:19:TYR:O	1:I:24:ARG:HB2	2.15	0.44
1:K:229:ARG:HG2	1:K:230:TYR:H	1.82	0.44
1:K:313:GLU:OE2	1:K:316:ARG:NH2	2.41	0.44
1:L:192:LYS:HE3	1:L:193:MSE:O	2.17	0.44
1:Q:140:ILE:HD12	1:Q:175:ARG:NE	2.33	0.44
1:R:287:TYR:CE2	1:R:291:MSE:HG3	2.52	0.44
1:A:277:ILE:O	1:A:281:ARG:HB2	2.16	0.44
1:B:20:ILE:HG22	1:B:20:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:HIS:CD2	1:C:132:ASP:OD1	2.67	0.44
1:C:22:ALA:O	1:C:26:PHE:HD2	1.97	0.44
1:C:260:TYR:HA	1:C:263:LYS:HG2	2.00	0.44
1:B:55:ARG:HD2	1:E:323:GLY:C	2.38	0.44
1:F:192:LYS:HB3	1:F:192:LYS:HE2	1.34	0.44
1:I:277:ILE:O	1:I:281:ARG:HB2	2.17	0.44
1:J:42:GLN:HB2	1:J:80:GLN:OE1	2.17	0.44
1:M:45:ILE:C	1:M:47:VAL:N	2.71	0.44
1:N:26:PHE:O	1:N:30:GLN:HB3	2.16	0.44
1:P:249:SER:OG	1:P:251:GLN:HG2	2.18	0.44
1:R:148:LYS:HB2	1:R:148:LYS:HE2	1.88	0.44
1:R:162:ASN:CA	1:R:166:GLY:O	2.64	0.44
1:R:19:TYR:CD2	1:R:24:ARG:HG3	2.53	0.44
1:F:184:MSE:CE	1:F:189:PRO:O	2.65	0.44
1:G:134:LEU:HB3	1:G:169:PHE:HD1	1.80	0.44
1:H:148:LYS:HE2	1:H:148:LYS:HB2	1.43	0.44
1:H:16:ILE:O	1:H:20:ILE:HB	2.18	0.44
1:H:253:ILE:O	1:H:257:GLU:HG3	2.17	0.44
1:K:8:ILE:HB	1:K:61:LEU:HD21	1.99	0.44
1:L:72:PRO:HB3	1:L:299:VAL:HG13	1.99	0.44
1:M:150:HIS:O	1:M:154:THR:CG2	2.65	0.44
1:M:48:TRP:O	1:M:49:GLN:HG2	2.18	0.44
1:O:195:LYS:HB3	1:O:195:LYS:HE3	1.57	0.44
1:O:209:ASP:OD1	1:O:209:ASP:N	2.50	0.44
1:P:94:GLN:HA	1:P:97:VAL:CG1	2.46	0.44
1:Q:182:ARG:O	1:Q:184:MSE:HE2	2.17	0.44
1:A:201:LYS:CB	1:A:201:LYS:NZ	2.81	0.44
1:B:5:PHE:HB2	1:B:138:THR:HG21	2.00	0.44
1:C:25:GLN:H	1:C:25:GLN:CD	2.21	0.44
1:C:50:ASP:HA	1:C:51:PRO:HD3	1.85	0.44
1:H:8:ILE:HB	1:H:61:LEU:HD21	2.00	0.44
1:H:96:ILE:HD13	1:H:96:ILE:N	2.32	0.44
1:I:119:SER:O	1:I:122:LEU:HB2	2.16	0.44
1:I:130:ALA:HB1	1:I:154:THR:HB	1.99	0.44
1:I:297:ASP:OD2	1:L:326:ARG:NH1	2.39	0.44
1:I:29:LEU:HD11	1:I:177:PRO:HB2	1.99	0.44
1:K:287:TYR:CZ	1:K:291:MSE:HE3	2.51	0.44
1:K:71:ASP:HA	1:K:72:PRO:HD2	1.81	0.44
1:L:5:PHE:CB	1:L:138:THR:HG21	2.43	0.44
1:N:199:ASN:HD22	1:N:201:LYS:H	1.65	0.44
1:N:40:VAL:HG23	1:N:40:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:59:ARG:CG	1:N:59:ARG:NH1	2.79	0.44
1:Q:43:HIS:HE1	1:Q:132:ASP:OD2	1.99	0.44
1:Q:151:ILE:HG21	1:Q:174:ALA:HB2	2.00	0.44
1:Q:215:LYS:HE2	1:Q:215:LYS:HB3	1.64	0.44
1:R:168:LEU:HA	1:R:168:LEU:HD23	1.82	0.44
1:R:56:GLN:HG2	1:R:60:ARG:NH2	2.32	0.44
1:A:125:TYR:N	1:A:126:PRO:HD2	2.32	0.44
1:B:118:VAL:HG12	1:E:99:ILE:CD1	2.48	0.44
1:E:141:VAL:HG12	1:E:143:VAL:HG13	2.00	0.44
1:L:182:ARG:HG2	1:L:184:MSE:HE1	2.00	0.44
1:L:313:GLU:HA	1:L:313:GLU:OE1	2.17	0.44
1:M:199:ASN:C	1:M:199:ASN:HD22	2.20	0.44
1:M:276:VAL:O	1:M:278:GLU:N	2.51	0.44
1:M:213:ILE:CD1	1:M:280:LEU:HD12	2.47	0.44
1:N:260:TYR:HA	1:N:263:LYS:HE3	2.00	0.44
1:O:205:THR:CG2	1:O:206:LEU:N	2.80	0.44
1:O:26:PHE:HA	1:O:29:LEU:HB2	1.99	0.44
1:P:218:LYS:HG2	1:P:219:SER:N	2.32	0.44
1:Q:199:ASN:HD22	1:Q:201:LYS:H	1.62	0.44
1:R:160:ARG:HG3	1:R:160:ARG:O	2.17	0.44
1:R:296:LEU:HA	1:R:296:LEU:HD12	1.71	0.44
1:A:130:ALA:HB1	1:A:154:THR:HB	2.00	0.44
1:A:106:THR:N	1:A:149:GLN:OE1	2.45	0.44
1:A:272:LEU:HA	1:A:275:VAL:HG13	1.99	0.44
4:B:1003:AMP:H8	4:B:1003:AMP:C5'	2.30	0.44
1:D:313:GLU:OE1	1:D:313:GLU:HA	2.18	0.44
1:G:59:ARG:NH1	1:G:297:ASP:OD1	2.44	0.44
1:I:176:ILE:O	1:I:176:ILE:HG13	2.18	0.44
1:I:278:GLU:CD	1:I:281:ARG:NH2	2.71	0.44
1:J:162:ASN:O	1:J:166:GLY:HA2	2.17	0.44
1:K:199:ASN:HA	1:K:200:PRO:HD2	1.80	0.44
1:K:230:TYR:CE1	1:K:239:SER:HB2	2.53	0.44
1:L:27:VAL:HG12	1:L:27:VAL:O	2.18	0.44
1:M:141:VAL:HA	1:M:142:PRO:HD2	1.90	0.44
1:O:183:ILE:HB	4:O:1003:AMP:N1	2.32	0.44
1:O:194:SER:O	1:O:197:ASP:HB2	2.18	0.44
1:B:238:ILE:HA	1:B:238:ILE:HD13	1.71	0.44
1:B:2:LYS:CD	1:B:2:LYS:N	2.80	0.44
1:B:40:VAL:HA	1:B:80:GLN:OE1	2.18	0.44
1:D:188:ASP:C	1:D:188:ASP:OD1	2.57	0.44
1:E:190:THR:CG2	1:O:48:TRP:CE3	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:THR:O	1:E:216:LYS:HB2	2.18	0.44
1:F:25:GLN:CD	1:F:25:GLN:N	2.72	0.44
4:I:1003:AMP:C8	4:I:1003:AMP:C5'	3.01	0.44
1:L:241:LEU:HA	1:L:241:LEU:HD12	1.78	0.44
1:M:205:THR:CG2	1:M:206:LEU:N	2.81	0.44
1:M:25:GLN:NE2	1:M:178:LYS:O	2.50	0.44
1:N:251:GLN:OE1	1:N:259:GLN:NE2	2.47	0.44
1:N:228:ILE:HD13	1:N:265:TYR:CE1	2.52	0.44
1:Q:168:LEU:HD21	1:Q:317:LYS:HB3	2.00	0.44
1:Q:258:ARG:O	1:Q:261:GLU:HB3	2.17	0.44
1:R:76:THR:HG23	1:R:306:LYS:HE3	2.00	0.44
1:O:91:TRP:NE1	1:R:42:GLN:HB3	2.33	0.44
1:R:60:ARG:HG3	1:R:287:TYR:OH	2.18	0.44
1:A:225:GLU:O	1:A:227:THR:HG23	2.18	0.43
1:B:96:ILE:HD11	1:B:157:LEU:HD22	2.00	0.43
1:E:105:MSE:CA	1:E:105:MSE:CE	2.96	0.43
1:H:146:ASP:OD1	1:H:146:ASP:N	2.49	0.43
1:I:147:GLN:O	1:I:150:HIS:HB2	2.18	0.43
1:L:295:GLU:O	1:L:299:VAL:HG23	2.18	0.43
1:M:175:ARG:O	1:M:177:PRO:HD3	2.18	0.43
1:N:245:TYR:CD2	1:N:256:LEU:HD22	2.51	0.43
1:P:129:MSE:O	1:P:129:MSE:HG3	2.16	0.43
1:Q:157:LEU:HD21	1:Q:160:ARG:NH2	2.32	0.43
1:Q:281:ARG:N	1:Q:282:PRO:HD2	2.33	0.43
1:R:78:PHE:N	1:R:78:PHE:CD1	2.86	0.43
1:B:230:TYR:CD1	1:B:239:SER:CB	3.01	0.43
1:D:213:ILE:O	1:D:217:ILE:HG12	2.18	0.43
1:F:164:ARG:HE	1:F:164:ARG:HB2	1.60	0.43
1:G:17:GLY:HA2	1:G:183:ILE:HG13	2.00	0.43
1:H:158:ALA:CB	1:H:171:ILE:CD1	2.97	0.43
1:H:318:MSE:O	1:H:322:MSE:HG3	2.17	0.43
1:I:22:ALA:O	1:I:26:PHE:CD2	2.70	0.43
1:L:59:ARG:HH11	1:L:59:ARG:HG3	1.82	0.43
1:N:122:LEU:HA	1:N:122:LEU:HD13	1.71	0.43
1:O:126:PRO:CB	1:O:127:PRO:CD	2.96	0.43
1:P:216:LYS:CG	1:P:216:LYS:O	2.66	0.43
1:Q:238:ILE:HD11	1:Q:265:TYR:CE1	2.54	0.43
1:Q:281:ARG:HB3	1:Q:282:PRO:CD	2.48	0.43
1:R:228:ILE:CG1	1:R:260:TYR:HB3	2.47	0.43
1:B:254:GLU:O	1:B:258:ARG:CG	2.65	0.43
1:B:308:ASN:O	1:B:312:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:PRO:N	1:C:127:PRO:HD2	2.33	0.43
1:C:199:ASN:HD22	1:C:200:PRO:N	2.16	0.43
1:C:201:LYS:HE3	1:C:201:LYS:HB3	1.57	0.43
1:D:168:LEU:CD2	1:D:314:MSE:SE	3.16	0.43
1:E:126:PRO:CB	1:E:127:PRO:CD	2.96	0.43
1:G:206:LEU:HD23	1:G:206:LEU:HA	1.84	0.43
1:I:193:MSE:HB3	4:I:1003:AMP:N6	2.33	0.43
1:J:176:ILE:HB	1:J:179:VAL:HG13	2.00	0.43
1:O:155:ARG:O	1:O:159:GLU:HB2	2.18	0.43
1:O:96:ILE:O	1:O:160:ARG:NH1	2.50	0.43
1:Q:106:THR:HG22	1:Q:107:GLN:N	2.33	0.43
1:Q:193:MSE:HE2	1:Q:203:TYR:HA	2.00	0.43
1:A:136:TYR:HB2	1:A:138:THR:HG22	2.00	0.43
1:C:188:ASP:HA	1:C:189:PRO:HD2	1.85	0.43
1:C:199:ASN:HD22	1:C:200:PRO:CD	2.31	0.43
1:E:107:GLN:H	1:E:107:GLN:HE21	1.65	0.43
1:F:176:ILE:HA	1:F:177:PRO:HD3	1.85	0.43
1:H:186:LEU:HB2	1:H:201:LYS:O	2.19	0.43
1:J:281:ARG:HB3	1:J:282:PRO:HD3	2.00	0.43
1:K:27:VAL:O	1:K:30:GLN:HG2	2.19	0.43
1:L:210:ALA:HB1	1:L:277:ILE:HD13	2.00	0.43
1:L:20:ILE:HD13	1:L:247:THR:OG1	2.18	0.43
1:M:147:GLN:O	1:M:150:HIS:HB2	2.18	0.43
1:N:147:GLN:OE1	1:N:150:HIS:HD2	2.01	0.43
1:P:253:ILE:O	1:P:257:GLU:HB2	2.17	0.43
1:P:217:ILE:HD11	1:P:276:VAL:HG21	2.00	0.43
1:M:211:LYS:HB2	1:Q:1:MSE:HG3	2.00	0.43
1:R:71:ASP:HA	1:R:72:PRO:HD2	1.81	0.43
1:R:94:GLN:HA	1:R:97:VAL:CG1	2.48	0.43
1:B:200:PRO:HA	1:B:203:TYR:CZ	2.54	0.43
1:C:241:LEU:HB3	1:C:268:PHE:HE2	1.84	0.43
1:E:19:TYR:O	1:E:24:ARG:HB3	2.19	0.43
1:F:20:ILE:HD13	1:F:247:THR:OG1	2.19	0.43
1:G:197:ASP:HA	1:G:198:PRO:HD2	1.73	0.43
1:G:213:ILE:HD11	1:G:280:LEU:HD12	2.01	0.43
1:H:150:HIS:O	1:H:154:THR:CG2	2.65	0.43
1:J:126:PRO:CB	1:J:127:PRO:HD3	2.44	0.43
1:N:278:GLU:OE1	1:N:278:GLU:HA	2.18	0.43
4:P:1003:AMP:H5'2	4:P:1003:AMP:N9	2.33	0.43
1:P:197:ASP:HA	1:P:198:PRO:HD2	1.81	0.43
1:P:245:TYR:CD1	1:P:272:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:HIS:O	1:C:56:GLN:HB2	2.19	0.43
1:F:136:TYR:HD1	1:F:310:VAL:HG11	1.84	0.43
1:H:195:LYS:HG2	3:H:1002:PO4:P	2.59	0.43
1:I:160:ARG:HB2	1:I:160:ARG:HE	1.73	0.43
1:I:25:GLN:OE1	1:I:176:ILE:HD11	2.19	0.43
1:I:42:GLN:HB2	1:I:80:GLN:OE1	2.19	0.43
1:J:185:SER:CA	1:J:188:ASP:O	2.66	0.43
1:K:239:SER:O	1:K:240:ASN:C	2.56	0.43
1:K:245:TYR:O	1:K:249:SER:N	2.52	0.43
1:K:258:ARG:CA	1:K:261:GLU:HG3	2.48	0.43
1:K:96:ILE:O	1:K:160:ARG:NH1	2.48	0.43
1:L:243:ASN:OD1	1:L:253:ILE:HD11	2.19	0.43
1:M:23:LEU:HD21	1:M:65:TYR:OH	2.18	0.43
1:M:64:LEU:HD21	1:M:287:TYR:CE1	2.54	0.43
1:N:295:GLU:O	1:N:299:VAL:HG23	2.19	0.43
1:P:228:ILE:CD1	1:P:228:ILE:N	2.82	0.43
1:Q:281:ARG:CG	1:Q:281:ARG:NH1	2.79	0.43
1:Q:59:ARG:CZ	1:Q:296:LEU:HD23	2.48	0.43
1:A:55:ARG:HD2	1:D:325:GLY:O	2.18	0.43
1:F:205:THR:HG22	1:F:208:ASP:N	2.34	0.43
1:G:151:ILE:HA	1:G:154:THR:HG23	2.01	0.43
1:I:89:ALA:HB2	1:I:135:LEU:HD21	1.99	0.43
1:J:125:TYR:CG	1:J:126:PRO:HD3	2.54	0.43
1:M:106:THR:H	1:M:149:GLN:HE22	1.67	0.43
1:O:19:TYR:HE1	1:O:68:VAL:CG1	2.25	0.43
1:P:218:LYS:CG	1:P:219:SER:N	2.80	0.43
1:P:298:ARG:HH11	1:P:298:ARG:HG3	1.82	0.43
1:R:29:LEU:HD22	1:R:33:TYR:HE1	1.82	0.43
1:A:59:ARG:NH1	1:A:59:ARG:CG	2.81	0.43
1:C:238:ILE:HA	1:C:238:ILE:HD13	1.77	0.43
1:F:32:GLU:HG2	1:F:32:GLU:H	1.64	0.43
1:H:86:HIS:CD2	1:H:132:ASP:HA	2.54	0.43
1:K:206:LEU:N	1:K:206:LEU:HD23	2.33	0.43
1:M:168:LEU:O	1:M:168:LEU:HD12	2.18	0.43
1:M:320:GLN:HE21	1:M:320:GLN:HB2	1.56	0.43
1:O:289:HIS:C	1:O:289:HIS:ND1	2.71	0.43
1:P:181:ALA:CB	1:P:243:ASN:HD22	2.11	0.43
1:B:32:GLU:HG2	1:B:33:TYR:CE1	2.54	0.43
1:B:8:ILE:CD1	1:B:65:TYR:OH	2.67	0.43
1:H:80:GLN:NE2	1:H:132:ASP:OD1	2.52	0.43
1:K:239:SER:HA	1:K:242:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:320:GLN:HA	1:K:55:ARG:NH2	2.34	0.43
1:L:238:ILE:HD13	1:L:238:ILE:HA	1.72	0.43
1:M:118:VAL:HB	1:P:99:ILE:CG1	2.48	0.43
1:M:92:MSE:O	1:M:96:ILE:HG23	2.18	0.43
1:O:192:LYS:HG2	4:O:1003:AMP:N6	2.34	0.43
1:P:142:PRO:CA	1:P:175:ARG:O	2.40	0.43
1:P:249:SER:HB2	1:P:251:GLN:HG2	1.99	0.43
1:R:213:ILE:O	1:R:217:ILE:HG13	2.19	0.43
1:C:41:ASP:N	1:C:41:ASP:OD1	2.52	0.43
1:D:210:ALA:HA	1:D:213:ILE:HD12	2.01	0.43
1:D:23:LEU:CD1	1:D:65:TYR:CE2	3.01	0.43
1:O:122:LEU:HA	1:O:122:LEU:HD12	1.87	0.43
4:P:1003:AMP:C5'	4:P:1003:AMP:N9	2.79	0.43
1:Q:40:VAL:HG23	1:Q:40:VAL:O	2.19	0.43
1:Q:94:GLN:HG2	1:Q:127:PRO:HG2	2.01	0.43
1:R:161:PHE:CD2	1:R:161:PHE:C	2.92	0.43
1:R:225:GLU:OE2	1:R:225:GLU:O	2.37	0.43
1:D:197:ASP:HA	1:D:198:PRO:HD3	1.83	0.42
1:E:106:THR:H	1:E:149:GLN:NE2	2.16	0.42
1:E:186:LEU:HD12	1:E:201:LYS:O	2.19	0.42
1:E:238:ILE:O	1:E:241:LEU:HD23	2.19	0.42
1:F:230:TYR:CD2	1:F:239:SER:HB3	2.54	0.42
1:G:71:ASP:HA	1:G:72:PRO:HD2	1.77	0.42
1:I:274:GLN:O	1:I:278:GLU:HB2	2.19	0.42
1:K:188:ASP:HA	1:K:189:PRO:HD2	1.84	0.42
1:M:293:SER:OG	1:M:294:GLU:N	2.52	0.42
1:P:160:ARG:HB2	1:P:160:ARG:HE	1.59	0.42
1:P:267:VAL:CG2	1:P:268:PHE:N	2.82	0.42
1:M:55:ARG:HH22	1:P:320:GLN:HA	1.84	0.42
1:N:55:ARG:HD2	1:Q:325:GLY:O	2.19	0.42
1:A:134:LEU:HB3	1:A:169:PHE:HD1	1.74	0.42
1:A:56:GLN:O	1:A:60:ARG:HG3	2.19	0.42
1:C:42:GLN:HB3	1:F:91:TRP:NE1	2.34	0.42
1:D:281:ARG:N	1:D:282:PRO:HD2	2.34	0.42
1:F:199:ASN:HD21	1:F:201:LYS:HB2	1.83	0.42
1:F:23:LEU:HD21	1:F:68:VAL:HG11	2.00	0.42
1:F:245:TYR:HH	1:F:260:TYR:HH	1.62	0.42
1:F:301:ASP:O	1:F:305:GLU:HB2	2.19	0.42
1:F:39:ILE:HG23	1:F:61:LEU:HD23	2.00	0.42
1:F:40:VAL:HG23	1:F:40:VAL:O	2.19	0.42
1:G:4:ILE:HD12	1:G:33:TYR:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:GLN:HG2	1:H:178:LYS:CB	2.49	0.42
1:I:125:TYR:CD2	1:I:126:PRO:HD3	2.53	0.42
1:J:197:ASP:HA	1:J:198:PRO:HD3	1.88	0.42
1:G:55:ARG:NH2	1:J:320:GLN:HA	2.33	0.42
1:K:165:TYR:CE1	1:K:321:ALA:O	2.72	0.42
1:K:134:LEU:CB	1:K:169:PHE:HE1	2.28	0.42
1:K:65:TYR:O	1:K:70:ILE:HB	2.20	0.42
4:L:1003:AMP:H8	4:L:1003:AMP:O1P	2.00	0.42
1:L:254:GLU:HA	1:L:257:GLU:OE1	2.19	0.42
1:M:185:SER:OG	1:M:187:VAL:CG2	2.63	0.42
1:N:59:ARG:HH11	1:N:59:ARG:HG3	1.84	0.42
1:B:289:HIS:C	1:B:289:HIS:ND1	2.72	0.42
1:C:71:ASP:HA	1:C:72:PRO:HD2	1.79	0.42
1:E:253:ILE:HA	1:E:256:LEU:HB3	2.01	0.42
1:E:287:TYR:C	1:E:289:HIS:H	2.23	0.42
1:G:101:GLU:CD	1:G:160:ARG:NH2	2.70	0.42
1:I:192:LYS:HG2	1:I:193:MSE:N	2.35	0.42
1:I:263:LYS:N	1:I:263:LYS:CD	2.80	0.42
1:O:280:LEU:O	1:O:284:GLN:HB2	2.20	0.42
1:P:39:ILE:HG12	1:P:61:LEU:HD23	2.00	0.42
1:R:106:THR:CB	1:R:149:GLN:HE22	2.32	0.42
1:R:214:GLU:CB	1:R:273:ALA:HB1	2.47	0.42
1:R:99:ILE:HG12	1:R:99:ILE:H	1.30	0.42
1:A:281:ARG:HB3	1:A:282:PRO:HD3	2.01	0.42
1:B:238:ILE:HG13	1:B:265:TYR:HE1	1.83	0.42
1:E:267:VAL:CG1	1:E:268:PHE:N	2.80	0.42
1:F:203:TYR:O	1:F:216:LYS:NZ	2.43	0.42
1:J:177:PRO:C	1:J:178:LYS:HG2	2.39	0.42
1:J:212:THR:CG2	1:J:216:LYS:HE3	2.49	0.42
1:J:319:GLU:HB3	1:J:324:LEU:HB2	2.02	0.42
1:M:203:TYR:O	1:M:216:LYS:NZ	2.46	0.42
1:N:281:ARG:N	1:N:282:PRO:HD2	2.35	0.42
1:O:182:ARG:HB3	1:O:184:MSE:HE1	2.01	0.42
1:Q:129:MSE:O	1:Q:132:ASP:HB2	2.20	0.42
1:Q:188:ASP:HA	1:Q:189:PRO:HD2	1.77	0.42
1:O:91:TRP:CZ2	1:R:128:LEU:HD22	2.55	0.42
1:R:215:LYS:HD2	1:R:215:LYS:C	2.39	0.42
4:B:1003:AMP:C8	4:B:1003:AMP:C5'	2.97	0.42
1:C:124:THR:HG21	1:F:124:THR:HG21	2.01	0.42
1:C:56:GLN:HB3	1:C:60:ARG:NH2	2.35	0.42
1:D:126:PRO:CB	1:D:127:PRO:HD3	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:THR:CG2	1:D:94:GLN:HE22	2.23	0.42
1:E:26:PHE:CD1	1:E:37:PHE:CE2	3.06	0.42
1:E:279:THR:O	1:E:282:PRO:HG2	2.19	0.42
1:H:245:TYR:CD2	1:H:268:PHE:CE1	3.07	0.42
1:H:294:GLU:H	1:H:294:GLU:HG3	1.48	0.42
1:H:325:GLY:O	1:K:55:ARG:HD2	2.19	0.42
1:I:176:ILE:C	1:I:176:ILE:HD12	2.40	0.42
1:J:281:ARG:HB3	1:J:282:PRO:CD	2.50	0.42
1:K:129:MSE:O	1:K:132:ASP:HB2	2.19	0.42
1:L:281:ARG:HB3	1:L:282:PRO:HD3	2.00	0.42
1:M:199:ASN:CG	1:M:201:LYS:HG2	2.34	0.42
1:M:99:ILE:CG2	1:M:99:ILE:O	2.60	0.42
1:N:315:VAL:O	1:N:319:GLU:HG3	2.19	0.42
1:O:248:LEU:HD23	1:O:248:LEU:HA	1.56	0.42
1:O:326:ARG:HH12	1:R:300:LEU:CB	2.30	0.42
1:O:94:GLN:O	1:O:97:VAL:HG12	2.19	0.42
1:P:15:THR:HB	1:P:193:MSE:SE	2.70	0.42
1:P:253:ILE:O	1:P:257:GLU:CB	2.68	0.42
1:P:53:GLU:O	1:P:57:ASN:HB2	2.18	0.42
1:R:185:SER:OG	1:R:187:VAL:HG22	2.20	0.42
1:B:320:GLN:HE22	1:E:55:ARG:HH21	1.66	0.42
1:D:229:ARG:HB3	1:D:229:ARG:HE	1.67	0.42
1:E:26:PHE:HA	1:E:29:LEU:HB2	2.01	0.42
1:F:256:LEU:O	1:F:260:TYR:HD2	2.02	0.42
1:H:228:ILE:O	1:H:228:ILE:HG22	2.19	0.42
1:L:318:MSE:O	1:L:322:MSE:HG3	2.19	0.42
1:M:135:LEU:HD13	1:M:311:ALA:HB1	2.02	0.42
1:M:44:ALA:O	1:M:49:GLN:NE2	2.43	0.42
1:O:213:ILE:HG23	1:O:276:VAL:HG11	2.01	0.42
1:O:251:GLN:HB3	1:O:255:GLU:CD	2.40	0.42
1:P:168:LEU:HD23	1:P:168:LEU:HA	1.77	0.42
1:P:22:ALA:O	1:P:26:PHE:CD2	2.73	0.42
1:P:85:ALA:HB1	1:P:315:VAL:CG2	2.50	0.42
1:R:185:SER:OG	1:R:202:ALA:CB	2.55	0.42
1:C:126:PRO:CB	1:C:127:PRO:CD	2.95	0.42
