



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:36 PM UTC

PDB ID : 3FI0 / pdb_00003fi0
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 types of validation reports are described at

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

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

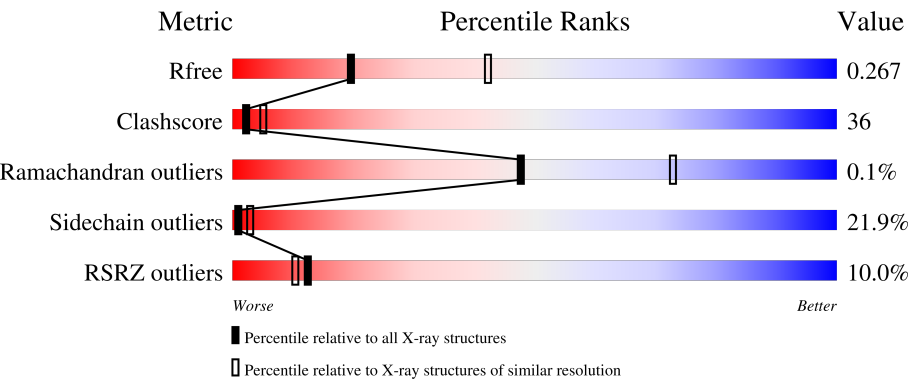
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

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Mol	Chain	Length	Quality of chain
1	E	326	
1	F	326	
1	G	326	
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	E	1003	-	-	-	X
4	AMP	G	1003	-	-	X	-
4	AMP	H	1003	-	-	-	X
4	AMP	K	1003	-	-	-	X
4	AMP	O	1003	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AMP	P	1003	-	-	X	X
4	AMP	R	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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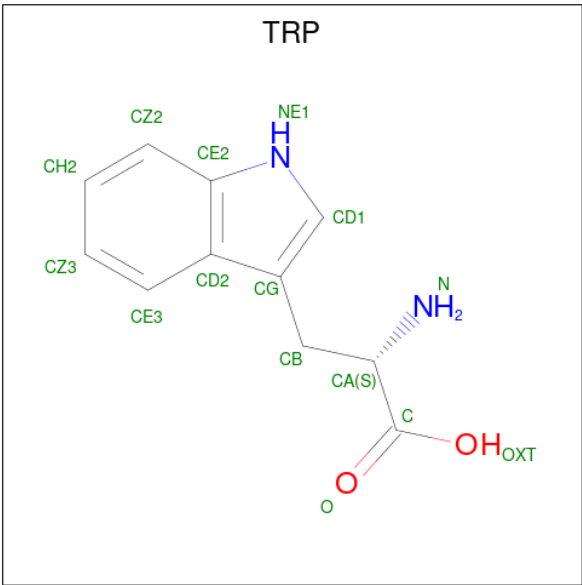
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	R	290	Total	C	N	O	S	Se	0	0	0
			2322	1473	399	437	3	10			

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 (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



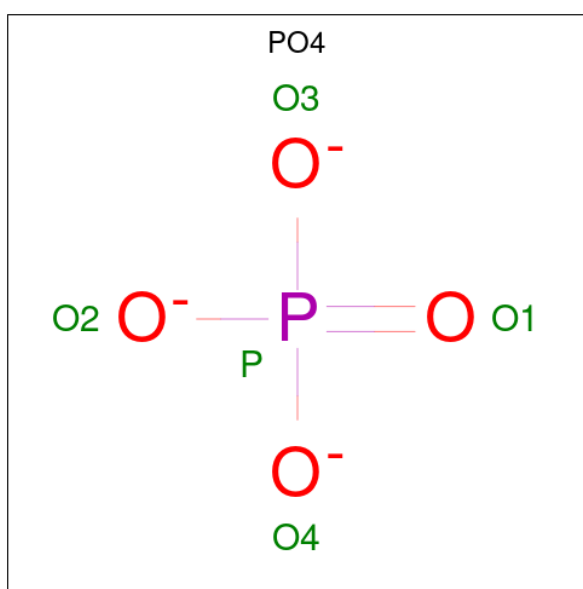
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	F	1	Total	C	N	O	0	0
			15	11	2	2		
2	G	1	Total	C	N	O	0	0
			15	11	2	2		
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 (CCD ID: PO4) (formula: O₄P).



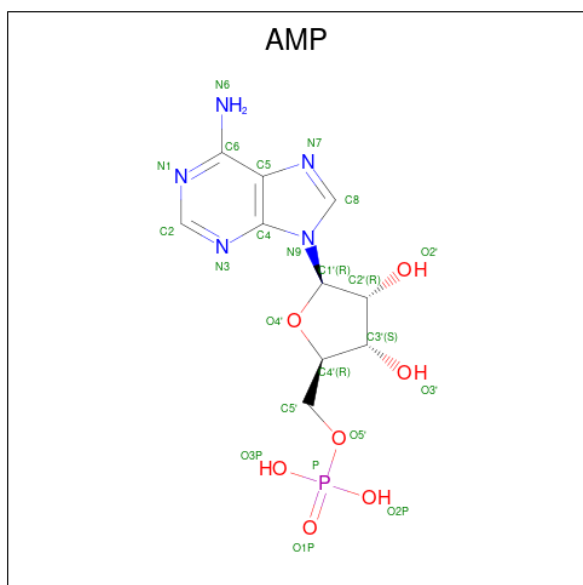
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		

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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 (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).

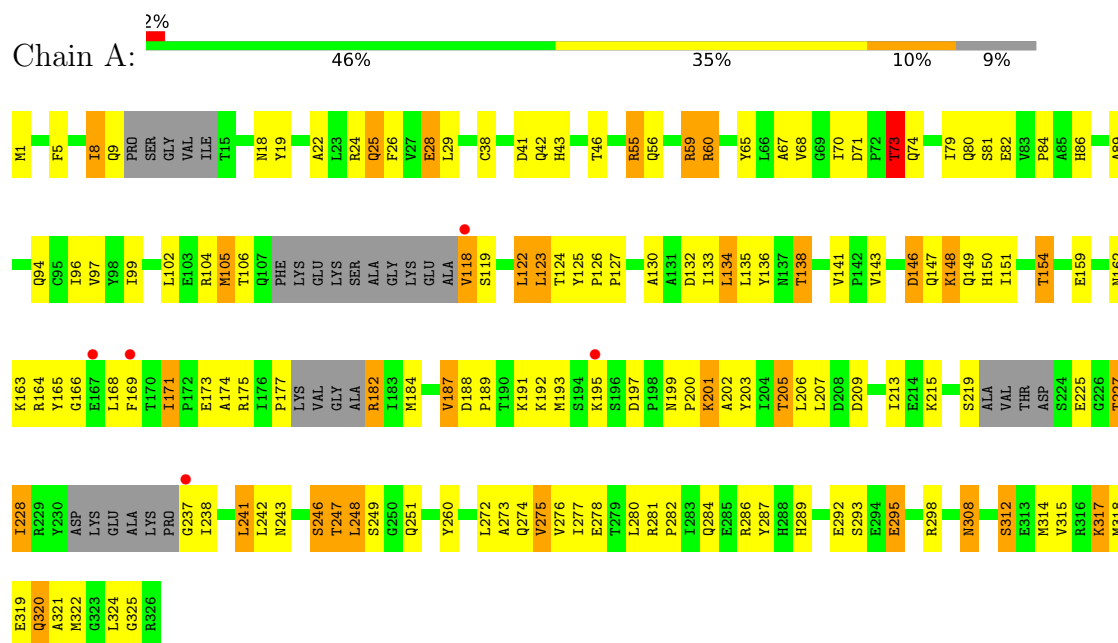


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	D	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	E	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	F	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	G	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	H	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

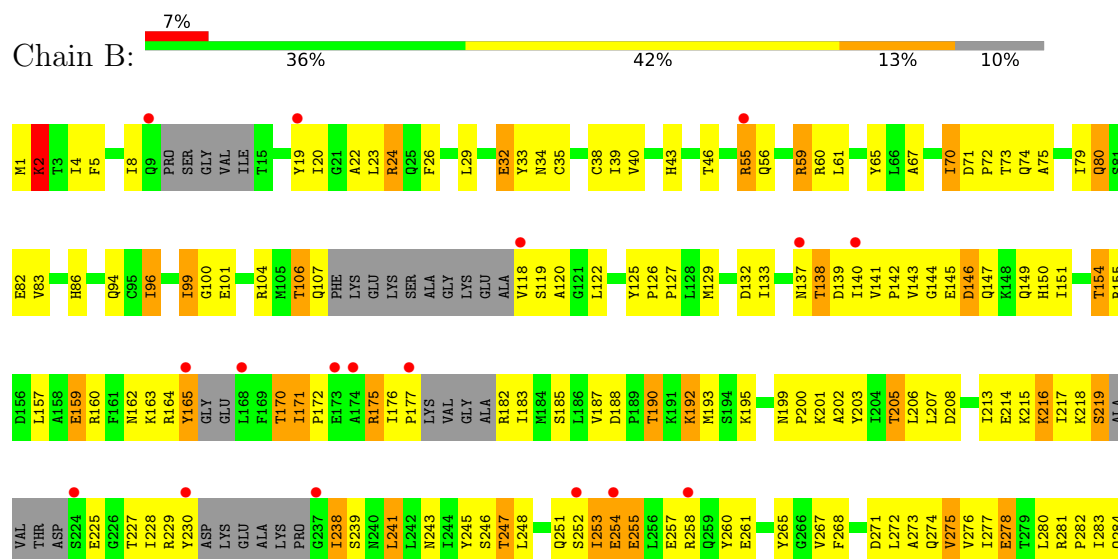
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tryptophanyl-tRNA synthetase

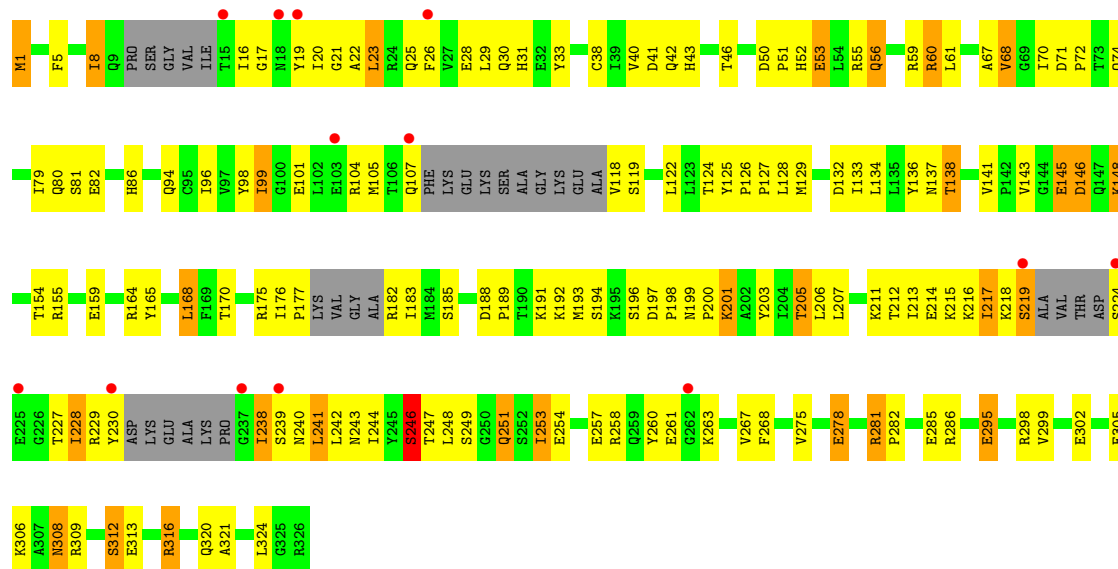
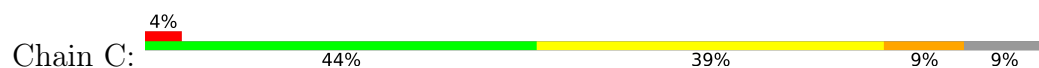


• Molecule 1: Tryptophanyl-tRNA synthetase

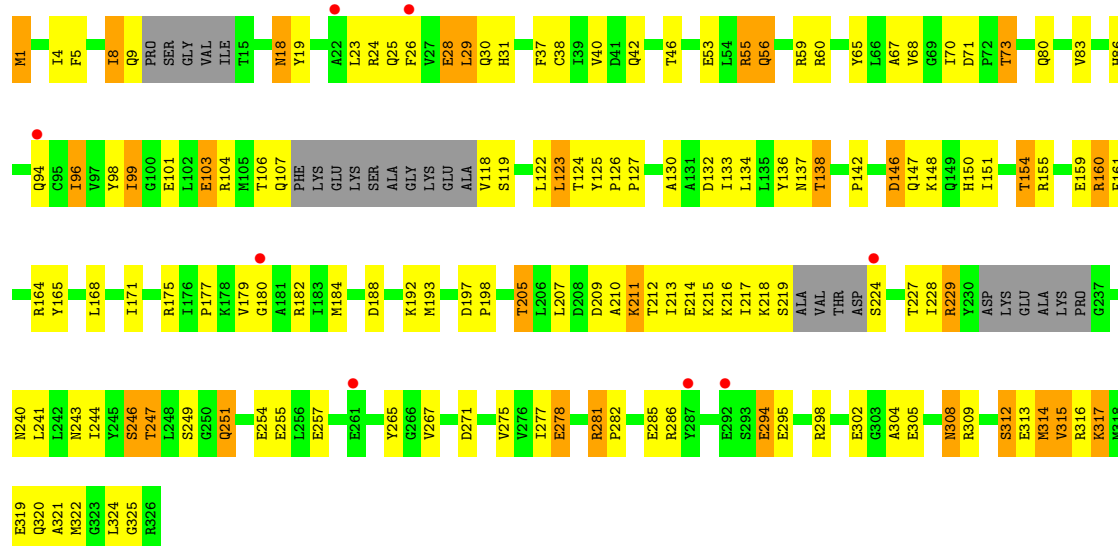




• Molecule 1: Tryptophanyl-tRNA synthetase

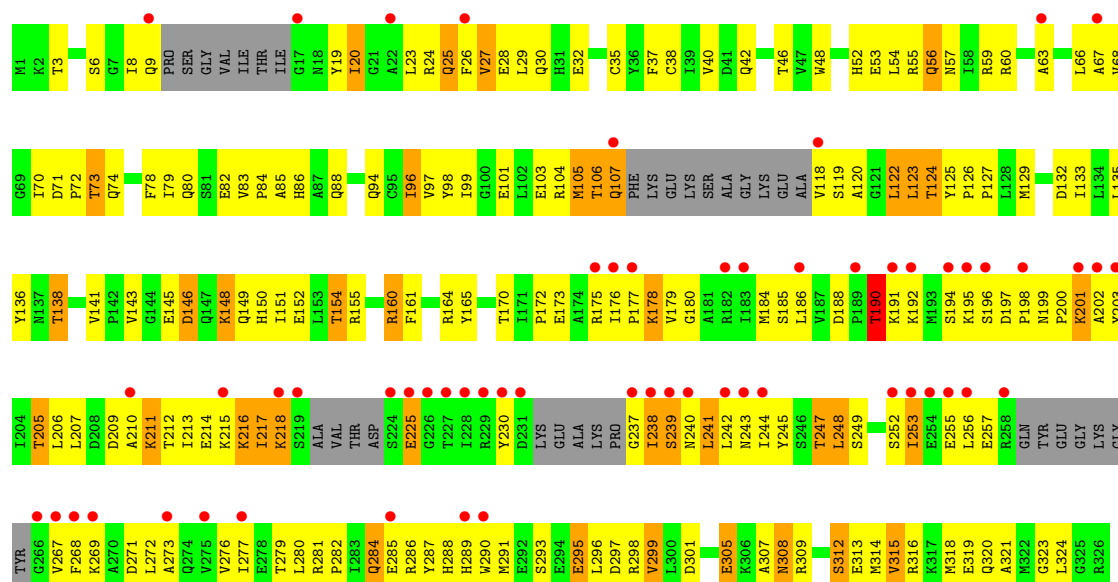


• Molecule 1: Tryptophanyl-tRNA synthetase

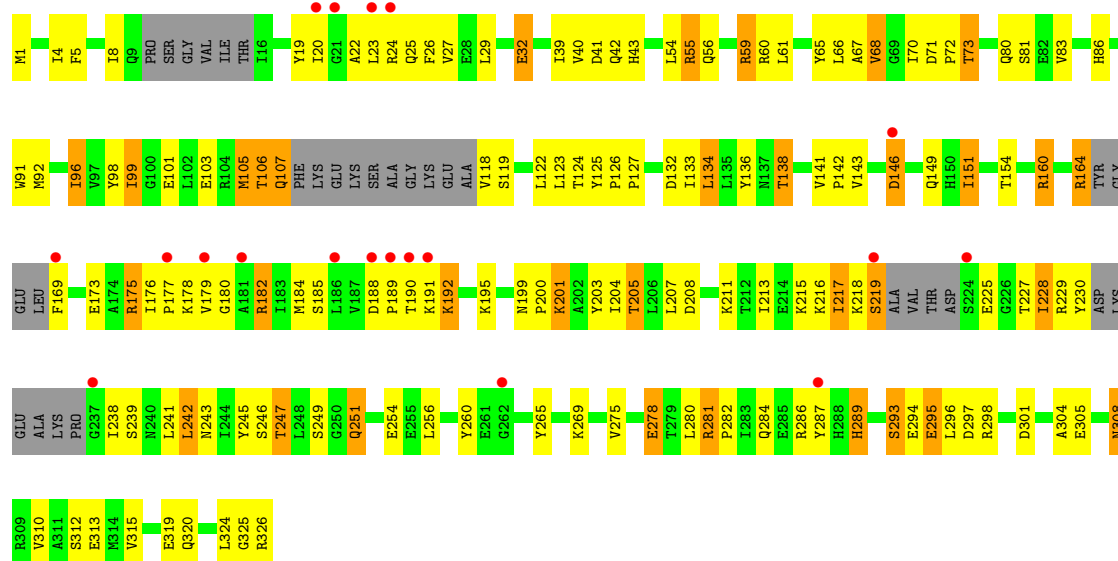
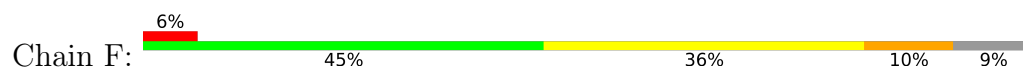


• Molecule 1: Tryptophanyl-tRNA synthetase

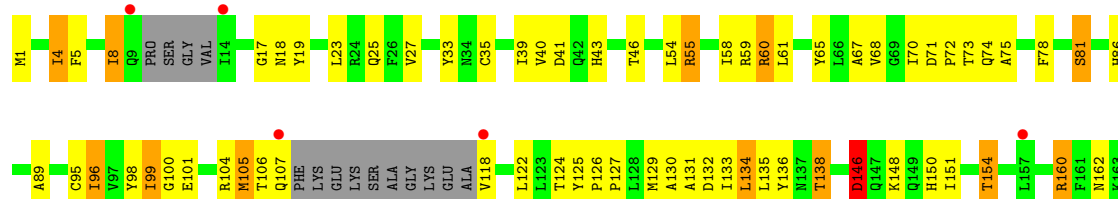


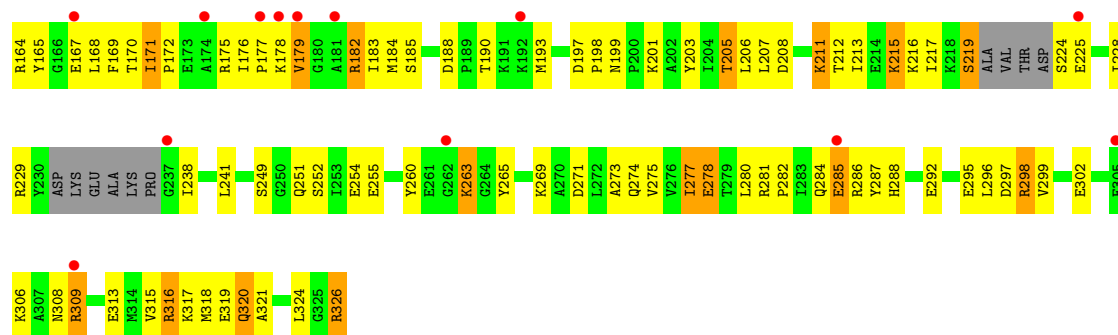


• Molecule 1: Tryptophanyl-tRNA synthetase

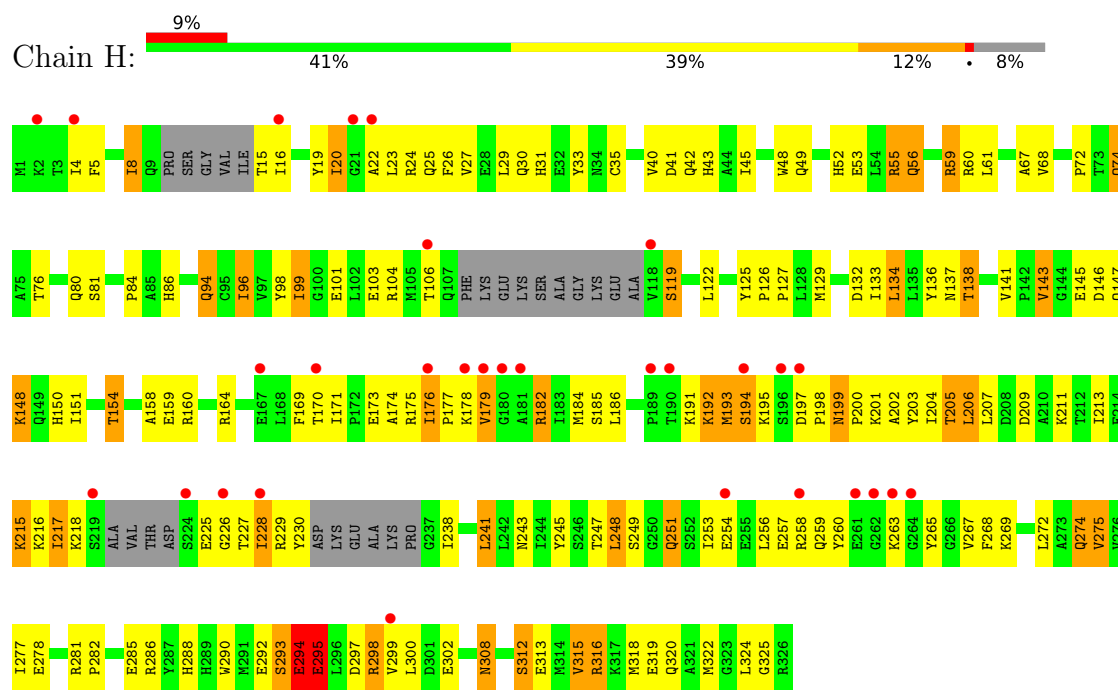


• Molecule 1: Tryptophanyl-tRNA synthetase

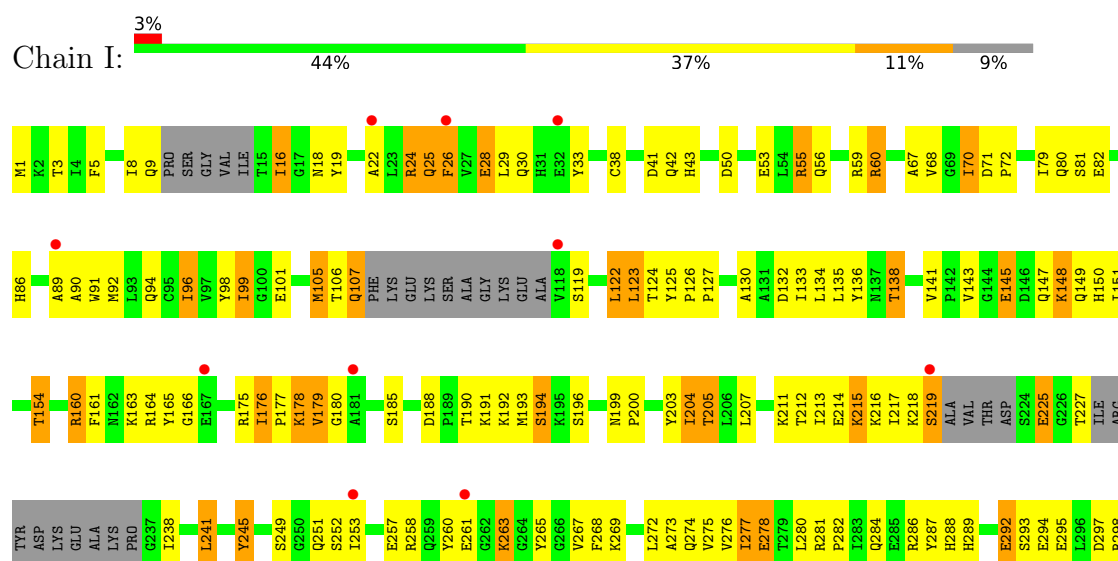




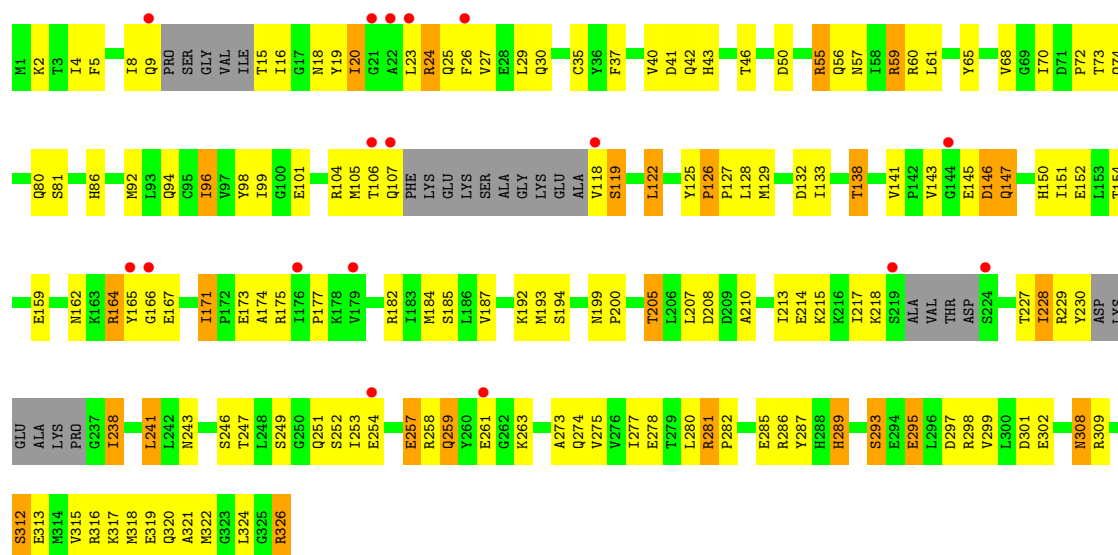
• Molecule 1: Tryptophanyl-tRNA synthetase



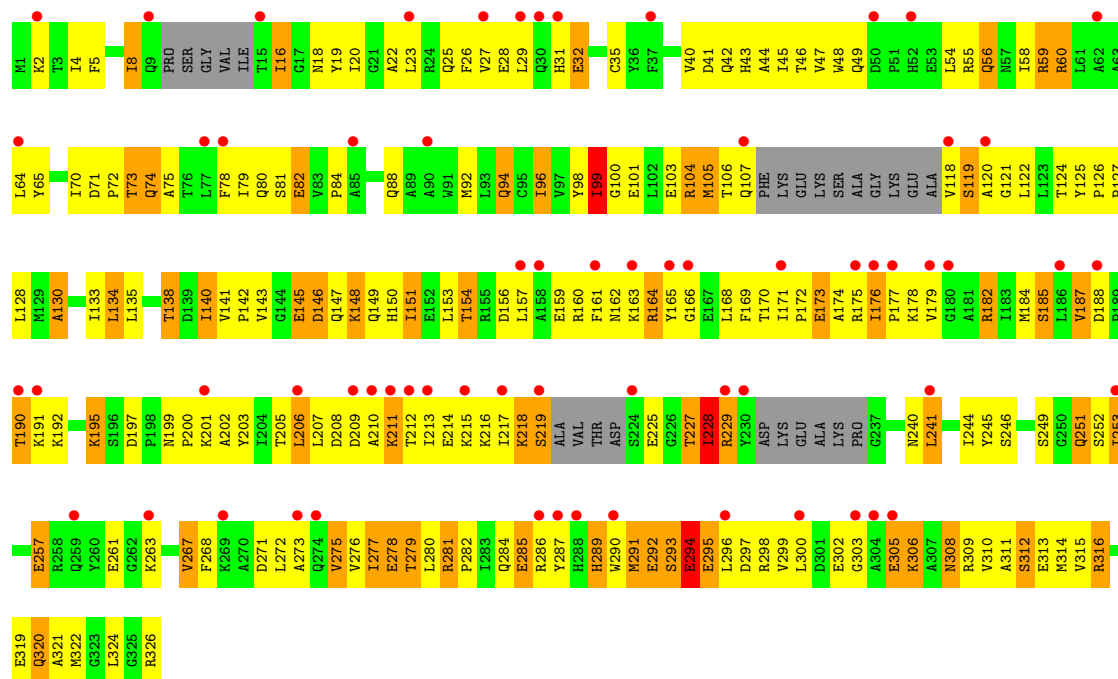
• Molecule 1: Tryptophanyl-tRNA synthetase



