



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:36 PM UTC

PDB ID : 1OB5 / pdb_00001ob5
Title : T. aquaticus elongation factor EF-Tu complexed with the antibiotic enacyloxin IIa, a GTP analog, and Phe-tRNA
Authors : Dahlberg, C.; Nielsen, R.C.; Parmeggiani, A.; Nyborg, J.; Nissen, P.
Deposited on : 2003-01-24
Resolution : 3.10 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

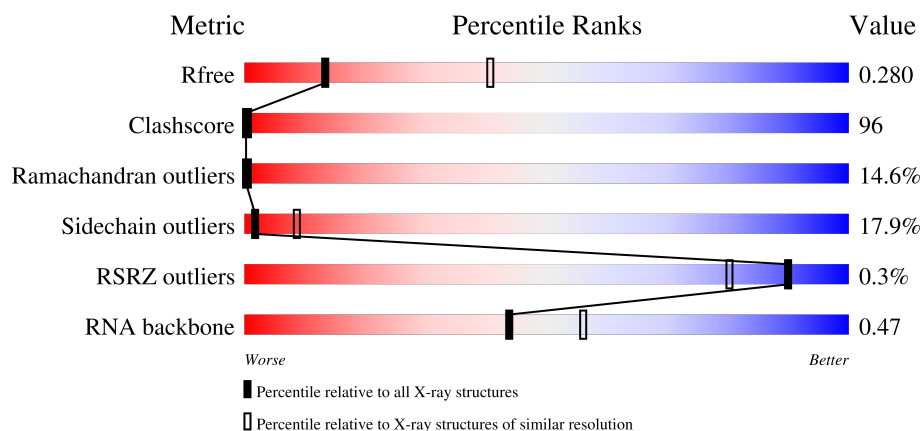
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



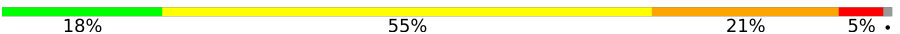
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	405	10% 59% 24% 5%
1	C	405	10% 59% 24% 5%
1	E	405	11% 59% 24% 5%
2	B	78	18% 55% 21% 5%

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Mol	Chain	Length	Quality of chain
2	D	78	
2	F	78	

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
2	PHA	B	77	-	-	X	-
2	M2G	D	26	-	-	X	-
2	PHA	D	77	-	-	X	-
2	M2G	F	26	-	-	X	-
2	PHA	F	77	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14547 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.

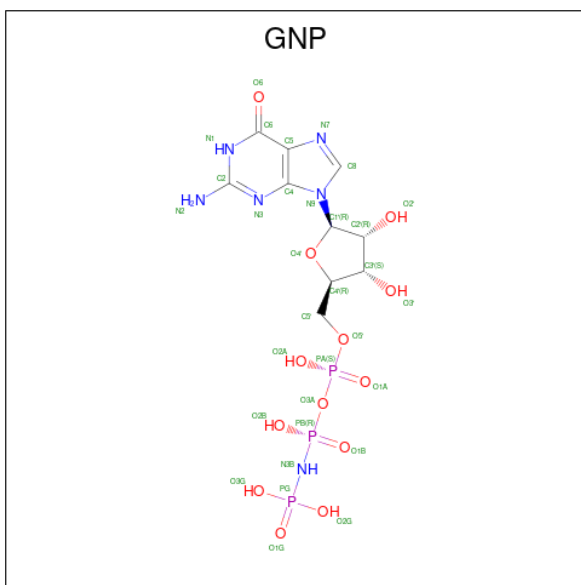
- Molecule 1 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3106	1961	542	591	12			
1	C	400	Total	C	N	O	S	0	0	0
			3106	1961	542	591	12			
1	E	400	Total	C	N	O	S	0	0	0
			3106	1961	542	591	12			

- Molecule 2 is a RNA chain called TRANSFER-RNA, PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	77	Total	C	N	O	P	0	0	0
			1663	755	295	537	76			
2	D	77	Total	C	N	O	P	0	0	0
			1663	755	295	537	76			
2	F	77	Total	C	N	O	P	0	0	0
			1663	755	295	537	76			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

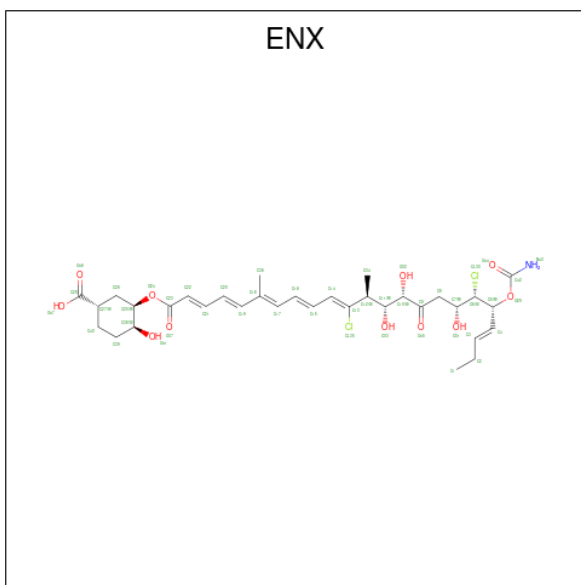


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	C	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	E	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

- Molecule 5 is ENACYLOXIN IIA (CCD ID: ENX) (formula: $\text{C}_{33}\text{H}_{45}\text{Cl}_2\text{NO}_{11}$).

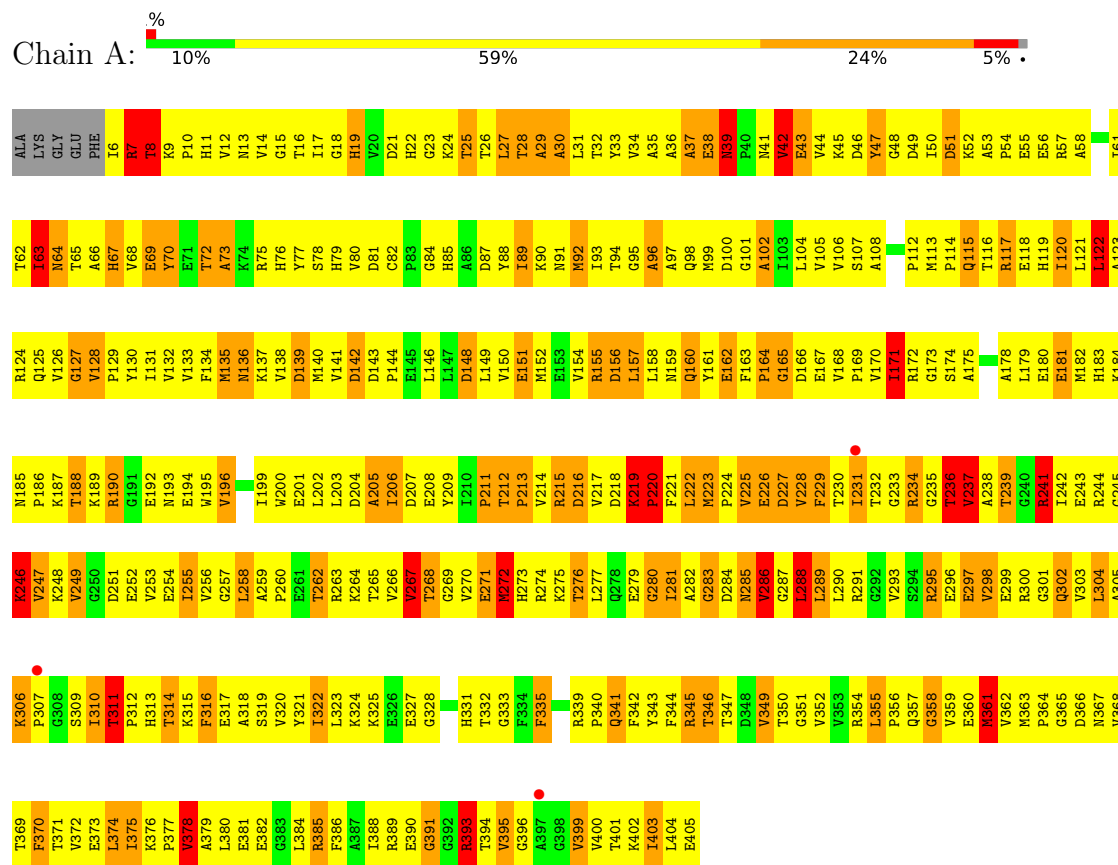


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 47	C 33	Cl 2	N 1	O 11	0	0
5	C	1	Total 47	C 33	Cl 2	N 1	O 11	0	0
5	E	1	Total 47	C 33	Cl 2	N 1	O 11	0	0

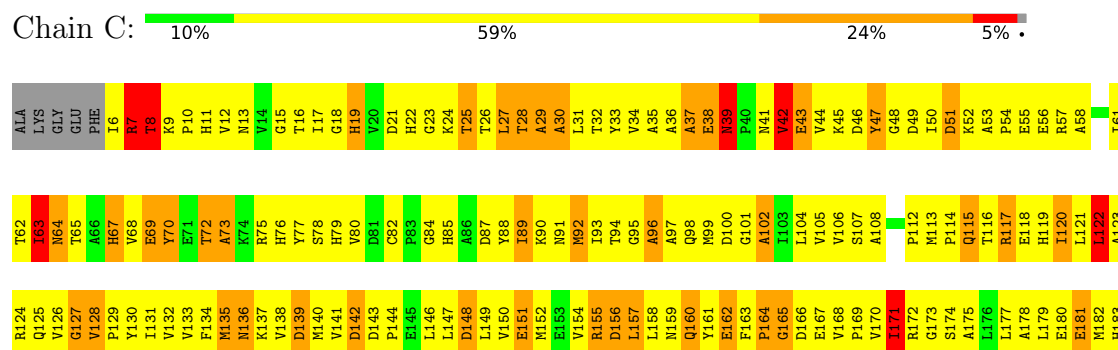
3 Residue-property plots

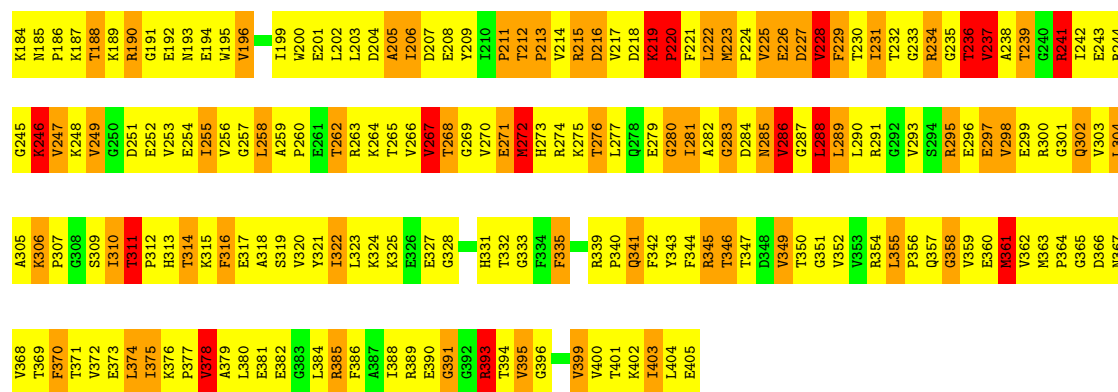
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ELONGATION FACTOR TU



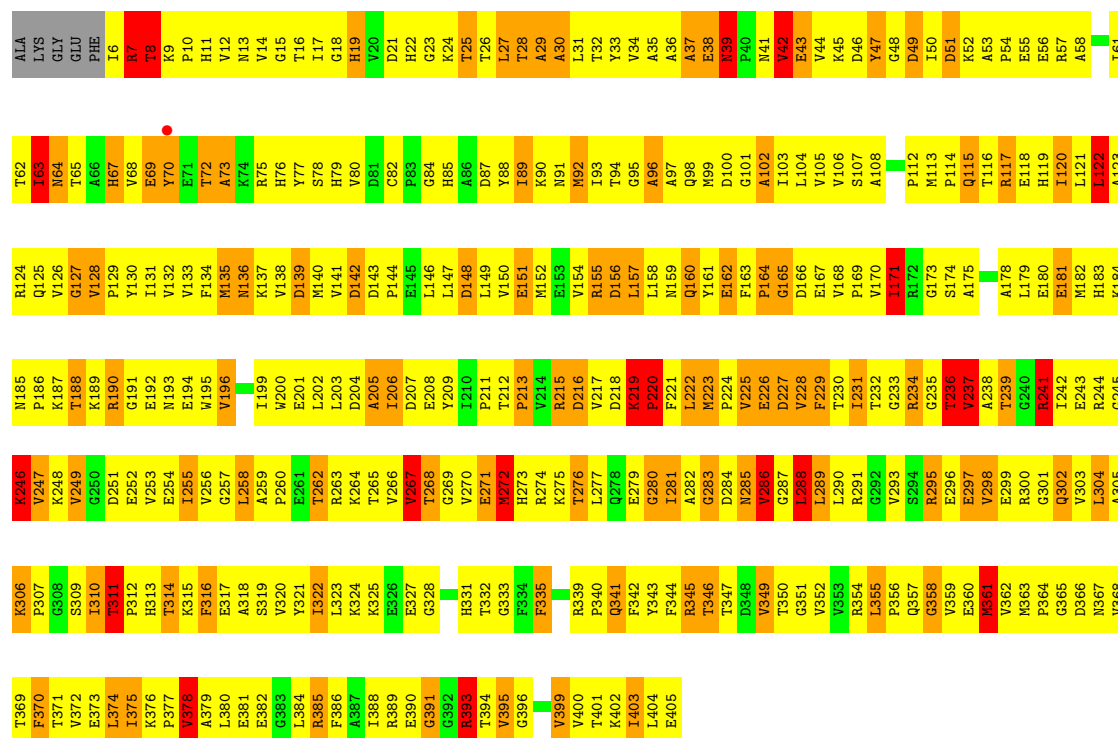
• Molecule 1: ELONGATION FACTOR TU





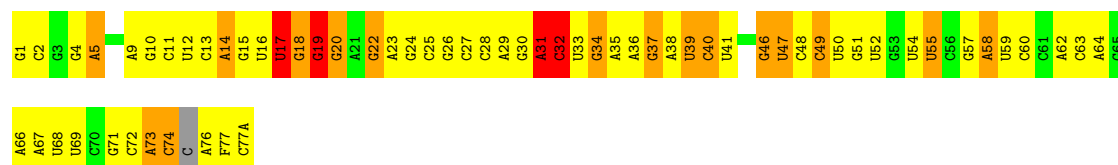
• Molecule 1: ELONGATION FACTOR TU

Chain E: 11% 59% 24% 5%



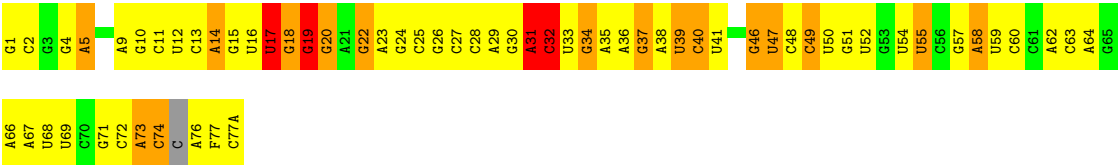
• Molecule 2: TRANSFER-RNA, PHE

Chain B: 18% 55% 21% 5%



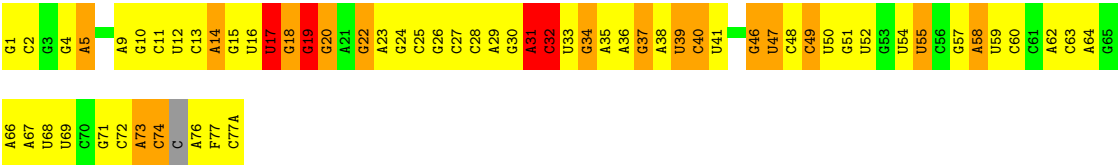
• Molecule 2: TRANSFER-RNA, PHE

Chain D: 18% 55% 21% 5% •



• Molecule 2: TRANSFER-RNA, PHE

Chain F: 18% 55% 21% 5% •



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.57Å 122.33Å 135.68Å 90.00° 121.30° 90.00°	Depositor
Resolution (Å)	29.54 – 3.10 29.54 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.54-3.10) 97.5 (29.54-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.280 , 0.294 0.260 , 0.280	Depositor DCC
R_{free} test set	1725 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 261.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.448 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.449 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14547	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHA, MG, 5MC, OMC, 2MG, GNP, YG, PSU, M2G, 5MU, 7MG, ENX, H2U, 1MA, OMC

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	0.72	1/3165 (0.0%)	1.32	46/4294 (1.1%)
1	C	0.72	1/3165 (0.0%)	1.32	46/4294 (1.1%)
1	E	0.72	1/3165 (0.0%)	1.32	46/4294 (1.1%)
2	B	0.58	0/1485	0.89	4/2307 (0.2%)
2	D	0.58	0/1485	0.89	4/2307 (0.2%)
2	F	0.58	0/1485	0.89	4/2307 (0.2%)
All	All	0.68	3/13950 (0.0%)	1.19	150/19803 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	4
2	D	0	4
2	F	0	4
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	MET	SD-CE	5.50	1.93	1.79
1	A	272	MET	SD-CE	5.46	1.93	1.79
1	E	272	MET	SD-CE	5.46	1.93	1.79

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	CA-C-N	10.06	132.42	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	C-N-CA	10.06	132.42	119.84
1	C	219	LYS	CA-C-N	10.05	132.40	119.84
1	C	219	LYS	C-N-CA	10.05	132.40	119.84
1	E	219	LYS	CA-C-N	10.04	132.39	119.84
1	E	219	LYS	C-N-CA	10.04	132.39	119.84
1	C	63	ILE	N-CA-C	-9.86	103.08	111.56
1	A	63	ILE	N-CA-C	-9.85	103.09	111.56
1	E	63	ILE	N-CA-C	-9.83	103.11	111.56
1	E	155	ARG	N-CA-C	-9.58	100.79	111.14
1	A	155	ARG	N-CA-C	-9.56	100.81	111.14
1	C	155	ARG	N-CA-C	-9.55	100.83	111.14
1	A	247	VAL	N-CA-C	9.08	122.50	107.24
1	C	247	VAL	N-CA-C	9.08	122.49	107.24
1	E	247	VAL	N-CA-C	9.07	122.48	107.24
1	C	151	GLU	N-CA-C	-8.82	103.10	114.04
1	A	151	GLU	N-CA-C	-8.82	103.10	114.04
1	E	151	GLU	N-CA-C	-8.81	103.11	114.04
1	A	205	ALA	N-CA-C	-8.36	103.67	114.04
1	C	205	ALA	N-CA-C	-8.36	103.67	114.04
1	E	205	ALA	N-CA-C	-8.35	103.69	114.04
1	A	378	VAL	N-CA-C	8.06	119.20	107.75
1	C	378	VAL	N-CA-C	8.05	119.18	107.75
1	E	378	VAL	N-CA-C	8.03	119.16	107.75
2	D	19	G	C2'-C3'-O3'	-7.85	101.92	113.70
2	F	19	G	C2'-C3'-O3'	-7.85	101.92	113.70
2	B	19	G	C2'-C3'-O3'	-7.85	101.92	113.70
1	A	304	LEU	N-CA-C	-7.47	98.83	109.96
1	E	304	LEU	N-CA-C	-7.45	98.86	109.96
1	C	304	LEU	N-CA-C	-7.45	98.86	109.96
1	C	43	GLU	N-CA-C	7.38	120.62	109.63
1	A	43	GLU	N-CA-C	7.37	120.61	109.63
1	E	43	GLU	N-CA-C	7.36	120.59	109.63
1	E	393	ARG	N-CA-C	7.36	119.23	108.86
1	A	148	ASP	N-CA-C	-7.35	102.87	111.03
1	C	393	ARG	N-CA-C	7.35	119.22	108.86
1	E	148	ASP	N-CA-C	-7.34	102.88	111.03
1	A	393	ARG	N-CA-C	7.33	119.20	108.86
1	C	148	ASP	N-CA-C	-7.33	102.89	111.03
1	A	73	ALA	N-CA-C	-6.97	100.96	111.34
1	E	73	ALA	N-CA-C	-6.96	100.97	111.34
1	C	73	ALA	N-CA-C	-6.93	101.01	111.34
1	A	288	LEU	N-CA-C	6.74	120.66	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	288	LEU	N-CA-C	6.73	120.65	109.95
1	C	288	LEU	N-CA-C	6.72	120.63	109.95
1	A	355	LEU	CA-C-N	6.71	126.69	119.78
1	A	355	LEU	C-N-CA	6.71	126.69	119.78
1	C	355	LEU	CA-C-N	6.69	126.67	119.78
1	C	355	LEU	C-N-CA	6.69	126.67	119.78
1	E	355	LEU	CA-C-N	6.68	126.66	119.78
1	E	355	LEU	C-N-CA	6.68	126.66	119.78
1	E	136	ASN	N-CA-C	6.64	120.22	110.59
1	A	136	ASN	N-CA-C	6.63	120.21	110.59
1	C	136	ASN	N-CA-C	6.63	120.20	110.59
1	E	180	GLU	N-CA-C	-6.51	105.33	113.28
1	C	180	GLU	N-CA-C	-6.50	105.34	113.28
1	A	180	GLU	N-CA-C	-6.49	105.36	113.28
1	E	295	ARG	N-CA-C	-6.45	104.33	111.36
1	C	295	ARG	N-CA-C	-6.44	104.34	111.36
1	A	295	ARG	N-CA-C	-6.43	104.35	111.36
1	C	120	ILE	N-CA-C	-6.43	103.54	110.23
1	A	120	ILE	N-CA-C	-6.42	103.56	110.23
1	C	237	VAL	N-CA-C	6.41	117.70	108.48
1	E	237	VAL	N-CA-C	6.40	117.70	108.48
1	A	237	VAL	N-CA-C	6.40	117.69	108.48
1	E	120	ILE	N-CA-C	-6.40	103.58	110.23
1	E	41	ASN	N-CA-C	-6.36	103.97	111.03
1	A	41	ASN	N-CA-C	-6.36	103.97	111.03
1	C	41	ASN	N-CA-C	-6.34	104.00	111.03
1	C	25	THR	N-CA-C	6.25	118.10	111.28
1	C	349	VAL	N-CA-C	6.25	117.13	108.12
1	E	25	THR	N-CA-C	6.25	118.10	111.28
1	E	349	VAL	N-CA-C	6.25	117.12	108.12
1	A	349	VAL	N-CA-C	6.25	117.11	108.12
1	A	212	THR	N-CA-C	6.24	115.49	108.25
1	C	212	THR	N-CA-C	6.23	115.48	108.25
1	E	212	THR	N-CA-C	6.23	115.48	108.25
1	A	25	THR	N-CA-C	6.23	118.07	111.28
1	C	227	ASP	N-CA-C	6.23	118.32	108.79
1	A	227	ASP	N-CA-C	6.21	118.30	108.79
1	C	29	ALA	N-CA-C	-6.21	104.51	111.28
1	A	29	ALA	N-CA-C	-6.21	104.51	111.28
1	E	227	ASP	N-CA-C	6.20	118.28	108.79
1	E	29	ALA	N-CA-C	-6.19	104.53	111.28
1	A	102	ALA	N-CA-C	6.05	118.27	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	102	ALA	N-CA-C	6.05	118.27	109.07
1	E	102	ALA	N-CA-C	6.03	118.23	109.07
1	C	361	MET	N-CA-C	6.02	117.28	107.23
1	A	361	MET	N-CA-C	6.00	117.26	107.23
1	A	252	GLU	N-CA-C	-5.99	101.17	110.10
1	E	252	GLU	N-CA-C	-5.99	101.17	110.10
1	E	361	MET	N-CA-C	5.98	117.22	107.23
1	C	252	GLU	N-CA-C	-5.98	101.19	110.10
2	F	22	G	N9-C1'-C2'	5.94	120.90	112.00
2	B	22	G	N9-C1'-C2'	5.93	120.90	112.00
2	D	22	G	N9-C1'-C2'	5.92	120.88	112.00
1	A	39	ASN	CA-C-N	5.83	125.93	119.87
1	A	39	ASN	C-N-CA	5.83	125.93	119.87
1	C	39	ASN	CA-C-N	5.82	125.92	119.87
1	C	39	ASN	C-N-CA	5.82	125.92	119.87
1	E	39	ASN	CA-C-N	5.80	125.90	119.87
1	E	39	ASN	C-N-CA	5.80	125.90	119.87
1	C	128	VAL	CA-C-N	5.72	126.99	119.84
1	C	128	VAL	C-N-CA	5.72	126.99	119.84
1	A	128	VAL	CA-C-N	5.71	126.97	119.84
1	A	128	VAL	C-N-CA	5.71	126.97	119.84
1	E	128	VAL	CA-C-N	5.71	126.97	119.84
1	E	128	VAL	C-N-CA	5.71	126.97	119.84
1	C	88	TYR	N-CA-C	5.70	119.83	112.41
1	A	88	TYR	N-CA-C	5.70	119.81	112.41
1	E	88	TYR	N-CA-C	5.68	119.80	112.41
1	A	228	VAL	N-CA-C	5.67	115.84	108.35
1	E	228	VAL	N-CA-C	5.67	115.84	108.35
1	C	228	VAL	N-CA-C	5.66	115.82	108.35
1	C	325	LYS	N-CA-C	-5.66	105.20	111.71
1	A	325	LYS	N-CA-C	-5.64	105.22	111.71
1	E	325	LYS	N-CA-C	-5.61	105.26	111.71
1	C	188	THR	N-CA-C	-5.57	102.03	110.28
1	A	188	THR	N-CA-C	-5.57	102.04	110.28
1	E	196	VAL	N-CA-C	-5.56	106.02	112.98
1	E	188	THR	N-CA-C	-5.56	102.06	110.28
1	E	15	GLY	N-CA-C	5.55	118.69	110.63
1	A	196	VAL	N-CA-C	-5.55	106.04	112.98
1	C	196	VAL	N-CA-C	-5.54	106.05	112.98
1	A	15	GLY	N-CA-C	5.54	118.66	110.63
1	C	15	GLY	N-CA-C	5.53	118.65	110.63
2	D	47	U	N1-C1'-C2'	5.52	120.28	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	47	U	N1-C1'-C2'	5.52	120.28	112.00
2	B	47	U	N1-C1'-C2'	5.51	120.26	112.00
1	E	127	GLY	N-CA-C	5.45	122.79	115.59
1	A	220	PRO	N-CA-C	5.44	123.67	112.47
1	C	127	GLY	N-CA-C	5.43	122.76	115.59
1	A	127	GLY	N-CA-C	5.43	122.75	115.59
1	C	220	PRO	N-CA-C	5.43	123.65	112.47
1	E	220	PRO	N-CA-C	5.42	123.64	112.47
1	A	311	THR	N-CA-C	5.36	121.66	109.81
1	C	311	THR	N-CA-C	5.36	121.65	109.81
1	E	311	THR	N-CA-C	5.36	121.64	109.81
1	E	122	LEU	N-CA-C	-5.26	105.45	111.07
1	C	122	LEU	N-CA-C	-5.25	105.45	111.07
1	A	122	LEU	N-CA-C	-5.25	105.46	111.07
2	F	47	U	C4'-C3'-O3'	-5.21	105.19	113.00
2	B	47	U	C4'-C3'-O3'	-5.19	105.21	113.00
2	D	47	U	C4'-C3'-O3'	-5.17	105.24	113.00
1	E	388	ILE	N-CA-C	5.13	115.50	108.12
1	A	388	ILE	N-CA-C	5.12	115.50	108.12
1	C	314	THR	N-CA-C	-5.12	107.10	113.55
1	A	314	THR	N-CA-C	-5.11	107.11	113.55
1	E	314	THR	N-CA-C	-5.09	107.13	113.55
1	C	388	ILE	N-CA-C	5.09	115.45	108.12

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	31	A	Sidechain
2	B	38	A	Sidechain
2	B	51	G	Sidechain
2	B	52	U	Sidechain
2	D	31	A	Sidechain
2	D	38	A	Sidechain
2	D	51	G	Sidechain
2	D	52	U	Sidechain
2	F	31	A	Sidechain
2	F	38	A	Sidechain
2	F	51	G	Sidechain
2	F	52	U	Sidechain

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	3106	0	3122	769	2
1	C	3106	0	3122	760	2
1	E	3106	0	3122	765	2
2	B	1663	0	869	132	0
2	D	1663	0	869	137	0
2	F	1663	0	869	139	0
3	A	32	0	13	7	0
3	C	32	0	13	7	0
3	E	32	0	13	8	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	47	0	45	5	0
5	C	47	0	45	5	0
5	E	47	0	45	5	0
All	All	14547	0	12147	2570	3

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 96.