1:E:9:GLN:HE21	1:E:9:GLN:CA	2.32	0.42
1:F:5:PHE:O	1:F:142:PRO:HD2	2.19	0.42
1:H:184:MSE:O	1:H:193:MSE:HE3	2.20	0.42
1:H:200:PRO:HA	1:H:203:TYR:CE2	2.55	0.42
1:I:124:THR:CB	1:L:94:GLN:NE2	2.82	0.42
1:K:268:PHE:CD1	1:K:268:PHE:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:214:GLU:O	1:L:218:LYS:HG3	2.19	0.42
1:M:5:PHE:HB2	1:M:138:THR:CG2	2.44	0.42
1:N:125:TYR:CG	1:N:126:PRO:HD3	2.55	0.42
1:O:225:GLU:O	1:O:227:THR:HG23	2.19	0.42
1:P:3:THR:HG22	1:P:138:THR:HB	2.00	0.42
1:R:106:THR:N	1:R:149:GLN:HE22	2.14	0.42
1:R:205:THR:O	1:R:207:LEU:N	2.53	0.42
1:R:272:LEU:CD1	1:R:272:LEU:C	2.84	0.42
1:A:71:ASP:HB3	1:A:74:GLN:CB	2.50	0.42
1:C:281:ARG:N	1:C:282:PRO:HD2	2.33	0.42
1:C:28:GLU:HA	1:C:31:HIS:CD2	2.44	0.42
1:E:29:LEU:CD1	1:E:177:PRO:HB2	2.48	0.42
1:E:66:LEU:HD13	1:E:290:TRP:CD2	2.55	0.42
1:G:285:GLU:OE1	1:G:285:GLU:HA	2.19	0.42
1:J:38:CYS:SG	1:J:80:GLN:HB2	2.60	0.42
1:K:258:ARG:O	1:K:261:GLU:CG	2.59	0.42
1:K:261:GLU:C	1:K:263:LYS:HD2	2.38	0.42
1:M:141:VAL:HG12	1:M:143:VAL:HG13	2.01	0.42
1:P:230:TYR:CD2	1:P:253:ILE:HD13	2.55	0.42
1:R:209:ASP:O	1:R:213:ILE:HG13	2.20	0.42
1:A:199:ASN:HA	1:A:200:PRO:HD3	1.83	0.42
1:A:29:LEU:HD11	1:A:177:PRO:HB2	2.01	0.42
1:A:165:TYR:HB3	1:A:321:ALA:HB1	2.01	0.42
1:E:106:THR:H	1:E:149:GLN:HE22	1.68	0.42
1:G:265:TYR:O	1:G:269:LYS:HG3	2.20	0.42
1:H:211:LYS:O	1:H:215:LYS:HG2	2.19	0.42
1:I:207:LEU:HD23	1:I:207:LEU:HA	1.89	0.42
1:L:15:THR:N	1:L:18:ASN:HD22	2.18	0.42
1:L:65:TYR:O	1:L:70:ILE:HB	2.20	0.42
1:M:210:ALA:HB2	1:M:277:ILE:HG23	2.02	0.42
1:O:201:LYS:HA	1:O:216:LYS:HE2	2.01	0.42
1:O:281:ARG:N	1:O:282:PRO:CD	2.83	0.42
1:P:97:VAL:HG21	1:P:102:LEU:HD21	2.01	0.42
1:R:281:ARG:HB3	1:R:282:PRO:CD	2.49	0.42
1:R:291:MSE:C	1:R:291:MSE:HE3	2.40	0.42
1:C:16:ILE:O	1:C:20:ILE:HG13	2.20	0.42
1:D:182:ARG:HG2	1:D:184:MSE:CE	2.49	0.42
1:E:3:THR:HG22	1:E:138:THR:HB	2.01	0.42
1:G:126:PRO:CB	1:G:127:PRO:CD	2.97	0.42
1:H:94:GLN:HG3	1:H:127:PRO:HG2	2.02	0.42
1:H:199:ASN:HD21	1:H:201:LYS:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:ASP:OD2	1:H:81:SER:HB3	2.19	0.42
1:I:92:MSE:O	1:I:96:ILE:HG23	2.20	0.42
1:J:130:ALA:HB1	1:J:154:THR:HB	2.00	0.42
1:J:304:ALA:O	1:J:308:ASN:HB2	2.19	0.42
1:K:56:GLN:NE2	1:K:56:GLN:CA	2.78	0.42
1:L:86:HIS:CD2	1:L:132:ASP:OD1	2.71	0.42
1:L:24:ARG:CG	1:L:24:ARG:HH11	2.33	0.42
1:M:276:VAL:O	1:M:279:THR:N	2.48	0.42
1:N:238:ILE:HD11	1:N:265:TYR:CD1	2.55	0.42
1:O:129:MSE:O	1:O:133:ILE:HD12	2.20	0.42
1:D:305:GLU:HB3	1:O:267:VAL:CG2	2.50	0.42
1:P:189:PRO:C	1:P:191:LYS:H	2.24	0.42
4:Q:1003:AMP:O5'	4:Q:1003:AMP:H8	2.03	0.42
1:Q:148:LYS:HE3	1:Q:148:LYS:HB3	1.31	0.42
1:C:197:ASP:HA	1:C:198:PRO:HD3	1.83	0.41
1:E:197:ASP:HB3	1:E:202:ALA:CB	2.49	0.41
1:E:290:TRP:CZ3	1:E:299:VAL:HG21	2.55	0.41
1:F:228:ILE:H	1:F:228:ILE:HG12	1.59	0.41
1:G:101:GLU:O	1:G:105:MSE:HE3	2.20	0.41
1:G:65:TYR:O	1:G:70:ILE:HB	2.20	0.41
1:H:249:SER:OG	1:H:251:GLN:CG	2.68	0.41
1:M:249:SER:OG	1:M:251:GLN:HG3	2.21	0.41
1:M:290:TRP:C	1:M:292:GLU:H	2.23	0.41
1:P:245:TYR:HA	1:P:272:LEU:HD11	1.98	0.41
1:R:228:ILE:CG2	1:R:260:TYR:O	2.68	0.41
1:A:189:PRO:HB3	1:A:237:GLY:HA2	2.01	0.41
1:A:205:THR:CG2	1:A:206:LEU:N	2.82	0.41
1:C:211:LYS:CE	1:C:215:LYS:HD2	2.51	0.41
4:D:1003:AMP:H2'	4:D:1003:AMP:O2P	2.20	0.41
1:E:286:ARG:O	1:E:289:HIS:N	2.53	0.41
1:E:29:LEU:HA	1:E:29:LEU:HD23	1.86	0.41
1:F:319:GLU:HB3	1:F:324:LEU:HB2	2.02	0.41
1:J:165:TYR:HB3	1:J:321:ALA:HB1	2.02	0.41
1:J:281:ARG:N	1:J:282:PRO:HD2	2.34	0.41
1:L:278:GLU:HA	1:L:278:GLU:OE1	2.19	0.41
1:M:141:VAL:O	1:M:174:ALA:CA	2.64	0.41
1:P:94:GLN:CA	1:P:97:VAL:HG12	2.49	0.41
1:B:200:PRO:O	1:B:216:LYS:HE2	2.20	0.41
1:B:86:HIS:HD2	1:B:132:ASP:HA	1.84	0.41
1:E:218:LYS:HB2	1:E:218:LYS:HE3	1.83	0.41
1:F:105:MSE:CA	1:F:105:MSE:CE	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:PRO:HB2	1:F:127:PRO:HD3	2.02	0.41
1:F:134:LEU:CB	1:F:169:PHE:CE1	2.97	0.41
1:H:126:PRO:CB	1:H:127:PRO:CD	2.96	0.41
1:J:177:PRO:C	1:J:178:LYS:CG	2.88	0.41
1:K:322:MSE:HE2	1:K:322:MSE:HB3	1.88	0.41
1:L:182:ARG:O	1:L:184:MSE:HE2	2.20	0.41
1:M:130:ALA:CB	1:M:154:THR:HB	2.50	0.41
1:M:64:LEU:CD2	1:M:287:TYR:CE1	3.02	0.41
1:N:118:VAL:HB	1:Q:99:ILE:HG13	2.01	0.41
1:P:192:LYS:HZ3	4:P:1003:AMP:H5'1	1.85	0.41
1:P:125:TYR:N	1:P:126:PRO:HD3	2.29	0.41
1:P:105:MSE:HE1	1:P:149:GLN:O	2.19	0.41
1:Q:241:LEU:HB3	1:Q:268:PHE:HE2	1.85	0.41
1:N:55:ARG:HH21	1:Q:320:GLN:NE2	2.18	0.41
1:Q:93:LEU:HD23	1:Q:96:ILE:HD13	2.02	0.41
1:R:251:GLN:HB3	1:R:256:LEU:HD12	2.01	0.41
1:R:96:ILE:O	1:R:160:ARG:NH1	2.51	0.41
1:D:86:HIS:CE1	1:D:136:TYR:OH	2.74	0.41
1:D:28:GLU:HG2	1:D:28:GLU:H	1.79	0.41
1:H:29:LEU:HD11	1:H:177:PRO:HB2	1.99	0.41
1:I:147:GLN:OE1	1:I:150:HIS:HD2	2.03	0.41
1:J:86:HIS:HE1	1:J:136:TYR:OH	2.04	0.41
1:J:192:LYS:HE3	1:J:192:LYS:HB3	1.33	0.41
1:J:59:ARG:HH11	1:J:59:ARG:HG3	1.85	0.41
1:K:187:VAL:HG13	1:K:202:ALA:HA	2.02	0.41
1:K:78:PHE:N	1:K:78:PHE:CD1	2.88	0.41
1:L:119:SER:O	1:L:122:LEU:HB2	2.21	0.41
1:M:306:LYS:O	1:M:310:VAL:HG23	2.21	0.41
1:N:152:GLU:HA	1:N:152:GLU:OE1	2.20	0.41
1:O:313:GLU:OE2	1:O:317:LYS:HE3	2.21	0.41
1:P:216:LYS:O	1:P:216:LYS:HG3	2.21	0.41
1:R:282:PRO:HB2	1:R:286:ARG:HH21	1.85	0.41
1:D:123:LEU:HD23	1:D:124:THR:HG23	2.02	0.41
1:D:165:TYR:CD2	1:D:321:ALA:O	2.74	0.41
1:E:85:ALA:O	1:E:135:LEU:HD11	2.20	0.41
1:E:184:MSE:HA	1:E:192:LYS:HA	2.03	0.41
1:H:192:LYS:O	1:H:193:MSE:C	2.59	0.41
1:I:289:HIS:O	1:I:293:SER:HB2	2.21	0.41
1:J:34:ASN:HA	1:J:34:ASN:HD22	1.77	0.41
1:L:27:VAL:CG1	1:L:27:VAL:O	2.69	0.41
1:I:326:ARG:NH2	1:L:301:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:56:GLN:CD	1:M:60:ARG:NH2	2.74	0.41
1:P:76:THR:HG23	1:P:306:LYS:HE3	2.03	0.41
1:M:55:ARG:NH2	1:P:320:GLN:HA	2.36	0.41
1:R:213:ILE:HG21	1:R:277:ILE:HG13	2.02	0.41
1:A:122:LEU:HD13	1:A:122:LEU:HA	1.79	0.41
1:C:230:TYR:CD1	1:C:239:SER:HB3	2.55	0.41
1:E:83:VAL:HG13	1:E:308:ASN:ND2	2.36	0.41
1:L:175:ARG:O	1:L:175:ARG:HG2	2.18	0.41
1:L:199:ASN:ND2	1:L:200:PRO:HD2	2.31	0.41
1:L:205:THR:O	1:L:208:ASP:HB2	2.21	0.41
1:P:213:ILE:O	1:P:217:ILE:HG13	2.21	0.41
1:B:129:MSE:HG3	2:B:1001:TRP:NE1	2.36	0.41
1:D:171:ILE:N	1:D:171:ILE:CD1	2.83	0.41
1:D:209:ASP:O	1:D:209:ASP:OD1	2.39	0.41
1:H:192:LYS:O	1:H:194:SER:N	2.53	0.41
1:J:295:GLU:O	1:J:299:VAL:HG23	2.20	0.41
1:K:258:ARG:C	1:K:261:GLU:HG3	2.37	0.41
1:L:129:MSE:O	1:L:132:ASP:HB2	2.21	0.41
1:N:168:LEU:HD22	1:N:314:MSE:SE	2.71	0.41
3:O:1002:PO4:O3	4:O:1003:AMP:O1P	2.39	0.41
1:O:71:ASP:HA	1:O:72:PRO:HD2	1.81	0.41
1:P:169:PHE:HE1	1:P:314:MSE:HE3	1.84	0.41
1:Q:205:THR:CG2	1:Q:206:LEU:N	2.83	0.41
1:Q:313:GLU:OE1	1:Q:313:GLU:HA	2.20	0.41
1:R:289:HIS:O	1:R:293:SER:N	2.53	0.41
1:D:209:ASP:OD1	1:D:209:ASP:C	2.59	0.41
1:D:42:GLN:HB2	1:D:80:GLN:OE1	2.21	0.41
1:F:160:ARG:HB2	1:F:160:ARG:HE	1.72	0.41
1:H:15:THR:CB	1:H:204:ILE:O	2.63	0.41
1:H:238:ILE:HD13	1:H:238:ILE:HA	1.92	0.41
1:J:59:ARG:CG	1:J:59:ARG:NH1	2.80	0.41
1:L:141:VAL:N	1:L:173:GLU:O	2.48	0.41
1:L:29:LEU:CD1	1:L:177:PRO:HG2	2.50	0.41
1:N:176:ILE:CG2	1:N:179:VAL:HG13	2.51	0.41
1:P:99:ILE:O	1:P:103:GLU:HG3	2.20	0.41
1:P:205:THR:HG22	1:P:207:LEU:N	2.25	0.41
1:P:217:ILE:CD1	1:P:273:ALA:HA	2.50	0.41
1:B:175:ARG:C	1:B:176:ILE:CG1	2.89	0.41
1:C:145:GLU:O	1:C:148:LYS:HB3	2.21	0.41
1:C:23:LEU:HG	1:C:68:VAL:HG11	2.02	0.41
1:E:238:ILE:O	1:E:239:SER:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:ARG:CG	1:G:184:MSE:HE1	2.41	0.41
1:J:243:ASN:O	1:J:247:THR:HG23	2.21	0.41
1:K:190:THR:O	1:K:190:THR:HG22	2.21	0.41
1:M:241:LEU:HA	1:M:241:LEU:HD12	1.88	0.41
1:M:293:SER:OG	1:M:295:GLU:N	2.54	0.41
1:N:25:GLN:HG2	1:N:178:LYS:HB2	2.01	0.41
1:P:19:TYR:HA	1:P:23:LEU:HB3	2.02	0.41
1:P:245:TYR:O	1:P:249:SER:OG	2.37	0.41
1:Q:40:VAL:HG11	2:Q:1001:TRP:CD1	2.55	0.41
1:Q:122:LEU:HA	1:Q:122:LEU:HD13	1.84	0.41
1:Q:242:LEU:O	1:Q:246:SER:HB3	2.21	0.41
1:Q:30:GLN:O	1:Q:74:GLN:HG3	2.20	0.41
1:R:188:ASP:OD2	1:R:190:THR:HB	2.21	0.41
1:D:53:GLU:OE1	1:D:53:GLU:HA	2.21	0.41
1:E:191:LYS:HG2	1:E:192:LYS:N	2.36	0.41
1:C:99:ILE:HG13	1:F:118:VAL:HB	2.03	0.41
1:F:71:ASP:HA	1:F:72:PRO:HD2	1.86	0.41
4:H:1003:AMP:H4'	4:H:1003:AMP:O1P	2.21	0.41
1:J:205:THR:C	1:J:207:LEU:N	2.74	0.41
1:J:94:GLN:HA	1:J:97:VAL:HG12	2.02	0.41
1:L:281:ARG:CG	1:L:281:ARG:NH1	2.78	0.41
1:M:128:LEU:O	1:M:128:LEU:HD12	2.21	0.41
1:N:125:TYR:N	1:N:126:PRO:HD2	2.36	0.41
1:N:146:ASP:OD1	1:N:146:ASP:N	2.36	0.41
1:Q:140:ILE:HD12	1:Q:175:ARG:HG2	2.01	0.41
1:R:209:ASP:O	1:R:212:THR:N	2.54	0.41
1:R:260:TYR:N	1:R:260:TYR:CD2	2.89	0.41
1:A:150:HIS:O	1:A:154:THR:CG2	2.69	0.41
1:A:67:ALA:HB2	1:A:287:TYR:HA	2.03	0.41
1:D:212:THR:CG2	1:D:216:LYS:HD2	2.39	0.41
1:F:293:SER:OG	1:F:295:GLU:HB2	2.21	0.41
1:H:300:LEU:HD23	1:H:300:LEU:HA	1.95	0.41
1:I:106:THR:O	1:I:107:GLN:C	2.59	0.41
1:I:194:SER:HB2	3:I:1002:PO4:O2	2.21	0.41
1:N:245:TYR:CD2	1:N:256:LEU:CD2	3.04	0.41
1:O:193:MSE:CA	4:O:1003:AMP:N6	2.83	0.41
1:P:245:TYR:CG	1:P:272:LEU:HD13	2.51	0.41
1:P:279:THR:O	1:P:282:PRO:CD	2.64	0.41
1:Q:98:TYR:HB2	1:Q:101:GLU:HG3	2.03	0.41
1:R:146:ASP:N	1:R:146:ASP:OD1	2.53	0.41
1:R:137:ASN:ND2	1:R:170:THR:OG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:241:LEU:O	1:R:244:ILE:N	2.54	0.41
1:O:320:GLN:OE1	1:R:55:ARG:NH2	2.54	0.41
1:C:316:ARG:CG	1:C:316:ARG:NH2	2.77	0.40
1:E:71:ASP:HB3	1:E:74:GLN:CB	2.50	0.40
1:F:228:ILE:HD13	1:F:265:TYR:CD1	2.55	0.40
1:G:282:PRO:HB2	1:G:286:ARG:HH21	1.86	0.40
1:H:119:SER:HB2	1:K:95:CYS:O	2.21	0.40
1:I:29:LEU:CD1	1:I:177:PRO:HB2	2.51	0.40
1:J:65:TYR:O	1:J:70:ILE:HB	2.21	0.40
1:M:276:VAL:C	1:M:278:GLU:N	2.73	0.40
1:N:86:HIS:CD2	1:N:132:ASP:OD1	2.74	0.40
1:O:175:ARG:NH2	1:O:177:PRO:CG	2.84	0.40
1:P:122:LEU:O	1:P:125:TYR:CE1	2.74	0.40
1:P:230:TYR:CD1	1:P:230:TYR:C	2.94	0.40
1:Q:97:VAL:CG1	1:Q:97:VAL:O	2.69	0.40
1:A:199:ASN:ND2	1:A:201:LYS:HG3	2.36	0.40
1:A:228:ILE:HG13	1:A:260:TYR:HB3	2.03	0.40
1:B:146:ASP:OD1	1:B:146:ASP:N	2.41	0.40
1:G:162:ASN:CG	1:G:167:GLU:HA	2.41	0.40
1:H:245:TYR:HD2	1:H:268:PHE:CE1	2.39	0.40
1:I:29:LEU:O	1:I:33:TYR:HB2	2.21	0.40
1:N:19:TYR:HE1	1:N:68:VAL:HG13	1.86	0.40
1:O:195:LYS:HG3	1:O:196:SER:N	2.36	0.40
1:O:246:SER:HB2	1:O:251:GLN:O	2.21	0.40
1:O:213:ILE:CD1	1:O:280:LEU:HD12	2.51	0.40
1:O:59:ARG:CG	1:O:60:ARG:N	2.83	0.40
1:P:248:LEU:CD1	1:P:248:LEU:H	2.29	0.40
1:Q:229:ARG:HE	1:Q:229:ARG:HB3	1.38	0.40
1:Q:41:ASP:N	1:Q:41:ASP:OD1	2.55	0.40
1:R:21:GLY:HA3	4:R:1003:AMP:N3	2.36	0.40
1:A:123:LEU:HG	1:A:123:LEU:O	2.20	0.40
1:B:38:CYS:SG	1:B:80:GLN:CB	3.09	0.40
1:E:105:MSE:HA	1:E:105:MSE:CE	2.47	0.40
1:F:207:LEU:HD11	1:F:287:TYR:CZ	2.57	0.40
1:F:242:LEU:O	1:F:246:SER:HB3	2.22	0.40
1:G:224:SER:HB2	1:I:166:GLY:H	1.83	0.40
1:J:50:ASP:OD2	1:J:51:PRO:HD2	2.21	0.40
1:K:126:PRO:HD2	1:K:127:PRO:HD2	2.03	0.40
1:M:105:MSE:O	1:M:106:THR:C	2.59	0.40
1:M:126:PRO:CB	1:M:127:PRO:CD	2.96	0.40
1:M:199:ASN:HD22	1:M:200:PRO:N	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:ILE:HG12	1:N:140:ILE:HB	2.04	0.40
1:O:242:LEU:HA	1:O:242:LEU:HD23	1.91	0.40
1:O:24:ARG:HH11	1:O:24:ARG:CB	2.35	0.40
1:Q:140:ILE:HD13	1:Q:175:ARG:CZ	2.52	0.40
1:Q:197:ASP:HA	1:Q:198:PRO:HD3	1.89	0.40
1:R:64:LEU:O	1:R:67:ALA:HB3	2.21	0.40
1:A:151:ILE:HA	1:A:154:THR:HG23	2.03	0.40
1:A:70:ILE:HD13	1:A:70:ILE:HA	1.87	0.40
1:C:16:ILE:HA	1:C:19:TYR:CB	2.52	0.40
1:E:281:ARG:N	1:E:282:PRO:CD	2.84	0.40
1:E:30:GLN:HG3	1:E:74:GLN:HG3	1.96	0.40
1:E:78:PHE:CD1	1:E:78:PHE:N	2.89	0.40
1:G:130:ALA:HB2	1:G:154:THR:HB	2.02	0.40
1:H:40:VAL:HG23	1:H:40:VAL:O	2.21	0.40
1:I:86:HIS:HE1	1:I:136:TYR:OH	2.04	0.40
1:K:302:GLU:O	1:K:306:LYS:HG3	2.21	0.40
1:N:125:TYR:CD2	1:N:126:PRO:HD3	2.57	0.40
1:N:150:HIS:O	1:N:154:THR:CG2	2.68	0.40
1:N:43:HIS:O	1:N:46:THR:OG1	2.31	0.40
1:O:252:SER:OG	1:O:255:GLU:HB3	2.22	0.40
1:Q:168:LEU:HA	1:Q:168:LEU:HD23	1.91	0.40
1:Q:176:ILE:HA	1:Q:177:PRO:HD3	1.89	0.40
1:R:184:MSE:HB3	1:R:184:MSE:HE2	1.61	0.40
1:R:59:ARG:HH22	1:R:297:ASP:CG	2.23	0.40
1:B:252:SER:OG	1:B:255:GLU:HB2	2.22	0.40
1:G:104:ARG:HH11	1:G:104:ARG:HD3	1.77	0.40
1:J:185:SER:O	1:J:188:ASP:O	2.39	0.40
1:K:242:LEU:HD23	1:K:242:LEU:HA	1.87	0.40
1:K:41:ASP:N	1:K:41:ASP:OD1	2.55	0.40
1:P:184:MSE:N	1:P:240:ASN:HD21	2.19	0.40
1:Q:4:ILE:HD13	1:Q:140:ILE:CG2	2.52	0.40
1:R:25:GLN:N	1:R:25:GLN:CD	2.71	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	285/326 (87%)	273 (96%)	11 (4%)	1 (0%)	34	60
1	B	281/326 (86%)	266 (95%)	14 (5%)	1 (0%)	34	60
1	C	285/326 (87%)	273 (96%)	12 (4%)	0	100	100
1	D	291/326 (89%)	282 (97%)	9 (3%)	0	100	100
1	E	281/326 (86%)	252 (90%)	29 (10%)	0	100	100
1	F	284/326 (87%)	276 (97%)	8 (3%)	0	100	100
1	G	292/326 (90%)	272 (93%)	20 (7%)	0	100	100
1	H	291/326 (89%)	278 (96%)	12 (4%)	1 (0%)	41	66
1	I	288/326 (88%)	279 (97%)	9 (3%)	0	100	100
1	J	291/326 (89%)	277 (95%)	14 (5%)	0	100	100
1	K	284/326 (87%)	269 (95%)	15 (5%)	0	100	100
1	L	291/326 (89%)	283 (97%)	8 (3%)	0	100	100
1	M	291/326 (89%)	269 (92%)	19 (6%)	3 (1%)	15	37
1	N	291/326 (89%)	281 (97%)	10 (3%)	0	100	100
1	O	291/326 (89%)	277 (95%)	14 (5%)	0	100	100
1	P	283/326 (87%)	256 (90%)	27 (10%)	0	100	100
1	Q	291/326 (89%)	277 (95%)	14 (5%)	0	100	100
1	R	276/326 (85%)	260 (94%)	16 (6%)	0	100	100
All	All	5167/5868 (88%)	4900 (95%)	261 (5%)	6 (0%)	51	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	GLY
1	H	193	MSE
1	M	291	MSE
1	A	246	SER
1	M	105	MSE
1	M	277	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 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	257/268 (96%)	219 (85%)	38 (15%)	3	7
1	B	256/268 (96%)	202 (79%)	54 (21%)	1	3
1	C	257/268 (96%)	211 (82%)	46 (18%)	2	4
1	D	259/268 (97%)	216 (83%)	43 (17%)	2	5
1	E	253/268 (94%)	208 (82%)	45 (18%)	2	4
1	F	255/268 (95%)	203 (80%)	52 (20%)	1	3
1	G	260/268 (97%)	219 (84%)	41 (16%)	2	6
1	H	259/268 (97%)	214 (83%)	45 (17%)	2	5
1	I	256/268 (96%)	203 (79%)	53 (21%)	1	3
1	J	259/268 (97%)	207 (80%)	52 (20%)	1	3
1	K	254/268 (95%)	210 (83%)	44 (17%)	2	5
1	L	259/268 (97%)	219 (85%)	40 (15%)	2	7
1	M	259/268 (97%)	202 (78%)	57 (22%)	1	2
1	N	259/268 (97%)	221 (85%)	38 (15%)	3	7
1	O	259/268 (97%)	194 (75%)	65 (25%)	0	1
1	P	255/268 (95%)	200 (78%)	55 (22%)	1	3
1	Q	259/268 (97%)	199 (77%)	60 (23%)	1	2
1	R	252/268 (94%)	196 (78%)	56 (22%)	1	2
All	All	4627/4824 (96%)	3743 (81%)	884 (19%)	1	4