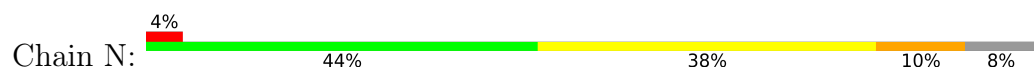


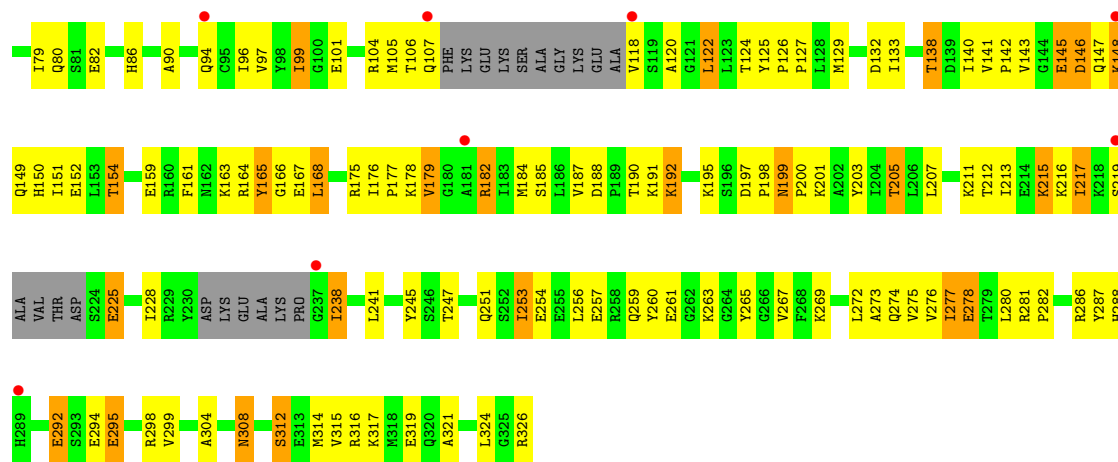


• Molecule 1: Tryptophanyl-tRNA synthetase

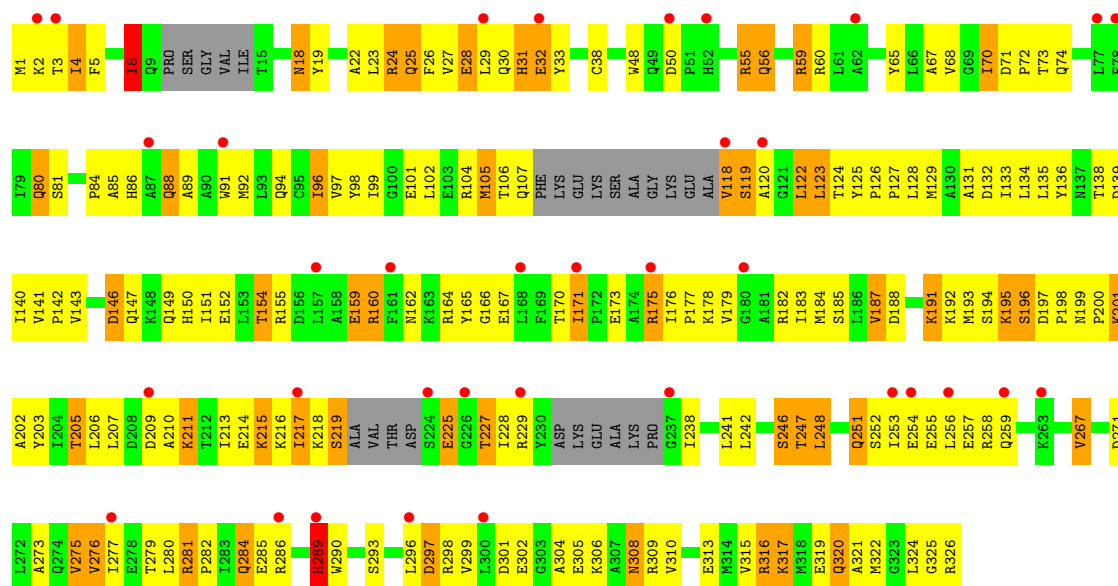


• Molecule 1: Tryptophanyl-tRNA synthetase

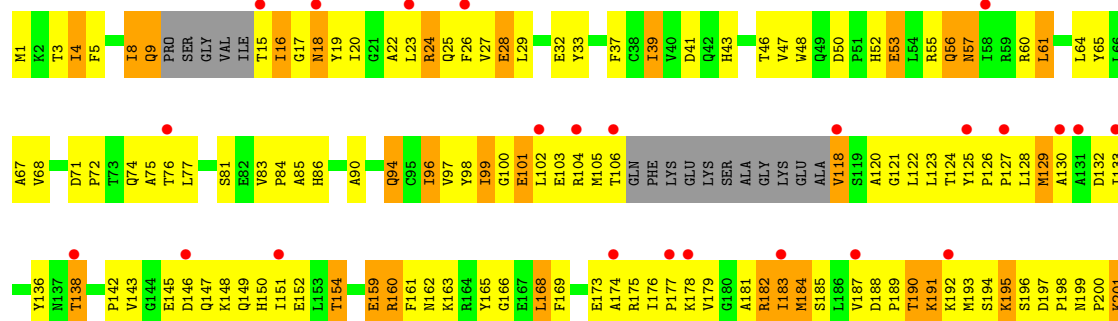


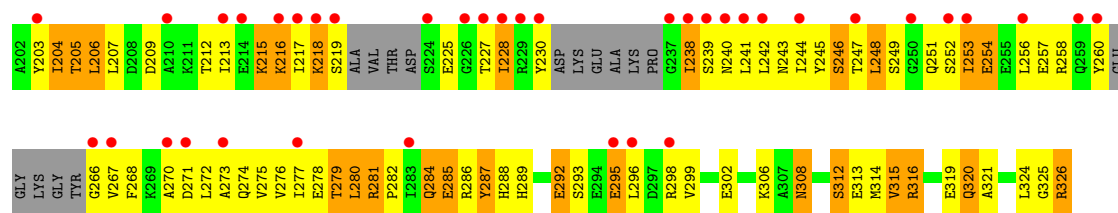


• Molecule 1: Tryptophanyl-tRNA synthetase

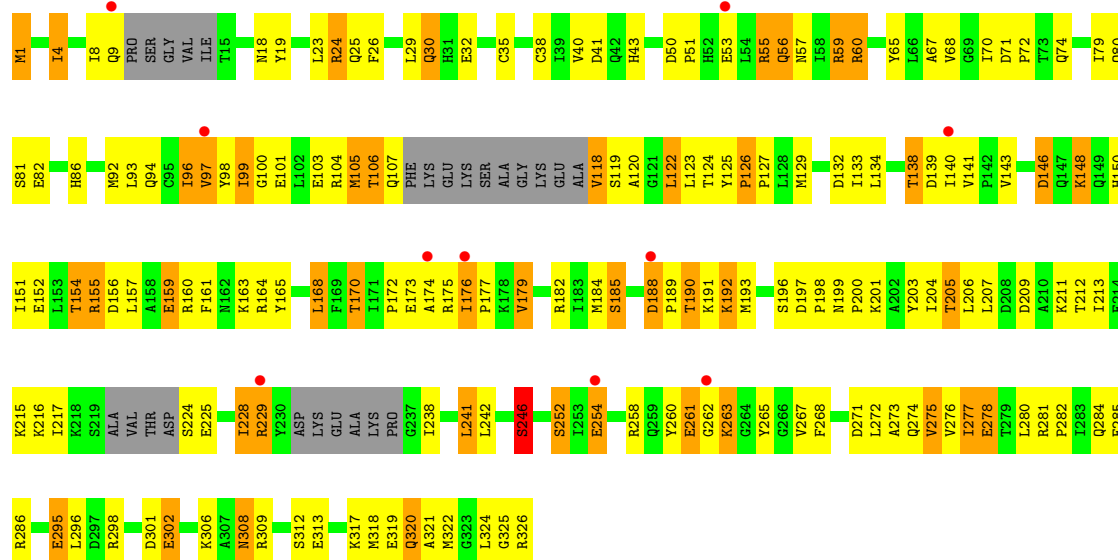


• Molecule 1: Tryptophanyl-tRNA synthetase

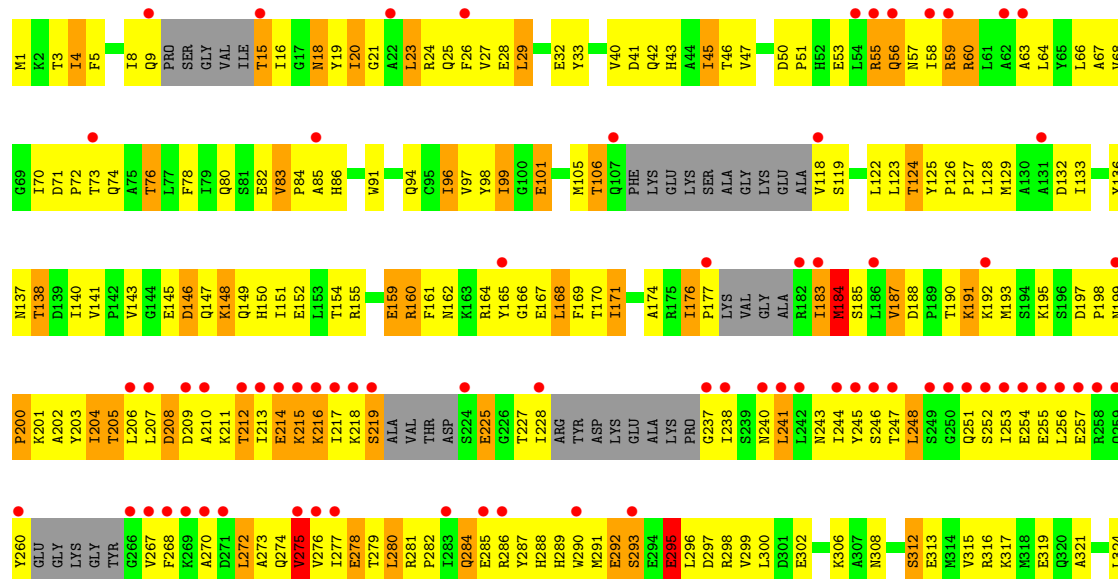




● Molecule 1: Tryptophanyl-tRNA synthetase



● Molecule 1: Tryptophanyl-tRNA synthetase



C325
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 25.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (25.00-2.70) 98.8 (25.00-2.70)	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 0.254 , 0.267	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)	0.34 , 56.4	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, AMP

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	0.46	0/2414	0.89	6/3242 (0.2%)
1	B	0.37	0/2400	0.87	4/3222 (0.1%)
1	C	0.40	0/2414	0.92	5/3242 (0.2%)
1	D	0.40	0/2440	0.90	7/3278 (0.2%)
1	E	0.37	0/2371	0.91	8/3184 (0.3%)
1	F	0.36	0/2398	0.87	1/3219 (0.0%)
1	G	0.37	0/2448	0.91	5/3289 (0.2%)
1	H	0.37	0/2440	0.90	7/3278 (0.2%)
1	I	0.39	0/2408	0.91	6/3235 (0.2%)
1	J	0.38	0/2440	0.88	2/3278 (0.1%)
1	K	0.35	0/2398	0.88	6/3220 (0.2%)
1	L	0.39	0/2440	0.93	7/3278 (0.2%)
1	M	0.36	0/2440	0.91	11/3278 (0.3%)
1	N	0.38	0/2440	0.91	9/3278 (0.3%)
1	O	0.37	0/2440	0.94	9/3278 (0.3%)
1	P	0.33	0/2391	0.95	12/3212 (0.4%)
1	Q	0.39	0/2440	0.96	9/3278 (0.3%)
1	R	0.36	0/2350	0.90	11/3156 (0.3%)
All	All	0.38	0/43512	0.91	125/58445 (0.2%)

There are no bond length outliers.

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	225	GLU	N-CA-C	8.88	120.96	111.28
1	P	190	THR	N-CA-C	-8.71	103.73	112.97
1	P	295	GLU	N-CA-C	-8.15	103.32	113.18
1	K	73	THR	N-CA-C	-7.84	102.82	111.36
1	I	294	GLU	N-CA-C	-7.56	104.08	113.38
1	H	295	GLU	N-CA-C	-7.46	103.08	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	246	SER	N-CA-C	7.38	119.11	111.14
1	B	46	THR	N-CA-C	-7.36	104.27	113.18
1	L	228	ILE	N-CA-C	7.22	113.93	106.21
1	K	242	LEU	N-CA-C	-7.13	102.70	111.40
1	M	294	GLU	N-CA-C	-7.09	104.27	114.12
1	A	28	GLU	N-CA-C	7.07	119.06	111.36
1	B	35	CYS	N-CA-C	7.04	120.93	109.59
1	K	257	GLU	N-CA-C	-7.03	103.61	111.28
1	G	46	THR	N-CA-C	-6.97	104.25	112.89
1	N	166	GLY	N-CA-C	-6.89	102.69	111.72
1	M	228	ILE	N-CA-C	6.87	113.56	106.21
1	L	46	THR	N-CA-C	-6.86	104.78	113.01
1	N	46	THR	N-CA-C	-6.86	104.92	113.28
1	O	134	LEU	N-CA-C	6.83	118.73	111.28
1	L	147	GLN	N-CA-C	-6.82	104.57	113.17
1	R	184	MSE	N-CA-C	6.80	120.13	110.14
1	C	295	GLU	N-CA-C	-6.76	104.51	112.89
1	M	35	CYS	N-CA-C	6.74	120.82	109.76
1	M	99	ILE	CB-CA-C	-6.74	100.98	110.95
1	N	50	ASP	N-CA-C	-6.74	101.30	109.72
1	R	183	ILE	N-CA-C	6.70	119.08	109.51
1	A	295	GLU	N-CA-C	-6.68	104.61	112.89
1	P	46	THR	N-CA-C	-6.64	104.66	112.89
1	A	134	LEU	N-CA-C	6.63	120.23	111.75
1	R	275	VAL	CB-CA-C	-6.60	103.37	112.02
1	R	208	ASP	N-CA-C	-6.59	102.31	110.41
1	E	73	THR	N-CA-C	-6.51	102.67	112.04
1	H	294	GLU	N-CA-C	-6.40	104.73	113.30
1	E	46	THR	N-CA-C	-6.36	105.49	113.18
1	R	46	THR	N-CA-C	-6.29	105.66	113.15
1	O	289	HIS	N-CA-C	-6.24	104.10	111.03
1	D	73	THR	N-CA-C	-6.24	104.37	112.23
1	J	134	LEU	N-CA-C	6.23	119.72	111.75
1	B	2	LYS	N-CA-C	6.21	119.47	110.28
1	E	190	THR	N-CA-C	-6.17	105.51	113.16
1	P	94	GLN	N-CA-C	-6.16	105.03	112.54
1	P	285	GLU	N-CA-C	6.08	118.82	111.40
1	D	46	THR	N-CA-C	-6.05	105.16	112.54
1	C	46	THR	N-CA-C	-6.04	105.17	112.54
1	M	46	THR	N-CA-C	-5.97	106.08	113.19
1	Q	57	ASN	N-CA-C	-5.97	104.70	112.23
1	P	57	ASN	N-CA-C	-5.96	105.10	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	73	THR	N-CA-C	-5.95	104.87	111.36
1	Q	262	GLY	N-CA-C	-5.95	107.44	115.36
1	I	149	GLN	N-CA-C	-5.94	104.89	111.36
1	L	126	PRO	N-CA-C	5.93	117.94	110.70
1	G	146	ASP	N-CA-C	-5.90	105.34	112.54
1	E	54	LEU	CB-CA-C	-5.87	101.92	110.96
1	C	246	SER	N-CA-C	5.86	117.66	111.28
1	R	200	PRO	N-CA-C	-5.84	107.05	114.35
1	K	258	ARG	N-CA-C	5.81	117.70	111.36
1	R	29	LEU	N-CA-C	-5.81	106.19	113.28
1	L	50	ASP	N-CA-C	-5.75	101.25	109.24
1	F	134	LEU	N-CA-C	5.74	119.10	111.75
1	M	134	LEU	N-CA-C	5.74	118.27	111.33
1	A	248	LEU	N-CA-C	-5.73	106.12	113.23
1	K	46	THR	N-CA-C	-5.71	106.27	113.18
1	Q	126	PRO	N-CA-C	5.70	117.66	110.70
1	P	187	VAL	N-CA-C	-5.70	105.01	113.39
1	D	246	SER	N-CA-C	5.68	117.55	111.36
1	M	306	LYS	N-CA-C	-5.68	105.00	111.14
1	D	294	GLU	N-CA-C	-5.68	106.33	113.20
1	O	310	VAL	N-CA-C	5.65	115.85	110.42
1	P	287	TYR	N-CA-C	-5.64	104.14	111.02
1	N	225	GLU	N-CA-C	5.64	117.88	111.11
1	Q	170	THR	CA-C-N	-5.64	118.77	122.60
1	Q	170	THR	C-N-CA	-5.64	118.77	122.60
1	O	50	ASP	N-CA-C	-5.63	102.69	109.72
1	O	276	VAL	N-CA-C	-5.62	105.13	110.42
1	G	124	THR	N-CA-C	5.61	119.82	112.92
1	I	134	LEU	N-CA-C	5.61	118.16	111.71
1	H	104	ARG	N-CA-C	-5.60	106.40	113.18
1	R	124	THR	N-CA-C	5.60	120.11	112.88
1	J	46	THR	N-CA-C	-5.59	105.72	112.54
1	K	299	VAL	N-CA-C	-5.59	104.07	111.05
1	O	256	LEU	CB-CA-C	-5.58	102.09	110.90
1	M	153	LEU	N-CA-C	5.57	117.16	111.14
1	M	295	GLU	N-CA-C	-5.56	106.34	113.01
1	N	190	THR	N-CA-C	-5.55	106.55	113.38
1	D	134	LEU	N-CA-C	5.50	118.03	111.71
1	O	320	GLN	N-CA-C	-5.47	105.40	111.36
1	N	167	GLU	N-CA-C	5.46	117.60	109.25
1	G	35	CYS	N-CA-C	5.45	118.37	109.59
1	M	130	ALA	N-CA-C	-5.45	104.75	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	134	LEU	N-CA-C	5.44	117.97	111.71
1	E	54	LEU	N-CA-C	5.44	116.90	110.97
1	H	35	CYS	N-CA-C	5.40	118.62	109.76
1	Q	35	CYS	N-CA-C	5.38	118.59	109.76
1	P	184	MSE	N-CA-C	5.37	118.75	110.42
1	Q	134	LEU	N-CA-C	5.37	118.62	111.75
1	A	73	THR	N-CA-C	-5.33	106.04	112.54
1	A	46	THR	N-CA-C	-5.32	106.62	113.01
1	N	215	LYS	N-CA-C	-5.30	105.40	111.07
1	B	287	TYR	N-CA-C	-5.30	104.75	111.11
1	R	295	GLU	CB-CA-C	-5.29	100.51	110.67
1	H	20	ILE	N-CA-C	-5.29	105.28	113.16
1	G	134	LEU	N-CA-C	5.28	117.03	111.28
1	C	168	LEU	N-CA-CB	-5.26	101.60	110.49
1	I	180	GLY	N-CA-C	-5.25	104.57	112.60
1	I	245	TYR	N-CA-C	5.24	116.99	111.28
1	M	252	SER	N-CA-CB	-5.24	102.44	111.55
1	O	8	ILE	N-CA-C	5.18	115.52	107.28
1	P	61	LEU	N-CA-C	5.17	116.92	111.28
1	P	50	ASP	N-CA-C	-5.15	101.22	109.04
1	C	134	LEU	N-CA-C	5.12	118.31	111.75
1	E	97	VAL	N-CA-C	-5.12	104.47	110.05
1	N	165	TYR	N-CA-C	5.11	119.52	113.28
1	N	295	GLU	N-CA-C	-5.11	106.31	112.54
1	R	66	LEU	N-CA-C	-5.10	105.63	111.14
1	D	317	LYS	N-CA-C	-5.08	105.83	112.23
1	D	18	ASN	N-CA-C	5.07	116.62	111.14
1	E	155	ARG	N-CA-C	-5.07	105.84	112.23
1	L	35	CYS	N-CA-C	5.07	117.50	109.24
1	H	143	VAL	N-CA-C	5.06	117.00	108.81
1	P	83	VAL	N-CA-C	-5.05	103.14	108.15
1	I	190	THR	N-CA-C	-5.04	107.30	113.50
1	E	35	CYS	N-CA-C	5.03	118.01	109.76
1	R	293	SER	N-CA-C	-5.03	104.22	110.41
1	O	256	LEU	N-CA-C	5.01	116.56	111.14

