Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 09:53 pm GMT

PDB ID	:	1OB5
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 (i) 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 (i)) were used in the production of this report:

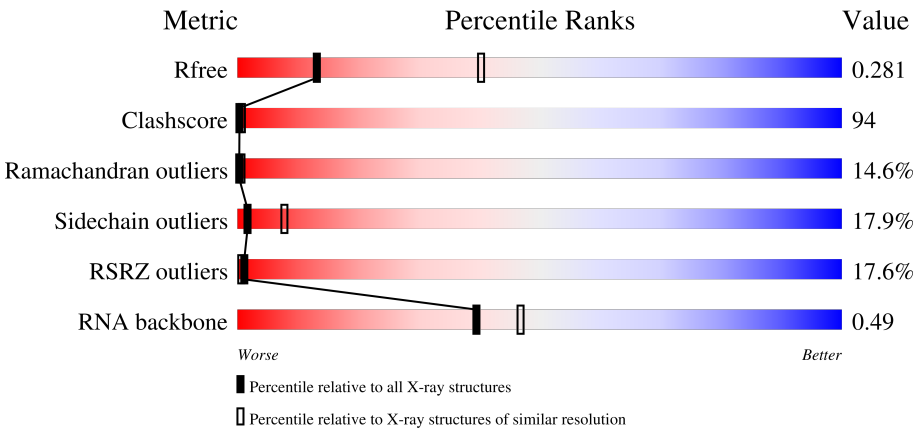
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 <=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	20% 13% 63% 20%
1	C	405	20% 12% 64% 19%
1	E	405	20% 13% 63% 20%
2	B	78	17% 54% 26%

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Mol	Chain	Length	Quality of chain
2	D	78	17% 53% 27%
2	F	78	17% 54% 26%

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	X
2	M2G	D	26	-	-	X	-
2	PHA	D	77	-	-	X	-
2	M2G	F	26	-	-	X	-
2	PHA	F	77	-	-	X	X
5	ENX	A	1408	-	-	-	X
5	ENX	C	1408	-	-	-	X
5	ENX	E	1408	-	-	-	X

2 Entry composition (i)

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.

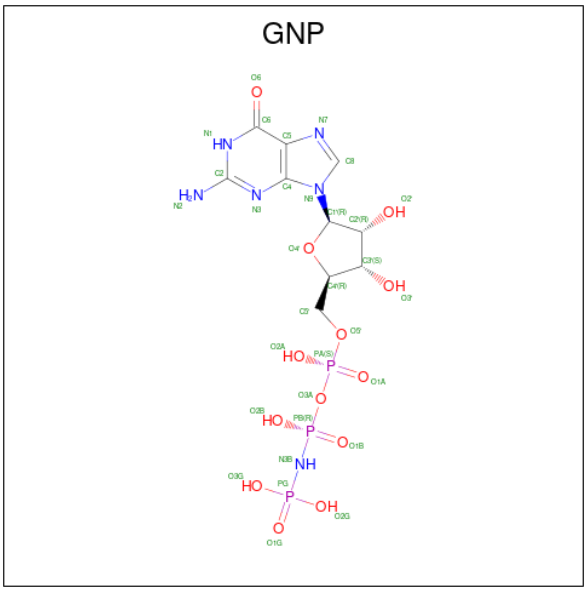
- Molecule 1 is a protein called ELONGATION FACTOR TU.

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

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

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

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



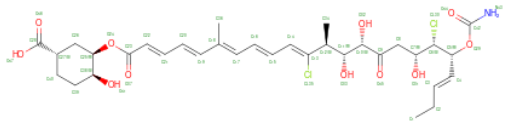
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	32	10	6	13	3	0	0
3	C	1	32	10	6	13	3	0	0
3	E	1	32	10	6	13	3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is ENACYLOXIN IIA (three-letter code: ENX) (formula: $C_{33}H_{45}Cl_2NO_{11}$).