All (2570) 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:A:368:VAL:HG22	1:A:369:THR:H	1.03	1.19
1:A:221:PHE:HB3	1:A:306:LYS:H	1.08	1.19
1:A:234:ARG:HB2	1:A:234:ARG:HH11	1.04	1.16
1:C:75:ARG:HH21	1:C:207:ASP:HA	1.04	1.15
1:C:234:ARG:HH11	1:C:234:ARG:HB2	1.04	1.14
1:A:263:ARG:HD3	1:A:293:VAL:HG12	1.26	1.14
2:F:13:C:H2'	2:F:14:A:H5''	1.23	1.14
1:A:75:ARG:HH21	1:A:207:ASP:HA	1.04	1.14
1:E:368:VAL:HG22	1:E:369:THR:H	1.03	1.13
1:C:313:HIS:HB2	1:C:380:LEU:HD23	1.31	1.13
1:C:368:VAL:HG22	1:C:369:THR:H	1.03	1.12
1:E:221:PHE:HB3	1:E:306:LYS:H	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:GLY:O	1:E:346:THR:HG21	1.50	1.11
1:A:301:GLY:O	1:A:346:THR:HG21	1.50	1.11
1:A:99:MET:HE1	1:A:102:ALA:HB2	1.13	1.11
1:C:221:PHE:HB3	1:C:306:LYS:H	1.08	1.11
1:C:99:MET:HE1	1:C:102:ALA:HB2	1.13	1.11
1:C:263:ARG:HD3	1:C:293:VAL:HG12	1.26	1.10
1:C:301:GLY:O	1:C:346:THR:HG21	1.50	1.10
2:D:13:C:H2'	2:D:14:A:H5''	1.23	1.10
1:E:75:ARG:HH21	1:E:207:ASP:HA	1.04	1.10
2:B:13:C:H2'	2:B:14:A:H5''	1.23	1.09
1:E:234:ARG:HB2	1:E:234:ARG:HH11	1.04	1.09
1:C:222:LEU:CD1	1:C:244:ARG:H	1.66	1.09
1:A:171:ILE:HD12	1:A:171:ILE:H	1.17	1.08
1:E:171:ILE:H	1:E:171:ILE:HD12	1.16	1.08
1:E:36:ALA:HA	1:E:42:VAL:HB	1.36	1.08
1:A:222:LEU:CD1	1:A:244:ARG:H	1.66	1.07
1:E:222:LEU:CD1	1:E:244:ARG:H	1.66	1.07
1:E:263:ARG:HD3	1:E:293:VAL:HG12	1.27	1.07
1:E:313:HIS:HB2	1:E:380:LEU:HD23	1.31	1.07
1:A:247:VAL:HG11	1:A:288:LEU:HD22	1.37	1.06
1:E:247:VAL:HG11	1:E:288:LEU:HD22	1.37	1.06
1:A:313:HIS:HB2	1:A:380:LEU:HD23	1.31	1.06
1:E:99:MET:HE1	1:E:102:ALA:HB2	1.13	1.06
1:A:36:ALA:HA	1:A:42:VAL:HB	1.36	1.05
1:C:171:ILE:H	1:C:171:ILE:HD12	1.17	1.05
1:A:52:LYS:NZ	2:B:74:C:H4'	1.72	1.04
1:E:52:LYS:NZ	2:F:74:C:H4'	1.72	1.04
1:C:36:ALA:HA	1:C:42:VAL:HB	1.37	1.04
1:E:339:ARG:HD2	1:E:352:VAL:HG22	1.39	1.04
1:A:52:LYS:HD2	2:B:74:C:H5'	1.39	1.04
1:A:339:ARG:HD2	1:A:352:VAL:HG22	1.39	1.04
1:C:339:ARG:HD2	1:C:352:VAL:HG22	1.39	1.04
1:E:52:LYS:HD2	2:F:74:C:H5'	1.39	1.03
1:C:52:LYS:NZ	2:D:74:C:H4'	1.72	1.03
1:A:149:LEU:HA	1:A:152:MET:HE3	1.41	1.03
1:E:149:LEU:HA	1:E:152:MET:HE3	1.41	1.02
1:A:354:ARG:HB3	1:A:354:ARG:HH11	1.25	1.02
2:D:10:2MG:HM22	2:D:25:C:O2	1.60	1.01
1:C:247:VAL:HG11	1:C:288:LEU:HD22	1.37	1.01
1:C:354:ARG:HB3	1:C:354:ARG:HH11	1.25	1.01
2:B:10:2MG:HM22	2:B:25:C:O2	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:2MG:HM23	2:D:26:M2G:H1'	1.01	1.00
1:A:266:VAL:O	1:A:290:LEU:HA	1.62	1.00
1:E:222:LEU:HD11	1:E:244:ARG:H	1.25	1.00
2:B:10:2MG:HM23	2:B:26:M2G:H1'	1.01	1.00
2:F:10:2MG:HM22	2:F:25:C:O2	1.60	1.00
1:C:52:LYS:HD2	2:D:74:C:H5'	1.39	0.99
1:C:266:VAL:O	1:C:290:LEU:HA	1.62	0.99
1:A:246:LYS:HG2	1:A:281:ILE:HA	1.44	0.99
1:C:149:LEU:HA	1:C:152:MET:HE3	1.41	0.99
1:C:234:ARG:HD3	1:C:234:ARG:N	1.78	0.98
2:F:10:2MG:HM23	2:F:26:M2G:H1'	1.01	0.98
1:A:222:LEU:HD11	1:A:244:ARG:H	1.25	0.98
1:C:246:LYS:HG2	1:C:281:ILE:HA	1.44	0.98
1:E:124:ARG:HG3	1:E:161:TYR:HB3	1.46	0.98
1:E:266:VAL:O	1:E:290:LEU:HA	1.62	0.98
2:F:11:C:H2'	2:F:12:U:H6	1.27	0.98
1:E:246:LYS:HG2	1:E:281:ILE:HA	1.44	0.97
1:A:346:THR:HG23	1:A:347:THR:H	1.29	0.97
1:C:241:ARG:HD3	1:C:283:GLY:HA2	1.44	0.97
1:C:124:ARG:HG3	1:C:161:TYR:HB3	1.46	0.97
2:D:4:G:H2'	2:D:5:A:H5''	1.44	0.97
1:A:402:LYS:HG2	1:A:403:ILE:H	1.27	0.97
1:E:234:ARG:HD3	1:E:234:ARG:N	1.78	0.97
1:C:222:LEU:HD11	1:C:244:ARG:H	1.25	0.96
1:A:241:ARG:HD3	1:A:283:GLY:HA2	1.44	0.96
1:C:402:LYS:HG2	1:C:403:ILE:H	1.27	0.96
1:E:241:ARG:HD3	1:E:283:GLY:HA2	1.44	0.96
1:E:354:ARG:HB3	1:E:354:ARG:HH11	1.25	0.96
2:B:31:A:H5'	2:B:31:A:H8	1.28	0.96
1:A:124:ARG:HG3	1:A:161:TYR:HB3	1.46	0.96
1:C:215:ARG:HG3	1:C:282:ALA:HB1	1.48	0.96
1:C:346:THR:HG23	1:C:347:THR:H	1.29	0.95
2:F:4:G:H2'	2:F:5:A:H5''	1.45	0.95
2:B:4:G:H2'	2:B:5:A:H5''	1.45	0.95
1:E:158:LEU:O	1:E:163:PHE:HB2	1.67	0.95
1:A:234:ARG:HD3	1:A:234:ARG:N	1.78	0.95
2:B:11:C:H2'	2:B:12:U:H6	1.27	0.95
1:A:75:ARG:NH2	1:A:207:ASP:HA	1.82	0.95
1:E:402:LYS:HG2	1:E:403:ILE:H	1.27	0.95
2:D:31:A:H5'	2:D:31:A:H8	1.28	0.95
1:C:354:ARG:HB3	1:C:354:ARG:NH1	1.82	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LEU:O	1:C:163:PHE:HB2	1.67	0.94
1:A:158:LEU:O	1:A:163:PHE:HB2	1.67	0.94
1:A:215:ARG:HG3	1:A:282:ALA:HB1	1.48	0.94
1:A:222:LEU:O	1:A:222:LEU:HD13	1.68	0.94
1:E:7:ARG:NH2	1:E:277:LEU:HD21	1.83	0.94
1:E:346:THR:HG23	1:E:347:THR:H	1.29	0.94
2:D:11:C:H2'	2:D:12:U:H6	1.27	0.94
2:D:13:C:C2'	2:D:14:A:H5''	1.98	0.94
1:C:247:VAL:HG21	1:C:267:VAL:HG11	1.48	0.94
1:E:75:ARG:NH2	1:E:207:ASP:HA	1.82	0.94
2:B:13:C:C2'	2:B:14:A:H5''	1.98	0.94
1:C:75:ARG:NH2	1:C:207:ASP:HA	1.82	0.94
1:E:222:LEU:O	1:E:222:LEU:HD13	1.68	0.94
1:C:341:GLN:HA	1:C:350:THR:HA	1.49	0.94
1:E:215:ARG:HG3	1:E:282:ALA:HB1	1.49	0.93
1:C:350:THR:HB	1:C:375:ILE:HD13	1.49	0.93
2:F:13:C:C2'	2:F:14:A:H5''	1.98	0.93
2:F:31:A:H5'	2:F:31:A:H8	1.28	0.93
1:A:7:ARG:NH2	1:A:277:LEU:HD21	1.83	0.93
1:C:222:LEU:O	1:C:222:LEU:HD13	1.68	0.93
1:C:289:LEU:HD23	1:C:290:LEU:H	1.31	0.93
1:A:289:LEU:HD23	1:A:290:LEU:H	1.31	0.93
1:C:7:ARG:NH2	1:C:277:LEU:HD21	1.83	0.93
1:A:354:ARG:HB3	1:A:354:ARG:NH1	1.82	0.93
1:E:354:ARG:HB3	1:E:354:ARG:NH1	1.82	0.93
1:A:247:VAL:HG21	1:A:267:VAL:HG11	1.48	0.93
1:E:341:GLN:HA	1:E:350:THR:HA	1.49	0.93
1:E:247:VAL:HG21	1:E:267:VAL:HG11	1.48	0.92
1:A:350:THR:HB	1:A:375:ILE:HD13	1.49	0.92
1:E:350:THR:HB	1:E:375:ILE:HD13	1.49	0.92
1:E:289:LEU:HD23	1:E:290:LEU:H	1.31	0.92
1:E:267:VAL:HA	1:E:290:LEU:HD23	1.52	0.92
1:A:267:VAL:HA	1:A:290:LEU:HD23	1.52	0.92
1:E:234:ARG:HH11	1:E:234:ARG:CB	1.82	0.92
1:E:389:ARG:HG2	1:E:394:THR:HA	1.53	0.91
1:A:356:PRO:HD2	1:A:359:VAL:HG22	1.53	0.91
1:A:43:GLU:HG2	1:A:44:VAL:H	1.35	0.91
1:A:389:ARG:HG2	1:A:394:THR:HA	1.53	0.91
1:C:389:ARG:HG2	1:C:394:THR:HA	1.53	0.91
1:E:43:GLU:HG2	1:E:44:VAL:H	1.35	0.91
1:C:267:VAL:HA	1:C:290:LEU:HD23	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:MET:C	1:C:92:MET:HE2	1.96	0.90
1:C:234:ARG:HH11	1:C:234:ARG:CB	1.82	0.90
1:A:234:ARG:HH11	1:A:234:ARG:CB	1.82	0.90
1:E:368:VAL:HG22	1:E:369:THR:N	1.86	0.90
1:A:341:GLN:HA	1:A:350:THR:HA	1.49	0.90
1:C:391:GLY:HA2	2:D:64:A:C4'	2.02	0.90
1:E:356:PRO:HD2	1:E:359:VAL:HG22	1.53	0.90
1:A:343:TYR:CE1	1:A:389:ARG:HB2	2.07	0.90
1:E:343:TYR:CE1	1:E:389:ARG:HB2	2.07	0.90
1:C:343:TYR:CE1	1:C:389:ARG:HB2	2.07	0.90
1:A:215:ARG:NH1	1:A:283:GLY:HA3	1.87	0.89
1:E:391:GLY:HA2	2:F:64:A:C4'	2.02	0.89
2:D:10:2MG:HM23	2:D:26:M2G:C1'	1.97	0.89
1:A:391:GLY:HA2	2:B:64:A:C4'	2.02	0.89
1:A:393:ARG:HH21	1:A:393:ARG:HB3	1.37	0.89
1:E:215:ARG:NH1	1:E:283:GLY:HA3	1.87	0.89
1:C:356:PRO:HD2	1:C:359:VAL:HG22	1.53	0.89
1:E:92:MET:C	1:E:92:MET:HE2	1.96	0.89
2:D:10:2MG:CM2	2:D:26:M2G:H1'	1.97	0.89
1:A:92:MET:HE2	1:A:92:MET:C	1.96	0.89
1:C:43:GLU:HG2	1:C:44:VAL:H	1.35	0.89
1:E:286:VAL:HG23	1:E:287:GLY:H	1.37	0.88
1:C:393:ARG:HH21	1:C:393:ARG:HB3	1.37	0.88
1:A:368:VAL:HG22	1:A:369:THR:N	1.86	0.88
2:B:10:2MG:HM23	2:B:26:M2G:C1'	1.97	0.88
1:C:215:ARG:NH1	1:C:283:GLY:HA3	1.87	0.88
1:A:227:ASP:HB3	1:A:239:THR:HG23	1.56	0.88
1:E:393:ARG:HB3	1:E:393:ARG:HH21	1.37	0.88
1:A:368:VAL:CG2	1:A:369:THR:H	1.87	0.88
1:E:227:ASP:HB3	1:E:239:THR:HG23	1.56	0.88
1:A:286:VAL:HG23	1:A:287:GLY:H	1.37	0.87
1:C:234:ARG:HB2	1:C:234:ARG:NH1	1.89	0.87
1:C:286:VAL:HG23	1:C:287:GLY:H	1.37	0.87
1:C:274:ARG:NH1	2:D:76:A:H5'	1.90	0.87
1:C:227:ASP:HB3	1:C:239:THR:HG23	1.56	0.87
1:E:258:LEU:HD21	1:E:347:THR:HG21	1.56	0.87
1:E:274:ARG:NH1	2:F:76:A:H5'	1.90	0.87
2:B:10:2MG:CM2	2:B:26:M2G:H1'	1.98	0.87
1:E:52:LYS:HD2	2:F:74:C:C5'	2.05	0.87
1:A:52:LYS:HD2	2:B:74:C:C5'	2.05	0.87
1:A:234:ARG:HB2	1:A:234:ARG:NH1	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:MET:HE3	1:C:304:LEU:HD12	1.57	0.87
1:E:234:ARG:HB2	1:E:234:ARG:NH1	1.89	0.87
1:E:241:ARG:HD2	1:E:241:ARG:O	1.75	0.87
1:A:221:PHE:HB3	1:A:306:LYS:N	1.90	0.86
1:A:258:LEU:HD11	1:A:301:GLY:HA3	1.55	0.86
1:A:274:ARG:NH1	2:B:76:A:H5'	1.89	0.86
1:C:258:LEU:HD11	1:C:301:GLY:HA3	1.55	0.86
1:A:184:LYS:O	1:A:186:PRO:HD3	1.75	0.86
1:C:368:VAL:HG22	1:C:369:THR:N	1.86	0.86
1:A:24:LYS:HA	1:A:105:VAL:HG21	1.58	0.86
1:C:391:GLY:HA2	2:D:64:A:H4'	1.55	0.86
1:E:241:ARG:HD2	1:E:241:ARG:C	2.01	0.86
1:A:223:MET:HE3	1:A:304:LEU:HD12	1.57	0.86
1:C:258:LEU:HD21	1:C:347:THR:HG21	1.56	0.86
1:E:24:LYS:HA	1:E:105:VAL:HG21	1.58	0.86
1:E:258:LEU:HD11	1:E:301:GLY:HA3	1.55	0.86
2:D:27:C:H2'	2:D:28:C:C6	2.11	0.85
1:E:391:GLY:HA2	2:F:64:A:H4'	1.55	0.85
2:B:27:C:H2'	2:B:28:C:C6	2.11	0.85
1:C:286:VAL:HG23	1:C:287:GLY:N	1.90	0.85
1:E:221:PHE:HB3	1:E:306:LYS:N	1.90	0.85
1:A:241:ARG:HD2	1:A:241:ARG:C	2.01	0.85
2:F:27:C:H2'	2:F:28:C:C6	2.11	0.85
1:C:241:ARG:HD2	1:C:241:ARG:C	2.01	0.85
1:C:52:LYS:HD2	2:D:74:C:C5'	2.05	0.85
1:C:221:PHE:HB3	1:C:306:LYS:N	1.90	0.85
1:E:184:LYS:O	1:E:186:PRO:HD3	1.75	0.85
1:A:258:LEU:HD21	1:A:347:THR:HG21	1.56	0.85
1:E:36:ALA:HA	1:E:42:VAL:CB	2.06	0.85
1:E:223:MET:HE3	1:E:304:LEU:HD12	1.57	0.85
2:F:10:2MG:CM2	2:F:26:M2G:H1'	1.98	0.85
1:A:36:ALA:HA	1:A:42:VAL:CB	2.06	0.85
1:A:241:ARG:HD2	1:A:241:ARG:O	1.75	0.85
1:A:391:GLY:HA2	2:B:64:A:H4'	1.55	0.85
1:C:34:VAL:HG11	1:C:199:ILE:HG21	1.58	0.85
1:C:241:ARG:HD2	1:C:241:ARG:O	1.75	0.85
1:C:24:LYS:HA	1:C:105:VAL:HG21	1.58	0.85
1:E:350:THR:O	1:E:375:ILE:HG12	1.77	0.84
1:A:34:VAL:HG11	1:A:199:ILE:HG21	1.58	0.84
1:A:286:VAL:HG23	1:A:287:GLY:N	1.90	0.84
1:E:286:VAL:HG23	1:E:287:GLY:N	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LEU:HD12	1:A:396:GLY:HA2	1.60	0.84
1:E:108:ALA:HB2	1:E:135:MET:HG2	1.60	0.84
1:C:184:LYS:O	1:C:186:PRO:HD3	1.75	0.84
1:E:121:LEU:HB2	1:E:161:TYR:CE1	2.13	0.84
1:C:34:VAL:HG11	1:C:199:ILE:CG2	2.08	0.84
1:C:36:ALA:HA	1:C:42:VAL:CB	2.06	0.84
1:C:323:LEU:HD12	1:C:396:GLY:HA2	1.59	0.84
1:E:34:VAL:HG11	1:E:199:ILE:HG21	1.58	0.84
1:A:108:ALA:HB2	1:A:135:MET:HG2	1.60	0.84
1:C:108:ALA:HB2	1:C:135:MET:HG2	1.59	0.84
1:C:350:THR:O	1:C:375:ILE:HG12	1.77	0.84
1:C:315:LYS:O	1:C:316:PHE:HB3	1.78	0.84
1:E:323:LEU:HD12	1:E:396:GLY:HA2	1.59	0.84
1:E:271:GLU:H	2:F:76:A:H2	1.25	0.84
1:A:271:GLU:H	2:B:76:A:H2	1.25	0.84
1:A:121:LEU:HB2	1:A:161:TYR:CE1	2.12	0.83
1:A:350:THR:O	1:A:375:ILE:HG12	1.77	0.83
1:C:121:LEU:HB2	1:C:161:TYR:CE1	2.12	0.83
1:A:21:ASP:H	3:A:1406:GNP:HNB3	1.24	0.83
1:E:34:VAL:HG11	1:E:199:ILE:CG2	2.08	0.83
1:E:315:LYS:O	1:E:316:PHE:HB3	1.78	0.83
1:A:34:VAL:HG11	1:A:199:ILE:CG2	2.08	0.83
1:A:315:LYS:O	1:A:316:PHE:HB3	1.78	0.82
1:E:21:ASP:H	3:E:1406:GNP:HNB3	1.24	0.82
2:D:11:C:H2'	2:D:12:U:C6	2.14	0.82
1:C:113:MET:HB3	1:C:114:PRO:HD2	1.62	0.82
1:E:254:GLU:HB3	1:E:262:THR:HG22	1.61	0.82
2:B:11:C:H2'	2:B:12:U:C6	2.14	0.82
2:F:11:C:H2'	2:F:12:U:C6	2.14	0.82
1:A:254:GLU:HB3	1:A:262:THR:HG22	1.61	0.82
1:A:184:LYS:HE2	1:A:184:LYS:HA	1.62	0.81
1:A:378:VAL:HG12	1:A:380:LEU:CD2	2.10	0.81
1:E:171:ILE:HD12	1:E:171:ILE:N	1.96	0.81
1:A:113:MET:HB3	1:A:114:PRO:HD2	1.62	0.81
1:C:21:ASP:H	3:C:1406:GNP:HNB3	1.24	0.81
1:C:343:TYR:HE1	1:C:389:ARG:HB2	1.45	0.81
1:C:247:VAL:CG2	1:C:267:VAL:HG11	2.10	0.81
1:C:378:VAL:HG12	1:C:380:LEU:CD2	2.10	0.81
1:E:343:TYR:HE1	1:E:389:ARG:HB2	1.45	0.81
2:F:10:2MG:HM23	2:F:26:M2G:C1'	1.98	0.81
1:C:271:GLU:H	2:D:76:A:H2	1.25	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:ASP:C	1:E:219:LYS:HD2	2.06	0.81
1:A:270:VAL:O	1:A:270:VAL:HG12	1.81	0.81
1:E:368:VAL:CG2	1:E:369:THR:H	1.87	0.81
1:C:249:VAL:HG22	1:C:270:VAL:HB	1.62	0.80
1:A:274:ARG:CZ	2:B:76:A:H5'	2.11	0.80
1:C:63:ILE:HG12	1:C:64:ASN:N	1.96	0.80
1:E:113:MET:HB3	1:E:114:PRO:HD2	1.62	0.80
1:A:223:MET:CE	1:A:304:LEU:HD12	2.11	0.80
1:A:249:VAL:HG22	1:A:270:VAL:HB	1.62	0.80
1:E:249:VAL:HG22	1:E:270:VAL:HB	1.62	0.80
1:E:274:ARG:CZ	2:F:76:A:H5'	2.11	0.80
1:A:67:HIS:CD2	2:B:77:PHA:HZ	2.17	0.80
1:C:12:VAL:HG21	1:C:75:ARG:HD2	1.63	0.80
1:C:171:ILE:HD12	1:C:171:ILE:N	1.96	0.80
1:E:378:VAL:HG12	1:E:380:LEU:CD2	2.10	0.80
1:E:52:LYS:HZ2	2:F:74:C:H4'	1.44	0.80
1:E:247:VAL:CG2	1:E:267:VAL:HG11	2.11	0.80
1:C:223:MET:CE	1:C:304:LEU:HD12	2.11	0.80
1:A:63:ILE:HG12	1:A:64:ASN:N	1.96	0.80
1:A:247:VAL:CG2	1:A:267:VAL:HG11	2.11	0.80
1:C:221:PHE:CB	1:C:306:LYS:H	1.93	0.80
1:C:368:VAL:CG2	1:C:369:THR:H	1.87	0.80
1:C:52:LYS:HZ2	2:D:74:C:H4'	1.47	0.80
1:C:56:GLU:HG2	1:C:63:ILE:HG23	1.63	0.80
1:C:218:ASP:C	1:C:219:LYS:HD2	2.06	0.80
2:F:15:G:H2'	2:F:16:H2U:H62	1.64	0.80
2:B:15:G:H2'	2:B:16:H2U:H62	1.64	0.79
2:B:31:A:H5'	2:B:31:A:C8	2.15	0.79
1:E:184:LYS:HE2	1:E:184:LYS:HA	1.61	0.79
1:A:12:VAL:HG21	1:A:75:ARG:HD2	1.63	0.79
1:A:56:GLU:HG2	1:A:63:ILE:HG23	1.63	0.79
1:A:218:ASP:C	1:A:219:LYS:HD2	2.06	0.79
1:C:315:LYS:HD3	1:C:405:GLU:HB3	1.64	0.79
1:E:231:ILE:HG21	2:F:76:A:H8	1.48	0.79
1:C:92:MET:HE2	1:C:92:MET:O	1.83	0.79
1:C:254:GLU:HB3	1:C:262:THR:HG22	1.61	0.79
2:D:4:G:C2'	2:D:5:A:H5''	2.12	0.79
1:E:270:VAL:O	1:E:270:VAL:HG12	1.81	0.79
2:F:74:C:H3'	2:F:77(A):C:C6	2.18	0.79
1:A:231:ILE:HG21	2:B:76:A:H8	1.48	0.79
1:A:316:PHE:HD1	1:A:317:GLU:O	1.66	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ARG:CZ	2:D:76:A:H5'	2.11	0.79
1:E:12:VAL:HG21	1:E:75:ARG:HD2	1.63	0.79
1:E:67:HIS:CD2	2:F:77:PHA:HZ	2.17	0.79
2:F:31:A:H5'	2:F:31:A:C8	2.15	0.79
1:C:67:HIS:CD2	2:D:77:PHA:HZ	2.17	0.79
2:D:31:A:H5'	2:D:31:A:C8	2.16	0.79
1:E:92:MET:HE2	1:E:92:MET:O	1.83	0.79
1:E:316:PHE:HD1	1:E:317:GLU:O	1.66	0.79
1:C:184:LYS:HA	1:C:184:LYS:HE2	1.62	0.79
1:C:270:VAL:O	1:C:270:VAL:HG12	1.81	0.79
1:E:223:MET:CE	1:E:304:LEU:HD12	2.11	0.79
1:A:343:TYR:HE1	1:A:389:ARG:HB2	1.45	0.79
1:C:235:GLY:O	1:C:236:THR:HG23	1.83	0.79
2:D:25:C:H2'	2:D:26:M2G:O4'	1.83	0.79
1:E:63:ILE:HG12	1:E:64:ASN:N	1.96	0.79
1:A:52:LYS:HZ2	2:B:74:C:H4'	1.47	0.79
1:E:69:GLU:O	1:E:70:TYR:HB3	1.83	0.79
1:E:235:GLY:O	1:E:236:THR:HG23	1.83	0.79
1:A:92:MET:HE2	1:A:92:MET:O	1.83	0.78
1:C:316:PHE:HD1	1:C:317:GLU:O	1.66	0.78
1:C:324:LYS:HG2	1:C:365:GLY:HA2	1.66	0.78
1:A:171:ILE:HD12	1:A:171:ILE:N	1.96	0.78
1:A:221:PHE:CB	1:A:306:LYS:H	1.93	0.78
1:A:315:LYS:HD3	1:A:405:GLU:HB3	1.64	0.78
1:C:231:ILE:HG21	2:D:76:A:H8	1.48	0.78
2:F:4:G:C2'	2:F:5:A:H5''	2.12	0.78
2:F:25:C:H2'	2:F:26:M2G:O4'	1.83	0.78
2:D:15:G:H2'	2:D:16:H2U:H62	1.64	0.78
1:A:33:TYR:HB3	1:A:182:MET:HB3	1.66	0.78
2:B:25:C:H2'	2:B:26:M2G:O4'	1.83	0.78
2:B:74:C:H3'	2:B:77(A):C:C6	2.18	0.78
1:C:215:ARG:CG	1:C:282:ALA:HB1	2.14	0.78
1:A:378:VAL:HG12	1:A:380:LEU:HD22	1.65	0.78
2:D:74:C:H3'	2:D:77(A):C:C6	2.18	0.78
1:E:324:LYS:HG2	1:E:365:GLY:HA2	1.66	0.78
1:E:378:VAL:HG12	1:E:380:LEU:HD22	1.65	0.78
1:A:36:ALA:C	1:A:38:GLU:H	1.92	0.78
1:A:215:ARG:CG	1:A:282:ALA:HB1	2.14	0.78
1:A:324:LYS:HG2	1:A:365:GLY:HA2	1.66	0.78
1:A:18:GLY:H	1:A:24:LYS:HD3	1.49	0.77
1:E:18:GLY:H	1:E:24:LYS:HD3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ASP:O	1:E:57:ARG:HG3	1.84	0.77
1:E:315:LYS:HD3	1:E:405:GLU:HB3	1.64	0.77
1:A:69:GLU:O	1:A:70:TYR:HB3	1.83	0.77
1:E:56:GLU:HG2	1:E:63:ILE:HG23	1.63	0.77
1:A:46:ASP:O	1:A:49:ASP:HB2	1.84	0.77
2:B:4:G:C2'	2:B:5:A:H5''	2.13	0.77
1:C:33:TYR:HB3	1:C:182:MET:HB3	1.66	0.77
1:C:18:GLY:H	1:C:24:LYS:HD3	1.49	0.77
1:E:36:ALA:C	1:E:38:GLU:H	1.92	0.77
1:A:51:ASP:O	1:A:57:ARG:HG3	1.84	0.77
1:A:157:LEU:HA	1:A:160:GLN:NE2	2.00	0.77
1:E:157:LEU:HA	1:E:160:GLN:NE2	2.00	0.77
1:A:63:ILE:HD12	2:B:2:C:H4'	1.66	0.77
1:A:235:GLY:O	1:A:236:THR:HG23	1.83	0.77
1:A:316:PHE:HE1	1:A:318:ALA:HB2	1.50	0.77
1:C:171:ILE:H	1:C:171:ILE:CD1	1.95	0.77
1:E:33:TYR:HB3	1:E:182:MET:HB3	1.66	0.77
2:B:27:C:H2'	2:B:28:C:H6	1.50	0.77
1:C:46:ASP:O	1:C:49:ASP:HB2	1.84	0.77
1:E:46:ASP:O	1:E:49:ASP:HB2	1.84	0.77
1:E:221:PHE:CB	1:E:306:LYS:H	1.93	0.77
1:C:63:ILE:HD12	2:D:2:C:H4'	1.66	0.77
1:C:289:LEU:CD2	1:C:290:LEU:H	1.98	0.77
1:E:120:ILE:O	1:E:123:ALA:HB3	1.85	0.77
1:E:26:THR:C	1:E:28:THR:H	1.93	0.76
1:A:171:ILE:H	1:A:171:ILE:CD1	1.95	0.76
1:C:51:ASP:O	1:C:57:ARG:HG3	1.84	0.76
1:C:157:LEU:HA	1:C:160:GLN:NE2	2.00	0.76
1:C:389:ARG:HG2	1:C:394:THR:CA	2.16	0.76
1:A:26:THR:C	1:A:28:THR:H	1.93	0.76
1:C:69:GLU:O	1:C:70:TYR:HB3	1.83	0.76
1:C:223:MET:HE1	1:C:238:ALA:HB3	1.68	0.76
1:C:286:VAL:CG2	1:C:287:GLY:N	2.48	0.76
1:C:378:VAL:HG12	1:C:380:LEU:HD22	1.65	0.76
1:E:215:ARG:CG	1:E:282:ALA:HB1	2.14	0.76
1:E:271:GLU:OE1	1:E:274:ARG:HA	1.86	0.76
2:F:27:C:H2'	2:F:28:C:H6	1.50	0.76
2:B:23:A:H2'	2:B:24:G:C8	2.21	0.76
1:C:316:PHE:HE1	1:C:318:ALA:HB2	1.50	0.76
1:C:331:HIS:CD2	1:C:332:THR:HG23	2.21	0.76
2:D:23:A:H2'	2:D:24:G:C8	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:VAL:CG2	1:E:287:GLY:N	2.48	0.76
1:A:289:LEU:CD2	1:A:290:LEU:H	1.99	0.76
1:C:26:THR:C	1:C:28:THR:H	1.93	0.76
1:E:289:LEU:CD2	1:E:290:LEU:H	1.99	0.76
1:A:120:ILE:O	1:A:123:ALA:HB3	1.85	0.75
1:E:171:ILE:H	1:E:171:ILE:CD1	1.94	0.75
1:E:99:MET:CE	1:E:102:ALA:HB2	2.07	0.75
2:D:27:C:H2'	2:D:28:C:H6	1.50	0.75
1:E:331:HIS:CD2	1:E:332:THR:HG23	2.21	0.75
1:A:215:ARG:HG3	1:A:282:ALA:CB	2.17	0.75
1:A:271:GLU:OE1	1:A:274:ARG:HA	1.86	0.75
1:A:286:VAL:CG2	1:A:287:GLY:N	2.48	0.75
1:C:34:VAL:HA	1:C:182:MET:HE2	1.68	0.75
1:C:120:ILE:O	1:C:123:ALA:HB3	1.85	0.75
1:A:389:ARG:HG2	1:A:394:THR:CA	2.16	0.75
1:C:36:ALA:C	1:C:38:GLU:H	1.92	0.75
1:C:271:GLU:OE1	1:C:274:ARG:HA	1.86	0.75
2:F:36:A:H2'	2:F:37:YG:H8	1.51	0.75
1:C:231:ILE:HG21	2:D:76:A:C8	2.22	0.75
2:F:23:A:H2'	2:F:24:G:C8	2.21	0.75
1:C:215:ARG:HG3	1:C:282:ALA:CB	2.17	0.75
1:E:63:ILE:HD12	2:F:2:C:H4'	1.66	0.75
1:A:155:ARG:HD3	1:A:166:ASP:HA	1.69	0.75
1:A:249:VAL:HG13	1:A:267:VAL:O	1.87	0.75
1:E:34:VAL:HG22	1:E:196:VAL:HG13	1.69	0.75
1:E:389:ARG:HG2	1:E:394:THR:CA	2.15	0.75
1:A:219:LYS:HD2	1:A:219:LYS:N	2.02	0.74
1:E:223:MET:HE1	1:E:238:ALA:HB3	1.68	0.74
1:E:316:PHE:HE1	1:E:318:ALA:HB2	1.50	0.74
1:A:34:VAL:HA	1:A:182:MET:HE2	1.68	0.74
1:A:34:VAL:HG22	1:A:196:VAL:HG13	1.69	0.74
1:A:389:ARG:CG	1:A:394:THR:HA	2.17	0.74
1:E:215:ARG:HG3	1:E:282:ALA:CB	2.17	0.74
1:C:263:ARG:CD	1:C:293:VAL:HG12	2.14	0.74
1:A:331:HIS:CD2	1:A:332:THR:HG23	2.21	0.74
1:C:222:LEU:HD12	1:C:244:ARG:H	1.52	0.74
1:A:231:ILE:HG21	2:B:76:A:C8	2.22	0.74
1:C:34:VAL:HG22	1:C:196:VAL:HG13	1.69	0.74
1:E:249:VAL:HG13	1:E:267:VAL:O	1.87	0.74
1:E:389:ARG:CG	1:E:394:THR:HA	2.17	0.74
2:B:36:A:H2'	2:B:37:YG:H8	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:A:H2'	2:B:37:YG:C8	2.22	0.74
1:C:289:LEU:HD12	2:D:76:A:N6	2.03	0.74
1:C:354:ARG:HH11	1:C:354:ARG:CB	1.99	0.74
1:A:122:LEU:O	1:A:126:VAL:HG22	1.87	0.74
1:A:354:ARG:HH11	1:A:354:ARG:CB	1.99	0.74
1:C:64:ASN:HD21	2:D:1:G:H1'	1.53	0.74
1:C:219:LYS:HD2	1:C:219:LYS:N	2.02	0.74
1:C:239:THR:HB	2:D:77:PHA:HD1	1.69	0.74
2:F:36:A:H2'	2:F:37:YG:C8	2.22	0.74
1:A:223:MET:HE1	1:A:238:ALA:HB3	1.68	0.74
1:E:64:ASN:HD21	2:F:1:G:H1'	1.53	0.74
1:A:17:ILE:HG13	1:A:17:ILE:O	1.87	0.74
1:C:122:LEU:O	1:C:126:VAL:HG22	1.87	0.74
1:C:233:GLY:C	1:C:234:ARG:HD3	2.13	0.74
1:C:389:ARG:CG	1:C:394:THR:HA	2.17	0.74
1:E:34:VAL:HA	1:E:182:MET:HE2	1.68	0.74
1:A:64:ASN:HD21	2:B:1:G:H1'	1.53	0.73
2:D:36:A:H2'	2:D:37:YG:C8	2.22	0.73
1:E:219:LYS:HD2	1:E:219:LYS:N	2.02	0.73
1:E:231:ILE:HG21	2:F:76:A:C8	2.22	0.73
1:E:289:LEU:HD12	2:F:76:A:N6	2.03	0.73
1:C:155:ARG:HD3	1:C:166:ASP:HA	1.69	0.73
1:E:239:THR:HB	2:F:77:PHA:HD1	1.69	0.73
1:A:289:LEU:HD12	2:B:76:A:N6	2.03	0.73
1:E:222:LEU:HD12	1:E:244:ARG:H	1.52	0.73
1:C:284:ASP:O	1:C:286:VAL:HG12	1.89	0.73
1:E:327:GLU:HA	5:E:1408:ENX:H19	1.70	0.73
1:C:246:LYS:HG2	1:C:281:ILE:CA	2.18	0.73
2:D:36:A:H2'	2:D:37:YG:H8	1.52	0.73
1:E:17:ILE:O	1:E:17:ILE:HG13	1.87	0.73
1:E:122:LEU:O	1:E:126:VAL:HG22	1.87	0.73
1:A:246:LYS:HG2	1:A:281:ILE:CA	2.18	0.73
1:C:249:VAL:HG13	1:C:267:VAL:O	1.87	0.73
1:E:222:LEU:O	1:E:242:ILE:HG23	1.89	0.73
1:E:284:ASP:O	1:E:286:VAL:HG12	1.89	0.73
1:A:267:VAL:HG13	1:A:288:LEU:HD13	1.72	0.72
1:A:284:ASP:O	1:A:286:VAL:HG12	1.89	0.72
2:F:9:A:H5'	2:F:46:7MG:H1'	1.71	0.72
1:C:199:ILE:O	1:C:202:LEU:HB3	1.89	0.72
1:A:233:GLY:C	1:A:234:ARG:HD3	2.13	0.72
1:C:17:ILE:HG13	1:C:17:ILE:O	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:VAL:HG13	1:C:288:LEU:HD13	1.71	0.72
1:E:155:ARG:HD3	1:E:166:ASP:HA	1.69	0.72
1:A:52:LYS:HZ3	2:B:74:C:H4'	1.54	0.72
1:C:222:LEU:O	1:C:242:ILE:HG23	1.89	0.72
1:C:402:LYS:HG2	1:C:403:ILE:N	2.04	0.72
1:E:354:ARG:HH11	1:E:354:ARG:CB	1.99	0.72
1:A:356:PRO:HD2	1:A:359:VAL:CG2	2.19	0.72
2:B:9:A:H5'	2:B:46:7MG:H1'	1.71	0.72
1:C:222:LEU:HD12	1:C:244:ARG:O	1.90	0.72
1:E:402:LYS:HG2	1:E:403:ILE:N	2.04	0.72
1:A:99:MET:CE	1:A:102:ALA:HB2	2.07	0.72
2:D:37:YG:H141	2:D:37:YG:H192	1.72	0.72
1:E:267:VAL:HG13	1:E:288:LEU:HD13	1.71	0.72
1:A:190:ARG:NH1	1:A:200:TRP:HB3	2.04	0.71
1:A:222:LEU:HD12	1:A:244:ARG:H	1.52	0.71
1:A:239:THR:HB	2:B:77:PHA:HD1	1.69	0.71
1:C:249:VAL:HG13	1:C:269:GLY:H	1.55	0.71
1:C:306:LYS:HD2	1:C:306:LYS:C	2.15	0.71
1:E:306:LYS:HD2	1:E:306:LYS:C	2.15	0.71
1:A:222:LEU:O	1:A:242:ILE:HG23	1.89	0.71
1:A:327:GLU:HA	5:A:1408:ENX:H19	1.70	0.71
1:C:356:PRO:HD2	1:C:359:VAL:CG2	2.19	0.71
1:E:246:LYS:HA	1:E:280:GLY:O	1.90	0.71
1:A:92:MET:HG3	1:A:119:HIS:CE1	2.25	0.71
2:B:37:YG:H192	2:B:37:YG:H141	1.72	0.71
1:E:233:GLY:C	1:E:234:ARG:HD3	2.13	0.71
1:E:263:ARG:CD	1:E:293:VAL:HG12	2.14	0.71
1:E:356:PRO:HD2	1:E:359:VAL:CG2	2.19	0.71
1:E:190:ARG:NH1	1:E:200:TRP:HB3	2.05	0.71
1:E:199:ILE:O	1:E:202:LEU:HB3	1.89	0.71
1:C:316:PHE:CD1	1:C:317:GLU:O	2.44	0.71
1:A:222:LEU:HD12	1:A:244:ARG:O	1.90	0.71
1:C:190:ARG:NH1	1:C:200:TRP:HB3	2.05	0.71
1:E:246:LYS:HG2	1:E:281:ILE:CA	2.18	0.71
1:E:92:MET:HG3	1:E:119:HIS:CE1	2.25	0.71
1:A:9:LYS:HB3	1:A:10:PRO:CD	2.21	0.71
1:C:92:MET:HG3	1:C:119:HIS:CE1	2.25	0.71
1:C:327:GLU:HA	5:C:1408:ENX:H19	1.70	0.71
2:D:9:A:H5'	2:D:46:7MG:H1'	1.71	0.71
2:F:37:YG:H141	2:F:37:YG:H192	1.72	0.71
1:A:247:VAL:C	1:A:279:GLU:HG3	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LEU:HD11	1:C:244:ARG:N	2.05	0.71
1:A:263:ARG:CD	1:A:293:VAL:HG12	2.15	0.71
1:E:61:ILE:HD12	1:E:61:ILE:O	1.91	0.71
1:E:222:LEU:HD12	1:E:244:ARG:O	1.90	0.71
1:C:246:LYS:HA	1:C:280:GLY:O	1.90	0.70
1:C:247:VAL:C	1:C:279:GLU:HG3	2.16	0.70
1:A:43:GLU:CG	1:A:44:VAL:H	2.05	0.70
1:E:316:PHE:CD1	1:E:317:GLU:O	2.44	0.70
1:A:199:ILE:O	1:A:202:LEU:HB3	1.89	0.70
1:A:246:LYS:HA	1:A:280:GLY:O	1.90	0.70
1:A:249:VAL:HG13	1:A:269:GLY:H	1.55	0.70
1:A:306:LYS:C	1:A:306:LYS:HD2	2.15	0.70
1:A:253:VAL:O	1:A:264:LYS:HG3	1.92	0.70
1:A:254:GLU:HA	1:A:263:ARG:O	1.92	0.70
1:A:350:THR:HB	1:A:375:ILE:CD1	2.21	0.70
1:C:149:LEU:CA	1:C:152:MET:HE3	2.21	0.70
1:E:9:LYS:HB3	1:E:10:PRO:CD	2.21	0.70
1:C:9:LYS:HB3	1:C:10:PRO:CD	2.21	0.70
1:C:52:LYS:HZ3	2:D:74:C:H4'	1.54	0.70
1:E:36:ALA:CA	1:E:42:VAL:HB	2.19	0.70
1:E:249:VAL:HG22	1:E:270:VAL:CG2	2.22	0.70
1:E:249:VAL:HG13	1:E:269:GLY:H	1.55	0.70
1:C:254:GLU:HA	1:C:263:ARG:O	1.92	0.70
1:E:247:VAL:C	1:E:279:GLU:HG3	2.16	0.70
1:A:316:PHE:CD1	1:A:317:GLU:O	2.44	0.70
1:C:350:THR:HB	1:C:375:ILE:CD1	2.21	0.70
1:E:254:GLU:HA	1:E:263:ARG:O	1.92	0.70
1:A:16:THR:HG23	1:A:79:HIS:HE1	1.57	0.69
1:A:132:VAL:HG12	1:A:169:PRO:HD2	1.73	0.69
1:E:132:VAL:HG12	1:E:169:PRO:HD2	1.73	0.69
1:E:253:VAL:O	1:E:264:LYS:HG3	1.92	0.69
1:E:404:LEU:O	1:E:405:GLU:HB2	1.92	0.69
1:A:85:HIS:HD2	1:A:87:ASP:HB2	1.56	0.69
1:C:249:VAL:HG22	1:C:270:VAL:CG2	2.22	0.69
1:C:271:GLU:HB2	2:D:76:A:N3	2.08	0.69
1:C:16:THR:HG23	1:C:79:HIS:HE1	1.57	0.69
1:C:39:ASN:HB2	1:C:42:VAL:HG23	1.74	0.69
1:C:150:VAL:O	1:C:150:VAL:HG12	1.92	0.69
1:C:256:VAL:HB	1:C:303:VAL:HG23	1.74	0.69
1:A:19:HIS:HA	1:A:115:GLN:HB2	1.74	0.69
1:A:256:VAL:HB	1:A:303:VAL:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ILE:HD12	1:C:61:ILE:O	1.91	0.69
1:C:404:LEU:O	1:C:405:GLU:HB2	1.92	0.69
1:A:169:PRO:HD3	1:A:209:TYR:CE1	2.28	0.69
1:A:271:GLU:HB2	2:B:76:A:N3	2.08	0.69
1:E:39:ASN:HB2	1:E:42:VAL:HG23	1.74	0.69
1:A:138:VAL:HG22	1:A:173:GLY:O	1.93	0.69
1:A:236:THR:O	1:A:289:LEU:HA	1.93	0.69
1:A:249:VAL:HG22	1:A:270:VAL:CG2	2.22	0.69
1:C:132:VAL:HG12	1:C:169:PRO:HD2	1.73	0.69
1:C:253:VAL:O	1:C:264:LYS:HG3	1.92	0.69
1:E:16:THR:HG23	1:E:79:HIS:HE1	1.56	0.69
1:E:85:HIS:HD2	1:E:87:ASP:HB2	1.56	0.69
1:A:61:ILE:O	1:A:61:ILE:HD12	1.91	0.69
1:C:215:ARG:HH11	1:C:283:GLY:HA3	1.58	0.69
1:E:355:LEU:HD22	1:E:359:VAL:HG21	1.75	0.69
1:A:404:LEU:O	1:A:405:GLU:HB2	1.92	0.69
1:C:85:HIS:HD2	1:C:87:ASP:HB2	1.56	0.69
1:C:138:VAL:HG22	1:C:173:GLY:O	1.93	0.69
1:A:222:LEU:HD11	1:A:244:ARG:N	2.05	0.69
1:C:355:LEU:HD22	1:C:359:VAL:HG21	1.75	0.69
1:E:271:GLU:HB2	2:F:76:A:N3	2.07	0.69
1:E:236:THR:O	1:E:289:LEU:HA	1.93	0.69
1:C:32:THR:HG21	1:C:45:LYS:HB2	1.75	0.68
1:C:222:LEU:HD11	1:C:243:GLU:HB3	1.75	0.68
1:C:236:THR:O	1:C:289:LEU:HA	1.93	0.68
1:E:222:LEU:HD11	1:E:243:GLU:HB3	1.75	0.68
2:D:30:G:H2'	2:D:31:A:C5'	2.23	0.68
1:E:380:LEU:CB	1:E:403:ILE:HD11	2.23	0.68
1:A:17:ILE:HG22	1:A:82:CYS:SG	2.34	0.68
1:C:164:PRO:HB2	1:C:168:VAL:HG13	1.76	0.68
1:C:380:LEU:CB	1:C:403:ILE:HD11	2.24	0.68
1:E:164:PRO:HB2	1:E:168:VAL:HG13	1.76	0.68
1:C:227:ASP:HB3	1:C:239:THR:CG2	2.24	0.68
2:F:30:G:H2'	2:F:31:A:C5'	2.23	0.68
1:A:249:VAL:HG22	1:A:270:VAL:CB	2.23	0.68
1:A:402:LYS:HG2	1:A:403:ILE:N	2.04	0.68
1:C:249:VAL:HG22	1:C:270:VAL:CB	2.23	0.68
1:C:402:LYS:CG	1:C:403:ILE:H	2.05	0.68
1:A:125:GLN:NE2	1:A:394:THR:HB	2.08	0.68
1:A:222:LEU:HD11	1:A:243:GLU:HB3	1.75	0.68
1:A:355:LEU:HD22	1:A:359:VAL:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:HIS:HA	1:C:115:GLN:HB2	1.74	0.68
1:C:95:GLY:O	1:C:97:ALA:N	2.27	0.68
1:E:222:LEU:HD22	1:E:224:PRO:HD3	1.75	0.68
1:A:380:LEU:CB	1:A:403:ILE:HD11	2.24	0.68
2:B:30:G:C2'	2:B:31:A:H5''	2.24	0.68
1:E:32:THR:HG21	1:E:45:LYS:HB2	1.75	0.68
1:A:164:PRO:HB2	1:A:168:VAL:HG13	1.76	0.68
1:C:151:GLU:HG3	1:C:170:VAL:HG21	1.76	0.68
1:E:150:VAL:O	1:E:150:VAL:HG12	1.92	0.68
1:A:133:VAL:HG21	1:A:154:VAL:HG11	1.76	0.68
1:E:138:VAL:HG22	1:E:173:GLY:O	1.93	0.68
1:A:39:ASN:HB2	1:A:42:VAL:HG23	1.74	0.68
2:D:30:G:C2'	2:D:31:A:H5''	2.24	0.68
1:E:151:GLU:HG3	1:E:170:VAL:HG21	1.76	0.68
1:E:169:PRO:HD3	1:E:209:TYR:CE1	2.28	0.68
1:A:95:GLY:O	1:A:97:ALA:N	2.27	0.67
1:C:169:PRO:HD3	1:C:209:TYR:CE1	2.28	0.67
1:E:125:GLN:NE2	1:E:394:THR:HB	2.08	0.67
1:A:222:LEU:HD22	1:A:224:PRO:HD3	1.75	0.67
2:B:30:G:H2'	2:B:31:A:C5'	2.23	0.67
1:C:125:GLN:NE2	1:C:394:THR:HB	2.08	0.67
1:E:350:THR:HB	1:E:375:ILE:CD1	2.21	0.67
1:C:17:ILE:HG22	1:C:82:CYS:SG	2.34	0.67
1:C:136:ASN:CG	1:C:137:LYS:N	2.52	0.67
1:C:290:LEU:HB2	1:C:293:VAL:CG2	2.24	0.67
1:C:281:ILE:HG13	1:C:284:ASP:OD2	1.95	0.67
1:E:227:ASP:HB3	1:E:239:THR:CG2	2.24	0.67
1:E:249:VAL:HG22	1:E:270:VAL:CB	2.23	0.67
1:E:256:VAL:HB	1:E:303:VAL:HG23	1.74	0.67
1:A:150:VAL:O	1:A:150:VAL:HG12	1.92	0.67
1:E:19:HIS:HA	1:E:115:GLN:HB2	1.74	0.67
1:E:136:ASN:CG	1:E:137:LYS:N	2.52	0.67
1:E:281:ILE:HG13	1:E:284:ASP:OD2	1.95	0.67
1:C:222:LEU:HD22	1:C:224:PRO:HD3	1.75	0.67
1:E:268:THR:HG21	1:E:291:ARG:NH2	2.10	0.67
2:F:72:C:H2'	2:F:73:A:O4'	1.95	0.67
1:A:151:GLU:HG3	1:A:170:VAL:HG21	1.76	0.67
1:A:227:ASP:HB3	1:A:239:THR:CG2	2.24	0.67
1:E:95:GLY:O	1:E:97:ALA:N	2.27	0.67
1:E:222:LEU:HD11	1:E:244:ARG:N	2.05	0.67
2:F:30:G:C2'	2:F:31:A:H5''	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:ILE:HG22	1:E:82:CYS:SG	2.34	0.67
1:E:402:LYS:CG	1:E:403:ILE:H	2.05	0.67
1:A:32:THR:HG21	1:A:45:LYS:HB2	1.75	0.67
1:A:36:ALA:CA	1:A:42:VAL:HB	2.19	0.66
1:A:149:LEU:CA	1:A:152:MET:HE3	2.21	0.66
1:A:290:LEU:HB2	1:A:293:VAL:CG2	2.24	0.66
1:E:133:VAL:HG21	1:E:154:VAL:HG11	1.76	0.66
1:E:312:PRO:HA	1:E:378:VAL:O	1.96	0.66
1:A:268:THR:HG21	1:A:291:ARG:NH2	2.10	0.66
1:A:355:LEU:HD21	1:A:362:VAL:CG2	2.25	0.66
1:E:290:LEU:HB2	1:E:293:VAL:CG2	2.24	0.66