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	202	0
1	C	2383	0	2390	130	0
1	D	2408	0	2421	131	0
1	E	2342	0	2355	227	0
1	F	2368	0	2384	140	0
1	G	2416	0	2432	141	0
1	H	2408	0	2421	160	0
1	I	2377	0	2388	142	0
1	J	2408	0	2421	146	0
1	K	2367	0	2382	210	0
1	L	2408	0	2421	123	0
1	M	2408	0	2421	269	0
1	N	2408	0	2421	146	0
1	O	2408	0	2421	202	0
1	P	2361	0	2378	365	0
1	Q	2408	0	2421	178	0
1	R	2322	0	2333	285	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
2	Q	15	0	9	1	0
2	R	15	0	9	0	0
3	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	7	0
4	B	23	0	12	4	0
4	C	23	0	12	2	0
4	D	23	0	12	3	0
4	E	23	0	12	1	0
4	F	23	0	12	2	0
4	G	23	0	12	7	0
4	H	23	0	12	0	0
4	I	23	0	12	3	0
4	J	23	0	12	3	0
4	K	23	0	12	1	0
4	L	23	0	12	0	0
4	M	23	0	12	5	0
4	N	23	0	12	1	0
4	O	23	0	12	17	0
4	P	23	0	12	7	0
4	Q	23	0	12	2	0
4	R	23	0	12	3	0
All	All	43727	0	43558	3170	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 (3170) 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:H	1:E:20:ILE:HD12	1.02	1.12
1:P:253:ILE:HG22	1:P:254:GLU:CD	1.75	1.11
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:228:ILE:HG22	1:P:238:ILE:HD11	1.33	1.07
1:P:245:TYR:HB2	1:P:272:LEU:HD13	1.12	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
1:P:245:TYR:CB	1:P:272:LEU:HD13	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:24:ARG:HG2	1:I:24:ARG:HH11	1.19	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: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:Q:140:ILE:CD1	1:Q:175:ARG:CG	2.32	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:I:258:ARG:O	1:I:261:GLU:HG2	1.60	1.00
1:R:260:TYR:CD1	1:R:268:PHE:HD1	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:260:TYR:C	1:I:263:LYS:HG2	1.91	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:P:124:THR:C	1:P:126:PRO:HD2	1.90	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:E:184:MSE:HE3	1:E:191:LYS:C	1.91	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:HH11	1:I:24:ARG:CG	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:H	1:F:107:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:18:ASN:HA	4:O:1003:AMP:H1'	1.51	0.92
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: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:K:25:GLN:O	1:K:29:LEU:HG	1.71	0.90
1:M:140:ILE:HG12	1:M:175:ARG:HB3	1.51	0.90
3:M:1002:PO4:O2	4:M:1003:AMP:H8	1.54	0.90
1:Q:94:GLN:O	1:Q:97:VAL:HG12	1.72	0.90
1:K:56:GLN:HA	1:K:56:GLN:HE21	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:HH11	1:H:182:ARG:HG3	1.36	0.88
1:D:126:PRO:HB2	1:D:127:PRO:HD3	1.56	0.88
1:K:124:THR:C	1:K:126:PRO:HD2	1.98	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
1:N:176:ILE:O	1:N:179:VAL:HG22	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:E:241:LEU:HD22	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:184:MSE:CE	1:E:191:LYS:C	2.50	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:B:254:GLU:H	1:B:254:GLU:CD	1.84	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:121:GLY:O	1:P:125:TYR:HB3	1.75	0.85
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:HD13	1:G:171:ILE:H	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:NE2	1:Q:107:GLN:H	1.76	0.83
1:K:241:LEU:HD12	1:K:241:LEU:N	1.90	0.83
1:K:260:TYR:CA	1:K:263:LYS:HD3	2.07	0.83
1:L:281:ARG:HH11	1:L:281:ARG:HG3	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:245:TYR:HE1	1:K:275:VAL:HG11	1.42	0.83
1:K:260:TYR:HA	1:K:263:LYS:CD	2.06	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:M:295:GLU:O	1:M:299:VAL:HG23	1.80	0.81
1:N:50:ASP:HB3	1:N:53:GLU:CG	2.09	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:OE1	1:P:295:GLU:HA	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
1:N:245:TYR:HD1	1:N:272:LEU:HD13	1.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:25:GLN:HG2	1:P:178:LYS:CB	2.11	0.81
1:P:238:ILE:HD12	1:P:238:ILE:O	1.80	0.81
1:B:175:ARG:HG3	1:B:176:ILE:N	1.93	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: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:H:199:ASN:C	1:H:199:ASN:HD22	1.89	0.80
1:P:20:ILE:CD1	1:P:183:ILE:HD11	2.11	0.80
1:P:126:PRO:CD	1:P:127:PRO:CD	2.60	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:84:PRO:HD2	1:R:308:ASN:HD21	1.46	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:E:213:ILE:HD13	1:E:276:VAL:HG12	1.64	0.80
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
1:F:134:LEU:HB3	1:F:169:PHE:CE1	2.16	0.79
1:J:205:THR:HG22	1:J:207:LEU:H	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:24:ARG:HH11	1:P:24:ARG:HG2	1.47	0.79
1:A:308:ASN:O	1:A:312:SER:HB2	1.83	0.79
1:H:22:ALA:O	1:H:26:PHE:CD2	2.36	0.79
1:H:176:ILE:HB	1:H:179:VAL:HG13	1.64	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
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:24:ARG:HH11	1:P:24:ARG:CG	1.96	0.79
1:P:248:LEU:HD12	1:P:248:LEU:N	1.97	0.79
1:P:253:ILE:HG22	1:P:254:GLU:OE1	1.83	0.79
1:R:225:GLU:CD	1:R:227:THR:HG23	2.08	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:HG2	1:M:281:ARG:HH11	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: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:84:PRO:HD2	1:P:308:ASN:HD21	1.49	0.78
1:P:126:PRO:CD	1:P:127:PRO:HD3	2.14	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:K:124:THR:C	1:K:126:PRO:CD	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:228:ILE:CG2	1:P:238:ILE:CD1	2.62	0.77
1:M:211:LYS:HD3	1:Q:1:MSE:HG2	1.66	0.77
1:P:253:ILE:CB	1:P:254:GLU:OE1	2.32	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:55:ARG:NH2	1:L:320:GLN:NE2	2.33	0.77
1:I:126:PRO:HB2	1:I:127:PRO:HD3	1.66	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:124:THR:HG21	1:D:94:GLN:HE22	1.48	0.76
1:A:168:LEU:HD11	1:A:317:LYS:HD2	1.66	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:98:TYR:HB2	1:O:101:GLU:HG3	1.68	0.75
1:O:182:ARG:O	1:O:184:MSE:HE2	1.87	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:HH11	1:N:24:ARG:CG	1.99	0.75
1:P:245:TYR:HA	1:P:272:LEU:CD1	2.16	0.75
1:R:41:ASP:HB3	1:R:58:ILE:HD11	1.66	0.75
1:R:145:GLU:HG2	1:R:145:GLU:O	1.86	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
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:P:253:ILE:CG2	1:P:254:GLU:CD	2.59	0.75
1:B:187:VAL:CG2	1:B:202:ALA:HB2	2.16	0.75
1:G:171:ILE:N	1:G:171:ILE:CD1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:124:THR:OG1	1:L:94:GLN:NE2	2.21	0.74
1:O:143:VAL:HG21	1:O:151:ILE:HD11	1.70	0.74
1:P:238:ILE:O	1:P:238:ILE:CD1	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:O:118:VAL:O	1:R:99:ILE:HG12	1.88	0.73
1:P:145:GLU:H	1:P:145:GLU:CD	1.96	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: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
1:C:28:GLU:HA	1:C:31:HIS:HD2	1.54	0.73
1:F:107:GLN:HE21	1:F:107:GLN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:55:ARG:NH2	1:F:320:GLN:HE22	1.87	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: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:HH11	1:A:281:ARG:HG3	1.54	0.72
1:G:309:ARG:HB3	1:G:309:ARG:CZ	2.19	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:8:ILE:HD12	1:J:65:TYR:OH	1.90	0.71
1:J:308:ASN:O	1:J:312:SER:HB2	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:HE2	1:E:105:MSE:HA	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:R:25:GLN:CD	1:R:25:GLN:H	1.97	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:19:TYR:HA	1:G:23:LEU:HB3	1.72	0.71
1:G:175:ARG:O	1:G:177:PRO:HD3	1.91	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:M:188:ASP:CG	1:M:190:THR:HB	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:67:ALA:O	1:H:286:ARG:NH1	2.24	0.70
1:H:182:ARG:HH11	1:H:182:ARG:CG	2.03	0.70
1:M:5:PHE:HB2	1:M:138:THR:HG21	1.72	0.70
1:R:206:LEU:C	1:R:207:LEU:HD23	2.16	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:P:254:GLU:CD	1:P:254:GLU:N	2.49	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:C:320:GLN:NE2	1:F:55:ARG:HH22	1.90	0.70
1:D:133:ILE:O	1:D:138:THR:HG23	1.92	0.70
1:K:98:TYR:HB2	1:K:101:GLU:HG3	1.73	0.70
1:K:238:ILE:O	1:K:241:LEU:CD1	2.39	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
1:G:101:GLU:CD	1:G:160:ARG:HH22	2.00	0.69
1:M:308:ASN:O	1:M:312:SER:HB2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:272:LEU:HD12	1:R:272:LEU:C	2.18	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:O:120:ALA:HA	1:R:99:ILE:HD13	1.74	0.69
1:P:241:LEU:HD22	1:P:272:LEU:CD2	2.23	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: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:K:295:GLU:HG2	1:K:298:ARG:NH1	2.07	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: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
1:B:72:PRO:HB3	1:B:299:VAL:CG1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ARG:HG3	1:B:281:ARG:HH11	1.58	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:O	1:R:291:MSE:HE3	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:HH11	1:M:281:ARG:CG	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:HG3	1:F:175:ARG:O	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:71:ASP:HB3	1:B:74:GLN:HB3	1.75	0.68
1:B:151:ILE:HA	1:B:154:THR:HG23	1.76	0.68
1:E:107:GLN:CD	1:E:150:HIS:HE2	2.02	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
1:O:71:ASP:OD2	1:O:74:GLN:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:THR:HG22	1:E:207:LEU:N	2.09	0.68
1:G:313:GLU:HG3	1:G:317:LYS:HZ3	1.58	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
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:Q:107:GLN:H	1:Q:107:GLN:CD	2.01	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
1:D:168:LEU:HD21	1:D:314:MSE:SE	2.45	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:P:245:TYR:HD1	1:P:272:LEU:HD12	1.60	0.66
1:R:23:LEU:O	1:R:26:PHE:HB2	1.95	0.66
1:R:199:ASN:OD1	1:R:201:LYS:N	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:M:32:GLU:O	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:N	1:E:241:LEU:CD2	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:B:281:ARG:HG3	1:B:281:ARG:NH1	2.10	0.65
1:I:324:LEU:O	1:L:55:ARG:NH1	2.29	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: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:P:161:PHE:C	1:P:161:PHE:CD2	2.73	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:71:ASP:HB3	1:P:74:GLN:HB3	1.78	0.65
1:P:284:GLN:O	1:P:288:HIS:ND1	2.28	0.65
1:R:98:TYR:HB2	1:R:101:GLU:CG	2.27	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ARG:HG2	1:B:287:TYR:OH	1.94	0.65
1:B:260:TYR:OH	1:B:271:ASP:CG	2.39	0.65
1:G:67:ALA:O	1:G:286:ARG:NH1	2.29	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:N:99:ILE:HG12	1:Q:118:VAL:O	1.96	0.65
1:P:64:LEU:HD21	1:P:207:LEU:HD21	1.78	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: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
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:99:ILE:HG13	1:L:118:VAL:HB	1.79	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
1:K:106:THR:CB	1:K:149:GLN:HE22	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ALA:O	1:B:286:ARG:NH1	2.30	0.64
1:B:252:SER:O	1:B:255:GLU:CB	2.46	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:M:211:LYS:CD	1:Q:1:MSE:HG2	2.27	0.64
1:N:281:ARG:HB3	1:N:282:PRO:HD3	1.77	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:Q:176:ILE:O	1:Q:176:ILE:HG13	1.91	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:56:GLN:O	1:D:60:ARG:HG3	1.97	0.64
1:D:205:THR:CG2	1:D:207:LEU:H	2.10	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: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:P:228:ILE:HG23	1:P:238:ILE:CD1	2.28	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:118:VAL:HG12	1:R:99:ILE:CD1	2.26	0.64
1:O:146:ASP:OD1	1:O:146:ASP:N	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:E:184:MSE:CE	1:E:191:LYS:CA	2.75	0.64
1:G:295:GLU:OE2	1:G:298:ARG:NH1	2.30	0.64
1:H:199:ASN:HD22	1:H:200:PRO:N	1.95	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:28:GLU:HA	1:O:31:HIS:HE1	1.62	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:Q:280:LEU:O	1:Q:284:GLN:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:O	1:B:24:ARG:HG2	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:19:TYR:O	1:H:24:ARG:HB2	1.97	0.64
1:H:182:ARG:HG3	1:H:182:ARG:NH1	2.12	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:HD13	1:A:171:ILE:N	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:HE2	1:F:105:MSE:CA	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
1:K:238:ILE:C	1:K:241:LEU:CD1	2.71	0.63
1:L:274:GLN:O	1:L:278:GLU:HG2	1.99	0.63
1:M:59:ARG:CZ	1:M:296:LEU:HD23	2.28	0.63
1:M:140:ILE:HD11	1:M:175:ARG:HD3	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:55:ARG:HH22	1:L:320:GLN:NE2	1.93	0.63
1:K:22:ALA:O	1:K:26:PHE:CE2	2.50	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:HD2	1:B:2:LYS:N	2.13	0.63
1:C:193:MSE:HB3	4:C:1003:AMP:N6	2.14	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:B:320:GLN:HE22	1:E:55:ARG:NH2	1.96	0.63
1:E:245:TYR:HA	1:E:272:LEU:HD13	1.78	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:H:324:LEU:O	1:K:55:ARG:NH1	2.32	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: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:79:ILE:HB	1:M:82:GLU:HG3	1.81	0.62
1:M:165:TYR:CE1	1:M:322:MSE:HG2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:124:THR:C	1:K:127:PRO:HD2	2.24	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:M:271:ASP:OD1	1:Q:309:ARG:NE	2.32	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:O:254:GLU:H	1:O:254:GLU:CD	2.07	0.62
1:Q:182:ARG:HE	1:Q:184:MSE:HE1	1.64	0.62
1:R:19:TYR:CE2	1:R:24:ARG:CG	2.83	0.62
1:R:106:THR:H	1:R:149:GLN:HE22	1.48	0.62
1:E:179:VAL:HG12	1:E:180:GLY:O	2.00	0.62
1:J:86:HIS:HD2	1:J:132:ASP:OD1	1.82	0.62
1:J:187:VAL:HG22	1:J:202:ALA:CB	2.29	0.62
1:M:200:PRO:O	1:M:216:LYS:NZ	2.32	0.62
1:N:205:THR:HG22	1:N:207:LEU:N	2.09	0.62
1:O:30:GLN:OE1	1:O:71:ASP:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:105:MSE:HE2	1:O:105:MSE:CA	2.28	0.62
1:P:195:LYS:HZ2	1:P:195:LYS:HB3	1.64	0.62
1:P:206:LEU:HD23	1:P:206:LEU:N	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:H:230:TYR:CD1	1:H:230:TYR:C	2.78	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:16:ILE:CD1	1:P:193:MSE:HE1	2.26	0.61
1:P:126:PRO:HD2	1:P:127:PRO:CD	2.30	0.61
1:P:308:ASN:O	1:P:312:SER:HB2	1.99	0.61
1:R:29:LEU:CD1	1:R:177:PRO:HG2	2.29	0.61
1:R:106:THR:H	1:R:149:GLN:NE2	1.98	0.61
1:A:274:GLN:O	1:A:278:GLU:HG2	2.00	0.61
1:K:7:GLY:C	1:K:8:ILE:HD13	2.25	0.61
1:K:176:ILE:O	1:K:179:VAL:HG22	2.01	0.61
1:O:325:GLY:C	1:O:326:ARG:HG3	2.24	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:245:TYR:HD1	1:P:272:LEU:HA	1.65	0.61
1:P:251:GLN:HG3	1:P:256:LEU:HD11	1.82	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:M:55:ARG:HD2	1:P:325:GLY:O	2.01	0.61
1:P:266:GLY:O	1:P:270:ALA:HB2	2.00	0.61
1:R:162:ASN:HA	1:R:166:GLY:O	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:ND1	1:O:31:HIS:N	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:D:5:PHE:HB2	1:D:138:THR:HG21	1.82	0.60
1:D:254:GLU:H	1:D:254:GLU:CD	2.08	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:P:175:ARG:HG2	1:P:176:ILE:N	2.14	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:M:45:ILE:C	1:M:47:VAL:H	2.10	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:120:ALA:HB2	1:P:102:LEU:CD1	2.30	0.60
1:M:241:LEU:HB3	1:M:268:PHE:CE2	2.33	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:27:VAL:HG23	1:R:28:GLU:HG2	1.83	0.60
1:R:43:HIS:HE1	1:R:132:ASP:OD2	1.84	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:Q:94:GLN:C	1:Q:97:VAL:HG12	2.25	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:315:VAL:O	1:E:319:GLU:HG3	2.02	0.60
1:G:105:MSE:HA	1:G:105:MSE:HE2	1.83	0.60
1:K:86:HIS:HD2	1:K:132:ASP:OD1	1.85	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:HH21	1:C:316:ARG:CG	2.13	0.59
1:K:287:TYR:CZ	1:K:291:MSE:CE	2.85	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:48:TRP:CZ2	1:K:164:ARG:NH1	2.70	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: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:26:PHE:CD1	1:E:37:PHE:HE2	2.20	0.59
1:E:125:TYR:N	1:E:126:PRO:HD2	2.17	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:P:280:LEU:C	1:P:282:PRO:HD2	2.28	0.59
1:A:133:ILE:O	1:A:138:THR:HG23	2.03	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:199:ASN:HD22	1:C:199:ASN:C	2.11	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:M:42:GLN:HB2	1:M:80:GLN:OE1	2.03	0.58
1:M:209:ASP:OD1	1:M:212:THR:CB	2.50	0.58
1:Q:38:CYS:SG	1:Q:80:GLN:HB2	2.43	0.58
1:A:105:MSE:HA	1:A:105:MSE:CE	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:E:253:ILE:O	1:E:253:ILE:CG1	2.49	0.58
1:G:105:MSE:HE2	1:G:105:MSE:CA	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:HD13	1:K:183:ILE:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:71:ASP:O	1:P:75:ALA:N	2.36	0.58
1:P:126:PRO:CG	1:P:127:PRO:CD	2.76	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:56:GLN:NE2	1:M:60:ARG:NH2	2.52	0.58
1:M:281:ARG:N	1:M:282:PRO:HD2	2.18	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:72:PRO:HB3	1:O:299:VAL:HG13	1.85	0.58
1:O:273:ALA:O	1:O:277:ILE:HG13	2.03	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
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:5:PHE:HB2	1:H:138:THR:HG21	1.86	0.57
1:H:59:ARG:NH2	1:H:297:ASP:OD1	2.27	0.57
1:H:277:ILE:O	1:H:281:ARG:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:Q:24:ARG:HH11	2.17	0.57
1:Q:281:ARG:HG3	1:Q:281:ARG:NH1	2.14	0.57
1:B:205:THR:HG22	1:B:207:LEU:H	1.69	0.57
1:E:96:ILE:O	1:E:160:ARG:NH1	2.37	0.57
1:E:176:ILE:HB	1:E:179:VAL:HG22	1.85	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:O	1:M:295:GLU:HG3	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:O:175:ARG:HH22	1:O:177:PRO:HB3	1.66	0.57
1:P:9:GLN:HA	1:P:9:GLN:HE21	1.68	0.57
1:R:141:VAL:HG12	1:R:143:VAL:HG13	1.86	0.57
1:B:199:ASN:HD22	1:B:199:ASN:C	2.11	0.57
1:C:126:PRO:HB2	1:C:127:PRO:CD	2.33	0.57
1:D:278:GLU:OE1	1:D:278:GLU:HA	2.04	0.57
1:L:165:TYR:HB3	1:L:321:ALA:HB1	1.85	0.57
1:M:48:TRP:C	1:M:49:GLN:HG2	2.28	0.57
1:N:254:GLU:CD	1:N:254:GLU:H	2.12	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:79:ILE:HB	1:J:82:GLU:HG3	1.87	0.57
1:J:185:SER:O	1:J:189:PRO:HA	2.04	0.57
1:M:22:ALA:O	1:M:26:PHE:CD2	2.57	0.57
1:M:98:TYR:N	1:M:101:GLU:OE1	2.22	0.57
1:P:145:GLU:OE1	1:P:145:GLU:N	2.33	0.57
1:H:30:GLN:O	1:H:74:GLN:NE2	2.38	0.57
1:H:199:ASN:ND2	1:H:199:ASN:C	2.62	0.57
1:I:38:CYS:SG	1:I:80:GLN:HB2	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:A:146:ASP:N	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:HE3	1:R:291:MSE:HA	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:OD1	1:G:146:ASP:N	2.29	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: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:OD1	1:E:146:ASP:N	2.36	0.57
1:I:326:ARG:NH1	1:L:297:ASP:OD2	2.35	0.57
1:L:133:ILE:O	1:L:138:THR:HG23	2.04	0.57
1:M:8:ILE:HD12	1:M:65:TYR:CZ	2.40	0.57
1:M:311:ALA:O	1:M:314:MSE:N	2.38	0.57
1:P:247:THR:OG1	1:P:248:LEU:CD1	2.51	0.57
1:R:19:TYR:CE2	1:R:24:ARG:HG2	2.40	0.57
1:R:184:MSE:HE3	1:R:192:LYS:CA	2.35	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
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:71:ASP:HB3	1:A:74:GLN:HB2	1.87	0.56
1:A:168:LEU:O	1:A:314:MSE:HE1	2.06	0.56
1:B:94:GLN:NE2	1:E:124:THR:CB	2.68	0.56
1:B:315:VAL:O	1:B:319:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:HIS:HD2	1:F:132:ASP:OD1	1.88	0.56
1:F:184:MSE:HE2	1:F:189:PRO:O	2.05	0.56
1:N:176:ILE:HB	1:N:179:VAL:HG13	1.86	0.56
1:P:3:THR:HB	1:P:138:THR:HA	1.87	0.56
1:P:16:ILE:HG12	1:P:17:GLY:H	1.69	0.56
1:P:18:ASN:ND2	1:P:18:ASN:C	2.56	0.56
1:P:125:TYR:C	1:P:127:PRO:HD2	2.30	0.56
1:Q:139:ASP:OD1	1:Q:170:THR:HG21	2.04	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:R:171:ILE:HD13	1:R:171:ILE:N	2.19	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:HH11	1:O:24:ARG:CG	2.19	0.56
1:P:248:LEU:N	1:P:248:LEU:CD1	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:29:LEU:HD11	1:R:177:PRO:HG2	1.87	0.56
1:R:195:LYS:HG2	3:R:1002:PO4:O1	2.05	0.56
1:G:199:ASN:HD22	1:G:199:ASN:C	2.14	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:O	1:R:145:GLU:CG	2.53	0.56
1:B:137:ASN:HB3	1:B:170:THR:HG21	1.87	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:24:ARG:HG3	1:L:25:GLN:N	2.19	0.56
1:L:258:ARG:O	1:L:261:GLU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:165:TYR:CB	1:R:321:ALA:HB1	2.32	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:105:MSE:HA	1:M:149:GLN:NE2	2.22	0.55
1:M:125:TYR:N	1:M:126:PRO:CD	2.69	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:R:279:THR:C	1:R:282:PRO:HD2	2.30	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:H:295:GLU:HA	1:H:295:GLU:OE2	2.05	0.55
1:I:101:GLU:O	1:I:105:MSE:HE2	2.06	0.55
1:M:228:ILE:O	1:M:228:ILE:HG22	2.05	0.55
1:E:133:ILE:O	1:E:138:THR:HG23	2.06	0.55
1:F:27:VAL:O	1:F:27:VAL:HG12	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:HG23	1:M:40:VAL:O	2.07	0.55
1:N:141:VAL:HG12	1:N:143:VAL:HG13	1.88	0.55
1:O:55:ARG:NH1	1:R:324:LEU:O	2.39	0.55
1:R:105:MSE:HE1	1:R:150:HIS:CA	2.34	0.55
1:G:170:THR:O	1:G:172:PRO:HD3	2.06	0.55
1:G:278:GLU:OE1	1:G:278:GLU:HA	2.05	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:79:ILE:HB	1:N:82:GLU:HG3	1.87	0.55
1:N:199:ASN:ND2	1:N:201:LYS:HB2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:I:26:PHE:HD2	2.04	0.55
1:J:145:GLU:C	1:J:147:GLN:H	2.14	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:B:326:ARG:NH2	1:E:301:ASP:OD1	2.29	0.55
1:D:228:ILE:HD13	1:D:265:TYR:CE1	2.42	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: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:86:HIS:HD2	1:P:132:ASP:OD1	1.90	0.55
1:P:169:PHE:CD1	1:P:314:MSE:HE3	2.42	0.55
1:P:241:LEU:HD22	1:P:272:LEU:HD23	1.89	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:D:175:ARG:C	1:D:177:PRO:HD3	2.32	0.55
1:E:244:ILE:O	1:E:248:LEU:HB2	2.06	0.55
1:F:65:TYR:O	1:F:70:ILE:HB	2.06	0.55
1:F:146:ASP:OD1	1:F:146:ASP:N	2.31	0.55
1:G:129:MSE:O	1:G:132:ASP:HB2	2.06	0.55
1:H:175:ARG:O	1:H:177:PRO:HD3	2.07	0.55
1:H:195:LYS:N	3:H:1002:PO4:O2	2.29	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:L:230:TYR:C	1:L:230:TYR:CD1	2.85	0.55
1:M:275:VAL:O	1:M:279:THR:OG1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:99:ILE:O	1:Q:103:GLU:HG3	2.07	0.55
1:A:55:ARG:HH22	1:D:320:GLN:NE2	2.05	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: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:HE2	1:E:105:MSE:CA	2.36	0.54
1:M:41:ASP:OD1	1:M:80:GLN:HB3	2.08	0.54
1:M:313:GLU:OE2	1:M:316:ARG:NH2	2.40	0.54
1:P:289:HIS:O	1:P:293:SER:HB2	2.06	0.54
1:Q:125:TYR:CG	1:Q:126:PRO:HD3	2.42	0.54
1:Q:182:ARG:HA	4:Q:1003:AMP:H2	1.72	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: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:M:190:THR:HG22	1:M:191:LYS:N	2.22	0.54
1:N:120:ALA:HB3	1:Q:97:VAL:HG12	1.88	0.54
1:O:24:ARG:NH2	1:O:247:THR:O	2.40	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:A:199:ASN:HD22	1:A:200:PRO:CD	2.19	0.54
1:B:29:LEU:HD11	1:B:177:PRO:CB	2.27	0.54
1:B:260:TYR:HE1	1:B:271:ASP:OD2	1.91	0.54
1:C:129:MSE:HE3	2:C:1001:TRP:CZ3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:F:59:ARG:HH11	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:Q:199:ASN:C	1:Q:199:ASN:HD22	2.15	0.54
1:R:225:GLU:CD	1:R:227:THR:CG2	2.81	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:E:145:GLU:HG3	1:E:145:GLU:O	2.06	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:OE1	1:A:278:GLU:HA	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:N:124:THR:HG21	1:Q:124:THR:HG21	1.90	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: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:99:ILE:HG12	1:E:118:VAL:O	2.07	0.54
1:B:133:ILE:O	1:B:138:THR:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:238:ILE:C	1:E:241:LEU:HD23	2.34	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:8:ILE:HD12	1:P:65:TYR:OH	2.07	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: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:41:ASP:OD2	1:A:81:SER:HB3	2.08	0.53
1:A:148:LYS:O	1:A:148:LYS:HG2	2.08	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:N	1:I:26:PHE:CD2	2.75	0.53
1:K:126:PRO:CD	1:K:127:PRO:HD2	2.39	0.53
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:P:215:LYS:HE2	1:P:215:LYS:C	2.34	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:185:SER:C	1:F:188:ASP:O	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:199:ASN:HD22	1:I:199:ASN:C	2.14	0.53
1:M:195:LYS:C	1:M:197:ASP:H	2.16	0.53
1:O:19:TYR:CE2	1:O:24:ARG:CD	2.92	0.53
1:O:195:LYS:CG	1:O:196:SER:N	2.72	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:72:PRO:HB3	1:C:299:VAL:HG13	1.91	0.53
1:C:125:TYR:CG	1:C:126:PRO:HD3	2.44	0.53
1:E:40:VAL:HG23	1:E:40:VAL:O	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:86:HIS:HE1	1:O:136:TYR:OH	1.91	0.53
1:O:118:VAL:CG1	1:R:99:ILE:HD11	2.35	0.53
1:O:125:TYR:N	1:O:126:PRO:CD	2.70	0.53
1:P:248:LEU:HD12	1:P:248:LEU:H	1.70	0.53
1:R:40:VAL:O	1:R:40:VAL:HG23	2.09	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: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:G:176:ILE:O	1:G:179:VAL:HG22	2.09	0.53
1:H:72:PRO:HB3	1:H:299:VAL:HG13	1.90	0.53
1:K:8:ILE:HD13	1:K:8:ILE:N	2.23	0.53
1:K:287:TYR:CE1	1:K:291:MSE:HE2	2.43	0.53
1:L:128:LEU:HD12	1:L:128:LEU:O	2.09	0.53
1:M:205:THR:CG2	1:M:207:LEU:H	2.07	0.53
1:P:126:PRO:HD2	1:P:127:PRO:HD2	1.90	0.53
1:R:85:ALA:HB1	1:R:315:VAL:HG21	1.91	0.53
1:R:205:THR:HG22	1:R:207:LEU:N	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:HIS:HE1	1:A:132:ASP:OD2	1.91	0.52
1:B:40:VAL:O	1:B:40:VAL:HG23	2.09	0.52
1:B:243:ASN:O	1:B:247:THR:OG1	2.25	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:N	1:G:78:PHE:CD1	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:225:GLU:CD	1:P:227:THR:OG1	2.52	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: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:H:31:HIS:HA	1:H:74:GLN:NE2	2.24	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: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:2:LYS:O	1:O:33:TYR:HB3	2.10	0.52
1:O:22:ALA:O	1:O:26:PHE:CE1	2.63	0.52
1:O:175:ARG:NH2	1:O:177:PRO:CA	2.72	0.52
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:O	1:E:253:ILE:HG13	2.10	0.52
1:H:19:TYR:HA	1:H:23:LEU:HB3	1.90	0.52
1:J:145:GLU:C	1:J:147:GLN:N	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:ARG:HG3	1:D:281:ARG:NH1	2.25	0.52
1:E:313:GLU:CD	1:E:316:ARG:HE	2.18	0.52
1:F:106:THR:HG22	1:F:107:GLN:N	2.25	0.52
1:L:258:ARG:O	1:L:259:GLN:C	2.51	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:CD2	1:P:161:PHE:O	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:OE1	1:J:313:GLU:HA	2.10	0.52
1:L:23:LEU:HD11	1:L:65:TYR:CE2	2.45	0.52
1:N:326:ARG:NH2	1:Q:301:ASP:OD1	2.43	0.52
1:P:124:THR:C	1:P:127:PRO:HD2	2.35	0.52
1:P:127:PRO:O	1:P:130:ALA:HB3	2.09	0.52
1:A:22:ALA:C	1:A:25:GLN:HE21	2.18	0.52
3:E:1002:PO4:O2	4:E:1003:AMP:O5'	2.28	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:295:GLU:O	1:P:299:VAL:HG23	2.10	0.52
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:F:199:ASN:C	1:F:199:ASN:HD22	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N	1:H:228:ILE:CD1	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:HH11	1:F:59:ARG:HG3	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:53:GLU:HA	1:C:53:GLU:OE2	2.09	0.51
1:C:146:ASP:OD1	1:C:146:ASP:N	2.39	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:H:29:LEU:HD22	1:H:33:TYR:HE1	1.74	0.51
1:J:152:GLU:OE1	1:J:152:GLU:HA	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
1:A:134:LEU:HB3	1:A:169:PHE:CE1	2.45	0.51
1:C:295:GLU:HA	1:C:295:GLU:OE2	2.10	0.51
1:E:38:CYS:SG	1:E:80:GLN:HB2	2.50	0.51
1:I:24:ARG:HH11	1:I:24:ARG:CB	2.23	0.51
1:I:193:MSE:HE2	1:I:203:TYR:HA	1.93	0.51
1:M:73:THR:OG1	1:M:74:GLN:N	2.44	0.51
1:M:245:TYR:HB2	1:M:272:LEU:HD13	1.91	0.51
1:O:297:ASP:O	1:O:301:ASP:OD1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:184:MSE:H	1:P:240:ASN:ND2	2.08	0.51
1:R:19:TYR:CD2	1:R:24:ARG:CG	2.94	0.51
1:R:187:VAL:HG22	1:R:202:ALA:HB1	1.84	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:9:GLN:HA	1:E:9:GLN:NE2	2.26	0.51
1:E:164:ARG:HD3	1:E:165:TYR:CE2	2.46	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:213:ILE:HD12	1:Q:277:ILE:HG13	1.92	0.51
1:Q:252:SER:OG	1:Q:254:GLU:HG2	2.09	0.51
1:R:205:THR:C	1:R:207:LEU:H	2.17	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:71:ASP:OD1	1:J:72:PRO:HD2	2.10	0.51
1:J:134:LEU:HB3	1:J:169:PHE:HD1	1.76	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
1:P:159:GLU:OE2	1:P:163:LYS:HE3	2.09	0.51
3:P:1002:PO4:O1	4:P:1003:AMP:O1P	2.28	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:HD13	1:B:171:ILE:N	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:O:29:LEU:O	1:O:30:GLN:C	2.54	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
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:43:HIS:HE1	1:G:132:ASP:OD2	1.93	0.51
1:G:130:ALA:CB	1:G:154:THR:HB	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:8:ILE:HD12	1:M:65:TYR:OH	2.10	0.51
1:M:55:ARG:HH22	1:P:320:GLN:CD	2.18	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:D:254:GLU:CD	1:D:254:GLU:N	2.69	0.51
1:H:313:GLU:OE1	1:H:313:GLU:HA	2.10	0.51
1:I:79:ILE:HB	1:I:82:GLU:HG3	1.93	0.51
1:K:155:ARG:NH1	1:K:171:ILE:CG2	2.74	0.51
1:K:165:TYR:CE1	1:K:322:MSE:HA	2.45	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:27:VAL:HG13	1:P:28:GLU:OE1	2.10	0.51
1:P:238:ILE:CD1	1:P:268:PHE:CE2	2.94	0.51
1:R:295:GLU:HA	1:R:295:GLU:OE2	2.10	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:43:HIS:CE1	1:R:132:ASP:OD2	2.64	0.51
1:R:162:ASN:HD21	1:R:169:PHE:H	1.59	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:H:45:ILE:HG21	1:K:322:MSE:HE2	1.93	0.50
1:I:5:PHE:CB	1:I:138:THR:HG21	2.41	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
1:R:187:VAL:CG1	1:R:199:ASN:ND2	2.75	0.50
1:B:23:LEU:HD12	1:B:23:LEU:O	2.12	0.50
1:B:29:LEU:CD1	1:B:177:PRO:CB	2.75	0.50
1:B:59:ARG:HH11	1:B:59:ARG:CG	2.24	0.50
1:B:238:ILE:CG1	1:B:265:TYR:CE1	2.95	0.50
1:B:252:SER:O	1:B:255:GLU:HB3	2.11	0.50
1:B:313:GLU:O	1:B:317:LYS:HG3	2.10	0.50
1:D:151:ILE:O	1:D:155:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:THR:O	1:F:107:GLN:C	2.53	0.50
1:F:182:ARG:NH1	1:F:192:LYS:CD	2.65	0.50
1:G:197:ASP:C	1:G:199:ASN:H	2.20	0.50
1:H:101:GLU:CD	1:H:160:ARG:HH22	2.18	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:86:HIS:HE1	1:D:136:TYR:OH	1.94	0.50
1:D:193:MSE:HB3	4:D:1003:AMP:N6	2.25	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:B:159:GLU:O	1:B:163:LYS:HG3	2.11	0.50
1:D:281:ARG:HG3	1:D:281:ARG:HH11	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:22:ALA:O	1:J:25:GLN:HG2	2.10	0.50
1:J:133:ILE:O	1:J:138:THR:HG23	2.11	0.50
1:K:122:LEU:O	1:K:125:TYR:CE1	2.63	0.50
1:M:43:HIS:CE1	1:M:128:LEU:HG	2.46	0.50
1:M:100:GLY:O	1:M:104:ARG:HG3	2.11	0.50
1:M:199:ASN:CG	1:M:201:LYS:HG2	2.34	0.50
1:N:200:PRO:O	1:N:216:LYS:NZ	2.35	0.50
1:P:24:ARG:HH11	1:P:24:ARG:CB	2.24	0.50
1:A:19:TYR:CZ	1:A:24:ARG:HD2	2.46	0.50
1:A:130:ALA:CB	1:A:154:THR:HB	2.42	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
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
3:N:1002:PO4:O1	4:N:1003:AMP:O1P	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:8:ILE:HD12	1:O:65:TYR:HH	1.76	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:K:258:ARG:C	1:K:261:GLU:HG3	2.37	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:184:MSE:H	1:P:240:ASN:HD21	1.59	0.50
1:P:199:ASN:ND2	1:P:201:LYS:HB2	2.26	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:86:HIS:HD2	1:E:132:ASP:OD1	1.95	0.50
1:E:126:PRO:HB2	1:E:127:PRO:CD	2.42	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:M:290:TRP:C	1:M:292:GLU:N	2.69	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:R:257:GLU:O	1:R:260:TYR:C	2.54	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:26:PHE:HA	1:O:29:LEU:HD12	1.93	0.50
1:O:124:THR:HG21	1:R:124:THR:HG21	1.93	0.50
1:P:9:GLN:HA	1:P:9:GLN:NE2	2.26	0.50
1:P:213:ILE:CG2	1:P:217:ILE:HD12	2.42	0.50
1:P:254:GLU:OE1	1:P:254:GLU:N	2.44	0.50
1:Q:182:ARG:NE	1:Q:184:MSE:HE1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:Q:146:ASP:N	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
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:R:45:ILE:C	1:R:47:VAL:H	2.19	0.49
1:B:22:ALA:HB1	1:B:26:PHE:HE2	1.77	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: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:OD1	1:K:146:ASP:N	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: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:101:GLU:CD	1:G:160:ARG:NH2	2.70	0.49
1:G:126:PRO:HB2	1:G:127:PRO:CD	2.37	0.49
1:J:26:PHE:CE2	1:J:29:LEU:HD12	2.48	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:105:MSE:HE1	1:K:150:HIS:ND1	2.27	0.49
1:P:41:ASP:OD2	1:P:81:SER:HB3	2.12	0.49
1:P:215:LYS:O	1:P:215:LYS:CE	2.61	0.49
1:R:59:ARG:HH11	1:R:59:ARG:CG	2.26	0.49
1:B:238:ILE:HD11	1:B:265:TYR:CD1	2.48	0.49
1:B:281:ARG:HH11	1:B:281:ARG:CG	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:HH11	1:J:59:ARG:CG	2.25	0.49
1:L:9:GLN:HG2	1:L:40:VAL:CG2	2.42	0.49
1:L:59:ARG:HH11	1:L:59:ARG:CG	2.25	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:71:ASP:O	1:B:75:ALA:N	2.40	0.49
1:B:205:THR:HG22	1:B:208:ASP:H	1.75	0.49
1:E:48:TRP:HB2	1:O:188:ASP:OD1	2.13	0.49
1:E:170:THR:O	1:E:172:PRO:HD3	2.12	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:59:ARG:CG	1:A:59:ARG:HH11	2.26	0.49
1:A:199:ASN:HD21	1:A:201:LYS:HG3	1.78	0.49
1:B:55:ARG:HD2	1:E:323:GLY:C	2.38	0.49
1:H:23:LEU:HD12	1:H:23:LEU:C	2.38	0.49
1:J:27:VAL:O	1:J:27:VAL:HG12	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:N	1:O:171:ILE:CD1	2.76	0.49
1:Q:26:PHE:HA	1:Q:29:LEU:HB2	1.95	0.49
1:R:41:ASP:CB	1:R:58:ILE:HD11	2.39	0.49
1:R:162:ASN:O	1:R:166:GLY:O	2.31	0.49
1:C:5:PHE:CB	1:C:138:THR:HG21	2.43	0.49
1:C:99:ILE:HG12	1:F:118:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:VAL:HB	1:F:99:ILE:HG13	1.93	0.49
1:D:228:ILE:HD11	1:D:265:TYR:HD1	1.78	0.49
1:F:105:MSE:HE2	1:F:105:MSE:N	2.28	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:N:99:ILE:CD1	1:Q:120:ALA:HA	2.42	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: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:C:25:GLN:H	1:C:25:GLN:CD	2.21	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:K:155:ARG:HG2	1:K:171:ILE:HG23	1.95	0.49
1:O:5:PHE:CZ	1:O:38:CYS:HB2	2.48	0.49
1:O:193:MSE:CA	4:O:1003:AMP:HN61	2.25	0.49
1:P:245:TYR:CE2	1:P:256:LEU:HD13	2.46	0.49
1:R:183:ILE:C	1:R:184:MSE:HG2	2.33	0.49
1:A:159:GLU:HG3	1:A:163:LYS:HE2	1.95	0.48
1:B:245:TYR:HD1	1:B:245:TYR:O	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
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:I:278:GLU:CD	1:I:281:ARG:NH2	2.71	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: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
1:Q:238:ILE:CD1	1:Q:265:TYR:CE1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:25:GLN:CD	1:F:25:GLN:N	2.72	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:199:ASN:HD22	1:M:199:ASN:C	2.20	0.48
4:M:1003:AMP:O1P	4:M:1003:AMP:O3'	2.29	0.48
1:N:304:ALA:O	1:N:308:ASN:HB2	2.13	0.48
1:P:298:ARG:HG3	1:P:298:ARG:NH1	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:OD1	1:D:146:ASP:N	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:197:ASP:C	1:G:199:ASN:N	2.69	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:3:THR:HB	1:R:138:THR:HA	1.95	0.48
1:R:240:ASN:O	1:R:243:ASN:HB2	2.11	0.48
1:C:320:GLN:HE22	1:F:55:ARG:NH2	2.07	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: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:K:261:GLU:C	1:K:263:LYS:HD2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:325:GLY:O	1:D:55:ARG:HD2	2.12	0.48
1:D:151:ILE:HA	1:D:154:THR:HG23	1.95	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:H:119:SER:HA	1:K:97:VAL:O	2.14	0.48
1:J:199:ASN:HD22	1:J:200:PRO:HD2	1.78	0.48
1:N:120:ALA:CB	1:Q:97:VAL:CG1	2.91	0.48
1:O:29:LEU:O	1:O:32:GLU:N	2.41	0.48
1:O:254:GLU:OE1	1:O:254:GLU:N	2.47	0.48
1:Q:140:ILE:CD1	1:Q:175:ARG:O	2.61	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:22:ALA:O	1:P:26:PHE:HD2	1.95	0.48
1:P:212:THR:O	1:P:216:LYS:HB3	2.13	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:25:GLN:H	1:A:25:GLN:CD	2.21	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:84:PRO:HD2	1:E:308:ASN:HD21	1.78	0.48
1:E:205:THR:CG2	1:E:207:LEU:H	2.15	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:K:239:SER:O	1:K:240:ASN:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:86:HIS:CD2	1:B:132:ASP:HA	2.49	0.47
1:G:54:LEU:O	1:G:58:ILE:HG13	2.13	0.47
1:G:224:SER:CB	1:I:166:GLY:N	2.77	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:O:289:HIS:ND1	1:O:289:HIS:C	2.71	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:71:ASP:OD1	1:E:72:PRO:HD2	2.15	0.47
1:E:293:SER:OG	1:E:295:GLU:HB2	2.14	0.47
1:F:41:ASP:OD2	1:F:81:SER:HB3	2.13	0.47
1:F:313:GLU:HA	1:F:313:GLU:OE1	2.15	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: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:83:VAL:HG13	1:D:308:ASN:HA	1.97	0.47
1:D:304:ALA:O	1:D:308:ASN:HB2	2.14	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:O	1:K:167:GLU:HG2	2.13	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:161:PHE:C	1:R:161:PHE:CD2	2.92	0.47
1:R:313:GLU:OE2	1:R:316:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:4:ILE:HD11	1:O:33:TYR:CG	2.48	0.47
1:O:25:GLN:O	1:O:29:LEU:HG	2.13	0.47
1:R:215:LYS:HD2	1:R:215:LYS:C	2.39	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
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:Q:101:GLU:O	1:Q:105:MSE:HE3	2.15	0.47
1:Q:175:ARG:HG3	1:Q:175:ARG:O	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
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:289:HIS:ND1	1:B:289:HIS:C	2.72	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:E:287:TYR:C	1:E:289:HIS:H	2.23	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:N	1:I:263:LYS:HD2	2.29	0.47
1:J:24:ARG:O	1:J:24:ARG:HG3	2.14	0.47
1:J:125:TYR:CD2	1:J:126:PRO:HD3	2.49	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:38:CYS:SG	1:A:80:GLN:HB2	2.54	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:B:272:LEU:O	1:B:276:VAL:HG23	2.14	0.47
1:C:55:ARG:HD2	1:F:325:GLY:O	2.15	0.47
1:C:137:ASN:ND2	1:C:170:THR:OG1	2.37	0.47
1:C:194:SER:O	1:C:197:ASP:HB2	2.15	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:89:ALA:HB2	1:G:135:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:LYS:O	1:G:211:LYS:HG3	2.14	0.47
1:H:256:LEU:O	1:H:260:TYR:HD2	1.97	0.47
1:I:176:ILE:C	1:I:176:ILE:HD12	2.40	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: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: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:P:185:SER:HB3	1:P:188:ASP:O	2.14	0.47
1:P:194:SER:HA	3:P:1002:PO4:O4	2.15	0.47
1:P:195:LYS:HB3	3:P:1002:PO4:O2	2.15	0.47
1:Q:56:GLN:O	1:Q:60:ARG:HB2	2.15	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:A:124:THR:CG2	1:D:124:THR:HG21	2.41	0.47
1:C:128:LEU:HD22	1:F:91:TRP:CE2	2.50	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:137:ASN:ND2	1:H:170:THR:HG23	2.27	0.47
1:H:158:ALA:HB3	1:H:171:ILE:HD12	1.95	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:OE1	1:L:152:GLU:HA	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:O:251:GLN:HB3	1:O:255:GLU:CD	2.40	0.47
1:P:161:PHE:C	1:P:161:PHE:HD2	2.22	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:3:THR:HB	1:J:138:THR:HA	1.97	0.47
1:J:123:LEU:O	1:J:123:LEU:HG	2.15	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:CA	1:O:105:MSE:CE	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:56:GLN:HG2	1:R:60:ARG:HH21	1.80	0.47
1:R:272:LEU:C	1:R:272:LEU:CD1	2.84	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
1:G:95:CYS:O	1:J:119:SER:OG	2.29	0.47
1:H:42:GLN:HB2	1:H:80:GLN:OE1	2.14	0.47
1:H:315:VAL:O	1:H:319:GLU:HG3	2.15	0.47
1:I:25:GLN:OE1	1:I:178:LYS:O	2.33	0.47
1:J:124:THR:O	1:J:124:THR:OG1	2.32	0.47
1:J:177:PRO:C	1:J:178:LYS:HG2	2.39	0.47
4:M:1003:AMP:P	4:M:1003:AMP:H3'	2.55	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:R:205:THR:C	1:R:207:LEU:N	2.69	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:NH1	1:G:309:ARG:HB3	2.30	0.46
1:H:228:ILE:N	1:H:228:ILE:HD12	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:291:MSE:HE3	1:R:291:MSE:C	2.40	0.46
1:D:228:ILE:CD1	1:D:265:TYR:CD1	2.98	0.46
1:F:107:GLN:NE2	1:F:107:GLN:N	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:85:ALA:HA	1:O:88:GLN:HG3	1.96	0.46
1:O:319:GLU:HB3	1:O:324:LEU:HB2	1.96	0.46
1:P:9:GLN:HE21	1:P:9:GLN:CA	2.23	0.46
1:P:189:PRO:C	1:P:191:LYS:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:290:TRP:C	1:M:292:GLU:H	2.23	0.46
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:59:ARG:HH22	1:R:297:ASP:CG	2.23	0.46
1:R:213:ILE:HD13	1:R:277:ILE:HG12	1.92	0.46
1:B:65:TYR:O	1:B:70:ILE:HB	2.15	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: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:HA	1:M:74:GLN:HE21	1.81	0.46
1:O:175:ARG:CG	1:O:175:ARG:NH2	2.78	0.46
1:P:209:ASP:OD1	1:P:212:THR:OG1	2.30	0.46
1:C:1:MSE:CG	1:D:211:LYS:HD2	2.29	0.46
1:C:227:THR:HG21	1:C:229:ARG:CZ	2.46	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:I:225:GLU:HG3	1:N:163:LYS:HD3	1.98	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: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:G:211:LYS:HD2	1:K:1:MSE:CG	2.45	0.46
1:J:177:PRO:C	1:J:178:LYS:CG	2.88	0.46
1:K:40:VAL:HG23	1:K:40:VAL:O	2.15	0.46
1:L:40:VAL:HG23	1:L:40:VAL:O	2.16	0.46
1:L:289:HIS:O	1:L:293:SER:HB3	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLN:HE21	1:D:55:ARG:HH22	1.45	0.46
1:H:192:LYS:O	1:H:193:MSE:C	2.59	0.46
1:K:105:MSE:CE	1:K:150:HIS:CE1	2.99	0.46
1:M:56:GLN:CD	1:M:60:ARG:NH2	2.74	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
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
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
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:33:TYR:CD1	1:O:33:TYR:N	2.84	0.46
1:O:326:ARG:NH1	1:R:300:LEU:CB	2.79	0.46
1:P:64:LEU:HG	1:P:287:TYR:CD1	2.51	0.46
1:P:193:MSE:HB3	4:P:1003:AMP:HN62	1.77	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:32:GLU:CG	1:B:33:TYR:CE1	2.99	0.46
1:B:175:ARG:C	1:B:176:ILE:CG1	2.89	0.46
1:B:238:ILE:HD11	1:B:265:TYR:CE1	2.50	0.46
1:E:9:GLN:HA	1:E:9:GLN:HE21	1.81	0.46
1:F:25:GLN:HB3	1:F:178:LYS:HB2	1.98	0.46
1:G:295:GLU:O	1:G:295:GLU:HG2	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:4:ILE:HD12	1:P:33:TYR:CD2	2.51	0.46
1:P:26:PHE:HZ	1:P:142:PRO:CB	2.29	0.46
1:R:51:PRO:O	1:R:55:ARG:HB2	2.15	0.46
1:A:26:PHE:HA	1:A:29:LEU:HB2	1.98	0.46
1:A:281:ARG:HH11	1:A:281:ARG:CG	2.26	0.46
1:B:175:ARG:CG	1:B:176:ILE:N	2.66	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:26:PHE:O	1:N:30:GLN:N	2.48	0.46
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:A:242:LEU:O	1:A:246:SER:HB3	2.16	0.45
1:B:59:ARG:CG	1:B:59:ARG:NH1	2.79	0.45
1:E:238:ILE:O	1:E:239:SER:C	2.59	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:63:ALA:CB	1:E:291:MSE:SE	3.14	0.45
1:E:126:PRO:N	1:E:127:PRO:CD	2.79	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:J:205:THR:C	1:J:207:LEU:N	2.74	0.45
1:O:4:ILE:HG22	1:O:142:PRO:HD3	1.98	0.45
1:O:18:ASN:OD1	4:O:1003:AMP:O4'	2.34	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:42:GLN:HB2	1:A:80:GLN:OE1	2.16	0.45
1:A:213:ILE:HD11	1:A:280:LEU:HD12	1.98	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:I:106:THR:O	1:I:107:GLN:C	2.59	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:5:PHE:CE1	1:P:132:ASP:HB3	2.52	0.45
1:P:101:GLU:O	1:P:105:MSE:CG	2.60	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:120:ALA:HA	1:E:99:ILE:CG1	2.47	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:F:191:LYS:HE2	1:F:191:LYS:HB3	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:320:GLN:O	1:J:320:GLN:HG3	2.13	0.45
1:K:86:HIS:HE1	1:K:136:TYR:OH	2.00	0.45
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:D:209:ASP:OD1	1:D:209:ASP:C	2.59	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:105:MSE:O	1:M:106:THR:C	2.59	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:P:230:TYR:CD1	1:P:230:TYR:C	2.94	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:8:ILE:HD13	1:B:65:TYR:OH	2.16	0.45
1:B:241:LEU:HD12	1:B:241:LEU:HA	1.73	0.45
1:D:136:TYR:HB2	1:D:138:THR:HG22	1.98	0.45
1:E:123:LEU:O	1:E:123:LEU:HG	2.17	0.45
1:G:162:ASN:CG	1:G:167:GLU:HA	2.41	0.45
1:I:105:MSE:HE2	1:I:105:MSE:HB2	1.78	0.45
1:M:164:ARG:NH2	1:P:48:TRP:CD2	2.84	0.45
1:P:25:GLN:O	1:P:29:LEU:HG	2.17	0.45
1:P:238:ILE:O	1:P:242:LEU:HG	2.16	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: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:40:VAL:HG23	1:D:40:VAL:O	2.17	0.45
1:D:182:ARG:HD3	1:D:184:MSE:HE1	1.99	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:HD12	1:L:122:LEU:HA	1.84	0.45
1:M:45:ILE:C	1:M:47:VAL:N	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:ILE:CG1	1:Q:118:VAL:O	2.63	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:Q:24:ARG:HH11	1:Q:24:ARG:HG2	1.78	0.45
1:Q:192:LYS:HE2	1:Q:192:LYS:HB3	1.55	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:49:GLN:O	1:K:164:ARG:NH2	2.45	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:I:249:SER:HB2	1:I:251:GLN:CG	2.46	0.45
1:J:241:LEU:HD12	1:J:241:LEU:HA	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:71:ASP:O	1:K:75:ALA:N	2.31	0.45
1:K:237:GLY:C	1:K:241:LEU:HD11	2.35	0.45
1:K:256:LEU:HD22	1:K:260:TYR:CD1	2.52	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: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:P:181:ALA:CB	1:P:243:ASN:ND2	2.73	0.45
1:Q:161:PHE:CD2	1:Q:161:PHE:C	2.95	0.45
1:R:155:ARG:O	1:R:159:GLU:HB2	2.17	0.45
1:R:302:GLU:O	1:R:306:LYS:HG3	2.17	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:60:ARG:HG2	1:I:287:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:ASN:O	1:J:166:GLY:N	2.50	0.45
1:L:59:ARG:CG	1:L:59:ARG:NH1	2.79	0.45
1:M:72:PRO:HG3	1:M:299:VAL:HG11	1.99	0.45
1:M:253:ILE:O	1:M:257:GLU:OE1	2.34	0.45
1:N:86:HIS:HD2	1:N:132:ASP:OD1	2.00	0.45
1:P:142:PRO:C	1:P:176:ILE:HG12	2.41	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:N	1:R:171:ILE:CD1	2.80	0.45
1:B:129:MSE:O	1:B:132:ASP:HB2	2.16	0.44
1:B:183:ILE:N	4:B:1003:AMP:N1	2.55	0.44
1:D:192:LYS:HE2	1:D:192:LYS:HB3	1.82	0.44
1:J:161:PHE:C	1:J:161:PHE:CD2	2.95	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:24:ARG:O	1:P:27:VAL:HG12	2.17	0.44
1:P:162:ASN:O	1:P:166:GLY:CA	2.65	0.44
1:P:199:ASN:C	1:P:201:LYS:N	2.76	0.44
1:P:245:TYR:CA	1:P:272:LEU:HD11	2.45	0.44
1:Q:26:PHE:HD2	1:Q:29:LEU:HD12	1.82	0.44
1:R:105:MSE:O	1:R:106:THR:C	2.60	0.44
1:A:188:ASP:OD2	1:A:191:LYS:HB2	2.17	0.44
1:B:325:GLY:C	1:B:326:ARG:HG3	2.42	0.44
1:G:41:ASP:CG	1:G:81:SER:HB3	2.41	0.44
1:G:55:ARG:HD2	1:J:325:GLY:O	2.17	0.44
1:H:25:GLN:HG2	1:H:178:LYS:HB2	1.98	0.44
1:J:41:ASP:CG	1:J:81:SER:HB3	2.41	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: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: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: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:41:ASP:N	1:H:41:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:ASP:HA	1:H:198:PRO:HD3	1.52	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:P:325:GLY:C	1:P:326:ARG:HG2	2.42	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:O	1:B:20:ILE:HG22	2.18	0.44
1:C:22:ALA:O	1:C:26:PHE:HD2	1.97	0.44
1:C:86:HIS:CD2	1:C:132:ASP:OD1	2.67	0.44
1:C:260:TYR:HA	1:C:263:LYS:HG2	2.00	0.44
1:E:184:MSE:HE1	1:E:191:LYS:C	2.41	0.44
1:F:192:LYS:HE2	1:F:192:LYS:HB3	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: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:19:TYR:CD2	1:R:24:ARG:HG3	2.53	0.44
1:R:148:LYS:HE2	1:R:148:LYS:HB2	1.88	0.44
1:R:162:ASN:CA	1:R:166:GLY:O	2.64	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:16:ILE:O	1:H:20:ILE:HB	2.18	0.44
1:H:148:LYS:HB2	1:H:148:LYS:HE2	1.43	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:48:TRP:O	1:M:49:GLN:HG2	2.18	0.44
1:M:150:HIS:O	1:M:154:THR:CG2	2.65	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: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:29:LEU:HD11	1:I:177:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:71:ASP:HA	1:K:72:PRO:HD2	1.81	0.44
1:K:158:ALA:O	1:K:162:ASN:CG	2.60	0.44
1:K:287:TYR:CZ	1:K:291:MSE:HE3	2.51	0.44
1:L:5:PHE:CB	1:L:138:THR:HG21	2.43	0.44
1:N:40:VAL:HG23	1:N:40:VAL:O	2.18	0.44
1:N:59:ARG:CG	1:N:59:ARG:NH1	2.79	0.44
1:N:199:ASN:HD22	1:N:201:LYS:H	1.65	0.44
1:O:74:GLN:HG3	1:O:74:GLN:O	2.17	0.44
1:P:188:ASP:OD1	1:P:190:THR:OG1	2.34	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:56:GLN:HG2	1:R:60:ARG:NH2	2.32	0.44
1:R:168:LEU:HD23	1:R:168:LEU:HA	1.82	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:E:161:PHE:C	1:E:161:PHE:CD2	2.95	0.44
1:J:294:GLU:C	1:J:296:LEU:N	2.76	0.44
1:L:182:ARG:HG2	1:L:184:MSE:HE1	2.00	0.44
1:L:313:GLU:OE1	1:L:313:GLU:HA	2.17	0.44
1:M:25:GLN:C	1:M:29:LEU:HG	2.43	0.44
1:M:213:ILE:CD1	1:M:280:LEU:HD12	2.47	0.44
1:M:276:VAL:O	1:M:278:GLU:N	2.51	0.44
1:N:260:TYR:HA	1:N:263:LYS:HE3	2.00	0.44
1:O:26:PHE:HA	1:O:29:LEU:HB2	1.99	0.44
1:O:205:THR:CG2	1:O:206:LEU:N	2.80	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:O	1:R:160:ARG:HG3	2.17	0.44
1:R:296:LEU:HD12	1:R:296:LEU:HA	1.71	0.44
1:A:106:THR:N	1:A:149:GLN:OE1	2.45	0.44
1:A:130:ALA:HB1	1:A:154:THR:HB	2.00	0.44
1:A:272:LEU:HA	1:A:275:VAL:HG13	1.99	0.44
1:B:162:ASN:C	1:B:165:TYR:O	2.61	0.44
1:D:188:ASP:C	1:D:188:ASP:OD1	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:176:ILE:HG13	1:I:176:ILE:O	2.18	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:O	1:L:27:VAL:HG12	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:2:LYS:N	1:B:2:LYS:CD	2.80	0.44
1:B:40:VAL:HA	1:B:80:GLN:OE1	2.18	0.44
1:B:238:ILE:HD13	1:B:238:ILE:HA	1.71	0.44
1:E:190:THR:CG2	1:O:48:TRP:CE3	3.01	0.44
1:E:212:THR:O	1:E:216:LYS:HB2	2.18	0.44
1:L:241:LEU:HD12	1:L:241:LEU:HA	1.78	0.44
1:M:25:GLN:NE2	1:M:178:LYS:O	2.50	0.44
1:M:205:THR:CG2	1:M:206:LEU:N	2.81	0.44
1:N:228:ILE:HD13	1:N:265:TYR:CE1	2.52	0.44
1:N:251:GLN:OE1	1:N:259:GLN:NE2	2.47	0.44
1:O:91:TRP:NE1	1:R:42:GLN:HB3	2.33	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:60:ARG:HG3	1:R:287:TYR:OH	2.18	0.44
1:R:76:THR:HG23	1:R:306:LYS:HE3	2.00	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:HG3	1:P:129:MSE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:ALA:O	1:I:26:PHE:CD2	2.70	0.43
1:J:263:LYS:HZ3	1:J:263:LYS:HG3	1.72	0.43
1:L:59:ARG:HH11	1:L:59:ARG:HG3	1.82	0.43
1:M:290:TRP:O	1:M:291:MSE:C	2.60	0.43
1:N:122:LEU:HD13	1:N:122:LEU:HA	1.71	0.43
1:O:126:PRO:CB	1:O:127:PRO:CD	2.96	0.43
1:P:216:LYS:O	1:P:216:LYS:CG	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
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:HB3	1:C:201:LYS:HE3	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:J:194:SER:OG	3:J:1002:PO4:O4	2.32	0.43
1:O:96:ILE:O	1:O:160:ARG:NH1	2.50	0.43
1:O:155:ARG:O	1:O:159:GLU:HB2	2.18	0.43
1:P:225:GLU:CD	1:P:227:THR:HG1	2.24	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:20:ILE:HD13	1:L:247:THR:OG1	2.18	0.43
1:L:210:ALA:HB1	1:L:277:ILE:HD13	2.00	0.43
1:M:147:GLN:O	1:M:150:HIS:HB2	2.18	0.43
1:M:211:LYS:HB2	1:Q:1:MSE:HG3	2.00	0.43
1:N:147:GLN:OE1	1:N:150:HIS:HD2	2.01	0.43
1:P:217:ILE:HD11	1:P:276:VAL:HG21	2.00	0.43
1:P:253:ILE:O	1:P:257:GLU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:106:THR:H	1:E:149:GLN:CD	2.26	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
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
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: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:I:160:ARG:HE	1:I:160:ARG:HB2	1.73	0.43
1:J:185:SER:CA	1:J:188:ASP:O	2.66	0.43
1:J:205:THR:C	1:J:207:LEU:H	2.27	0.43
1:K:96:ILE:O	1:K:160:ARG:NH1	2.48	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: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:N	1:P:228:ILE:CD1	2.82	0.43
1:Q:59:ARG:CZ	1:Q:296:LEU:HD23	2.48	0.43
1:Q:281:ARG:NH1	1:Q:281:ARG:CG	2.79	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:HG3	1:P:298:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:29:LEU:HD22	1:R:33:TYR:HE1	1.82	0.43
1:A:59:ARG:CG	1:A:59:ARG:NH1	2.81	0.43
1:C:238:ILE:HA	1:C:238:ILE:HD13	1.77	0.43
1:F:32:GLU:H	1:F:32:GLU:HG2	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:HD12	1:M:168:LEU:O	2.18	0.43
1:M:320:GLN:HE21	1:M:320:GLN:HB2	1.56	0.43
1:P:181:ALA:CB	1:P:243:ASN:HD22	2.11	0.43
1:B:8:ILE:CD1	1:B:65:TYR:OH	2.67	0.43
1:B:32:GLU:HG2	1:B:33:TYR:CE1	2.54	0.43
1:E:184:MSE:CE	1:E:190:THR:C	2.92	0.43
1:H:80:GLN:NE2	1:H:132:ASP:OD1	2.52	0.43
1:H:320:GLN:HA	1:K:55:ARG:NH2	2.34	0.43
1:K:239:SER:HA	1:K:242:LEU:HD12	2.01	0.43
1:L:238:ILE:HD13	1:L:238:ILE:HA	1.72	0.43
1:M:55:ARG:NH2	1:P:320:GLN:CD	2.77	0.43
1:M:92:MSE:O	1:M:96:ILE:HG23	2.18	0.43
1:M:118:VAL:HB	1:P:99:ILE:CG1	2.48	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:23:LEU:CD1	1:D:65:TYR:CE2	3.01	0.43
1:D:210:ALA:HA	1:D:213:ILE:HD12	2.01	0.43
1:E:245:TYR:CD1	1:E:245:TYR:C	2.97	0.43
1:M:276:VAL:C	1:M:278:GLU:N	2.73	0.43
1:O:122:LEU:HD12	1:O:122:LEU:HA	1.87	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: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:199:ASN:ND2	1:I:199:ASN:C	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:55:ARG:HH22	1:P:320:GLN:HA	1.84	0.42
1:M:293:SER:OG	1:M:294:GLU:N	2.52	0.42
1:N:55:ARG:HD2	1:Q:325:GLY:O	2.19	0.42
1:P:160:ARG:HE	1:P:160:ARG:HB2	1.59	0.42
1:P:267:VAL:CG2	1:P:268:PHE:N	2.82	0.42
1:A:56:GLN:O	1:A:60:ARG:HG3	2.19	0.42
1:A:134:LEU:HB3	1:A:169:PHE:HD1	1.74	0.42
1:B:175:ARG:C	1:B:176:ILE:HG13	2.44	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:23:LEU:HD21	1:F:68:VAL:HG11	2.00	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:F:199:ASN:HD21	1:F:201:LYS:HB2	1.83	0.42
1:F:301:ASP:O	1:F:305:GLU:HB2	2.19	0.42
1:G:4:ILE:HD12	1:G:33:TYR:CG	2.54	0.42
1:G:55:ARG:NH2	1:J:320:GLN:HA	2.33	0.42
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:I:161:PHE:C	1:I:161:PHE:CD2	2.98	0.42
1:J:197:ASP:HA	1:J:198:PRO:HD3	1.88	0.42
1:K:65:TYR:O	1:K:70:ILE:HB	2.20	0.42
1:K:134:LEU:CB	1:K:169:PHE:HE1	2.28	0.42
1:K:165:TYR:CE1	1:K:321:ALA:O	2.72	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:101:GLU:CD	1:B:160:ARG:HH22	2.27	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: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:J:185:SER:C	1:J:188:ASP:O	2.62	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:99:ILE:HG12	1:R:99:ILE:H	1.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:TYR:O	1:F:216:LYS:NZ	2.43	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:N:281:ARG:N	1:N:282:PRO:HD2	2.35	0.42
1:O:91:TRP:CZ2	1:R:128:LEU:HD22	2.55	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:R:71:ASP:OD2	1:R:73:THR:OG1	2.27	0.42
1:A:124:THR:CG2	1:D:94:GLN:HE22	2.23	0.42
1:C:56:GLN:HB3	1:C:60:ARG:NH2	2.35	0.42
1:C:124:THR:HG21	1:F:124:THR:HG21	2.01	0.42
1:D:126:PRO:CB	1:D:127:PRO:HD3	2.37	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: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:99:ILE:O	1:M:99:ILE:CG2	2.60	0.42
1:M:165:TYR:CD1	1:M:321:ALA:C	2.96	0.42
1:N:254:GLU:CD	1:N:254:GLU:N	2.76	0.42
1:N:315:VAL:O	1:N:319:GLU:HG3	2.19	0.42
1:O:94:GLN:O	1:O:97:VAL:HG12	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:P:15:THR:HB	1:P:193:MSE:SE	2.70	0.42
1:P:53:GLU:O	1:P:57:ASN:HB2	2.18	0.42
1:P:253:ILE:O	1:P:257:GLU:CB	2.68	0.42
1:Q:106:THR:O	1:Q:107:GLN:C	2.62	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:HE	1:D:229:ARG:HB3	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:HG22	1:H:228:ILE:O	2.19	0.42
1:L:318:MSE:O	1:L:322:MSE:HG3	2.19	0.42
1:M:44:ALA:O	1:M:49:GLN:NE2	2.43	0.42
1:M:135:LEU:HD13	1:M:311:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:213:ILE:HG23	1:O:276:VAL:HG11	2.01	0.42
1:O:275:VAL:O	1:O:279:THR:OG1	2.29	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:P:168:LEU:HD23	1:P:168:LEU:HA	1.77	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
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:Q:209:ASP:OD1	1:Q:212:THR:OG1	2.31	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:A:71:ASP:HB3	1:A:74:GLN:CB	2.50	0.42
1:C:28:GLU:HA	1:C:31:HIS:CD2	2.44	0.42
1:C:281:ARG:N	1:C:282:PRO:HD2	2.33	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: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: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:A:199:ASN:HA	1:A:200:PRO:HD3	1.83	0.42
1:C:254:GLU:N	1:C:254:GLU:CD	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:TYR:O	1:L:70:ILE:HB	2.20	0.42
1:L:107:GLN:CD	1:L:107:GLN:H	2.28	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:P:254:GLU:C	1:P:256:LEU:N	2.76	0.42
1:R:281:ARG:HB3	1:R:282:PRO:CD	2.49	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:D:305:GLU:HB3	1:O:267:VAL:CG2	2.50	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:41:ASP:OD2	1:H:81:SER:HB3	2.19	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
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:24:ARG:HH11	1:L:24:ARG:CG	2.33	0.42
1:L:86:HIS:CD2	1:L:132:ASP:OD1	2.71	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: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:65:TYR:O	1:G:70:ILE:HB	2.20	0.41
1:G:101:GLU:O	1:G:105:MSE:HE3	2.20	0.41
1:H:249:SER:OG	1:H:251:GLN:CG	2.68	0.41
1:M:119:SER:C	1:M:121:GLY:N	2.76	0.41
1:M:249:SER:OG	1:M:251:GLN:HG3	2.21	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
1:D:161:PHE:CD2	1:D:161:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:LEU:HD23	1:E:29:LEU:HA	1.86	0.41
1:E:286:ARG:O	1:E:289:HIS:N	2.53	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:OE1	1:L:278:GLU:HA	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:P:125:TYR:C	1:P:125:TYR:CD2	2.98	0.41
1:B:86:HIS:HD2	1:B:132:ASP:HA	1.84	0.41
1:B:200:PRO:O	1:B:216:LYS:HE2	2.20	0.41
1:E:218:LYS:HE3	1:E:218:LYS:HB2	1.83	0.41
1:F:105:MSE:CA	1:F:105:MSE:CE	2.95	0.41
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:I:123:LEU:O	1:I:123:LEU:HG	2.16	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:64:LEU:CD2	1:M:287:TYR:CE1	3.02	0.41
1:M:130:ALA:CB	1:M:154:THR:HB	2.50	0.41
1:N:55:ARG:HH21	1:Q:320:GLN:NE2	2.18	0.41
1:N:118:VAL:HB	1:Q:99:ILE:HG13	2.01	0.41
1:P:105:MSE:HE1	1:P:149:GLN:O	2.19	0.41
1:P:125:TYR:N	1:P:126:PRO:HD3	2.29	0.41
1:P:192:LYS:HZ3	4:P:1003:AMP:H5'1	1.85	0.41
1:Q:93:LEU:HD23	1:Q:96:ILE:HD13	2.02	0.41
1:Q:241:LEU:HB3	1:Q:268:PHE:HE2	1.85	0.41
1:R:96:ILE:O	1:R:160:ARG:NH1	2.51	0.41
1:R:251:GLN:HB3	1:R:256:LEU:HD12	2.01	0.41
1:D:28:GLU:H	1:D:28:GLU:HG2	1.79	0.41
1:D:86:HIS:CE1	1:D:136:TYR:OH	2.74	0.41
1:E:269:LYS:C	1:E:271:ASP:N	2.77	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:59:ARG:HH11	1:J:59:ARG:HG3	1.85	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:K:78:PHE:N	1:K:78:PHE:CD1	2.88	0.41
1:K:187:VAL:HG13	1:K:202:ALA:HA	2.02	0.41
1:L:119:SER:O	1:L:122:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:306:LYS:O	1:M:310:VAL:HG23	2.21	0.41
1:N:152:GLU:OE1	1:N:152:GLU:HA	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:A:125:TYR:CD1	1:A:125:TYR:C	2.98	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:E:245:TYR:HD1	1:E:245:TYR:C	2.28	0.41
1:I:289:HIS:O	1:I:293:SER:HB2	2.21	0.41
1:I:326:ARG:NH2	1:L:301:ASP:OD1	2.53	0.41
1:J:34:ASN:HD22	1:J:34:ASN:HA	1.77	0.41
1:L:27:VAL:O	1:L:27:VAL:CG1	2.69	0.41
1:M:55:ARG:NH2	1:P:320:GLN:HA	2.36	0.41
1:P:76:THR:HG23	1:P:306:LYS:HE3	2.03	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:I:26:PHE:C	1:I:28:GLU:N	2.77	0.41
1:J:120:ALA:C	1:J:124:THR:HG23	2.44	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:8:ILE:C	1:B:40:VAL:HG22	2.46	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:OD1	1:D:209:ASP:O	2.39	0.41
1:H:192:LYS:O	1:H:194:SER:N	2.53	0.41
1:J:254:GLU:N	1:J:254:GLU:CD	2.78	0.41
1:J:295:GLU:O	1:J:299:VAL:HG23	2.20	0.41
1:L:129:MSE:O	1:L:132:ASP:HB2	2.21	0.41
1:N:161:PHE:CD2	1:N:161:PHE:C	2.99	0.41
1:N:168:LEU:HD22	1:N:314:MSE:SE	2.71	0.41
1:O:71:ASP:HA	1:O:72:PRO:HD2	1.81	0.41
1:O:296:LEU:C	1:O:298:ARG:N	2.75	0.41
3:O:1002:PO4:O3	4:O:1003:AMP:O1P	2.39	0.41
1:P:56:GLN:CD	1:P:60:ARG:NH2	2.78	0.41
1:P:169:PHE:HE1	1:P:314:MSE:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:205:THR:CG2	1:Q:206:LEU:N	2.83	0.41
1:Q:313:GLU:HA	1:Q:313:GLU:OE1	2.20	0.41
1:R:289:HIS:O	1:R:293:SER:N	2.53	0.41
1:D:42:GLN:HB2	1:D:80:GLN:OE1	2.21	0.41
1:F:160:ARG:HE	1:F:160:ARG:HB2	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:29:LEU:CD1	1:L:177:PRO:HG2	2.50	0.41
1:L:141:VAL:N	1:L:173:GLU:O	2.48	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:C:23:LEU:HG	1:C:68:VAL:HG11	2.02	0.41
1:C:99:ILE:HG13	1:F:118:VAL:HB	2.03	0.41
1:C:145:GLU:O	1:C:148:LYS:HB3	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:F:71:ASP:HA	1:F:72:PRO:HD2	1.86	0.41
1:G:182:ARG:CG	1:G:184:MSE:HE1	2.41	0.41
1:J:94:GLN:HA	1:J:97:VAL:HG12	2.02	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:K:214:GLU:O	1:K:215:LYS:C	2.63	0.41
1:L:281:ARG:NH1	1:L:281:ARG:CG	2.78	0.41
1:M:128:LEU:O	1:M:128:LEU:HD12	2.21	0.41
1:M:241:LEU:HD12	1:M:241:LEU:HA	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: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:O:195:LYS:C	1:O:197:ASP:H	2.28	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:30:GLN:O	1:Q:74:GLN:HG3	2.20	0.41
1:Q:40:VAL:HG11	2:Q:1001:TRP:CD1	2.55	0.41
1:Q:107:GLN:CD	1:Q:107:GLN:N	2.75	0.41
1:Q:122:LEU:HD13	1:Q:122:LEU:HA	1.84	0.41
1:Q:125:TYR:CD1	1:Q:125:TYR:C	2.99	0.41
1:Q:140:ILE:HD12	1:Q:175:ARG:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:242:LEU:O	1:Q:246:SER:HB3	2.21	0.41
1:R:45:ILE:C	1:R:47:VAL:N	2.79	0.41
1:R:188:ASP:OD2	1:R:190:THR:HB	2.21	0.41
1:R:209:ASP:O	1:R:212:THR:N	2.54	0.41
1:R:260:TYR:CD2	1:R:260:TYR:N	2.89	0.41
1:A:67:ALA:HB2	1:A:287:TYR:HA	2.03	0.41
1:A:150:HIS:O	1:A:154:THR:CG2	2.69	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: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:O:320:GLN:OE1	1:R:55:ARG:NH2	2.54	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:25:GLN:CD	1:R:25:GLN:N	2.71	0.41
1:R:137:ASN:ND2	1:R:170:THR:OG1	2.51	0.41
1:R:146:ASP:OD1	1:R:146:ASP:N	2.53	0.41
1:R:241:LEU:O	1:R:244:ILE:N	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: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:Q:97:VAL:CG1	1:Q:97:VAL:O	2.69	0.40
1:Q:199:ASN:ND2	1:Q:199:ASN:C	2.79	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: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:M:188:ASP:CG	1:M:190:THR:H	2.29	0.40
1:N:19:TYR:HE1	1:N:68:VAL:HG13	1.86	0.40
1:O:59:ARG:CG	1:O:60:ARG:N	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:195:LYS:HG3	1:O:196:SER:N	2.36	0.40
1:O:213:ILE:CD1	1:O:280:LEU:HD12	2.51	0.40
1:O:246:SER:HB2	1:O:251:GLN:O	2.21	0.40
1:P:248:LEU:CD1	1:P:248:LEU:H	2.29	0.40
1:Q:41:ASP:OD1	1:Q:41:ASP:N	2.55	0.40
1:Q:229:ARG:HE	1:Q:229:ARG:HB3	1.38	0.40
1:R:21:GLY:HA3	4:R:1003:AMP:N3	2.36	0.40
1:A:123:LEU:O	1:A:123:LEU:HG	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:104:ARG:O	1:G:105:MSE:C	2.64	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: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
1:N:4:ILE:HG12	1:N:140:ILE:HB	2.04	0.40
1:N:18:ASN:O	1:N:19:TYR:C	2.63	0.40
1:O:24:ARG:HH11	1:O:24:ARG:CB	2.35	0.40
1:O:242:LEU:HD23	1:O:242:LEU:HA	1.91	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:70:ILE:HD13	1:A:70:ILE:HA	1.87	0.40
1:A:151:ILE:HA	1:A:154:THR:HG23	2.03	0.40
1:C:16:ILE:HA	1:C:19:TYR:CB	2.52	0.40
1:E:27:VAL:HG13	1:E:28:GLU:CD	2.47	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:E:281:ARG:N	1:E:282:PRO:CD	2.84	0.40
1:G:130:ALA:HB2	1:G:154:THR:HB	2.02	0.40
1:G:131:ALA:O	1:G:132:ASP:C	2.64	0.40
1:H:29:LEU:C	1:H:31:HIS:H	2.29	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:I:278:GLU:CD	1:I:281:ARG:HH22	2.30	0.40
1:K:302:GLU:O	1:K:306:LYS:HG3	2.21	0.40
1:N:43:HIS:O	1:N:46:THR:OG1	2.31	0.40
1:N:125:TYR:CD2	1:N:126:PRO:HD3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:150:HIS:O	1:N:154:THR:CG2	2.68	0.40
1:O:252:SER:OG	1:O:255:GLU:HB3	2.22	0.40
1:Q:168:LEU:HD23	1:Q:168:LEU:HA	1.91	0.40
1:Q:176:ILE:HA	1:Q:177:PRO:HD3	1.89	0.40
1:R:184:MSE:HE2	1:R:184:MSE:HB3	1.61	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:41:ASP:OD1	1:K:41:ASP:N	2.55	0.40
1:K:242:LEU:HA	1:K:242:LEU:HD23	1.87	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