All (884) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	8	ILE
1	A	9	GLN
1	A	25	GLN
1	A	28	GLU
1	A	55	ARG

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Mol	Chain	Res	Type
1	A	59	ARG
1	A	60	ARG
1	A	73	THR
1	A	99	ILE
1	A	104	ARG
1	A	105	MSE
1	A	119	SER
1	A	122	LEU
1	A	138	THR
1	A	146	ASP
1	A	148	LYS
1	A	154	THR
1	A	164	ARG
1	A	173	GLU
1	A	175	ARG
1	A	182	ARG
1	A	197	ASP
1	A	199	ASN
1	A	201	LYS
1	A	205	THR
1	A	219	SER
1	A	228	ILE
1	A	238	ILE
1	A	241	LEU
1	A	245	TYR
1	A	247	THR
1	A	275	VAL
1	A	292	GLU
1	A	308	ASN
1	A	312	SER
1	A	317	LYS
1	A	320	GLN
1	B	2	LYS
1	B	24	ARG
1	B	32	GLU
1	B	55	ARG
1	B	59	ARG
1	B	70	ILE
1	B	73	THR
1	B	80	GLN
1	B	81	SER
1	B	96	ILE

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Mol	Chain	Res	Type
1	B	99	ILE
1	B	106	THR
1	B	119	SER
1	B	122	LEU
1	B	138	THR
1	B	145	GLU
1	B	146	ASP
1	B	154	THR
1	B	159	GLU
1	B	164	ARG
1	B	165	TYR
1	B	170	THR
1	B	171	ILE
1	B	175	ARG
1	B	185	SER
1	B	190	THR
1	B	192	LYS
1	B	195	LYS
1	B	199	ASN
1	B	205	THR
1	B	206	LEU
1	B	219	SER
1	B	225	GLU
1	B	227	THR
1	B	228	ILE
1	B	229	ARG
1	B	238	ILE
1	B	241	LEU
1	B	245	TYR
1	B	246	SER
1	B	247	THR
1	B	254	GLU
1	B	255	GLU
1	B	261	GLU
1	B	267	VAL
1	B	278	GLU
1	B	284	GLN
1	B	285	GLU
1	B	286	ARG
1	B	289	HIS
1	B	292	GLU
1	B	308	ASN

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Mol	Chain	Res	Type
1	B	312	SER
1	B	316	ARG
1	C	1	MSE
1	C	8	ILE
1	C	23	LEU
1	C	24	ARG
1	C	53	GLU
1	C	55	ARG
1	C	56	GLN
1	C	59	ARG
1	C	70	ILE
1	C	96	ILE
1	C	99	ILE
1	C	107	GLN
1	C	119	SER
1	C	122	LEU
1	C	138	THR
1	C	145	GLU
1	C	146	ASP
1	C	148	LYS
1	C	154	THR
1	C	164	ARG
1	C	168	LEU
1	C	175	ARG
1	C	182	ARG
1	C	185	SER
1	C	196	SER
1	C	199	ASN
1	C	201	LYS
1	C	217	ILE
1	C	219	SER
1	C	224	SER
1	C	238	ILE
1	C	241	LEU
1	C	245	TYR
1	C	246	SER
1	C	252	SER
1	C	253	ILE
1	C	267	VAL
1	C	275	VAL
1	C	278	GLU
1	C	281	ARG

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Mol	Chain	Res	Type
1	C	285	GLU
1	C	302	GLU
1	C	305	GLU
1	C	308	ASN
1	C	312	SER
1	C	316	ARG
1	D	1	MSE
1	D	8	ILE
1	D	9	GLN
1	D	28	GLU
1	D	29	LEU
1	D	55	ARG
1	D	56	GLN
1	D	59	ARG
1	D	96	ILE
1	D	99	ILE
1	D	107	GLN
1	D	122	LEU
1	D	137	ASN
1	D	138	THR
1	D	146	ASP
1	D	148	LYS
1	D	154	THR
1	D	159	GLU
1	D	160	ARG
1	D	164	ARG
1	D	185	SER
1	D	199	ASN
1	D	205	THR
1	D	211	LYS
1	D	219	SER
1	D	224	SER
1	D	225	GLU
1	D	229	ARG
1	D	241	LEU
1	D	245	TYR
1	D	247	THR
1	D	255	GLU
1	D	278	GLU
1	D	281	ARG
1	D	285	GLU
1	D	294	GLU

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Mol	Chain	Res	Type
1	D	302	GLU
1	D	308	ASN
1	D	309	ARG
1	D	312	SER
1	D	314	MSE
1	D	316	ARG
1	D	317	LYS
1	E	6	SER
1	E	20	ILE
1	E	23	LEU
1	E	25	GLN
1	E	27	VAL
1	E	32	GLU
1	E	53	GLU
1	E	55	ARG
1	E	56	GLN
1	E	96	ILE
1	E	104	ARG
1	E	105	MSE
1	E	106	THR
1	E	107	GLN
1	E	122	LEU
1	E	124	THR
1	E	138	THR
1	E	148	LYS
1	E	154	THR
1	E	160	ARG
1	E	173	GLU
1	E	175	ARG
1	E	178	LYS
1	E	201	LYS
1	E	206	LEU
1	E	211	LYS
1	E	215	LYS
1	E	218	LYS
1	E	225	GLU
1	E	238	ILE
1	E	239	SER
1	E	241	LEU
1	E	245	TYR
1	E	247	THR
1	E	248	LEU

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Mol	Chain	Res	Type
1	E	253	ILE
1	E	258	ARG
1	E	284	GLN
1	E	285	GLU
1	E	295	GLU
1	E	299	VAL
1	E	308	ASN
1	E	309	ARG
1	E	312	SER
1	E	320	GLN
1	F	1	MSE
1	F	8	ILE
1	F	18	ASN
1	F	24	ARG
1	F	32	GLU
1	F	34	ASN
1	F	55	ARG
1	F	56	GLN
1	F	59	ARG
1	F	60	ARG
1	F	73	THR
1	F	96	ILE
1	F	99	ILE
1	F	105	MSE
1	F	107	GLN
1	F	119	SER
1	F	122	LEU
1	F	123	LEU
1	F	138	THR
1	F	146	ASP
1	F	151	ILE
1	F	154	THR
1	F	160	ARG
1	F	164	ARG
1	F	175	ARG
1	F	182	ARG
1	F	188	ASP
1	F	190	THR
1	F	192	LYS
1	F	199	ASN
1	F	205	THR
1	F	211	LYS

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Mol	Chain	Res	Type
1	F	217	ILE
1	F	218	LYS
1	F	219	SER
1	F	225	GLU
1	F	227	THR
1	F	228	ILE
1	F	229	ARG
1	F	238	ILE
1	F	241	LEU
1	F	242	LEU
1	F	245	TYR
1	F	247	THR
1	F	251	GLN
1	F	254	GLU
1	F	278	GLU
1	F	281	ARG
1	F	289	HIS
1	F	293	SER
1	F	308	ASN
1	F	326	ARG
1	G	1	MSE
1	G	4	ILE
1	G	8	ILE
1	G	25	GLN
1	G	55	ARG
1	G	60	ARG
1	G	73	THR
1	G	74	GLN
1	G	78	PHE
1	G	81	SER
1	G	96	ILE
1	G	99	ILE
1	G	106	THR
1	G	107	GLN
1	G	122	LEU
1	G	138	THR
1	G	146	ASP
1	G	148	LYS
1	G	154	THR
1	G	164	ARG
1	G	171	ILE
1	G	182	ARG

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Mol	Chain	Res	Type
1	G	185	SER
1	G	199	ASN
1	G	205	THR
1	G	211	LYS
1	G	215	LYS
1	G	219	SER
1	G	229	ARG
1	G	241	LEU
1	G	245	TYR
1	G	254	GLU
1	G	263	LYS
1	G	277	ILE
1	G	278	GLU
1	G	285	GLU
1	G	298	ARG
1	G	308	ASN
1	G	309	ARG
1	G	320	GLN
1	G	326	ARG
1	H	8	ILE
1	H	9	GLN
1	H	53	GLU
1	H	55	ARG
1	H	56	GLN
1	H	59	ARG
1	H	76	THR
1	H	94	GLN
1	H	96	ILE
1	H	99	ILE
1	H	106	THR
1	H	119	SER
1	H	122	LEU
1	H	138	THR
1	H	148	LYS
1	H	154	THR
1	H	159	GLU
1	H	164	ARG
1	H	173	GLU
1	H	176	ILE
1	H	179	VAL
1	H	182	ARG
1	H	191	LYS

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Mol	Chain	Res	Type
1	H	192	LYS
1	H	194	SER
1	H	199	ASN
1	H	215	LYS
1	H	217	ILE
1	H	218	LYS
1	H	225	GLU
1	H	227	THR
1	H	228	ILE
1	H	241	LEU
1	H	245	TYR
1	H	251	GLN
1	H	267	VAL
1	H	274	GLN
1	H	293	SER
1	H	294	GLU
1	H	295	GLU
1	H	302	GLU
1	H	305	GLU
1	H	308	ASN
1	H	312	SER
1	H	316	ARG
1	I	1	MSE
1	I	8	ILE
1	I	9	GLN
1	I	16	ILE
1	I	24	ARG
1	I	25	GLN
1	I	26	PHE
1	I	28	GLU
1	I	50	ASP
1	I	53	GLU
1	I	55	ARG
1	I	56	GLN
1	I	59	ARG
1	I	60	ARG
1	I	70	ILE
1	I	81	SER
1	I	96	ILE
1	I	99	ILE
1	I	107	GLN
1	I	122	LEU

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Mol	Chain	Res	Type
1	I	138	THR
1	I	148	LYS
1	I	154	THR
1	I	160	ARG
1	I	164	ARG
1	I	176	ILE
1	I	178	LYS
1	I	179	VAL
1	I	182	ARG
1	I	191	LYS
1	I	192	LYS
1	I	194	SER
1	I	196	SER
1	I	199	ASN
1	I	211	LYS
1	I	215	LYS
1	I	219	SER
1	I	225	GLU
1	I	227	THR
1	I	238	ILE
1	I	241	LEU
1	I	245	TYR
1	I	252	SER
1	I	263	LYS
1	I	267	VAL
1	I	278	GLU
1	I	292	GLU
1	I	295	GLU
1	I	302	GLU
1	I	308	ASN
1	I	312	SER
1	I	314	MSE
1	I	320	GLN
1	J	1	MSE
1	J	8	ILE
1	J	9	GLN
1	J	23	LEU
1	J	24	ARG
1	J	28	GLU
1	J	55	ARG
1	J	56	GLN
1	J	59	ARG

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Mol	Chain	Res	Type
1	J	60	ARG
1	J	81	SER
1	J	94	GLN
1	J	96	ILE
1	J	99	ILE
1	J	104	ARG
1	J	105	MSE
1	J	106	THR
1	J	122	LEU
1	J	124	THR
1	J	138	THR
1	J	145	GLU
1	J	146	ASP
1	J	148	LYS
1	J	154	THR
1	J	159	GLU
1	J	160	ARG
1	J	164	ARG
1	J	175	ARG
1	J	178	LYS
1	J	179	VAL
1	J	190	THR
1	J	192	LYS
1	J	199	ASN
1	J	205	THR
1	J	215	LYS
1	J	219	SER
1	J	225	GLU
1	J	227	THR
1	J	229	ARG
1	J	238	ILE
1	J	239	SER
1	J	241	LEU
1	J	245	TYR
1	J	277	ILE
1	J	278	GLU
1	J	281	ARG
1	J	308	ASN
1	J	309	ARG
1	J	312	SER
1	J	315	VAL
1	J	320	GLN

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Mol	Chain	Res	Type
1	J	326	ARG
1	K	8	ILE
1	K	16	ILE
1	K	23	LEU
1	K	24	ARG
1	K	53	GLU
1	K	55	ARG
1	K	56	GLN
1	K	60	ARG
1	K	94	GLN
1	K	96	ILE
1	K	99	ILE
1	K	119	SER
1	K	122	LEU
1	K	138	THR
1	K	145	GLU
1	K	146	ASP
1	K	149	GLN
1	K	154	THR
1	K	164	ARG
1	K	175	ARG
1	K	179	VAL
1	K	182	ARG
1	K	187	VAL
1	K	191	LYS
1	K	192	LYS
1	K	195	LYS
1	K	196	SER
1	K	199	ASN
1	K	204	ILE
1	K	205	THR
1	K	206	LEU
1	K	211	LYS
1	K	215	LYS
1	K	218	LYS
1	K	219	SER
1	K	241	LEU
1	K	256	LEU
1	K	259	GLN
1	K	267	VAL
1	K	295	GLU
1	K	308	ASN

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Mol	Chain	Res	Type
1	K	312	SER
1	K	320	GLN
1	K	322	MSE
1	L	2	LYS
1	L	20	ILE
1	L	24	ARG
1	L	25	GLN
1	L	55	ARG
1	L	56	GLN
1	L	59	ARG
1	L	60	ARG
1	L	81	SER
1	L	96	ILE
1	L	99	ILE
1	L	119	SER
1	L	122	LEU
1	L	138	THR
1	L	145	GLU
1	L	146	ASP
1	L	154	THR
1	L	159	GLU
1	L	164	ARG
1	L	167	GLU
1	L	175	ARG
1	L	182	ARG
1	L	194	SER
1	L	199	ASN
1	L	205	THR
1	L	227	THR
1	L	228	ILE
1	L	238	ILE
1	L	241	LEU
1	L	245	TYR
1	L	246	SER
1	L	252	SER
1	L	285	GLU
1	L	289	HIS
1	L	293	SER
1	L	295	GLU
1	L	308	ASN
1	L	309	ARG
1	L	312	SER

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Mol	Chain	Res	Type
1	L	316	ARG
1	M	8	ILE
1	M	16	ILE
1	M	18	ASN
1	M	32	GLU
1	M	56	GLN
1	M	59	ARG
1	M	60	ARG
1	M	73	THR
1	M	74	GLN
1	M	94	GLN
1	M	96	ILE
1	M	99	ILE
1	M	107	GLN
1	M	119	SER
1	M	122	LEU
1	M	138	THR
1	M	140	ILE
1	M	146	ASP
1	M	148	LYS
1	M	151	ILE
1	M	154	THR
1	M	164	ARG
1	M	171	ILE
1	M	173	GLU
1	M	176	ILE
1	M	182	ARG
1	M	185	SER
1	M	187	VAL
1	M	190	THR
1	M	195	LYS
1	M	199	ASN
1	M	206	LEU
1	M	211	LYS
1	M	219	SER
1	M	227	THR
1	M	229	ARG
1	M	241	LEU
1	M	245	TYR
1	M	246	SER
1	M	251	GLN
1	M	253	ILE