1:A:356:PRO:HD3	1:A:370:PHE:HB3	1.76	0.66
2:B:58:1MA:H5''	2:F:34:OMG:O6	1.95	0.66
1:C:355:LEU:HD21	1:C:362:VAL:CG2	2.25	0.66
1:E:104:LEU:HG	1:E:106:VAL:CG2	2.26	0.66
1:E:306:LYS:HD2	1:E:306:LYS:O	1.95	0.66
1:A:372:VAL:HG12	1:A:373:GLU:N	2.09	0.66
1:C:61:ILE:HG22	3:C:1406:GNP:O3G	1.96	0.66
1:C:268:THR:HG21	1:C:291:ARG:NH2	2.10	0.66
1:C:306:LYS:HD2	1:C:306:LYS:O	1.95	0.66
1:C:356:PRO:HD3	1:C:370:PHE:HB3	1.77	0.66
1:E:356:PRO:HD3	1:E:370:PHE:HB3	1.76	0.66
2:B:29:A:H61	2:B:41:U:H3	1.44	0.66
1:C:344:PHE:HE2	1:C:386:PHE:CB	2.09	0.66
2:D:72:C:H2'	2:D:73:A:O4'	1.95	0.66
1:A:29:ALA:C	1:A:31:LEU:H	2.04	0.66
1:A:104:LEU:HG	1:A:106:VAL:CG2	2.26	0.66
1:A:189:LYS:O	1:A:192:GLU:HB2	1.96	0.66
1:A:215:ARG:HH11	1:A:283:GLY:HA3	1.58	0.66
1:A:223:MET:HE1	1:A:238:ALA:O	1.95	0.66
1:A:236:THR:H	1:A:289:LEU:CD2	2.09	0.66
1:C:75:ARG:HH21	1:C:207:ASP:CA	1.96	0.66
1:C:99:MET:CE	1:C:102:ALA:HB2	2.07	0.66
1:E:344:PHE:HE2	1:E:386:PHE:CB	2.09	0.66
1:A:313:HIS:HB2	1:A:380:LEU:CD2	2.19	0.66
2:B:37:YG:H1'	2:B:37:YG:H31	1.78	0.66
1:E:236:THR:H	1:E:289:LEU:CD2	2.09	0.66
1:E:293:VAL:HG23	1:E:293:VAL:O	1.96	0.66
1:E:372:VAL:HG12	1:E:373:GLU:N	2.09	0.66
1:A:136:ASN:CG	1:A:137:LYS:N	2.52	0.66
1:A:312:PRO:HA	1:A:378:VAL:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:LYS:O	1:C:192:GLU:HB2	1.96	0.66
1:A:402:LYS:CG	1:A:403:ILE:H	2.05	0.66
2:B:72:C:H2'	2:B:73:A:O4'	1.95	0.66
1:C:133:VAL:HG21	1:C:154:VAL:HG11	1.76	0.66
1:C:223:MET:HE1	1:C:238:ALA:O	1.95	0.66
1:C:372:VAL:HG12	1:C:373:GLU:N	2.09	0.66
1:E:223:MET:HE1	1:E:238:ALA:O	1.95	0.66
2:F:37:YG:H1'	2:F:37:YG:H31	1.78	0.66
1:A:281:ILE:HG13	1:A:284:ASP:OD2	1.95	0.65
1:A:306:LYS:HD2	1:A:306:LYS:O	1.95	0.65
1:C:104:LEU:HG	1:C:106:VAL:CG2	2.26	0.65
1:C:236:THR:H	1:C:289:LEU:CD2	2.09	0.65
1:E:29:ALA:C	1:E:31:LEU:H	2.04	0.65
1:E:47:TYR:C	1:E:49:ASP:H	2.05	0.65
1:E:52:LYS:HZ3	2:F:74:C:H4'	1.57	0.65
1:E:169:PRO:HB2	1:E:171:ILE:HD11	1.79	0.65
1:E:355:LEU:HD21	1:E:362:VAL:CG2	2.25	0.65
1:E:149:LEU:CA	1:E:152:MET:HE3	2.21	0.65
1:C:43:GLU:CG	1:C:44:VAL:H	2.05	0.65
1:C:157:LEU:HA	1:C:160:GLN:HE21	1.61	0.65
1:C:29:ALA:C	1:C:31:LEU:H	2.04	0.65
1:C:169:PRO:HB2	1:C:171:ILE:HD11	1.78	0.65
1:E:61:ILE:HG22	3:E:1406:GNP:O3G	1.96	0.65
1:A:157:LEU:HA	1:A:160:GLN:HE21	1.61	0.65
1:A:293:VAL:HG23	1:A:293:VAL:O	1.96	0.65
1:C:231:ILE:HD11	1:C:237:VAL:HG12	1.79	0.65
2:F:26:M2G:HM12	2:F:27:C:H1'	1.78	0.65
1:A:231:ILE:HG12	2:B:76:A:C8	2.32	0.65
1:A:246:LYS:HB2	1:A:246:LYS:NZ	2.12	0.65
1:E:215:ARG:HH11	1:E:283:GLY:HA3	1.58	0.65
1:E:246:LYS:HB2	1:E:246:LYS:NZ	2.12	0.65
2:D:37:YG:H31	2:D:37:YG:H1'	1.78	0.65
1:E:124:ARG:CG	1:E:161:TYR:HB3	2.25	0.65
1:A:26:THR:O	1:A:28:THR:N	2.29	0.65
1:A:255:ILE:HG22	1:A:302:GLN:HB2	1.79	0.65
1:A:380:LEU:HB2	1:A:403:ILE:HD11	1.79	0.65
1:C:223:MET:HE1	1:C:238:ALA:CB	2.27	0.65
1:C:312:PRO:HA	1:C:378:VAL:O	1.96	0.65
1:E:231:ILE:HG12	2:F:76:A:C8	2.32	0.65
1:A:344:PHE:HE2	1:A:386:PHE:CB	2.09	0.65
2:B:32:OMC:HM22	2:B:33:U:H5'	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:LYS:O	1:E:192:GLU:HB2	1.96	0.65
1:A:61:ILE:HG22	3:A:1406:GNP:O3G	1.96	0.64
1:C:95:GLY:C	1:C:97:ALA:H	2.05	0.64
1:C:246:LYS:HB2	1:C:246:LYS:NZ	2.12	0.64
1:E:33:TYR:HA	1:E:36:ALA:HB3	1.79	0.64
1:E:380:LEU:HB2	1:E:403:ILE:HD11	1.79	0.64
1:A:95:GLY:C	1:A:97:ALA:H	2.05	0.64
1:C:26:THR:O	1:C:28:THR:N	2.29	0.64
1:C:255:ILE:HG22	1:C:302:GLN:HB2	1.79	0.64
1:E:320:VAL:HG12	1:E:322:ILE:HD12	1.79	0.64
1:A:391:GLY:HA2	2:B:64:A:O4'	1.97	0.64
1:C:33:TYR:HA	1:C:36:ALA:HB3	1.78	0.64
1:A:33:TYR:HA	1:A:36:ALA:HB3	1.79	0.64
1:A:113:MET:HB3	1:A:114:PRO:CD	2.27	0.64
1:C:293:VAL:HG23	1:C:293:VAL:O	1.96	0.64
2:D:26:M2G:HM12	2:D:27:C:H1'	1.78	0.64
2:F:29:A:H61	2:F:41:U:H3	1.44	0.64
2:B:26:M2G:HM12	2:B:27:C:H1'	1.78	0.64
1:C:380:LEU:HB2	1:C:403:ILE:HD11	1.79	0.64
1:E:95:GLY:C	1:E:97:ALA:H	2.05	0.64
1:A:169:PRO:HB2	1:A:171:ILE:HD11	1.79	0.64
1:C:231:ILE:HG12	2:D:76:A:C8	2.32	0.64
1:C:267:VAL:HG12	1:C:270:VAL:HG22	1.80	0.64
1:C:320:VAL:HG12	1:C:322:ILE:HD12	1.79	0.64
2:D:29:A:H61	2:D:41:U:H3	1.44	0.64
1:C:47:TYR:C	1:C:49:ASP:H	2.04	0.64
1:C:246:LYS:HB2	1:C:246:LYS:HZ2	1.63	0.64
1:E:43:GLU:CG	1:E:44:VAL:H	2.05	0.64
1:E:223:MET:HE1	1:E:238:ALA:CB	2.27	0.64
1:E:231:ILE:HD11	1:E:237:VAL:HG12	1.79	0.64
1:A:231:ILE:HD11	1:A:237:VAL:HG12	1.78	0.64
1:E:113:MET:HB3	1:E:114:PRO:CD	2.28	0.64
1:A:267:VAL:HG12	1:A:270:VAL:HG22	1.80	0.64
1:A:289:LEU:CD2	1:A:290:LEU:N	2.61	0.64
1:C:289:LEU:HD23	1:C:290:LEU:N	2.10	0.64
2:F:32:OMC:HM22	2:F:33:U:H5'	1.79	0.64
1:A:223:MET:HE1	1:A:238:ALA:CB	2.27	0.63
1:A:229:PHE:O	1:A:236:THR:HG22	1.99	0.63
1:A:363:MET:HE3	1:A:364:PRO:HD2	1.79	0.63
1:C:229:PHE:O	1:C:236:THR:HG22	1.98	0.63
2:F:4:G:H2'	2:F:5:A:C5'	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:VAL:HG12	1:A:322:ILE:HD12	1.79	0.63
2:D:36:A:N6	2:D:37:YG:H193	2.13	0.63
1:E:26:THR:O	1:E:28:THR:N	2.29	0.63
1:E:255:ILE:HG22	1:E:302:GLN:HB2	1.79	0.63
1:E:289:LEU:HD23	1:E:290:LEU:N	2.10	0.63
1:E:363:MET:HE3	1:E:364:PRO:HD2	1.79	0.63
1:A:187:LYS:HB3	1:A:189:LYS:NZ	2.13	0.63
1:A:220:PRO:HB3	1:A:306:LYS:CE	2.28	0.63
1:C:124:ARG:CG	1:C:161:TYR:HB3	2.25	0.63
1:C:220:PRO:HB3	1:C:306:LYS:CE	2.28	0.63
1:C:391:GLY:HA2	2:D:64:A:O4'	1.97	0.63
1:A:47:TYR:C	1:A:49:ASP:H	2.04	0.63
1:C:187:LYS:HB3	1:C:189:LYS:NZ	2.13	0.63
1:C:249:VAL:HG12	1:C:268:THR:HA	1.80	0.63
2:D:32:OMC:HM22	2:D:33:U:H5'	1.79	0.63
1:E:391:GLY:HA2	2:F:64:A:O4'	1.97	0.63
1:C:289:LEU:CD2	1:C:290:LEU:N	2.61	0.63
1:E:220:PRO:HB3	1:E:306:LYS:CE	2.28	0.63
1:E:187:LYS:HB3	1:E:189:LYS:NZ	2.13	0.63
1:A:16:THR:HG23	1:A:79:HIS:CE1	2.33	0.63
1:C:255:ILE:HG22	1:C:302:GLN:CB	2.29	0.63
2:D:19:G:H5''	2:D:20:G:H5'	1.81	0.63
1:A:47:TYR:O	1:A:49:ASP:N	2.32	0.63
1:E:157:LEU:HA	1:E:160:GLN:HE21	1.61	0.63
1:A:124:ARG:CG	1:A:161:TYR:HB3	2.25	0.62
1:C:113:MET:HB3	1:C:114:PRO:CD	2.27	0.62
1:C:363:MET:HE3	1:C:364:PRO:HD2	1.79	0.62
1:E:34:VAL:CG1	1:E:199:ILE:HG21	2.29	0.62
1:E:229:PHE:O	1:E:236:THR:HG22	1.98	0.62
2:B:4:G:H2'	2:B:5:A:C5'	2.25	0.62
1:A:92:MET:HG3	1:A:119:HIS:NE2	2.15	0.62
1:E:16:THR:HG23	1:E:79:HIS:CE1	2.33	0.62
1:E:47:TYR:O	1:E:49:ASP:N	2.32	0.62
1:A:34:VAL:CG1	1:A:199:ILE:HG21	2.29	0.62
1:A:104:LEU:O	1:A:106:VAL:HG23	2.00	0.62
1:C:47:TYR:O	1:C:49:ASP:N	2.32	0.62
1:C:67:HIS:HB3	1:C:80:VAL:HG13	1.80	0.62
1:C:92:MET:HG3	1:C:119:HIS:NE2	2.15	0.62
2:D:30:G:H2'	2:D:31:A:H5'	1.81	0.62
2:B:19:G:H5''	2:B:20:G:H5'	1.81	0.62
1:E:249:VAL:HG12	1:E:268:THR:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:VAL:HG12	1:E:270:VAL:HG22	1.80	0.62
1:A:251:ASP:O	1:A:253:VAL:HG13	2.00	0.62
1:A:314:THR:HG22	1:A:373:GLU:OE2	2.00	0.62
1:C:6:ILE:N	1:C:277:LEU:HD13	2.15	0.62
1:C:120:ILE:HD12	1:C:157:LEU:HD23	1.81	0.62
1:C:134:PHE:CD1	1:C:202:LEU:HD22	2.35	0.62
1:E:289:LEU:CD2	1:E:290:LEU:N	2.61	0.62
1:E:315:LYS:O	1:E:316:PHE:CB	2.48	0.62
1:A:67:HIS:HB3	1:A:80:VAL:HG13	1.80	0.62
1:A:120:ILE:HD12	1:A:157:LEU:HD23	1.81	0.62
2:B:36:A:N6	2:B:37:YG:H193	2.13	0.62
1:A:255:ILE:HG22	1:A:302:GLN:CB	2.29	0.62
1:A:372:VAL:CG1	1:A:373:GLU:N	2.63	0.62
1:C:314:THR:HG22	1:C:373:GLU:OE2	2.00	0.62
2:D:37:YG:H141	2:D:37:YG:C19	2.30	0.62
1:E:251:ASP:O	1:E:253:VAL:HG13	2.00	0.62
2:F:35:A:O2'	2:F:36:A:H5'	2.00	0.62
1:A:134:PHE:CD1	1:A:202:LEU:HD22	2.35	0.62
1:C:16:THR:HG23	1:C:79:HIS:CE1	2.33	0.62
1:C:36:ALA:CA	1:C:42:VAL:HB	2.20	0.62
1:C:104:LEU:O	1:C:106:VAL:HG23	2.00	0.62
1:E:255:ILE:HG22	1:E:302:GLN:CB	2.29	0.62
1:E:372:VAL:CG1	1:E:373:GLU:N	2.63	0.62
2:B:30:G:H2'	2:B:31:A:H5'	1.81	0.62
1:E:314:THR:HG22	1:E:373:GLU:OE2	2.00	0.62
2:F:30:G:H2'	2:F:31:A:H5'	1.81	0.62
2:F:31:A:O2'	2:F:32:OMC:H5''	2.00	0.62
1:A:205:ALA:HA	1:A:208:GLU:HB3	1.82	0.61
1:C:251:ASP:O	1:C:253:VAL:HG13	2.00	0.61
1:C:344:PHE:CE2	1:C:386:PHE:CB	2.83	0.61
2:D:35:A:O2'	2:D:36:A:H5'	2.00	0.61
1:E:6:ILE:N	1:E:277:LEU:HD13	2.15	0.61
1:A:249:VAL:HG12	1:A:268:THR:HA	1.80	0.61
1:A:266:VAL:CG1	1:A:268:THR:HG23	2.30	0.61
1:A:361:MET:HE2	1:A:363:MET:SD	2.40	0.61
1:C:39:ASN:N	1:C:39:ASN:ND2	2.48	0.61
1:E:134:PHE:CD1	1:E:202:LEU:HD22	2.35	0.61
1:E:361:MET:HE2	1:E:363:MET:SD	2.40	0.61
2:F:36:A:N6	2:F:37:YG:H193	2.13	0.61
1:A:163:PHE:O	1:A:165:GLY:N	2.33	0.61
2:B:35:A:O2'	2:B:36:A:H5'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:PHE:CE1	1:C:237:VAL:HG13	2.35	0.61
1:C:361:MET:HE2	1:C:363:MET:SD	2.40	0.61
1:E:54:PRO:HG2	2:F:73:A:H4'	1.82	0.61
1:E:67:HIS:HB3	1:E:80:VAL:HG13	1.80	0.61
1:E:229:PHE:CE1	1:E:237:VAL:HG13	2.35	0.61
1:E:344:PHE:CD1	1:E:378:VAL:HG11	2.36	0.61
2:F:74:C:H3'	2:F:77(A):C:C5	2.35	0.61
1:A:6:ILE:N	1:A:277:LEU:HD13	2.15	0.61
1:A:75:ARG:HH21	1:A:207:ASP:CA	1.96	0.61
2:B:37:YG:H141	2:B:37:YG:C19	2.30	0.61
1:C:403:ILE:O	1:C:404:LEU:HD23	2.00	0.61
1:A:28:THR:HG23	1:A:68:VAL:HG21	1.83	0.61
1:A:96:ALA:HA	1:A:99:MET:HG2	1.83	0.61
1:C:163:PHE:O	1:C:165:GLY:N	2.33	0.61
1:E:163:PHE:O	1:E:165:GLY:N	2.33	0.61
1:E:344:PHE:CE2	1:E:386:PHE:CB	2.83	0.61
1:A:315:LYS:O	1:A:316:PHE:CB	2.48	0.61
1:A:344:PHE:CD1	1:A:378:VAL:HG11	2.36	0.61
1:C:28:THR:HG23	1:C:68:VAL:HG21	1.83	0.61
1:C:138:VAL:O	1:C:141:VAL:N	2.34	0.61
1:C:315:LYS:O	1:C:316:PHE:CB	2.48	0.61
1:E:120:ILE:HD12	1:E:157:LEU:HD23	1.81	0.61
1:E:403:ILE:O	1:E:404:LEU:HD23	2.00	0.61
1:A:24:LYS:N	1:A:105:VAL:HG11	2.16	0.61
1:A:222:LEU:CD1	1:A:244:ARG:N	2.51	0.61
1:C:266:VAL:CG1	1:C:268:THR:HG23	2.30	0.61
2:D:31:A:O2'	2:D:32:OMC:H5''	2.00	0.61
1:E:136:ASN:CG	1:E:137:LYS:H	2.09	0.61
1:E:226:GLU:OE2	1:E:227:ASP:HB2	2.00	0.61
1:A:135:MET:HE2	1:A:150:VAL:O	2.01	0.61
1:A:203:LEU:C	1:A:205:ALA:H	2.09	0.61
1:A:229:PHE:CE1	1:A:237:VAL:HG13	2.35	0.61
2:B:74:C:H3'	2:B:77(A):C:C5	2.35	0.61
1:E:135:MET:HE2	1:E:150:VAL:O	2.01	0.61
1:A:84:GLY:O	1:A:115:GLN:HG2	2.01	0.61
1:A:226:GLU:OE2	1:A:227:ASP:HB2	2.00	0.61
1:C:344:PHE:CD1	1:C:378:VAL:HG11	2.35	0.61
1:C:372:VAL:CG1	1:C:373:GLU:N	2.63	0.61
1:E:92:MET:HG3	1:E:119:HIS:NE2	2.14	0.61
1:A:138:VAL:O	1:A:141:VAL:N	2.34	0.61
1:C:108:ALA:CB	1:C:135:MET:HG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:HIS:HB2	1:C:380:LEU:CD2	2.19	0.61
1:E:104:LEU:O	1:E:106:VAL:HG23	2.00	0.61
1:A:241:ARG:HA	1:A:285:ASN:HA	1.83	0.60
1:A:281:ILE:HD12	1:A:282:ALA:HB3	1.83	0.60
1:A:344:PHE:CE2	1:A:386:PHE:CB	2.83	0.60
1:A:404:LEU:O	1:A:405:GLU:CB	2.49	0.60
1:C:24:LYS:N	1:C:105:VAL:HG11	2.16	0.60
1:C:84:GLY:O	1:C:115:GLN:HG2	2.01	0.60
1:C:155:ARG:NH2	1:C:170:VAL:HG23	2.16	0.60
1:C:226:GLU:OE2	1:C:227:ASP:HB2	2.00	0.60
1:C:286:VAL:CG2	1:C:288:LEU:HD23	2.31	0.60
1:E:28:THR:HG23	1:E:68:VAL:HG21	1.83	0.60
1:E:138:VAL:O	1:E:141:VAL:N	2.34	0.60
1:C:203:LEU:C	1:C:205:ALA:H	2.09	0.60
1:C:346:THR:HG23	1:C:347:THR:N	2.09	0.60
1:E:33:TYR:HB3	1:E:182:MET:CB	2.31	0.60
1:E:155:ARG:NH2	1:E:170:VAL:HG23	2.17	0.60
1:E:200:TRP:O	1:E:203:LEU:N	2.35	0.60
1:E:205:ALA:HA	1:E:208:GLU:HB3	1.82	0.60
2:B:31:A:O2'	2:B:32:OMC:H5''	2.00	0.60
1:E:24:LYS:N	1:E:105:VAL:HG11	2.16	0.60
1:A:39:ASN:N	1:A:39:ASN:ND2	2.48	0.60
1:A:244:ARG:NH2	1:A:381:GLU:OE2	2.34	0.60
1:A:350:THR:H	1:A:375:ILE:HD11	1.66	0.60
1:C:33:TYR:HB3	1:C:182:MET:CB	2.31	0.60
2:D:74:C:H3'	2:D:77(A):C:C5	2.35	0.60
1:E:52:LYS:HD2	2:F:74:C:C4'	2.31	0.60
1:E:323:LEU:HD12	1:E:396:GLY:CA	2.30	0.60
2:F:37:YG:H141	2:F:37:YG:C19	2.30	0.60
1:A:200:TRP:O	1:A:203:LEU:N	2.35	0.60
1:A:403:ILE:O	1:A:404:LEU:HD23	2.01	0.60
1:E:350:THR:H	1:E:375:ILE:HD11	1.66	0.60
1:A:136:ASN:CG	1:A:137:LYS:H	2.09	0.60
1:A:324:LYS:HG2	1:A:365:GLY:CA	2.31	0.60
1:A:393:ARG:HB3	1:A:393:ARG:NH2	2.14	0.60
1:C:52:LYS:HD2	2:D:74:C:C4'	2.31	0.60
1:C:96:ALA:HA	1:C:99:MET:HG2	1.83	0.60
1:C:135:MET:HE2	1:C:150:VAL:O	2.01	0.60
1:C:222:LEU:CD1	1:C:244:ARG:N	2.51	0.60
1:C:222:LEU:HD12	1:C:244:ARG:C	2.27	0.60
1:C:350:THR:H	1:C:375:ILE:HD11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:MET:O	1:E:225:VAL:N	2.35	0.60
1:E:229:PHE:N	1:E:229:PHE:CD1	2.70	0.60
2:F:19:G:H5''	2:F:20:G:H5'	1.81	0.60
1:A:222:LEU:HD12	1:A:244:ARG:C	2.27	0.60
1:A:223:MET:O	1:A:225:VAL:N	2.35	0.60
1:C:98:GLN:NE2	1:C:224:PRO:HB2	2.17	0.60
1:C:205:ALA:HA	1:C:208:GLU:HB3	1.82	0.60
1:C:223:MET:O	1:C:225:VAL:N	2.35	0.60
1:E:27:LEU:HG	1:E:27:LEU:O	2.02	0.60
1:E:266:VAL:CG1	1:E:268:THR:HG23	2.30	0.60
1:E:317:GLU:HB3	1:E:402:LYS:HB3	1.84	0.60
1:E:324:LYS:HG2	1:E:365:GLY:CA	2.31	0.60
1:A:27:LEU:O	1:A:27:LEU:HG	2.02	0.60
1:A:124:ARG:HD3	1:A:161:TYR:O	2.02	0.60
1:A:270:VAL:O	1:A:271:GLU:O	2.20	0.60
1:A:286:VAL:CG2	1:A:288:LEU:HD23	2.31	0.60
1:C:27:LEU:O	1:C:27:LEU:HG	2.02	0.60
1:C:54:PRO:HG2	2:D:73:A:H4'	1.82	0.60
1:C:136:ASN:CG	1:C:137:LYS:H	2.09	0.60
1:C:227:ASP:CB	1:C:239:THR:HG23	2.31	0.60
1:C:254:GLU:HG3	1:C:307:PRO:HG3	1.84	0.60
2:D:4:G:H2'	2:D:5:A:C5'	2.25	0.60
1:E:227:ASP:CB	1:E:239:THR:HG23	2.31	0.60
1:E:281:ILE:HD12	1:E:282:ALA:HB3	1.83	0.60
1:E:286:VAL:CG2	1:E:288:LEU:HD23	2.31	0.60
1:A:54:PRO:HG2	2:B:73:A:H4'	1.83	0.60
1:C:270:VAL:O	1:C:271:GLU:O	2.20	0.60
1:E:96:ALA:HA	1:E:99:MET:HG2	1.83	0.60
1:E:244:ARG:NH2	1:E:381:GLU:OE2	2.34	0.60
1:E:254:GLU:HG3	1:E:307:PRO:HG3	1.84	0.60
1:A:13:ASN:HB2	1:A:100:ASP:OD1	2.02	0.60
1:E:39:ASN:N	1:E:39:ASN:ND2	2.48	0.60
1:E:270:VAL:O	1:E:271:GLU:O	2.20	0.60
1:E:313:HIS:HB2	1:E:380:LEU:CD2	2.19	0.60
1:E:313:HIS:CB	1:E:380:LEU:HD23	2.20	0.60
1:C:124:ARG:HD3	1:C:161:TYR:O	2.02	0.59
1:C:159:ASN:OD1	1:C:165:GLY:HA3	2.02	0.59
1:C:200:TRP:O	1:C:203:LEU:N	2.35	0.59
1:C:317:GLU:HB3	1:C:402:LYS:HB3	1.84	0.59
1:E:84:GLY:O	1:E:115:GLN:HG2	2.01	0.59
1:E:222:LEU:HD12	1:E:244:ARG:C	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:NH2	1:A:170:VAL:HG23	2.16	0.59
1:A:246:LYS:HB2	1:A:246:LYS:HZ2	1.66	0.59
1:C:13:ASN:HB2	1:C:100:ASP:OD1	2.02	0.59
1:C:323:LEU:HD12	1:C:396:GLY:CA	2.30	0.59
2:F:39:PSU:H2'	2:F:40:5MC:C6	2.38	0.59
1:A:254:GLU:HG3	1:A:307:PRO:HG3	1.84	0.59
1:A:346:THR:HG23	1:A:347:THR:N	2.09	0.59
2:B:39:PSU:H2'	2:B:40:5MC:C6	2.38	0.59
1:C:244:ARG:NH2	1:C:381:GLU:OE2	2.34	0.59
1:A:217:VAL:HG13	1:A:282:ALA:HB2	1.85	0.59
1:C:241:ARG:HA	1:C:285:ASN:HA	1.83	0.59
1:C:378:VAL:HG12	1:C:380:LEU:HD21	1.84	0.59
1:E:187:LYS:HB3	1:E:189:LYS:HZ2	1.68	0.59
1:E:222:LEU:CD1	1:E:244:ARG:N	2.51	0.59
1:A:227:ASP:CB	1:A:239:THR:HG23	2.31	0.59
1:C:34:VAL:CG1	1:C:199:ILE:HG21	2.29	0.59
1:C:217:VAL:HG13	1:C:282:ALA:HB2	1.85	0.59
1:C:281:ILE:HD12	1:C:282:ALA:HB3	1.83	0.59
2:D:39:PSU:H2'	2:D:40:5MC:C6	2.37	0.59
1:E:31:LEU:HD13	1:E:70:TYR:CE2	2.37	0.59
1:E:98:GLN:NE2	1:E:224:PRO:HB2	2.17	0.59
1:E:190:ARG:HH12	1:E:200:TRP:HB3	1.68	0.59
2:B:4:G:C3'	2:B:5:A:H5''	2.32	0.59
1:E:13:ASN:HB2	1:E:100:ASP:OD1	2.02	0.59
1:E:124:ARG:HD3	1:E:161:TYR:O	2.02	0.59
1:A:195:TRP:O	1:A:199:ILE:HD13	2.03	0.59
2:B:15:G:H2'	2:B:16:H2U:C6	2.33	0.59
1:C:225:VAL:HG12	1:C:300:ARG:HA	1.85	0.59
1:C:229:PHE:N	1:C:229:PHE:CD1	2.70	0.59
1:C:324:LYS:HG2	1:C:365:GLY:CA	2.31	0.59
1:C:404:LEU:O	1:C:405:GLU:CB	2.49	0.59
2:D:4:G:C3'	2:D:5:A:H5''	2.32	0.59
1:E:7:ARG:C	1:E:8:THR:HG22	2.28	0.59
1:E:241:ARG:HA	1:E:285:ASN:HA	1.83	0.59
1:A:159:ASN:OD1	1:A:165:GLY:HA3	2.02	0.59
1:A:378:VAL:HG12	1:A:380:LEU:HD21	1.84	0.59
1:E:225:VAL:HG12	1:E:300:ARG:HA	1.85	0.59
1:E:378:VAL:HG12	1:E:380:LEU:HD21	1.84	0.59
2:F:4:G:C3'	2:F:5:A:H5''	2.32	0.59
1:A:33:TYR:HB3	1:A:182:MET:CB	2.31	0.59
1:A:52:LYS:HD2	2:B:74:C:C4'	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:VAL:HG13	1:E:282:ALA:HB2	1.85	0.59
1:E:371:THR:HG22	1:E:372:VAL:N	2.18	0.59
2:F:17:H2U:O2'	2:F:18:G:OP1	2.20	0.59
1:A:7:ARG:C	1:A:8:THR:HG22	2.28	0.59
1:A:31:LEU:HD13	1:A:70:TYR:CE2	2.38	0.59
1:A:108:ALA:CB	1:A:135:MET:HG2	2.31	0.59
1:C:31:LEU:HD13	1:C:70:TYR:CE2	2.38	0.59
1:C:47:TYR:C	1:C:49:ASP:N	2.61	0.59
1:C:341:GLN:H	1:C:341:GLN:CD	2.11	0.59
1:E:43:GLU:HG2	1:E:44:VAL:N	2.13	0.59
1:E:75:ARG:HH21	1:E:207:ASP:CA	1.96	0.59
1:E:203:LEU:C	1:E:205:ALA:H	2.09	0.59
1:A:98:GLN:NE2	1:A:224:PRO:HB2	2.17	0.58
1:C:7:ARG:C	1:C:8:THR:HG22	2.28	0.58
1:E:52:LYS:CE	2:F:74:C:H4'	2.33	0.58
1:E:239:THR:CB	2:F:77:PHA:HD1	2.33	0.58
1:E:341:GLN:CD	1:E:341:GLN:H	2.11	0.58
1:A:229:PHE:CD1	1:A:229:PHE:N	2.70	0.58
1:A:371:THR:HG22	1:A:372:VAL:N	2.18	0.58
1:C:382:GLU:HA	1:C:400:VAL:O	2.03	0.58
1:C:393:ARG:HB3	1:C:393:ARG:NH2	2.14	0.58
1:E:159:ASN:OD1	1:E:165:GLY:HA3	2.02	0.58
1:E:195:TRP:O	1:E:199:ILE:HD13	2.03	0.58
1:C:313:HIS:CD2	1:C:403:ILE:HD13	2.38	0.58
2:D:15:G:H2'	2:D:16:H2U:C6	2.33	0.58
1:E:171:ILE:HG12	1:E:202:LEU:HA	1.86	0.58
1:E:299:GLU:O	1:E:302:GLN:OE1	2.21	0.58
1:E:313:HIS:CD2	1:E:403:ILE:HD13	2.38	0.58
1:A:115:GLN:O	1:A:116:THR:C	2.45	0.58
1:C:371:THR:HG22	1:C:372:VAL:N	2.18	0.58
1:E:146:LEU:O	1:E:150:VAL:HG23	2.04	0.58
2:F:26:M2G:H2'	2:F:26:M2G:N3	2.18	0.58
1:E:47:TYR:C	1:E:49:ASP:N	2.61	0.58
1:E:222:LEU:CD1	1:E:222:LEU:O	2.49	0.58
1:A:146:LEU:O	1:A:150:VAL:HG23	2.04	0.58
1:E:115:GLN:O	1:E:116:THR:C	2.45	0.58
1:A:217:VAL:HG11	1:A:281:ILE:HB	1.86	0.58
1:A:317:GLU:HB3	1:A:402:LYS:HB3	1.84	0.58
1:A:382:GLU:HA	1:A:400:VAL:O	2.03	0.58
1:E:26:THR:HG22	1:E:175:ALA:HB1	1.86	0.58
1:E:404:LEU:O	1:E:405:GLU:CB	2.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HH12	1:A:200:TRP:HB3	1.67	0.58
2:B:17:H2U:O2'	2:B:18:G:OP1	2.20	0.58
1:C:223:MET:CG	1:C:242:ILE:HG12	2.34	0.58
2:D:34:OMG:O6	2:F:58:1MA:H5''	2.04	0.58
1:A:171:ILE:HG12	1:A:202:LEU:HA	1.86	0.58
1:A:313:HIS:CD2	1:A:403:ILE:HD13	2.38	0.58
1:C:195:TRP:O	1:C:199:ILE:HD13	2.03	0.58
2:D:30:G:H2'	2:D:31:A:H5''	1.86	0.58
1:A:323:LEU:HD12	1:A:396:GLY:CA	2.30	0.58
1:A:341:GLN:H	1:A:341:GLN:CD	2.11	0.58
1:E:94:THR:O	1:E:97:ALA:HB3	2.04	0.58
1:E:382:GLU:HA	1:E:400:VAL:O	2.03	0.58
1:A:52:LYS:CE	2:B:74:C:H4'	2.33	0.57
1:A:68:VAL:HG23	1:A:68:VAL:O	2.04	0.57
1:C:130:TYR:O	1:C:131:ILE:HD13	2.04	0.57
1:A:225:VAL:HG12	1:A:300:ARG:HA	1.85	0.57
1:C:31:LEU:HD13	1:C:70:TYR:CZ	2.40	0.57
1:C:52:LYS:CE	2:D:74:C:H4'	2.33	0.57
1:C:94:THR:O	1:C:97:ALA:HB3	2.04	0.57
1:E:130:TYR:O	1:E:131:ILE:HD13	2.04	0.57
1:A:31:LEU:HD13	1:A:70:TYR:CZ	2.40	0.57
1:A:94:THR:O	1:A:97:ALA:HB3	2.04	0.57
1:A:257:GLY:O	1:A:259:ALA:N	2.37	0.57
1:A:311:THR:HG22	1:A:312:PRO:HD2	1.87	0.57
1:C:115:GLN:O	1:C:116:THR:C	2.45	0.57
1:C:146:LEU:O	1:C:150:VAL:HG23	2.04	0.57
1:C:299:GLU:O	1:C:302:GLN:OE1	2.21	0.57
1:E:217:VAL:HG11	1:E:281:ILE:HB	1.86	0.57
1:E:223:MET:CG	1:E:242:ILE:HG12	2.34	0.57
1:A:63:ILE:CG1	1:A:64:ASN:N	2.67	0.57
1:C:239:THR:CB	2:D:77:PHA:HD1	2.33	0.57
1:E:257:GLY:O	1:E:259:ALA:N	2.37	0.57
1:A:286:VAL:O	2:B:77:PHA:HB3	2.05	0.57
1:C:217:VAL:HG11	1:C:281:ILE:HB	1.86	0.57
1:C:257:GLY:O	1:C:259:ALA:N	2.37	0.57
2:D:66:A:H2'	2:D:67:A:C8	2.40	0.57
1:A:299:GLU:O	1:A:302:GLN:OE1	2.21	0.57
1:A:322:ILE:HD12	1:A:322:ILE:N	2.19	0.57
1:C:171:ILE:HG12	1:C:202:LEU:HA	1.86	0.57
1:C:190:ARG:HH12	1:C:200:TRP:HB3	1.67	0.57
1:C:286:VAL:O	2:D:77:PHA:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:VAL:HG12	1:E:134:PHE:N	2.20	0.57
1:A:247:VAL:CA	1:A:279:GLU:HG3	2.34	0.57
1:A:273:HIS:O	1:A:274:ARG:HB2	2.05	0.57
1:E:108:ALA:O	1:E:141:VAL:HG21	2.04	0.57
1:E:273:HIS:O	1:E:274:ARG:HB2	2.05	0.57
1:A:108:ALA:O	1:A:141:VAL:HG21	2.04	0.57
1:A:130:TYR:O	1:A:131:ILE:HD13	2.04	0.57
1:A:223:MET:CG	1:A:242:ILE:HG12	2.34	0.57
2:B:69:U:O5'	2:B:69:U:H6	1.87	0.57
1:C:108:ALA:O	1:C:141:VAL:HG21	2.04	0.57
1:E:63:ILE:CG1	1:E:64:ASN:N	2.67	0.57
1:E:68:VAL:HG23	1:E:68:VAL:O	2.04	0.57
1:E:113:MET:O	1:E:116:THR:HB	2.05	0.57
1:E:149:LEU:O	1:E:149:LEU:HD12	2.05	0.57
1:E:247:VAL:CA	1:E:279:GLU:HG3	2.34	0.57
1:A:133:VAL:HG12	1:A:134:PHE:N	2.20	0.57
1:C:273:HIS:O	1:C:274:ARG:HB2	2.05	0.57
2:D:26:M2G:H2'	2:D:26:M2G:N3	2.18	0.57
1:E:108:ALA:CB	1:E:135:MET:HG2	2.31	0.57
1:E:322:ILE:HD12	1:E:322:ILE:N	2.19	0.57
2:F:66:A:H2'	2:F:67:A:C8	2.40	0.57
1:A:43:GLU:HG2	1:A:44:VAL:N	2.13	0.56
1:A:222:LEU:CD1	1:A:222:LEU:O	2.49	0.56
1:A:229:PHE:HB2	2:B:77(A):C:O2'	2.05	0.56
1:A:321:TYR:CE2	1:A:323:LEU:HA	2.40	0.56
1:C:68:VAL:O	1:C:68:VAL:HG23	2.04	0.56
1:E:31:LEU:HD13	1:E:70:TYR:CZ	2.39	0.56
1:E:187:LYS:O	1:E:189:LYS:HD2	2.05	0.56
1:E:246:LYS:HB2	1:E:246:LYS:HZ2	1.70	0.56
1:E:286:VAL:O	2:F:77:PHA:HB3	2.05	0.56
1:E:311:THR:HG22	1:E:312:PRO:HD2	1.87	0.56
1:E:321:TYR:CE2	1:E:323:LEU:HA	2.40	0.56
2:F:69:U:H6	2:F:69:U:O5'	1.87	0.56
1:A:149:LEU:HD12	1:A:149:LEU:O	2.05	0.56
2:B:26:M2G:H2'	2:B:26:M2G:N3	2.18	0.56
1:C:26:THR:HG22	1:C:175:ALA:HB1	1.86	0.56
1:C:220:PRO:HB2	1:C:309:SER:OG	2.05	0.56
1:C:311:THR:HG22	1:C:312:PRO:HD2	1.87	0.56
2:F:15:G:H2'	2:F:16:H2U:C6	2.33	0.56
1:A:26:THR:HG22	1:A:175:ALA:HB1	1.86	0.56
1:A:29:ALA:O	1:A:31:LEU:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:A:H2'	2:B:67:A:C8	2.40	0.56
1:C:247:VAL:CA	1:C:279:GLU:HG3	2.34	0.56
1:C:322:ILE:HD12	1:C:322:ILE:N	2.19	0.56
1:E:63:ILE:CD1	2:F:2:C:H4'	2.35	0.56
1:E:380:LEU:HB3	1:E:403:ILE:HD11	1.88	0.56
1:C:229:PHE:HB2	2:D:77(A):C:O2'	2.05	0.56
1:C:289:LEU:HD12	2:D:76:A:H61	1.71	0.56
2:D:69:U:O5'	2:D:69:U:H6	1.87	0.56
1:E:215:ARG:CD	1:E:282:ALA:HB1	2.36	0.56
1:A:215:ARG:CD	1:A:282:ALA:HB1	2.36	0.56
1:C:133:VAL:HG12	1:C:134:PHE:N	2.20	0.56
1:C:149:LEU:HD12	1:C:149:LEU:O	2.05	0.56
1:C:222:LEU:CD1	1:C:222:LEU:O	2.49	0.56
1:C:316:PHE:CE1	1:C:318:ALA:HB2	2.38	0.56
1:E:229:PHE:HB2	2:F:77(A):C:O2'	2.06	0.56
1:E:380:LEU:HA	1:E:384:LEU:CD1	2.36	0.56
1:A:256:VAL:HG22	1:A:262:THR:HG23	1.87	0.56
1:A:265:THR:HB	1:A:293:VAL:HG13	1.87	0.56
1:C:187:LYS:O	1:C:189:LYS:HD2	2.05	0.56
1:E:256:VAL:HG22	1:E:262:THR:HG23	1.88	0.56
1:A:32:THR:O	1:A:33:TYR:HD1	1.89	0.56
1:C:113:MET:O	1:C:116:THR:HB	2.05	0.56
1:E:217:VAL:CG1	1:E:282:ALA:H	2.19	0.56
1:A:113:MET:O	1:A:116:THR:HB	2.05	0.56
1:A:380:LEU:HA	1:A:384:LEU:CD1	2.36	0.56
1:C:53:ALA:HB3	1:C:56:GLU:HB2	1.88	0.56
1:C:265:THR:HB	1:C:293:VAL:HG13	1.87	0.56
1:A:53:ALA:HB3	1:A:56:GLU:HB2	1.88	0.56
1:A:217:VAL:CG1	1:A:282:ALA:H	2.19	0.56
1:A:228:VAL:HG21	1:A:298:VAL:O	2.06	0.56
1:A:400:VAL:HG12	1:A:402:LYS:O	2.06	0.56
1:C:18:GLY:N	1:C:24:LYS:HD3	2.20	0.56
1:C:32:THR:O	1:C:33:TYR:HD1	1.89	0.56
1:E:228:VAL:HG21	1:E:298:VAL:O	2.06	0.56
2:F:30:G:H2'	2:F:31:A:H5''	1.86	0.56
1:C:113:MET:HE3	1:C:114:PRO:HD2	1.88	0.55
1:C:265:THR:OG1	1:C:266:VAL:N	2.39	0.55
2:D:9:A:H5'	2:D:46:7MG:C1'	2.36	0.55
1:E:113:MET:HE3	1:E:114:PRO:HD2	1.88	0.55
1:E:251:ASP:HB2	1:E:267:VAL:HG21	1.89	0.55
2:F:9:A:H5'	2:F:46:7MG:C1'	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:TYR:C	1:A:49:ASP:N	2.61	0.55
1:A:187:LYS:O	1:A:189:LYS:HD2	2.05	0.55
1:A:220:PRO:HB2	1:A:309:SER:OG	2.05	0.55
1:C:43:GLU:HG2	1:C:44:VAL:N	2.13	0.55
1:C:185:ASN:HB3	1:C:188:THR:OG1	2.07	0.55
1:C:217:VAL:CG1	1:C:282:ALA:H	2.19	0.55
1:A:239:THR:CB	2:B:77:PHA:HD1	2.33	0.55
1:C:251:ASP:HB2	1:C:267:VAL:HG21	1.89	0.55
1:E:32:THR:O	1:E:33:TYR:HD1	1.89	0.55
1:E:53:ALA:HB3	1:E:56:GLU:HB2	1.88	0.55
1:E:140:MET:HE2	1:E:140:MET:HA	1.89	0.55
1:E:346:THR:HG23	1:E:347:THR:N	2.09	0.55
1:E:400:VAL:HG12	1:E:402:LYS:O	2.06	0.55
1:C:215:ARG:CD	1:C:282:ALA:HB1	2.36	0.55
1:C:321:TYR:CE2	1:C:323:LEU:HA	2.40	0.55
1:E:265:THR:HB	1:E:293:VAL:HG13	1.87	0.55
1:E:390:GLU:O	1:E:391:GLY:C	2.50	0.55
2:F:30:G:C2'	2:F:31:A:C5'	2.85	0.55
1:A:229:PHE:CD1	1:A:237:VAL:HG13	2.42	0.55
1:A:356:PRO:HG3	1:A:370:PHE:HA	1.89	0.55
1:C:140:MET:HE2	1:C:140:MET:HA	1.89	0.55
1:C:380:LEU:HA	1:C:384:LEU:CD1	2.36	0.55
1:E:185:ASN:HB3	1:E:188:THR:OG1	2.07	0.55
1:A:140:MET:HA	1:A:140:MET:HE2	1.89	0.55
1:A:165:GLY:O	1:A:168:VAL:HG22	2.07	0.55
1:A:185:ASN:HB3	1:A:188:THR:OG1	2.07	0.55
1:A:380:LEU:HB3	1:A:403:ILE:HD11	1.88	0.55
1:C:63:ILE:CD1	2:D:2:C:H4'	2.36	0.55
1:C:356:PRO:C	1:C:358:GLY:H	2.15	0.55
1:C:400:VAL:HG12	1:C:402:LYS:O	2.06	0.55
1:E:61:ILE:CD1	1:E:63:ILE:HG22	2.37	0.55
2:F:14:A:O2'	2:F:15:G:H5'	2.07	0.55
1:A:25:THR:OG1	3:A:1406:GNP:O2B	2.25	0.55
1:A:113:MET:HE3	1:A:114:PRO:HD2	1.89	0.55
1:C:61:ILE:HD12	1:C:61:ILE:C	2.32	0.55
1:C:256:VAL:HG22	1:C:262:THR:HG23	1.88	0.55
1:E:163:PHE:C	1:E:165:GLY:H	2.15	0.55
1:E:220:PRO:HB2	1:E:309:SER:OG	2.05	0.55
1:E:393:ARG:HB3	1:E:393:ARG:NH2	2.14	0.55
1:C:163:PHE:C	1:C:165:GLY:H	2.15	0.55
1:C:165:GLY:O	1:C:168:VAL:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:A:N6	2:F:41:U:H3	2.05	0.55
1:A:265:THR:OG1	1:A:266:VAL:N	2.39	0.55
1:E:18:GLY:N	1:E:24:LYS:HD3	2.20	0.55
1:E:248:LYS:O	1:E:249:VAL:C	2.50	0.55
1:E:322:ILE:N	1:E:322:ILE:CD1	2.70	0.55
1:A:34:VAL:HG11	1:A:199:ILE:HG22	1.89	0.55
1:A:63:ILE:CD1	2:B:2:C:H4'	2.35	0.55
1:A:390:GLU:O	1:A:391:GLY:C	2.50	0.55
1:E:67:HIS:CD2	1:E:67:HIS:H	2.25	0.55
1:E:231:ILE:O	1:E:234:ARG:CZ	2.55	0.55
1:E:355:LEU:HD21	1:E:362:VAL:HG21	1.88	0.55
1:A:161:TYR:O	1:A:162:GLU:C	2.50	0.54
1:C:38:GLU:O	1:C:39:ASN:O	2.25	0.54
1:C:161:TYR:O	1:C:162:GLU:C	2.50	0.54
1:C:231:ILE:O	1:C:234:ARG:CZ	2.55	0.54
2:D:17:H2U:O2'	2:D:18:G:OP1	2.20	0.54
2:D:29:A:N6	2:D:41:U:H3	2.05	0.54
1:A:38:GLU:O	1:A:39:ASN:O	2.25	0.54
1:A:61:ILE:CD1	1:A:63:ILE:HG22	2.37	0.54
1:A:163:PHE:C	1:A:165:GLY:H	2.15	0.54
1:C:228:VAL:HG21	1:C:298:VAL:O	2.06	0.54
1:C:271:GLU:HB2	2:D:76:A:O2'	2.07	0.54
1:C:248:LYS:O	1:C:249:VAL:C	2.50	0.54
1:C:322:ILE:N	1:C:322:ILE:CD1	2.70	0.54
1:C:390:GLU:O	1:C:391:GLY:C	2.50	0.54
2:D:14:A:O2'	2:D:15:G:H5'	2.07	0.54
1:A:67:HIS:CD2	1:A:67:HIS:H	2.25	0.54
1:A:89:ILE:HG22	1:A:93:ILE:HG13	1.90	0.54
1:A:231:ILE:O	1:A:234:ARG:CZ	2.55	0.54
1:A:322:ILE:N	1:A:322:ILE:CD1	2.70	0.54
2:B:29:A:N6	2:B:41:U:H3	2.05	0.54
1:C:25:THR:OG1	3:C:1406:GNP:O2B	2.25	0.54
1:C:355:LEU:HD21	1:C:362:VAL:HG21	1.88	0.54
1:C:380:LEU:HB3	1:C:403:ILE:HD11	1.88	0.54
1:C:381:GLU:O	1:C:384:LEU:HB2	2.08	0.54
1:E:29:ALA:O	1:E:31:LEU:N	2.35	0.54
1:E:67:HIS:CD2	1:E:67:HIS:N	2.76	0.54
1:E:161:TYR:O	1:E:162:GLU:C	2.50	0.54
1:E:165:GLY:O	1:E:168:VAL:HG22	2.07	0.54
1:E:231:ILE:CG1	1:E:237:VAL:HG12	2.38	0.54
1:E:289:LEU:HD12	2:F:76:A:H61	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:CG1	1:A:237:VAL:HG12	2.38	0.54
1:A:271:GLU:HB2	2:B:76:A:O2'	2.07	0.54
2:B:34:OMG:O6	2:D:58:1MA:H5''	2.08	0.54
1:C:189:LYS:N	1:C:192:GLU:OE1	2.35	0.54
1:E:144:PRO:C	1:E:146:LEU:H	2.15	0.54
1:A:289:LEU:HD23	1:A:290:LEU:N	2.10	0.54
1:A:355:LEU:HD21	1:A:362:VAL:HG21	1.88	0.54
2:B:9:A:H5'	2:B:46:7MG:C1'	2.35	0.54
2:B:30:G:C2'	2:B:31:A:C5'	2.85	0.54
2:B:30:G:H2'	2:B:31:A:H5''	1.85	0.54
1:C:136:ASN:ND2	1:C:137:LYS:HG3	2.23	0.54
1:C:178:ALA:HB2	1:C:195:TRP:HB3	1.90	0.54
1:E:178:ALA:HB2	1:E:195:TRP:HB3	1.90	0.54
1:E:265:THR:CG2	1:E:290:LEU:HD13	2.38	0.54
1:E:229:PHE:CD1	1:E:237:VAL:HG13	2.42	0.54
1:E:356:PRO:C	1:E:358:GLY:H	2.15	0.54
1:E:381:GLU:O	1:E:384:LEU:HB2	2.08	0.54
1:A:313:HIS:CB	1:A:380:LEU:HD23	2.20	0.54
2:B:14:A:O2'	2:B:15:G:H5'	2.07	0.54
1:C:11:HIS:CD2	1:C:284:ASP:HA	2.43	0.54
1:C:144:PRO:C	1:C:146:LEU:H	2.14	0.54
1:C:356:PRO:HG3	1:C:370:PHE:HA	1.89	0.54
1:E:38:GLU:O	1:E:39:ASN:O	2.25	0.54
1:A:248:LYS:O	1:A:249:VAL:C	2.50	0.54
1:A:251:ASP:HB2	1:A:267:VAL:HG21	1.89	0.54
1:A:356:PRO:C	1:A:358:GLY:H	2.15	0.54
1:C:61:ILE:CD1	1:C:63:ILE:HG22	2.37	0.54
1:E:25:THR:OG1	3:E:1406:GNP:O2B	2.25	0.54
1:E:290:LEU:HB2	1:E:293:VAL:HG21	1.90	0.54
1:A:61:ILE:HD12	1:A:61:ILE:C	2.32	0.54
1:A:144:PRO:C	1:A:146:LEU:H	2.14	0.54
1:A:220:PRO:HB3	1:A:306:LYS:HE2	1.90	0.54
1:C:229:PHE:CD1	1:C:237:VAL:HG13	2.42	0.54
1:C:313:HIS:CB	1:C:380:LEU:HD23	2.20	0.54
1:E:11:HIS:CD2	1:E:284:ASP:HA	2.43	0.54
1:E:113:MET:H	1:E:116:THR:CB	2.21	0.54
1:E:136:ASN:ND2	1:E:137:LYS:HG3	2.23	0.54
1:E:265:THR:OG1	1:E:266:VAL:N	2.39	0.54
1:A:141:VAL:HG13	1:A:146:LEU:HD23	1.91	0.53
1:A:178:ALA:HB2	1:A:195:TRP:HB3	1.90	0.53