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%)	30	54
1	B	281/326 (86%)	266 (95%)	14 (5%)	1 (0%)	30	54
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%)	36	60
1	I	288/326 (88%)	279 (97%)	9 (3%)	0	100	100
1	J	291/326 (89%)	277 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	12	32
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%)	48	73

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%)	210 (82%)	47 (18%)	2	5
1	B	256/268 (96%)	194 (76%)	62 (24%)	1	2
1	C	257/268 (96%)	206 (80%)	51 (20%)	1	4
1	D	259/268 (97%)	205 (79%)	54 (21%)	1	3
1	E	253/268 (94%)	197 (78%)	56 (22%)	1	3
1	F	255/268 (95%)	197 (77%)	58 (23%)	1	3
1	G	260/268 (97%)	212 (82%)	48 (18%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	259/268 (97%)	206 (80%)	53 (20%)	1	3
1	I	256/268 (96%)	196 (77%)	60 (23%)	1	2
1	J	259/268 (97%)	198 (76%)	61 (24%)	1	2
1	K	254/268 (95%)	203 (80%)	51 (20%)	1	4
1	L	259/268 (97%)	212 (82%)	47 (18%)	2	5
1	M	259/268 (97%)	194 (75%)	65 (25%)	0	2
1	N	259/268 (97%)	210 (81%)	49 (19%)	1	4
1	O	259/268 (97%)	188 (73%)	71 (27%)	0	1
1	P	255/268 (95%)	194 (76%)	61 (24%)	1	2
1	Q	259/268 (97%)	196 (76%)	63 (24%)	1	2
1	R	252/268 (94%)	191 (76%)	61 (24%)	1	2
All	All	4627/4824 (96%)	3609 (78%)	1018 (22%)	1	3

All (1018) 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
1	A	59	ARG
1	A	60	ARG
1	A	68	VAL
1	A	73	THR
1	A	96	ILE
1	A	99	ILE
1	A	104	ARG
1	A	105	MSE
1	A	118	VAL
1	A	119	SER
1	A	122	LEU
1	A	123	LEU
1	A	138	THR
1	A	146	ASP
1	A	148	LYS
1	A	154	THR

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Mol	Chain	Res	Type
1	A	164	ARG
1	A	171	ILE
1	A	173	GLU
1	A	175	ARG
1	A	182	ARG
1	A	187	VAL
1	A	192	LYS
1	A	197	ASP
1	A	201	LYS
1	A	205	THR
1	A	215	LYS
1	A	219	SER
1	A	227	THR
1	A	228	ILE
1	A	238	ILE
1	A	241	LEU
1	A	247	THR
1	A	275	VAL
1	A	292	GLU
1	A	295	GLU
1	A	298	ARG
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	56	GLN
1	B	59	ARG
1	B	70	ILE
1	B	73	THR
1	B	80	GLN
1	B	96	ILE
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

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Mol	Chain	Res	Type
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	205	THR
1	B	206	LEU
1	B	216	LYS
1	B	217	ILE
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	247	THR
1	B	248	LEU
1	B	253	ILE
1	B	254	GLU
1	B	255	GLU
1	B	261	GLU
1	B	267	VAL
1	B	275	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	296	LEU
1	B	298	ARG
1	B	302	GLU
1	B	305	GLU
1	B	308	ASN
1	B	312	SER

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Mol	Chain	Res	Type
1	B	315	VAL
1	B	316	ARG
1	B	317	LYS
1	C	1	MSE
1	C	8	ILE
1	C	23	LEU
1	C	53	GLU
1	C	56	GLN
1	C	59	ARG
1	C	60	ARG
1	C	68	VAL
1	C	70	ILE
1	C	94	GLN
1	C	96	ILE
1	C	99	ILE
1	C	104	ARG
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	176	ILE
1	C	182	ARG
1	C	185	SER
1	C	196	SER
1	C	201	LYS
1	C	205	THR
1	C	217	ILE
1	C	219	SER
1	C	224	SER
1	C	228	ILE
1	C	238	ILE
1	C	241	LEU
1	C	246	SER
1	C	248	LEU
1	C	251	GLN

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Mol	Chain	Res	Type
1	C	253	ILE
1	C	267	VAL
1	C	275	VAL
1	C	278	GLU
1	C	281	ARG
1	C	285	GLU
1	C	298	ARG
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	4	ILE
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	68	VAL
1	D	96	ILE
1	D	99	ILE
1	D	103	GLU
1	D	104	ARG
1	D	106	THR
1	D	107	GLN
1	D	118	VAL
1	D	122	LEU
1	D	123	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	205	THR
1	D	211	LYS
1	D	215	LYS

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Mol	Chain	Res	Type
1	D	219	SER
1	D	224	SER
1	D	227	THR
1	D	229	ARG
1	D	241	LEU
1	D	247	THR
1	D	251	GLN
1	D	255	GLU
1	D	257	GLU
1	D	275	VAL
1	D	278	GLU
1	D	281	ARG
1	D	285	GLU
1	D	294	GLU
1	D	295	GLU
1	D	298	ARG
1	D	302	GLU
1	D	308	ASN
1	D	309	ARG
1	D	312	SER
1	D	314	MSE
1	D	315	VAL
1	D	316	ARG
1	D	317	LYS
1	E	6	SER
1	E	8	ILE
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	56	GLN
1	E	70	ILE
1	E	94	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	123	LEU