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Mol	Chain	Res	Type
1	M	257	GLU
1	M	267	VAL
1	M	278	GLU
1	M	279	THR
1	M	281	ARG
1	M	289	HIS
1	M	292	GLU
1	M	293	SER
1	M	294	GLU
1	M	297	ASP
1	M	305	GLU
1	M	308	ASN
1	M	312	SER
1	M	316	ARG
1	M	320	GLN
1	M	326	ARG
1	N	1	MSE
1	N	8	ILE
1	N	24	ARG
1	N	53	GLU
1	N	55	ARG
1	N	59	ARG
1	N	96	ILE
1	N	99	ILE
1	N	107	GLN
1	N	122	LEU
1	N	129	MSE
1	N	138	THR
1	N	145	GLU
1	N	146	ASP
1	N	149	GLN
1	N	154	THR
1	N	164	ARG
1	N	168	LEU
1	N	179	VAL
1	N	182	ARG
1	N	187	VAL
1	N	191	LYS
1	N	192	LYS
1	N	195	LYS
1	N	199	ASN
1	N	211	LYS

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Mol	Chain	Res	Type
1	N	215	LYS
1	N	217	ILE
1	N	219	SER
1	N	225	GLU
1	N	241	LEU
1	N	253	ILE
1	N	278	GLU
1	N	292	GLU
1	N	294	GLU
1	N	308	ASN
1	N	312	SER
1	N	316	ARG
1	O	1	MSE
1	O	4	ILE
1	O	8	ILE
1	O	18	ASN
1	O	23	LEU
1	O	24	ARG
1	O	25	GLN
1	O	28	GLU
1	O	31	HIS
1	O	32	GLU
1	O	34	ASN
1	O	55	ARG
1	O	56	GLN
1	O	59	ARG
1	O	70	ILE
1	O	81	SER
1	O	96	ILE
1	O	99	ILE
1	O	105	MSE
1	O	106	THR
1	O	107	GLN
1	O	119	SER
1	O	122	LEU
1	O	123	LEU
1	O	146	ASP
1	O	148	LYS
1	O	152	GLU
1	O	154	THR
1	O	159	GLU
1	O	160	ARG

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Mol	Chain	Res	Type
1	O	164	ARG
1	O	167	GLU
1	O	171	ILE
1	O	173	GLU
1	O	175	ARG
1	O	179	VAL
1	O	187	VAL
1	O	191	LYS
1	O	195	LYS
1	O	196	SER
1	O	199	ASN
1	O	205	THR
1	O	211	LYS
1	O	215	LYS
1	O	217	ILE
1	O	219	SER
1	O	225	GLU
1	O	227	THR
1	O	229	ARG
1	O	241	LEU
1	O	245	TYR
1	O	246	SER
1	O	247	THR
1	O	251	GLN
1	O	259	GLN
1	O	267	VAL
1	O	281	ARG
1	O	284	GLN
1	O	285	GLU
1	O	289	HIS
1	O	293	SER
1	O	297	ASP
1	O	305	GLU
1	O	308	ASN
1	O	316	ARG
1	P	1	MSE
1	P	8	ILE
1	P	9	GLN
1	P	16	ILE
1	P	18	ASN
1	P	24	ARG
1	P	28	GLU

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Mol	Chain	Res	Type
1	P	32	GLU
1	P	47	VAL
1	P	53	GLU
1	P	55	ARG
1	P	56	GLN
1	P	96	ILE
1	P	99	ILE
1	P	101	GLU
1	P	118	VAL
1	P	129	MSE
1	P	138	THR
1	P	146	ASP
1	P	154	THR
1	P	159	GLU
1	P	160	ARG
1	P	161	PHE
1	P	168	LEU
1	P	173	GLU
1	P	182	ARG
1	P	183	ILE
1	P	191	LYS
1	P	195	LYS
1	P	196	SER
1	P	199	ASN
1	P	201	LYS
1	P	205	THR
1	P	215	LYS
1	P	216	LYS
1	P	218	LYS
1	P	228	ILE
1	P	238	ILE
1	P	246	SER
1	P	248	LEU
1	P	252	SER
1	P	253	ILE
1	P	254	GLU
1	P	279	THR
1	P	280	LEU
1	P	281	ARG
1	P	284	GLN
1	P	285	GLU
1	P	292	GLU

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Mol	Chain	Res	Type
1	P	296	LEU
1	P	302	GLU
1	P	308	ASN
1	P	312	SER
1	P	320	GLN
1	P	326	ARG
1	Q	1	MSE
1	Q	4	ILE
1	Q	8	ILE
1	Q	9	GLN
1	Q	18	ASN
1	Q	24	ARG
1	Q	25	GLN
1	Q	30	GLN
1	Q	32	GLU
1	Q	53	GLU
1	Q	55	ARG
1	Q	56	GLN
1	Q	59	ARG
1	Q	60	ARG
1	Q	68	VAL
1	Q	96	ILE
1	Q	97	VAL
1	Q	99	ILE
1	Q	105	MSE
1	Q	118	VAL
1	Q	119	SER
1	Q	122	LEU
1	Q	138	THR
1	Q	146	ASP
1	Q	148	LYS
1	Q	154	THR
1	Q	155	ARG
1	Q	159	GLU
1	Q	164	ARG
1	Q	167	GLU
1	Q	168	LEU
1	Q	173	GLU
1	Q	176	ILE
1	Q	179	VAL
1	Q	185	SER
1	Q	188	ASP

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Mol	Chain	Res	Type
1	Q	190	THR
1	Q	192	LYS
1	Q	196	SER
1	Q	199	ASN
1	Q	205	THR
1	Q	217	ILE
1	Q	224	SER
1	Q	228	ILE
1	Q	229	ARG
1	Q	241	LEU
1	Q	245	TYR
1	Q	246	SER
1	Q	252	SER
1	Q	261	GLU
1	Q	267	VAL
1	Q	274	GLN
1	Q	277	ILE
1	Q	278	GLU
1	Q	295	GLU
1	Q	302	GLU
1	Q	308	ASN
1	Q	312	SER
1	Q	320	GLN
1	Q	326	ARG
1	R	1	MSE
1	R	4	ILE
1	R	8	ILE
1	R	9	GLN
1	R	15	THR
1	R	18	ASN
1	R	23	LEU
1	R	32	GLU
1	R	55	ARG
1	R	56	GLN
1	R	59	ARG
1	R	60	ARG
1	R	76	THR
1	R	96	ILE
1	R	99	ILE
1	R	101	GLU
1	R	106	THR
1	R	119	SER

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Mol	Chain	Res	Type
1	R	122	LEU
1	R	138	THR
1	R	146	ASP
1	R	148	LYS
1	R	154	THR
1	R	159	GLU
1	R	160	ARG
1	R	161	PHE
1	R	164	ARG
1	R	167	GLU
1	R	168	LEU
1	R	171	ILE
1	R	176	ILE
1	R	182	ARG
1	R	184	MSE
1	R	187	VAL
1	R	191	LYS
1	R	197	ASP
1	R	204	ILE
1	R	212	THR
1	R	214	GLU
1	R	215	LYS
1	R	216	LYS
1	R	219	SER
1	R	225	GLU
1	R	241	LEU
1	R	245	TYR
1	R	248	LEU
1	R	272	LEU
1	R	275	VAL
1	R	278	GLU
1	R	284	GLN
1	R	286	ARG
1	R	292	GLU
1	R	295	GLU
1	R	297	ASP
1	R	298	ARG
1	R	312	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (191) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	18	ASN
1	A	25	GLN
1	A	34	ASN
1	A	43	HIS
1	A	52	HIS
1	A	86	HIS
1	A	94	GLN
1	A	150	HIS
1	A	199	ASN
1	A	284	GLN
1	A	308	ASN
1	A	320	GLN
1	B	18	ASN
1	B	25	GLN
1	B	34	ASN
1	B	43	HIS
1	B	86	HIS
1	B	94	GLN
1	B	107	GLN
1	B	137	ASN
1	B	199	ASN
1	B	284	GLN
1	B	308	ASN
1	B	320	GLN
1	C	9	GLN
1	C	31	HIS
1	C	34	ASN
1	C	43	HIS
1	C	86	HIS
1	C	137	ASN
1	C	150	HIS
1	C	199	ASN
1	C	284	GLN
1	C	308	ASN
1	C	320	GLN
1	D	18	ASN
1	D	34	ASN
1	D	43	HIS
1	D	86	HIS
1	D	94	GLN
1	D	107	GLN
1	D	150	HIS

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Mol	Chain	Res	Type
1	D	199	ASN
1	D	284	GLN
1	D	320	GLN
1	E	9	GLN
1	E	34	ASN
1	E	86	HIS
1	E	288	HIS
1	E	308	ASN
1	E	320	GLN
1	F	18	ASN
1	F	34	ASN
1	F	43	HIS
1	F	86	HIS
1	F	107	GLN
1	F	137	ASN
1	F	150	HIS
1	F	199	ASN
1	F	308	ASN
1	F	320	GLN
1	G	18	ASN
1	G	25	GLN
1	G	34	ASN
1	G	43	HIS
1	G	86	HIS
1	G	107	GLN
1	G	150	HIS
1	G	199	ASN
1	G	259	GLN
1	G	308	ASN
1	G	320	GLN
1	H	9	GLN
1	H	31	HIS
1	H	34	ASN
1	H	43	HIS
1	H	52	HIS
1	H	56	GLN
1	H	86	HIS
1	H	137	ASN
1	H	150	HIS
1	H	199	ASN
1	H	308	ASN
1	H	320	GLN

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Mol	Chain	Res	Type
1	I	9	GLN
1	I	18	ASN
1	I	34	ASN
1	I	43	HIS
1	I	86	HIS
1	I	107	GLN
1	I	150	HIS
1	I	199	ASN
1	I	259	GLN
1	I	284	GLN
1	J	34	ASN
1	J	43	HIS
1	J	56	GLN
1	J	86	HIS
1	J	199	ASN
1	J	259	GLN
1	J	284	GLN
1	J	308	ASN
1	K	9	GLN
1	K	18	ASN
1	K	34	ASN
1	K	43	HIS
1	K	56	GLN
1	K	86	HIS
1	K	149	GLN
1	K	150	HIS
1	K	199	ASN
1	K	320	GLN
1	L	25	GLN
1	L	34	ASN
1	L	43	HIS
1	L	86	HIS
1	L	94	GLN
1	L	107	GLN
1	L	150	HIS
1	L	199	ASN
1	L	308	ASN
1	L	320	GLN
1	M	9	GLN
1	M	18	ASN
1	M	31	HIS
1	M	34	ASN

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Mol	Chain	Res	Type
1	M	56	GLN
1	M	74	GLN
1	M	86	HIS
1	M	94	GLN
1	M	137	ASN
1	M	199	ASN
1	M	259	GLN
1	M	284	GLN
1	M	288	HIS
1	M	308	ASN
1	M	320	GLN
1	N	9	GLN
1	N	34	ASN
1	N	43	HIS
1	N	52	HIS
1	N	86	HIS
1	N	94	GLN
1	N	107	GLN
1	N	150	HIS
1	N	199	ASN
1	N	251	GLN
1	N	259	GLN
1	N	284	GLN
1	O	9	GLN
1	O	34	ASN
1	O	86	HIS
1	O	107	GLN
1	O	150	HIS
1	O	199	ASN
1	O	259	GLN
1	P	9	GLN
1	P	34	ASN
1	P	86	HIS
1	P	150	HIS
1	P	199	ASN
1	P	240	ASN
1	P	308	ASN
1	P	320	GLN
1	Q	9	GLN
1	Q	25	GLN
1	Q	34	ASN
1	Q	43	HIS

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Mol	Chain	Res	Type
1	Q	86	HIS
1	Q	94	GLN
1	Q	107	GLN
1	Q	150	HIS
1	Q	199	ASN
1	Q	251	GLN
1	Q	259	GLN
1	Q	308	ASN
1	Q	320	GLN
1	R	18	ASN
1	R	34	ASN
1	R	43	HIS
1	R	57	ASN
1	R	74	GLN
1	R	80	GLN
1	R	86	HIS
1	R	107	GLN
1	R	137	ASN
1	R	149	GLN
1	R	150	HIS
1	R	240	ASN
1	R	308	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

54 ligands are modelled in this entry.

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	PO4	N	1002	-	4,4,4	1.95	1 (25%)	6,6,6	0.47	0
4	AMP	K	1003	-	22,25,25	1.03	1 (4%)	25,38,38	1.01	2 (8%)
3	PO4	Q	1002	-	4,4,4	1.94	1 (25%)	6,6,6	0.40	0
4	AMP	C	1003	-	22,25,25	1.14	2 (9%)	25,38,38	0.87	1 (4%)
3	PO4	G	1002	-	4,4,4	1.95	1 (25%)	6,6,6	0.46	0
4	AMP	E	1003	-	22,25,25	1.11	2 (9%)	25,38,38	1.05	1 (4%)
4	AMP	G	1003	-	22,25,25	1.15	2 (9%)	25,38,38	0.94	2 (8%)
3	PO4	F	1002	-	4,4,4	1.84	1 (25%)	6,6,6	0.46	0
3	PO4	R	1002	-	4,4,4	1.78	1 (25%)	6,6,6	0.41	0
4	AMP	M	1003	-	22,25,25	0.80	0	25,38,38	1.80	8 (32%)
3	PO4	H	1002	-	4,4,4	2.00	1 (25%)	6,6,6	0.46	0
4	AMP	O	1003	-	22,25,25	1.16	2 (9%)	25,38,38	1.51	3 (12%)
3	PO4	I	1002	-	4,4,4	1.96	1 (25%)	6,6,6	0.37	0
3	PO4	P	1002	-	4,4,4	1.81	1 (25%)	6,6,6	0.91	0
4	AMP	Q	1003	-	22,25,25	1.13	2 (9%)	25,38,38	1.07	2 (8%)
4	AMP	D	1003	-	22,25,25	1.11	2 (9%)	25,38,38	0.88	1 (4%)
3	PO4	J	1002	-	4,4,4	2.08	1 (25%)	6,6,6	0.73	0
4	AMP	L	1003	-	22,25,25	1.08	2 (9%)	25,38,38	1.07	1 (4%)
3	PO4	O	1002	-	4,4,4	1.95	1 (25%)	6,6,6	0.46	0
4	AMP	N	1003	-	22,25,25	1.38	3 (13%)	25,38,38	1.35	4 (16%)
4	AMP	H	1003	-	22,25,25	1.11	2 (9%)	25,38,38	1.82	6 (24%)
4	AMP	P	1003	-	22,25,25	0.96	2 (9%)	25,38,38	1.44	5 (20%)
4	AMP	R	1003	-	22,25,25	1.12	2 (9%)	25,38,38	1.00	1 (4%)
3	PO4	B	1002	-	4,4,4	1.96	1 (25%)	6,6,6	0.52	0
4	AMP	F	1003	-	22,25,25	1.16	2 (9%)	25,38,38	1.10	1 (4%)
3	PO4	E	1002	-	4,4,4	2.12	1 (25%)	6,6,6	0.54	0
3	PO4	C	1002	-	4,4,4	1.98	1 (25%)	6,6,6	0.46	0
4	AMP	B	1003	-	22,25,25	1.11	2 (9%)	25,38,38	0.97	1 (4%)
3	PO4	L	1002	-	4,4,4	1.99	1 (25%)	6,6,6	0.63	0
4	AMP	I	1003	-	22,25,25	1.13	2 (9%)	25,38,38	1.21	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	M	1002	-	4,4,4	1.75	0	6,6,6	0.81	0
3	PO4	K	1002	-	4,4,4	1.86	1 (25%)	6,6,6	0.48	0
4	AMP	J	1003	-	22,25,25	1.06	1 (4%)	25,38,38	0.97	1 (4%)
4	AMP	A	1003	-	22,25,25	1.33	2 (9%)	25,38,38	1.52	3 (12%)
3	PO4	D	1002	-	4,4,4	1.85	1 (25%)	6,6,6	0.41	0
3	PO4	A	1002	-	4,4,4	1.94	1 (25%)	6,6,6	0.58	0

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
4	AMP	N	1003	-	-	3/6/26/26	0/3/3/3
4	AMP	M	1003	-	-	4/6/26/26	0/3/3/3
4	AMP	H	1003	-	-	6/6/26/26	0/3/3/3
4	AMP	O	1003	-	-	2/6/26/26	0/3/3/3
4	AMP	J	1003	-	-	5/6/26/26	0/3/3/3
4	AMP	I	1003	-	-	4/6/26/26	0/3/3/3
4	AMP	P	1003	-	-	4/6/26/26	0/3/3/3
4	AMP	R	1003	-	-	2/6/26/26	0/3/3/3
4	AMP	Q	1003	-	-	3/6/26/26	0/3/3/3
4	AMP	C	1003	-	-	4/6/26/26	0/3/3/3
4	AMP	D	1003	-	-	6/6/26/26	0/3/3/3
4	AMP	K	1003	-	-	3/6/26/26	0/3/3/3
4	AMP	F	1003	-	-	5/6/26/26	0/3/3/3
4	AMP	E	1003	-	-	1/6/26/26	0/3/3/3
4	AMP	G	1003	-	-	4/6/26/26	0/3/3/3
4	AMP	B	1003	-	-	5/6/26/26	0/3/3/3
4	AMP	A	1003	-	-	6/6/26/26	0/3/3/3
4	AMP	L	1003	-	-	6/6/26/26	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	AMP	O4'-C1'	4.30	1.47	1.41
4	N	1003	AMP	O4'-C1'	4.26	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1003	AMP	O4'-C1'	4.02	1.46	1.41
4	G	1003	AMP	O4'-C1'	4.00	1.46	1.41
4	Q	1003	AMP	O4'-C1'	3.88	1.46	1.41
4	C	1003	AMP	O4'-C1'	3.85	1.46	1.41
4	F	1003	AMP	O4'-C1'	3.85	1.46	1.41
4	D	1003	AMP	O4'-C1'	3.77	1.46	1.41
4	J	1003	AMP	O4'-C1'	3.75	1.46	1.41
4	R	1003	AMP	O4'-C1'	3.70	1.46	1.41
4	B	1003	AMP	O4'-C1'	3.60	1.46	1.41
4	L	1003	AMP	O4'-C1'	3.56	1.46	1.41
3	E	1002	PO4	P-O1	3.44	1.58	1.50
3	I	1002	PO4	P-O1	3.42	1.58	1.50
4	K	1003	AMP	O4'-C1'	3.31	1.45	1.41
3	L	1002	PO4	P-O1	3.29	1.58	1.50
3	H	1002	PO4	P-O1	3.29	1.58	1.50
3	B	1002	PO4	P-O1	3.28	1.58	1.50
3	G	1002	PO4	P-O1	3.28	1.58	1.50
3	C	1002	PO4	P-O1	3.28	1.58	1.50
3	J	1002	PO4	P-O1	3.27	1.58	1.50
3	N	1002	PO4	P-O1	3.22	1.58	1.50
4	E	1003	AMP	O4'-C1'	3.22	1.45	1.41
3	Q	1002	PO4	P-O1	3.21	1.58	1.50
3	A	1002	PO4	P-O1	3.21	1.58	1.50
3	D	1002	PO4	P-O1	3.19	1.58	1.50
3	O	1002	PO4	P-O1	3.18	1.58	1.50
4	O	1003	AMP	O4'-C1'	3.14	1.45	1.41
3	F	1002	PO4	P-O1	3.05	1.58	1.50
3	P	1002	PO4	P-O1	3.02	1.57	1.50
3	K	1002	PO4	P-O1	3.01	1.57	1.50
3	R	1002	PO4	P-O1	2.95	1.57	1.50
4	A	1003	AMP	C8-N7	-2.75	1.29	1.34
4	O	1003	AMP	C2-N3	2.71	1.36	1.32
4	H	1003	AMP	O4'-C1'	2.69	1.44	1.41
4	P	1003	AMP	O4'-C1'	2.50	1.44	1.41
4	H	1003	AMP	C2-N3	2.48	1.36	1.32
4	E	1003	AMP	C2-N3	2.45	1.36	1.32
4	N	1003	AMP	C8-N7	-2.39	1.30	1.34
4	N	1003	AMP	C2-N3	2.38	1.35	1.32
4	R	1003	AMP	C2-N3	2.34	1.35	1.32
4	Q	1003	AMP	C2-N3	2.32	1.35	1.32
4	F	1003	AMP	C2-N3	2.32	1.35	1.32
4	L	1003	AMP	C2-N3	2.29	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	AMP	C2-N3	2.27	1.35	1.32
4	D	1003	AMP	C2-N3	2.20	1.35	1.32
4	C	1003	AMP	C2-N3	2.20	1.35	1.32
4	G	1003	AMP	C2-N3	2.15	1.35	1.32
4	I	1003	AMP	C2-N3	2.06	1.35	1.32
4	P	1003	AMP	C2-N3	2.04	1.35	1.32

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1003	AMP	O4'-C1'-C2'	-5.72	98.56	106.93
4	A	1003	AMP	P-O5'-C5'	-4.40	106.17	118.30
4	P	1003	AMP	O3P-P-O5'	4.20	117.91	106.73
4	O	1003	AMP	C4-C5-N7	4.17	113.75	109.40
4	M	1003	AMP	N3-C2-N1	-4.04	122.36	128.68
4	O	1003	AMP	C3'-C2'-C1'	3.57	106.35	100.98
4	H	1003	AMP	O5'-P-O1P	3.24	115.56	106.47
4	F	1003	AMP	C3'-C2'-C1'	3.20	105.79	100.98
4	I	1003	AMP	P-O5'-C5'	-3.18	109.54	118.30
4	A	1003	AMP	C3'-C2'-C1'	3.17	105.75	100.98
4	E	1003	AMP	C3'-C2'-C1'	3.00	105.50	100.98
4	H	1003	AMP	C3'-C2'-C1'	2.94	105.40	100.98
4	M	1003	AMP	C1'-N9-C4	-2.93	121.50	126.64
4	P	1003	AMP	C3'-C2'-C1'	2.75	105.11	100.98
4	M	1003	AMP	O4'-C1'-C2'	2.74	110.94	106.93
4	R	1003	AMP	C3'-C2'-C1'	2.73	105.09	100.98
4	Q	1003	AMP	C3'-C2'-C1'	2.71	105.05	100.98
4	K	1003	AMP	C3'-C2'-C1'	2.66	104.98	100.98
4	M	1003	AMP	N6-C6-N1	2.62	124.02	118.57
4	N	1003	AMP	C2'-C3'-C4'	-2.62	97.55	102.64
4	P	1003	AMP	O4'-C1'-C2'	-2.57	103.17	106.93
4	H	1003	AMP	C5-C6-N6	2.51	124.17	120.35
4	G	1003	AMP	C3'-C2'-C1'	2.50	104.74	100.98
4	J	1003	AMP	C5-C6-N6	2.46	124.09	120.35
4	M	1003	AMP	O3'-C3'-C2'	-2.45	103.89	111.82
4	N	1003	AMP	O4'-C1'-C2'	-2.39	103.43	106.93
4	B	1003	AMP	C3'-C2'-C1'	2.37	104.54	100.98
4	L	1003	AMP	C5-C6-N6	2.31	123.86	120.35
4	Q	1003	AMP	C5-C6-N6	2.29	123.83	120.35
4	N	1003	AMP	C4-C5-N7	2.23	111.72	109.40
4	D	1003	AMP	C5-C6-N6	2.20	123.70	120.35
4	O	1003	AMP	O4'-C4'-C3'	2.20	109.46	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1003	AMP	O4'-C4'-C3'	2.15	109.37	105.11
4	M	1003	AMP	C2-N1-C6	2.15	122.43	118.75
4	A	1003	AMP	O2'-C2'-C3'	-2.13	104.95	111.82
4	H	1003	AMP	O4'-C4'-C5'	2.12	116.34	109.37
4	I	1003	AMP	C5-C6-N6	2.10	123.55	120.35
4	P	1003	AMP	C5-C6-N6	2.08	123.52	120.35
4	N	1003	AMP	C5'-C4'-C3'	-2.07	107.42	115.18
4	C	1003	AMP	C5-C6-N6	2.05	123.47	120.35
4	P	1003	AMP	O4'-C4'-C5'	2.05	116.10	109.37
4	K	1003	AMP	C5-C6-N6	2.04	123.46	120.35
4	H	1003	AMP	C2'-C3'-C4'	-2.04	98.67	102.64
4	M	1003	AMP	C3'-C2'-C1'	2.03	104.03	100.98
4	G	1003	AMP	C5-C6-N6	2.02	123.42	120.35
4	I	1003	AMP	O3P-P-O5'	2.01	112.07	106.73