ENX



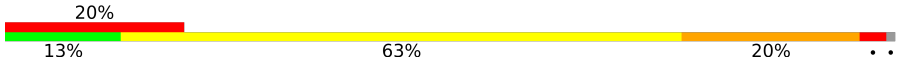
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	A	1	47	33	2	1	11	0	0
			Total	C	Cl	N	O		
5	C	1	47	33	2	1	11	0	0
			Total	C	Cl	N	O		
5	E	1	47	33	2	1	11	0	0

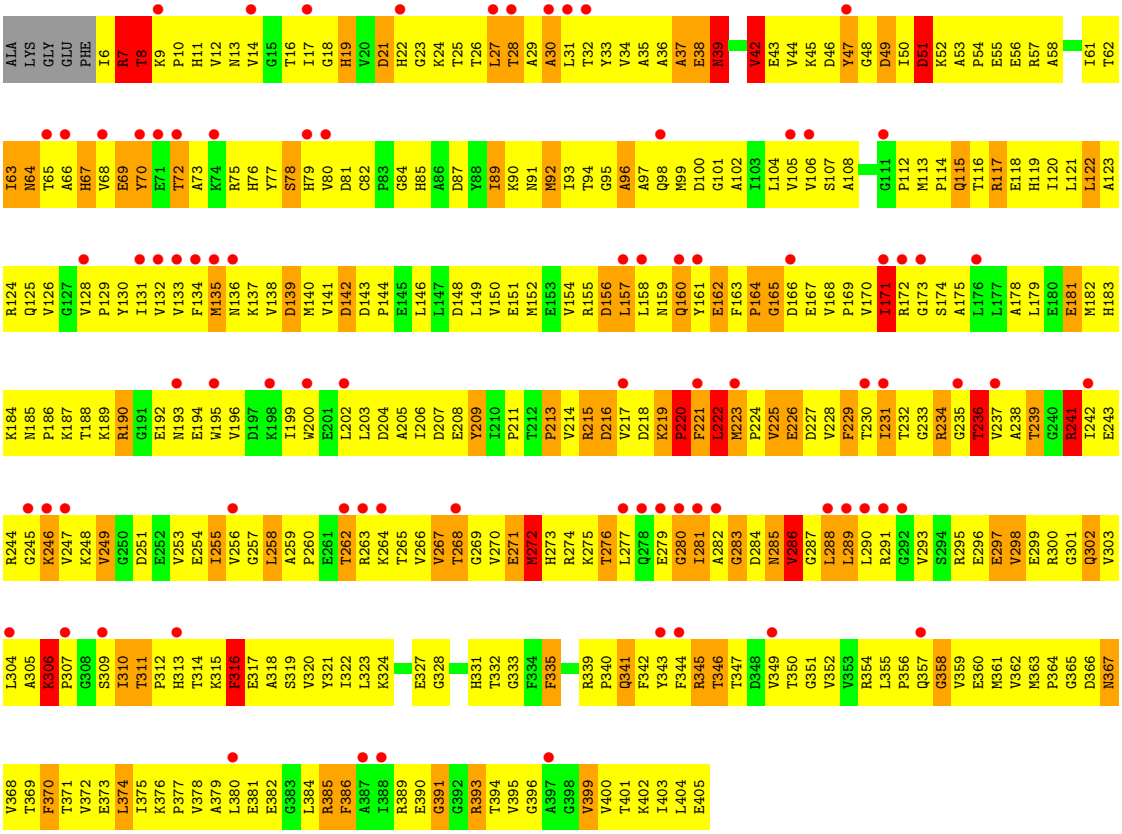
3 Residue-property plots (i)