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Mol	Chain	Res	Type
1	E	124	THR
1	E	129	MSE
1	E	138	THR
1	E	146	ASP
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	190	THR
1	E	196	SER
1	E	201	LYS
1	E	205	THR
1	E	206	LEU
1	E	211	LYS
1	E	214	GLU
1	E	215	LYS
1	E	216	LYS
1	E	217	ILE
1	E	218	LYS
1	E	225	GLU
1	E	238	ILE
1	E	239	SER
1	E	241	LEU
1	E	247	THR
1	E	248	LEU
1	E	253	ILE
1	E	284	GLN
1	E	285	GLU
1	E	295	GLU
1	E	299	VAL
1	E	305	GLU
1	E	308	ASN
1	E	309	ARG
1	E	312	SER
1	E	315	VAL
1	E	320	GLN
1	F	1	MSE
1	F	4	ILE
1	F	8	ILE
1	F	32	GLU

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Mol	Chain	Res	Type
1	F	54	LEU
1	F	55	ARG
1	F	56	GLN
1	F	59	ARG
1	F	60	ARG
1	F	68	VAL
1	F	73	THR
1	F	96	ILE
1	F	99	ILE
1	F	105	MSE
1	F	106	THR
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	149	GLN
1	F	151	ILE
1	F	154	THR
1	F	160	ARG
1	F	164	ARG
1	F	173	GLU
1	F	175	ARG
1	F	182	ARG
1	F	190	THR
1	F	192	LYS
1	F	195	LYS
1	F	201	LYS
1	F	204	ILE
1	F	205	THR
1	F	211	LYS
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	238	ILE
1	F	241	LEU
1	F	242	LEU
1	F	243	ASN

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Mol	Chain	Res	Type
1	F	247	THR
1	F	251	GLN
1	F	254	GLU
1	F	275	VAL
1	F	278	GLU
1	F	281	ARG
1	F	289	HIS
1	F	293	SER
1	F	295	GLU
1	F	298	ARG
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	27	VAL
1	G	55	ARG
1	G	60	ARG
1	G	68	VAL
1	G	73	THR
1	G	74	GLN
1	G	81	SER
1	G	96	ILE
1	G	99	ILE
1	G	105	MSE
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	160	ARG
1	G	164	ARG
1	G	171	ILE
1	G	178	LYS
1	G	179	VAL
1	G	182	ARG
1	G	185	SER
1	G	205	THR
1	G	211	LYS

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Mol	Chain	Res	Type
1	G	215	LYS
1	G	219	SER
1	G	228	ILE
1	G	229	ARG
1	G	238	ILE
1	G	241	LEU
1	G	254	GLU
1	G	263	LYS
1	G	275	VAL
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	316	ARG
1	G	320	GLN
1	G	326	ARG
1	H	4	ILE
1	H	8	ILE
1	H	53	GLU
1	H	55	ARG
1	H	56	GLN
1	H	59	ARG
1	H	74	GLN
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	205	THR
1	H	206	LEU
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	229	ARG
1	H	241	LEU
1	H	248	LEU
1	H	251	GLN
1	H	259	GLN
1	H	267	VAL
1	H	274	GLN
1	H	275	VAL
1	H	285	GLU
1	H	293	SER
1	H	294	GLU
1	H	295	GLU
1	H	298	ARG
1	H	302	GLU
1	H	308	ASN
1	H	312	SER
1	H	315	VAL
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

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Mol	Chain	Res	Type
1	I	60	ARG
1	I	68	VAL
1	I	70	ILE
1	I	96	ILE
1	I	99	ILE
1	I	105	MSE
1	I	107	GLN
1	I	122	LEU
1	I	123	LEU
1	I	138	THR
1	I	145	GLU
1	I	148	LYS
1	I	154	THR
1	I	160	ARG
1	I	164	ARG
1	I	175	ARG
1	I	176	ILE
1	I	178	LYS
1	I	179	VAL
1	I	191	LYS
1	I	194	SER
1	I	196	SER
1	I	204	ILE
1	I	205	THR
1	I	211	LYS
1	I	215	LYS
1	I	217	ILE
1	I	219	SER
1	I	225	GLU
1	I	227	THR
1	I	238	ILE
1	I	241	LEU
1	I	252	SER
1	I	263	LYS
1	I	267	VAL
1	I	275	VAL
1	I	277	ILE
1	I	278	GLU
1	I	284	GLN
1	I	292	GLU
1	I	295	GLU
1	I	298	ARG

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Mol	Chain	Res	Type
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	4	ILE
1	J	8	ILE
1	J	9	GLN
1	J	20	ILE
1	J	23	LEU
1	J	24	ARG
1	J	28	GLU
1	J	55	ARG
1	J	56	GLN
1	J	59	ARG
1	J	60	ARG
1	J	68	VAL
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	123	LEU
1	J	124	THR
1	J	137	ASN
1	J	138	THR
1	J	146	ASP
1	J	148	LYS
1	J	152	GLU
1	J	154	THR
1	J	159	GLU
1	J	160	ARG
1	J	163	LYS
1	J	164	ARG
1	J	175	ARG
1	J	178	LYS
1	J	179	VAL
1	J	190	THR

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Mol	Chain	Res	Type
1	J	192	LYS
1	J	205	THR
1	J	215	LYS
1	J	217	ILE
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	263	LYS
1	J	275	VAL
1	J	277	ILE
1	J	278	GLU
1	J	281	ARG
1	J	285	GLU
1	J	305	GLU
1	J	308	ASN
1	J	309	ARG
1	J	312	SER
1	J	315	VAL
1	J	320	GLN
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	82	GLU
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

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Mol	Chain	Res	Type
1	K	154	THR
1	K	164	ARG
1	K	175	ARG
1	K	179	VAL
1	K	183	ILE
1	K	187	VAL
1	K	190	THR
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	217	ILE
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	275	VAL
1	K	280	LEU
1	K	289	HIS
1	K	295	GLU
1	K	308	ASN
1	K	312	SER
1	K	317	LYS
1	K	320	GLN
1	K	322	MSE
1	L	2	LYS
1	L	4	ILE
1	L	20	ILE
1	L	24	ARG
1	L	55	ARG
1	L	56	GLN
1	L	59	ARG
1	L	68	VAL
1	L	96	ILE

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Mol	Chain	Res	Type
1	L	99	ILE
1	L	104	ARG
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	171	ILE
1	L	175	ARG
1	L	194	SER
1	L	205	THR
1	L	215	LYS
1	L	217	ILE
1	L	227	THR
1	L	228	ILE
1	L	229	ARG
1	L	238	ILE
1	L	241	LEU
1	L	246	SER
1	L	252	SER
1	L	257	GLU
1	L	259	GLN
1	L	263	LYS
1	L	275	VAL
1	L	281	ARG
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
1	L	316	ARG
1	L	326	ARG
1	M	2	LYS
1	M	8	ILE
1	M	16	ILE
1	M	18	ASN

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Mol	Chain	Res	Type
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	82	GLU
1	M	94	GLN
1	M	96	ILE
1	M	99	ILE
1	M	104	ARG
1	M	107	GLN
1	M	119	SER
1	M	122	LEU
1	M	138	THR
1	M	140	ILE
1	M	145	GLU
1	M	146	ASP
1	M	148	LYS
1	M	151	ILE
1	M	154	THR
1	M	157	LEU
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	206	LEU
1	M	211	LYS
1	M	217	ILE
1	M	218	LYS
1	M	219	SER
1	M	227	THR
1	M	228	ILE
1	M	229	ARG
1	M	241	LEU
1	M	246	SER
1	M	251	GLN

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Mol	Chain	Res	Type
1	M	253	ILE
1	M	257	GLU
1	M	267	VAL
1	M	275	VAL
1	M	278	GLU
1	M	279	THR
1	M	281	ARG
1	M	285	GLU
1	M	289	HIS
1	M	292	GLU
1	M	293	SER
1	M	294	GLU
1	M	305	GLU
1	M	308	ASN
1	M	312	SER
1	M	315	VAL
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	28	GLU
1	N	53	GLU
1	N	55	ARG
1	N	59	ARG
1	N	68	VAL
1	N	96	ILE
1	N	99	ILE
1	N	104	ARG
1	N	106	THR
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	148	LYS
1	N	149	GLN
1	N	154	THR
1	N	164	ARG
1	N	168	LEU

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Mol	Chain	Res	Type
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	205	THR
1	N	211	LYS
1	N	215	LYS
1	N	217	ILE
1	N	219	SER
1	N	225	GLU
1	N	238	ILE
1	N	241	LEU
1	N	253	ILE
1	N	261	GLU
1	N	267	VAL
1	N	275	VAL
1	N	277	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	55	ARG
1	O	56	GLN
1	O	59	ARG
1	O	70	ILE
1	O	80	GLN
1	O	81	SER

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Mol	Chain	Res	Type
1	O	88	GLN
1	O	96	ILE
1	O	99	ILE
1	O	104	ARG
1	O	105	MSE
1	O	106	THR
1	O	107	GLN
1	O	118	VAL
1	O	119	SER
1	O	122	LEU
1	O	123	LEU
1	O	146	ASP
1	O	152	GLU
1	O	154	THR
1	O	159	GLU
1	O	160	ARG
1	O	164	ARG
1	O	167	GLU
1	O	171	ILE
1	O	173	GLU
1	O	175	ARG
1	O	176	ILE
1	O	179	VAL
1	O	187	VAL
1	O	191	LYS
1	O	195	LYS
1	O	196	SER
1	O	201	LYS
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	238	ILE
1	O	241	LEU
1	O	246	SER
1	O	247	THR
1	O	248	LEU
1	O	251	GLN

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Mol	Chain	Res	Type
1	O	259	GLN
1	O	267	VAL
1	O	275	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	O	317	LYS
1	P	1	MSE
1	P	4	ILE
1	P	8	ILE
1	P	9	GLN
1	P	16	ILE
1	P	18	ASN
1	P	24	ARG
1	P	28	GLU
1	P	32	GLU
1	P	39	ILE
1	P	43	HIS
1	P	47	VAL
1	P	53	GLU
1	P	56	GLN
1	P	68	VAL
1	P	96	ILE
1	P	99	ILE
1	P	101	GLU
1	P	118	VAL
1	P	123	LEU
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	168	LEU
1	P	173	GLU
1	P	182	ARG

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Mol	Chain	Res	Type
1	P	183	ILE
1	P	191	LYS
1	P	195	LYS
1	P	196	SER
1	P	201	LYS
1	P	204	ILE
1	P	205	THR
1	P	206	LEU
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
1	P	296	LEU
1	P	302	GLU
1	P	308	ASN
1	P	312	SER
1	P	315	VAL
1	P	316	ARG
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

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Mol	Chain	Res	Type
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	106	THR
1	Q	118	VAL
1	Q	119	SER
1	Q	122	LEU
1	Q	123	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	168	LEU
1	Q	173	GLU
1	Q	176	ILE
1	Q	179	VAL
1	Q	185	SER
1	Q	188	ASP
1	Q	190	THR
1	Q	192	LYS
1	Q	196	SER
1	Q	204	ILE
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	246	SER
1	Q	252	SER
1	Q	254	GLU
1	Q	261	GLU
1	Q	263	LYS

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Mol	Chain	Res	Type
1	Q	267	VAL
1	Q	274	GLN
1	Q	275	VAL
1	Q	277	ILE
1	Q	278	GLU
1	Q	285	GLU
1	Q	295	GLU
1	Q	302	GLU
1	Q	308	ASN
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	20	ILE
1	R	23	LEU
1	R	32	GLU
1	R	45	ILE
1	R	55	ARG
1	R	56	GLN
1	R	59	ARG
1	R	60	ARG
1	R	70	ILE
1	R	76	THR
1	R	82	GLU
1	R	83	VAL
1	R	96	ILE
1	R	99	ILE
1	R	101	GLU
1	R	106	THR
1	R	118	VAL
1	R	119	SER
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

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Mol	Chain	Res	Type
1	R	164	ARG
1	R	167	GLU
1	R	168	LEU
1	R	171	ILE
1	R	176	ILE
1	R	184	MSE
1	R	187	VAL
1	R	191	LYS
1	R	197	ASP
1	R	204	ILE
1	R	205	THR
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	280	LEU
1	R	284	GLN
1	R	292	GLU
1	R	295	GLU
1	R	298	ARG
1	R	312	SER
1	R	317	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (211) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	18	ASN
1	A	31	HIS
1	A	34	ASN
1	A	52	HIS
1	A	74	GLN
1	A	86	HIS
1	A	94	GLN

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Mol	Chain	Res	Type
1	A	150	HIS
1	A	199	ASN
1	A	251	GLN
1	A	259	GLN
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	251	GLN
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	56	GLN
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	56	GLN
1	D	86	HIS
1	D	94	GLN
1	D	107	GLN
1	D	150	HIS
1	D	199	ASN
1	D	308	ASN

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Mol	Chain	Res	Type
1	D	320	GLN
1	E	9	GLN
1	E	34	ASN
1	E	42	GLN
1	E	86	HIS
1	E	251	GLN
1	E	288	HIS
1	E	308	ASN
1	E	320	GLN
1	F	18	ASN
1	F	34	ASN
1	F	42	GLN
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	42	GLN
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

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Mol	Chain	Res	Type
1	H	243	ASN
1	H	308	ASN
1	H	320	GLN
1	I	9	GLN
1	I	18	ASN
1	I	34	ASN
1	I	74	GLN
1	I	86	HIS
1	I	107	GLN
1	I	150	HIS
1	I	199	ASN
1	I	308	ASN
1	J	34	ASN
1	J	42	GLN
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	31	HIS
1	K	34	ASN
1	K	42	GLN
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	308	ASN
1	K	320	GLN
1	L	25	GLN
1	L	34	ASN
1	L	56	GLN
1	L	86	HIS
1	L	94	GLN
1	L	107	GLN
1	L	150	HIS
1	L	199	ASN

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Mol	Chain	Res	Type
1	L	284	GLN
1	L	308	ASN
1	L	320	GLN
1	M	9	GLN
1	M	25	GLN
1	M	31	HIS
1	M	34	ASN
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	107	GLN
1	N	150	HIS
1	N	199	ASN
1	N	251	GLN
1	N	259	GLN
1	N	284	GLN
1	N	308	ASN
1	O	9	GLN
1	O	25	GLN
1	O	34	ASN
1	O	52	HIS
1	O	56	GLN
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

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Mol	Chain	Res	Type
1	P	150	HIS
1	P	199	ASN
1	P	284	GLN
1	P	308	ASN
1	P	320	GLN
1	Q	9	GLN
1	Q	25	GLN
1	Q	34	ASN
1	Q	43	HIS
1	Q	52	HIS
1	Q	74	GLN
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	9	GLN
1	R	18	ASN
1	R	34	ASN
1	R	42	GLN
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	1002	-	4,4,4	2.04	1 (25%)	6,6,6	0.55	0
4	AMP	C	1003	-	25,25,25	0.67	0	37,38,38	0.74	0
2	TRP	N	1001	-	15,16,16	0.66	0	18,22,22	0.40	0
2	TRP	H	1001	-	15,16,16	0.72	0	18,22,22	0.41	0
4	AMP	Q	1003	-	25,25,25	0.66	0	37,38,38	0.74	0
2	TRP	C	1001	-	15,16,16	0.67	0	18,22,22	0.40	0
2	TRP	P	1001	-	15,16,16	0.76	0	18,22,22	0.43	0
3	PO4	F	1002	-	4,4,4	1.91	1 (25%)	6,6,6	0.49	0
4	AMP	L	1003	-	25,25,25	0.64	0	37,38,38	0.77	0
4	AMP	K	1003	-	25,25,25	0.63	0	37,38,38	0.80	0
3	PO4	C	1002	-	4,4,4	2.05	1 (25%)	6,6,6	0.49	0
4	AMP	O	1003	-	25,25,25	0.74	0	37,38,38	1.29	5 (13%)
3	PO4	I	1002	-	4,4,4	2.03	1 (25%)	6,6,6	0.39	0
2	TRP	F	1001	-	15,16,16	0.76	0	18,22,22	0.41	0
4	AMP	I	1003	-	25,25,25	0.63	1 (4%)	37,38,38	0.86	1 (2%)
4	AMP	R	1003	-	25,25,25	0.66	0	37,38,38	0.76	0
2	TRP	E	1001	-	15,16,16	0.69	0	18,22,22	0.40	0
3	PO4	J	1002	-	4,4,4	2.15	1 (25%)	6,6,6	0.77	0
3	PO4	Q	1002	-	4,4,4	2.01	1 (25%)	6,6,6	0.42	0
4	AMP	B	1003	-	25,25,25	0.68	0	37,38,38	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	R	1002	-	4,4,4	1.84	1 (25%)	6,6,6	0.44	0
4	AMP	N	1003	-	25,25,25	0.83	1 (4%)	37,38,38	1.06	2 (5%)
2	TRP	G	1001	-	15,16,16	0.66	0	18,22,22	0.39	0
2	TRP	Q	1001	-	15,16,16	0.66	0	18,22,22	0.39	0
3	PO4	N	1002	-	4,4,4	2.02	1 (25%)	6,6,6	0.50	0
2	TRP	M	1001	-	15,16,16	0.67	0	18,22,22	0.40	0
2	TRP	K	1001	-	15,16,16	0.68	0	18,22,22	0.38	0
3	PO4	H	1002	-	4,4,4	2.07	1 (25%)	6,6,6	0.49	0
4	AMP	P	1003	-	25,25,25	0.62	0	37,38,38	1.23	4 (10%)
3	PO4	M	1002	-	4,4,4	1.80	1 (25%)	6,6,6	0.85	0
2	TRP	B	1001	-	15,16,16	0.75	0	18,22,22	0.41	0
2	TRP	A	1001	-	15,16,16	0.68	0	18,22,22	0.39	0
4	AMP	A	1003	-	25,25,25	0.88	1 (4%)	37,38,38	1.17	6 (16%)
4	AMP	H	1003	-	25,25,25	0.78	0	37,38,38	1.47	6 (16%)
4	AMP	J	1003	-	25,25,25	0.57	0	37,38,38	0.75	0
2	TRP	D	1001	-	15,16,16	0.78	0	18,22,22	0.44	0
3	PO4	G	1002	-	4,4,4	2.02	1 (25%)	6,6,6	0.49	0
4	AMP	E	1003	-	25,25,25	0.68	0	37,38,38	0.83	1 (2%)
3	PO4	L	1002	-	4,4,4	2.06	1 (25%)	6,6,6	0.66	0
2	TRP	L	1001	-	15,16,16	0.66	0	18,22,22	0.41	0
4	AMP	G	1003	-	25,25,25	0.69	1 (4%)	37,38,38	0.69	0
4	AMP	M	1003	-	25,25,25	1.34	4 (16%)	37,38,38	2.22	17 (45%)
2	TRP	I	1001	-	15,16,16	0.66	0	18,22,22	0.39	0
2	TRP	O	1001	-	15,16,16	0.65	0	18,22,22	0.41	0
3	PO4	A	1002	-	4,4,4	2.01	1 (25%)	6,6,6	0.62	0
3	PO4	E	1002	-	4,4,4	2.20	1 (25%)	6,6,6	0.57	0
3	PO4	K	1002	-	4,4,4	1.93	1 (25%)	6,6,6	0.52	0
4	AMP	D	1003	-	25,25,25	0.65	0	37,38,38	0.66	0
3	PO4	O	1002	-	4,4,4	2.02	1 (25%)	6,6,6	0.49	0
3	PO4	D	1002	-	4,4,4	1.92	1 (25%)	6,6,6	0.43	0
4	AMP	F	1003	-	25,25,25	0.69	0	37,38,38	0.79	1 (2%)
2	TRP	J	1001	-	15,16,16	0.67	0	18,22,22	0.41	0
2	TRP	R	1001	-	15,16,16	0.67	0	18,22,22	0.40	0
3	PO4	P	1002	-	4,4,4	1.88	1 (25%)	6,6,6	0.95	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	C	1003	-	-	4/10/26/26	0/3/3/3
2	TRP	N	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	H	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	Q	1003	-	-	3/10/26/26	0/3/3/3
2	TRP	C	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	P	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	L	1003	-	-	6/10/26/26	0/3/3/3
4	AMP	K	1003	-	-	3/10/26/26	0/3/3/3
4	AMP	O	1003	-	-	2/10/26/26	0/3/3/3
2	TRP	F	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	I	1003	-	-	4/10/26/26	0/3/3/3
4	AMP	R	1003	-	-	2/10/26/26	0/3/3/3
2	TRP	E	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	B	1003	-	-	5/10/26/26	0/3/3/3
4	AMP	N	1003	-	-	3/10/26/26	0/3/3/3
2	TRP	G	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	Q	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	M	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	K	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	P	1003	-	-	6/10/26/26	0/3/3/3
2	TRP	B	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	A	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	A	1003	-	-	6/10/26/26	0/3/3/3
4	AMP	H	1003	-	-	6/10/26/26	0/3/3/3
4	AMP	J	1003	-	-	5/10/26/26	0/3/3/3
2	TRP	D	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	E	1003	-	-	1/10/26/26	0/3/3/3
2	TRP	L	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	G	1003	-	-	4/10/26/26	0/3/3/3
4	AMP	M	1003	-	-	4/10/26/26	0/3/3/3
2	TRP	I	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	O	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	D	1003	-	-	6/10/26/26	0/3/3/3
4	AMP	F	1003	-	-	5/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRP	J	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	R	1001	-	-	2/8/8/8	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1003	AMP	C5-C4	3.72	1.45	1.39
3	E	1002	PO4	P-O1	3.58	1.58	1.50
3	I	1002	PO4	P-O1	3.56	1.58	1.50
3	L	1002	PO4	P-O1	3.43	1.58	1.50
3	H	1002	PO4	P-O1	3.43	1.58	1.50
3	B	1002	PO4	P-O1	3.42	1.58	1.50
3	C	1002	PO4	P-O1	3.41	1.58	1.50
3	G	1002	PO4	P-O1	3.41	1.58	1.50
3	J	1002	PO4	P-O1	3.40	1.58	1.50
3	N	1002	PO4	P-O1	3.36	1.58	1.50
3	Q	1002	PO4	P-O1	3.34	1.58	1.50
3	A	1002	PO4	P-O1	3.34	1.58	1.50
3	D	1002	PO4	P-O1	3.32	1.58	1.50
3	O	1002	PO4	P-O1	3.31	1.58	1.50
3	F	1002	PO4	P-O1	3.18	1.58	1.50
3	P	1002	PO4	P-O1	3.15	1.57	1.50
3	K	1002	PO4	P-O1	3.15	1.57	1.50
3	R	1002	PO4	P-O1	3.08	1.57	1.50
4	M	1003	AMP	C5-N7	-2.80	1.34	1.39
4	M	1003	AMP	C4-N9	-2.71	1.32	1.37
4	M	1003	AMP	C8-N7	2.29	1.36	1.31
4	A	1003	AMP	O4'-C1'	2.20	1.47	1.42
4	N	1003	AMP	O4'-C1'	2.18	1.47	1.42
3	M	1002	PO4	P-O4	-2.05	1.48	1.54
4	I	1003	AMP	O4'-C1'	2.03	1.46	1.42
4	G	1003	AMP	O4'-C1'	2.01	1.46	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1003	AMP	C4'-O4'-C1'	-4.66	99.17	109.47
4	M	1003	AMP	C5-C4-N3	-4.62	120.35	126.72
4	M	1003	AMP	C4-N9-C8	4.40	110.36	105.74
4	M	1003	AMP	N3-C4-N9	4.39	134.63	127.17
4	P	1003	AMP	O3P-P-O5'	4.31	117.91	106.67
4	M	1003	AMP	N3-C2-N1	-4.11	122.36	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1003	AMP	O4'-C1'-C2'	-3.76	98.56	106.62
4	M	1003	AMP	C2'-C1'-N9	-3.74	104.02	113.30
4	M	1003	AMP	C2-N3-C4	3.50	120.39	111.83
4	H	1003	AMP	O5'-P-O1P	3.38	115.56	106.44
4	M	1003	AMP	N9-C8-N7	-3.09	109.55	113.94
4	O	1003	AMP	C4-C5-N7	2.77	113.75	110.58
4	N	1003	AMP	C2'-C3'-C4'	-2.62	97.55	102.61
4	O	1003	AMP	C3'-C2'-C1'	2.59	106.35	101.46
4	M	1003	AMP	N6-C6-N1	2.53	124.02	118.38
4	O	1003	AMP	C5-C4-N9	-2.51	103.07	105.81
4	M	1003	AMP	O3'-C3'-C2'	-2.47	103.89	111.82
4	P	1003	AMP	C4'-O4'-C1'	-2.44	104.08	109.47
4	P	1003	AMP	O4'-C1'-N9	-2.40	103.48	108.09
4	A	1003	AMP	C2'-C1'-N9	-2.33	107.53	113.30
4	M	1003	AMP	C5-N7-C8	2.31	107.08	103.45
4	M	1003	AMP	C5-C6-N6	-2.31	117.57	123.29
4	F	1003	AMP	C3'-C2'-C1'	2.29	105.79	101.46
4	M	1003	AMP	C4-C5-N7	-2.27	107.99	110.58
4	A	1003	AMP	C3'-C2'-C1'	2.26	105.75	101.46
4	M	1003	AMP	C2-N1-C6	2.25	122.43	118.73
4	M	1003	AMP	C4-N9-C1'	-2.19	121.50	126.63
4	H	1003	AMP	O4'-C4'-C5'	2.19	116.34	109.33
4	O	1003	AMP	O4'-C4'-C3'	2.17	109.46	105.15
4	N	1003	AMP	C5'-C4'-C3'	-2.16	107.42	115.21
4	A	1003	AMP	C5-C4-N9	-2.15	103.47	105.81
4	A	1003	AMP	O2'-C2'-C3'	-2.14	104.95	111.82
4	E	1003	AMP	C3'-C2'-C1'	2.13	105.50	101.46
4	M	1003	AMP	O4'-C4'-C3'	2.12	109.37	105.15
4	P	1003	AMP	O4'-C4'-C5'	2.11	116.10	109.33
4	H	1003	AMP	C3'-C2'-C1'	2.08	105.40	101.46
4	I	1003	AMP	O3P-P-O5'	2.07	112.07	106.67
4	A	1003	AMP	O5'-P-O1P	2.05	111.98	106.44
4	H	1003	AMP	C2'-C3'-C4'	-2.04	98.67	102.61
4	O	1003	AMP	N3-C4-N9	2.03	130.63	127.17
4	A	1003	AMP	O4'-C4'-C5'	2.02	115.82	109.33
4	M	1003	AMP	O4'-C1'-C2'	2.02	110.94	106.62
4	M	1003	AMP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (111) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	A	1003	AMP	O4'-C4'-C5'-O5'
4	K	1003	AMP	O4'-C4'-C5'-O5'
4	Q	1003	AMP	O4'-C4'-C5'-O5'
4	C	1003	AMP	C3'-C4'-C5'-O5'
4	L	1003	AMP	C3'-C4'-C5'-O5'
4	N	1003	AMP	C3'-C4'-C5'-O5'
4	C	1003	AMP	O4'-C4'-C5'-O5'
4	M	1003	AMP	O4'-C4'-C5'-O5'
4	R	1003	AMP	O4'-C4'-C5'-O5'
4	L	1003	AMP	C4'-C5'-O5'-P
4	N	1003	AMP	O4'-C4'-C5'-O5'
4	R	1003	AMP	C3'-C4'-C5'-O5'
4	P	1003	AMP	C2'-C1'-N9-C4
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	P	1003	AMP	C2'-C1'-N9-C8
4	J	1003	AMP	O4'-C4'-C5'-O5'
4	M	1003	AMP	C3'-C4'-C5'-O5'
4	C	1003	AMP	C5'-O5'-P-O3P
4	J	1003	AMP	C3'-C4'-C5'-O5'
2	M	1001	TRP	O-C-CA-CB
2	N	1001	TRP	O-C-CA-CB
2	P	1001	TRP	O-C-CA-CB
4	K	1003	AMP	C5'-O5'-P-O1P
4	Q	1003	AMP	C5'-O5'-P-O1P
2	A	1001	TRP	OXT-C-CA-CB
2	B	1001	TRP	OXT-C-CA-CB
2	C	1001	TRP	O-C-CA-CB
2	D	1001	TRP	O-C-CA-CB
2	E	1001	TRP	OXT-C-CA-CB
2	F	1001	TRP	O-C-CA-CB
2	G	1001	TRP	O-C-CA-CB
2	H	1001	TRP	OXT-C-CA-CB
2	I	1001	TRP	O-C-CA-CB
2	J	1001	TRP	O-C-CA-CB
2	K	1001	TRP	O-C-CA-CB
2	L	1001	TRP	O-C-CA-CB
2	O	1001	TRP	O-C-CA-CB
2	Q	1001	TRP	O-C-CA-CB
2	R	1001	TRP	O-C-CA-CB
4	G	1003	AMP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	1001	TRP	O-C-CA-CB
2	B	1001	TRP	O-C-CA-CB
2	C	1001	TRP	OXT-C-CA-CB
2	D	1001	TRP	OXT-C-CA-CB
2	E	1001	TRP	O-C-CA-CB
2	F	1001	TRP	OXT-C-CA-CB
2	G	1001	TRP	OXT-C-CA-CB
2	H	1001	TRP	O-C-CA-CB
2	I	1001	TRP	OXT-C-CA-CB
2	J	1001	TRP	OXT-C-CA-CB
2	K	1001	TRP	OXT-C-CA-CB
2	L	1001	TRP	OXT-C-CA-CB
2	M	1001	TRP	OXT-C-CA-CB
2	N	1001	TRP	OXT-C-CA-CB
2	O	1001	TRP	OXT-C-CA-CB
2	P	1001	TRP	OXT-C-CA-CB
2	Q	1001	TRP	OXT-C-CA-CB
2	R	1001	TRP	OXT-C-CA-CB
4	B	1003	AMP	C4'-C5'-O5'-P
4	H	1003	AMP	C3'-C4'-C5'-O5'
4	A	1003	AMP	C4'-C5'-O5'-P
4	D	1003	AMP	C4'-C5'-O5'-P
4	J	1003	AMP	C5'-O5'-P-O3P
4	M	1003	AMP	C5'-O5'-P-O1P
4	B	1003	AMP	O4'-C4'-C5'-O5'
4	I	1003	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

36 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	PO4	1	0
4	C	1003	AMP	2	0
2	H	1001	TRP	1	0
4	Q	1003	AMP	2	0
2	C	1001	TRP	2	0
3	F	1002	PO4	2	0
4	K	1003	AMP	1	0
4	O	1003	AMP	17	0
3	I	1002	PO4	1	0
4	I	1003	AMP	3	0
4	R	1003	AMP	3	0

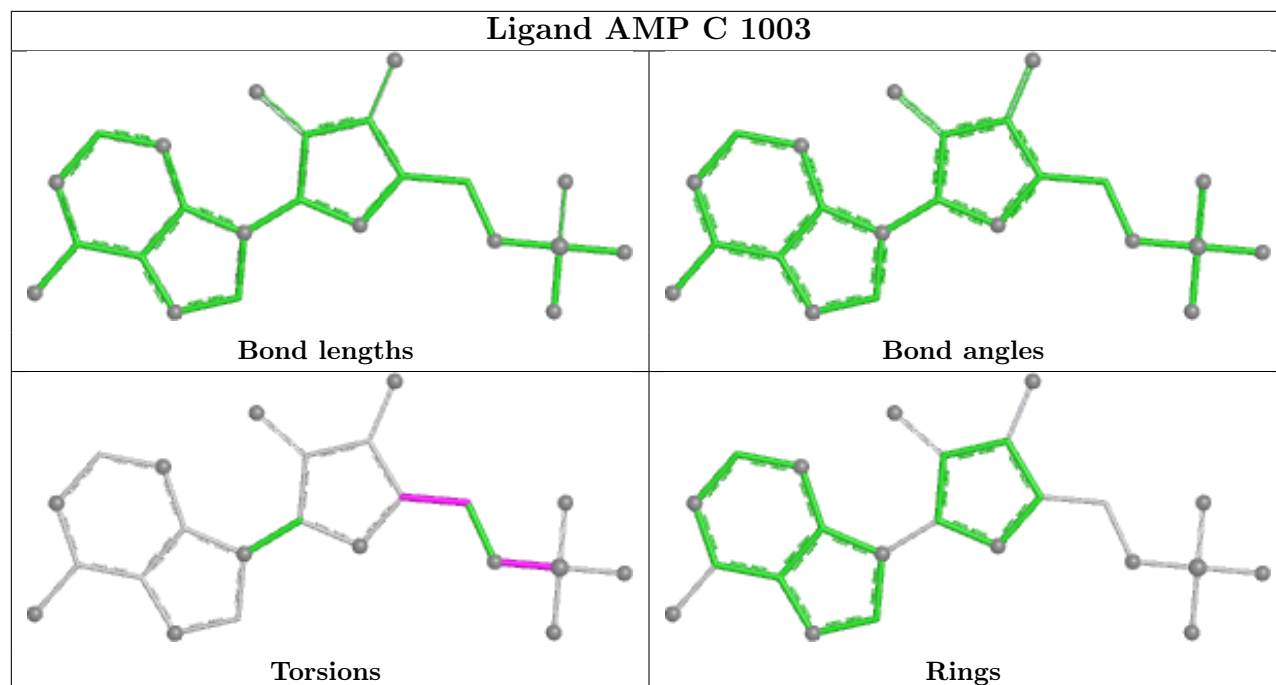
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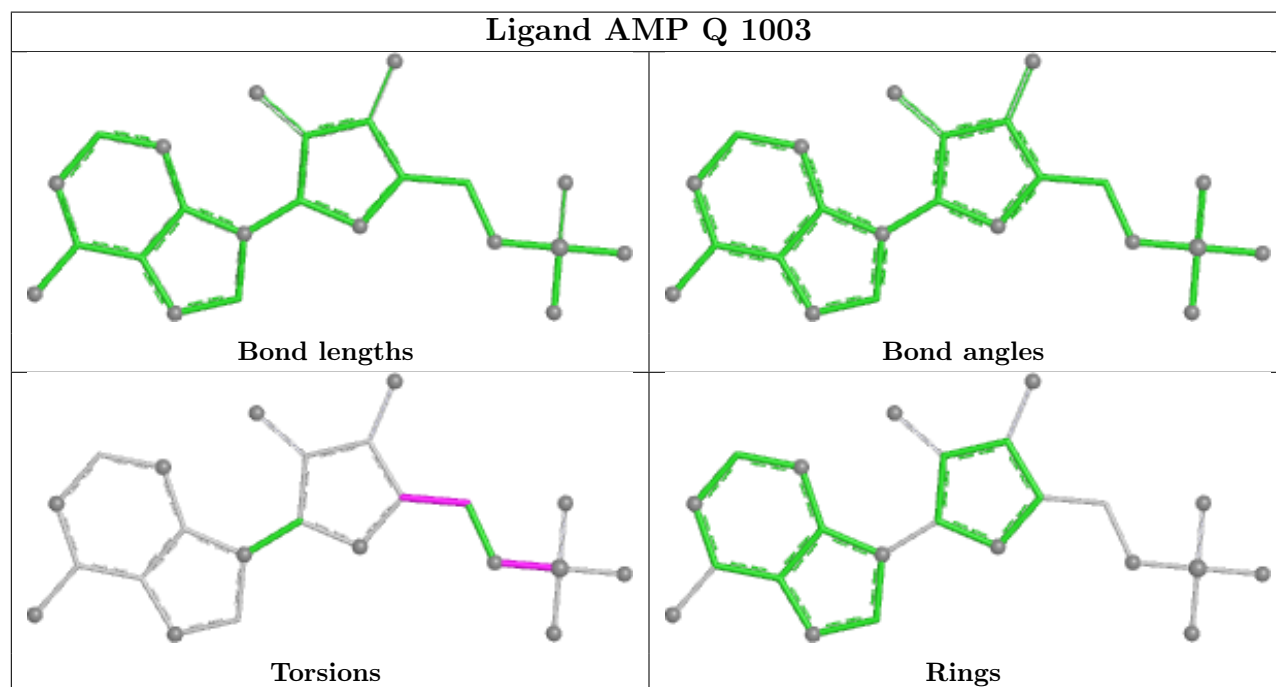
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1002	PO4	1	0
4	B	1003	AMP	4	0
3	R	1002	PO4	1	0
4	N	1003	AMP	1	0
2	G	1001	TRP	2	0
2	Q	1001	TRP	1	0
3	N	1002	PO4	2	0
3	H	1002	PO4	2	0
4	P	1003	AMP	7	0
3	M	1002	PO4	3	0
2	B	1001	TRP	1	0
4	A	1003	AMP	7	0
4	J	1003	AMP	3	0
3	G	1002	PO4	1	0
4	E	1003	AMP	1	0
4	G	1003	AMP	7	0
4	M	1003	AMP	5	0
3	A	1002	PO4	1	0
3	E	1002	PO4	3	0
3	K	1002	PO4	1	0
4	D	1003	AMP	3	0
3	O	1002	PO4	2	0
4	F	1003	AMP	2	0
2	J	1001	TRP	2	0
3	P	1002	PO4	7	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.