1:C:221:PHE:HE2	1:C:253:VAL:HG11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ILE:HD12	1:E:61:ILE:C	2.32	0.53
1:E:271:GLU:HB2	2:F:76:A:O2'	2.07	0.53
1:C:99:MET:HE3	1:C:101:GLY:O	2.08	0.53
1:C:335:PHE:N	1:C:335:PHE:CD1	2.77	0.53
1:E:89:ILE:CG2	1:E:93:ILE:HG13	2.39	0.53
1:E:231:ILE:CD1	1:E:237:VAL:HG12	2.38	0.53
1:A:290:LEU:HB2	1:A:293:VAL:HG21	1.90	0.53
1:A:295:ARG:C	1:A:297:GLU:H	2.17	0.53
1:A:381:GLU:O	1:A:384:LEU:HB2	2.08	0.53
1:C:385:ARG:HA	1:C:399:VAL:HG13	1.90	0.53
1:E:256:VAL:O	1:E:303:VAL:HG22	2.08	0.53
1:E:356:PRO:HG3	1:E:370:PHE:HA	1.89	0.53
1:A:265:THR:CG2	1:A:290:LEU:HD13	2.38	0.53
1:C:113:MET:H	1:C:116:THR:CB	2.21	0.53
1:C:159:ASN:O	1:C:161:TYR:N	2.42	0.53
1:C:249:VAL:CG1	1:C:267:VAL:O	2.57	0.53
1:E:220:PRO:HB3	1:E:306:LYS:HE2	1.90	0.53
1:E:385:ARG:HA	1:E:399:VAL:HG13	1.90	0.53
1:A:67:HIS:CD2	1:A:67:HIS:N	2.76	0.53
1:E:89:ILE:HG22	1:E:93:ILE:HG13	1.90	0.53
1:E:295:ARG:C	1:E:297:GLU:H	2.17	0.53
1:A:30:ALA:O	1:A:31:LEU:HD23	2.09	0.53
1:A:50:ILE:C	1:A:52:LYS:H	2.17	0.53
1:A:99:MET:HE3	1:A:101:GLY:O	2.08	0.53
1:A:113:MET:H	1:A:116:THR:CB	2.21	0.53
1:A:385:ARG:HA	1:A:399:VAL:HG13	1.90	0.53
1:C:231:ILE:CD1	1:C:237:VAL:HG12	2.38	0.53
1:C:231:ILE:CG1	1:C:237:VAL:HG12	2.38	0.53
1:C:256:VAL:O	1:C:303:VAL:HG22	2.09	0.53
1:E:89:ILE:O	1:E:90:LYS:C	2.51	0.53
1:E:133:VAL:CG1	1:E:134:PHE:N	2.72	0.53
1:E:301:GLY:O	1:E:346:THR:CG2	2.41	0.53
1:A:193:ASN:HB3	1:A:196:VAL:HB	1.91	0.53
1:A:316:PHE:CE1	1:A:318:ALA:HB2	2.38	0.53
1:A:335:PHE:N	1:A:335:PHE:CD1	2.77	0.53
1:C:67:HIS:CD2	1:C:67:HIS:H	2.25	0.53
1:C:67:HIS:CD2	1:C:67:HIS:N	2.76	0.53
1:C:89:ILE:O	1:C:90:LYS:C	2.51	0.53
1:C:247:VAL:O	1:C:279:GLU:HA	2.09	0.53
1:A:246:LYS:NZ	1:A:246:LYS:CB	2.72	0.53
1:A:339:ARG:HD2	1:A:352:VAL:CG2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:ARG:O	1:E:159:ASN:ND2	2.42	0.53
1:E:248:LYS:N	1:E:279:GLU:HG3	2.24	0.53
1:E:335:PHE:N	1:E:335:PHE:CD1	2.77	0.53
1:A:11:HIS:CD2	1:A:284:ASP:HA	2.43	0.53
1:A:223:MET:HG3	1:A:242:ILE:HG12	1.91	0.53
1:A:248:LYS:N	1:A:279:GLU:HG3	2.24	0.53
1:A:256:VAL:O	1:A:303:VAL:HG22	2.08	0.53
1:A:289:LEU:HD12	2:B:76:A:H61	1.71	0.53
1:C:193:ASN:HB3	1:C:196:VAL:HB	1.91	0.53
1:E:189:LYS:N	1:E:192:GLU:OE1	2.35	0.53
1:A:9:LYS:HB3	1:A:10:PRO:HD2	1.91	0.53
1:A:89:ILE:CG2	1:A:93:ILE:HG13	2.39	0.53
1:A:136:ASN:ND2	1:A:137:LYS:HG3	2.23	0.53
1:A:221:PHE:HE2	1:A:253:VAL:HG11	1.73	0.53
1:C:36:ALA:C	1:C:38:GLU:N	2.62	0.53
1:C:141:VAL:HG13	1:C:146:LEU:HD23	1.91	0.53
1:C:290:LEU:HB2	1:C:293:VAL:HG21	1.90	0.53
1:E:234:ARG:HH11	1:E:234:ARG:CG	2.22	0.53
1:A:155:ARG:O	1:A:159:ASN:ND2	2.42	0.52
1:A:156:ASP:HA	1:A:159:ASN:HD22	1.74	0.52
1:A:249:VAL:CG1	1:A:267:VAL:O	2.57	0.52
1:C:38:GLU:O	1:C:39:ASN:C	2.52	0.52
1:C:89:ILE:CG2	1:C:93:ILE:HG13	2.39	0.52
1:C:155:ARG:O	1:C:159:ASN:ND2	2.42	0.52
1:C:220:PRO:HB3	1:C:306:LYS:HE2	1.90	0.52
1:C:246:LYS:NZ	1:C:246:LYS:CB	2.72	0.52
1:C:248:LYS:O	1:C:249:VAL:O	2.28	0.52
2:D:32:OMC:C4	2:D:33:U:C5	2.96	0.52
1:E:76:HIS:CD2	1:E:77:TYR:N	2.77	0.52
1:E:223:MET:HG3	1:E:242:ILE:HG12	1.91	0.52
1:A:189:LYS:N	1:A:192:GLU:OE1	2.35	0.52
1:C:76:HIS:CD2	1:C:77:TYR:N	2.77	0.52
1:C:89:ILE:HG22	1:C:93:ILE:HG13	1.90	0.52
1:C:133:VAL:CG1	1:C:134:PHE:N	2.72	0.52
1:C:339:ARG:HD2	1:C:352:VAL:CG2	2.27	0.52
1:E:99:MET:HE3	1:E:101:GLY:O	2.08	0.52
1:A:220:PRO:O	1:A:245:GLY:HA2	2.09	0.52
1:A:222:LEU:O	1:A:222:LEU:HD22	2.10	0.52
2:B:40:5MC:H2'	2:B:41:U:C6	2.45	0.52
1:C:138:VAL:HG23	1:C:139:ASP:H	1.74	0.52
1:E:138:VAL:HG23	1:E:139:ASP:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:VAL:HG13	1:E:146:LEU:HD23	1.90	0.52
2:F:32:OMC:C4	2:F:33:U:C5	2.96	0.52
1:A:18:GLY:N	1:A:24:LYS:HD3	2.20	0.52
1:A:76:HIS:CD2	1:A:77:TYR:N	2.77	0.52
2:B:32:OMC:C4	2:B:33:U:C5	2.96	0.52
1:E:221:PHE:HE2	1:E:253:VAL:HG11	1.73	0.52
1:A:159:ASN:O	1:A:161:TYR:N	2.42	0.52
1:A:234:ARG:HH11	1:A:234:ARG:CG	2.22	0.52
1:C:125:GLN:HE22	1:C:394:THR:HB	1.75	0.52
1:C:223:MET:HG3	1:C:242:ILE:HG12	1.91	0.52
1:C:265:THR:CG2	1:C:290:LEU:HD13	2.38	0.52
1:E:50:ILE:C	1:E:52:LYS:H	2.17	0.52
1:E:159:ASN:O	1:E:161:TYR:N	2.42	0.52
1:E:247:VAL:O	1:E:279:GLU:HA	2.09	0.52
1:E:32:THR:CB	1:E:45:LYS:HB2	2.40	0.52
1:E:319:SER:N	1:E:401:THR:HG23	2.25	0.52
2:F:40:5MC:H2'	2:F:41:U:C6	2.45	0.52
1:A:38:GLU:O	1:A:39:ASN:C	2.52	0.52
1:A:133:VAL:CG1	1:A:134:PHE:N	2.72	0.52
1:A:247:VAL:O	1:A:279:GLU:HA	2.09	0.52
1:A:248:LYS:O	1:A:249:VAL:O	2.28	0.52
1:A:313:HIS:CE1	1:A:403:ILE:HD13	2.45	0.52
1:A:344:PHE:HE2	1:A:386:PHE:CG	2.28	0.52
1:C:235:GLY:HA3	1:C:289:LEU:HD21	1.92	0.52
1:A:39:ASN:HB2	1:A:42:VAL:CG2	2.39	0.52
1:A:89:ILE:O	1:A:90:LYS:C	2.51	0.52
1:C:30:ALA:O	1:C:31:LEU:HD23	2.09	0.52
1:C:156:ASP:HA	1:C:159:ASN:HD22	1.74	0.52
1:C:220:PRO:O	1:C:245:GLY:HA2	2.09	0.52
2:D:35:A:C2'	2:D:36:A:H5'	2.40	0.52
1:E:38:GLU:HB2	1:E:39:ASN:ND2	2.25	0.52
1:E:133:VAL:O	1:E:171:ILE:HD13	2.10	0.52
1:E:313:HIS:CE1	1:E:403:ILE:HD13	2.45	0.52
1:A:187:LYS:HB3	1:A:189:LYS:HZ2	1.74	0.52
1:A:393:ARG:HG2	1:A:394:THR:N	2.22	0.52
1:C:29:ALA:O	1:C:31:LEU:N	2.35	0.52
2:D:30:G:C2'	2:D:31:A:C5'	2.85	0.52
1:E:30:ALA:O	1:E:31:LEU:HD23	2.09	0.52
1:E:38:GLU:O	1:E:39:ASN:C	2.52	0.52
1:E:318:ALA:HA	1:E:401:THR:H	1.75	0.52
1:A:32:THR:CB	1:A:45:LYS:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLY:HA3	1:A:289:LEU:HD21	1.92	0.52
1:C:133:VAL:O	1:C:171:ILE:HD13	2.10	0.52
1:C:234:ARG:HH11	1:C:234:ARG:CG	2.22	0.52
2:F:47:U:O2	2:F:47:U:H2'	2.10	0.52
1:A:125:GLN:HE22	1:A:394:THR:HB	1.75	0.51
1:A:142:ASP:N	1:A:142:ASP:OD1	2.43	0.51
1:A:231:ILE:CD1	1:A:237:VAL:HG12	2.38	0.51
1:A:281:ILE:HD12	1:A:282:ALA:N	2.25	0.51
1:A:284:ASP:O	1:A:286:VAL:N	2.43	0.51
1:A:319:SER:N	1:A:401:THR:HG23	2.25	0.51
1:A:363:MET:HB2	1:A:366:ASP:CG	2.35	0.51
1:C:38:GLU:HB2	1:C:39:ASN:ND2	2.25	0.51
1:C:39:ASN:HB2	1:C:42:VAL:CG2	2.39	0.51
1:C:318:ALA:HA	1:C:401:THR:H	1.75	0.51
1:E:27:LEU:HD13	1:E:134:PHE:CE2	2.46	0.51
1:E:222:LEU:O	1:E:222:LEU:HD22	2.10	0.51
1:E:235:GLY:HA3	1:E:289:LEU:HD21	1.92	0.51
1:A:133:VAL:O	1:A:171:ILE:HD13	2.10	0.51
1:C:32:THR:CB	1:C:45:LYS:HB2	2.40	0.51
1:C:222:LEU:O	1:C:222:LEU:HD22	2.10	0.51
1:E:11:HIS:CE1	1:E:78:SER:HB2	2.45	0.51
1:E:246:LYS:NZ	1:E:246:LYS:CB	2.72	0.51
1:A:77:TYR:CZ	1:A:206:ILE:HG21	2.46	0.51
1:A:220:PRO:HB3	1:A:306:LYS:HE3	1.93	0.51
1:C:90:LYS:HE2	1:C:343:TYR:CE2	2.46	0.51
1:C:231:ILE:HD11	1:C:237:VAL:N	2.26	0.51
1:C:313:HIS:CE1	1:C:403:ILE:HD13	2.45	0.51
2:D:40:5MC:H2'	2:D:41:U:C6	2.45	0.51
2:D:47:U:H2'	2:D:47:U:O2	2.10	0.51
1:E:50:ILE:H	1:E:50:ILE:HD12	1.75	0.51
1:E:77:TYR:CZ	1:E:206:ILE:HG21	2.46	0.51
1:E:220:PRO:O	1:E:245:GLY:HA2	2.09	0.51
1:E:281:ILE:HD12	1:E:282:ALA:N	2.25	0.51
1:E:344:PHE:HE2	1:E:386:PHE:CG	2.28	0.51
2:F:35:A:C2'	2:F:36:A:H5'	2.40	0.51
1:A:138:VAL:HG23	1:A:139:ASP:H	1.74	0.51
1:A:231:ILE:HD11	1:A:237:VAL:N	2.26	0.51
1:C:142:ASP:OD1	1:C:142:ASP:N	2.43	0.51
1:C:316:PHE:HA	1:C:404:LEU:HG	1.93	0.51
2:D:14:A:C4	2:D:22:G:C2	2.99	0.51
1:E:9:LYS:HB3	1:E:10:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ASP:OD1	1:E:142:ASP:N	2.43	0.51
1:E:249:VAL:CG1	1:E:267:VAL:O	2.57	0.51
1:E:316:PHE:HA	1:E:404:LEU:HG	1.93	0.51
1:E:363:MET:HB2	1:E:366:ASP:CG	2.35	0.51
1:A:256:VAL:HB	1:A:303:VAL:CG2	2.41	0.51
1:A:378:VAL:HG13	1:A:379:ALA:N	2.26	0.51
2:B:47:U:O2	2:B:47:U:H2'	2.10	0.51
1:C:248:LYS:N	1:C:279:GLU:HG3	2.24	0.51
1:C:363:MET:HB2	1:C:366:ASP:CG	2.35	0.51
1:E:156:ASP:HA	1:E:159:ASN:HD22	1.74	0.51
1:E:270:VAL:O	1:E:270:VAL:CG1	2.52	0.51
1:E:403:ILE:C	1:E:404:LEU:HD23	2.36	0.51
1:A:38:GLU:HB2	1:A:39:ASN:ND2	2.25	0.51
1:A:139:ASP:OD2	1:A:140:MET:HE3	2.11	0.51
1:A:267:VAL:CG1	1:A:270:VAL:HG22	2.41	0.51
1:C:11:HIS:CE1	1:C:78:SER:HB2	2.46	0.51
1:C:272:MET:SD	1:C:273:HIS:CD2	3.04	0.51
1:E:39:ASN:HB2	1:E:42:VAL:CG2	2.39	0.51
1:E:248:LYS:O	1:E:249:VAL:O	2.28	0.51
1:A:50:ILE:H	1:A:50:ILE:HD12	1.75	0.51
1:A:249:VAL:HG13	1:A:269:GLY:N	2.25	0.51
1:A:371:THR:HG22	1:A:372:VAL:H	1.75	0.51
2:D:41:U:O5'	2:D:41:U:H6	1.94	0.51
2:D:74:C:O2	2:D:74:C:H2'	2.11	0.51
1:E:32:THR:CG2	1:E:45:LYS:HB2	2.41	0.51
1:E:236:THR:H	1:E:289:LEU:HD21	1.76	0.51
1:E:272:MET:SD	1:E:273:HIS:CD2	3.04	0.51
1:A:316:PHE:HA	1:A:404:LEU:HG	1.93	0.51
1:A:355:LEU:HD22	1:A:359:VAL:CG2	2.40	0.51
2:B:14:A:C4	2:B:22:G:C2	2.99	0.51
1:C:223:MET:N	1:C:304:LEU:O	2.43	0.51
1:C:295:ARG:C	1:C:297:GLU:H	2.17	0.51
1:C:319:SER:N	1:C:401:THR:HG23	2.25	0.51
1:C:390:GLU:O	1:C:391:GLY:O	2.29	0.51
1:E:231:ILE:HD11	1:E:237:VAL:N	2.26	0.51
2:F:14:A:C4	2:F:22:G:C2	2.99	0.51
1:A:324:LYS:HE2	1:A:327:GLU:OE1	2.11	0.51
1:C:50:ILE:HD12	1:C:50:ILE:H	1.75	0.51
1:C:281:ILE:HD12	1:C:282:ALA:N	2.25	0.51
1:C:313:HIS:NE2	1:C:403:ILE:HD13	2.26	0.51
1:C:403:ILE:C	1:C:404:LEU:HD23	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:ASN:HB3	1:E:196:VAL:HB	1.91	0.51
1:E:390:GLU:O	1:E:391:GLY:O	2.29	0.51
2:F:41:U:O5'	2:F:41:U:H6	1.94	0.51
1:A:318:ALA:HA	1:A:401:THR:H	1.75	0.51
2:B:74:C:H2'	2:B:74:C:O2	2.11	0.51
1:C:34:VAL:HG11	1:C:199:ILE:HG22	1.89	0.51
1:C:272:MET:HA	2:D:77:PHA:N	2.26	0.51
1:C:378:VAL:HG13	1:C:379:ALA:N	2.26	0.51
1:E:34:VAL:HG21	1:E:199:ILE:HG21	1.92	0.51
1:A:34:VAL:HG21	1:A:199:ILE:HG21	1.92	0.50
1:A:223:MET:SD	1:A:238:ALA:O	2.69	0.50
1:A:249:VAL:HA	1:A:270:VAL:CG2	2.41	0.50
1:C:222:LEU:HD12	1:C:244:ARG:N	2.23	0.50
1:E:393:ARG:HG2	1:E:394:THR:N	2.22	0.50
1:A:272:MET:HA	2:B:77:PHA:N	2.26	0.50
1:A:272:MET:SD	1:A:273:HIS:CD2	3.04	0.50
1:A:313:HIS:NE2	1:A:403:ILE:HD13	2.26	0.50
2:B:35:A:C2'	2:B:36:A:H5'	2.40	0.50
1:C:267:VAL:CG1	1:C:270:VAL:HG22	2.41	0.50
1:C:324:LYS:HE2	1:C:327:GLU:OE1	2.11	0.50
1:C:355:LEU:HD22	1:C:359:VAL:CG2	2.41	0.50
2:D:14:A:C1'	2:D:22:G:N2	2.75	0.50
1:E:19:His:HA	1:E:115:GLN:CB	2.41	0.50
1:E:193:ASN:OD1	1:E:196:VAL:HG23	2.12	0.50
1:E:220:PRO:HB3	1:E:306:LYS:HE3	1.93	0.50
1:E:324:LYS:HE2	1:E:327:GLU:OE1	2.11	0.50
1:A:32:THR:CG2	1:A:45:LYS:HB2	2.40	0.50
1:A:390:GLU:O	1:A:391:GLY:O	2.29	0.50
2:B:41:U:H6	2:B:41:U:O5'	1.94	0.50
1:C:32:THR:CG2	1:C:45:LYS:HB2	2.40	0.50
1:C:187:LYS:HB3	1:C:189:LYS:HZ2	1.76	0.50
1:C:256:VAL:HB	1:C:303:VAL:CG2	2.41	0.50
1:E:249:VAL:HA	1:E:270:VAL:CG2	2.41	0.50
1:E:267:VAL:CG1	1:E:270:VAL:HG22	2.41	0.50
1:E:361:MET:O	1:E:361:MET:HG2	2.12	0.50
1:E:378:VAL:HG13	1:E:379:ALA:N	2.26	0.50
1:A:90:LYS:HE2	1:A:343:TYR:CE2	2.45	0.50
1:C:9:LYS:HB3	1:C:10:PRO:HD2	1.91	0.50
1:C:33:TYR:CA	1:C:36:ALA:HB3	2.42	0.50
1:C:34:VAL:HG21	1:C:199:ILE:HG21	1.92	0.50
1:C:77:TYR:CZ	1:C:206:ILE:HG21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:MET:SD	1:C:238:ALA:O	2.69	0.50
1:C:344:PHE:HE2	1:C:386:PHE:CG	2.27	0.50
1:E:90:LYS:HE2	1:E:343:TYR:CE2	2.46	0.50
1:E:95:GLY:C	1:E:97:ALA:N	2.67	0.50
1:E:223:MET:SD	1:E:238:ALA:O	2.69	0.50
1:E:350:THR:N	1:E:375:ILE:HD11	2.27	0.50
1:A:222:LEU:HD22	1:A:222:LEU:C	2.37	0.50
1:C:139:ASP:OD2	1:C:140:MET:HE3	2.11	0.50
1:C:236:THR:H	1:C:289:LEU:HD21	1.76	0.50
1:C:249:VAL:HA	1:C:270:VAL:CG2	2.41	0.50
1:E:284:ASP:O	1:E:286:VAL:N	2.43	0.50
1:A:27:LEU:HD13	1:A:134:PHE:CE2	2.46	0.50
1:A:161:TYR:CD1	5:A:1408:ENX:H20	2.47	0.50
1:A:386:PHE:CD1	1:A:386:PHE:C	2.90	0.50
1:C:371:THR:HG22	1:C:372:VAL:H	1.75	0.50
1:E:355:LEU:HD22	1:E:359:VAL:CG2	2.40	0.50
1:A:344:PHE:HD1	1:A:378:VAL:HG11	1.77	0.50
1:A:403:ILE:C	1:A:404:LEU:HD23	2.36	0.50
1:E:144:PRO:C	1:E:146:LEU:N	2.70	0.50
1:E:151:GLU:O	1:E:155:ARG:HG3	2.12	0.50
2:B:14:A:C1'	2:B:22:G:N2	2.75	0.50
1:C:27:LEU:HD13	1:C:134:PHE:CE2	2.46	0.50
1:C:328:GLY:O	1:C:393:ARG:HG3	2.12	0.50
1:E:26:THR:C	1:E:28:THR:N	2.61	0.50
1:E:139:ASP:OD2	1:E:140:MET:HE3	2.11	0.50
1:E:222:LEU:HD22	1:E:222:LEU:C	2.37	0.50
1:E:251:ASP:HB2	1:E:267:VAL:CG2	2.42	0.50
1:E:267:VAL:HA	1:E:290:LEU:CD2	2.35	0.50
1:A:11:HIS:CE1	1:A:78:SER:HB2	2.46	0.50
1:A:115:GLN:NE2	1:A:118:GLU:OE1	2.45	0.50
1:A:144:PRO:C	1:A:146:LEU:N	2.70	0.50
1:A:236:THR:H	1:A:289:LEU:HD21	1.76	0.50
1:A:251:ASP:HB2	1:A:267:VAL:CG2	2.42	0.50
1:A:267:VAL:O	1:A:269:GLY:N	2.42	0.50
1:C:350:THR:N	1:C:375:ILE:HD11	2.27	0.50
1:E:39:ASN:O	1:E:42:VAL:HG23	2.12	0.50
1:E:163:PHE:C	1:E:165:GLY:N	2.69	0.50
1:E:249:VAL:HG13	1:E:269:GLY:N	2.25	0.50
1:E:272:MET:HA	2:F:77:PHA:N	2.26	0.50
1:A:33:TYR:CA	1:A:36:ALA:HB3	2.42	0.49
1:A:39:ASN:O	1:A:42:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:MET:HG2	1:A:361:MET:O	2.12	0.49
1:C:50:ILE:C	1:C:52:LYS:H	2.17	0.49
1:C:339:ARG:CD	1:C:352:VAL:HG22	2.27	0.49
1:C:386:PHE:C	1:C:386:PHE:CD1	2.90	0.49
1:E:115:GLN:NE2	1:E:118:GLU:OE1	2.45	0.49
1:E:313:HIS:NE2	1:E:403:ILE:HD13	2.26	0.49
1:C:19:HIS:HA	1:C:115:GLN:CB	2.41	0.49
1:C:113:MET:H	1:C:116:THR:HB	1.78	0.49
1:C:220:PRO:HB3	1:C:306:LYS:HE3	1.93	0.49
1:C:251:ASP:HB2	1:C:267:VAL:CG2	2.42	0.49
1:C:361:MET:O	1:C:361:MET:HG2	2.11	0.49
1:A:328:GLY:O	1:A:393:ARG:HG3	2.12	0.49
1:C:26:THR:C	1:C:28:THR:N	2.61	0.49
1:C:193:ASN:OD1	1:C:196:VAL:HG23	2.12	0.49
1:C:284:ASP:O	1:C:286:VAL:N	2.43	0.49
1:E:271:GLU:O	1:E:272:MET:CB	2.61	0.49
1:E:371:THR:HG22	1:E:372:VAL:H	1.75	0.49
1:E:386:PHE:CD1	1:E:386:PHE:C	2.90	0.49
1:A:113:MET:H	1:A:116:THR:HB	1.78	0.49
1:A:350:THR:N	1:A:375:ILE:HD11	2.27	0.49
1:C:24:LYS:HE2	1:C:82:CYS:O	2.13	0.49
1:C:39:ASN:O	1:C:42:VAL:HG23	2.12	0.49
1:C:223:MET:CE	1:C:238:ALA:O	2.60	0.49
1:E:204:ASP:O	1:E:208:GLU:HB2	2.13	0.49
1:E:339:ARG:CD	1:E:352:VAL:HG22	2.27	0.49
2:F:14:A:C1'	2:F:22:G:N2	2.74	0.49
2:F:74:C:O2	2:F:74:C:H2'	2.11	0.49
1:A:19:HIS:HA	1:A:115:GLN:CB	2.41	0.49
1:A:46:ASP:C	1:A:49:ASP:HB2	2.37	0.49
1:A:50:ILE:HG22	1:A:51:ASP:N	2.27	0.49
1:C:115:GLN:NE2	1:C:118:GLU:OE1	2.45	0.49
1:C:151:GLU:O	1:C:155:ARG:HG3	2.12	0.49
1:A:344:PHE:CE2	1:A:386:PHE:HB3	2.48	0.49
1:A:344:PHE:C	1:A:345:ARG:HG2	2.38	0.49
1:C:385:ARG:CA	1:C:399:VAL:HG13	2.43	0.49
1:E:28:THR:HG23	1:E:68:VAL:CG2	2.43	0.49
1:E:82:CYS:HB3	1:E:92:MET:HG2	1.95	0.49
2:F:59:U:O2'	2:F:60:C:H5'	2.13	0.49
1:A:121:LEU:O	1:A:125:GLN:HG3	2.13	0.49
1:A:271:GLU:O	1:A:272:MET:CB	2.61	0.49
1:A:281:ILE:HD12	1:A:282:ALA:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:PHE:CE1	1:A:378:VAL:HG11	2.48	0.49
1:C:161:TYR:CD1	5:C:1408:ENX:H20	2.47	0.49
1:C:204:ASP:O	1:C:208:GLU:HB2	2.13	0.49
1:E:24:LYS:HE2	1:E:82:CYS:O	2.13	0.49
1:E:223:MET:CE	1:E:238:ALA:O	2.60	0.49
1:A:39:ASN:ND2	1:A:42:VAL:HG21	2.27	0.49
1:A:151:GLU:O	1:A:155:ARG:HG3	2.12	0.49
1:A:217:VAL:HG21	1:A:246:LYS:HD3	1.95	0.49
1:C:28:THR:CG2	1:C:68:VAL:HG21	2.43	0.49
1:C:199:ILE:O	1:C:203:LEU:HD12	2.13	0.49
1:C:249:VAL:HG13	1:C:269:GLY:N	2.25	0.49
1:C:279:GLU:O	1:C:280:GLY:O	2.30	0.49
1:E:138:VAL:HG22	1:E:173:GLY:C	2.38	0.49
1:E:216:ASP:OD1	1:E:218:ASP:HB2	2.13	0.49
1:E:281:ILE:HD12	1:E:282:ALA:H	1.77	0.49
1:C:222:LEU:HD22	1:C:222:LEU:C	2.37	0.49
1:C:344:PHE:CE1	1:C:378:VAL:HG11	2.48	0.49
2:D:59:U:O2'	2:D:60:C:H5'	2.13	0.49
1:E:52:LYS:HD2	2:F:74:C:H4'	1.95	0.49
1:E:344:PHE:C	1:E:345:ARG:HG2	2.38	0.49
1:E:385:ARG:CA	1:E:399:VAL:HG13	2.43	0.49
1:A:223:MET:CE	1:A:238:ALA:O	2.60	0.49
1:A:279:GLU:O	1:A:280:GLY:O	2.30	0.49
1:C:121:LEU:O	1:C:125:GLN:HG3	2.13	0.49
1:C:179:LEU:HD12	1:C:179:LEU:O	2.13	0.49
1:C:279:GLU:O	1:C:280:GLY:C	2.56	0.49
1:C:344:PHE:C	1:C:345:ARG:HG2	2.38	0.49
1:E:23:GLY:O	1:E:24:LYS:C	2.56	0.49
1:E:113:MET:H	1:E:116:THR:HB	1.78	0.49
1:E:161:TYR:CD1	5:E:1408:ENX:H20	2.47	0.49
1:E:379:ALA:O	1:E:384:LEU:HD11	2.13	0.49
1:A:37:ALA:O	1:A:189:LYS:HE3	2.13	0.48
1:A:156:ASP:O	1:A:159:ASN:HB2	2.13	0.48
1:A:199:ILE:O	1:A:203:LEU:HD12	2.13	0.48
1:A:279:GLU:O	1:A:280:GLY:C	2.56	0.48
1:C:46:ASP:C	1:C:49:ASP:HB2	2.37	0.48
1:C:50:ILE:HG22	1:C:51:ASP:N	2.27	0.48
1:C:216:ASP:OD1	1:C:218:ASP:HB2	2.13	0.48
2:D:62:A:O2'	2:D:63:C:H5'	2.13	0.48
1:E:251:ASP:O	1:E:267:VAL:HG23	2.13	0.48
1:A:113:MET:HE3	1:A:114:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLY:O	1:C:24:LYS:C	2.56	0.48
1:C:29:ALA:HA	1:C:32:THR:OG1	2.13	0.48
1:C:39:ASN:ND2	1:C:42:VAL:HG21	2.27	0.48
1:E:29:ALA:HA	1:E:32:THR:OG1	2.13	0.48
1:E:134:PHE:O	1:E:136:ASN:N	2.46	0.48
1:E:279:GLU:O	1:E:280:GLY:C	2.56	0.48
1:E:328:GLY:O	1:E:393:ARG:HG3	2.12	0.48
2:F:32:OMC:CM2	2:F:33:U:H5'	2.44	0.48
1:C:12:VAL:CG2	1:C:75:ARG:HD2	2.40	0.48
1:C:163:PHE:C	1:C:165:GLY:N	2.69	0.48
1:C:217:VAL:CG1	1:C:282:ALA:HB2	2.44	0.48
1:C:247:VAL:N	1:C:279:GLU:HG3	2.29	0.48
1:E:12:VAL:CG2	1:E:75:ARG:HD2	2.40	0.48
1:E:39:ASN:ND2	1:E:42:VAL:HG21	2.27	0.48
1:E:143:ASP:O	1:E:146:LEU:HB3	2.14	0.48
1:E:299:GLU:O	1:E:300:ARG:C	2.57	0.48
1:E:344:PHE:CE2	1:E:386:PHE:HB3	2.48	0.48
1:A:28:THR:CG2	1:A:68:VAL:HG21	2.43	0.48
1:A:89:ILE:HD12	1:A:122:LEU:HD12	1.95	0.48
1:A:251:ASP:O	1:A:267:VAL:HG23	2.13	0.48
1:A:275:LYS:O	1:A:276:THR:C	2.56	0.48
1:A:281:ILE:HD12	1:A:282:ALA:CB	2.43	0.48
1:C:143:ASP:O	1:C:146:LEU:HB3	2.14	0.48
1:E:28:THR:CG2	1:E:68:VAL:HG21	2.43	0.48
1:E:33:TYR:CA	1:E:36:ALA:HB3	2.42	0.48
1:E:34:VAL:CB	1:E:199:ILE:HG21	2.44	0.48
1:E:46:ASP:C	1:E:49:ASP:HB2	2.37	0.48
1:E:156:ASP:O	1:E:159:ASN:HB2	2.14	0.48
1:A:24:LYS:HE2	1:A:82:CYS:O	2.13	0.48
1:A:341:GLN:HE21	1:A:390:GLU:HA	1.79	0.48
1:C:28:THR:HG23	1:C:68:VAL:CG2	2.43	0.48
1:C:95:GLY:C	1:C:97:ALA:N	2.67	0.48
1:C:134:PHE:O	1:C:136:ASN:N	2.46	0.48
1:C:281:ILE:HD12	1:C:282:ALA:H	1.78	0.48
1:C:341:GLN:HE21	1:C:390:GLU:HA	1.79	0.48
1:E:217:VAL:HG21	1:E:246:LYS:HD3	1.95	0.48
1:A:247:VAL:N	1:A:279:GLU:HG3	2.29	0.48
1:A:345:ARG:HG3	1:A:346:THR:H	1.78	0.48
1:C:345:ARG:HG3	1:C:346:THR:H	1.78	0.48
2:D:9:A:H4'	2:D:46:7MG:H4'	1.96	0.48
1:E:77:TYR:CE2	1:E:206:ILE:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:LEU:HD12	1:E:179:LEU:O	2.13	0.48
1:E:205:ALA:CA	1:E:208:GLU:HB3	2.43	0.48
1:E:281:ILE:HD12	1:E:282:ALA:CB	2.43	0.48
1:E:344:PHE:HD1	1:E:378:VAL:HG11	1.77	0.48
1:E:345:ARG:HG3	1:E:346:THR:H	1.78	0.48
1:A:134:PHE:O	1:A:136:ASN:N	2.46	0.48
1:A:193:ASN:OD1	1:A:196:VAL:HG23	2.12	0.48
1:A:217:VAL:CG1	1:A:282:ALA:HB2	2.44	0.48
1:C:37:ALA:O	1:C:189:LYS:HE3	2.13	0.48
1:C:344:PHE:HD1	1:C:378:VAL:HG11	1.77	0.48
1:E:102:ALA:H	1:E:131:ILE:HD13	1.79	0.48
1:E:199:ILE:O	1:E:203:LEU:HD12	2.13	0.48
1:E:256:VAL:HB	1:E:303:VAL:CG2	2.41	0.48
1:A:62:THR:HB	3:A:1406:GNP:O1G	2.14	0.48
1:A:102:ALA:H	1:A:131:ILE:HD13	1.79	0.48
1:A:179:LEU:HD12	1:A:179:LEU:O	2.13	0.48
1:A:216:ASP:OD1	1:A:218:ASP:HB2	2.13	0.48
2:B:59:U:O2'	2:B:60:C:H5'	2.13	0.48
1:C:52:LYS:HD2	2:D:74:C:H4'	1.95	0.48
1:C:251:ASP:O	1:C:267:VAL:HG23	2.13	0.48
2:D:32:OMC:CM2	2:D:33:U:H5'	2.44	0.48
1:E:113:MET:HE3	1:E:114:PRO:CD	2.43	0.48
1:A:82:CYS:HB3	1:A:92:MET:HG2	1.95	0.48
1:A:138:VAL:HG22	1:A:173:GLY:C	2.38	0.48
1:A:182:MET:SD	1:A:196:VAL:HG21	2.54	0.48
1:A:204:ASP:O	1:A:208:GLU:HB2	2.13	0.48
1:A:248:LYS:HG3	1:A:251:ASP:OD1	2.14	0.48
1:A:379:ALA:O	1:A:384:LEU:HD11	2.13	0.48
2:B:62:A:O2'	2:B:63:C:H5'	2.13	0.48
1:C:299:GLU:O	1:C:300:ARG:C	2.57	0.48
1:C:379:ALA:O	1:C:384:LEU:HD11	2.13	0.48
1:E:339:ARG:HD2	1:E:352:VAL:CG2	2.27	0.48
1:A:17:ILE:O	1:A:17:ILE:CG1	2.61	0.48
1:A:32:THR:C	1:A:36:ALA:HB2	2.39	0.48
1:A:36:ALA:C	1:A:38:GLU:N	2.62	0.48
1:A:266:VAL:O	1:A:290:LEU:HD23	2.14	0.48
2:B:32:OMC:CM2	2:B:33:U:H5'	2.44	0.48
1:C:203:LEU:C	1:C:205:ALA:N	2.72	0.48
1:C:269:GLY:O	1:C:289:LEU:N	2.44	0.48
1:C:271:GLU:O	1:C:272:MET:CB	2.60	0.48
1:C:281:ILE:HD12	1:C:282:ALA:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:PHE:CE2	1:C:386:PHE:HB3	2.48	0.48
1:E:37:ALA:O	1:E:189:LYS:HE3	2.13	0.48
1:E:125:GLN:HE22	1:E:394:THR:HB	1.75	0.48
1:E:344:PHE:CE1	1:E:378:VAL:HG11	2.48	0.48
1:A:29:ALA:HA	1:A:32:THR:OG1	2.13	0.47
1:A:156:ASP:O	1:A:160:GLN:HG3	2.14	0.47
1:A:241:ARG:C	1:A:241:ARG:CD	2.80	0.47
1:A:271:GLU:HG3	2:B:76:A:C2	2.49	0.47
1:A:299:GLU:O	1:A:300:ARG:C	2.57	0.47
1:C:190:ARG:NH1	1:C:200:TRP:CB	2.77	0.47
1:E:32:THR:C	1:E:36:ALA:HB2	2.39	0.47
1:E:50:ILE:HG22	1:E:51:ASP:N	2.27	0.47
1:E:89:ILE:HD12	1:E:122:LEU:HD12	1.95	0.47
1:E:121:LEU:O	1:E:125:GLN:HG3	2.13	0.47
1:E:182:MET:SD	1:E:196:VAL:HG21	2.54	0.47
1:E:217:VAL:HG11	1:E:246:LYS:HD3	1.96	0.47
1:E:369:THR:HG22	1:E:370:PHE:N	2.29	0.47
1:A:34:VAL:CB	1:A:199:ILE:HG21	2.44	0.47
1:A:203:LEU:C	1:A:205:ALA:N	2.72	0.47
1:C:82:CYS:HB3	1:C:92:MET:HG2	1.95	0.47
1:C:132:VAL:HG12	1:C:169:PRO:CD	2.44	0.47
1:C:144:PRO:C	1:C:146:LEU:N	2.70	0.47
1:C:156:ASP:O	1:C:159:ASN:HB2	2.13	0.47
1:C:156:ASP:O	1:C:160:GLN:HG3	2.14	0.47
1:C:271:GLU:HG3	2:D:76:A:C2	2.49	0.47
1:E:217:VAL:CG1	1:E:282:ALA:HB2	2.44	0.47
1:E:279:GLU:O	1:E:280:GLY:O	2.30	0.47
1:E:341:GLN:HE21	1:E:390:GLU:HA	1.79	0.47
2:F:49:5MC:C2	2:F:50:U:C5	3.02	0.47
1:A:23:GLY:O	1:A:24:LYS:C	2.56	0.47
1:A:36:ALA:O	1:A:38:GLU:N	2.47	0.47
1:A:221:PHE:CE2	1:A:253:VAL:HG11	2.50	0.47
1:A:385:ARG:CA	1:A:399:VAL:HG13	2.43	0.47
2:B:9:A:H4'	2:B:46:7MG:H4'	1.95	0.47
1:C:17:ILE:O	1:C:17:ILE:CG1	2.61	0.47
1:C:24:LYS:N	3:C:1406:GNP:O1B	2.47	0.47
1:C:138:VAL:HG22	1:C:173:GLY:C	2.38	0.47
1:C:205:ALA:CA	1:C:208:GLU:HB3	2.43	0.47
1:C:249:VAL:HA	1:C:270:VAL:HG21	1.95	0.47
1:C:266:VAL:O	1:C:290:LEU:HD23	2.14	0.47
2:D:34:OMG:C8	2:F:20:G:C6	3.01	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ALA:C	1:E:38:GLU:N	2.63	0.47
1:E:57:ARG:HB3	1:E:57:ARG:HH11	1.80	0.47
1:E:62:THR:HB	3:E:1406:GNP:O1G	2.14	0.47
1:E:91:ASN:O	1:E:92:MET:C	2.57	0.47
1:E:156:ASP:O	1:E:160:GLN:HG3	2.14	0.47
1:E:248:LYS:HG3	1:E:251:ASP:OD1	2.14	0.47
1:E:267:VAL:HG12	1:E:270:VAL:CG2	2.44	0.47
1:E:304:LEU:HD23	1:E:304:LEU:HA	1.63	0.47
2:F:62:A:O2'	2:F:63:C:H5'	2.13	0.47
1:A:184:LYS:HA	1:A:184:LYS:CE	2.39	0.47
1:A:301:GLY:O	1:A:346:THR:CG2	2.41	0.47
1:A:369:THR:HG22	1:A:370:PHE:N	2.29	0.47
2:B:49:5MC:C2	2:B:50:U:C5	3.02	0.47
1:C:112:PRO:HB3	1:C:116:THR:HG21	1.97	0.47
1:C:113:MET:HE3	1:C:114:PRO:CD	2.43	0.47
1:C:182:MET:SD	1:C:196:VAL:HG21	2.54	0.47
1:C:221:PHE:CE2	1:C:253:VAL:HG11	2.50	0.47
2:D:37:YG:H31	2:D:37:YG:C1'	2.44	0.47
2:D:67:A:H2'	2:D:68:U:C6	2.50	0.47
1:E:24:LYS:N	3:E:1406:GNP:O1B	2.47	0.47
1:E:203:LEU:C	1:E:205:ALA:N	2.72	0.47
1:E:247:VAL:N	1:E:279:GLU:HG3	2.29	0.47
1:E:249:VAL:HA	1:E:270:VAL:HG21	1.95	0.47
1:E:275:LYS:O	1:E:276:THR:C	2.56	0.47
1:E:361:MET:O	1:E:361:MET:CG	2.62	0.47
2:F:37:YG:H31	2:F:37:YG:C1'	2.44	0.47
1:A:132:VAL:HG12	1:A:169:PRO:CD	2.44	0.47
1:A:143:ASP:O	1:A:146:LEU:HB3	2.14	0.47
1:A:249:VAL:HA	1:A:270:VAL:HG21	1.95	0.47
1:A:344:PHE:C	1:A:345:ARG:CG	2.88	0.47
1:C:62:THR:HB	3:C:1406:GNP:O1G	2.14	0.47
1:C:89:ILE:HD12	1:C:122:LEU:HD12	1.95	0.47
1:C:248:LYS:HG3	1:C:251:ASP:OD1	2.14	0.47
1:E:223:MET:N	1:E:304:LEU:O	2.43	0.47
1:E:331:HIS:NE2	2:F:54:5MU:OP1	2.38	0.47
1:A:24:LYS:N	3:A:1406:GNP:O1B	2.47	0.47
1:A:91:ASN:O	1:A:92:MET:C	2.57	0.47
1:A:93:ILE:O	1:A:94:THR:C	2.58	0.47
1:A:112:PRO:HB3	1:A:116:THR:HG21	1.97	0.47
1:A:205:ALA:O	1:A:209:TYR:N	2.45	0.47
1:C:91:ASN:O	1:C:92:MET:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:LYS:O	1:C:276:THR:C	2.56	0.47
1:E:34:VAL:HG11	1:E:199:ILE:HG22	1.89	0.47
1:E:36:ALA:O	1:E:38:GLU:N	2.47	0.47
1:E:267:VAL:O	1:E:269:GLY:N	2.42	0.47
1:A:10:PRO:O	1:A:76:HIS:N	2.47	0.47
1:A:35:ALA:O	1:A:42:VAL:HG21	2.15	0.47
1:A:52:LYS:HD2	2:B:74:C:H4'	1.95	0.47
1:A:77:TYR:CE2	1:A:206:ILE:HG21	2.48	0.47
1:A:124:ARG:HD2	1:A:163:PHE:CZ	2.50	0.47
1:A:181:GLU:C	1:A:183:HIS:N	2.72	0.47
1:A:205:ALA:CA	1:A:208:GLU:HB3	2.43	0.47
1:A:266:VAL:HG12	1:A:268:THR:HG23	1.97	0.47
1:A:363:MET:HE3	1:A:363:MET:HB3	1.84	0.47
1:C:32:THR:C	1:C:36:ALA:HB2	2.39	0.47
1:C:34:VAL:CB	1:C:199:ILE:HG21	2.44	0.47
1:C:45:LYS:HG3	1:C:68:VAL:HB	1.97	0.47
1:C:57:ARG:HB3	1:C:57:ARG:HH11	1.80	0.47
1:C:77:TYR:CE2	1:C:206:ILE:HG21	2.48	0.47
1:C:217:VAL:HG21	1:C:246:LYS:HD3	1.95	0.47
1:C:247:VAL:HG21	1:C:267:VAL:CG1	2.34	0.47
1:C:403:ILE:CG2	1:C:404:LEU:N	2.77	0.47
1:E:93:ILE:O	1:E:94:THR:C	2.58	0.47
1:E:190:ARG:NH1	1:E:200:TRP:CB	2.77	0.47
1:E:274:ARG:CZ	2:F:76:A:C5'	2.89	0.47
1:E:316:PHE:CE1	1:E:318:ALA:HB2	2.38	0.47
2:F:9:A:H4'	2:F:46:7MG:H4'	1.95	0.47
1:A:136:ASN:HA	1:A:173:GLY:O	2.15	0.47
1:A:403:ILE:CG2	1:A:404:LEU:N	2.77	0.47
1:C:35:ALA:O	1:C:42:VAL:HG21	2.15	0.47
1:C:271:GLU:HA	1:C:276:THR:HA	1.97	0.47
1:E:121:LEU:HB2	1:E:161:TYR:HE1	1.75	0.47
1:E:124:ARG:HD2	1:E:163:PHE:CZ	2.50	0.47
1:E:184:LYS:C	1:E:186:PRO:HD3	2.40	0.47
1:E:242:ILE:HG13	1:E:286:VAL:HG13	1.97	0.47
1:C:102:ALA:H	1:C:131:ILE:HD13	1.79	0.47
1:E:45:LYS:HG3	1:E:68:VAL:HB	1.97	0.47
1:E:123:ALA:HA	1:E:126:VAL:CG2	2.45	0.47
1:E:301:GLY:HA2	1:E:346:THR:CG2	2.45	0.47
1:A:28:THR:HG23	1:A:68:VAL:CG2	2.43	0.47
1:A:45:LYS:HA	1:A:45:LYS:HD3	1.59	0.47
1:A:267:VAL:HG12	1:A:270:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:A:H2'	2:B:68:U:C6	2.50	0.47
1:C:123:ALA:HA	1:C:126:VAL:CG2	2.45	0.47
1:C:124:ARG:HD2	1:C:163:PHE:CZ	2.50	0.47
1:C:136:ASN:HA	1:C:173:GLY:O	2.15	0.47
1:C:344:PHE:C	1:C:345:ARG:CG	2.88	0.47
1:E:157:LEU:C	1:E:159:ASN:N	2.72	0.47
1:E:184:LYS:HA	1:E:184:LYS:CE	2.39	0.47
1:E:223:MET:HG2	1:E:242:ILE:HG12	1.97	0.47
1:E:395:VAL:CG2	1:E:396:GLY:N	2.78	0.47
1:E:403:ILE:CG2	1:E:404:LEU:N	2.77	0.47
2:F:67:A:H2'	2:F:68:U:C6	2.50	0.47
1:A:32:THR:O	1:A:36:ALA:CB	2.63	0.46
1:A:163:PHE:C	1:A:165:GLY:N	2.69	0.46
1:A:222:LEU:HD12	1:A:244:ARG:N	2.23	0.46
1:A:267:VAL:HA	1:A:290:LEU:CD2	2.35	0.46
1:A:361:MET:O	1:A:361:MET:CG	2.62	0.46
1:C:205:ALA:O	1:C:209:TYR:N	2.45	0.46
2:D:37:YG:C19	2:D:37:YG:C14	2.93	0.46
2:D:49:5MC:C2	2:D:50:U:C5	3.02	0.46
1:E:112:PRO:HB3	1:E:116:THR:HG21	1.97	0.46
1:E:271:GLU:HG3	2:F:76:A:C2	2.49	0.46
1:A:123:ALA:HA	1:A:126:VAL:CG2	2.45	0.46
1:C:32:THR:O	1:C:36:ALA:CB	2.63	0.46
1:C:369:THR:HG22	1:C:370:PHE:N	2.29	0.46
1:E:32:THR:O	1:E:36:ALA:CB	2.63	0.46
1:E:344:PHE:C	1:E:345:ARG:CG	2.88	0.46
1:A:157:LEU:C	1:A:159:ASN:N	2.72	0.46
1:A:223:MET:HG2	1:A:242:ILE:HG12	1.97	0.46
1:C:184:LYS:HA	1:C:184:LYS:CE	2.39	0.46
1:C:395:VAL:CG2	1:C:396:GLY:N	2.77	0.46
1:E:266:VAL:O	1:E:290:LEU:HD23	2.14	0.46
2:F:37:YG:C19	2:F:37:YG:C14	2.93	0.46
1:A:256:VAL:HG22	1:A:262:THR:CG2	2.45	0.46
1:A:301:GLY:HA2	1:A:346:THR:CG2	2.45	0.46
1:C:125:GLN:C	1:C:127:GLY:H	2.24	0.46
1:C:267:VAL:HG12	1:C:270:VAL:CG2	2.44	0.46
1:A:45:LYS:HG3	1:A:68:VAL:HB	1.97	0.46
1:A:231:ILE:HG12	1:A:237:VAL:HG12	1.97	0.46
1:A:316:PHE:HE2	1:A:374:LEU:HD21	1.81	0.46
1:A:395:VAL:CG2	1:A:396:GLY:N	2.77	0.46
1:C:36:ALA:O	1:C:38:GLU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ILE:HG13	1:C:286:VAL:HG13	1.97	0.46
1:C:266:VAL:HG12	1:C:268:THR:HG23	1.97	0.46
1:C:267:VAL:HA	1:C:290:LEU:CD2	2.35	0.46
1:C:267:VAL:O	1:C:269:GLY:N	2.41	0.46
1:C:301:GLY:O	1:C:346:THR:CG2	2.41	0.46
2:F:36:A:C2'	2:F:37:YG:H8	2.26	0.46
1:A:57:ARG:HB3	1:A:57:ARG:HH11	1.80	0.46
1:A:140:MET:HE2	1:A:140:MET:CA	2.46	0.46
1:C:18:GLY:O	1:C:24:LYS:HD3	2.16	0.46
1:C:32:THR:HG21	1:C:45:LYS:CB	2.44	0.46
1:C:32:THR:O	1:C:33:TYR:CD1	2.69	0.46
1:C:217:VAL:HG11	1:C:246:LYS:HD3	1.96	0.46
1:C:223:MET:HG2	1:C:242:ILE:HG12	1.97	0.46
1:C:241:ARG:HG2	1:C:283:GLY:O	2.16	0.46
1:E:35:ALA:O	1:E:42:VAL:HG21	2.15	0.46
1:E:117:ARG:O	1:E:118:GLU:C	2.59	0.46
1:E:221:PHE:CE2	1:E:253:VAL:HG11	2.50	0.46
1:E:229:PHE:CB	2:F:77(A):C:H1'	2.46	0.46
1:E:254:GLU:HB2	1:E:305:ALA:O	2.16	0.46
1:E:306:LYS:HE3	1:E:309:SER:OG	2.16	0.46
1:A:18:GLY:O	1:A:24:LYS:HD3	2.15	0.46
1:A:190:ARG:NH1	1:A:200:TRP:CB	2.77	0.46
1:A:242:ILE:HG13	1:A:286:VAL:HG13	1.97	0.46
1:A:369:THR:O	1:A:370:PHE:HB3	2.16	0.46
1:C:139:ASP:OD1	1:C:174:SER:HB2	2.16	0.46
1:C:369:THR:O	1:C:370:PHE:HB3	2.16	0.46
1:E:32:THR:O	1:E:33:TYR:CD1	2.69	0.46
1:E:136:ASN:HA	1:E:173:GLY:O	2.15	0.46
1:A:229:PHE:CB	2:B:77(A):C:H1'	2.46	0.46
1:A:263:ARG:CD	1:A:297:GLU:HB3	2.46	0.46