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1003	AMP	C5'-O5'-P-O1P
4	E	1003	AMP	C4'-C5'-O5'-P
4	G	1003	AMP	C5'-O5'-P-O2P
4	G	1003	AMP	C5'-O5'-P-O3P
4	M	1003	AMP	C4'-C5'-O5'-P
4	O	1003	AMP	O4'-C4'-C5'-O5'
4	O	1003	AMP	C3'-C4'-C5'-O5'
4	D	1003	AMP	C5'-O5'-P-O1P
4	D	1003	AMP	C5'-O5'-P-O2P
4	D	1003	AMP	C5'-O5'-P-O3P
4	D	1003	AMP	O4'-C4'-C5'-O5'
4	L	1003	AMP	C5'-O5'-P-O2P
4	L	1003	AMP	C5'-O5'-P-O3P
4	L	1003	AMP	O4'-C4'-C5'-O5'
4	N	1003	AMP	C4'-C5'-O5'-P
4	H	1003	AMP	C5'-O5'-P-O1P
4	H	1003	AMP	C5'-O5'-P-O2P
4	H	1003	AMP	C5'-O5'-P-O3P
4	H	1003	AMP	C4'-C5'-O5'-P
4	P	1003	AMP	C5'-O5'-P-O2P
4	P	1003	AMP	C5'-O5'-P-O3P
4	P	1003	AMP	C4'-C5'-O5'-P
4	F	1003	AMP	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
4	F	1003	AMP	C5'-O5'-P-O2P
4	F	1003	AMP	C5'-O5'-P-O3P
4	F	1003	AMP	O4'-C4'-C5'-O5'
4	F	1003	AMP	C3'-C4'-C5'-O5'
4	A	1003	AMP	C5'-O5'-P-O1P
4	A	1003	AMP	C5'-O5'-P-O2P
4	A	1003	AMP	C5'-O5'-P-O3P
4	B	1003	AMP	C5'-O5'-P-O1P
4	B	1003	AMP	C5'-O5'-P-O2P
4	B	1003	AMP	C5'-O5'-P-O3P
4	I	1003	AMP	C5'-O5'-P-O1P
4	I	1003	AMP	C5'-O5'-P-O2P
4	I	1003	AMP	C5'-O5'-P-O3P
4	J	1003	AMP	C5'-O5'-P-O1P
4	J	1003	AMP	C5'-O5'-P-O2P
4	C	1003	AMP	O4'-C4'-C5'-O5'
4	C	1003	AMP	C3'-C4'-C5'-O5'
4	K	1003	AMP	O4'-C4'-C5'-O5'
4	K	1003	AMP	C3'-C4'-C5'-O5'
4	M	1003	AMP	O4'-C4'-C5'-O5'
4	Q	1003	AMP	C3'-C4'-C5'-O5'
4	D	1003	AMP	C3'-C4'-C5'-O5'
4	L	1003	AMP	C3'-C4'-C5'-O5'
4	N	1003	AMP	O4'-C4'-C5'-O5'
4	N	1003	AMP	C3'-C4'-C5'-O5'
4	H	1003	AMP	O4'-C4'-C5'-O5'
4	A	1003	AMP	C3'-C4'-C5'-O5'
4	Q	1003	AMP	O4'-C4'-C5'-O5'
4	A	1003	AMP	O4'-C4'-C5'-O5'
4	M	1003	AMP	C3'-C4'-C5'-O5'
4	R	1003	AMP	O4'-C4'-C5'-O5'
4	L	1003	AMP	C4'-C5'-O5'-P
4	R	1003	AMP	C3'-C4'-C5'-O5'
4	G	1003	AMP	C5'-O5'-P-O1P
4	L	1003	AMP	C5'-O5'-P-O1P
4	P	1003	AMP	C5'-O5'-P-O1P
4	G	1003	AMP	O4'-C4'-C5'-O5'
4	J	1003	AMP	O4'-C4'-C5'-O5'
4	C	1003	AMP	C5'-O5'-P-O3P
4	B	1003	AMP	C4'-C5'-O5'-P
4	J	1003	AMP	C3'-C4'-C5'-O5'
4	K	1003	AMP	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
4	Q	1003	AMP	C5'-O5'-P-O1P
4	D	1003	AMP	C4'-C5'-O5'-P
4	B	1003	AMP	O4'-C4'-C5'-O5'
4	I	1003	AMP	O4'-C4'-C5'-O5'
4	A	1003	AMP	C4'-C5'-O5'-P
4	H	1003	AMP	C3'-C4'-C5'-O5'
4	J	1003	AMP	C5'-O5'-P-O3P
4	M	1003	AMP	C5'-O5'-P-O1P

There are no ring outliers.

31 monomers are involved in 122 short contacts:

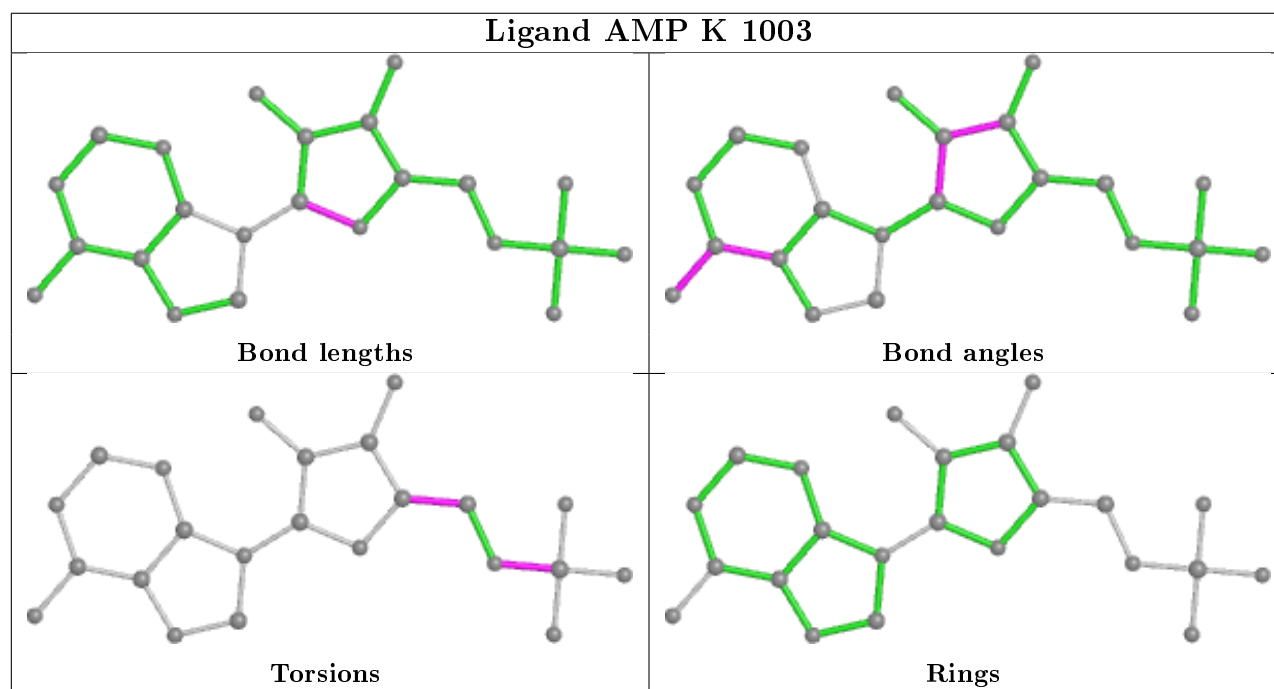
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1002	PO4	2	0
4	K	1003	AMP	4	0
4	C	1003	AMP	3	0
3	G	1002	PO4	1	0
4	E	1003	AMP	4	0
4	G	1003	AMP	9	0
3	F	1002	PO4	2	0
3	R	1002	PO4	1	0
4	M	1003	AMP	5	0
3	H	1002	PO4	2	0
4	O	1003	AMP	17	0
3	I	1002	PO4	1	0
3	P	1002	PO4	7	0
4	Q	1003	AMP	7	0
4	D	1003	AMP	5	0
4	L	1003	AMP	1	0
3	O	1002	PO4	2	0
4	N	1003	AMP	6	0
4	H	1003	AMP	1	0
4	P	1003	AMP	12	0
4	R	1003	AMP	4	0
3	B	1002	PO4	1	0
4	F	1003	AMP	2	0
3	E	1002	PO4	3	0
4	B	1003	AMP	8	0
4	I	1003	AMP	7	0
3	M	1002	PO4	3	0
3	K	1002	PO4	1	0
4	J	1003	AMP	3	0

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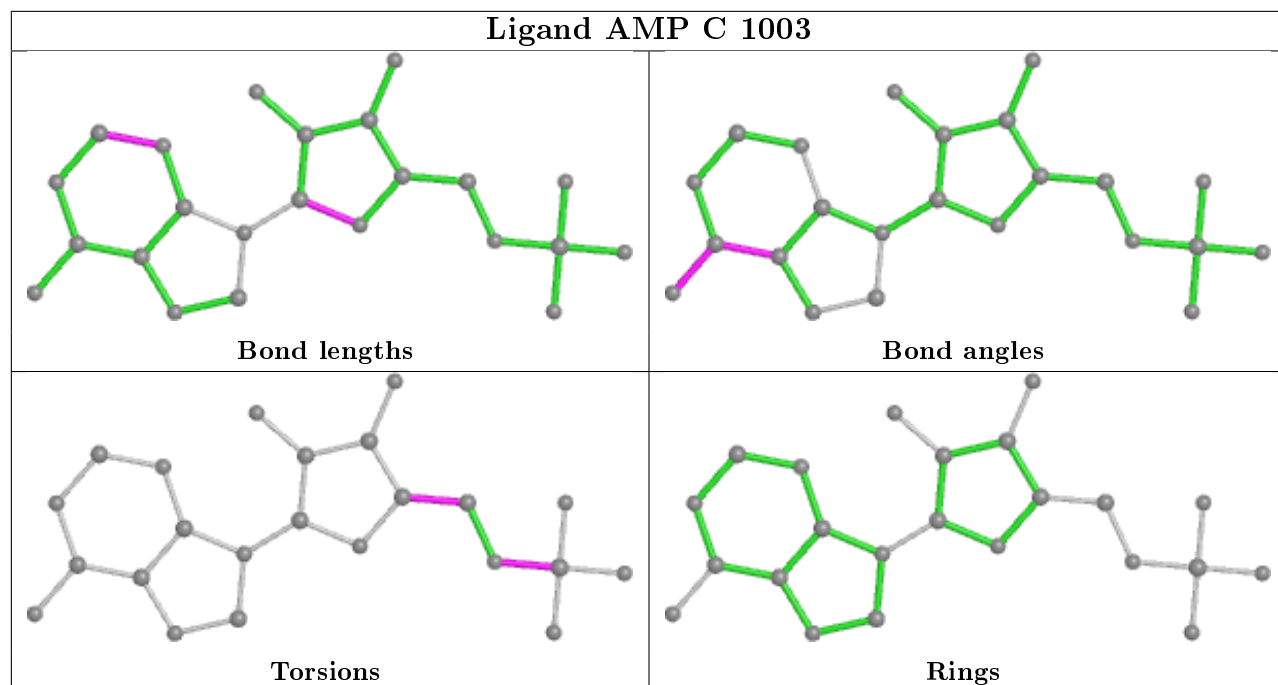
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	AMP	10	0
3	A	1002	PO4	1	0

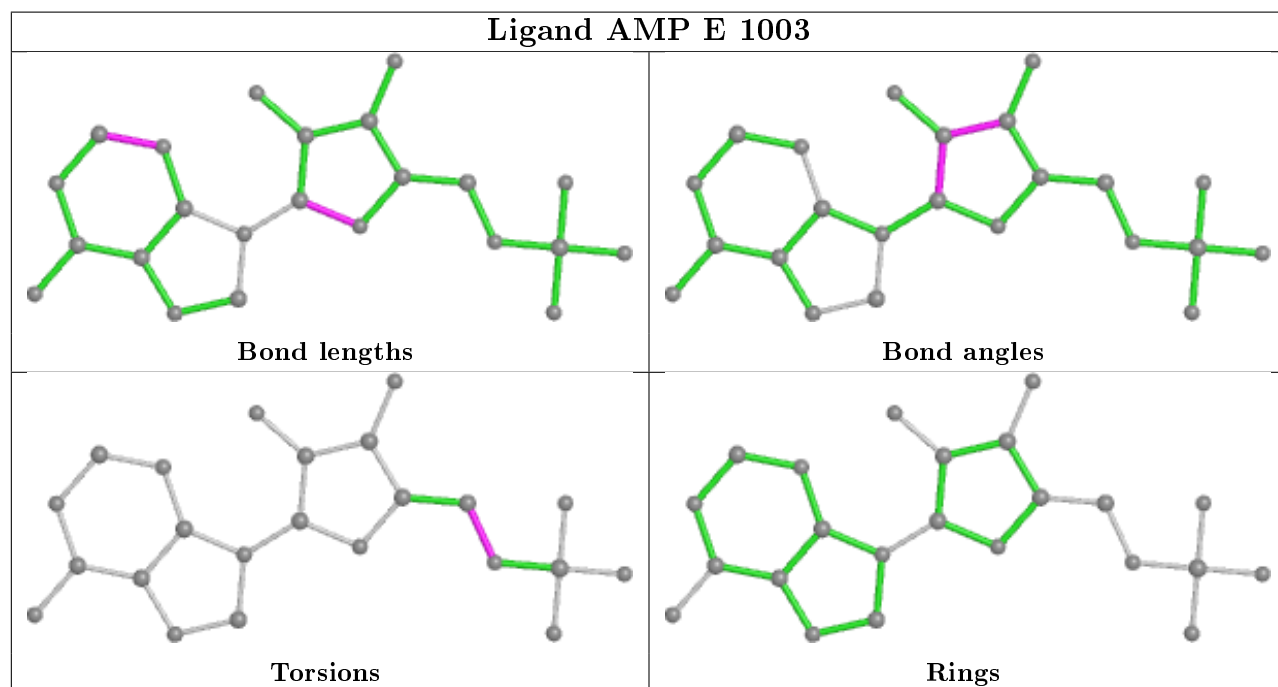
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