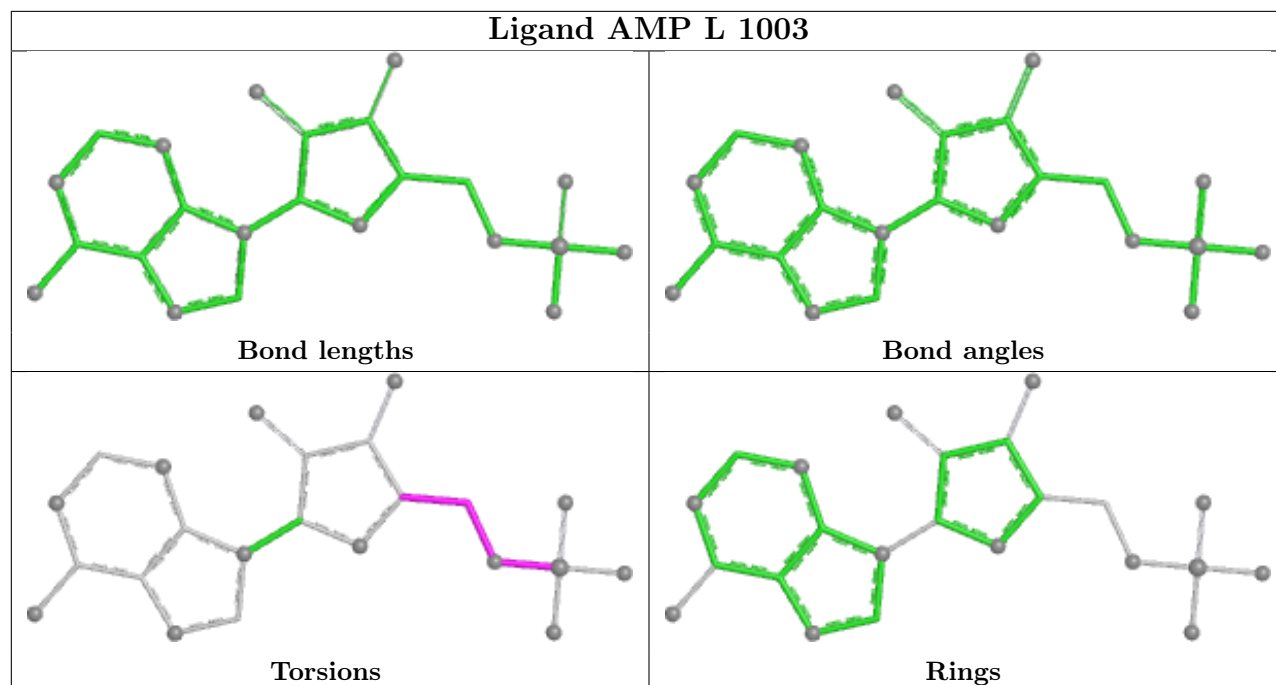
Ligand AMP C 1003



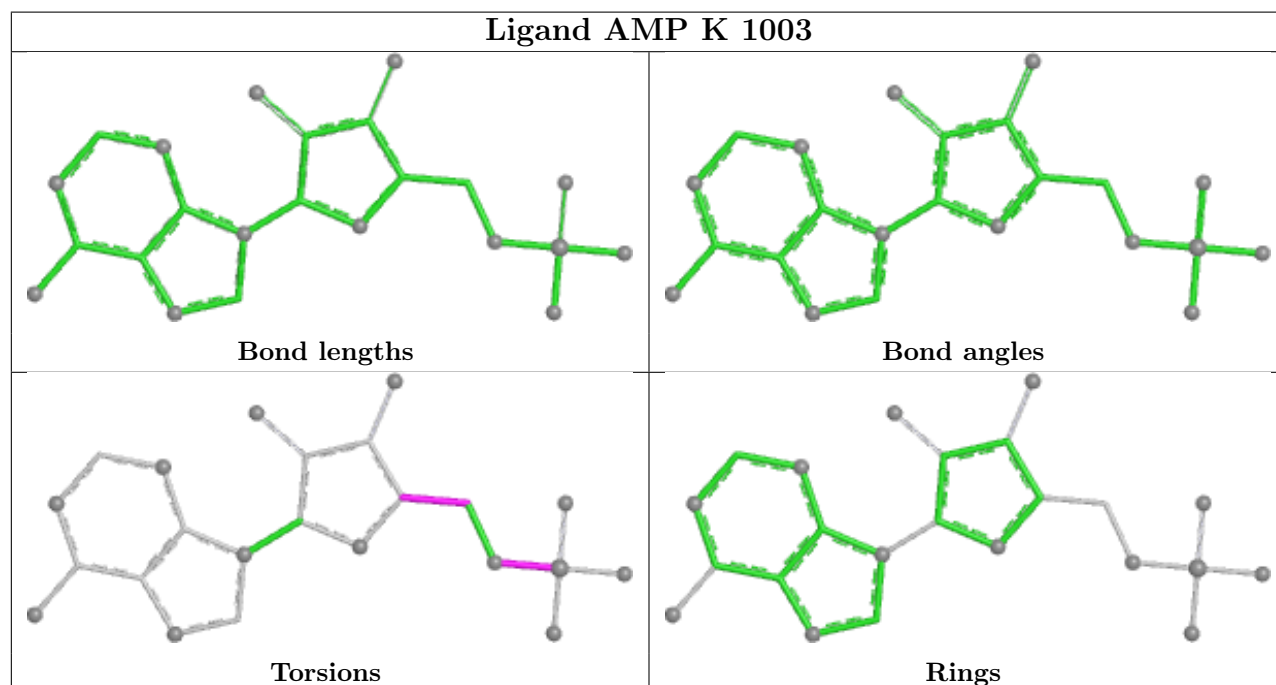
Ligand AMP Q 1003



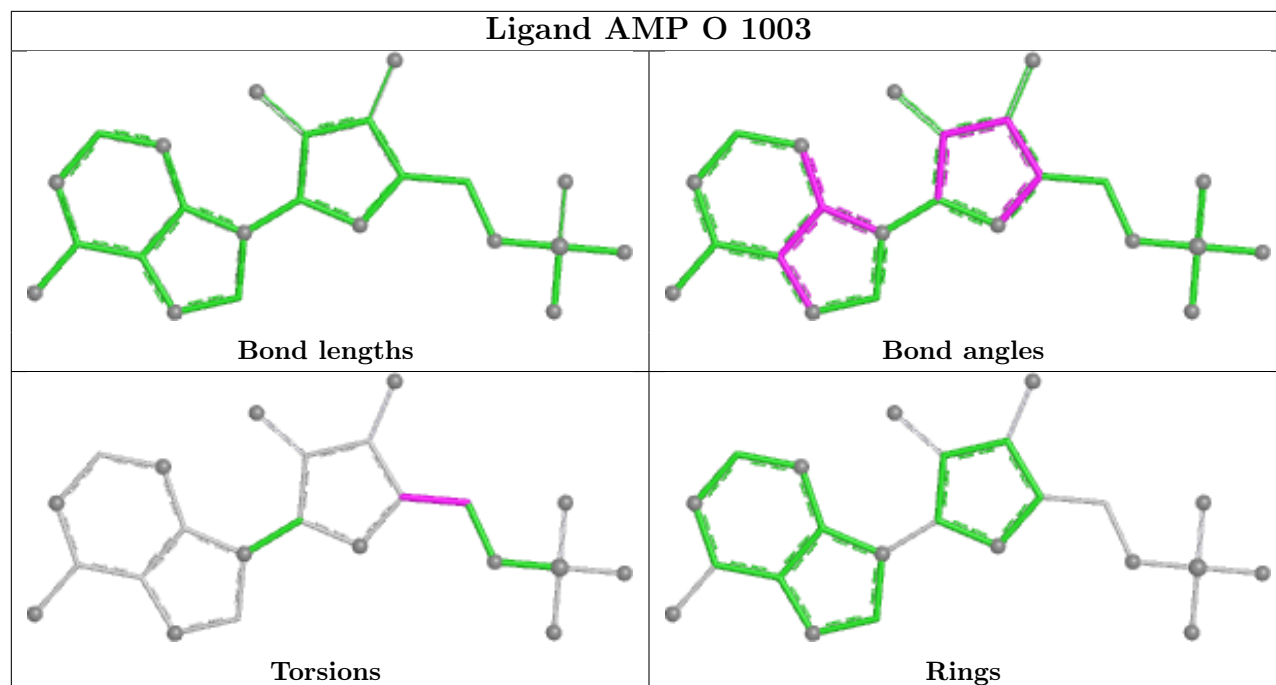
Ligand AMP L 1003



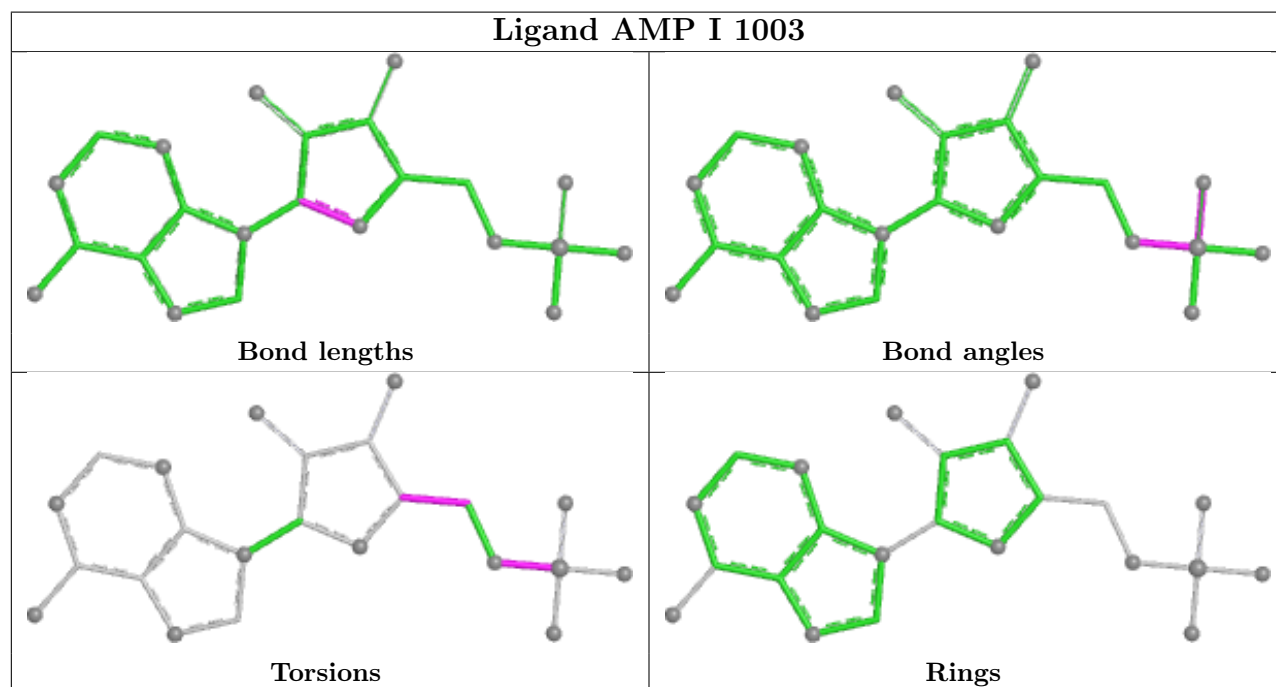
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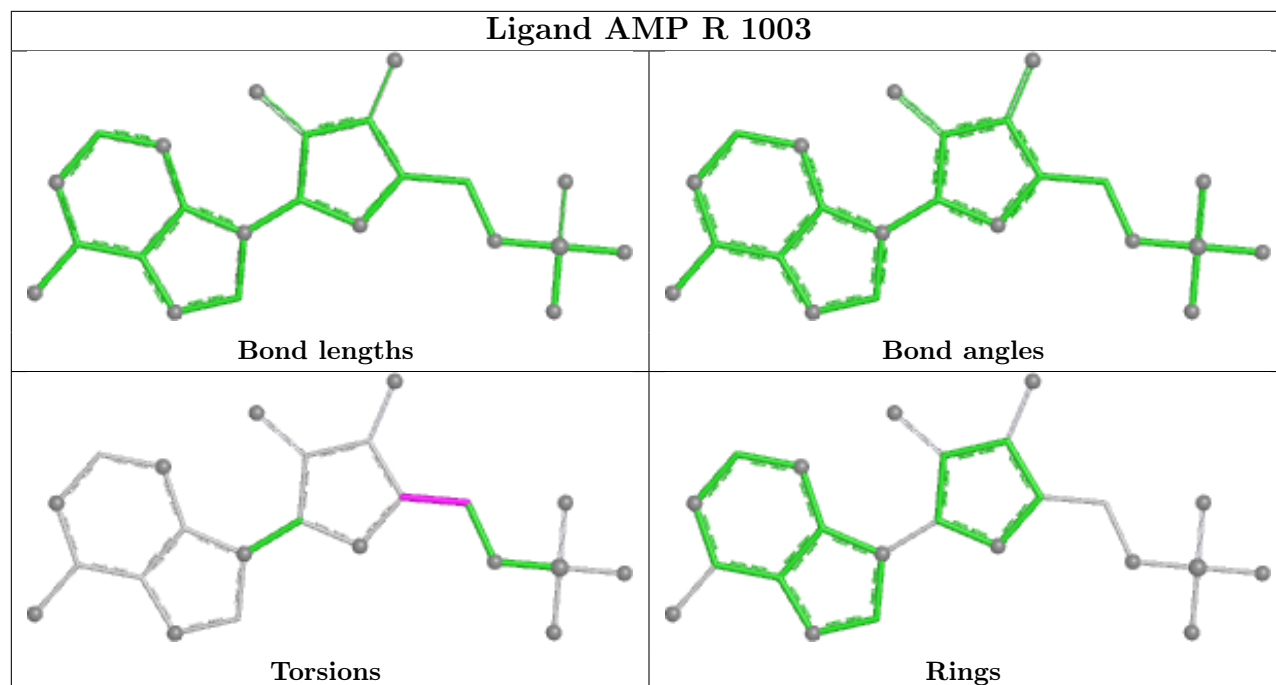
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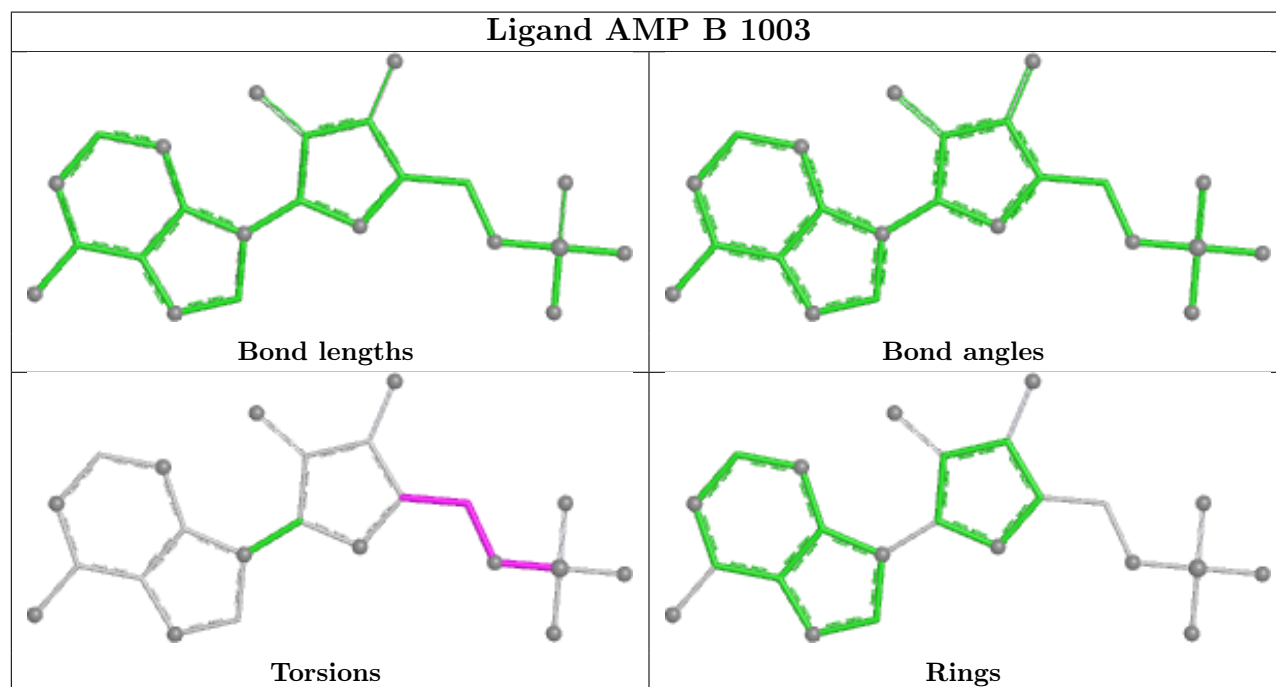
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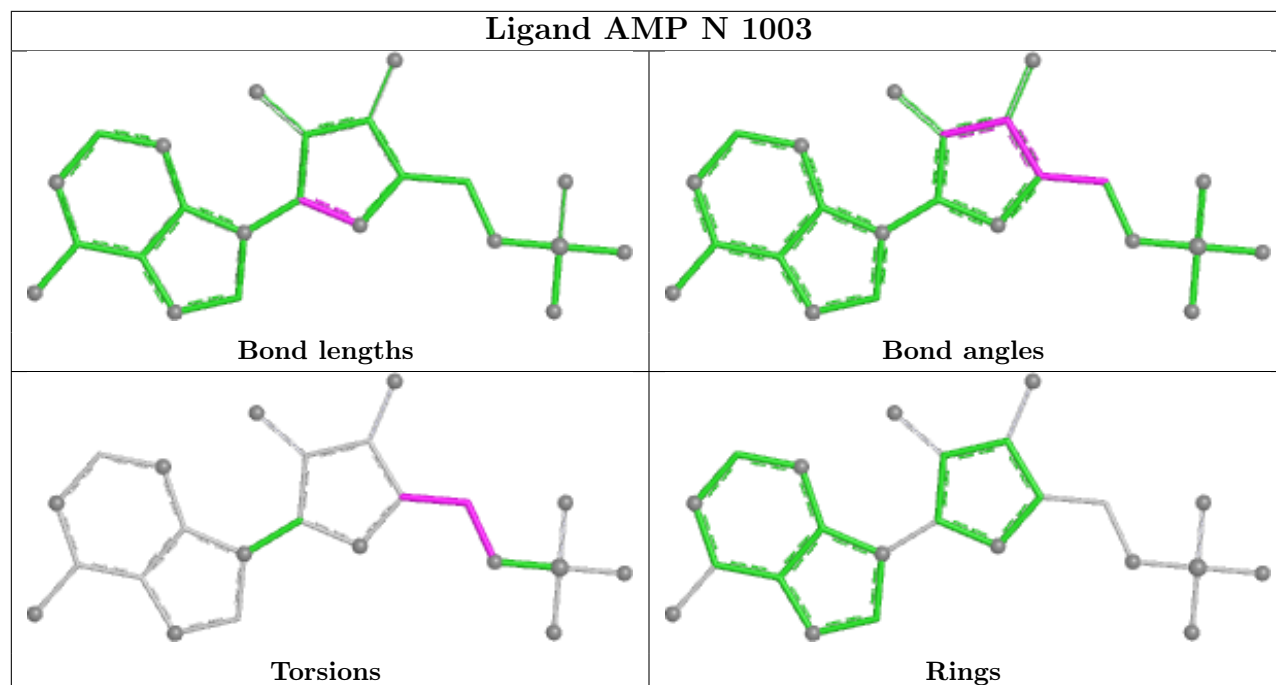
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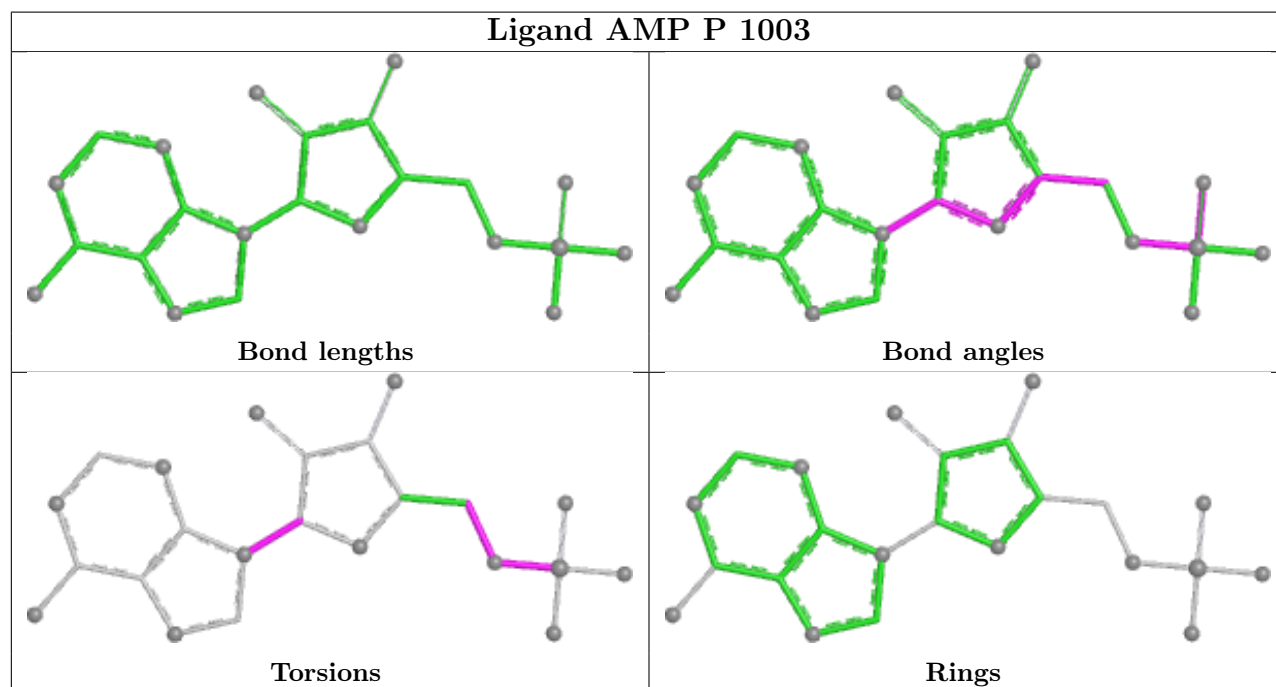
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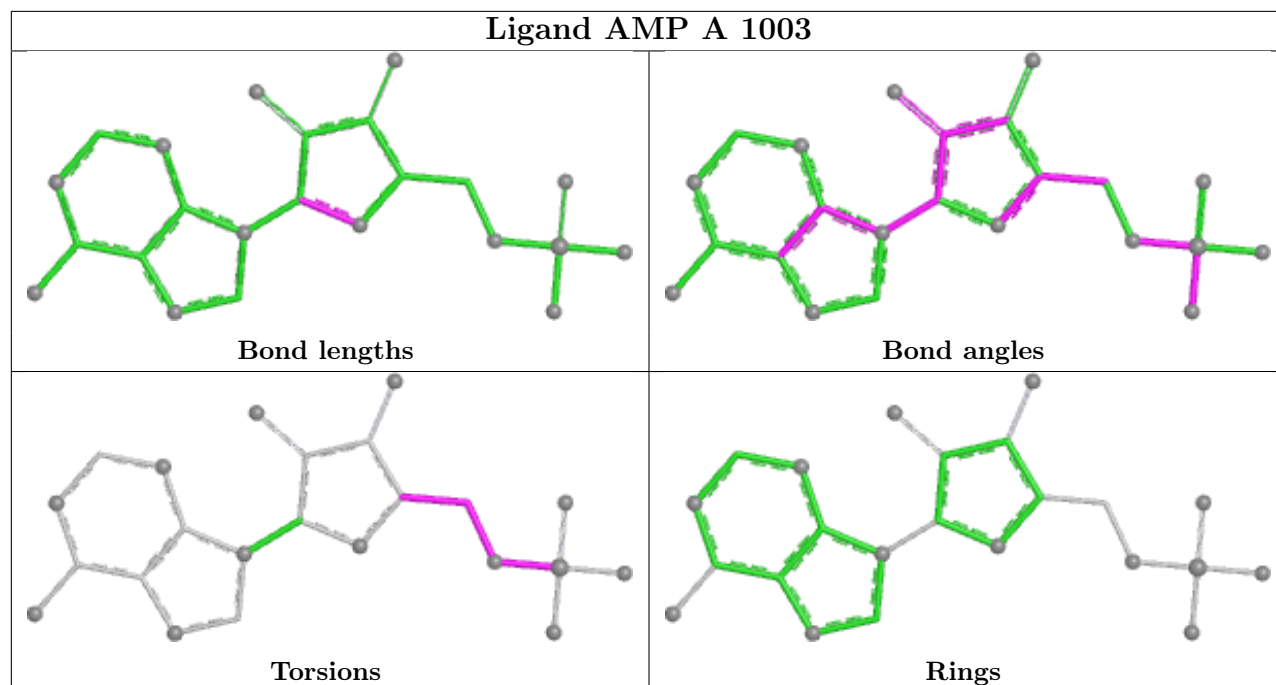
Ligand AMP N 1003



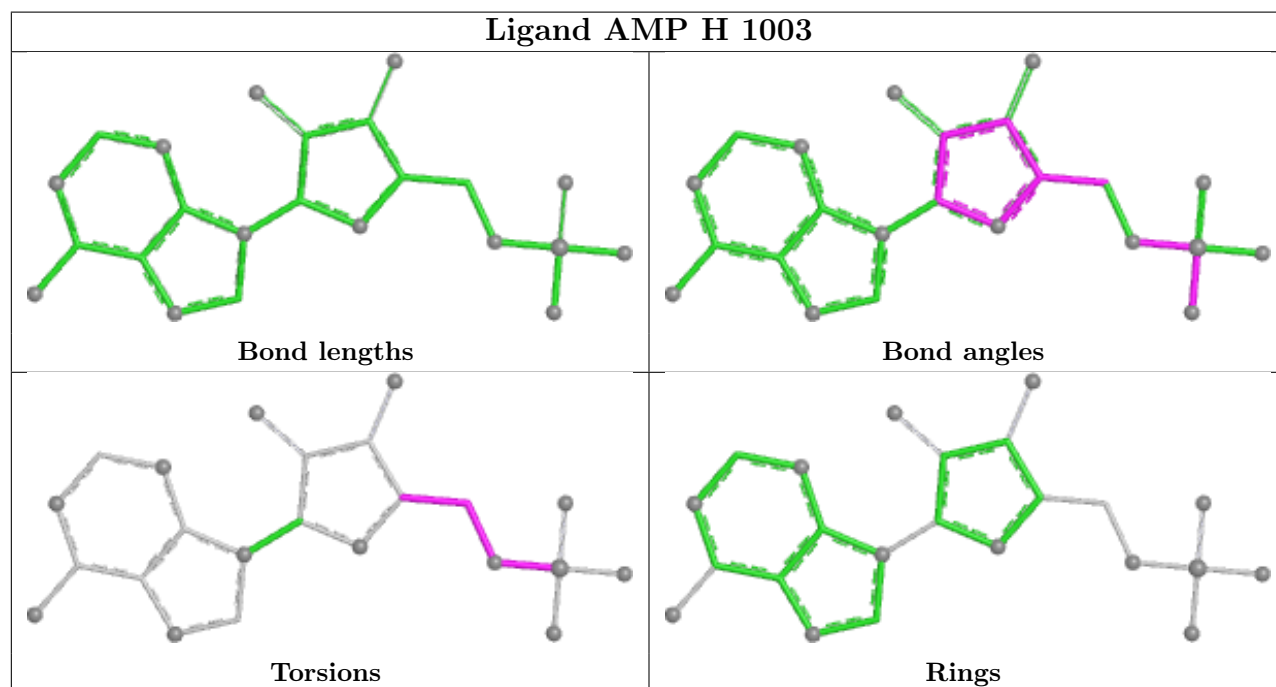
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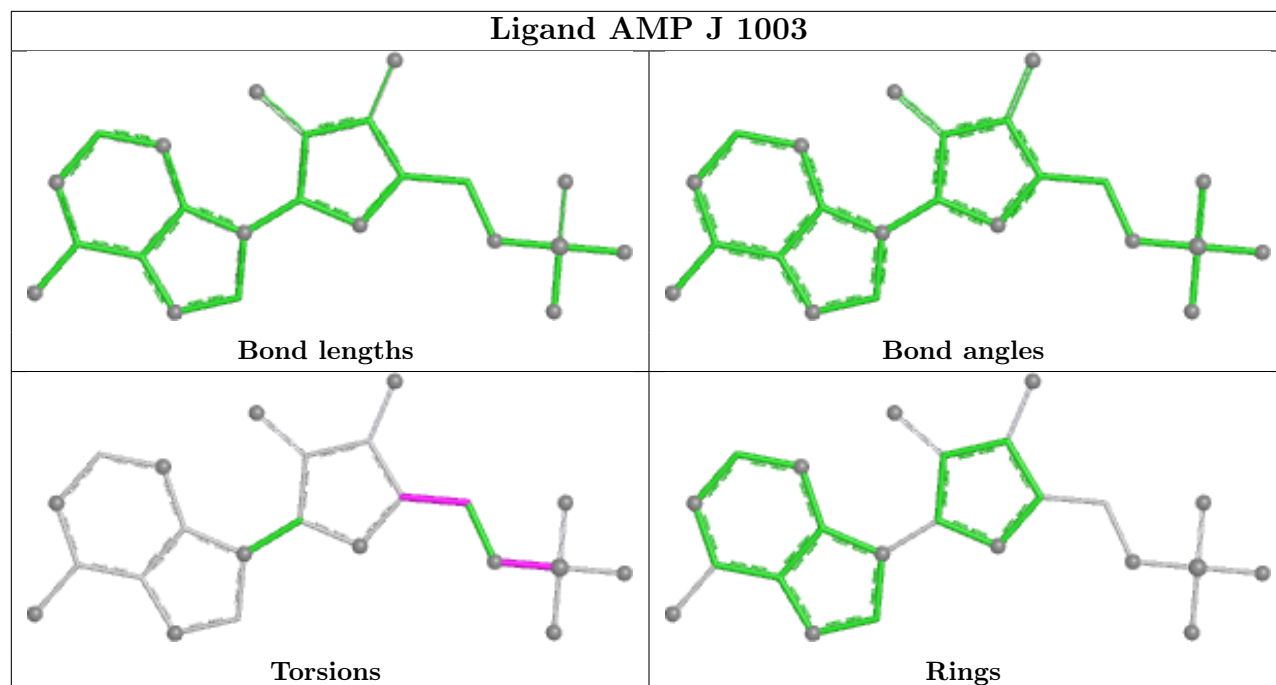
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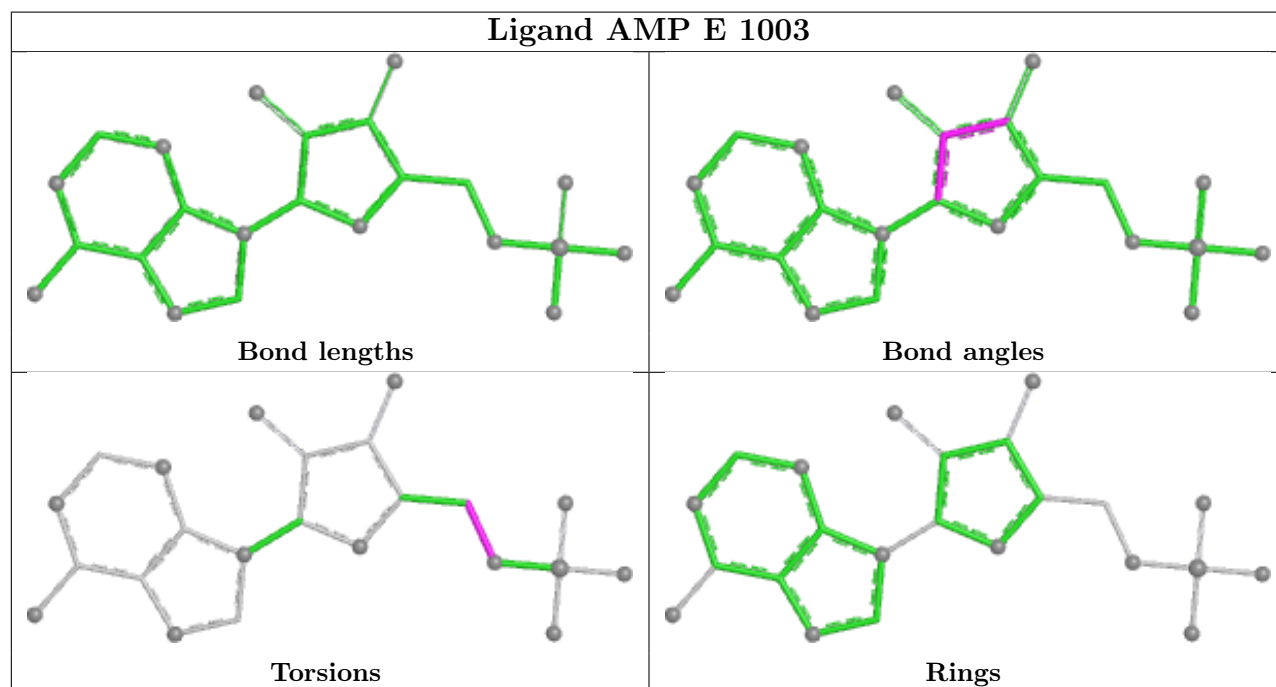
Ligand AMP H 1003