1:A:271:GLU:HA	1:A:276:THR:HA	1.97	0.46
1:A:306:LYS:HE3	1:A:309:SER:OG	2.16	0.46
1:A:376:LYS:HB3	1:A:377:PRO:CD	2.46	0.46
2:B:37:YG:H31	2:B:37:YG:C1'	2.45	0.46
1:C:10:PRO:O	1:C:76:HIS:N	2.47	0.46
1:C:138:VAL:HG23	1:C:139:ASP:N	2.31	0.46
1:C:181:GLU:C	1:C:183:HIS:N	2.72	0.46
1:C:263:ARG:CD	1:C:297:GLU:HB3	2.46	0.46
1:E:18:GLY:O	1:E:24:LYS:HD3	2.15	0.46
1:E:94:THR:O	1:E:95:GLY:C	2.58	0.46
1:E:258:LEU:CD1	1:E:301:GLY:HA3	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:THR:O	1:E:370:PHE:HB3	2.16	0.46
1:E:386:PHE:C	5:E:1408:ENX:CL30	2.96	0.46
1:A:217:VAL:HG11	1:A:246:LYS:HD3	1.96	0.46
1:A:226:GLU:C	1:A:226:GLU:CD	2.84	0.46
1:A:254:GLU:OE1	1:A:307:PRO:HA	2.16	0.46
1:A:305:ALA:HB1	1:A:309:SER:HB2	1.98	0.46
1:C:229:PHE:CB	2:D:77(A):C:H1'	2.46	0.46
1:C:246:LYS:HG2	1:C:281:ILE:CB	2.46	0.46
1:C:254:GLU:OE1	1:C:307:PRO:HA	2.16	0.46
1:C:306:LYS:HE3	1:C:309:SER:OG	2.16	0.46
1:C:376:LYS:HB3	1:C:377:PRO:CD	2.46	0.46
2:D:36:A:C2'	2:D:37:YG:H8	2.26	0.46
2:D:57:G:H2'	2:D:58:1MA:H5'	1.98	0.46
1:E:205:ALA:O	1:E:209:TYR:N	2.45	0.46
1:E:246:LYS:HG2	1:E:281:ILE:CB	2.46	0.46
1:E:256:VAL:HG22	1:E:262:THR:CG2	2.45	0.46
1:E:263:ARG:CD	1:E:297:GLU:HB3	2.46	0.46
1:E:376:LYS:HB3	1:E:377:PRO:CD	2.46	0.46
1:A:12:VAL:HB	1:A:77:TYR:CD1	2.51	0.46
1:A:72:THR:HG22	1:A:203:LEU:HD22	1.98	0.46
1:A:94:THR:O	1:A:95:GLY:C	2.58	0.46
1:A:133:VAL:HG21	1:A:154:VAL:CG1	2.46	0.46
1:A:138:VAL:HG23	1:A:139:ASP:N	2.31	0.46
1:A:245:GLY:O	1:A:246:LYS:HB2	2.16	0.46
2:B:57:G:H2'	2:B:58:1MA:H5'	1.98	0.46
1:C:52:LYS:CD	2:D:74:C:H4'	2.46	0.46
1:C:285:ASN:O	2:D:77:PHA:HB3	2.16	0.46
1:C:340:PRO:O	1:C:340:PRO:HG2	2.15	0.46
1:E:200:TRP:O	1:E:201:GLU:C	2.59	0.46
1:E:245:GLY:O	1:E:246:LYS:HB2	2.16	0.46
1:E:340:PRO:HG2	1:E:340:PRO:O	2.15	0.46
1:A:386:PHE:C	5:A:1408:ENX:CL30	2.96	0.45
1:C:256:VAL:HG22	1:C:262:THR:CG2	2.45	0.45
1:E:139:ASP:OD1	1:E:174:SER:HB2	2.16	0.45
1:E:269:GLY:O	1:E:289:LEU:N	2.44	0.45
1:E:271:GLU:HA	1:E:276:THR:HA	1.97	0.45
1:E:341:GLN:H	1:E:341:GLN:NE2	2.14	0.45
1:A:220:PRO:CB	1:A:309:SER:OG	2.64	0.45
1:A:331:HIS:NE2	2:B:54:5MU:OP1	2.38	0.45
1:C:200:TRP:O	1:C:201:GLU:C	2.59	0.45
1:C:231:ILE:HG12	1:C:237:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:GLY:O	1:C:246:LYS:HB2	2.16	0.45
1:C:316:PHE:CD1	1:C:317:GLU:N	2.84	0.45
1:E:130:TYR:HB3	1:E:209:TYR:HD2	1.82	0.45
1:E:132:VAL:HG12	1:E:169:PRO:CD	2.44	0.45
1:E:219:LYS:N	1:E:219:LYS:CD	2.72	0.45
1:E:226:GLU:CD	1:E:226:GLU:C	2.84	0.45
1:E:254:GLU:OE1	1:E:307:PRO:HA	2.16	0.45
1:E:316:PHE:HE2	1:E:374:LEU:HD21	1.81	0.45
1:C:12:VAL:HB	1:C:77:TYR:CD1	2.51	0.45
1:C:43:GLU:CG	1:C:44:VAL:N	2.77	0.45
1:C:93:ILE:O	1:C:94:THR:C	2.58	0.45
1:C:305:ALA:HB1	1:C:309:SER:HB2	1.98	0.45
1:C:344:PHE:CE1	1:C:380:LEU:HD11	2.52	0.45
1:C:386:PHE:C	5:C:1408:ENX:CL30	2.96	0.45
1:E:12:VAL:HB	1:E:77:TYR:CD1	2.51	0.45
1:E:72:THR:HG22	1:E:203:LEU:HD22	1.98	0.45
1:E:138:VAL:HG23	1:E:139:ASP:N	2.31	0.45
1:E:220:PRO:CB	1:E:309:SER:OG	2.64	0.45
1:E:269:GLY:HA3	1:E:289:LEU:HB3	1.99	0.45
1:E:306:LYS:C	1:E:306:LYS:CD	2.88	0.45
1:E:316:PHE:CD1	1:E:317:GLU:N	2.84	0.45
1:A:12:VAL:CG2	1:A:75:ARG:HD2	2.40	0.45
1:A:241:ARG:HG2	1:A:283:GLY:O	2.16	0.45
1:A:246:LYS:HG2	1:A:281:ILE:CB	2.46	0.45
1:A:341:GLN:H	1:A:341:GLN:NE2	2.14	0.45
1:C:72:THR:HG22	1:C:203:LEU:HD22	1.98	0.45
1:C:361:MET:O	1:C:361:MET:CG	2.62	0.45
1:E:52:LYS:CD	2:F:74:C:H4'	2.46	0.45
1:E:140:MET:HE2	1:E:140:MET:CA	2.46	0.45
1:E:266:VAL:HG12	1:E:268:THR:HG23	1.97	0.45
1:A:24:LYS:CE	1:A:82:CYS:O	2.65	0.45
1:A:31:LEU:C	1:A:33:TYR:H	2.25	0.45
1:A:184:LYS:C	1:A:186:PRO:HD3	2.40	0.45
1:A:269:GLY:HA3	1:A:289:LEU:HB3	1.99	0.45
1:C:157:LEU:C	1:C:159:ASN:N	2.72	0.45
1:E:24:LYS:CE	1:E:82:CYS:O	2.65	0.45
1:E:125:GLN:C	1:E:127:GLY:H	2.24	0.45
1:E:285:ASN:O	2:F:77:PHA:HB3	2.16	0.45
1:E:305:ALA:HB1	1:E:309:SER:HB2	1.98	0.45
1:A:130:TYR:HB3	1:A:209:TYR:HD2	1.82	0.45
1:A:223:MET:N	1:A:304:LEU:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:HB2	1:A:305:ALA:O	2.16	0.45
1:A:274:ARG:CZ	2:B:76:A:C5'	2.89	0.45
1:A:316:PHE:CD1	1:A:317:GLU:N	2.84	0.45
2:B:20:G:C6	2:F:34:OMG:C8	3.05	0.45
1:C:45:LYS:HD3	1:C:45:LYS:HA	1.60	0.45
1:C:226:GLU:C	1:C:226:GLU:CD	2.84	0.45
1:C:301:GLY:HA2	1:C:346:THR:CG2	2.45	0.45
1:E:181:GLU:C	1:E:183:HIS:N	2.72	0.45
1:E:215:ARG:HD2	1:E:282:ALA:HB1	1.98	0.45
1:E:241:ARG:HG2	1:E:283:GLY:O	2.16	0.45
1:E:335:PHE:CD2	1:E:361:MET:HB2	2.52	0.45
1:A:12:VAL:HG22	1:A:213:PRO:HG3	1.99	0.45
1:A:52:LYS:CD	2:B:74:C:H4'	2.46	0.45
1:A:119:HIS:O	1:A:120:ILE:C	2.59	0.45
1:A:266:VAL:O	1:A:290:LEU:CA	2.50	0.45
2:B:37:YG:C19	2:B:37:YG:C14	2.93	0.45
1:C:184:LYS:C	1:C:186:PRO:HD3	2.40	0.45
1:C:215:ARG:HD2	1:C:282:ALA:HB1	1.98	0.45
1:C:323:LEU:HD12	1:C:395:VAL:C	2.42	0.45
1:E:119:HIS:O	1:E:120:ILE:C	2.59	0.45
1:C:24:LYS:CE	1:C:82:CYS:O	2.65	0.45
1:E:45:LYS:HA	1:E:45:LYS:HD3	1.60	0.45
1:E:79:HIS:CD2	1:E:79:HIS:C	2.95	0.45
1:E:133:VAL:CG2	1:E:154:VAL:HG11	2.46	0.45
1:E:222:LEU:HD12	1:E:244:ARG:N	2.23	0.45
1:E:231:ILE:HG12	1:E:237:VAL:HG12	1.98	0.45
1:A:29:ALA:C	1:A:31:LEU:N	2.72	0.45
1:A:117:ARG:O	1:A:118:GLU:C	2.59	0.45
1:A:139:ASP:OD1	1:A:174:SER:HB2	2.16	0.45
1:A:340:PRO:O	1:A:340:PRO:HG2	2.15	0.45
1:C:12:VAL:HG22	1:C:213:PRO:HG3	1.99	0.45
1:C:79:HIS:CD2	1:C:79:HIS:C	2.95	0.45
1:C:104:LEU:HD23	1:C:133:VAL:HG22	1.99	0.45
1:C:130:TYR:HB3	1:C:209:TYR:HD2	1.82	0.45
1:C:254:GLU:HB2	1:C:305:ALA:O	2.16	0.45
1:C:335:PHE:CD2	1:C:361:MET:HB2	2.52	0.45
1:E:101:GLY:HA2	1:E:130:TYR:O	2.17	0.45
1:E:245:GLY:O	1:E:246:LYS:CB	2.65	0.45
1:A:227:ASP:O	1:A:238:ALA:HA	2.17	0.45
1:C:77:TYR:OH	1:C:206:ILE:HG22	2.17	0.45
1:C:117:ARG:O	1:C:118:GLU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:A:H1'	2:D:22:G:N2	2.32	0.45
2:D:34:OMG:N2	2:F:20:G:H1'	2.32	0.45
1:E:140:MET:HG2	3:E:1406:GNP:N2	2.32	0.45
1:E:301:GLY:O	1:E:302:GLN:O	2.35	0.45
1:A:140:MET:HG2	3:A:1406:GNP:N2	2.32	0.44
1:A:200:TRP:O	1:A:201:GLU:C	2.59	0.44
1:A:219:LYS:N	1:A:219:LYS:CD	2.72	0.44
1:A:249:VAL:CA	1:A:270:VAL:HG21	2.47	0.44
1:A:269:GLY:O	1:A:289:LEU:N	2.44	0.44
1:A:344:PHE:CE1	1:A:380:LEU:HD11	2.52	0.44
1:A:382:GLU:CG	1:A:402:LYS:HA	2.47	0.44
1:A:402:LYS:O	1:A:403:ILE:HG13	2.17	0.44
1:C:92:MET:HE2	1:C:93:ILE:N	2.32	0.44
1:E:76:HIS:CD2	1:E:77:TYR:H	2.35	0.44
1:E:247:VAL:HG21	1:E:267:VAL:CG1	2.34	0.44
1:E:249:VAL:CA	1:E:270:VAL:HG21	2.47	0.44
1:A:121:LEU:HB2	1:A:161:TYR:HE1	1.75	0.44
2:B:14:A:H1'	2:B:22:G:N2	2.32	0.44
1:C:119:HIS:O	1:C:120:ILE:C	2.59	0.44
1:C:229:PHE:CD2	2:D:77(A):C:H4'	2.53	0.44
1:C:245:GLY:O	1:C:246:LYS:CB	2.65	0.44
1:C:314:THR:CG2	1:C:373:GLU:OE2	2.65	0.44
1:E:77:TYR:OH	1:E:206:ILE:HG22	2.17	0.44
1:E:344:PHE:CE1	1:E:380:LEU:HD11	2.52	0.44
1:E:378:VAL:O	1:E:380:LEU:HD22	2.17	0.44
1:E:402:LYS:O	1:E:403:ILE:HG13	2.17	0.44
1:A:215:ARG:HD2	1:A:282:ALA:HB1	1.98	0.44
1:A:230:THR:HA	1:A:236:THR:CG2	2.47	0.44
1:A:284:ASP:O	1:A:286:VAL:CG1	2.63	0.44
1:A:378:VAL:O	1:A:380:LEU:HD22	2.17	0.44
1:C:140:MET:HE2	1:C:140:MET:CA	2.46	0.44
1:C:301:GLY:O	1:C:302:GLN:O	2.35	0.44
1:C:316:PHE:HE2	1:C:374:LEU:HD21	1.81	0.44
1:C:341:GLN:H	1:C:341:GLN:NE2	2.14	0.44
1:C:393:ARG:HG2	1:C:394:THR:N	2.22	0.44
1:E:227:ASP:O	1:E:238:ALA:HA	2.17	0.44
1:E:266:VAL:O	1:E:290:LEU:CA	2.50	0.44
1:E:284:ASP:O	1:E:286:VAL:CG1	2.63	0.44
2:F:57:G:H2'	2:F:58:1MA:H5'	1.98	0.44
1:A:7:ARG:O	1:A:8:THR:HG22	2.18	0.44
1:A:32:THR:HG21	1:A:45:LYS:CB	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TYR:OH	1:A:206:ILE:HG22	2.17	0.44
1:A:206:ILE:HG22	1:A:207:ASP:N	2.32	0.44
1:C:85:HIS:CD2	1:C:87:ASP:HB2	2.45	0.44
1:C:181:GLU:HG2	1:C:193:ASN:CG	2.43	0.44
1:C:230:THR:HA	1:C:236:THR:CG2	2.47	0.44
1:C:274:ARG:CZ	2:D:76:A:C5'	2.89	0.44
1:E:7:ARG:O	1:E:8:THR:HG22	2.17	0.44
1:E:32:THR:HG21	1:E:45:LYS:CB	2.44	0.44
1:E:248:LYS:C	1:E:249:VAL:O	2.61	0.44
2:F:26:M2G:H5'	2:F:27:C:OP2	2.18	0.44
1:A:159:ASN:O	1:A:160:GLN:C	2.61	0.44
1:A:323:LEU:HD12	1:A:395:VAL:C	2.42	0.44
1:C:94:THR:O	1:C:95:GLY:C	2.57	0.44
1:C:133:VAL:CG2	1:C:154:VAL:HG11	2.46	0.44
1:C:220:PRO:CB	1:C:309:SER:OG	2.64	0.44
1:C:249:VAL:CA	1:C:270:VAL:HG21	2.47	0.44
1:C:378:VAL:O	1:C:380:LEU:HD22	2.17	0.44
2:F:37:YG:C1'	2:F:37:YG:C3	2.96	0.44
1:A:75:ARG:NH2	1:A:207:ASP:CA	2.69	0.44
1:A:249:VAL:CG1	1:A:268:THR:HA	2.47	0.44
1:A:285:ASN:O	2:B:77:PHA:HB3	2.16	0.44
1:C:120:ILE:O	1:C:123:ALA:CB	2.61	0.44
2:D:26:M2G:H5'	2:D:27:C:OP2	2.18	0.44
2:F:14:A:H1'	2:F:22:G:N2	2.32	0.44
1:A:32:THR:O	1:A:33:TYR:CD1	2.69	0.44
1:A:125:GLN:C	1:A:127:GLY:H	2.24	0.44
1:A:229:PHE:CD2	2:B:77(A):C:H4'	2.53	0.44
1:C:266:VAL:O	1:C:290:LEU:CA	2.50	0.44
2:D:37:YG:C1'	2:D:37:YG:C3	2.96	0.44
1:E:181:GLU:HG2	1:E:193:ASN:CG	2.43	0.44
1:E:230:THR:HA	1:E:236:THR:CG2	2.47	0.44
1:E:316:PHE:O	1:E:371:THR:HG23	2.18	0.44
1:A:79:HIS:CD2	1:A:79:HIS:C	2.95	0.44
1:A:101:GLY:HA2	1:A:130:TYR:O	2.17	0.44
1:A:136:ASN:O	1:A:137:LYS:HB2	2.18	0.44
1:A:217:VAL:HB	1:A:246:LYS:HG3	2.00	0.44
1:A:245:GLY:O	1:A:246:LYS:CB	2.65	0.44
1:A:247:VAL:HG21	1:A:267:VAL:CG1	2.34	0.44
1:A:306:LYS:C	1:A:306:LYS:CD	2.88	0.44
1:A:335:PHE:CD2	1:A:361:MET:HB2	2.52	0.44
1:E:217:VAL:HB	1:E:246:LYS:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:PHE:CD2	2:F:77(A):C:H4'	2.53	0.44
1:E:323:LEU:HD12	1:E:395:VAL:C	2.42	0.44
1:E:382:GLU:CG	1:E:402:LYS:HA	2.47	0.44
1:A:181:GLU:HG2	1:A:193:ASN:CG	2.43	0.44
1:C:36:ALA:HA	1:C:42:VAL:CG1	2.48	0.44
1:C:50:ILE:O	1:C:52:LYS:N	2.42	0.44
1:C:140:MET:HG2	3:C:1406:GNP:N2	2.32	0.44
1:C:217:VAL:HB	1:C:246:LYS:HG3	2.00	0.44
1:C:227:ASP:O	1:C:238:ALA:HA	2.17	0.44
1:C:382:GLU:CG	1:C:402:LYS:HA	2.47	0.44
2:D:47:U:O2	2:D:47:U:C2'	2.66	0.44
1:E:72:THR:HG21	1:E:207:ASP:OD1	2.18	0.44
1:E:104:LEU:HD23	1:E:133:VAL:HG22	1.99	0.44
1:E:206:ILE:HG22	1:E:207:ASP:N	2.32	0.44
1:A:36:ALA:HA	1:A:42:VAL:CG1	2.48	0.43
1:A:221:PHE:HB3	1:A:305:ALA:HA	2.00	0.43
1:A:267:VAL:HG13	1:A:288:LEU:CD1	2.45	0.43
1:A:301:GLY:O	1:A:302:GLN:O	2.35	0.43
1:A:339:ARG:CD	1:A:352:VAL:HG22	2.27	0.43
1:C:269:GLY:HA3	1:C:289:LEU:HB3	1.99	0.43
1:E:168:VAL:HA	1:E:169:PRO:HD3	1.73	0.43
1:E:229:PHE:HB2	2:F:77(A):C:H1'	2.00	0.43
1:E:314:THR:CG2	1:E:373:GLU:OE2	2.65	0.43
1:A:76:HIS:CD2	1:A:77:TYR:H	2.36	0.43
1:A:316:PHE:O	1:A:371:THR:HG23	2.18	0.43
2:B:26:M2G:H5'	2:B:27:C:OP2	2.18	0.43
2:B:34:OMG:C8	2:D:20:G:C6	3.05	0.43
2:B:47:U:O2	2:B:47:U:C2'	2.66	0.43
2:B:48:C:OP2	2:B:48:C:H6	2.01	0.43
1:C:31:LEU:C	1:C:33:TYR:H	2.25	0.43
1:C:72:THR:HG21	1:C:207:ASP:OD1	2.18	0.43
1:C:159:ASN:O	1:C:160:GLN:C	2.61	0.43
1:C:248:LYS:C	1:C:249:VAL:O	2.61	0.43
1:C:301:GLY:C	1:C:346:THR:HG21	2.36	0.43
1:C:316:PHE:O	1:C:371:THR:HG23	2.18	0.43
1:E:136:ASN:O	1:E:137:LYS:HB2	2.18	0.43
1:E:271:GLU:CB	2:F:76:A:O2'	2.66	0.43
2:F:47:U:O2	2:F:47:U:C2'	2.66	0.43
1:A:120:ILE:O	1:A:123:ALA:CB	2.61	0.43
2:B:37:YG:C1'	2:B:37:YG:C3	2.96	0.43
1:C:229:PHE:HB2	2:D:77(A):C:H1'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:LEU:C	1:E:33:TYR:H	2.25	0.43
1:A:104:LEU:HD23	1:A:133:VAL:HG22	1.99	0.43
1:A:248:LYS:C	1:A:249:VAL:O	2.61	0.43
1:C:7:ARG:O	1:C:8:THR:HG22	2.18	0.43
1:C:271:GLU:CB	2:D:76:A:O2'	2.66	0.43
1:C:289:LEU:O	1:C:290:LEU:HD23	2.19	0.43
1:C:402:LYS:O	1:C:403:ILE:HG13	2.17	0.43
2:D:10:2MG:CM2	2:D:25:C:O2	2.50	0.43
2:D:48:C:OP2	2:D:48:C:H6	2.01	0.43
1:E:159:ASN:O	1:E:160:GLN:C	2.61	0.43
1:E:344:PHE:CE2	1:E:386:PHE:HB2	2.53	0.43
2:F:10:2MG:CM2	2:F:25:C:O2	2.50	0.43
1:A:72:THR:HG21	1:A:207:ASP:OD1	2.18	0.43
1:A:258:LEU:CD1	1:A:301:GLY:HA3	2.38	0.43
1:E:17:ILE:O	1:E:17:ILE:CG1	2.61	0.43
1:E:115:GLN:OE1	1:E:115:GLN:N	2.51	0.43
1:E:231:ILE:HB	1:E:234:ARG:NH2	2.34	0.43
1:E:289:LEU:O	1:E:290:LEU:HD23	2.19	0.43
1:E:372:VAL:CG1	1:E:373:GLU:H	2.32	0.43
2:F:25:C:C2'	2:F:26:M2G:O4'	2.62	0.43
2:F:48:C:OP2	2:F:48:C:H6	2.01	0.43
2:F:59:U:C4	2:F:60:C:N3	2.86	0.43
1:A:115:GLN:OE1	1:A:115:GLN:N	2.51	0.43
1:A:133:VAL:CG2	1:A:154:VAL:HG11	2.46	0.43
1:A:164:PRO:O	1:A:167:GLU:HB2	2.19	0.43
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.84	0.43
1:A:384:LEU:O	1:A:400:VAL:HG23	2.19	0.43
2:B:25:C:C4	2:B:26:M2G:N7	2.87	0.43
1:C:346:THR:CG2	1:C:347:THR:H	2.10	0.43
1:A:137:LYS:HA	3:A:1406:GNP:N1	2.34	0.43
2:B:4:G:H2'	2:B:5:A:O4'	2.19	0.43
2:B:59:U:C4	2:B:60:C:N3	2.86	0.43
1:C:101:GLY:HA2	1:C:130:TYR:O	2.17	0.43
1:C:115:GLN:N	1:C:115:GLN:OE1	2.51	0.43
1:C:339:ARG:HA	1:C:351:GLY:O	2.19	0.43
1:E:12:VAL:HG22	1:E:213:PRO:HG3	1.99	0.43
1:E:29:ALA:C	1:E:31:LEU:N	2.72	0.43
1:A:132:VAL:O	1:A:132:VAL:HG23	2.19	0.43
1:A:135:MET:HE1	1:A:151:GLU:HB2	2.01	0.43
1:A:168:VAL:HA	1:A:169:PRO:HD3	1.73	0.43
1:A:271:GLU:CB	2:B:76:A:O2'	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:HIS:CD2	1:C:77:TYR:H	2.36	0.43
2:D:25:C:C4	2:D:26:M2G:N7	2.87	0.43
1:C:55:GLU:O	1:C:56:GLU:C	2.62	0.43
1:C:231:ILE:HB	1:C:234:ARG:NH2	2.34	0.43
1:C:384:LEU:O	1:C:400:VAL:HG23	2.19	0.43
1:E:9:LYS:NZ	1:E:73:ALA:O	2.42	0.43
1:E:249:VAL:CG1	1:E:268:THR:HA	2.47	0.43
1:A:50:ILE:O	1:A:52:LYS:N	2.42	0.43
1:C:70:TYR:CD1	1:C:70:TYR:C	2.97	0.43
1:C:72:THR:OG1	1:C:73:ALA:N	2.52	0.43
1:C:121:LEU:HD22	5:C:1408:ENX:O41	2.19	0.43
1:C:134:PHE:CD2	1:C:136:ASN:HB2	2.54	0.43
1:C:178:ALA:O	1:C:182:MET:HG2	2.19	0.43
1:C:237:VAL:HA	1:C:288:LEU:O	2.19	0.43
1:C:271:GLU:HB3	1:C:272:MET:H	1.50	0.43
2:D:59:U:C4	2:D:60:C:N3	2.86	0.43
1:E:339:ARG:HA	1:E:351:GLY:O	2.19	0.43
1:E:363:MET:HE3	1:E:363:MET:HB3	1.84	0.43
1:E:395:VAL:HG23	1:E:396:GLY:N	2.34	0.43
2:F:25:C:C4	2:F:26:M2G:N7	2.87	0.43
1:A:34:VAL:HG21	1:A:199:ILE:HG12	2.00	0.42
1:A:46:ASP:O	1:A:50:ILE:HD12	2.19	0.42
1:A:234:ARG:NH1	1:A:234:ARG:CG	2.82	0.42
1:C:136:ASN:O	1:C:137:LYS:HB2	2.18	0.42
1:C:206:ILE:HG22	1:C:207:ASP:N	2.32	0.42
1:E:56:GLU:CG	1:E:63:ILE:HG23	2.44	0.42
1:E:255:ILE:HG23	1:E:304:LEU:CD2	2.49	0.42
1:E:316:PHE:CA	1:E:404:LEU:HG	2.49	0.42
1:A:178:ALA:O	1:A:182:MET:HG2	2.19	0.42
1:A:339:ARG:HA	1:A:351:GLY:O	2.19	0.42
1:A:344:PHE:CE2	1:A:386:PHE:HB2	2.53	0.42
2:B:20:G:H1'	2:F:34:OMG:N2	2.34	0.42
1:C:46:ASP:O	1:C:50:ILE:HD12	2.19	0.42
1:C:182:MET:SD	1:C:196:VAL:CG2	3.07	0.42
1:C:234:ARG:NH1	1:C:234:ARG:CG	2.82	0.42
1:E:34:VAL:HG21	1:E:199:ILE:HG12	2.00	0.42
1:E:137:LYS:HA	3:E:1406:GNP:N1	2.34	0.42
1:E:182:MET:SD	1:E:196:VAL:CG2	3.07	0.42
1:E:216:ASP:OD2	1:E:218:ASP:OD2	2.37	0.42
1:A:121:LEU:HD22	5:A:1408:ENX:O41	2.19	0.42
1:A:196:VAL:O	1:A:196:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PHE:CA	1:A:404:LEU:HG	2.49	0.42
1:C:38:GLU:HB2	1:C:39:ASN:H	1.60	0.42
1:C:255:ILE:HG23	1:C:304:LEU:CD2	2.49	0.42
1:C:344:PHE:CE2	1:C:386:PHE:HB2	2.53	0.42
1:C:395:VAL:HG23	1:C:396:GLY:N	2.34	0.42
1:E:36:ALA:HA	1:E:42:VAL:CG1	2.48	0.42
1:E:70:TYR:CD1	1:E:70:TYR:C	2.97	0.42
1:E:134:PHE:CD2	1:E:136:ASN:HB2	2.54	0.42
1:E:196:VAL:O	1:E:196:VAL:HG12	2.20	0.42
1:E:237:VAL:HA	1:E:288:LEU:O	2.19	0.42
1:E:384:LEU:O	1:E:400:VAL:HG23	2.19	0.42
1:A:18:GLY:O	1:A:19:HIS:O	2.38	0.42
2:B:19:G:H5''	2:B:20:G:C5'	2.47	0.42
1:E:23:GLY:C	1:E:105:VAL:HG11	2.44	0.42
1:E:46:ASP:O	1:E:50:ILE:HD12	2.19	0.42
1:E:85:HIS:CD2	1:E:87:ASP:HB2	2.46	0.42
1:E:121:LEU:HD22	5:E:1408:ENX:O41	2.19	0.42
1:E:221:PHE:HB3	1:E:305:ALA:HA	2.00	0.42
1:E:274:ARG:HH11	1:E:274:ARG:HG3	1.85	0.42
1:E:402:LYS:CG	1:E:403:ILE:N	2.72	0.42
2:F:19:G:H5''	2:F:20:G:C5'	2.47	0.42
1:A:55:GLU:HA	1:A:58:ALA:HB3	2.01	0.42
1:A:70:TYR:CD1	1:A:70:TYR:C	2.97	0.42
1:A:125:GLN:CD	1:A:394:THR:HB	2.45	0.42
1:A:150:VAL:O	1:A:150:VAL:CG1	2.65	0.42
1:A:185:ASN:HD22	1:A:188:THR:CA	2.33	0.42
1:A:255:ILE:HG23	1:A:304:LEU:CD2	2.49	0.42
1:A:274:ARG:HG3	1:A:274:ARG:HH11	1.85	0.42
1:A:281:ILE:CG1	1:A:282:ALA:N	2.81	0.42
1:C:34:VAL:HG21	1:C:199:ILE:HG12	2.00	0.42
2:D:39:PSU:O2'	2:D:40:5MC:H5'	2.20	0.42
1:E:125:GLN:CD	1:E:394:THR:HB	2.45	0.42
1:E:164:PRO:O	1:E:167:GLU:HB2	2.19	0.42
1:E:178:ALA:O	1:E:182:MET:HG2	2.19	0.42
1:E:234:ARG:NH1	1:E:234:ARG:CG	2.82	0.42
1:E:305:ALA:O	1:E:306:LYS:C	2.63	0.42
1:A:55:GLU:O	1:A:56:GLU:C	2.62	0.42
1:A:231:ILE:HB	1:A:234:ARG:NH2	2.34	0.42
1:A:328:GLY:HA2	5:A:1408:ENX:H402	2.02	0.42
2:B:34:OMG:H1'	2:B:34:OMG:HM23	1.80	0.42
1:C:25:THR:O	1:C:28:THR:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:VAL:CG1	1:C:268:THR:HA	2.47	0.42
1:C:320:VAL:O	1:C:367:ASN:ND2	2.53	0.42
2:D:4:G:H2'	2:D:5:A:O4'	2.19	0.42
2:D:19:G:H5''	2:D:20:G:C5'	2.47	0.42
2:D:22:G:O2'	2:D:23:A:O5'	2.34	0.42
2:D:25:C:C2'	2:D:26:M2G:O4'	2.62	0.42
1:E:135:MET:HE1	1:E:151:GLU:HB2	2.01	0.42
1:E:169:PRO:CB	1:E:171:ILE:HD11	2.49	0.42
1:E:277:LEU:HD12	1:E:277:LEU:HA	1.90	0.42
1:E:291:ARG:HH11	1:E:291:ARG:HG3	1.84	0.42
1:E:386:PHE:C	1:E:386:PHE:HD1	2.28	0.42
1:A:53:ALA:HA	1:A:54:PRO:HD3	1.89	0.42
1:A:92:MET:HE2	1:A:93:ILE:N	2.32	0.42
1:A:216:ASP:OD2	1:A:218:ASP:OD2	2.37	0.42
1:C:18:GLY:O	1:C:19:HIS:O	2.38	0.42
1:C:25:THR:OG1	1:C:62:THR:OG1	2.37	0.42
1:C:34:VAL:CA	1:C:182:MET:HE2	2.45	0.42
1:C:55:GLU:HA	1:C:58:ALA:HB3	2.01	0.42
1:C:164:PRO:O	1:C:167:GLU:HB2	2.19	0.42
1:C:216:ASP:OD2	1:C:218:ASP:OD2	2.37	0.42
1:C:221:PHE:HB3	1:C:305:ALA:HA	2.00	0.42
1:C:274:ARG:HG3	1:C:274:ARG:HH11	1.85	0.42
1:C:331:HIS:NE2	2:D:54:5MU:OP1	2.38	0.42
1:E:92:MET:HE2	1:E:93:ILE:N	2.32	0.42
1:E:220:PRO:O	1:E:244:ARG:O	2.38	0.42
1:E:221:PHE:CE2	1:E:253:VAL:CG1	3.03	0.42
2:F:2:C:H42	2:F:71:G:H1	1.68	0.42
1:A:165:GLY:O	1:A:168:VAL:CG2	2.68	0.42
1:A:182:MET:SD	1:A:196:VAL:CG2	3.07	0.42
1:A:314:THR:CG2	1:A:373:GLU:OE2	2.65	0.42
1:A:395:VAL:HG23	1:A:396:GLY:N	2.34	0.42
2:B:2:C:H42	2:B:71:G:H1	1.68	0.42
2:B:39:PSU:O2'	2:B:40:5MC:H5'	2.20	0.42
1:C:135:MET:HE1	1:C:151:GLU:HB2	2.01	0.42
1:C:137:LYS:HA	3:C:1406:GNP:N1	2.34	0.42
1:C:328:GLY:HA2	5:C:1408:ENX:H402	2.02	0.42
1:C:386:PHE:C	1:C:386:PHE:HD1	2.28	0.42
1:E:22:HIS:CD2	1:E:107:SER:HB2	2.55	0.42
1:A:22:HIS:CD2	1:A:107:SER:HB2	2.55	0.42
1:A:229:PHE:HB2	2:B:77(A):C:H1'	2.00	0.42
1:A:344:PHE:O	1:A:345:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:PHE:C	1:A:386:PHE:HD1	2.28	0.42
1:C:132:VAL:HG23	1:C:132:VAL:O	2.19	0.42
1:C:221:PHE:CE2	1:C:253:VAL:CG1	3.03	0.42
1:C:316:PHE:CA	1:C:404:LEU:HG	2.49	0.42
2:D:2:C:H42	2:D:71:G:H1	1.68	0.42
1:E:10:PRO:O	1:E:76:HIS:N	2.47	0.42
1:E:18:GLY:O	1:E:19:HIS:O	2.38	0.42
1:E:181:GLU:C	1:E:183:HIS:H	2.28	0.42
1:E:281:ILE:CG1	1:E:282:ALA:N	2.81	0.42
1:E:319:SER:H	1:E:401:THR:HG23	1.85	0.42
1:A:23:GLY:C	1:A:105:VAL:HG11	2.45	0.42
1:A:265:THR:HG1	1:A:291:ARG:C	2.27	0.42
1:A:310:ILE:HD12	1:A:381:GLU:HB2	2.02	0.42
1:A:342:PHE:HE1	1:A:351:GLY:HA3	1.85	0.42
1:C:200:TRP:HA	1:C:203:LEU:HD12	2.02	0.42
1:C:265:THR:HG1	1:C:291:ARG:C	2.27	0.42
1:C:305:ALA:O	1:C:306:LYS:C	2.63	0.42
2:D:19:G:H4'	2:D:20:G:O5'	2.20	0.42
2:F:22:G:HO2'	2:F:23:A:P	2.41	0.42
1:A:120:ILE:CD1	1:A:157:LEU:HD23	2.50	0.41
1:A:134:PHE:CD2	1:A:136:ASN:HB2	2.54	0.41
1:A:151:GLU:CG	1:A:170:VAL:HG21	2.48	0.41
1:A:289:LEU:O	1:A:290:LEU:HD23	2.19	0.41
2:B:18:G:O6	2:B:55:PSU:H1'	2.20	0.41
1:C:23:GLY:C	1:C:105:VAL:HG11	2.44	0.41
1:C:121:LEU:HB2	1:C:161:TYR:HE1	1.75	0.41
1:C:214:VAL:CG2	1:C:215:ARG:N	2.83	0.41
1:C:319:SER:H	1:C:401:THR:HG23	1.85	0.41
2:D:18:G:O6	2:D:55:PSU:H1'	2.20	0.41
1:E:55:GLU:HA	1:E:58:ALA:HB3	2.01	0.41
1:E:132:VAL:HG23	1:E:132:VAL:O	2.19	0.41
1:E:320:VAL:O	1:E:367:ASN:ND2	2.53	0.41
1:E:328:GLY:HA2	5:E:1408:ENX:H402	2.02	0.41
1:E:342:PHE:HE1	1:E:351:GLY:HA3	1.85	0.41
1:E:344:PHE:O	1:E:345:ARG:HG3	2.20	0.41
1:A:187:LYS:HB3	1:A:189:LYS:HZ1	1.83	0.41
1:A:221:PHE:CE2	1:A:253:VAL:CG1	3.03	0.41
1:A:305:ALA:O	1:A:306:LYS:C	2.63	0.41
1:A:320:VAL:O	1:A:367:ASN:ND2	2.53	0.41
1:C:125:GLN:CD	1:C:394:THR:HB	2.45	0.41
1:C:169:PRO:CB	1:C:171:ILE:HD11	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:PHE:HE2	1:C:386:PHE:HB2	1.85	0.41
1:C:344:PHE:O	1:C:345:ARG:HG3	2.20	0.41
1:C:372:VAL:CG1	1:C:373:GLU:H	2.32	0.41
1:E:25:THR:O	1:E:28:THR:HB	2.20	0.41
1:E:34:VAL:CA	1:E:182:MET:HE2	2.45	0.41
1:E:151:GLU:CG	1:E:170:VAL:HG21	2.48	0.41
1:E:248:LYS:CG	1:E:251:ASP:OD1	2.68	0.41
1:E:344:PHE:O	1:E:346:THR:N	2.53	0.41
2:F:4:G:H2'	2:F:5:A:O4'	2.19	0.41
1:A:72:THR:OG1	1:A:73:ALA:N	2.52	0.41
1:A:181:GLU:C	1:A:183:HIS:H	2.28	0.41
1:A:248:LYS:CG	1:A:251:ASP:OD1	2.68	0.41
1:A:265:THR:HG21	1:A:293:VAL:HG21	2.03	0.41
1:A:270:VAL:O	1:A:270:VAL:CG1	2.52	0.41
1:A:322:ILE:HA	1:A:396:GLY:HA3	2.03	0.41
1:C:22:HIS:CD2	1:C:107:SER:HB2	2.55	0.41
1:C:277:LEU:HD23	1:C:280:GLY:HA2	2.02	0.41
1:C:291:ARG:HH11	1:C:291:ARG:HG3	1.84	0.41
1:C:335:PHE:CE2	1:C:361:MET:SD	3.13	0.41
1:E:310:ILE:HD12	1:E:381:GLU:HB2	2.02	0.41
1:A:151:GLU:OE1	1:A:170:VAL:HB	2.21	0.41
1:A:235:GLY:O	1:A:236:THR:CG2	2.64	0.41
1:A:301:GLY:C	1:A:346:THR:HG21	2.35	0.41
1:E:263:ARG:HH11	1:E:263:ARG:HG3	1.86	0.41
1:E:320:VAL:HG12	1:E:322:ILE:CD1	2.49	0.41
2:F:14:A:H2'	2:F:15:G:O4'	2.21	0.41
2:F:63:C:H2'	2:F:64:A:O4'	2.20	0.41
1:A:9:LYS:NZ	1:A:73:ALA:O	2.42	0.41
1:A:14:VAL:O	1:A:79:HIS:HA	2.21	0.41
1:A:66:ALA:O	1:A:81:ASP:N	2.34	0.41
1:A:146:LEU:HD12	1:A:150:VAL:HG23	2.03	0.41
1:A:333:GLY:CA	1:A:362:VAL:O	2.69	0.41
1:A:335:PHE:CE2	1:A:361:MET:SD	3.13	0.41
1:C:310:ILE:HD12	1:C:381:GLU:HB2	2.02	0.41
1:C:333:GLY:CA	1:C:362:VAL:O	2.69	0.41
1:C:342:PHE:HE1	1:C:351:GLY:HA3	1.85	0.41
1:C:344:PHE:O	1:C:346:THR:N	2.53	0.41
1:C:363:MET:HB2	1:C:366:ASP:OD2	2.21	0.41
1:E:43:GLU:CG	1:E:44:VAL:N	2.77	0.41
1:E:55:GLU:O	1:E:56:GLU:C	2.62	0.41
1:E:277:LEU:HD23	1:E:280:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1:G:O2'	2:F:2:C:H5'	2.21	0.41
1:A:200:TRP:HA	1:A:203:LEU:HD12	2.02	0.41
1:A:241:ARG:HG3	1:A:241:ARG:NH1	2.36	0.41
1:C:133:VAL:HG21	1:C:154:VAL:CG1	2.46	0.41
1:C:141:VAL:HG11	1:C:147:LEU:HG	2.03	0.41
1:C:246:LYS:HB3	1:C:279:GLU:HG2	2.03	0.41
1:C:287:GLY:HA3	2:D:77:PHA:N	2.36	0.41
2:D:1:G:O2'	2:D:2:C:H5'	2.21	0.41
2:D:36:A:H2'	2:D:37:YG:O4'	2.21	0.41
1:E:141:VAL:HG11	1:E:147:LEU:HG	2.03	0.41
1:E:165:GLY:O	1:E:168:VAL:CG2	2.68	0.41
1:E:249:VAL:HG22	1:E:270:VAL:HG23	2.02	0.41
1:E:265:THR:HG1	1:E:266:VAL:H	1.68	0.41
1:A:25:THR:O	1:A:28:THR:HB	2.20	0.41
1:A:26:THR:C	1:A:28:THR:N	2.61	0.41
1:A:214:VAL:CG2	1:A:215:ARG:N	2.83	0.41
1:A:220:PRO:O	1:A:244:ARG:O	2.38	0.41
1:A:263:ARG:HH11	1:A:263:ARG:HG3	1.86	0.41
1:A:277:LEU:HD23	1:A:280:GLY:HA2	2.02	0.41
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.63	0.41
2:B:63:C:H2'	2:B:64:A:O4'	2.20	0.41
2:B:73:A:H2'	2:B:73:A:N3	2.35	0.41
1:C:57:ARG:HB3	1:C:57:ARG:NH1	2.36	0.41
1:C:146:LEU:HD12	1:C:150:VAL:HG23	2.03	0.41
1:C:181:GLU:C	1:C:183:HIS:H	2.28	0.41
1:C:185:ASN:HD22	1:C:188:THR:CA	2.33	0.41
1:E:151:GLU:OE1	1:E:170:VAL:HB	2.21	0.41
1:E:185:ASN:HD22	1:E:188:THR:CA	2.33	0.41
1:E:265:THR:HG21	1:E:290:LEU:HD13	2.02	0.41
1:E:267:VAL:HG13	1:E:288:LEU:CD1	2.45	0.41
1:E:322:ILE:HA	1:E:396:GLY:HA3	2.03	0.41
2:F:18:G:O6	2:F:55:PSU:H1'	2.20	0.41
1:A:249:VAL:HG22	1:A:270:VAL:HG23	2.02	0.41
1:A:363:MET:HB2	1:A:366:ASP:OD1	2.20	0.41
1:C:151:GLU:OE1	1:C:170:VAL:HB	2.21	0.41
1:C:257:GLY:O	1:C:258:LEU:C	2.64	0.41
2:D:14:A:H2'	2:D:15:G:O4'	2.21	0.41
1:E:14:VAL:O	1:E:79:HIS:HA	2.21	0.41
1:E:72:THR:OG1	1:E:73:ALA:N	2.52	0.41
2:F:39:PSU:O2'	2:F:40:5MC:H5'	2.20	0.41
1:A:50:ILE:HD12	1:A:50:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ALA:O	1:A:209:TYR:HB2	2.21	0.41
1:A:257:GLY:O	1:A:258:LEU:C	2.64	0.41
1:A:264:LYS:HE3	1:A:264:LYS:HB2	1.85	0.41
1:A:275:LYS:O	1:A:276:THR:O	2.39	0.41
1:A:287:GLY:HA3	2:B:77:PHA:N	2.36	0.41
1:A:320:VAL:HG12	1:A:322:ILE:CD1	2.49	0.41
2:B:1:G:O2'	2:B:2:C:H5'	2.21	0.41
2:B:19:G:H4'	2:B:20:G:O5'	2.20	0.41
1:C:168:VAL:HA	1:C:169:PRO:HD3	1.72	0.41
1:C:187:LYS:HB3	1:C:189:LYS:HZ1	1.81	0.41
1:C:196:VAL:O	1:C:196:VAL:HG12	2.20	0.41
1:C:219:LYS:N	1:C:219:LYS:CD	2.72	0.41
1:C:220:PRO:O	1:C:244:ARG:O	2.38	0.41
1:C:248:LYS:O	1:C:251:ASP:OD1	2.39	0.41
1:C:248:LYS:CG	1:C:251:ASP:OD1	2.68	0.41
1:C:284:ASP:O	1:C:286:VAL:CG1	2.63	0.41
2:D:39:PSU:C5	2:D:40:5MC:HM52	2.56	0.41
2:D:63:C:H2'	2:D:64:A:O4'	2.20	0.41
1:E:27:LEU:HB2	1:E:175:ALA:HB2	2.03	0.41
1:E:52:LYS:HE3	1:E:52:LYS:HB3	1.95	0.41
1:E:120:ILE:O	1:E:123:ALA:CB	2.61	0.41
1:E:146:LEU:HD12	1:E:150:VAL:HG23	2.03	0.41
1:E:231:ILE:HB	1:E:234:ARG:HH22	1.86	0.41
1:E:248:LYS:O	1:E:251:ASP:OD1	2.39	0.41
1:E:257:GLY:O	1:E:258:LEU:C	2.64	0.41
1:E:335:PHE:CE2	1:E:361:MET:SD	3.13	0.41
1:E:356:PRO:O	1:E:358:GLY:N	2.52	0.41
1:E:363:MET:HB2	1:E:366:ASP:OD2	2.21	0.41
2:F:34:OMG:HM23	2:F:34:OMG:H1'	1.80	0.41
2:F:34:OMG:C6	2:F:35:A:C5	3.09	0.41
2:F:36:A:H2'	2:F:37:YG:O4'	2.21	0.41
1:A:85:HIS:CD2	1:A:87:ASP:HB2	2.45	0.41
1:A:344:PHE:O	1:A:346:THR:N	2.53	0.41
2:B:14:A:H2'	2:B:15:G:O4'	2.21	0.41
1:C:61:ILE:HD12	1:C:63:ILE:HG22	2.03	0.41
1:C:165:GLY:O	1:C:168:VAL:CG2	2.68	0.41
1:C:363:MET:HE3	1:C:363:MET:HB3	1.84	0.41
1:E:24:LYS:HE3	1:E:84:GLY:N	2.36	0.41
1:E:67:HIS:H	1:E:67:HIS:HD2	1.67	0.41
1:E:241:ARG:HG3	1:E:241:ARG:NH1	2.36	0.41
1:A:93:ILE:HG12	1:A:122:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HG23	1:A:304:LEU:HD23	2.03	0.40
2:B:36:A:C2'	2:B:37:YG:H8	2.26	0.40
1:C:24:LYS:HE3	1:C:84:GLY:N	2.36	0.40
1:C:27:LEU:HB2	1:C:175:ALA:HB2	2.03	0.40
1:C:46:ASP:O	1:C:50:ILE:CD1	2.70	0.40
1:C:356:PRO:C	1:C:358:GLY:N	2.79	0.40
1:E:190:ARG:HG2	1:E:191:GLY:N	2.36	0.40
1:E:333:GLY:CA	1:E:362:VAL:O	2.69	0.40
2:F:19:G:H4'	2:F:20:G:O5'	2.20	0.40
1:A:363:MET:HB2	1:A:366:ASP:OD2	2.21	0.40
2:B:22:G:HO2'	2:B:23:A:P	2.42	0.40
1:C:226:GLU:CD	1:C:226:GLU:O	2.64	0.40
2:D:34:OMG:H1'	2:F:20:G:N7	2.37	0.40
1:E:114:PRO:HB2	1:E:115:GLN:OE1	2.21	0.40
1:E:275:LYS:O	1:E:276:THR:O	2.39	0.40
1:E:342:PHE:CE1	1:E:351:GLY:HA3	2.57	0.40
1:A:61:ILE:HD12	1:A:63:ILE:HG22	2.03	0.40
1:A:211:PRO:C	1:A:212:THR:HG23	2.46	0.40
1:A:237:VAL:HA	1:A:288:LEU:O	2.19	0.40
1:A:246:LYS:HB3	1:A:279:GLU:HG2	2.03	0.40
1:C:135:MET:HB3	1:C:172:ARG:HA	2.04	0.40
1:C:231:ILE:HB	1:C:234:ARG:HH22	1.86	0.40
1:C:363:MET:HB2	1:C:366:ASP:OD1	2.21	0.40
1:C:402:LYS:CG	1:C:403:ILE:N	2.72	0.40
1:E:226:GLU:CD	1:E:226:GLU:O	2.64	0.40
1:E:255:ILE:HG23	1:E:304:LEU:HD23	2.03	0.40
1:E:287:GLY:HA3	2:F:77:PHA:N	2.36	0.40
1:E:363:MET:HB2	1:E:366:ASP:OD1	2.20	0.40
1:A:29:ALA:O	1:A:32:THR:N	2.55	0.40
1:A:265:THR:HG21	1:A:290:LEU:HD13	2.02	0.40
1:A:372:VAL:CG1	1:A:373:GLU:H	2.32	0.40
1:C:33:TYR:HB3	1:C:182:MET:HG3	2.03	0.40
1:C:114:PRO:HB2	1:C:115:GLN:OE1	2.21	0.40
1:C:205:ALA:O	1:C:209:TYR:HB2	2.21	0.40
1:C:263:ARG:HH11	1:C:263:ARG:HG3	1.86	0.40
1:C:265:THR:HG21	1:C:293:VAL:HG21	2.02	0.40
1:E:220:PRO:CG	1:E:306:LYS:HE2	2.51	0.40
1:E:230:THR:HA	1:E:236:THR:HG22	2.04	0.40
1:E:253:VAL:CG2	1:E:265:THR:HG23	2.52	0.40
2:F:23:A:H2'	2:F:24:G:H8	1.83	0.40
1:A:24:LYS:HE3	1:A:84:GLY:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASP:O	1:A:50:ILE:CD1	2.69	0.40
1:A:57:ARG:HB3	1:A:57:ARG:NH1	2.36	0.40
1:A:67:HIS:H	1:A:67:HIS:HD2	1.67	0.40
1:A:135:MET:HB3	1:A:172:ARG:HA	2.04	0.40
1:A:220:PRO:CG	1:A:306:LYS:HE2	2.51	0.40
1:A:342:PHE:CE1	1:A:351:GLY:HA3	2.57	0.40
1:C:67:HIS:H	1:C:67:HIS:HD2	1.67	0.40
1:C:177:LEU:HD23	1:C:177:LEU:HA	1.85	0.40
1:C:190:ARG:HG2	1:C:191:GLY:N	2.36	0.40
1:C:211:PRO:C	1:C:212:THR:HG23	2.46	0.40
1:C:258:LEU:CD1	1:C:301:GLY:HA3	2.38	0.40
2:D:16:H2U:H2'	2:D:16:H2U:H61	1.91	0.40
2:D:34:OMG:C6	2:D:35:A:C5	3.09	0.40
1:E:140:MET:HG2	3:E:1406:GNP:HN21	1.87	0.40
1:E:158:LEU:HD23	1:E:158:LEU:HA	1.93	0.40
2:F:73:A:N3	2:F:73:A:H2'	2.35	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TYR:OH	1:C:148:ASP:OD1[3_545]	1.71	0.49
1:C:130:TYR:OH	1:E:148:ASP:OD1[1_565]	1.76	0.44
1:A:148:ASP:OD1	1:E:130:TYR:OH[3_555]	1.82	0.38