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

• Molecule 1: ELONGATION FACTOR TU

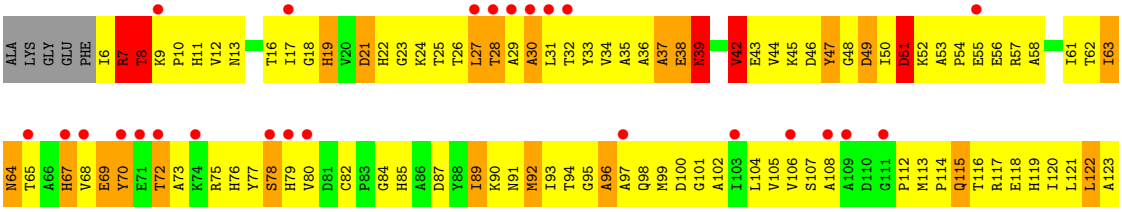
Chain A:

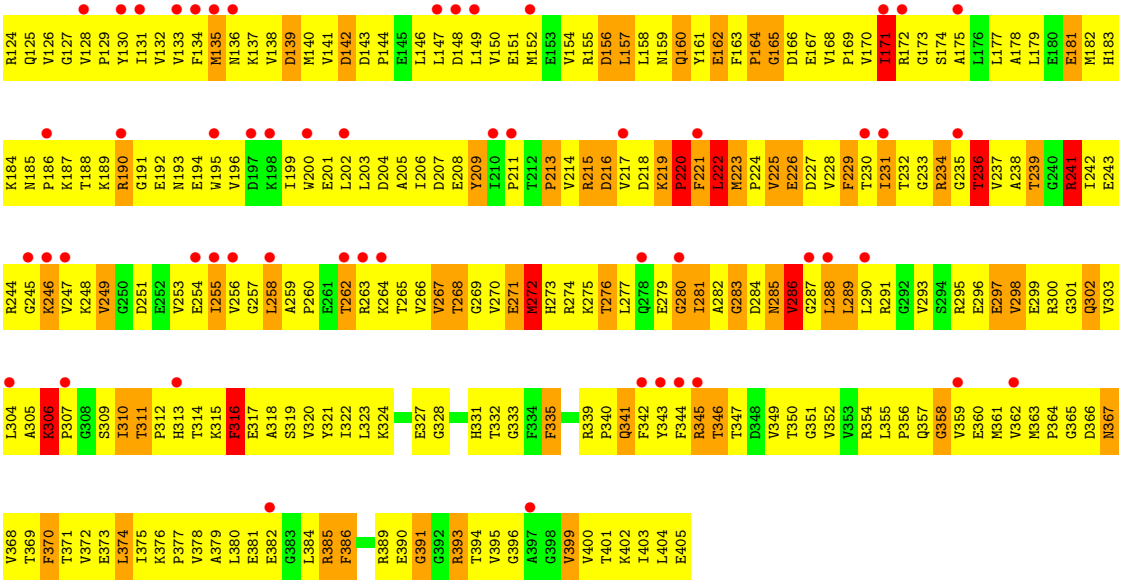




• Molecule 1: ELONGATION FACTOR TU

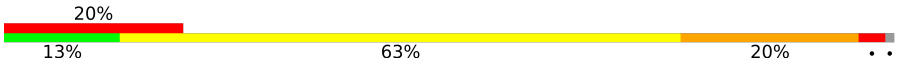
Chain C:

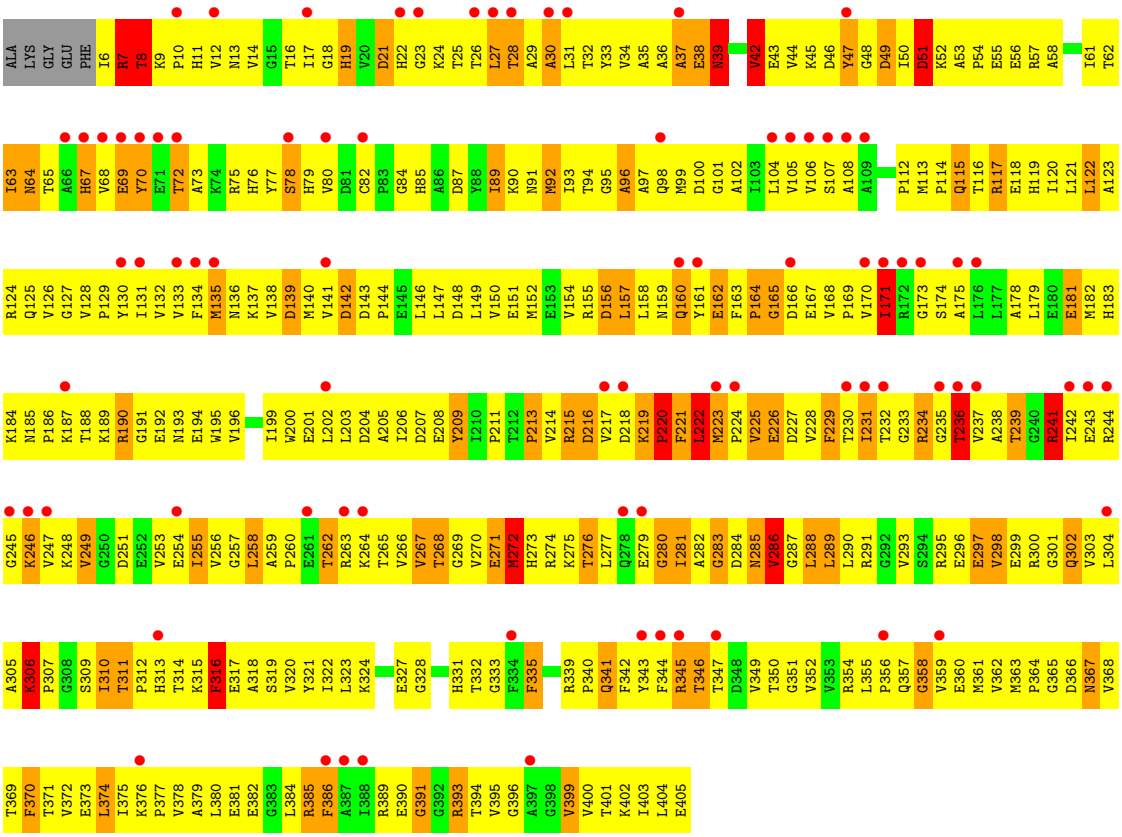




- Molecule 1: ELONGATION FACTOR TU

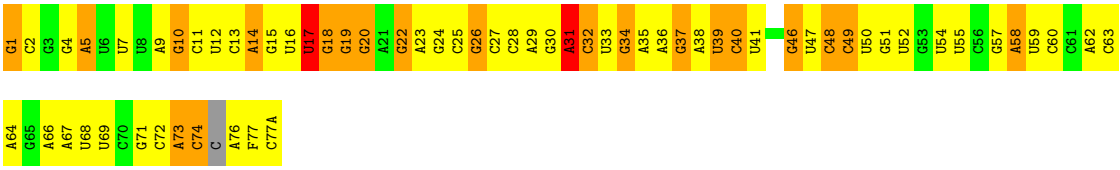
Chain E:





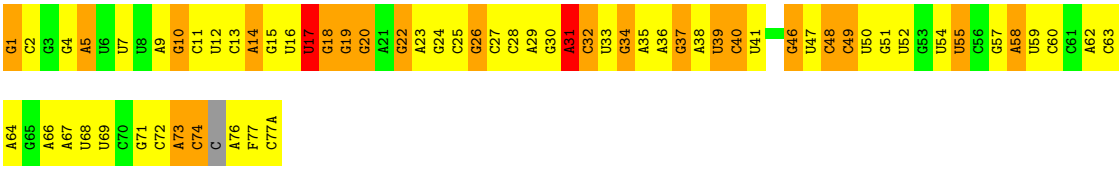
- Molecule 2: TRANSFER-RNA, PHE

Chain B:



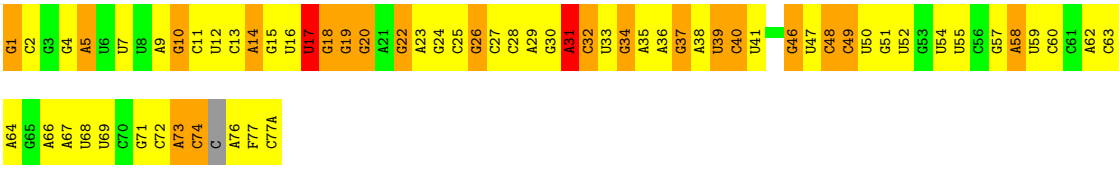
• Molecule 2: TRANSFER-RNA, PHE

Chain D:



• Molecule 2: TRANSFER-RNA, PHE

Chain F:



4 Data and refinement statistics (i)

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 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.54-3.10) 96.6 (29.54-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.280 , 0.294 0.261 , 0.281	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)	0.29 , 62.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	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	0.91	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.55	0/3165	0.86	1/4294 (0.0%)
1	C	0.55	0/3165	0.86	1/4294 (0.0%)
1	E	0.55	0/3165	0.86	1/4294 (0.0%)
2	B	0.81	1/1485 (0.1%)	0.87	2/2307 (0.1%)
2	D	0.81	1/1485 (0.1%)	0.87	2/2307 (0.1%)
2	F	0.81	1/1485 (0.1%)	0.87	2/2307 (0.1%)
All	All	0.65	3/13950 (0.0%)	0.86	9/19803 (0.0%)

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)
2	D	1	G	OP3-P	-6.99	1.52	1.61
2	B	1	G	OP3-P	-6.99	1.52	1.61
2	F	1	G	OP3-P	-6.96	1.52	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	48	C	O5'-P-OP2	-5.99	100.31	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	48	C	O5'-P-OP2	-5.97	100.33	105.70
2	F	48	C	O5'-P-OP2	-5.96	100.33	105.70
1	C	222	LEU	CA-CB-CG	5.51	127.97	115.30
1	E	222	LEU	CA-CB-CG	5.51	127.96	115.30
1	A	222	LEU	CA-CB-CG	5.50	127.96	115.30
2	F	22	G	N9-C1'-C2'	5.31	120.90	114.00
2	B	22	G	N9-C1'-C2'	5.31	120.90	114.00
2	D	22	G	N9-C1'-C2'	5.29	120.88	114.00

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 (i)

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	747	2
1	C	3106	0	3122	734	2
1	E	3106	0	3122	743	2
2	B	1663	0	869	133	0
2	D	1663	0	869	137	0
2	F	1663	0	869	140	0
3	A	32	0	13	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2502	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 94.