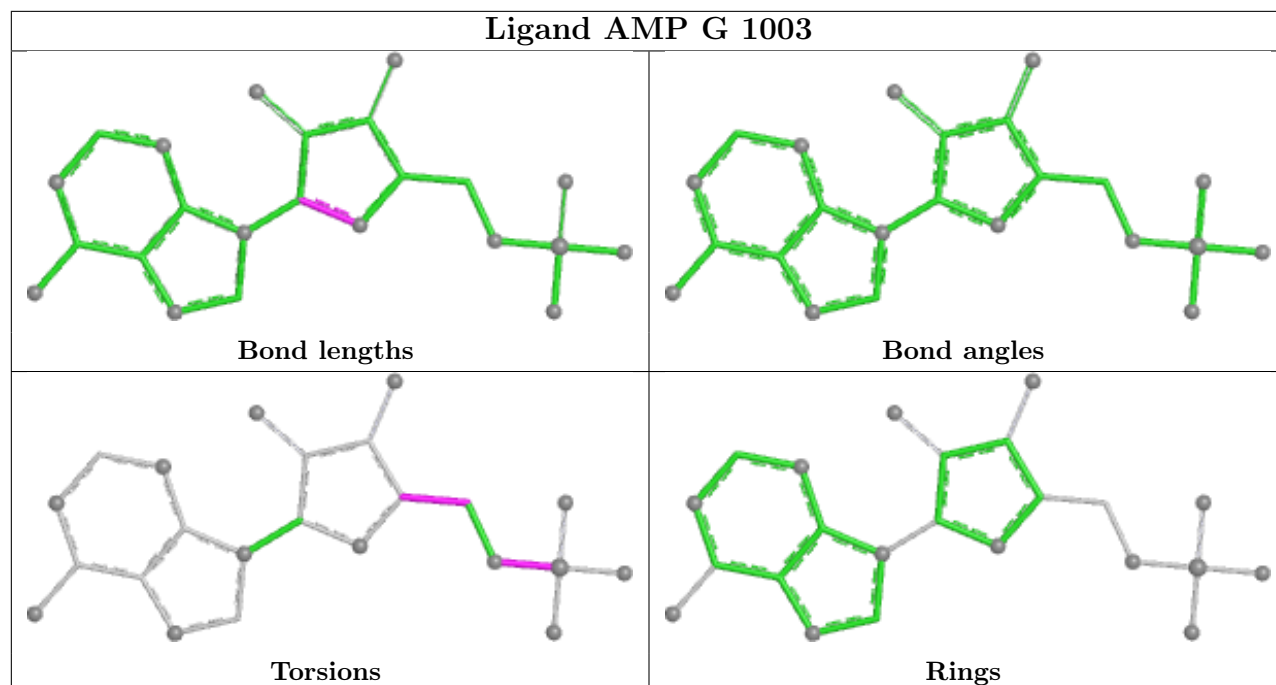
Ligand AMP J 1003



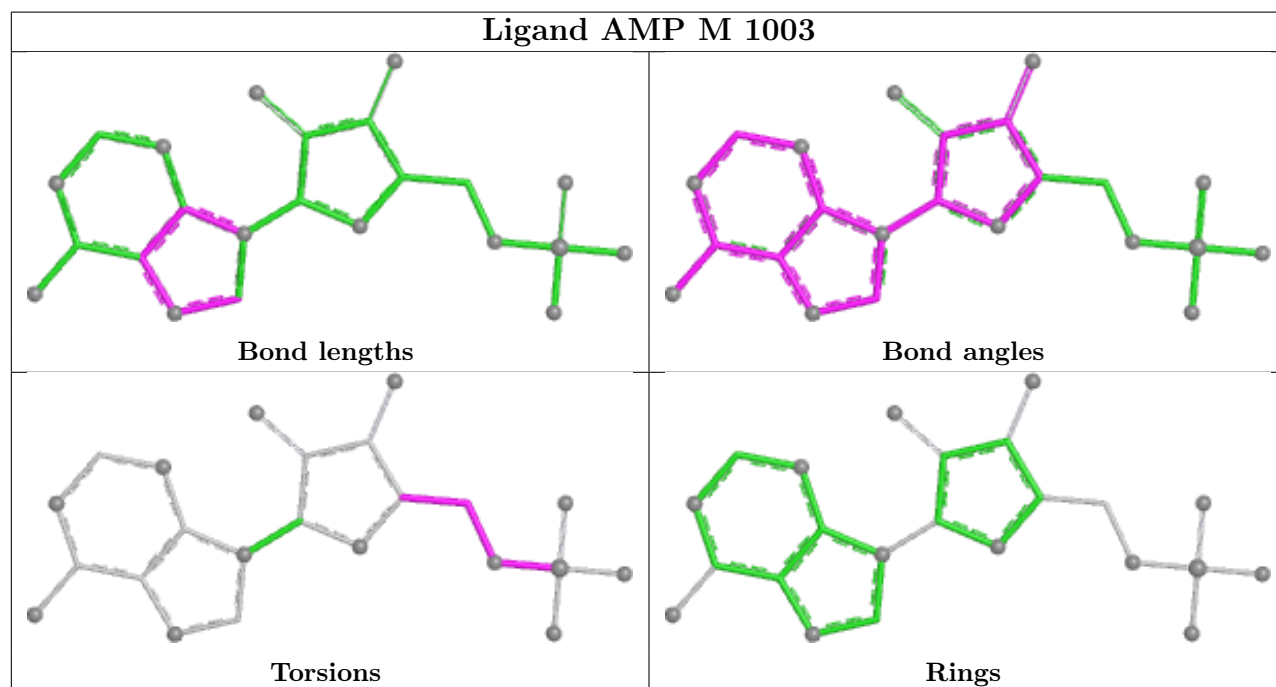
Ligand AMP E 1003

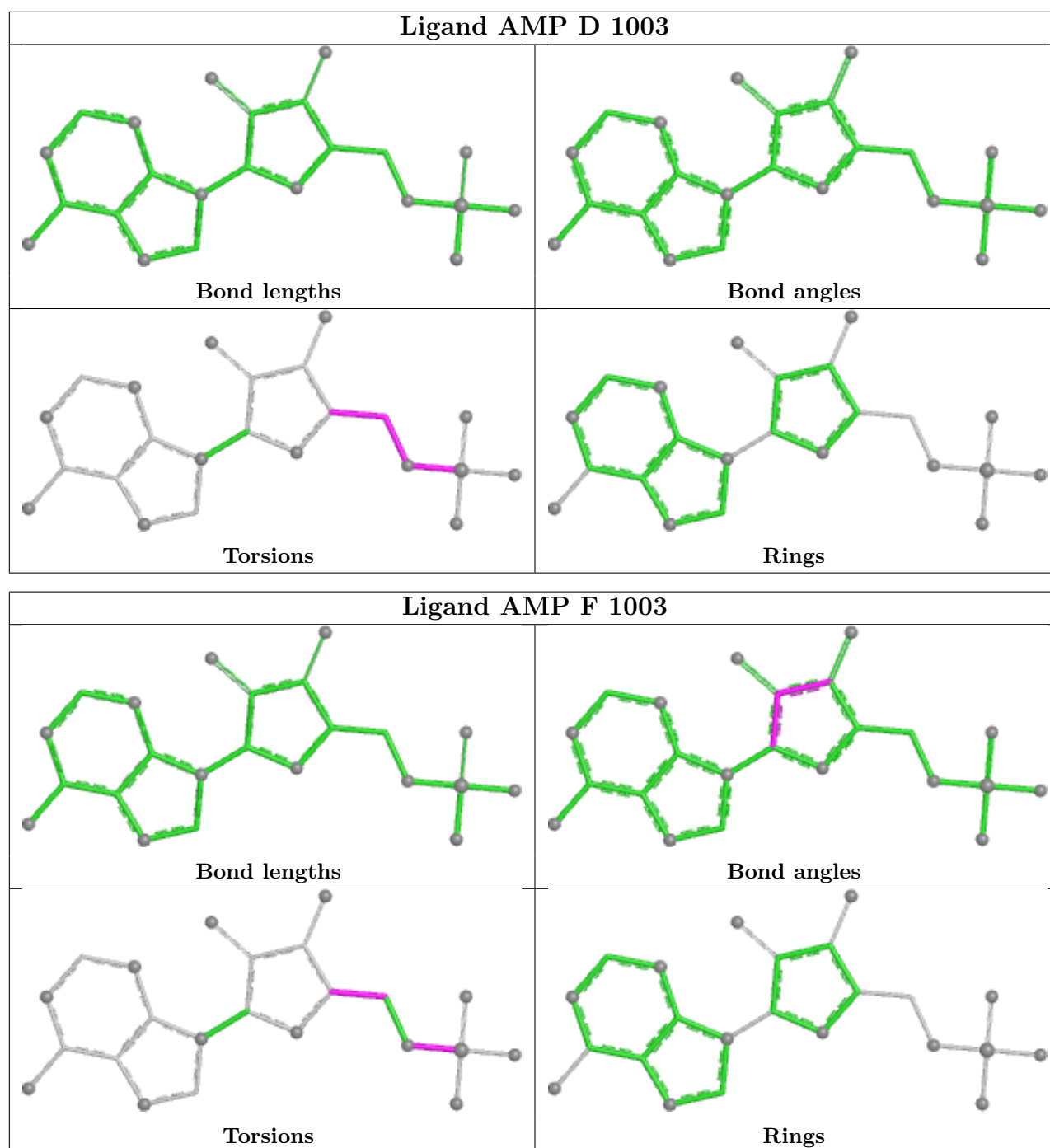


Ligand AMP G 1003



Ligand AMP M 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	287/326 (88%)	0.28	5 (1%) 69 67	23, 45, 67, 89	0
1	B	285/326 (87%)	0.77	22 (7%) 19 17	41, 56, 80, 95	0
1	C	287/326 (88%)	0.30	13 (4%) 38 34	28, 43, 63, 86	0
1	D	291/326 (89%)	0.33	8 (2%) 56 53	29, 43, 66, 87	0
1	E	283/326 (86%)	1.13	59 (20%) 2 2	37, 63, 100, 125	0
1	F	286/326 (87%)	0.57	19 (6%) 24 21	32, 50, 73, 91	0
1	G	292/326 (89%)	0.51	18 (6%) 26 23	36, 51, 76, 92	0
1	H	291/326 (89%)	0.73	30 (10%) 12 10	26, 54, 79, 96	0
1	I	288/326 (88%)	0.31	10 (3%) 47 43	28, 44, 69, 89	0
1	J	291/326 (89%)	0.31	15 (5%) 33 29	31, 44, 67, 91	0
1	K	286/326 (87%)	0.90	44 (15%) 5 4	29, 58, 95, 120	0
1	L	291/326 (89%)	0.32	17 (5%) 29 25	24, 42, 68, 83	0
1	M	291/326 (89%)	1.34	65 (22%) 2 2	49, 69, 93, 106	0
1	N	291/326 (89%)	0.33	13 (4%) 38 34	25, 43, 65, 92	0
1	O	291/326 (89%)	0.92	35 (12%) 9 7	44, 60, 85, 98	0
1	P	285/326 (87%)	1.24	62 (21%) 2 2	44, 69, 110, 135	0
1	Q	291/326 (89%)	0.34	10 (3%) 48 44	28, 43, 68, 86	0
1	R	280/326 (85%)	1.47	72 (25%) 1 1	27, 67, 118, 137	0
All	All	5187/5868 (88%)	0.67	517 (9%) 12 10	23, 52, 88, 137	0

All (517) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	252	SER	8.5
1	E	237	GLY	7.2
1	R	255	GLU	7.1

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Mol	Chain	Res	Type	RSRZ
1	R	256	LEU	6.5
1	P	237	GLY	6.2
1	C	19	TYR	5.9
1	R	58	ILE	5.9
1	E	194	SER	5.8
1	R	237	GLY	5.7
1	R	266	GLY	5.7
1	P	241	LEU	5.7
1	R	251	GLN	5.7
1	E	229	ARG	5.5
1	R	245	TYR	5.4
1	E	256	LEU	5.1
1	J	261	GLU	4.9
1	K	22	ALA	4.8
1	H	263	LYS	4.8
1	D	261	GLU	4.7
1	E	202	ALA	4.7
1	N	22	ALA	4.7
1	R	219	SER	4.7
1	P	260	TYR	4.7
1	P	219	SER	4.6
1	K	266	GLY	4.6
1	M	287	TYR	4.6
1	A	167	GLU	4.5
1	P	230	TYR	4.5
1	P	266	GLY	4.5
1	R	267	VAL	4.4
1	P	23	LEU	4.3
1	R	276	VAL	4.3
1	F	181	ALA	4.3
1	R	283	ILE	4.3
1	E	266	GLY	4.3
1	E	231	ASP	4.2
1	K	237	GLY	4.2
1	K	268	PHE	4.2
1	M	161	PHE	4.2
1	P	217	ILE	4.2
1	L	22	ALA	4.2
1	K	264	GLY	4.2
1	R	216	LYS	4.2
1	M	77	LEU	4.2
1	R	247	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	R	260	TYR	4.1
1	L	254	GLU	4.0
1	G	179	VAL	4.0
1	K	267	VAL	4.0
1	P	267	VAL	4.0
1	M	166	GLY	4.0
1	E	230	TYR	4.0
1	F	169	PHE	4.0
1	H	106	THR	4.0
1	O	263	LYS	4.0
1	P	239	SER	3.9
1	R	238	ILE	3.9
1	E	219	SER	3.9
1	A	118	VAL	3.9
1	P	224	SER	3.9
1	O	300	LEU	3.9
1	E	118	VAL	3.9
1	P	26	PHE	3.8
1	E	107	GLN	3.8
1	F	190	THR	3.8
1	H	196	SER	3.8
1	K	168	LEU	3.8
1	H	181	ALA	3.8
1	E	290	TRP	3.8
1	E	17	GLY	3.8
1	P	240	ASN	3.7
1	I	167	GLU	3.7
1	R	217	ILE	3.7
1	H	180	GLY	3.7
1	M	180	GLY	3.6
1	R	254	GLU	3.6
1	B	118	VAL	3.5
1	R	250	GLY	3.5
1	R	177	PRO	3.5
1	E	26	PHE	3.5
1	K	230	TYR	3.5
1	M	304	ALA	3.5
1	M	206	LEU	3.5
1	R	228	ILE	3.5
1	K	256	LEU	3.5
1	E	203	TYR	3.4
1	P	238	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	3.4
1	G	262	GLY	3.4
1	M	157	LEU	3.4
1	P	256	LEU	3.4
1	P	118	VAL	3.4
1	H	176	ILE	3.4
1	C	239	SER	3.4
1	R	269	LYS	3.4
1	C	15	THR	3.4
1	R	210	ALA	3.4
1	F	219	SER	3.3
1	G	237	GLY	3.3
1	R	131	ALA	3.3
1	N	26	PHE	3.3
1	R	26	PHE	3.3
1	K	228	ILE	3.3
1	P	218	LYS	3.3
1	E	285	GLU	3.3
1	K	248	LEU	3.3
1	G	118	VAL	3.3
1	K	26	PHE	3.3
1	E	225	GLU	3.3
1	H	226	GLY	3.3
1	E	191	LYS	3.3
1	O	161	PHE	3.3
1	F	224	SER	3.3
1	O	226	GLY	3.3
1	I	22	ALA	3.3
1	M	78	PHE	3.3
1	E	227	THR	3.2
1	K	263	LYS	3.2
1	M	165	TYR	3.2
1	P	226	GLY	3.2
1	E	176	ILE	3.2
1	M	118	VAL	3.2
1	E	186	LEU	3.2
1	E	9	GLN	3.2
1	M	286	ARG	3.2
1	Q	254	GLU	3.2
1	E	289	HIS	3.2
1	H	219	SER	3.2
1	O	118	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	188	ASP	3.2
1	K	271	ASP	3.2
1	I	181	ALA	3.2
1	O	224	SER	3.2
1	R	22	ALA	3.2
1	I	118	VAL	3.2
1	R	218	LYS	3.1
1	C	219	SER	3.1
1	H	224	SER	3.1
1	M	176	ILE	3.1
1	R	246	SER	3.1
1	B	165	TYR	3.1
1	R	240	ASN	3.1
1	F	237	GLY	3.1
1	K	219	SER	3.1
1	R	182	ARG	3.1
1	R	192	LYS	3.1
1	O	157	LEU	3.1
1	Q	9	GLN	3.1
1	C	262	GLY	3.1
1	M	217	ILE	3.1
1	O	120	ALA	3.1
1	H	299	VAL	3.1
1	K	265	TYR	3.1
1	H	254	GLU	3.1
1	K	225	GLU	3.1
1	K	285	GLU	3.1
1	R	285	GLU	3.1
1	P	106	THR	3.1
1	M	2	LYS	3.1
1	P	277	ILE	3.1
1	B	258	ARG	3.1
1	M	27	VAL	3.1
1	M	179	VAL	3.1
1	E	177	PRO	3.0
1	E	218	LYS	3.0
1	H	264	GLY	3.0
1	K	180	GLY	3.0
1	E	273	ALA	3.0
1	E	242	LEU	3.0
1	R	186	LEU	3.0
1	C	225	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	R	165	TYR	3.0
1	M	269	LYS	3.0
1	G	309	ARG	3.0
1	E	224	SER	3.0
1	I	219	SER	3.0
1	M	107	GLN	3.0
1	O	256	LEU	3.0
1	H	189	PRO	3.0
1	K	104	ARG	3.0
1	M	15	THR	3.0
1	P	130	ALA	3.0
1	P	174	ALA	3.0
1	R	85	ALA	3.0
1	F	191	LYS	2.9
1	L	219	SER	2.9
1	E	183	ILE	2.9
1	E	228	ILE	2.9
1	M	90	ALA	2.9
1	R	118	VAL	2.9
1	G	167	GLU	2.9
1	F	188	ASP	2.9
1	M	171	ILE	2.9
1	P	210	ALA	2.9
1	E	267	VAL	2.9
1	M	215	LYS	2.9
1	M	300	LEU	2.9
1	M	288	HIS	2.9
1	P	127	PRO	2.9
1	K	106	THR	2.9
1	G	157	LEU	2.9
1	M	120	ALA	2.9
1	M	263	LYS	2.9
1	B	177	PRO	2.8
1	B	9	GLN	2.8
1	F	21	GLY	2.8
1	M	50	ASP	2.8
1	R	54	LEU	2.8
1	J	189	PRO	2.8
1	R	244	ILE	2.8
1	R	215	LYS	2.8
1	P	15	THR	2.8
1	E	253	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	239	SER	2.8
1	P	192	LYS	2.8
1	L	166	GLY	2.8
1	M	303	GLY	2.8
1	K	227	THR	2.8
1	L	106	THR	2.8
1	K	165	TYR	2.8
1	N	118	VAL	2.8
1	N	181	ALA	2.8
1	O	87	ALA	2.8
1	P	131	ALA	2.8
1	R	275	VAL	2.8
1	K	229	ARG	2.8
1	R	213	ILE	2.8
1	E	240	ASN	2.8
1	N	237	GLY	2.8
1	F	179	VAL	2.8
1	I	261	GLU	2.8
1	K	261	GLU	2.8
1	R	59	ARG	2.8
1	P	228	ILE	2.7
1	M	224	SER	2.7
1	R	249	SER	2.7
1	E	243	ASN	2.7
1	E	210	ALA	2.7
1	F	177	PRO	2.7
1	G	177	PRO	2.7
1	R	107	GLN	2.7
1	B	140	ILE	2.7
1	O	253	ILE	2.7
1	P	242	LEU	2.7
1	B	289	HIS	2.7
1	M	273	ALA	2.7
1	M	177	PRO	2.7
1	L	9	GLN	2.7
1	M	9	GLN	2.7
1	M	211	LYS	2.7
1	M	253	ILE	2.7
1	O	217	ILE	2.7
1	B	254	GLU	2.7
1	K	270	ALA	2.7
1	M	212	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	97	VAL	2.7
1	M	23	LEU	2.7
1	O	29	LEU	2.7
1	P	250	GLY	2.7
1	H	261	GLU	2.7
1	G	178	LYS	2.7
1	M	201	LYS	2.7
1	O	2	LYS	2.7
1	R	62	ALA	2.7
1	D	94	GLN	2.6
1	C	230	TYR	2.6
1	P	58	ILE	2.6
1	P	298	ARG	2.6
1	E	201	LYS	2.6
1	E	196	SER	2.6
1	K	277	ILE	2.6
1	M	213	ILE	2.6
1	F	262	GLY	2.6
1	M	163	LYS	2.6
1	R	214	GLU	2.6
1	E	268	PHE	2.6
1	L	118	VAL	2.6
1	H	190	THR	2.6
1	R	212	THR	2.6
1	M	30	GLN	2.6
1	Q	176	ILE	2.6
1	N	23	LEU	2.6
1	H	258	ARG	2.6
1	K	255	GLU	2.6
1	H	170	THR	2.6
1	P	227	THR	2.6
1	K	238	ILE	2.6
1	R	183	ILE	2.6
1	O	77	LEU	2.6
1	P	216	LYS	2.6
1	G	225	GLU	2.6
1	K	273	ALA	2.6
1	L	26	PHE	2.6
1	M	158	ALA	2.6
1	G	9	GLN	2.6
1	K	25	GLN	2.6
1	E	252	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	224	SER	2.5
1	B	300	LEU	2.5
1	H	2	LYS	2.5
1	K	258	ARG	2.5
1	K	257	GLU	2.5
1	P	177	PRO	2.5
1	O	78	PHE	2.5
1	H	197	ASP	2.5
1	M	229	ARG	2.5
1	R	206	LEU	2.5
1	B	173	GLU	2.5
1	R	224	SER	2.5
1	P	146	ASP	2.5
1	B	19	TYR	2.5
1	M	37	PHE	2.5
1	R	73	THR	2.5
1	A	195	LYS	2.5
1	H	194	SER	2.5
1	M	241	LEU	2.5
1	P	252	SER	2.5
1	R	242	LEU	2.5
1	M	188	ASP	2.5
1	O	209	ASP	2.5
1	A	237	GLY	2.5
1	D	26	PHE	2.5
1	E	63	ALA	2.5
1	H	178	LYS	2.4
1	E	258	ARG	2.4
1	P	253	ILE	2.4
1	P	178	LYS	2.4
1	J	258	ARG	2.4
1	M	29	LEU	2.4
1	P	151	ILE	2.4
1	P	283	ILE	2.4
1	R	277	ILE	2.4
1	M	209	ASP	2.4
1	E	254	GLU	2.4
1	H	21	GLY	2.4
1	H	179	VAL	2.4
1	J	107	GLN	2.4
1	O	259	GLN	2.4
1	R	259	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	125	TYR	2.4
1	R	268	PHE	2.4
1	P	229	ARG	2.4
1	P	183	ILE	2.4
1	P	244	ILE	2.4
1	P	296	LEU	2.4
1	D	224	SER	2.4
1	M	290	TRP	2.4
1	O	254	GLU	2.4
1	K	250	GLY	2.4
1	N	94	GLN	2.4
1	B	230	TYR	2.4
1	H	22	ALA	2.4
1	O	62	ALA	2.4
1	R	63	ALA	2.4
1	R	286	ARG	2.4
1	F	20	ILE	2.4
1	O	168	LEU	2.4
1	P	102	LEU	2.4
1	R	207	LEU	2.4
1	P	214	GLU	2.4
1	L	144	GLY	2.4
1	Q	262	GLY	2.4
1	B	55	ARG	2.4
1	K	169	PHE	2.4
1	L	23	LEU	2.3
1	O	3	THR	2.3
1	N	52	HIS	2.3
1	B	308	ASN	2.3
1	C	103	GLU	2.3
1	E	182	ARG	2.3
1	R	258	ARG	2.3
1	C	26	PHE	2.3
1	B	296	LEU	2.3
1	R	253	ILE	2.3
1	B	137	ASN	2.3
1	B	292	GLU	2.3
1	M	191	LYS	2.3
1	N	219	SER	2.3
1	F	189	PRO	2.3
1	M	175	ARG	2.3
1	K	134	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	186	LEU	2.3
1	E	238	ILE	2.3
1	J	106	THR	2.3
1	J	167	GLU	2.3
1	P	295	GLU	2.3
1	K	239	SER	2.3
1	R	209	ASP	2.3
1	M	274	GLN	2.3
1	P	259	GLN	2.3
1	F	23	LEU	2.3
1	M	85	ALA	2.3
1	P	273	ALA	2.3
1	O	52	HIS	2.3
1	P	76	THR	2.3
1	K	287	TYR	2.3
1	G	305	GLU	2.3
1	H	167	GLU	2.3
1	E	175	ARG	2.3
1	M	219	SER	2.3
1	B	237	GLY	2.3
1	O	180	GLY	2.3
1	R	290	TRP	2.3
1	J	23	LEU	2.3
1	B	174	ALA	2.2
1	G	14	ILE	2.2
1	G	181	ALA	2.2
1	N	148	LYS	2.2
1	J	260	TYR	2.2
1	R	199	ASN	2.2
1	F	24	ARG	2.2
1	C	224	SER	2.2
1	M	64	LEU	2.2
1	E	192	LYS	2.2
1	E	215	LYS	2.2
1	J	169	PHE	2.2
1	E	255	GLU	2.2
1	M	230	TYR	2.2
1	L	224	SER	2.2
1	E	275	VAL	2.2
1	M	31	HIS	2.2
1	M	210	ALA	2.2
1	N	62	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	261	GLU	2.2
1	O	32	GLU	2.2
1	F	146	ASP	2.2
1	H	118	VAL	2.2
1	A	169	PHE	2.2
1	H	16	ILE	2.2
1	G	174	ALA	2.2
1	M	190	THR	2.2
1	R	15	THR	2.2
1	F	186	LEU	2.2
1	L	21	GLY	2.2
1	M	296	LEU	2.2
1	L	179	VAL	2.2
1	E	67	ALA	2.1
1	Q	174	ALA	2.1
1	K	279	THR	2.1
1	O	286	ARG	2.1
1	Q	229	ARG	2.1
1	J	18	ASN	2.1
1	D	287	TYR	2.1
1	E	269	LYS	2.1
1	P	18	ASN	2.1
1	P	203	TYR	2.1
1	O	237	GLY	2.1
1	I	253	ILE	2.1
1	D	292	GLU	2.1
1	Q	53	GLU	2.1
1	J	24	ARG	2.1
1	P	104	ARG	2.1
1	J	15	THR	2.1
1	B	168	LEU	2.1
1	C	18	ASN	2.1
1	R	9	GLN	2.1
1	L	165	TYR	2.1
1	E	244	ILE	2.1
1	L	176	ILE	2.1
1	P	271	ASP	2.1
1	Q	188	ASP	2.1
1	B	252	SER	2.1
1	R	257	GLU	2.1
1	O	175	ARG	2.1
1	E	195	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	192	LYS	2.1
1	K	269	LYS	2.1
1	C	107	GLN	2.1
1	G	107	GLN	2.1
1	M	259	GLN	2.1
1	J	237	GLY	2.1
1	O	277	ILE	2.1
1	P	213	ILE	2.1
1	I	26	PHE	2.1
1	E	22	ALA	2.1
1	P	270	ALA	2.1
1	R	270	ALA	2.1
1	R	293	SER	2.1
1	E	198	PRO	2.1
1	R	241	LEU	2.1
1	H	262	GLY	2.1
1	M	52	HIS	2.1
1	N	289	HIS	2.1
1	F	287	TYR	2.1
1	O	171	ILE	2.1
1	O	229	ARG	2.0
1	R	55	ARG	2.0
1	R	271	ASP	2.0
1	G	285	GLU	2.0
1	I	32	GLU	2.0
1	I	89	ALA	2.0
1	P	247	THR	2.0
1	E	189	PRO	2.0
1	R	56	GLN	2.0
1	D	180	GLY	2.0
1	E	226	GLY	2.0
1	H	4	ILE	2.0
1	P	133	ILE	2.0
1	Q	140	ILE	2.0
1	K	24	ARG	2.0
1	M	305	GLU	2.0
1	M	62	ALA	2.0
1	O	50	ASP	2.0
1	B	224	SER	2.0
1	O	91	TRP	2.0
1	P	138	THR	2.0
1	K	272	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	107	GLN	2.0
1	N	107	GLN	2.0
1	O	296	LEU	2.0
1	O	289	HIS	2.0
1	C	237	GLY	2.0
1	E	277	ILE	2.0
1	H	228	ILE	2.0
1	P	187	VAL	2.0
1	J	230	TYR	2.0
1	K	125	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AMP	M	1003	23/23	0.56	0.18	20,20,20,20	0
3	PO4	P	1002	5/5	0.62	0.23	104,107,110,111	5
4	AMP	O	1003	23/23	0.62	0.34	34,41,47,48	23
4	AMP	R	1003	23/23	0.64	0.52	49,56,66,68	23
4	AMP	K	1003	23/23	0.69	0.52	47,55,60,61	23
4	AMP	F	1003	23/23	0.72	0.34	39,47,56,58	23
3	PO4	R	1002	5/5	0.73	0.16	76,79,82,83	5
4	AMP	H	1003	23/23	0.73	0.41	45,50,52,53	23
4	AMP	B	1003	23/23	0.74	0.28	34,43,47,49	23
4	AMP	E	1003	23/23	0.74	0.49	42,50,56,57	23
4	AMP	P	1003	23/23	0.75	0.52	54,60,69,70	23
4	AMP	N	1003	23/23	0.76	0.26	19,29,47,48	23
4	AMP	I	1003	23/23	0.76	0.29	22,28,41,42	23