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	398/405 (98%)	250 (63%)	90 (23%)	58 (15%)	0 0
1	C	398/405 (98%)	250 (63%)	90 (23%)	58 (15%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	398/405 (98%)	250 (63%)	90 (23%)	58 (15%)	0	0
All	All	1194/1215 (98%)	750 (63%)	270 (23%)	174 (15%)	0	0

All (174) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	THR
1	A	19	HIS
1	A	27	LEU
1	A	39	ASN
1	A	47	TYR
1	A	72	THR
1	A	96	ALA
1	A	135	MET
1	A	160	GLN
1	A	220	PRO
1	A	232	THR
1	A	246	LYS
1	A	249	VAL
1	A	258	LEU
1	A	271	GLU
1	A	272	MET
1	A	280	GLY
1	A	302	GLN
1	A	316	PHE
1	A	391	GLY
1	C	7	ARG
1	C	8	THR
1	C	19	HIS
1	C	27	LEU
1	C	39	ASN
1	C	47	TYR
1	C	51	ASP
1	C	72	THR
1	C	96	ALA
1	C	135	MET
1	C	160	GLN
1	C	220	PRO
1	C	232	THR
1	C	246	LYS
1	C	249	VAL

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Mol	Chain	Res	Type
1	C	258	LEU
1	C	271	GLU
1	C	272	MET
1	C	280	GLY
1	C	302	GLN
1	C	316	PHE
1	C	391	GLY
1	E	7	ARG
1	E	8	THR
1	E	19	HIS
1	E	27	LEU
1	E	39	ASN
1	E	47	TYR
1	E	51	ASP
1	E	72	THR
1	E	96	ALA
1	E	135	MET
1	E	160	GLN
1	E	220	PRO
1	E	232	THR
1	E	246	LYS
1	E	249	VAL
1	E	258	LEU
1	E	271	GLU
1	E	272	MET
1	E	280	GLY
1	E	302	GLN
1	E	316	PHE
1	E	391	GLY
1	A	30	ALA
1	A	37	ALA
1	A	48	GLY
1	A	51	ASP
1	A	69	GLU
1	A	70	TYR
1	A	117	ARG
1	A	162	GLU
1	A	165	GLY
1	A	171	ILE
1	A	225	VAL
1	A	276	THR
1	A	345	ARG