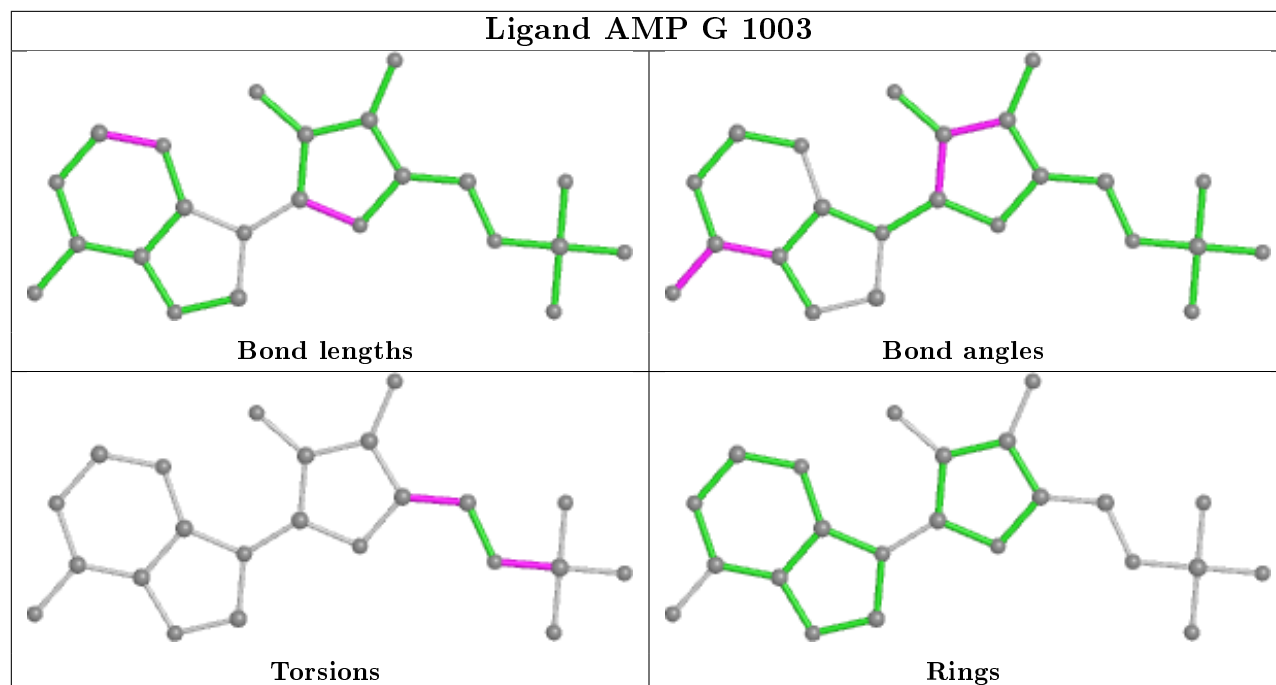
Ligand AMP C 1003



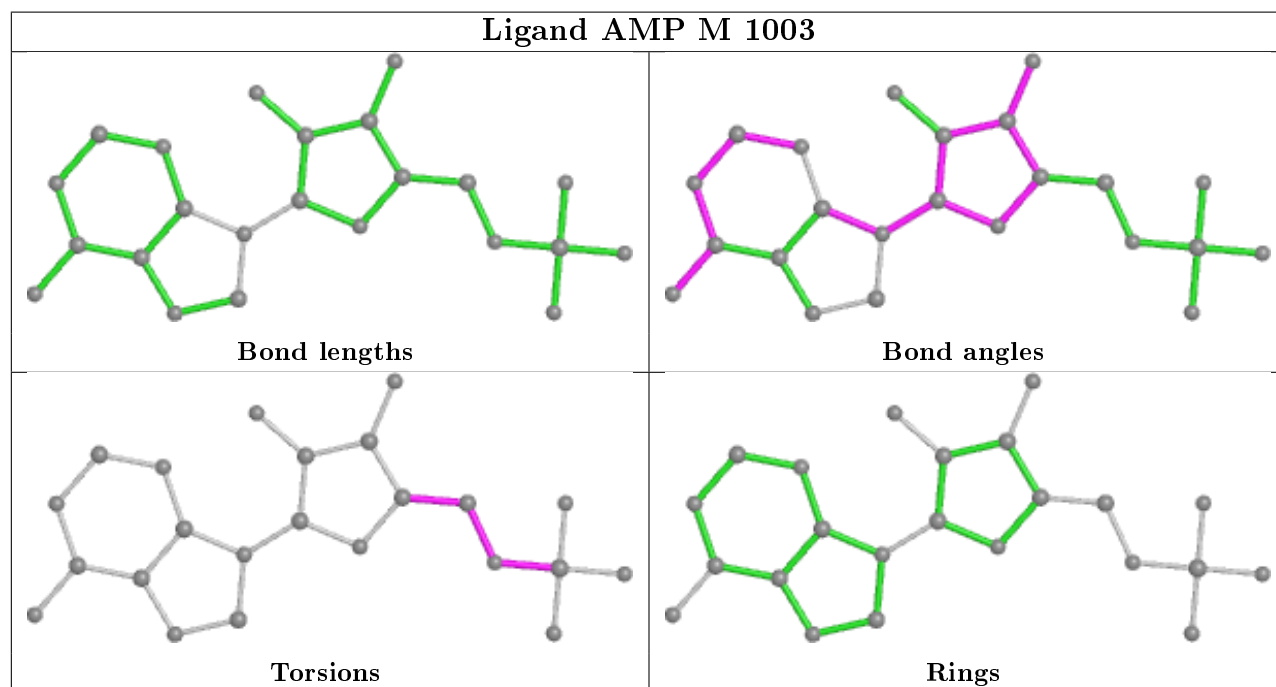
Ligand AMP E 1003



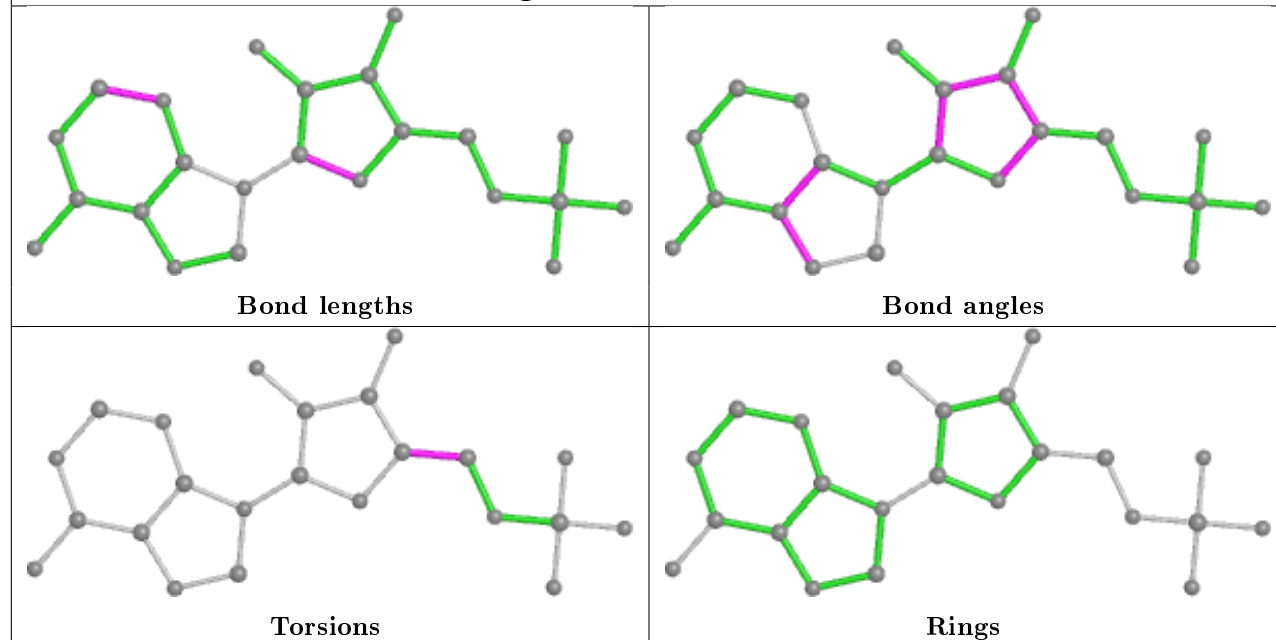
Ligand AMP G 1003



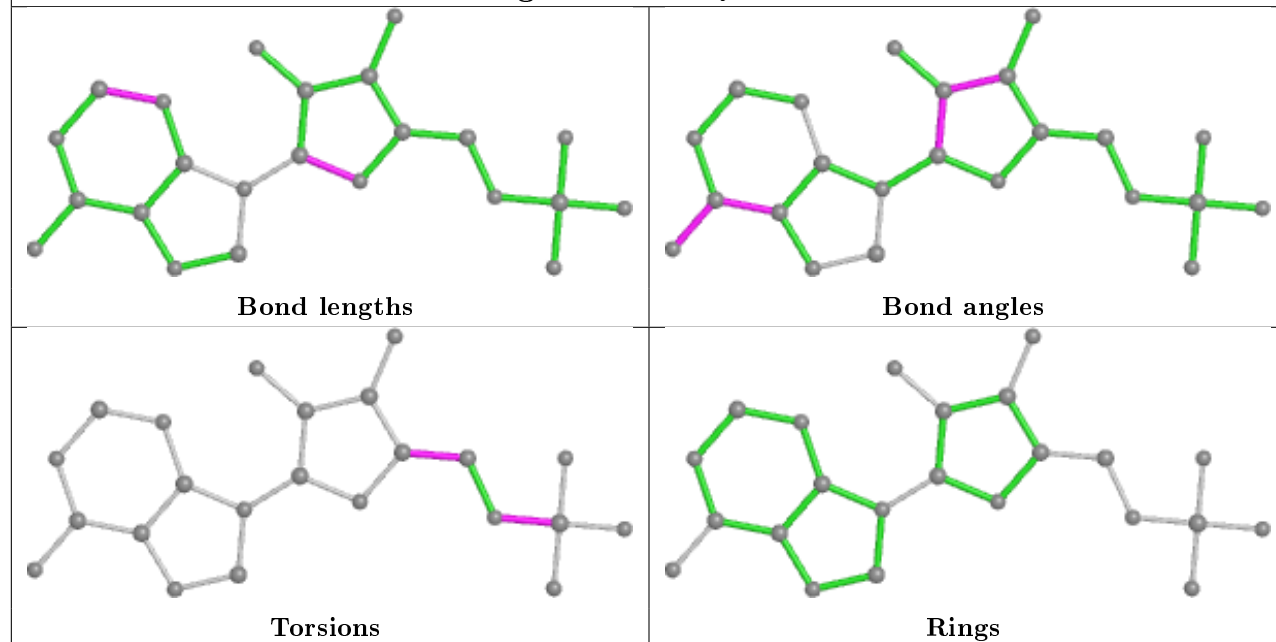
Ligand AMP M 1003



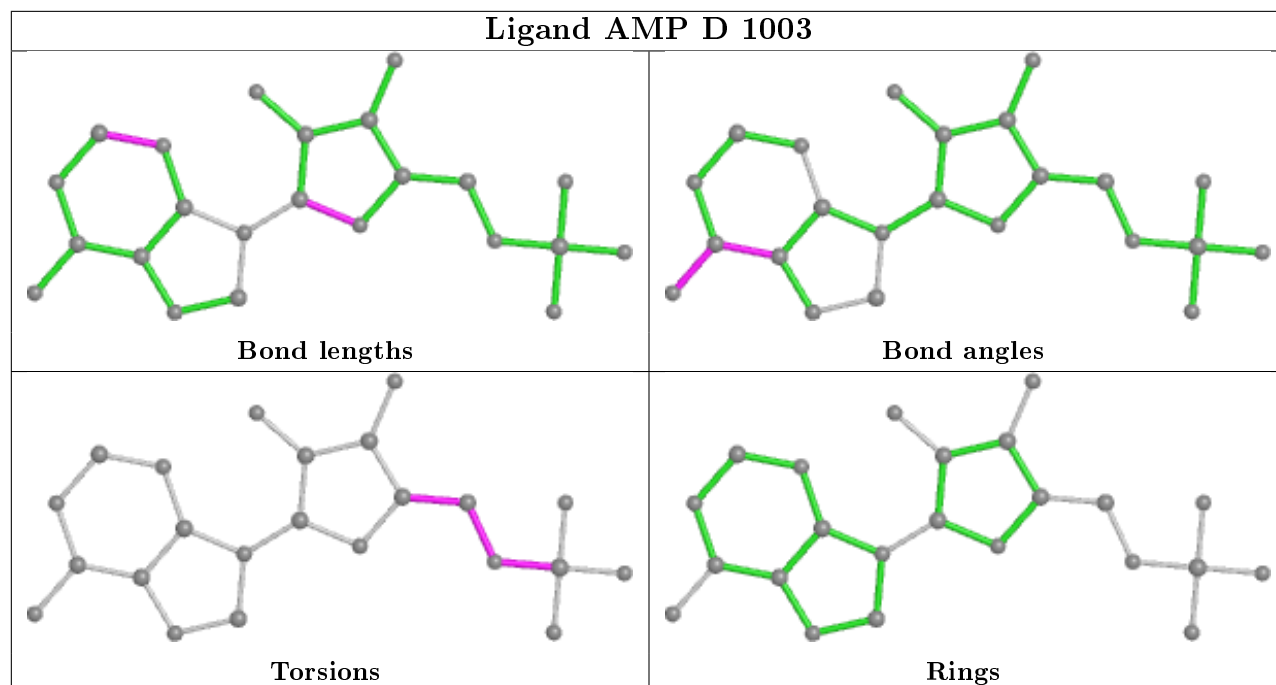
Ligand AMP O 1003



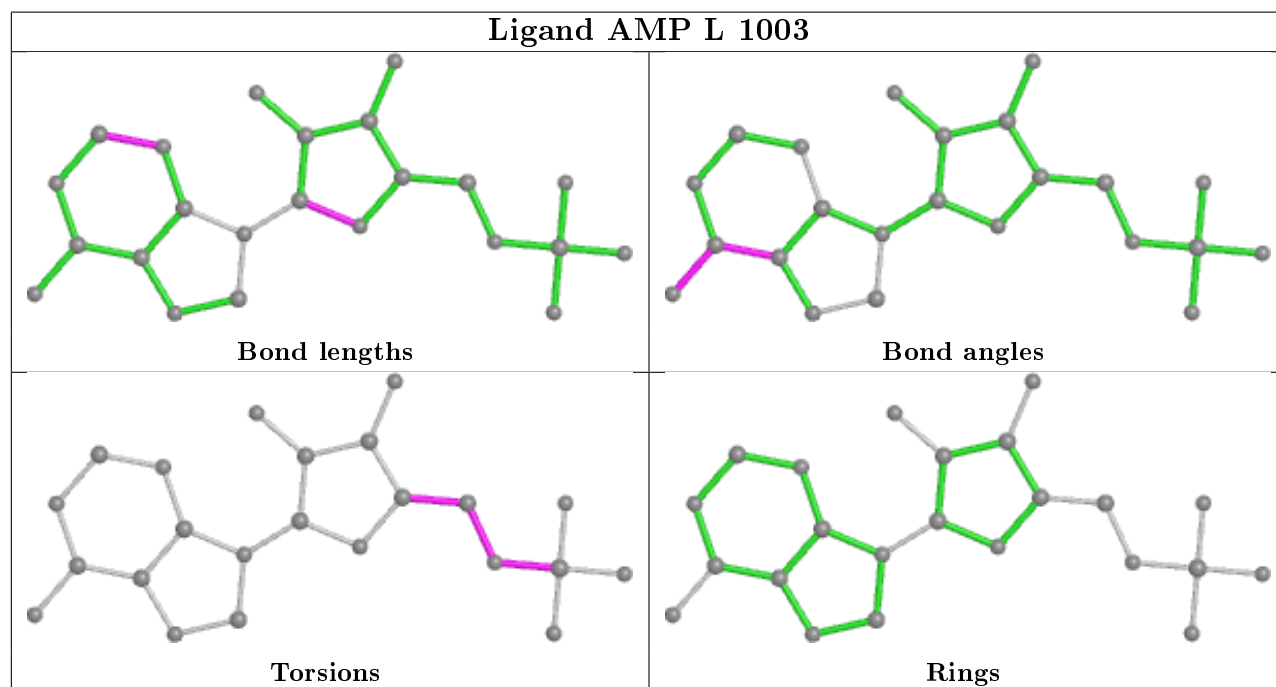
Ligand AMP Q 1003



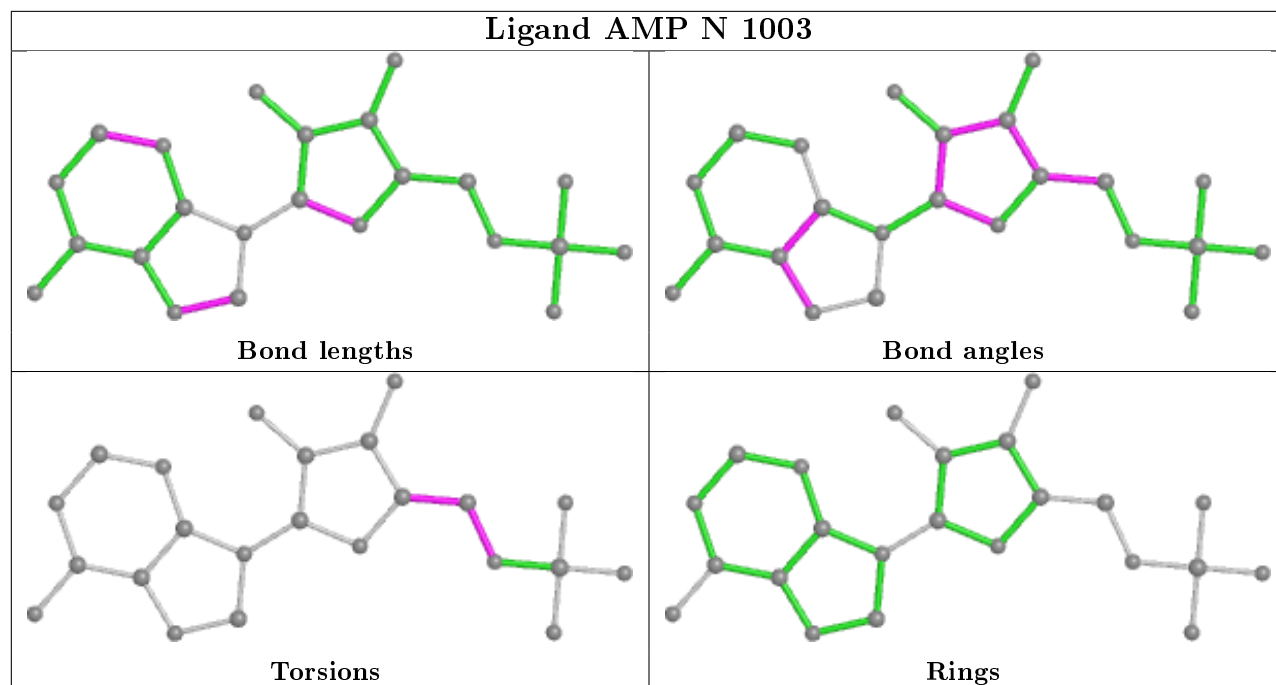
Ligand AMP D 1003



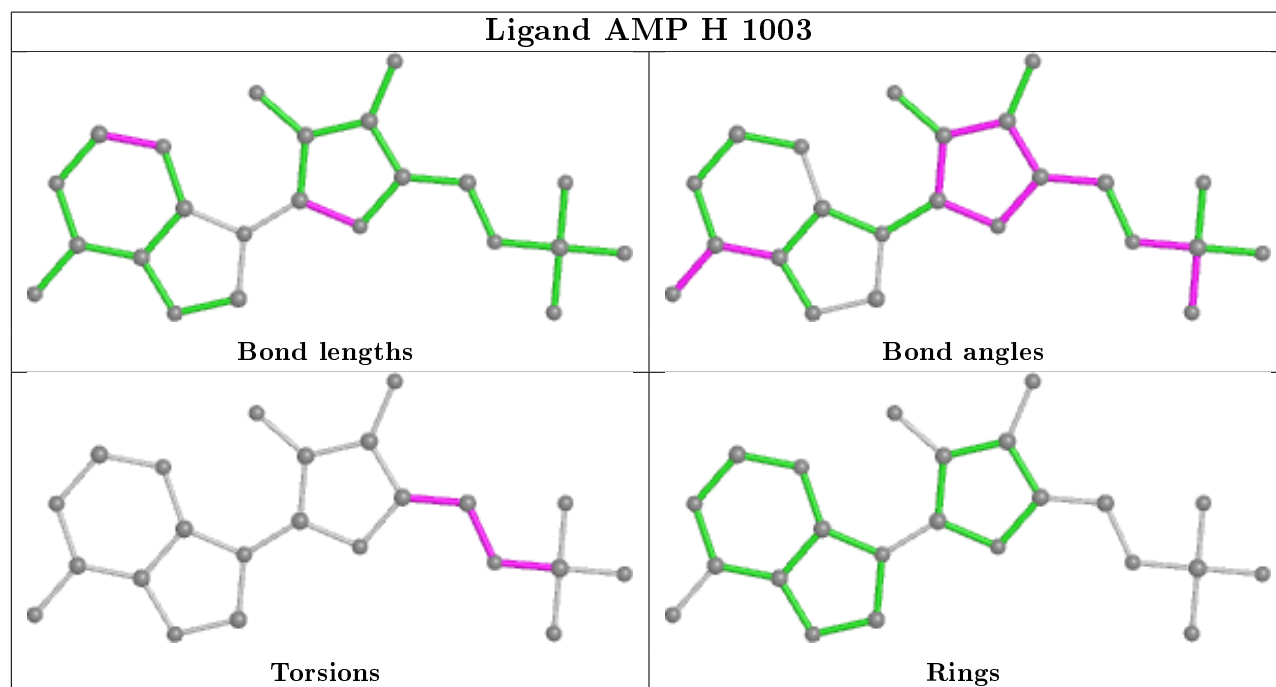
Ligand AMP L 1003



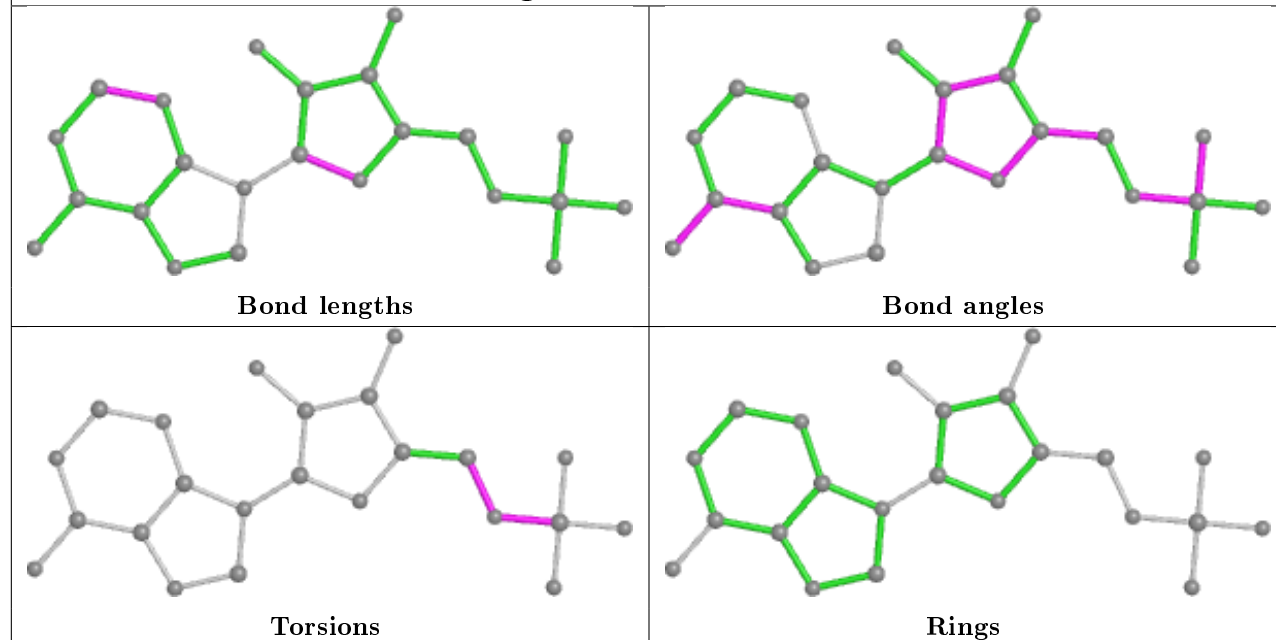
Ligand AMP N 1003



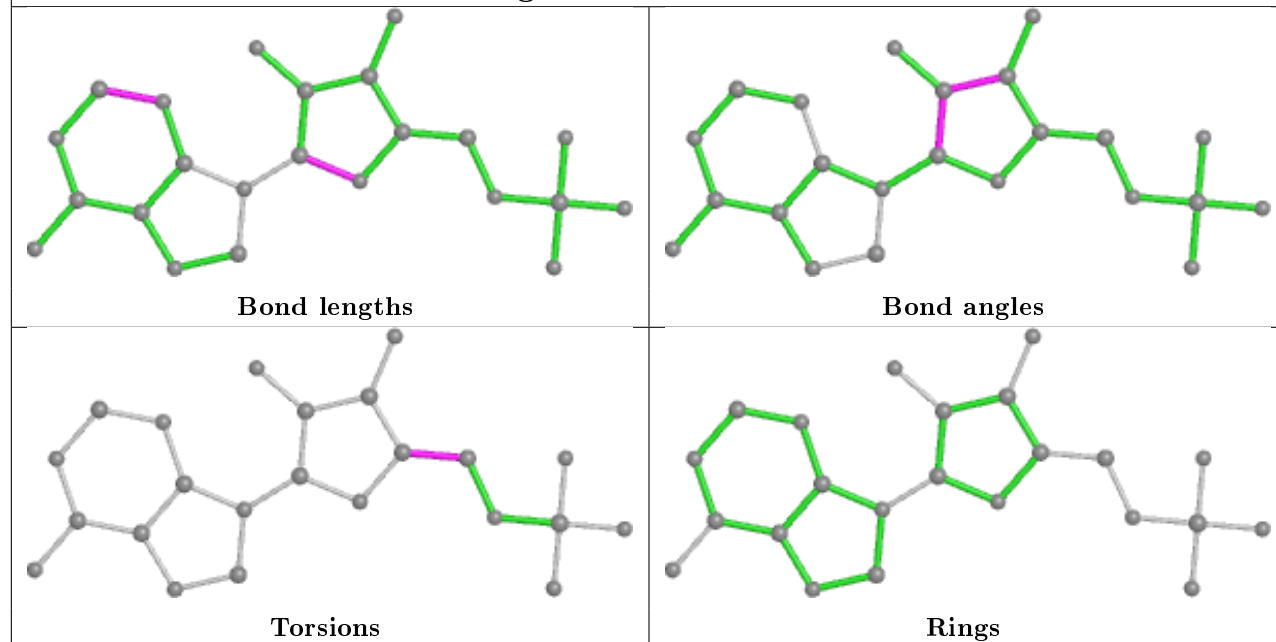
Ligand AMP H 1003



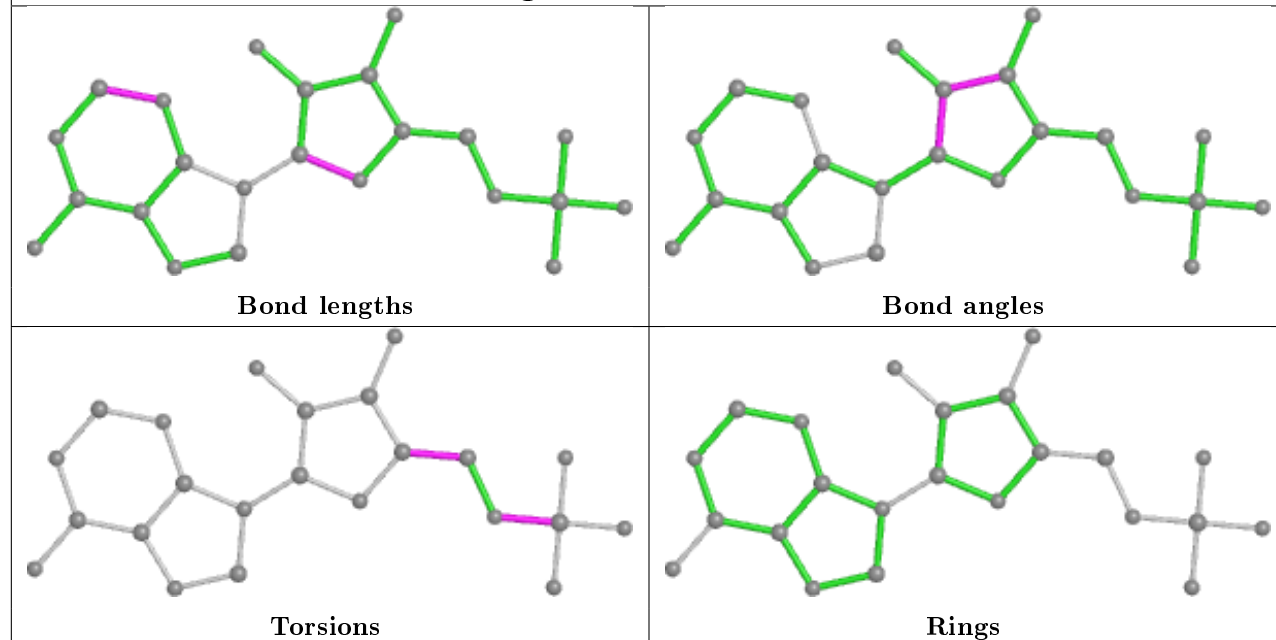
Ligand AMP P 1003



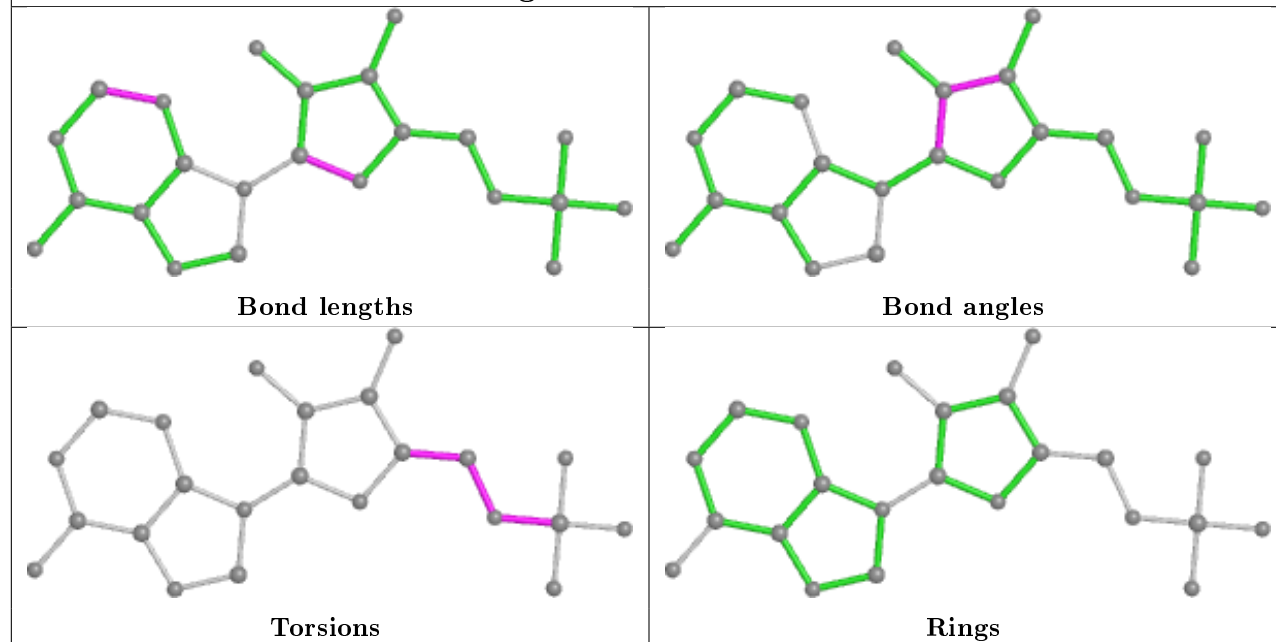
Ligand AMP R 1003



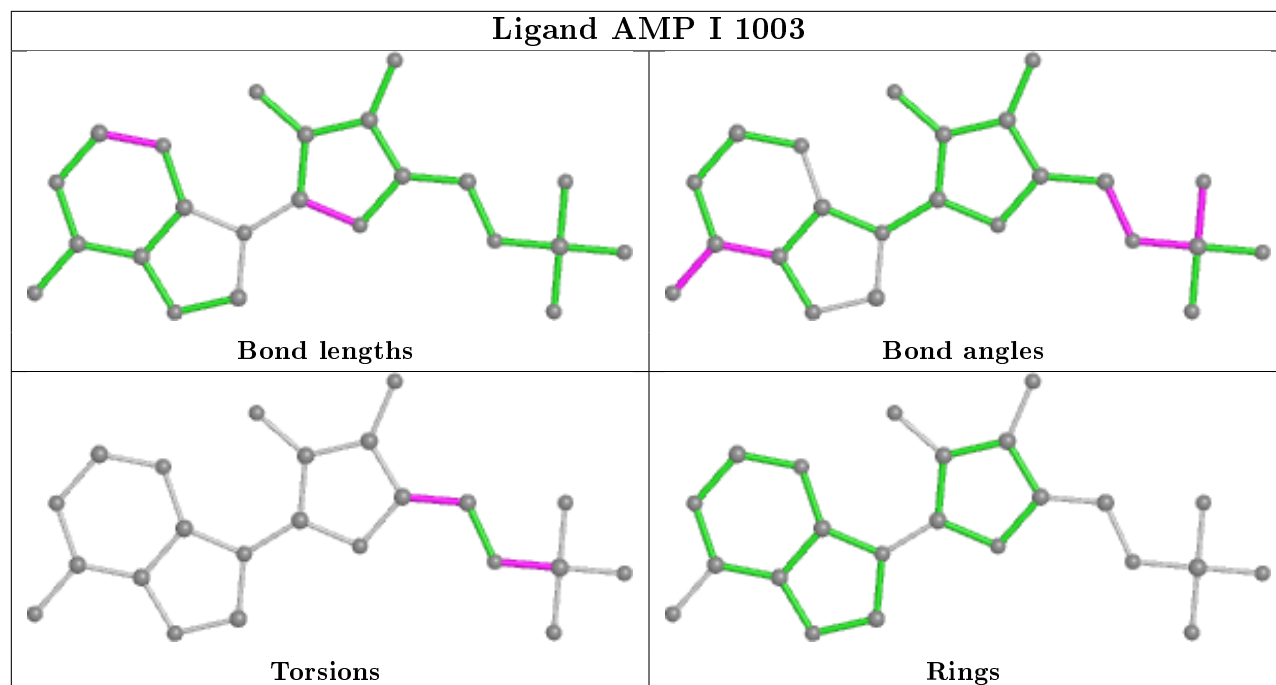
Ligand AMP F 1003



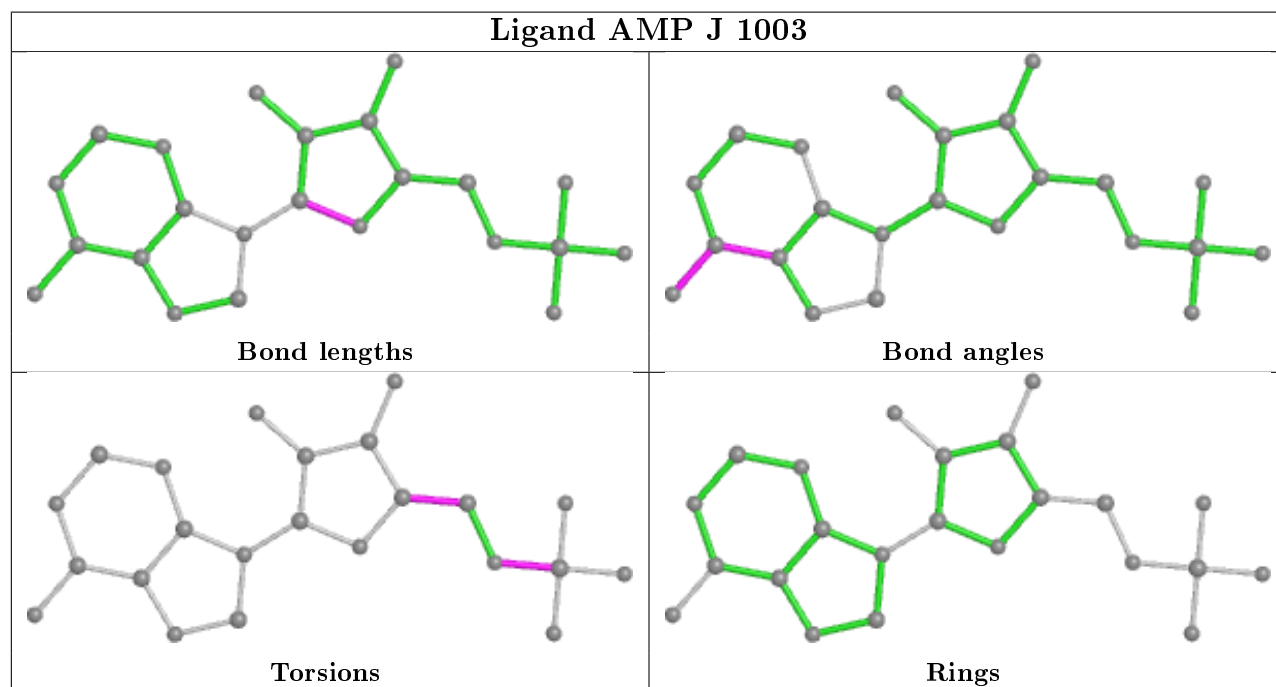
Ligand AMP B 1003

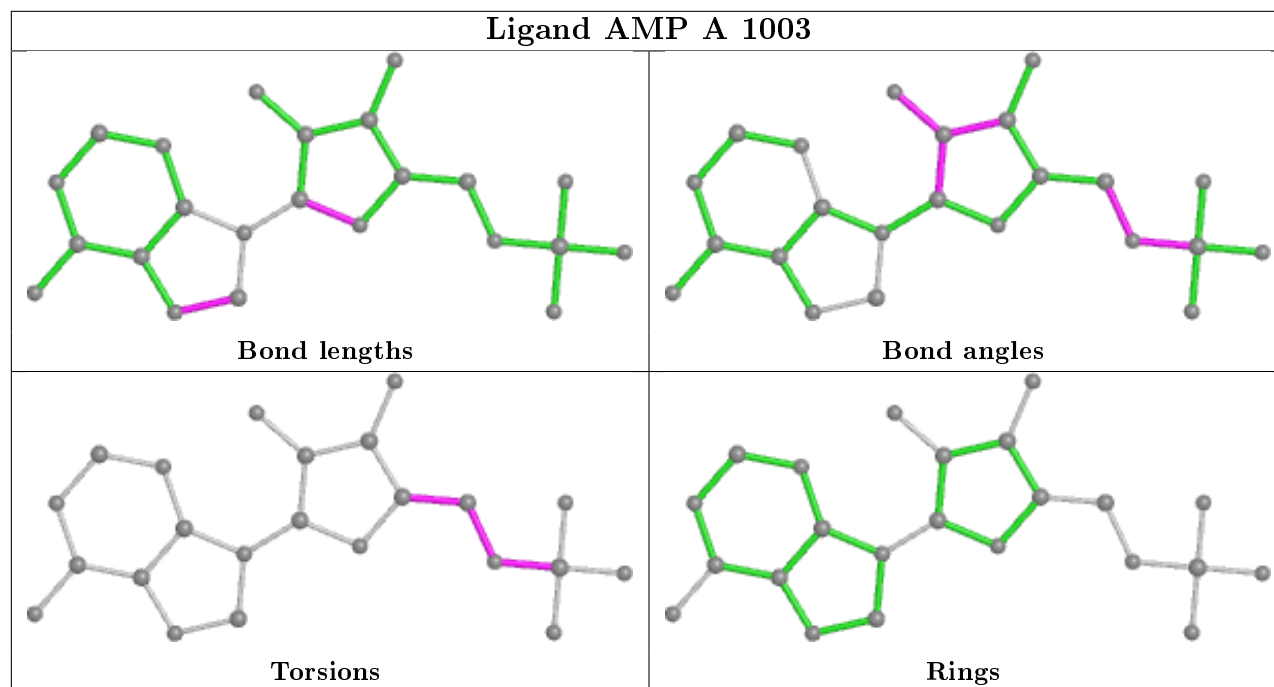


Ligand AMP I 1003



Ligand AMP J 1003





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