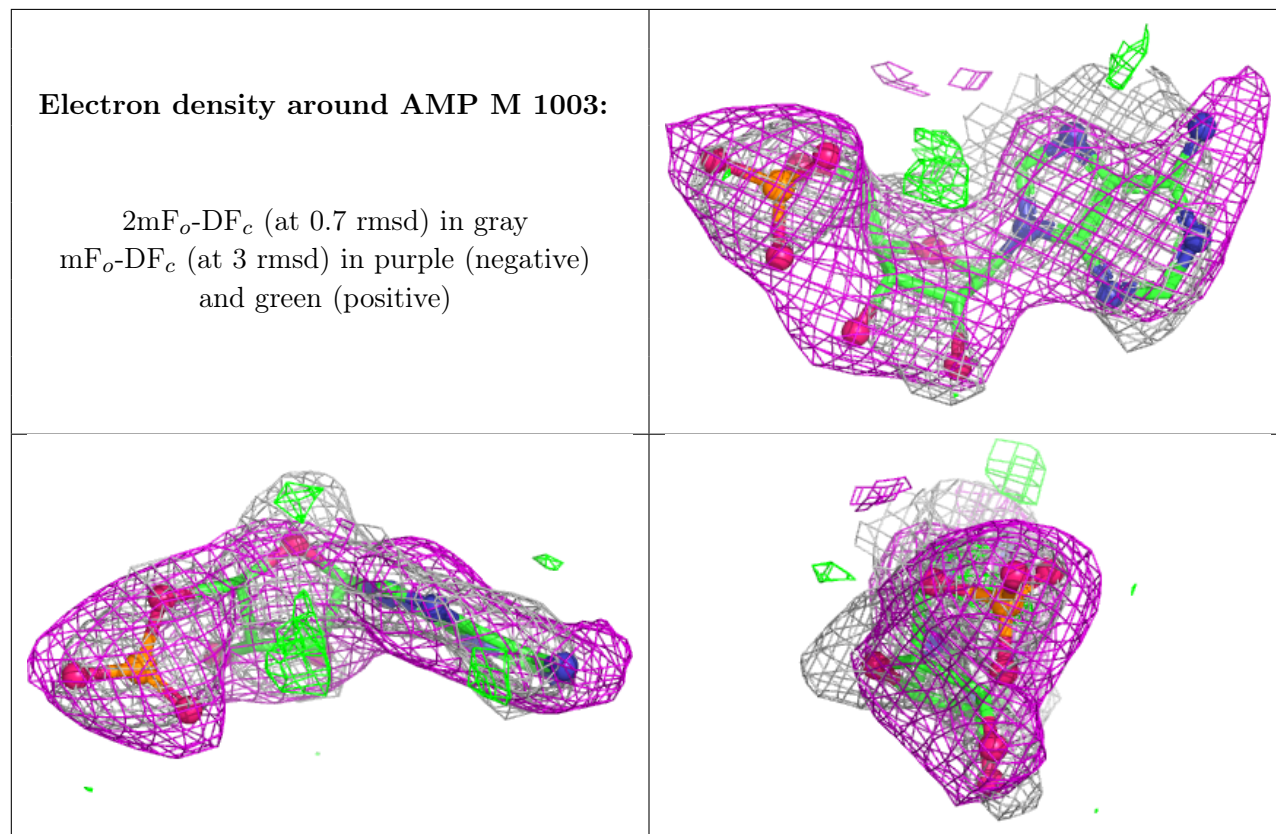
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AMP	D	1003	23/23	0.77	0.31	33,42,54,56	23
4	AMP	Q	1003	23/23	0.78	0.21	22,37,51,53	23
4	AMP	C	1003	23/23	0.78	0.28	21,30,43,44	23
3	PO4	E	1002	5/5	0.80	0.15	75,78,80,81	5
4	AMP	J	1003	23/23	0.81	0.29	29,37,48,49	23
3	PO4	O	1002	5/5	0.82	0.16	41,44,46,47	5
4	AMP	L	1003	23/23	0.82	0.24	24,37,46,47	23
3	PO4	K	1002	5/5	0.85	0.13	64,67,70,71	5
4	AMP	A	1003	23/23	0.85	0.24	38,41,48,50	23
2	TRP	B	1001	15/15	0.86	0.16	29,44,76,106	15
2	TRP	O	1001	15/15	0.86	0.15	24,42,70,106	15
2	TRP	M	1001	15/15	0.87	0.14	21,34,65,103	15
4	AMP	G	1003	23/23	0.88	0.19	41,47,51,53	23
2	TRP	R	1001	15/15	0.88	0.15	12,44,70,106	15
3	PO4	F	1002	5/5	0.89	0.10	51,54,58,60	0
3	PO4	G	1002	5/5	0.89	0.11	50,53,56,56	5
2	TRP	A	1001	15/15	0.89	0.14	22,34,61,104	15
2	TRP	L	1001	15/15	0.89	0.14	20,35,69,101	15
2	TRP	E	1001	15/15	0.90	0.13	5,25,52,93	15
3	PO4	H	1002	5/5	0.90	0.15	46,49,52,54	5
3	PO4	C	1002	5/5	0.90	0.13	42,45,48,49	5
2	TRP	P	1001	15/15	0.91	0.14	18,32,70,99	15
3	PO4	I	1002	5/5	0.91	0.10	47,50,53,53	5
2	TRP	H	1001	15/15	0.91	0.12	20,36,73,103	15
2	TRP	D	1001	15/15	0.91	0.12	11,32,64,100	15
2	TRP	F	1001	15/15	0.92	0.11	12,37,65,99	15
3	PO4	B	1002	5/5	0.92	0.10	48,51,54,54	5
2	TRP	N	1001	15/15	0.92	0.12	14,29,61,100	15
2	TRP	Q	1001	15/15	0.93	0.11	20,34,69,98	15
2	TRP	I	1001	15/15	0.93	0.10	16,37,63,103	15
2	TRP	J	1001	15/15	0.93	0.12	16,30,62,95	15
2	TRP	K	1001	15/15	0.93	0.11	16,32,62,101	15
3	PO4	J	1002	5/5	0.93	0.08	65,68,71,72	0
2	TRP	G	1001	15/15	0.93	0.11	23,46,73,106	15
3	PO4	N	1002	5/5	0.93	0.08	52,55,57,59	0
2	TRP	C	1001	15/15	0.94	0.10	20,37,69,101	15
3	PO4	M	1002	5/5	0.94	0.30	20,20,20,20	0
3	PO4	D	1002	5/5	0.94	0.10	51,54,56,59	0
3	PO4	L	1002	5/5	0.95	0.07	57,60,62,63	0
3	PO4	A	1002	5/5	0.95	0.13	39,43,45,45	5
3	PO4	Q	1002	5/5	0.96	0.07	34,37,40,42	5

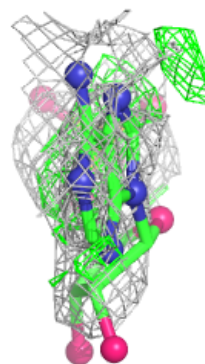
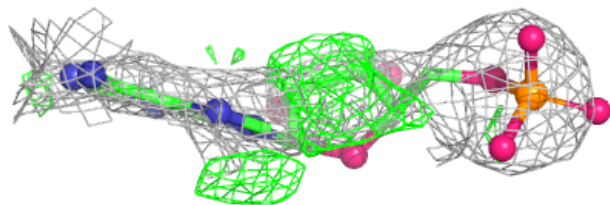
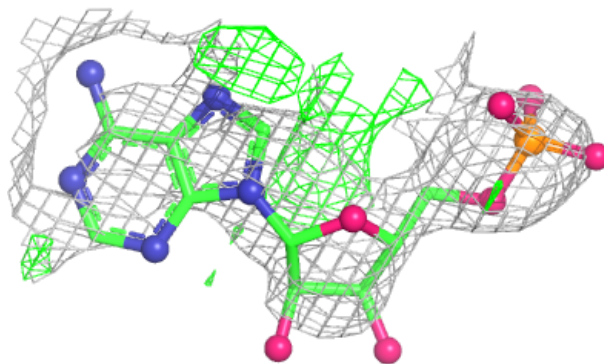
The following is a graphical depiction of the model fit to experimental electron density of all

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.



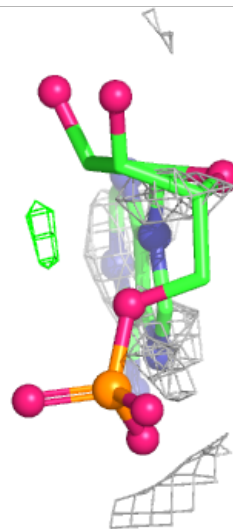
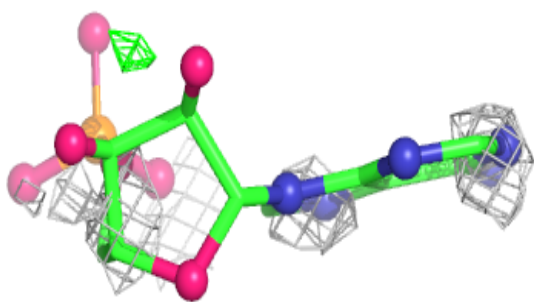
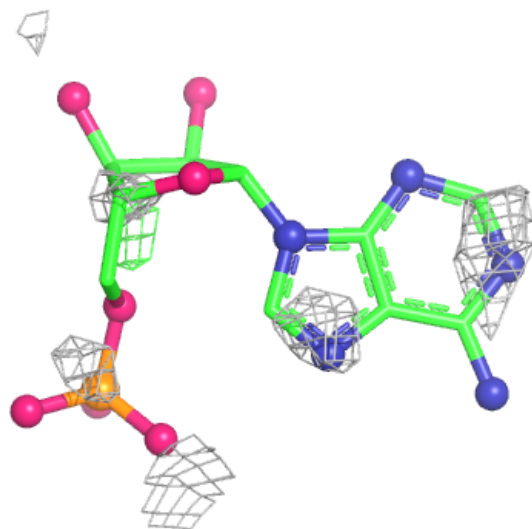
Electron density around AMP O 1003:

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



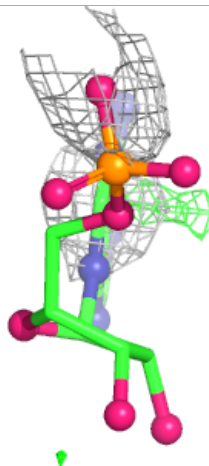
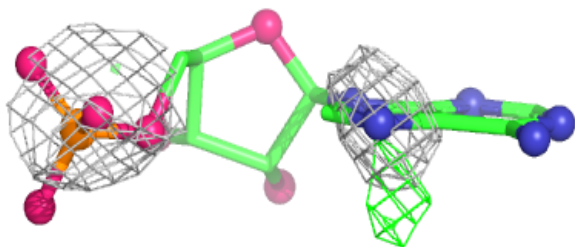
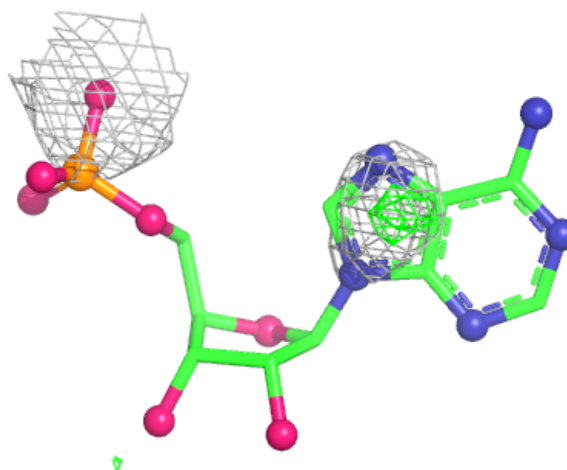
Electron density around AMP R 1003:

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



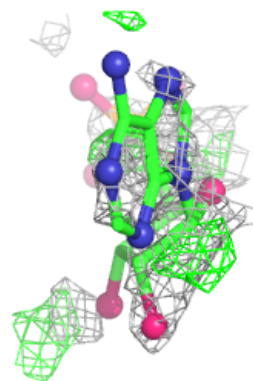
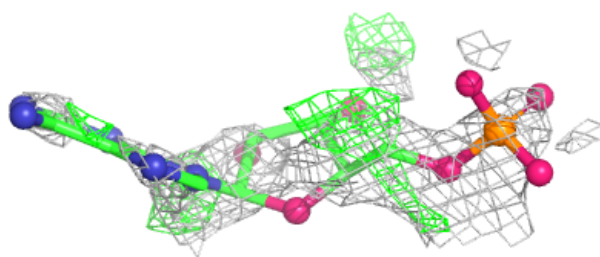
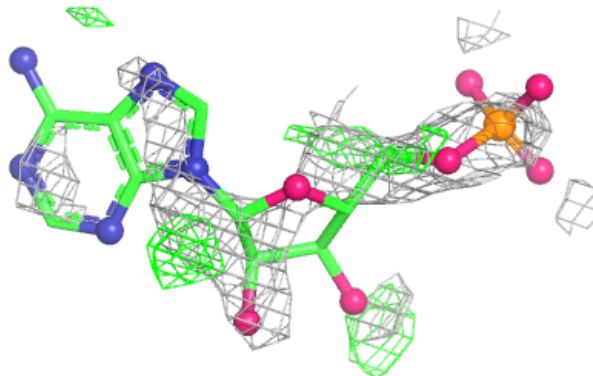
Electron density around AMP K 1003:

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



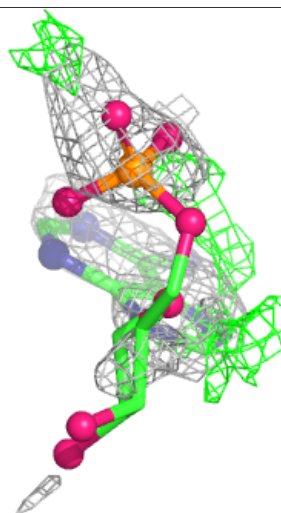
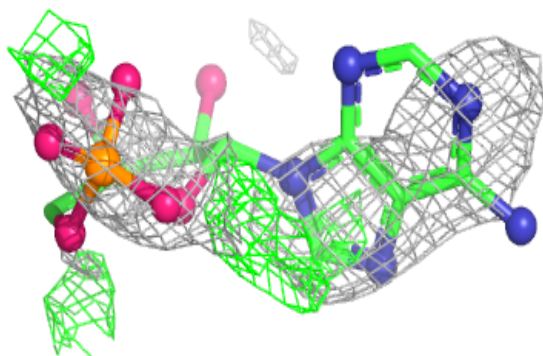
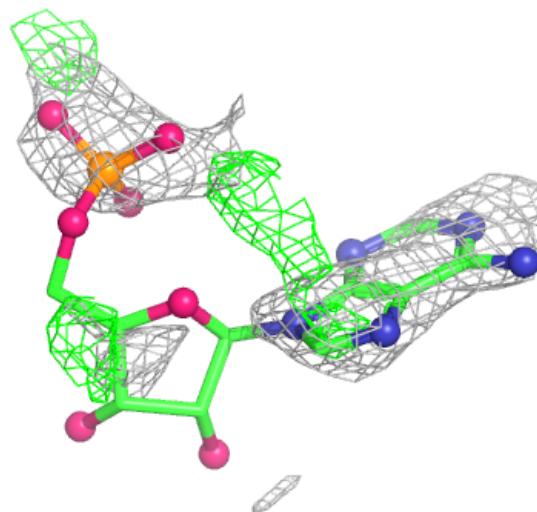
Electron density around AMP F 1003:

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



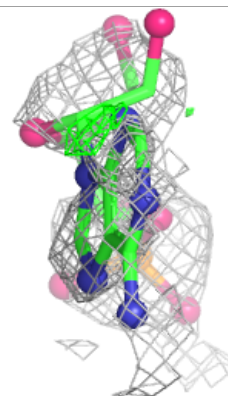
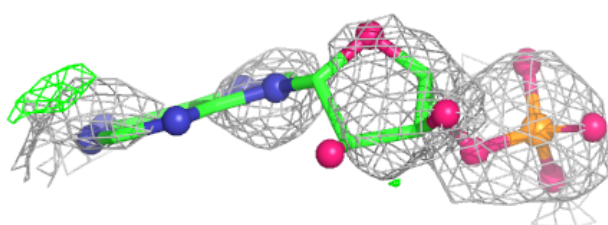
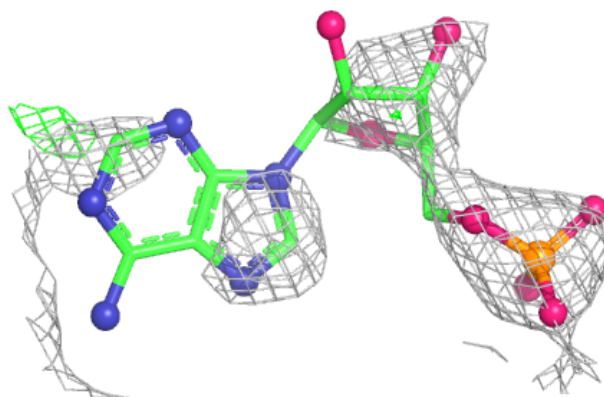
Electron density around AMP H 1003:

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

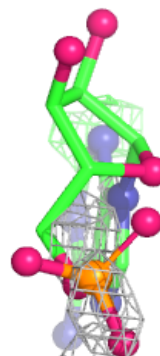
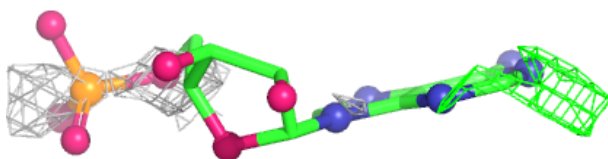
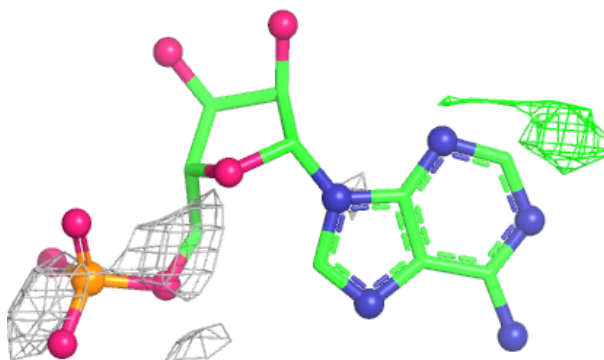


Electron density around AMP B 1003:

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

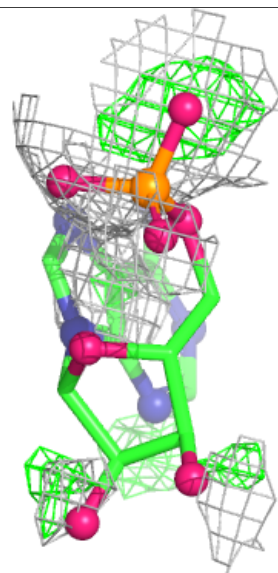
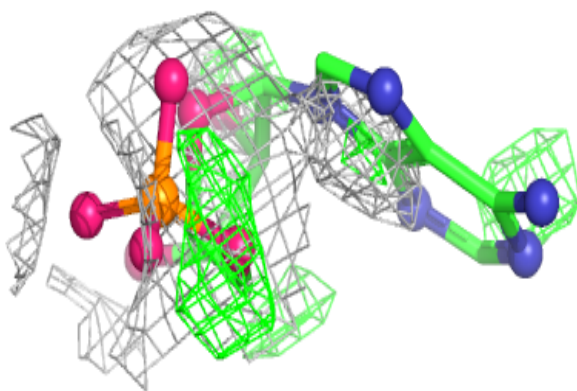
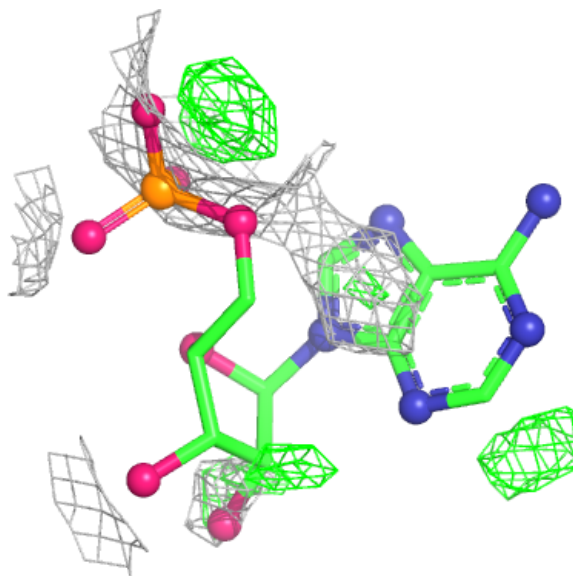
**Electron density around AMP E 1003:**

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



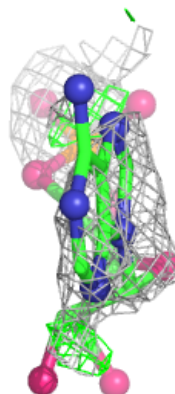
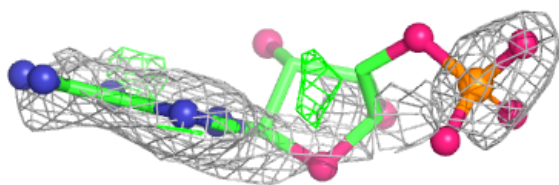
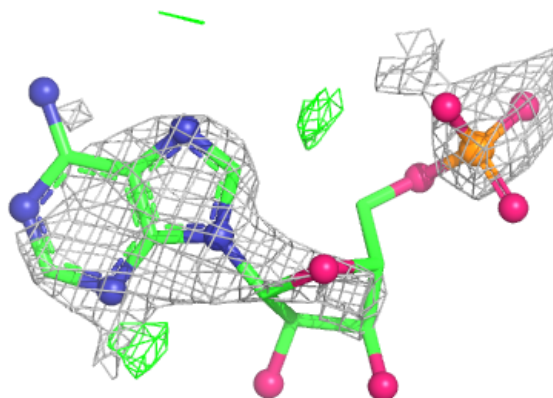
Electron density around AMP P 1003:

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

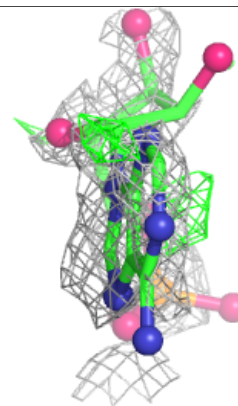
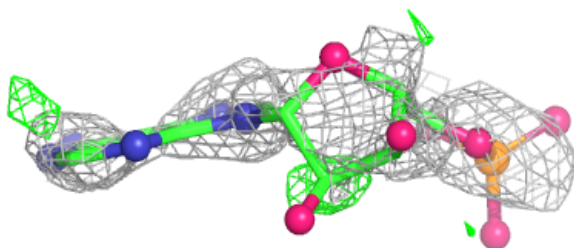
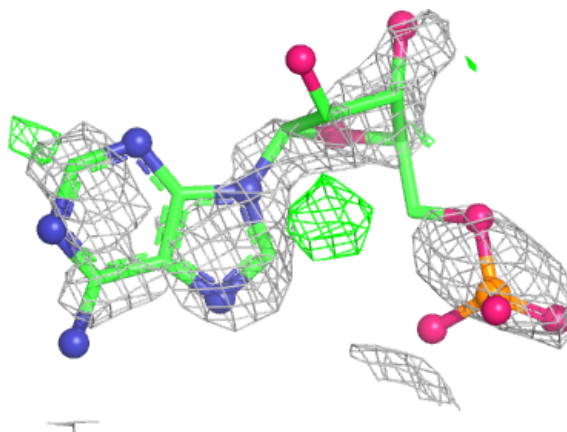


Electron density around AMP N 1003:

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

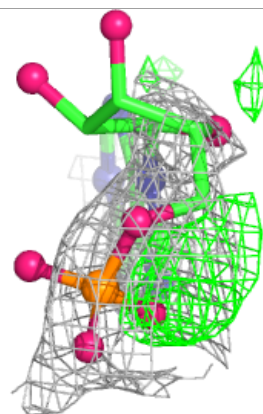
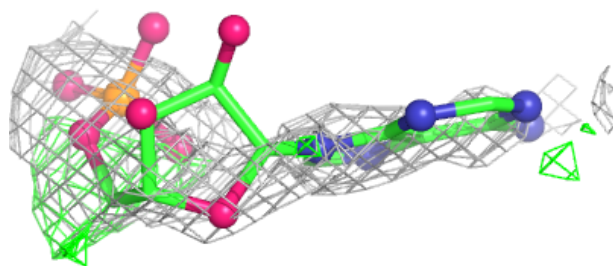
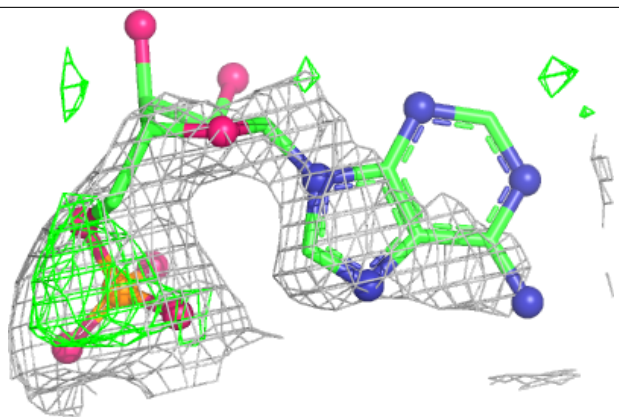
**Electron density around AMP I 1003:**

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

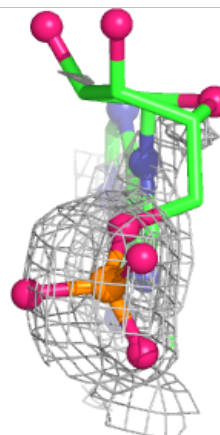
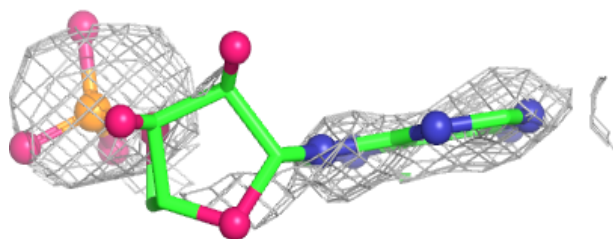
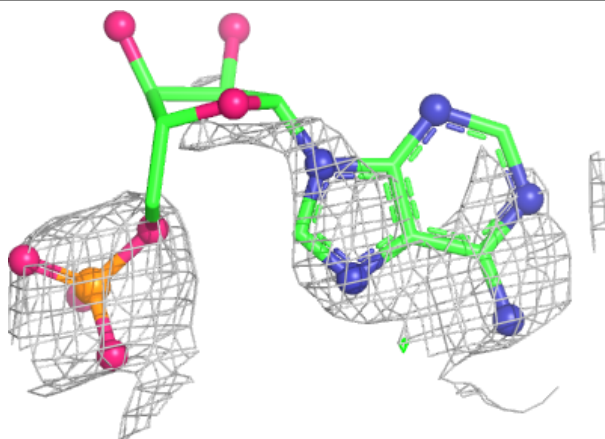


Electron density around AMP D 1003:

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

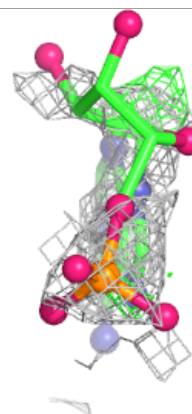
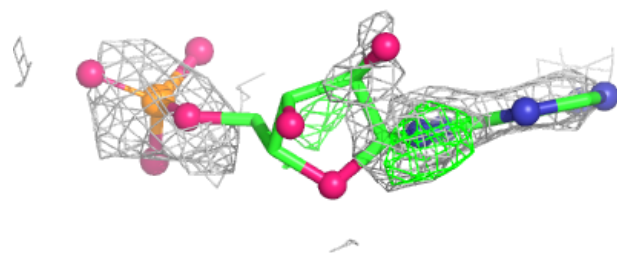
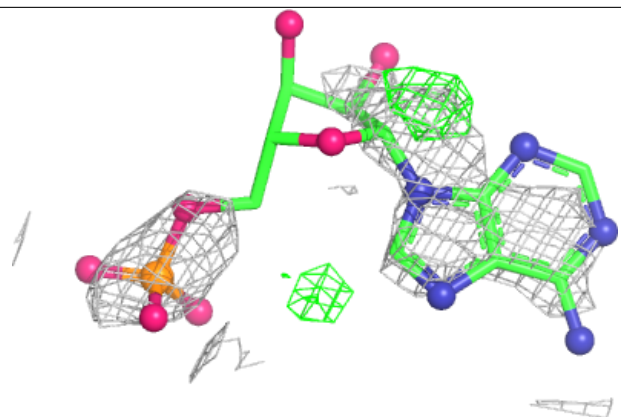
**Electron density around AMP Q 1003:**

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

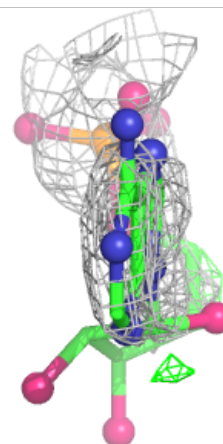
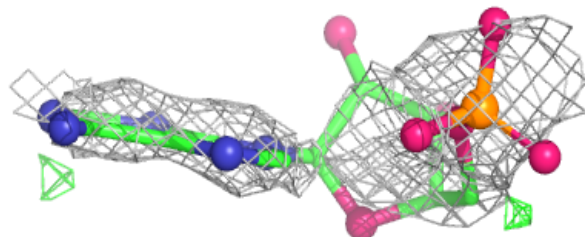
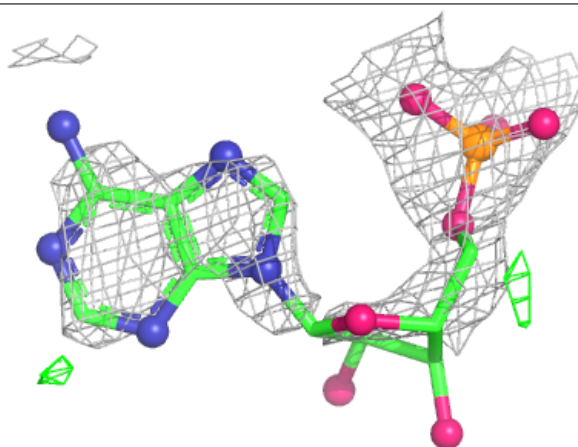


Electron density around AMP C 1003:

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

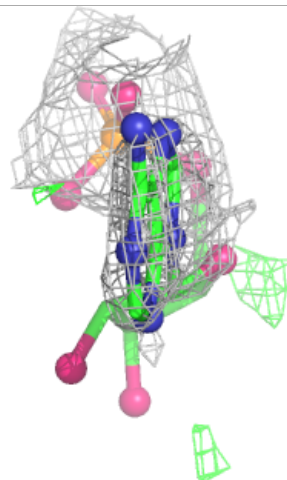
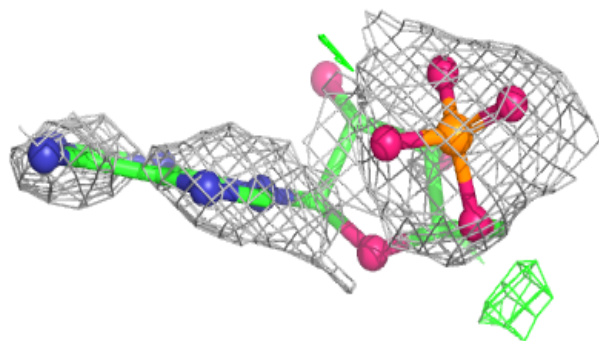
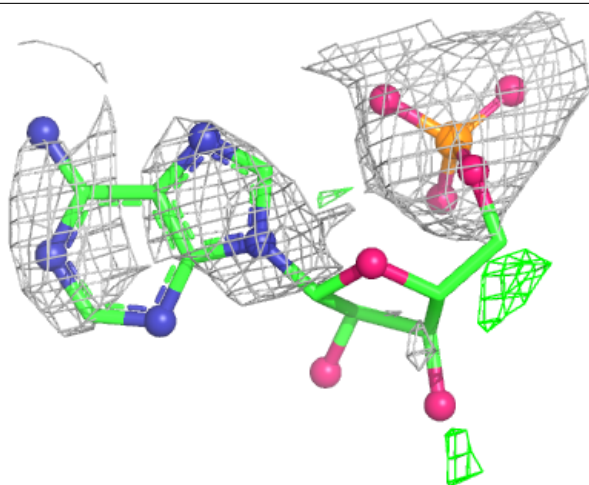
**Electron density around AMP J 1003:**

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



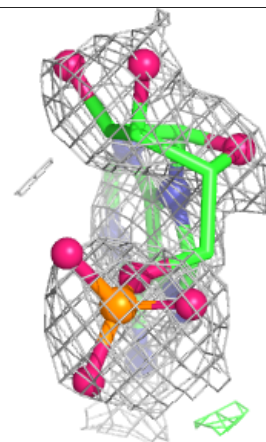
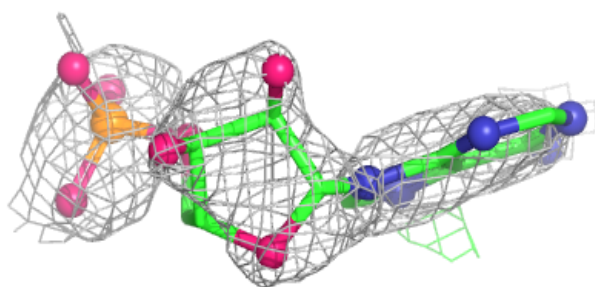
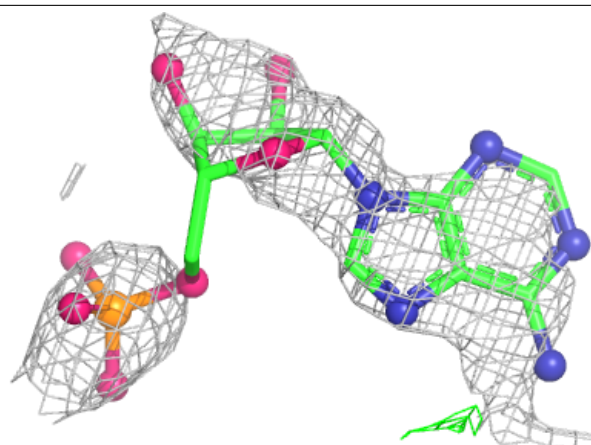
Electron density around AMP L 1003:

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

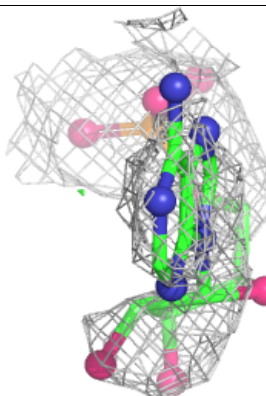
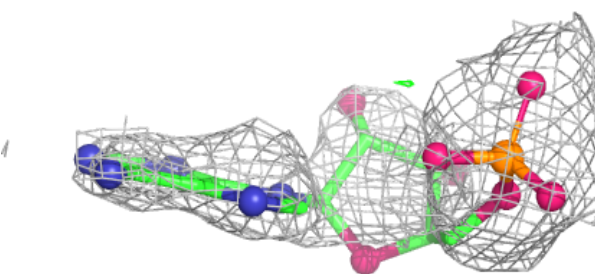
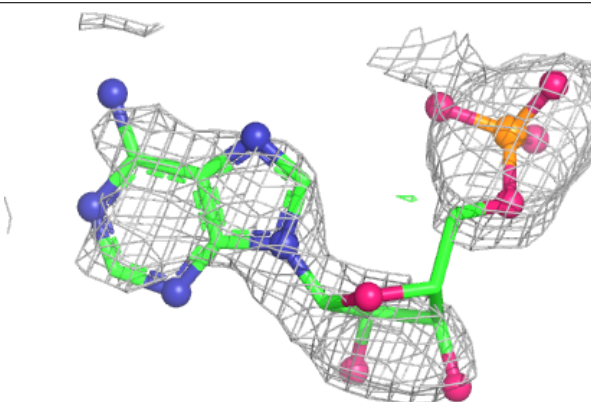


Electron density around AMP A 1003:

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

**Electron density around AMP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.