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Mol	Chain	Res	Type
1	A	346	THR
1	C	30	ALA
1	C	37	ALA
1	C	48	GLY
1	C	69	GLU
1	C	70	TYR
1	C	117	ARG
1	C	162	GLU
1	C	165	GLY
1	C	171	ILE
1	C	225	VAL
1	C	276	THR
1	C	345	ARG
1	C	346	THR
1	E	30	ALA
1	E	37	ALA
1	E	48	GLY
1	E	69	GLU
1	E	70	TYR
1	E	117	ARG
1	E	162	GLU
1	E	165	GLY
1	E	171	ILE
1	E	225	VAL
1	E	276	THR
1	E	345	ARG
1	E	346	THR
1	A	164	PRO
1	A	211	PRO
1	A	241	ARG
1	A	268	THR
1	A	283	GLY
1	A	357	GLN
1	A	370	PHE
1	C	164	PRO
1	C	211	PRO
1	C	241	ARG
1	C	268	THR
1	C	283	GLY
1	C	357	GLN
1	C	370	PHE
1	E	164	PRO

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Mol	Chain	Res	Type
1	E	211	PRO
1	E	241	ARG
1	E	268	THR
1	E	283	GLY
1	E	357	GLN
1	E	370	PHE
1	A	213	PRO
1	A	215	ARG
1	A	260	PRO
1	A	285	ASN
1	A	286	VAL
1	A	296	GLU
1	C	213	PRO
1	C	215	ARG
1	C	260	PRO
1	C	285	ASN
1	C	286	VAL
1	C	296	GLU
1	E	213	PRO
1	E	215	ARG
1	E	260	PRO
1	E	285	ASN
1	E	286	VAL
1	E	296	GLU
1	A	129	PRO
1	C	129	PRO
1	E	129	PRO
1	E	216	ASP
1	A	190	ARG
1	A	216	ASP
1	A	236	THR
1	A	310	ILE
1	C	190	ARG
1	C	216	ASP
1	C	236	THR
1	C	310	ILE
1	E	190	ARG
1	E	236	THR
1	E	310	ILE
1	A	298	VAL
1	A	306	LYS
1	C	298	VAL

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Mol	Chain	Res	Type
1	C	306	LYS
1	E	298	VAL
1	E	306	LYS
1	A	42	VAL
1	A	267	VAL
1	C	42	VAL
1	C	267	VAL
1	E	42	VAL
1	E	267	VAL
1	A	358	GLY
1	C	358	GLY
1	E	358	GLY

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	335/338 (99%)	276 (82%)	59 (18%)	2	9
1	C	335/338 (99%)	275 (82%)	60 (18%)	2	9
1	E	335/338 (99%)	274 (82%)	61 (18%)	2	8
All	All	1005/1014 (99%)	825 (82%)	180 (18%)	2	9

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	THR
1	A	28	THR
1	A	38	GLU
1	A	39	ASN
1	A	42	VAL
1	A	63	ILE
1	A	64	ASN
1	A	65	THR
1	A	67	HIS

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Mol	Chain	Res	Type
1	A	89	ILE
1	A	92	MET
1	A	115	GLN
1	A	122	LEU
1	A	128	VAL
1	A	139	ASP
1	A	142	ASP
1	A	156	ASP
1	A	157	LEU
1	A	171	ILE
1	A	181	GLU
1	A	194	GLU
1	A	206	ILE
1	A	219	LYS
1	A	220	PRO
1	A	222	LEU
1	A	223	MET
1	A	226	GLU
1	A	229	PHE
1	A	231	ILE
1	A	234	ARG
1	A	236	THR
1	A	237	VAL
1	A	239	THR
1	A	241	ARG
1	A	246	LYS
1	A	255	ILE
1	A	262	THR
1	A	267	VAL
1	A	281	ILE
1	A	286	VAL
1	A	288	LEU
1	A	289	LEU
1	A	297	GLU
1	A	311	THR
1	A	322	ILE
1	A	335	PHE
1	A	341	GLN
1	A	349	VAL
1	A	360	GLU
1	A	361	MET
1	A	374	LEU

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Mol	Chain	Res	Type
1	A	375	ILE
1	A	378	VAL
1	A	385	ARG
1	A	393	ARG
1	A	395	VAL
1	A	399	VAL
1	A	403	ILE
1	C	7	ARG
1	C	8	THR
1	C	28	THR
1	C	38	GLU
1	C	39	ASN
1	C	42	VAL
1	C	63	ILE
1	C	64	ASN
1	C	65	THR
1	C	67	HIS
1	C	89	ILE
1	C	92	MET
1	C	115	GLN
1	C	122	LEU
1	C	128	VAL
1	C	139	ASP
1	C	142	ASP
1	C	156	ASP
1	C	157	LEU
1	C	171	ILE
1	C	181	GLU
1	C	194	GLU
1	C	206	ILE
1	C	219	LYS
1	C	220	PRO
1	C	222	LEU
1	C	223	MET
1	C	226	GLU
1	C	228	VAL
1	C	229	PHE
1	C	231	ILE
1	C	234	ARG
1	C	236	THR
1	C	237	VAL
1	C	239	THR

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Mol	Chain	Res	Type
1	C	241	ARG
1	C	246	LYS
1	C	255	ILE
1	C	262	THR
1	C	267	VAL
1	C	281	ILE
1	C	286	VAL
1	C	288	LEU
1	C	289	LEU
1	C	297	GLU
1	C	311	THR
1	C	322	ILE
1	C	335	PHE
1	C	341	GLN
1	C	349	VAL
1	C	360	GLU
1	C	361	MET
1	C	374	LEU
1	C	375	ILE
1	C	378	VAL
1	C	385	ARG
1	C	393	ARG
1	C	395	VAL
1	C	399	VAL
1	C	403	ILE
1	E	7	ARG
1	E	8	THR
1	E	28	THR
1	E	38	GLU
1	E	39	ASN
1	E	42	VAL
1	E	49	ASP
1	E	63	ILE
1	E	64	ASN
1	E	65	THR
1	E	67	HIS
1	E	89	ILE
1	E	92	MET
1	E	103	ILE
1	E	115	GLN
1	E	122	LEU
1	E	128	VAL

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Mol	Chain	Res	Type
1	E	139	ASP
1	E	142	ASP
1	E	156	ASP
1	E	157	LEU
1	E	171	ILE
1	E	181	GLU
1	E	194	GLU
1	E	206	ILE
1	E	219	LYS
1	E	220	PRO
1	E	222	LEU
1	E	223	MET
1	E	226	GLU
1	E	229	PHE
1	E	231	ILE
1	E	234	ARG
1	E	236	THR
1	E	237	VAL
1	E	239	THR
1	E	241	ARG
1	E	246	LYS
1	E	255	ILE
1	E	262	THR
1	E	267	VAL
1	E	281	ILE
1	E	286	VAL
1	E	288	LEU
1	E	289	LEU
1	E	297	GLU
1	E	311	THR
1	E	322	ILE
1	E	335	PHE
1	E	341	GLN
1	E	349	VAL
1	E	360	GLU
1	E	361	MET
1	E	374	LEU
1	E	375	ILE
1	E	378	VAL
1	E	385	ARG
1	E	393	ARG
1	E	395	VAL

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Mol	Chain	Res	Type
1	E	399	VAL
1	E	403	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	39	ASN
1	A	41	ASN
1	A	64	ASN
1	A	67	HIS
1	A	76	HIS
1	A	79	HIS
1	A	85	HIS
1	A	91	ASN
1	A	159	ASN
1	A	185	ASN
1	A	273	HIS
1	A	278	GLN
1	A	285	ASN
1	A	341	GLN
1	A	367	ASN
1	C	11	HIS
1	C	39	ASN
1	C	41	ASN
1	C	64	ASN
1	C	67	HIS
1	C	76	HIS
1	C	79	HIS
1	C	85	HIS
1	C	91	ASN
1	C	159	ASN
1	C	185	ASN
1	C	273	HIS
1	C	278	GLN
1	C	285	ASN
1	C	341	GLN
1	C	367	ASN
1	E	11	HIS
1	E	39	ASN
1	E	41	ASN
1	E	64	ASN

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Mol	Chain	Res	Type
1	E	67	HIS
1	E	76	HIS
1	E	79	HIS
1	E	85	HIS
1	E	91	ASN
1	E	159	ASN
1	E	185	ASN
1	E	273	HIS
1	E	278	GLN
1	E	285	ASN
1	E	341	GLN
1	E	367	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	71/78 (91%)	10 (14%)	2 (2%)
2	D	71/78 (91%)	10 (14%)	2 (2%)
2	F	71/78 (91%)	10 (14%)	2 (2%)
All	All	213/234 (91%)	30 (14%)	6 (2%)

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	5	A
2	B	14	A
2	B	17	H2U
2	B	18	G
2	B	19	G
2	B	20	G
2	B	31	A
2	B	32	OMC
2	B	73	A
2	B	74	C
2	D	5	A
2	D	14	A
2	D	17	H2U
2	D	18	G
2	D	19	G
2	D	20	G
2	D	31	A

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Mol	Chain	Res	Type
2	D	32	OMC
2	D	73	A
2	D	74	C
2	F	5	A
2	F	14	A
2	F	17	H2U
2	F	18	G
2	F	19	G
2	F	20	G
2	F	31	A
2	F	32	OMC
2	F	73	A
2	F	74	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	17	H2U
2	B	19	G
2	D	17	H2U
2	D	19	G
2	F	17	H2U
2	F	19	G

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

45 non-standard protein/DNA/RNA residues 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
2	YG	B	37	2	38,42,43	1.67	7 (18%)	45,62,65	2.29	14 (31%)
2	OMG	B	34	2	23,26,27	0.59	0	32,38,41	0.70	2 (6%)
2	PSU	F	39	2	18,21,22	0.82	1 (5%)	21,30,33	1.03	3 (14%)
2	OMC	F	32	2	19,22,23	0.34	0	25,31,34	0.72	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PHA	D	77	2	10,11,11	0.68	0	8,13,13	0.22	0
2	5MC	F	40	2	19,22,23	0.52	0	26,32,35	0.82	1 (3%)
2	PHA	F	77	2	10,11,11	0.68	0	8,13,13	0.21	0
2	PSU	D	55	2	18,21,22	0.63	0	21,30,33	0.84	1 (4%)
2	M2G	F	26	2	24,27,28	0.48	0	33,40,43	0.43	0
2	M2G	D	26	2	24,27,28	0.49	0	33,40,43	0.43	0
2	5MU	B	54	2	19,22,23	0.62	0	27,32,35	0.45	0
2	2MG	B	10	2	23,26,27	0.52	0	33,38,41	0.49	0
2	7MG	B	46	2	23,26,27	2.78	3 (13%)	27,39,42	1.63	2 (7%)
2	1MA	F	58	2	21,25,26	0.87	2 (9%)	30,37,40	0.88	2 (6%)
2	5MC	D	49	2	19,22,23	0.49	0	26,32,35	0.75	1 (3%)
2	H2U	B	17	2	18,21,22	0.74	0	19,30,33	1.14	2 (10%)
2	H2U	B	16	2	18,21,22	0.62	0	19,30,33	0.76	0
2	OMC	B	32	2	19,22,23	0.34	0	25,31,34	0.72	1 (4%)
2	7MG	F	46	2	23,26,27	2.80	3 (13%)	27,39,42	1.64	2 (7%)
2	7MG	D	46	2	23,26,27	2.79	3 (13%)	27,39,42	1.63	2 (7%)
2	PSU	B	55	2	18,21,22	0.63	0	21,30,33	0.84	1 (4%)
2	M2G	B	26	2	24,27,28	0.49	0	33,40,43	0.43	0
2	YG	D	37	2	38,42,43	1.67	7 (18%)	45,62,65	2.29	14 (31%)
2	OMG	D	34	2	23,26,27	0.59	0	32,38,41	0.70	2 (6%)
2	5MU	F	54	2	19,22,23	0.61	0	27,32,35	0.45	0
2	PSU	D	39	2	18,21,22	0.82	1 (5%)	21,30,33	1.04	3 (14%)
2	PSU	F	55	2	18,21,22	0.63	0	21,30,33	0.84	1 (4%)
2	5MC	B	49	2	19,22,23	0.49	0	26,32,35	0.75	1 (3%)
2	H2U	F	17	2	18,21,22	0.74	0	19,30,33	1.14	2 (10%)
2	1MA	B	58	2	21,25,26	0.87	2 (9%)	30,37,40	0.87	2 (6%)
2	H2U	D	17	2	18,21,22	0.75	0	19,30,33	1.14	2 (10%)
2	2MG	F	10	2	23,26,27	0.52	0	33,38,41	0.50	0
2	2MG	D	10	2	23,26,27	0.53	0	33,38,41	0.49	0
2	5MC	D	40	2	19,22,23	0.52	0	26,32,35	0.83	1 (3%)
2	PSU	B	39	2	18,21,22	0.83	1 (5%)	21,30,33	1.03	3 (14%)
2	PHA	B	77	2	10,11,11	0.68	0	8,13,13	0.22	0
2	H2U	F	16	2	18,21,22	0.62	0	19,30,33	0.75	0
2	YG	F	37	2	38,42,43	1.67	7 (18%)	45,62,65	2.29	14 (31%)
2	5MC	B	40	2	19,22,23	0.52	0	26,32,35	0.83	1 (3%)
2	H2U	D	16	2	18,21,22	0.61	0	19,30,33	0.76	0
2	OMC	D	32	2	19,22,23	0.35	0	25,31,34	0.72	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	F	34	2	23,26,27	0.60	0	32,38,41	0.70	2 (6%)
2	1MA	D	58	2	21,25,26	0.87	2 (9%)	30,37,40	0.87	2 (6%)
2	5MC	F	49	2	19,22,23	0.49	0	26,32,35	0.76	1 (3%)
2	5MU	D	54	2	19,22,23	0.63	0	27,32,35	0.45	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
2	YG	B	37	2	-	7/24/42/43	0/4/4/4
2	OMG	B	34	2	-	1/9/27/28	0/3/3/3
2	PSU	F	39	2	-	0/7/25/26	0/2/2/2
2	OMC	F	32	2	-	0/9/27/28	0/2/2/2
2	PHA	D	77	2	-	1/5/6/6	0/1/1/1
2	5MC	F	40	2	-	0/7/25/26	0/2/2/2
2	PHA	F	77	2	-	1/5/6/6	0/1/1/1
2	PSU	D	55	2	-	1/7/25/26	0/2/2/2
2	M2G	F	26	2	-	2/11/29/30	0/3/3/3
2	M2G	D	26	2	-	2/11/29/30	0/3/3/3
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
2	2MG	B	10	2	-	0/9/27/28	0/3/3/3
2	7MG	B	46	2	-	0/7/37/38	0/3/3/3
2	1MA	F	58	2	-	0/7/25/26	0/3/3/3
2	5MC	D	49	2	-	1/7/25/26	0/2/2/2
2	H2U	B	17	2	-	3/7/38/39	0/2/2/2
2	H2U	B	16	2	-	1/7/38/39	0/2/2/2
2	OMC	B	32	2	-	0/9/27/28	0/2/2/2
2	7MG	F	46	2	-	0/7/37/38	0/3/3/3
2	7MG	D	46	2	-	0/7/37/38	0/3/3/3
2	PSU	B	55	2	-	1/7/25/26	0/2/2/2
2	M2G	B	26	2	-	2/11/29/30	0/3/3/3
2	YG	D	37	2	-	7/24/42/43	0/4/4/4
2	OMG	D	34	2	-	1/9/27/28	0/3/3/3
2	5MU	F	54	2	-	0/7/25/26	0/2/2/2
2	PSU	D	39	2	-	0/7/25/26	0/2/2/2
2	PSU	F	55	2	-	1/7/25/26	0/2/2/2
2	5MC	B	49	2	-	1/7/25/26	0/2/2/2
2	H2U	F	17	2	-	3/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1MA	B	58	2	-	0/7/25/26	0/3/3/3
2	H2U	D	17	2	-	3/7/38/39	0/2/2/2
2	2MG	F	10	2	-	0/9/27/28	0/3/3/3
2	2MG	D	10	2	-	0/9/27/28	0/3/3/3
2	5MC	D	40	2	-	0/7/25/26	0/2/2/2
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
2	PHA	B	77	2	-	1/5/6/6	0/1/1/1
2	H2U	F	16	2	-	1/7/38/39	0/2/2/2
2	YG	F	37	2	-	7/24/42/43	0/4/4/4
2	5MC	B	40	2	-	0/7/25/26	0/2/2/2
2	H2U	D	16	2	-	1/7/38/39	0/2/2/2
2	OMC	D	32	2	-	0/9/27/28	0/2/2/2
2	OMG	F	34	2	-	1/9/27/28	0/3/3/3
2	1MA	D	58	2	-	0/7/25/26	0/3/3/3
2	5MC	F	49	2	-	1/7/25/26	0/2/2/2
2	5MU	D	54	2	-	0/7/25/26	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	46	7MG	C8-N9	-12.78	1.37	1.45
2	D	46	7MG	C8-N9	-12.74	1.37	1.45
2	B	46	7MG	C8-N9	-12.71	1.37	1.45
2	D	37	YG	C15-N20	4.71	1.55	1.45
2	B	37	YG	C15-N20	4.68	1.55	1.45
2	F	37	YG	C15-N20	4.68	1.55	1.45
2	F	37	YG	C2-N3	-4.41	1.31	1.38
2	B	37	YG	C2-N3	-4.40	1.31	1.38
2	D	37	YG	C2-N3	-4.40	1.31	1.38
2	F	37	YG	C21-N20	3.37	1.43	1.34
2	B	37	YG	C21-N20	3.36	1.43	1.34
2	D	37	YG	C21-N20	3.34	1.43	1.34
2	F	37	YG	O23-C21	-3.32	1.28	1.34
2	B	37	YG	O23-C21	-3.28	1.28	1.34
2	D	37	YG	O23-C21	-3.26	1.28	1.34
2	D	37	YG	C13-C12	2.90	1.53	1.50
2	B	37	YG	C13-C12	2.86	1.53	1.50
2	F	37	YG	C13-C12	2.86	1.53	1.50
2	F	37	YG	O18-C16	-2.78	1.26	1.33
2	B	37	YG	O18-C16	-2.75	1.26	1.33
2	D	37	YG	O18-C16	-2.75	1.26	1.33
2	D	37	YG	C10-C11	-2.71	1.44	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	YG	C10-C11	-2.68	1.44	1.49
2	F	37	YG	C10-C11	-2.66	1.44	1.49
2	D	58	1MA	C6-N6	2.55	1.34	1.28
2	B	58	1MA	C6-N6	2.54	1.34	1.28
2	F	58	1MA	C6-N6	2.53	1.34	1.28
2	D	46	7MG	C5-N7	2.49	1.38	1.35
2	B	46	7MG	C8-N7	-2.46	1.30	1.42
2	D	46	7MG	C8-N7	-2.46	1.30	1.42
2	F	46	7MG	C8-N7	-2.46	1.30	1.42
2	B	46	7MG	C5-N7	2.45	1.38	1.35
2	F	46	7MG	C5-N7	2.45	1.38	1.35
2	B	39	PSU	C6-C5	-2.18	1.32	1.35
2	D	39	PSU	C6-C5	-2.17	1.32	1.35
2	F	39	PSU	C6-C5	-2.14	1.32	1.35
2	B	58	1MA	C2-N3	2.02	1.34	1.30
2	D	58	1MA	C2-N3	2.02	1.34	1.30
2	F	58	1MA	C2-N3	2.01	1.34	1.30

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	46	7MG	N9-C8-N7	6.48	112.55	103.37
2	B	46	7MG	N9-C8-N7	6.48	112.54	103.37
2	D	46	7MG	N9-C8-N7	6.47	112.54	103.37
2	F	37	YG	O23-C21-N20	5.91	120.71	110.77
2	B	37	YG	O23-C21-N20	5.91	120.71	110.77
2	D	37	YG	O23-C21-N20	5.88	120.66	110.77
2	D	37	YG	C5-C4-N3	4.92	127.99	123.99
2	B	37	YG	C5-C4-N3	4.91	127.98	123.99
2	F	37	YG	C5-C4-N3	4.89	127.97	123.99
2	D	37	YG	O23-C21-O22	-4.61	117.91	124.62
2	B	37	YG	O23-C21-O22	-4.61	117.91	124.62
2	F	37	YG	O23-C21-O22	-4.59	117.93	124.62
2	D	37	YG	O18-C16-C15	4.42	122.73	111.49
2	F	37	YG	O18-C16-C15	4.42	122.73	111.49
2	B	37	YG	O18-C16-C15	4.42	122.73	111.49
2	B	37	YG	C14-C15-C16	-4.41	98.05	110.38
2	F	37	YG	C14-C15-C16	-4.40	98.06	110.38
2	D	37	YG	C14-C15-C16	-4.40	98.06	110.38
2	F	37	YG	C11-C12-N1	-4.35	102.24	105.31
2	B	37	YG	C11-C12-N1	-4.35	102.24	105.31
2	D	37	YG	C11-C12-N1	-4.32	102.26	105.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	37	YG	C14-C13-C12	-4.23	104.71	113.36
2	F	37	YG	C14-C13-C12	-4.23	104.72	113.36
2	F	37	YG	C24-O23-C21	4.22	120.52	115.63
2	D	37	YG	C14-C13-C12	-4.22	104.73	113.36
2	B	37	YG	C24-O23-C21	4.20	120.50	115.63
2	D	37	YG	C24-O23-C21	4.19	120.48	115.63
2	F	46	7MG	C4-C5-N7	4.17	110.31	105.38
2	B	46	7MG	C4-C5-N7	4.17	110.30	105.38
2	D	46	7MG	C4-C5-N7	4.13	110.26	105.38
2	B	37	YG	N3-C2-N2	-3.90	121.24	126.62
2	D	37	YG	N3-C2-N2	-3.89	121.25	126.62
2	F	37	YG	N3-C2-N2	-3.85	121.32	126.62
2	D	40	5MC	CM5-C5-C6	-2.66	119.25	122.85
2	B	40	5MC	CM5-C5-C6	-2.65	119.26	122.85
2	F	40	5MC	CM5-C5-C6	-2.64	119.28	122.85
2	F	58	1MA	N1-C2-N3	2.59	129.07	126.00
2	D	34	OMG	O2'-C2'-C1'	2.54	113.81	108.99
2	B	34	OMG	O2'-C2'-C1'	2.54	113.80	108.99
2	D	58	1MA	N1-C2-N3	2.53	129.00	126.00
2	F	34	OMG	O2'-C2'-C1'	2.53	113.78	108.99
2	B	58	1MA	N1-C2-N3	2.52	128.99	126.00
2	B	49	5MC	C5-C6-N1	-2.41	120.69	123.31
2	F	49	5MC	C5-C6-N1	-2.41	120.70	123.31
2	D	49	5MC	C5-C6-N1	-2.37	120.74	123.31
2	D	58	1MA	O3'-C3'-C4'	-2.36	104.29	111.08
2	B	58	1MA	O3'-C3'-C4'	-2.36	104.31	111.08
2	F	58	1MA	O3'-C3'-C4'	-2.36	104.31	111.08
2	B	39	PSU	C6-C5-C4	2.34	119.75	118.17
2	D	39	PSU	C6-C5-C4	2.34	119.75	118.17
2	F	37	YG	C10-C11-N2	2.33	123.99	119.32
2	D	37	YG	O18-C16-O17	-2.32	119.33	123.85
2	D	37	YG	C10-C11-N2	2.32	123.97	119.32
2	B	37	YG	O18-C16-O17	-2.31	119.34	123.85
2	B	37	YG	C10-C11-N2	2.31	123.96	119.32
2	F	39	PSU	C6-C5-C4	2.31	119.73	118.17
2	F	37	YG	O18-C16-O17	-2.30	119.37	123.85
2	B	39	PSU	O4'-C1'-C2'	2.19	108.18	105.15
2	F	39	PSU	O4'-C1'-C2'	2.17	108.15	105.15
2	D	39	PSU	O4'-C1'-C2'	2.16	108.14	105.15
2	D	55	PSU	C6-C5-C4	2.14	119.62	118.17
2	F	37	YG	O22-C21-N20	-2.14	121.36	124.86
2	D	39	PSU	C6-N1-C2	-2.14	120.71	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	32	OMC	C2'-C1'-N1	-2.13	110.20	114.24
2	B	37	YG	O22-C21-N20	-2.13	121.38	124.86
2	F	17	H2U	N3-C2-N1	-2.13	114.51	116.65
2	B	32	OMC	C2'-C1'-N1	-2.12	110.21	114.24
2	D	32	OMC	C2'-C1'-N1	-2.11	110.23	114.24
2	B	17	H2U	N3-C2-N1	-2.11	114.52	116.65
2	D	17	H2U	N3-C2-N1	-2.11	114.53	116.65
2	F	55	PSU	C6-C5-C4	2.10	119.59	118.17
2	B	55	PSU	C6-C5-C4	2.10	119.59	118.17
2	D	37	YG	O22-C21-N20	-2.10	121.42	124.86
2	D	17	H2U	O3'-C3'-C2'	2.09	118.51	111.82
2	F	17	H2U	O3'-C3'-C2'	2.08	118.50	111.82
2	F	37	YG	C15-N20-C21	2.08	126.11	120.93
2	B	17	H2U	O3'-C3'-C2'	2.08	118.48	111.82
2	B	39	PSU	C6-N1-C2	-2.07	120.77	122.69
2	B	37	YG	C15-N20-C21	2.07	126.08	120.93
2	D	37	YG	C15-N20-C21	2.06	126.06	120.93
2	B	34	OMG	CM2-O2'-C2'	-2.06	109.19	114.47
2	D	34	OMG	CM2-O2'-C2'	-2.05	109.20	114.47
2	F	34	OMG	CM2-O2'-C2'	-2.05	109.20	114.47
2	F	37	YG	O17-C16-C15	-2.04	117.90	123.94
2	B	37	YG	O17-C16-C15	-2.03	117.93	123.94
2	D	37	YG	O17-C16-C15	-2.03	117.93	123.94
2	F	39	PSU	C6-N1-C2	-2.03	120.81	122.69

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	34	OMG	C1'-C2'-O2'-CM2
2	B	37	YG	C15-C16-O18-C19
2	B	37	YG	O17-C16-O18-C19
2	B	37	YG	N20-C21-O23-C24
2	B	37	YG	O22-C21-O23-C24
2	D	34	OMG	C1'-C2'-O2'-CM2
2	D	37	YG	C15-C16-O18-C19
2	D	37	YG	O17-C16-O18-C19
2	D	37	YG	N20-C21-O23-C24
2	D	37	YG	O22-C21-O23-C24
2	D	77	PHA	C-CA-CB-CG
2	F	34	OMG	C1'-C2'-O2'-CM2
2	F	37	YG	C15-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
2	F	37	YG	O17-C16-O18-C19
2	F	37	YG	N20-C21-O23-C24
2	F	37	YG	O22-C21-O23-C24
2	F	77	PHA	C-CA-CB-CG
2	B	37	YG	O23-C21-N20-C15
2	D	37	YG	O23-C21-N20-C15
2	F	37	YG	O23-C21-N20-C15
2	B	37	YG	O22-C21-N20-C15
2	D	37	YG	O22-C21-N20-C15
2	F	37	YG	O22-C21-N20-C15
2	B	17	H2U	C2'-C1'-N1-C6
2	D	17	H2U	C2'-C1'-N1-C6
2	F	17	H2U	C2'-C1'-N1-C6
2	B	77	PHA	C-CA-CB-CG
2	B	37	YG	C12-C13-C14-C15
2	D	37	YG	C12-C13-C14-C15
2	F	37	YG	C12-C13-C14-C15
2	B	55	PSU	O4'-C1'-C5-C4
2	D	55	PSU	O4'-C1'-C5-C4
2	F	55	PSU	O4'-C1'-C5-C4
2	B	17	H2U	C2'-C1'-N1-C2
2	D	17	H2U	C2'-C1'-N1-C2
2	F	17	H2U	C2'-C1'-N1-C2
2	B	17	H2U	C4'-C5'-O5'-P
2	B	26	M2G	C4'-C5'-O5'-P
2	D	17	H2U	C4'-C5'-O5'-P
2	D	26	M2G	C4'-C5'-O5'-P
2	F	17	H2U	C4'-C5'-O5'-P
2	F	26	M2G	C4'-C5'-O5'-P
2	F	16	H2U	C2'-C1'-N1-C6
2	B	26	M2G	C2'-C1'-N9-C4
2	D	26	M2G	C2'-C1'-N9-C4
2	F	26	M2G	C2'-C1'-N9-C4
2	B	49	5MC	C2'-C1'-N1-C2
2	D	49	5MC	C2'-C1'-N1-C2
2	F	49	5MC	C2'-C1'-N1-C2
2	B	16	H2U	C2'-C1'-N1-C6
2	D	16	H2U	C2'-C1'-N1-C6

There are no ring outliers.