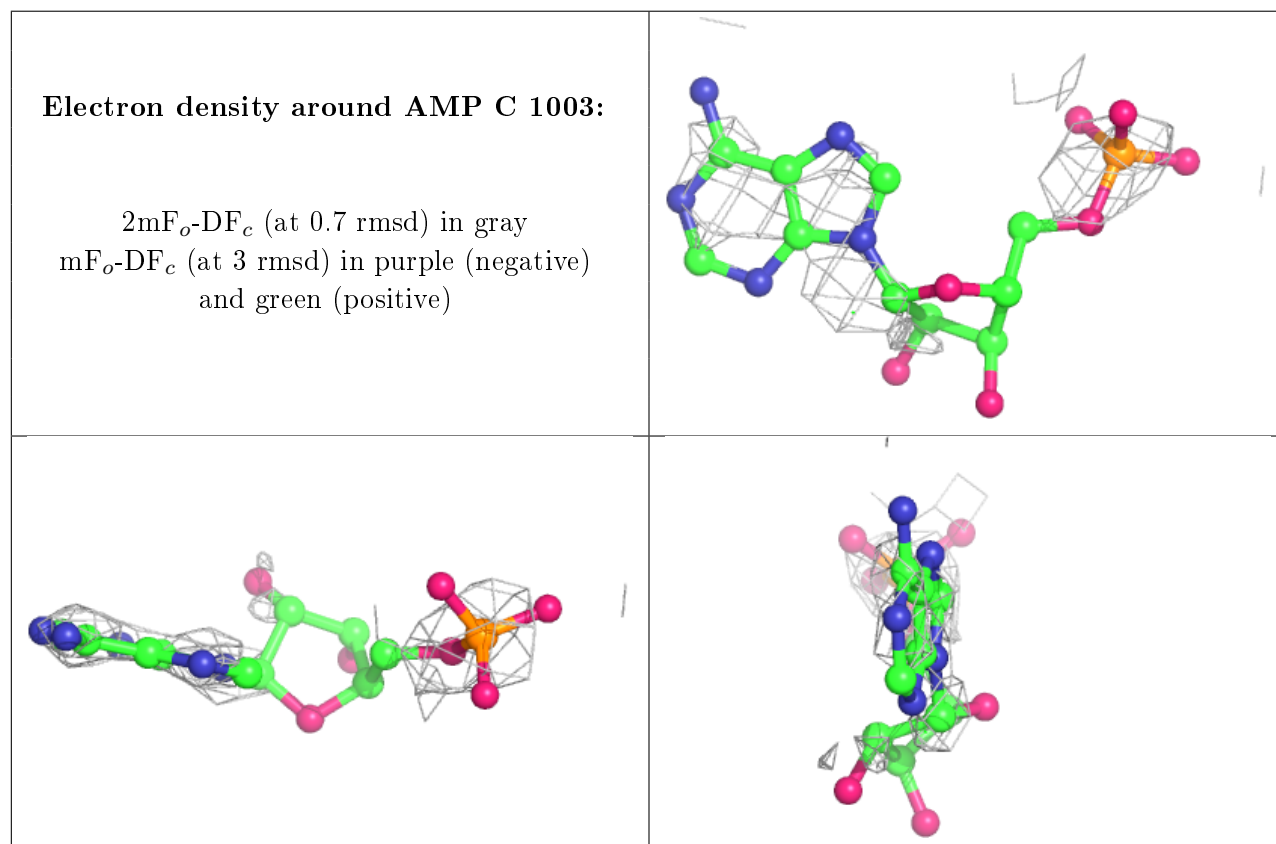
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

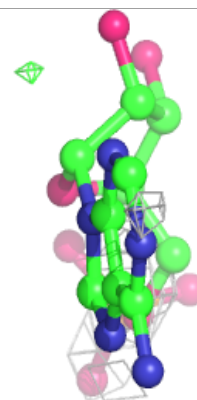
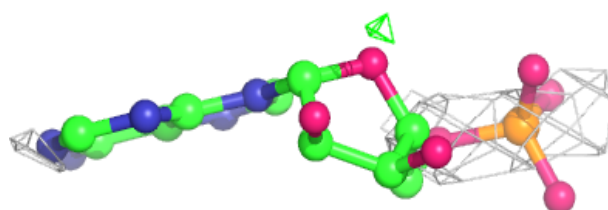
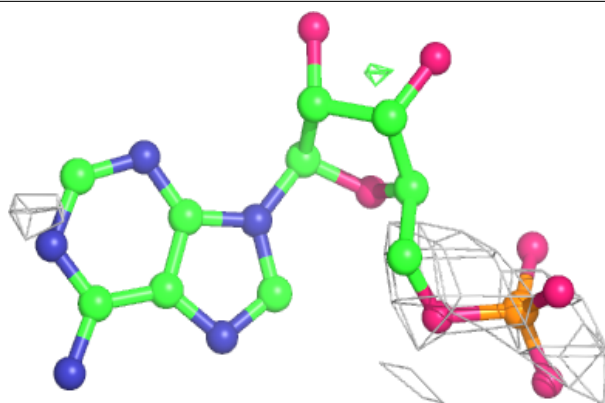
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

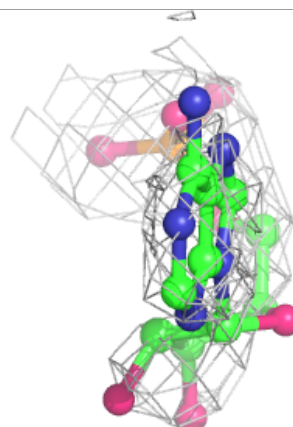
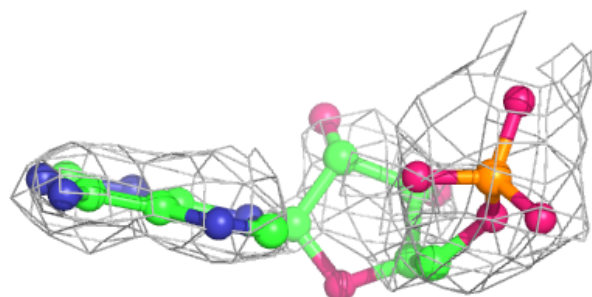
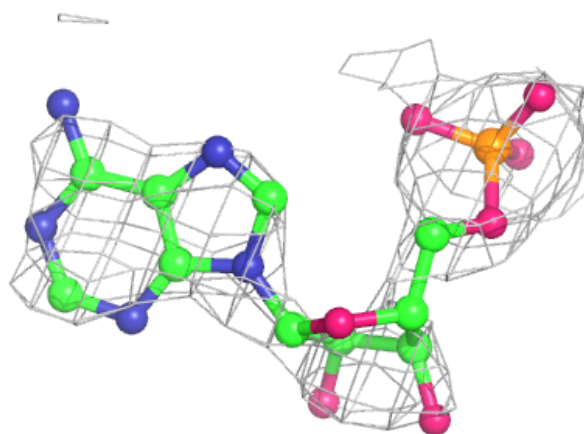


Electron density around AMP E 1003:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

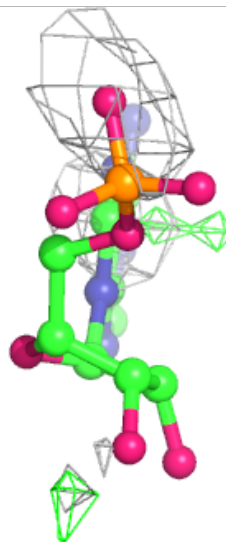
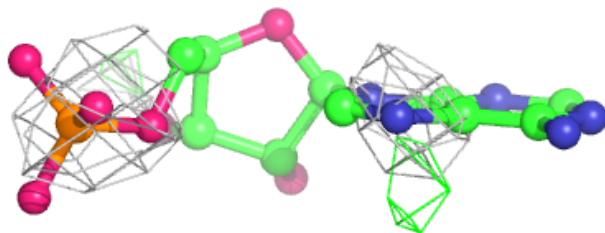
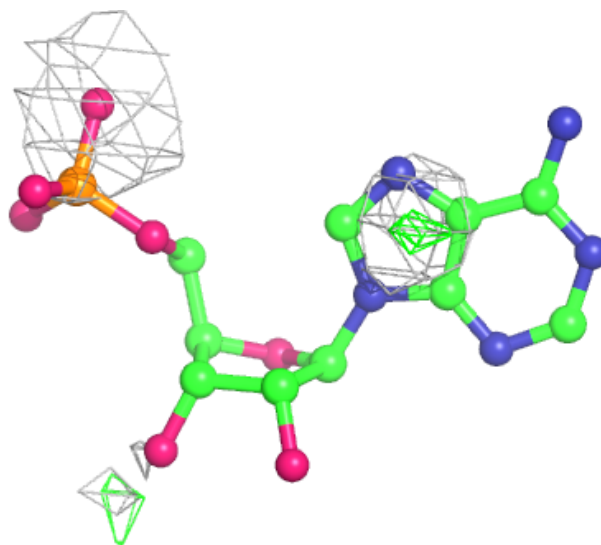
**Electron density around AMP G 1003:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



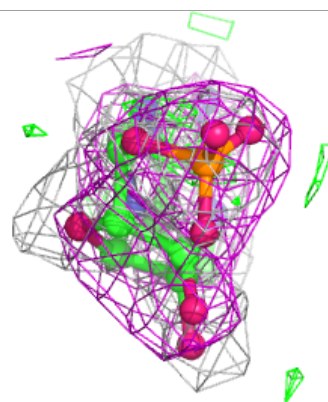
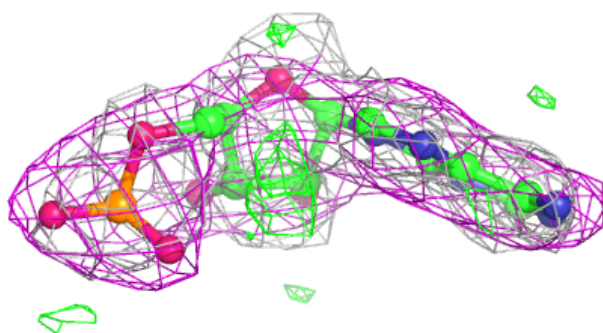
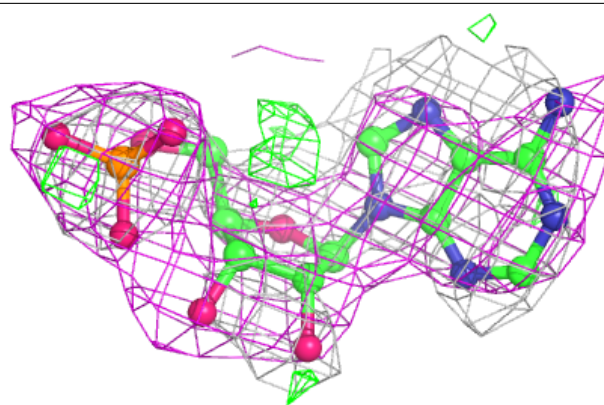
Electron density around AMP K 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

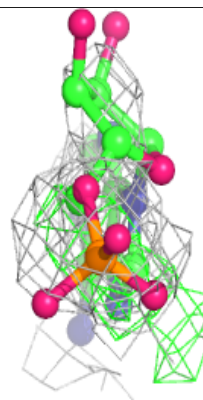
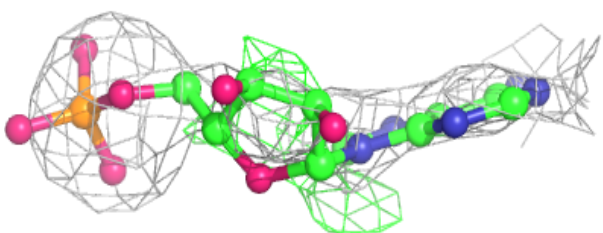
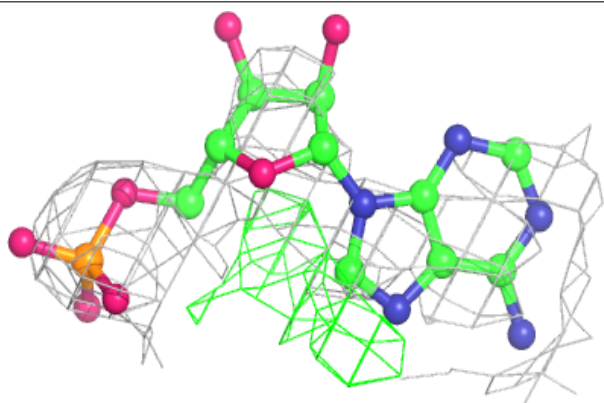