All (2502) 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
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:C:221:PHE:HB3	1:C:306:LYS:H	1.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:99:MET:HE3	1:A:102:ALA:HB2	1.40	1.03
1:C:52:LYS:NZ	2:D:74:C:H4'	1.72	1.03
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
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: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:99:MET:HE3	1:E:102:ALA:HB2	1.44	0.97
1:E:246:LYS:HG2	1:E:281:ILE:HA	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:368:VAL:HG22	1:C:369:THR:N	1.86	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:A:368:VAL:HG22	1:A:369:THR:N	1.86	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:PRO:HD2	1:C:359:VAL:HG22	1.53	0.89
2:D:10:2MG:CM2	2:D:26:M2G:H1'	1.97	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
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:C:99:MET:HE3	1:C:102:ALA:HB2	1.53	0.87
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
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:A:286:VAL:HG23	1:A:287:GLY:N	1.90	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:C:H2'	2:F:28:C:C6	2.11	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
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:O	1:C:241:ARG:HD2	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:E:286:VAL:HG23	1:E:287:GLY:N	1.90	0.84
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:99:MET:CE	1:C:102:ALA:HB2	2.07	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:E:99:MET:CE	1:E:102:ALA:HB2	2.07	0.83
1:A:21:ASP:H	3:A:1406:GNP:HNB3	1.24	0.83
1:A:99:MET:CE	1:A:102:ALA:HB2	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:37:YG:H1'	2:F:37:YG:H31	1.62	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:B:37:YG:H1'	2:B:37:YG:H31	1.62	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:241:ARG:HD2	1:C:241:ARG:C	2.01	0.81
1:C:343:TYR:HE1	1:C:389:ARG:HB2	1.45	0.81
1:E:241:ARG:HD2	1:E:241:ARG:C	2.01	0.81
2:D:37:YG:H31	2:D:37:YG:H1'	1.62	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
1:A:270:VAL:O	1:A:270:VAL:HG12	1.81	0.81
1:A:241:ARG:HD2	1:A:241:ARG:C	2.01	0.81
1:E:223:MET:CE	1:E:304:LEU:HD12	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:218:ASP:C	1:E:219:LYS:HD2	2.06	0.76
1:C:69:GLU:O	1:C:70:TYR:HB3	1.83	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
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: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
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:120:ILE:O	1:C:123:ALA:HB3	1.85	0.75
1:C:218:ASP:C	1:C:219:LYS:HD2	2.06	0.75
1:A:389:ARG:HG2	1:A:394:THR:CA	2.16	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:A:218:ASP:C	1:A:219:LYS:HD2	2.06	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:316:PHE:HE1	1:E:318:ALA:HB2	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:389:ARG:CG	1:C:394:THR:HA	2.17	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:A:36:ALA:C	1:A:38:GLU:H	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:VAL:HG13	1:C:267:VAL:O	1.87	0.73
2:F:37:YG:H31	2:F:37:YG:C1'	2.19	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:D:37:YG:H31	2:D:37:YG:C1'	2.19	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:C:17:ILE:HG13	1:C:17:ILE:O	1.87	0.72
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
2:B:37:YG:H31	2:B:37:YG:C1'	2.19	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
2:D:37:YG:H141	2:D:37:YG:H192	1.72	0.72
1:E:26:THR:C	1:E:28:THR:H	1.93	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: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: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:A:26:THR:C	1:A:28:THR:H	1.93	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:E:36:ALA:C	1:E:38:GLU:H	1.92	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:26:THR:C	1:C:28:THR:H	1.93	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: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: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: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:36:ALA:C	1:C:38:GLU:H	1.92	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: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:A:404:LEU:O	1:A:405:GLU:HB2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:233:GLY:C	1:C:234:ARG:HD3	2.13	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:A:223:MET:HE3	1:A:304:LEU:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:233:GLY:C	1:A:234:ARG:HD3	2.13	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: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:281:ILE:HG13	1:E:284:ASP:OD2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:372:VAL:HG12	1:A:373:GLU:N	2.09	0.67
1:E:223:MET:HE3	1:E:304:LEU:HD12	1.77	0.67
1:E:17:ILE:HG22	1:E:82:CYS:SG	2.34	0.67
1:E:233:GLY:C	1:E:234:ARG:HD3	2.13	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:C:223:MET:HE3	1:C:304:LEU:HD12	1.77	0.67
1:A:36:ALA:CA	1:A:42:VAL:HB	2.19	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:306:LYS:HD2	1:E:306:LYS:C	2.15	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:C:306:LYS:HD2	1:C:306:LYS:C	2.15	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:247:VAL:C	1:A:279:GLU:HG3	2.16	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