45 monomers are involved in 150 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	37	YG	10	0
2	B	34	OMG	3	0
2	F	39	PSU	2	0
2	F	32	OMC	4	0
2	D	77	PHA	7	0
2	F	40	5MC	3	0
2	F	77	PHA	7	0
2	D	55	PSU	1	0
2	F	26	M2G	9	0
2	D	26	M2G	9	0
2	B	54	5MU	1	0
2	B	10	2MG	4	0
2	B	46	7MG	3	0
2	F	58	1MA	2	0
2	D	49	5MC	1	0
2	B	17	H2U	1	0
2	B	16	H2U	2	0
2	B	32	OMC	4	0
2	F	46	7MG	3	0
2	D	46	7MG	3	0
2	B	55	PSU	1	0
2	B	26	M2G	8	0
2	D	37	YG	11	0
2	D	34	OMG	5	0
2	F	54	5MU	1	0
2	D	39	PSU	3	0
2	F	55	PSU	1	0
2	B	49	5MC	1	0
2	F	17	H2U	1	0
2	B	58	1MA	2	0
2	D	17	H2U	1	0
2	F	10	2MG	5	0
2	D	10	2MG	5	0
2	D	40	5MC	4	0
2	B	39	PSU	2	0
2	B	77	PHA	7	0
2	F	16	H2U	2	0
2	F	37	YG	11	0
2	B	40	5MC	3	0
2	D	16	H2U	3	0
2	D	32	OMC	4	0
2	F	34	OMG	5	0
2	D	58	1MA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	49	5MC	1	0
2	D	54	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GNP	A	1406	4	34,34,34	1.33	5 (14%)	47,54,54	1.40	5 (10%)
3	GNP	E	1406	4	34,34,34	1.34	5 (14%)	47,54,54	1.40	5 (10%)
5	ENX	A	1408	-	44,47,47	1.29	8 (18%)	45,62,62	1.46	9 (20%)
5	ENX	E	1408	-	44,47,47	1.29	8 (18%)	45,62,62	1.46	9 (20%)
3	GNP	C	1406	4	34,34,34	1.33	5 (14%)	47,54,54	1.40	5 (10%)
5	ENX	C	1408	-	44,47,47	1.29	8 (18%)	45,62,62	1.46	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GNP	A	1406	4	-	6/18/38/38	0/3/3/3
3	GNP	E	1406	4	-	6/18/38/38	0/3/3/3
5	ENX	A	1408	-	-	12/54/71/71	0/1/1/1
5	ENX	E	1408	-	-	12/54/71/71	0/1/1/1
3	GNP	C	1406	4	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ENX	C	1408	-	-	12/54/71/71	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1406	GNP	PG-O2G	-3.69	1.47	1.56
3	E	1406	GNP	PG-O2G	-3.67	1.47	1.56
3	A	1406	GNP	PG-O2G	-3.67	1.47	1.56
5	E	1408	ENX	C38-C25	3.32	1.57	1.52
5	A	1408	ENX	C38-C25	3.30	1.57	1.52
5	C	1408	ENX	C38-C25	3.28	1.57	1.52
5	A	1408	ENX	O24-C23	3.07	1.41	1.34
5	C	1408	ENX	O24-C23	3.06	1.41	1.34
5	E	1408	ENX	O24-C23	3.05	1.41	1.34
3	C	1406	GNP	PG-O1G	3.02	1.50	1.46
3	A	1406	GNP	PG-O1G	3.01	1.50	1.46
3	E	1406	GNP	PG-O1G	3.01	1.50	1.46
3	E	1406	GNP	C6-N1	2.59	1.43	1.38
3	C	1406	GNP	C6-N1	2.58	1.43	1.38
3	A	1406	GNP	C6-N1	2.57	1.43	1.38
5	C	1408	ENX	O29-C42	2.44	1.40	1.35
5	A	1408	ENX	O29-C42	2.41	1.40	1.35
5	E	1408	ENX	O29-C42	2.39	1.40	1.35
3	E	1406	GNP	C4-N3	2.24	1.39	1.34
3	A	1406	GNP	C4-N3	2.24	1.39	1.34
3	C	1406	GNP	C4-N3	2.21	1.39	1.34
5	E	1408	ENX	C8-C7	-2.15	1.50	1.53
5	A	1408	ENX	C8-C7	-2.13	1.50	1.53
5	C	1408	ENX	C8-C7	-2.12	1.50	1.53
5	E	1408	ENX	O44-C42	2.12	1.25	1.22
3	E	1406	GNP	PG-O3G	-2.10	1.51	1.56
5	E	1408	ENX	O47-C28	2.10	1.37	1.30
5	A	1408	ENX	O44-C42	2.09	1.25	1.22
3	A	1406	GNP	PG-O3G	-2.09	1.51	1.56
3	C	1406	GNP	PG-O3G	-2.08	1.51	1.56
5	C	1408	ENX	C42-N43	2.07	1.37	1.33
5	A	1408	ENX	O47-C28	2.07	1.37	1.30
5	C	1408	ENX	O47-C28	2.07	1.37	1.30
5	C	1408	ENX	C39-C38	2.05	1.55	1.52
5	A	1408	ENX	C42-N43	2.05	1.37	1.33
5	C	1408	ENX	O44-C42	2.04	1.25	1.22
5	E	1408	ENX	C42-N43	2.04	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1408	ENX	C39-C38	2.02	1.55	1.52
5	E	1408	ENX	C39-C38	2.01	1.55	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1406	GNP	O1G-PG-N3B	-5.11	104.24	111.77
3	A	1406	GNP	O1G-PG-N3B	-5.11	104.25	111.77
3	C	1406	GNP	O1G-PG-N3B	-5.10	104.25	111.77
3	C	1406	GNP	O2G-PG-O3G	4.08	118.56	107.59
3	A	1406	GNP	O2G-PG-O3G	4.08	118.56	107.59
3	E	1406	GNP	O2G-PG-O3G	4.08	118.55	107.59
5	C	1408	ENX	O24-C25-C38	3.88	112.76	106.74
5	A	1408	ENX	O24-C25-C38	3.88	112.76	106.74
5	E	1408	ENX	O24-C25-C38	3.87	112.75	106.74
5	E	1408	ENX	O47-C28-O46	-3.47	116.20	124.08
5	A	1408	ENX	O47-C28-O46	-3.46	116.22	124.08
5	C	1408	ENX	O47-C28-O46	-3.46	116.24	124.08
3	E	1406	GNP	O2G-PG-O1G	-3.07	105.75	113.45
3	A	1406	GNP	O2G-PG-O1G	-3.07	105.76	113.45
3	C	1406	GNP	O2G-PG-O1G	-3.05	105.79	113.45
3	E	1406	GNP	O4'-C1'-N9	2.72	114.53	108.36
3	C	1406	GNP	O4'-C1'-N9	2.72	114.53	108.36
3	A	1406	GNP	O4'-C1'-N9	2.71	114.49	108.36
5	E	1408	ENX	O24-C23-O37	-2.61	119.17	123.34
5	A	1408	ENX	O24-C23-O37	-2.60	119.17	123.34
5	C	1408	ENX	O24-C23-O37	-2.59	119.19	123.34
5	E	1408	ENX	C5-O29-C42	2.52	119.89	116.28
3	C	1406	GNP	O3G-PG-O1G	-2.50	107.17	113.45
5	A	1408	ENX	C5-O29-C42	2.50	119.87	116.28
5	C	1408	ENX	C5-O29-C42	2.49	119.85	116.28
5	E	1408	ENX	O33-C11-C10	-2.48	104.84	109.29
5	C	1408	ENX	O33-C11-C10	-2.47	104.85	109.29
3	A	1406	GNP	O3G-PG-O1G	-2.47	107.25	113.45
5	A	1408	ENX	O33-C11-C10	-2.47	104.86	109.29
3	E	1406	GNP	O3G-PG-O1G	-2.46	107.29	113.45
5	A	1408	ENX	C7-C8-C9	-2.35	109.03	114.27
5	C	1408	ENX	C7-C8-C9	-2.35	109.05	114.27
5	E	1408	ENX	C7-C8-C9	-2.34	109.08	114.27
5	E	1408	ENX	O46-C28-C27	2.28	128.91	122.86
5	A	1408	ENX	O46-C28-C27	2.27	128.89	122.86
5	C	1408	ENX	O46-C28-C27	2.27	128.87	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1408	ENX	C25-O24-C23	2.16	120.67	117.50
5	C	1408	ENX	C25-O24-C23	2.15	120.67	117.50
5	A	1408	ENX	C25-O24-C23	2.15	120.66	117.50
5	A	1408	ENX	C26-C25-C38	-2.13	108.84	111.07
5	E	1408	ENX	C26-C25-C38	-2.12	108.84	111.07
5	C	1408	ENX	C26-C25-C38	-2.10	108.87	111.07

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1406	GNP	PG-N3B-PB-O1B
3	A	1406	GNP	C5'-O5'-PA-O3A
3	A	1406	GNP	C5'-O5'-PA-O1A
3	A	1406	GNP	C5'-O5'-PA-O2A
3	C	1406	GNP	PG-N3B-PB-O1B
3	C	1406	GNP	C5'-O5'-PA-O3A
3	C	1406	GNP	C5'-O5'-PA-O1A
3	C	1406	GNP	C5'-O5'-PA-O2A
3	E	1406	GNP	PG-N3B-PB-O1B
3	E	1406	GNP	C5'-O5'-PA-O3A
3	E	1406	GNP	C5'-O5'-PA-O1A
3	E	1406	GNP	C5'-O5'-PA-O2A
5	A	1408	ENX	C3-C4-C5-C6
5	A	1408	ENX	C17-C18-C19-C20
5	A	1408	ENX	C18-C19-C20-C21
5	A	1408	ENX	C20-C21-C22-C23
5	A	1408	ENX	N43-C42-O29-C5
5	A	1408	ENX	O44-C42-O29-C5
5	C	1408	ENX	C3-C4-C5-C6
5	C	1408	ENX	C17-C18-C19-C20
5	C	1408	ENX	C18-C19-C20-C21
5	C	1408	ENX	C20-C21-C22-C23
5	C	1408	ENX	N43-C42-O29-C5
5	C	1408	ENX	O44-C42-O29-C5
5	E	1408	ENX	C3-C4-C5-C6
5	E	1408	ENX	C17-C18-C19-C20
5	E	1408	ENX	C18-C19-C20-C21
5	E	1408	ENX	C20-C21-C22-C23
5	E	1408	ENX	N43-C42-O29-C5
5	E	1408	ENX	O44-C42-O29-C5
5	A	1408	ENX	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
5	C	1408	ENX	C36-C18-C19-C20
5	E	1408	ENX	C36-C18-C19-C20
5	A	1408	ENX	C21-C22-C23-O24
5	C	1408	ENX	C21-C22-C23-O24
5	E	1408	ENX	C21-C22-C23-O24
5	A	1408	ENX	C21-C22-C23-O37
5	C	1408	ENX	C21-C22-C23-O37
5	E	1408	ENX	C21-C22-C23-O37
5	A	1408	ENX	C1-C2-C3-C4
5	C	1408	ENX	C1-C2-C3-C4
5	E	1408	ENX	C1-C2-C3-C4
5	A	1408	ENX	C9-C10-C11-O33
5	C	1408	ENX	C9-C10-C11-O33
5	E	1408	ENX	C9-C10-C11-O33
3	A	1406	GNP	O4'-C4'-C5'-O5'
3	C	1406	GNP	O4'-C4'-C5'-O5'
3	E	1406	GNP	O4'-C4'-C5'-O5'
3	A	1406	GNP	C3'-C4'-C5'-O5'
3	C	1406	GNP	C3'-C4'-C5'-O5'
3	E	1406	GNP	C3'-C4'-C5'-O5'
5	A	1408	ENX	C3-C4-C5-O29
5	C	1408	ENX	C3-C4-C5-O29
5	E	1408	ENX	C3-C4-C5-O29

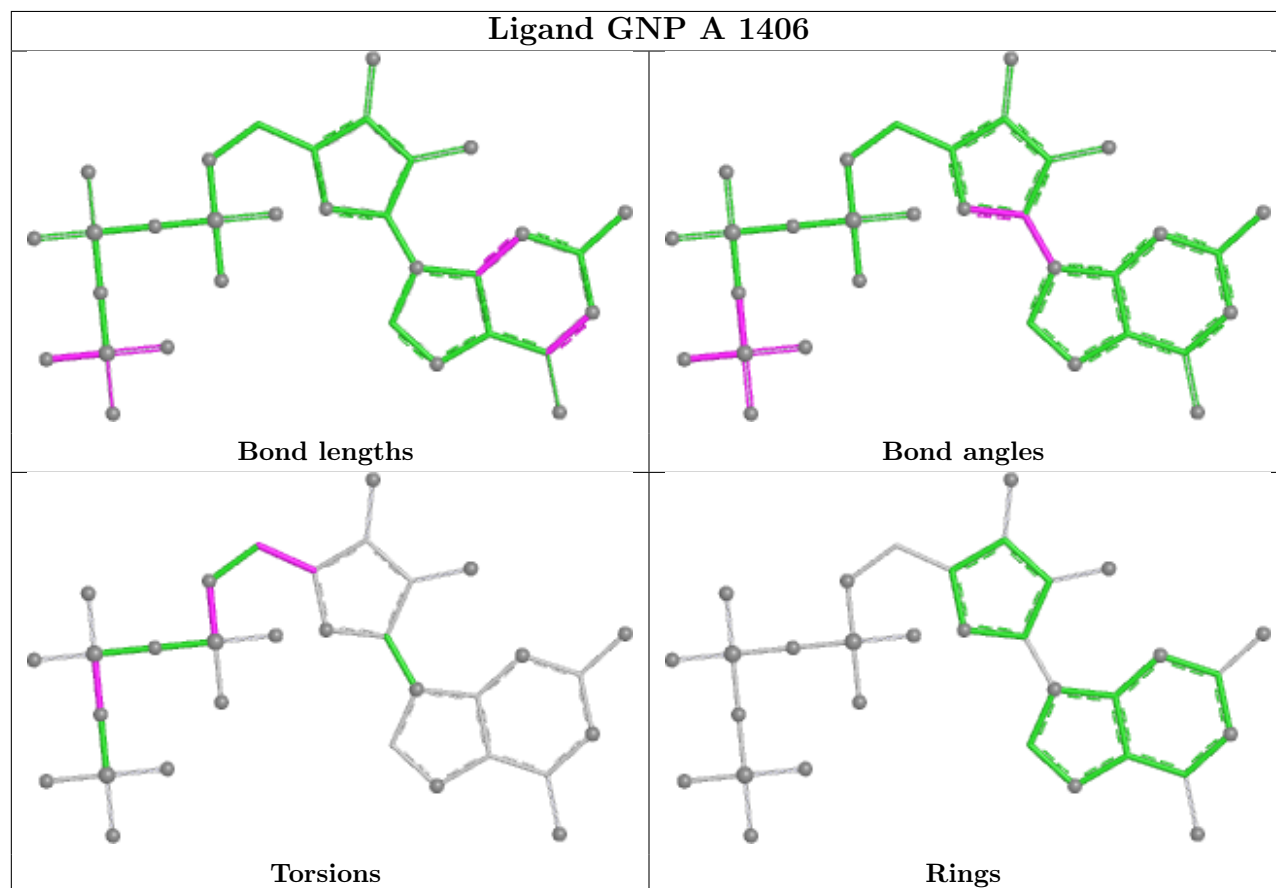
There are no ring outliers.

6 monomers are involved in 37 short contacts:

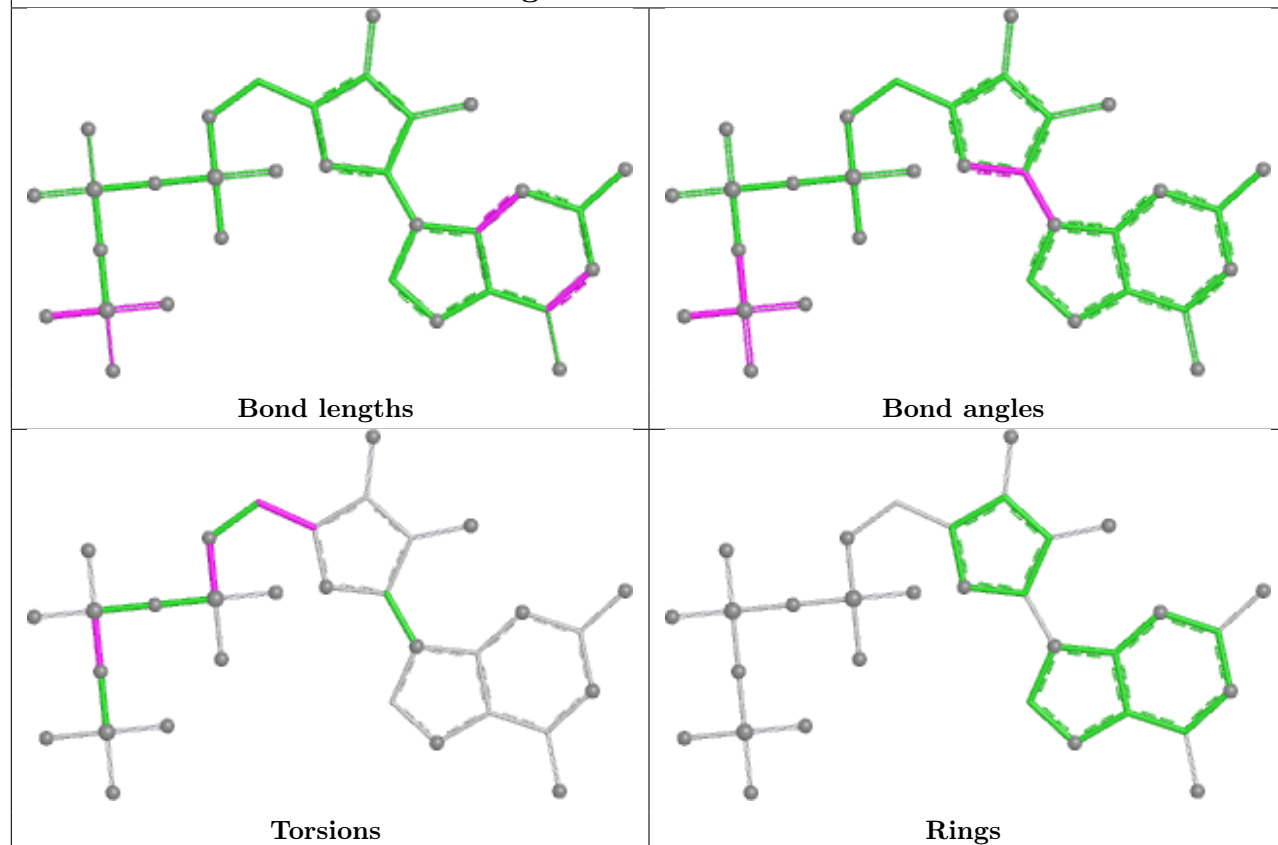
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1406	GNP	7	0
3	E	1406	GNP	8	0
5	A	1408	ENX	5	0
5	E	1408	ENX	5	0
3	C	1406	GNP	7	0
5	C	1408	ENX	5	0

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

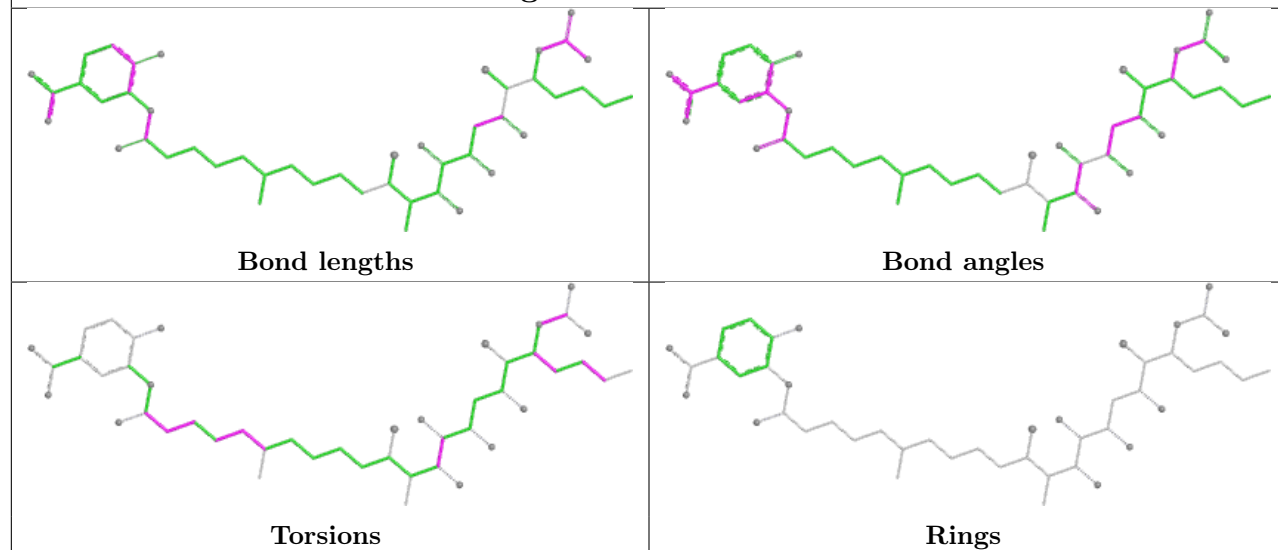
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



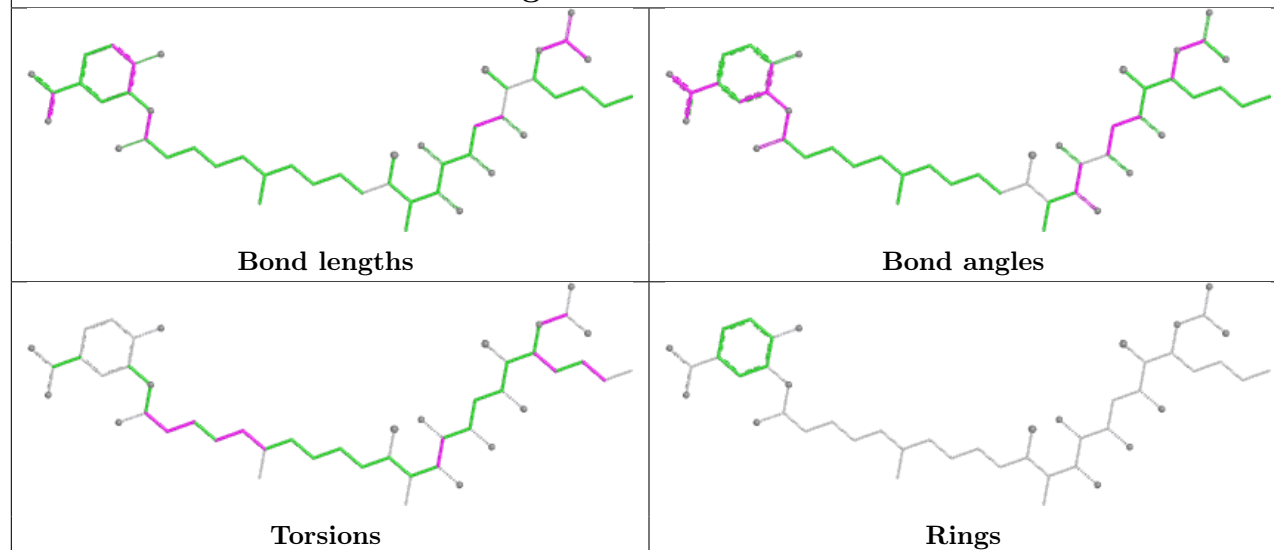
Ligand GNP E 1406



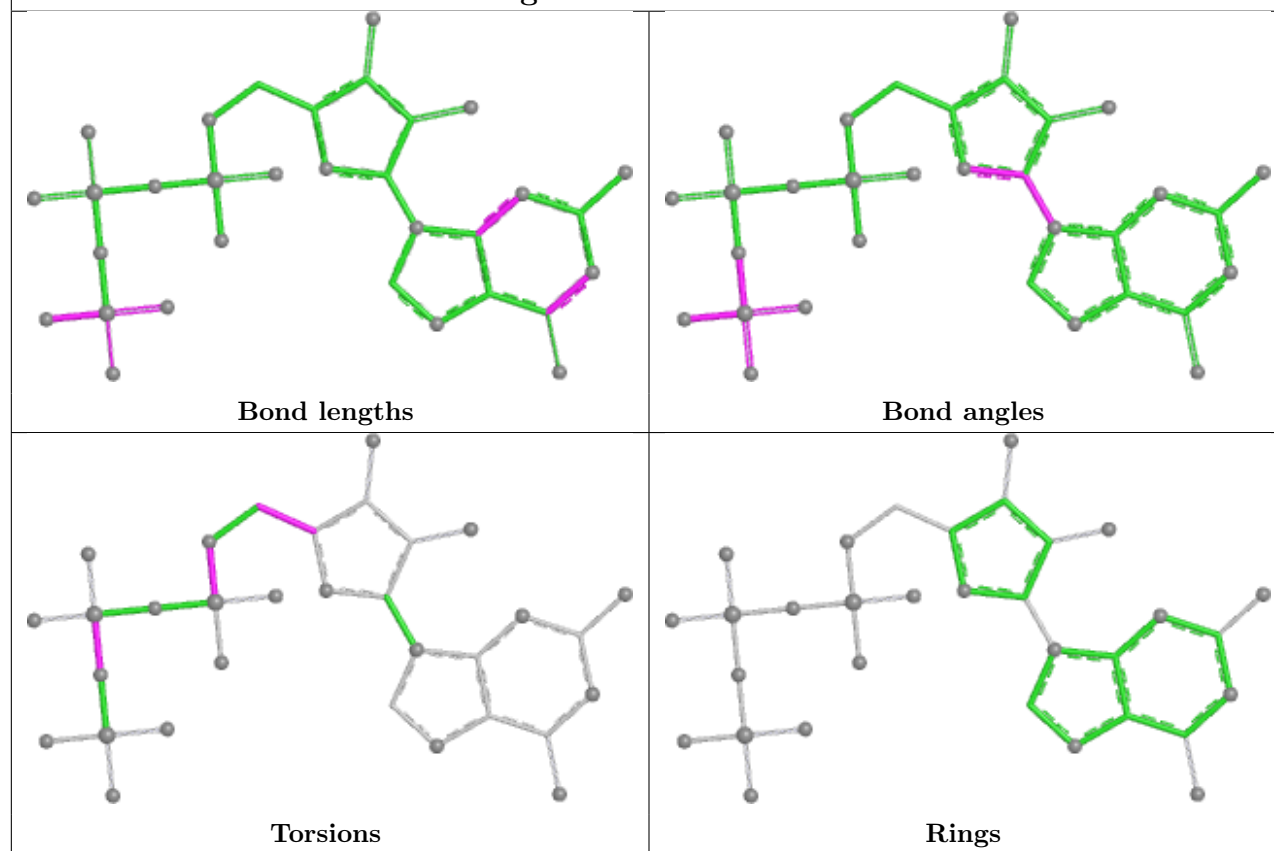
Ligand ENX A 1408

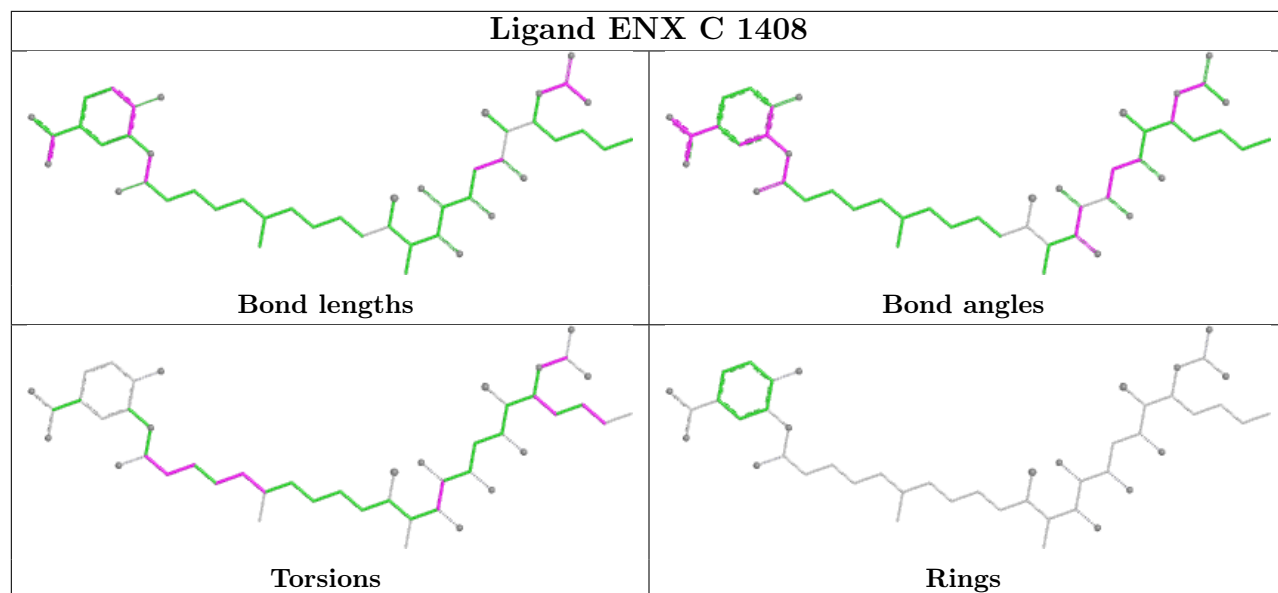


Ligand ENX E 1408



Ligand GNP C 1406





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	D	1
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	77:PHA	C	77(A):C	P	10.77
1	D	77:PHA	C	77(A):C	P	10.77
1	F	77:PHA	C	77(A):C	P	10.77

6 Fit of model and data [i](#)

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

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	400/405 (98%)	-1.08	3 (0%) 82 65	24, 83, 127, 155	0
1	C	400/405 (98%)	-1.12	0 100 100	24, 83, 127, 155	0
1	E	400/405 (98%)	-1.10	1 (0%) 90 80	24, 83, 127, 155	0
2	B	62/78 (79%)	-1.62	0 100 100	22, 62, 102, 111	0
2	D	62/78 (79%)	-1.71	0 100 100	22, 62, 102, 111	0
2	F	62/78 (79%)	-1.77	0 100 100	22, 62, 102, 111	0
All	All	1386/1449 (95%)	-1.18	4 (0%) 90 80	22, 80, 126, 155	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	TYR	2.6
1	A	231	ILE	2.3
1	A	307	PRO	2.1
1	A	397	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	M2G	B	26	25/26	0.98	0.05	67,87,114,121	0
2	PHA	B	77	11/11	0.98	0.14	98,114,124,126	0
2	2MG	D	10	24/25	0.98	0.05	76,85,97,103	0
2	H2U	D	16	20/21	0.98	0.04	50,92,109,111	0
2	H2U	D	17	20/21	0.98	0.04	91,123,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	H2U	F	17	20/21	0.98	0.04	91,123,146,146	0
2	M2G	F	26	25/26	0.98	0.05	67,87,114,121	0
2	PSU	B	39	20/21	0.99	0.04	16,36,50,54	0
2	5MC	B	40	21/22	0.99	0.03	23,42,56,65	0
2	7MG	B	46	24/25	0.99	0.04	25,53,93,99	0
2	5MC	B	49	21/22	0.99	0.04	19,28,35,50	0
2	5MU	B	54	21/22	0.99	0.05	3,28,45,54	0
2	PSU	B	55	20/21	0.99	0.04	18,38,54,57	0
2	1MA	B	58	23/24	0.99	0.06	6,25,34,37	0
2	H2U	B	16	20/21	0.99	0.05	50,92,109,111	0
2	H2U	B	17	20/21	0.99	0.04	91,123,146,146	0
2	2MG	B	10	24/25	0.99	0.04	76,85,97,103	0
2	OMC	B	32	21/22	0.99	0.04	44,63,73,89	0
2	M2G	D	26	25/26	0.99	0.05	67,87,114,121	0
2	OMC	D	32	21/22	0.99	0.04	44,63,73,89	0
2	OMG	D	34	24/25	0.99	0.04	2,29,39,50	0
2	YG	D	37	39/40	0.99	0.05	13,44,86,93	0
2	PSU	D	39	20/21	0.99	0.04	16,36,50,54	0
2	5MC	D	40	21/22	0.99	0.02	23,42,56,65	0
2	7MG	D	46	24/25	0.99	0.03	25,53,93,99	0
2	5MC	D	49	21/22	0.99	0.05	19,28,35,50	0
2	5MU	D	54	21/22	0.99	0.04	3,28,45,54	0
2	PSU	D	55	20/21	0.99	0.04	18,38,54,57	0
2	1MA	D	58	23/24	0.99	0.05	6,25,34,37	0
2	PHA	D	77	11/11	0.99	0.07	98,114,124,126	0
2	2MG	F	10	24/25	0.99	0.04	76,85,97,103	0
2	H2U	F	16	20/21	0.99	0.04	50,92,109,111	0
2	OMG	B	34	24/25	0.99	0.03	2,29,39,50	0
2	YG	B	37	39/40	0.99	0.05	13,44,86,93	0
2	OMC	F	32	21/22	0.99	0.04	44,63,73,89	0
2	OMG	F	34	24/25	0.99	0.03	2,29,39,50	0
2	YG	F	37	39/40	0.99	0.05	13,44,86,93	0
2	PSU	F	39	20/21	0.99	0.03	16,36,50,54	0
2	5MC	F	40	21/22	0.99	0.03	23,42,56,65	0
2	7MG	F	46	24/25	0.99	0.04	25,53,93,99	0
2	5MC	F	49	21/22	0.99	0.04	19,28,35,50	0
2	5MU	F	54	21/22	0.99	0.03	3,28,45,54	0
2	PSU	F	55	20/21	0.99	0.04	18,38,54,57	0
2	1MA	F	58	23/24	0.99	0.04	6,25,34,37	0
2	PHA	F	77	11/11	0.99	0.06	98,114,124,126	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

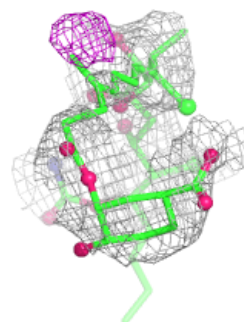
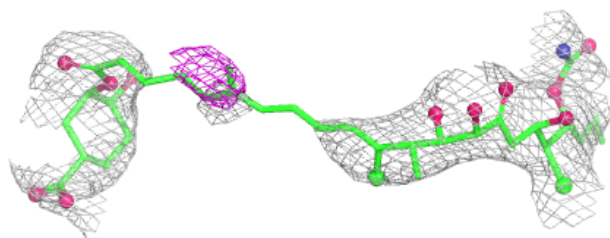
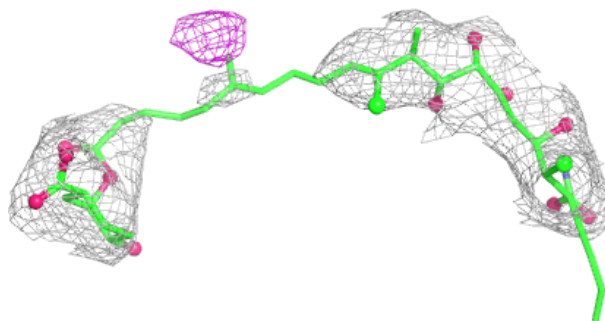
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	ENX	C	1408	47/47	0.98	0.06	45,74,86,109	0
5	ENX	E	1408	47/47	0.98	0.05	45,74,86,109	0
3	GNP	E	1406	32/32	0.99	0.04	47,70,85,90	0
4	MG	A	1407	1/1	0.99	0.03	57,57,57,57	0
4	MG	C	1407	1/1	0.99	0.02	57,57,57,57	0
4	MG	E	1407	1/1	0.99	0.04	57,57,57,57	0
5	ENX	A	1408	47/47	0.99	0.06	45,74,86,109	0
3	GNP	A	1406	32/32	0.99	0.04	47,70,85,90	0
3	GNP	C	1406	32/32	0.99	0.04	47,70,85,90	0

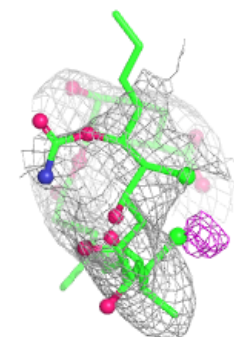
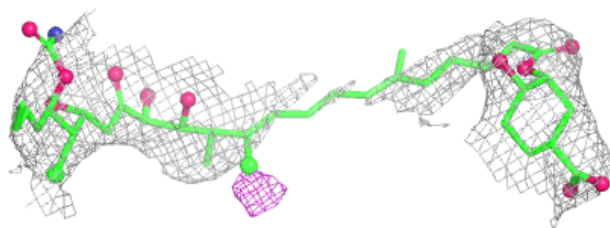
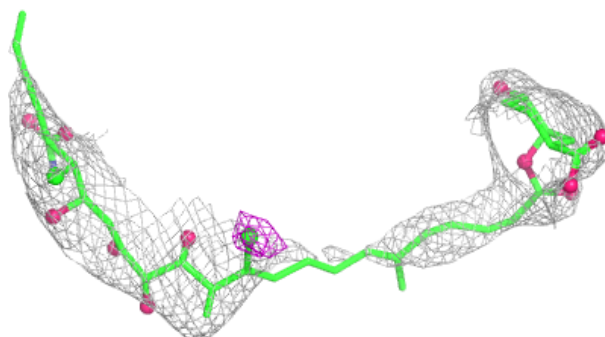
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ENX C 1408:

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

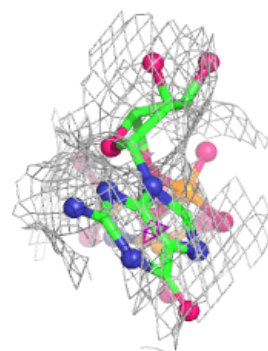
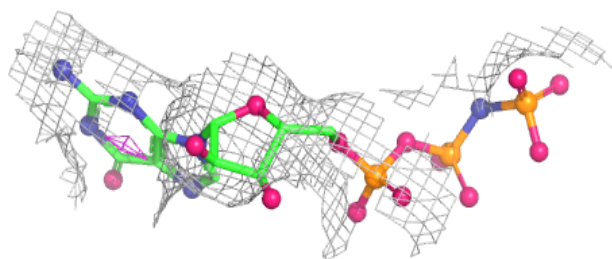
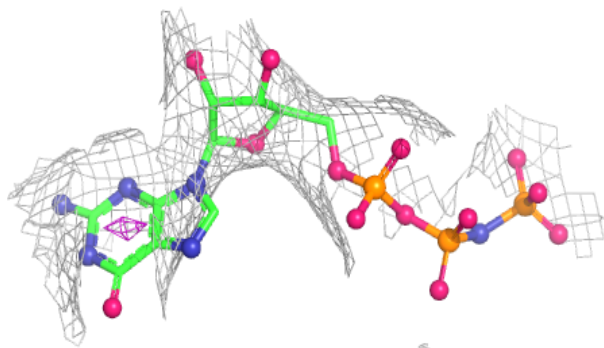
**Electron density around ENX E 1408:**

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

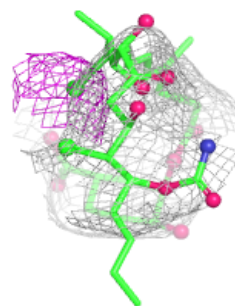
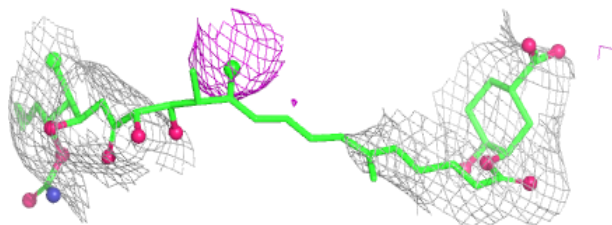
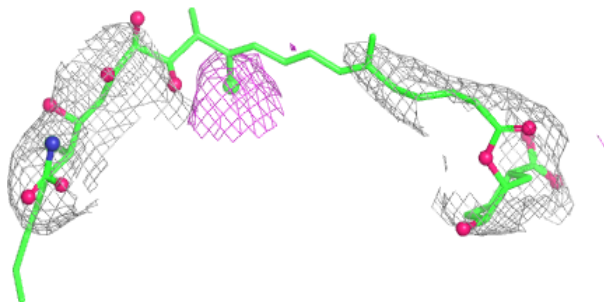


Electron density around GNP E 1406:

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

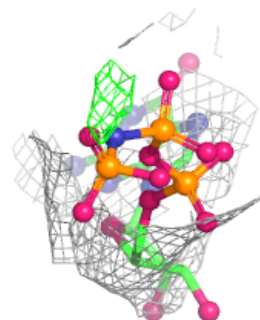
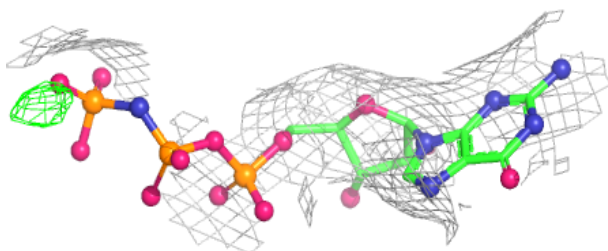
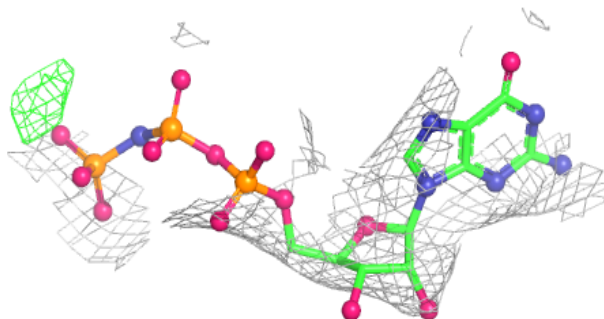
**Electron density around ENX A 1408:**

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

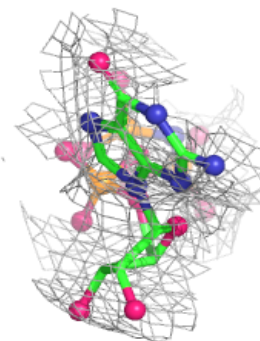
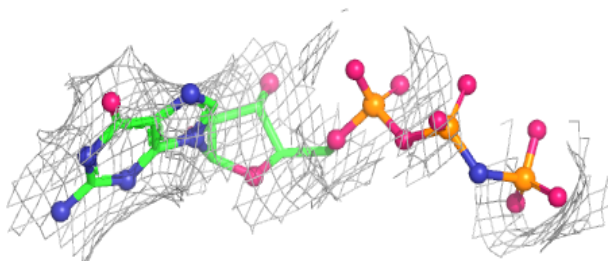
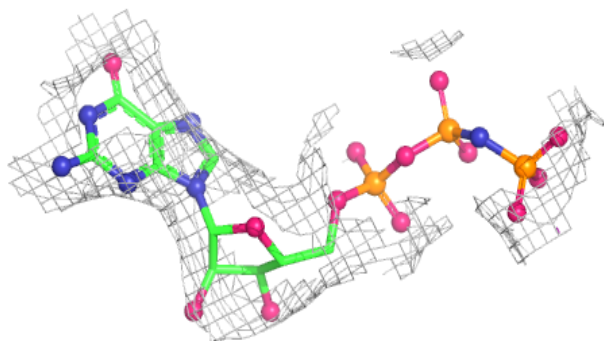


Electron density around GNP A 1406:

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

**Electron density around GNP C 1406:**

$2mF_o-DF_c$ (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.