Electron density around AMP M 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

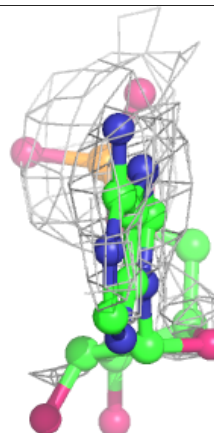
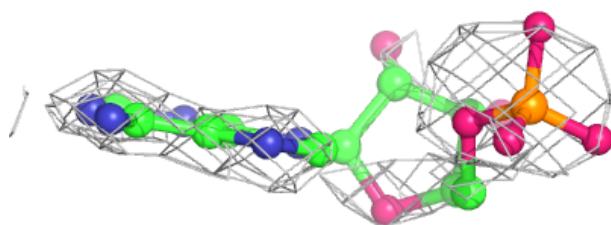
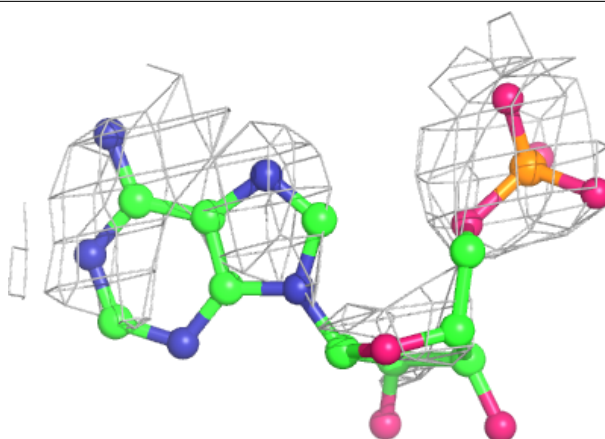
**Electron density around AMP O 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

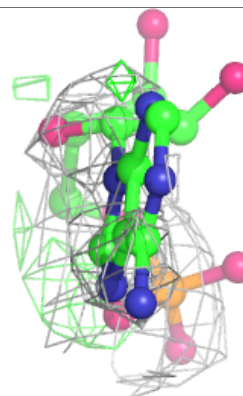
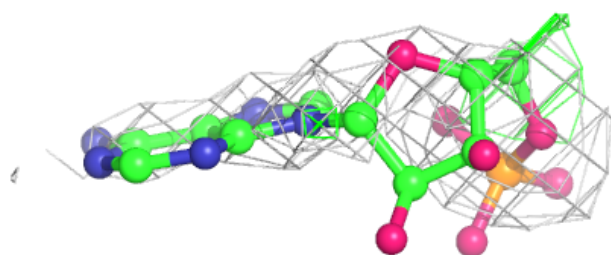
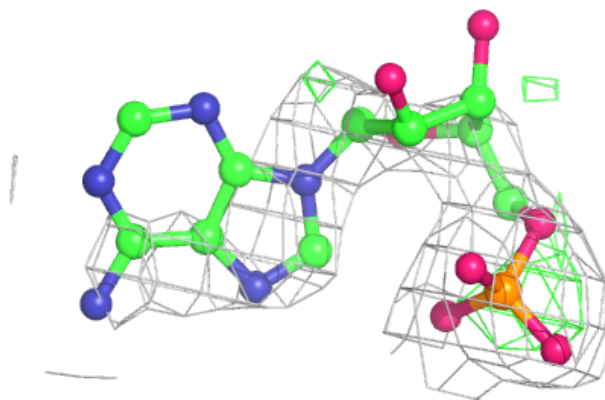


Electron density around AMP Q 1003:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

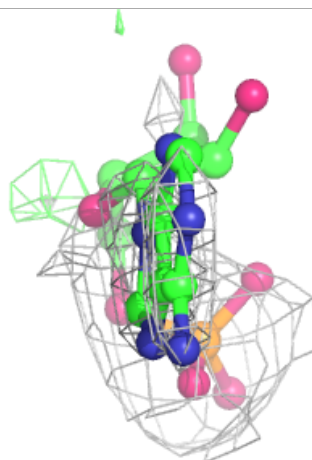
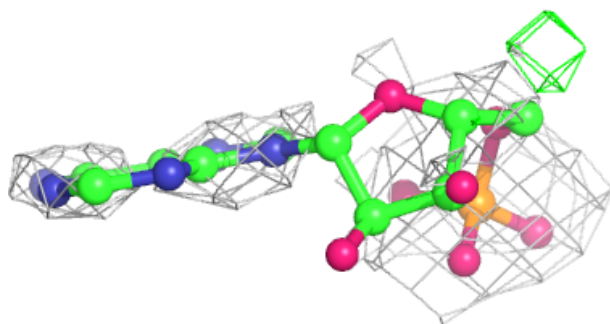
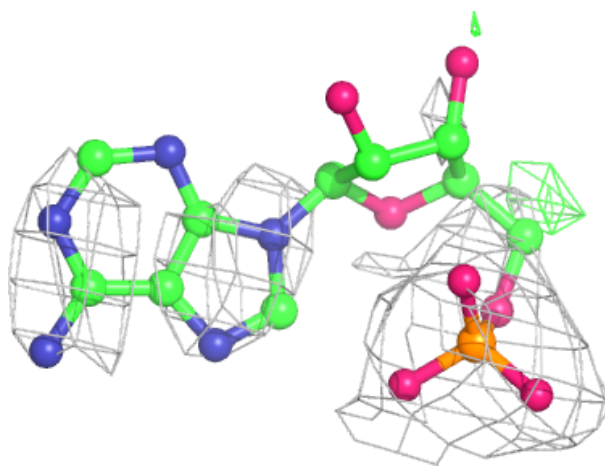
**Electron density around AMP D 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



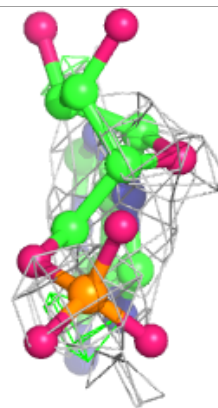
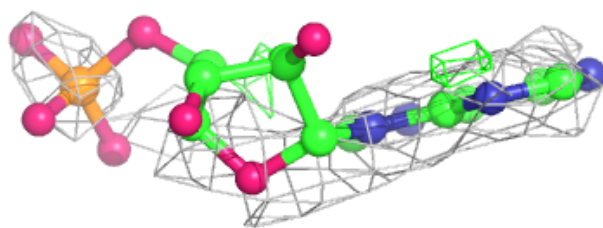
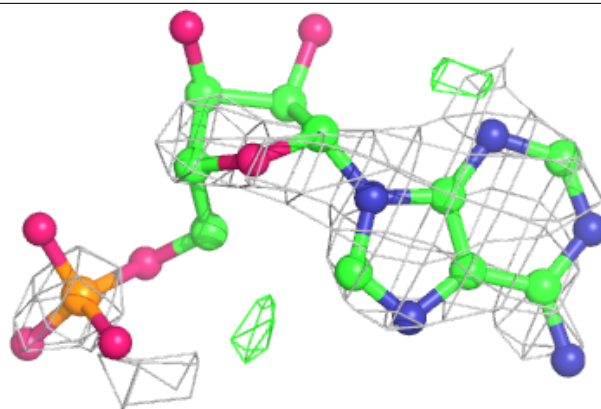
Electron density around AMP L 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



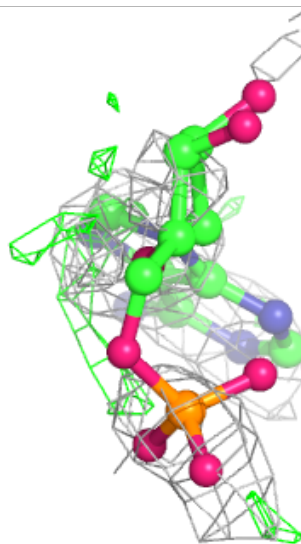
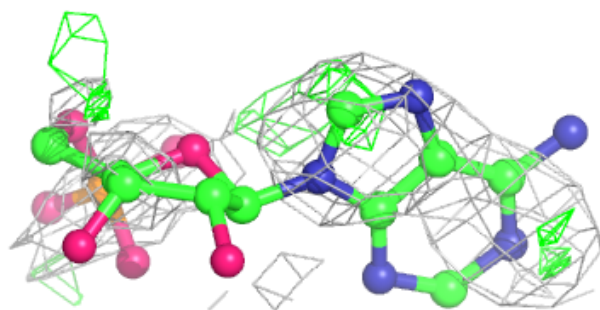
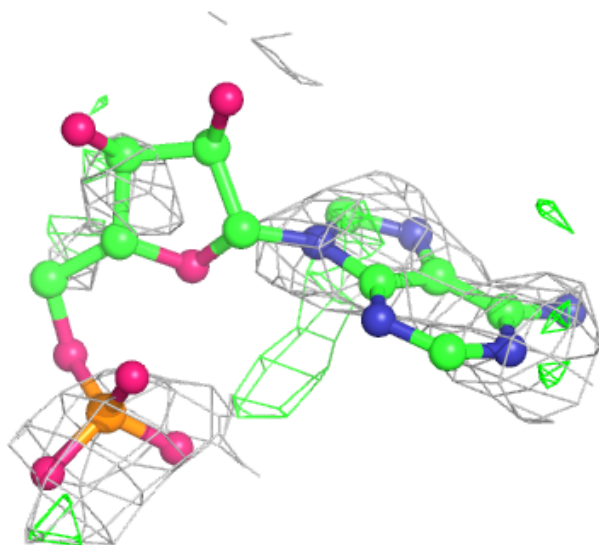
Electron density around AMP N 1003:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



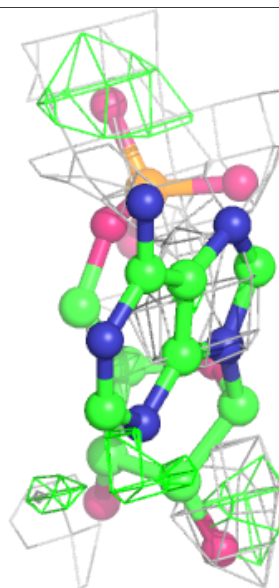
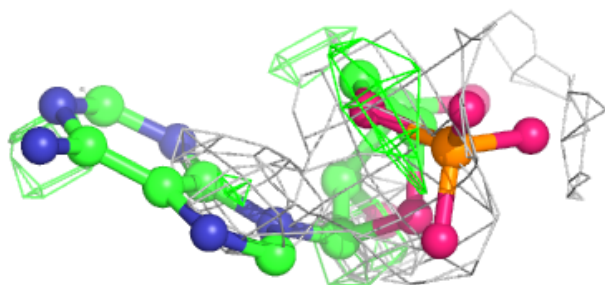
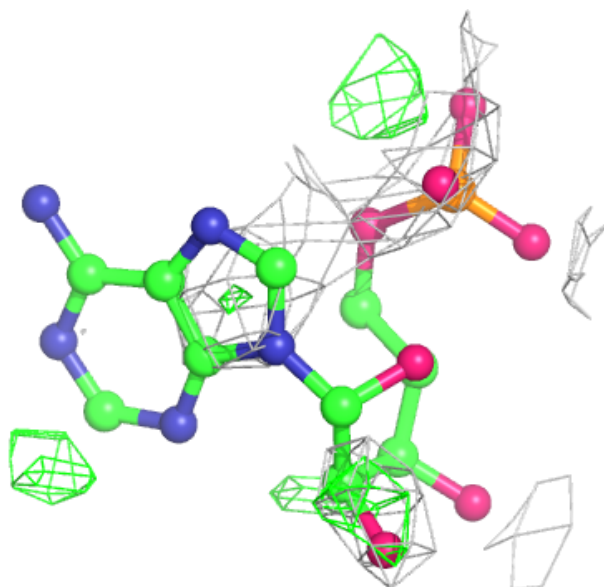
Electron density around AMP H 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



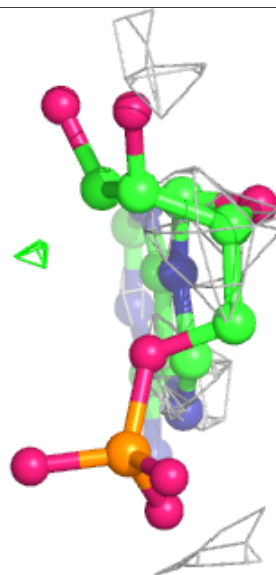
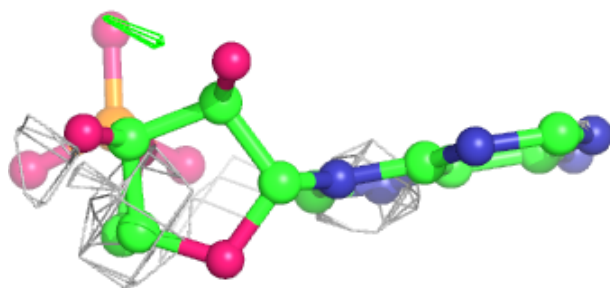
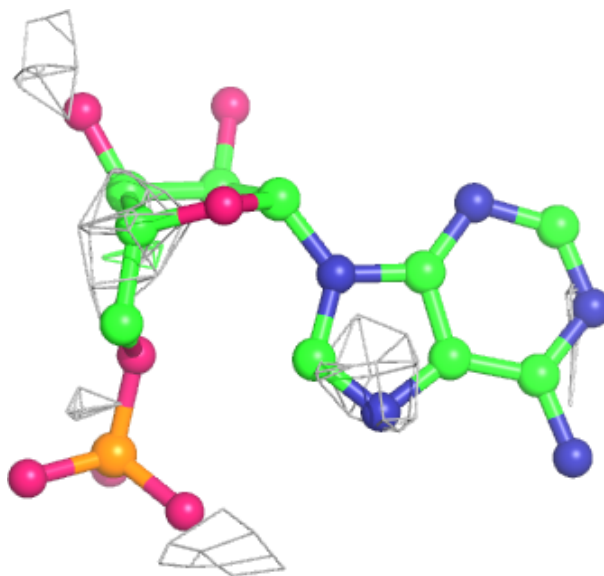
Electron density around AMP P 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



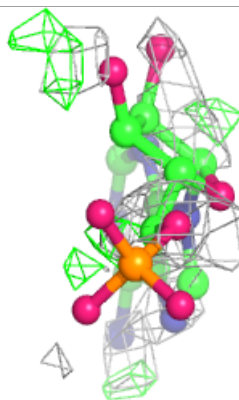
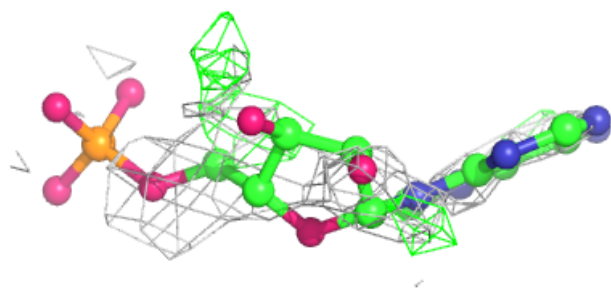
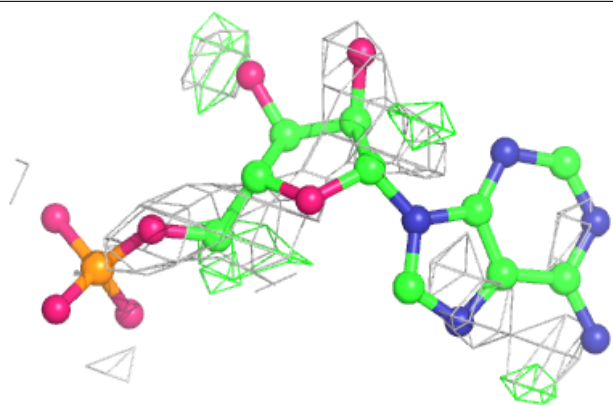
Electron density around AMP R 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

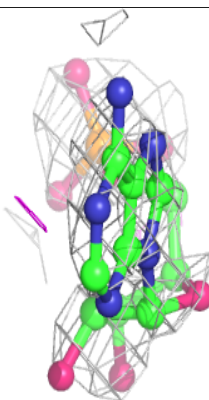
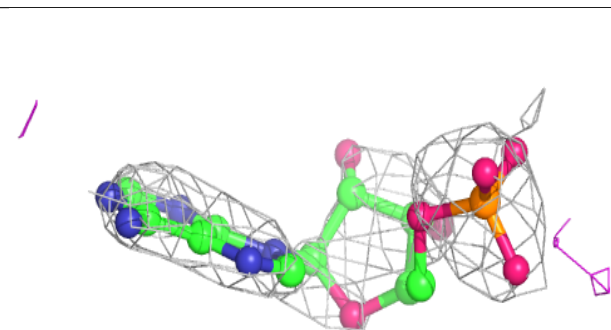
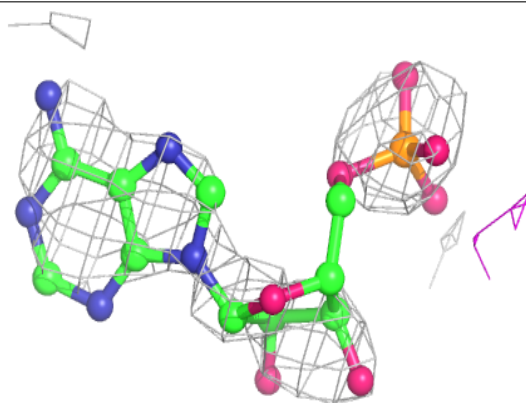


Electron density around AMP F 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

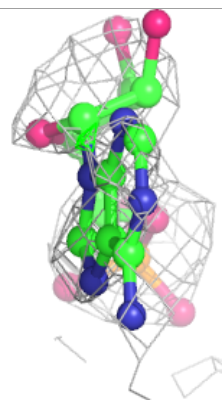
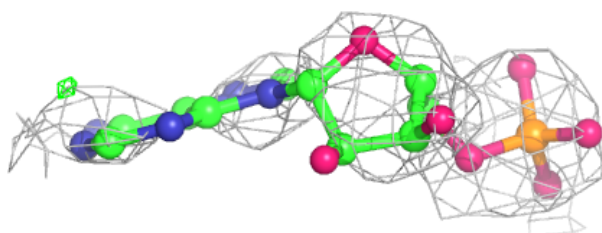
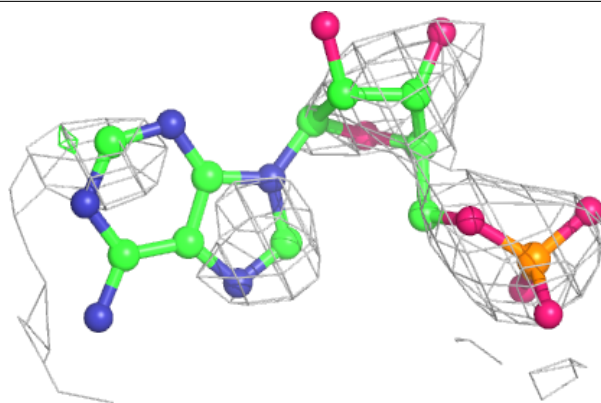
**Electron density around AMP A 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

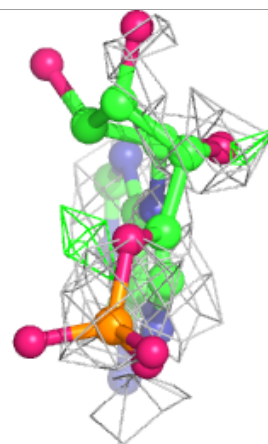
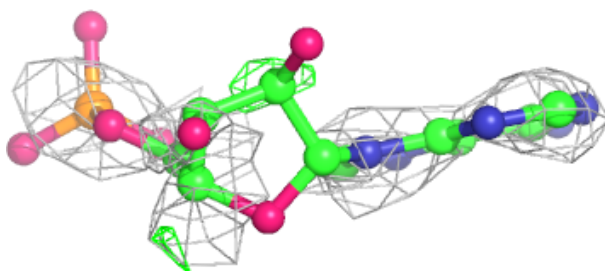
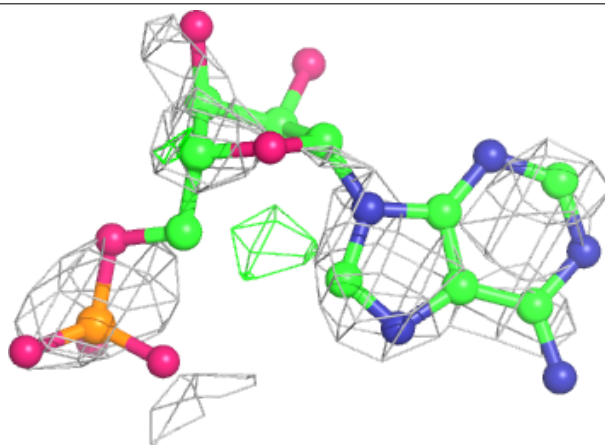


Electron density around AMP B 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

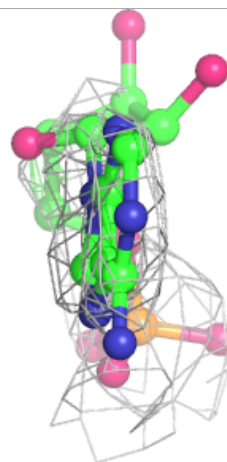
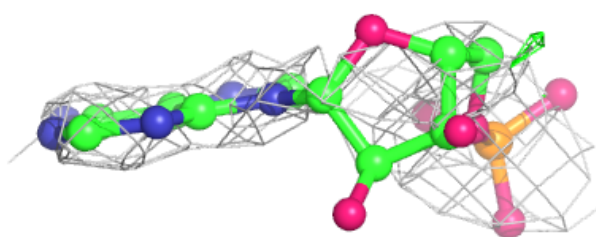
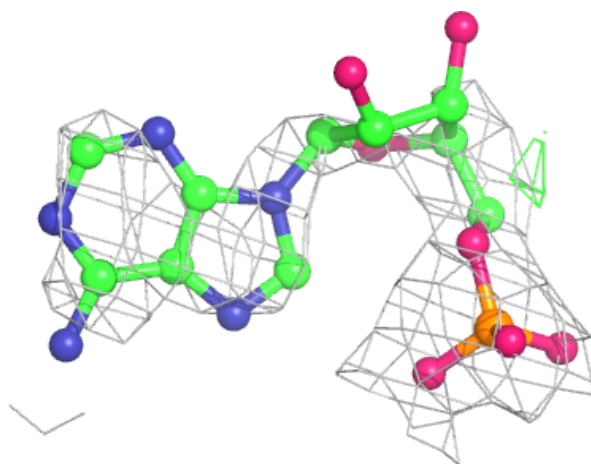
**Electron density around AMP I 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP J 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.