1:A:306:LYS:C	1:A:306:LYS:HD2	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HH11	1:A:283:GLY:HA3	1.58	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: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
1:E:236:THR:H	1:E:289:LEU:CD2	2.09	0.66
1:E:247:VAL:C	1:E:279:GLU:HG3	2.16	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:312:PRO:HA	1:A:378:VAL:O	1.96	0.66
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:372:VAL:HG12	1:C:373:GLU:N	2.09	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: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:363:MET:HE3	1:E:364:PRO:HD2	1.78	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: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:C:247:VAL:C	1:C:279:GLU:HG3	2.16	0.65
1:E:149:LEU:HA	1:E:152:MET:HE3	1.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:149:LEU:HA	1:C:152:MET:HE3	1.78	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: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
1:E:92:MET:HE1	1:E:93:ILE:HA	1.80	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: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:E:43:GLU:CG	1:E:44:VAL:H	2.05	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:229:PHE:O	1:A:236:THR:HG22	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:92:MET:HE1	1:A:93:ILE:HA	1.80	0.63
1:C:92:MET:HE1	1:C:93:ILE:HA	1.81	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:136:ASN:CG	1:C:137:LYS:N	2.52	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:E:346:THR:HG23	1:E:347:THR:N	2.09	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
1:E:136:ASN:CG	1:E:137:LYS:N	2.52	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: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
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
1:C:229:PHE:CE1	1:C:237:VAL:HG13	2.35	0.61
1:E:54:PRO:HG2	2:F:73:A:H4'	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:ALA:C	1:A:31:LEU:H	2.04	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:136:ASN:CG	1:A:137:LYS:N	2.52	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:226:GLU:OE2	1:E:227:ASP:HB2	2.00	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: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:29:ALA:C	1:E:31:LEU:H	2.04	0.61
1:E:47:TYR:C	1:E:49:ASP:H	2.05	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:29:ALA:C	1:C:31:LEU:H	2.04	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: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:222:LEU:CD1	1:C:244:ARG:N	2.51	0.60
1:C:350:THR:H	1:C:375:ILE:HD11	1.66	0.60
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:223:MET:O	1:A:225:VAL:N	2.35	0.60
1:A:346:THR:HG23	1:A:347:THR:N	2.09	0.60
1:C:98:GLN:NE2	1:C:224:PRO:HB2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:95:GLY:C	1:C:97:ALA:H	2.05	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:A:95:GLY:C	1:A:97:ALA:H	2.05	0.59
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:95:GLY:C	1:E:97:ALA:H	2.05	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: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:47:TYR:C	1:C:49:ASP:H	2.04	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: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:47:TYR:C	1:A:49:ASP:H	2.04	0.59
1:A:52:LYS:HD2	2:B:74:C:C4'	2.31	0.59
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
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:E:43:GLU:HG2	1:E:44:VAL:N	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ARG:HH21	1:E:207:ASP:CA	1.96	0.59
1:A:98:GLN:NE2	1:A:224:PRO:HB2	2.17	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: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:149:LEU:HA	1:A:152:MET:HE3	1.86	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: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: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:246:LYS:HB2	1:E:246:LYS:HZ2	1.68	0.58
1:E:404:LEU:O	1:E:405:GLU:CB	2.49	0.58
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: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:A:363:MET:HE3	1:A:364:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:246:LYS:HB2	1:C:246:LYS:HZ2	1.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:66:A:H2'	2:B:67:A:C8	2.40	0.56
1:C:223:MET:HE2	1:C:304:LEU:HD12	1.88	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:A:203:LEU:C	1:A:205:ALA:H	2.09	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:136:ASN:CG	1:E:137:LYS:H	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:136:ASN:CG	1:A:137:LYS:H	2.09	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:C:222:LEU:HD12	1:C:244:ARG:C	2.27	0.55
1:C:333:GLY:HA3	1:C:361:MET:HE3	1.87	0.55
1:A:222:LEU:HD12	1:A:244:ARG:C	2.27	0.55
1:A:239:THR:CB	2:B:77:PHA:HD1	2.33	0.55
1:C:136:ASN:CG	1:C:137:LYS:H	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:VAL:HG12	1:E:402:LYS:O	2.06	0.55
1:C:203:LEU:C	1:C:205:ALA:H	2.09	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
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: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: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: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:C:256:VAL:HG22	1:C:262:THR:HG23	1.88	0.55
1:E:203:LEU:C	1:E:205:ALA:H	2.09	0.55
1:E:220:PRO:HB2	1:E:309:SER:OG	2.05	0.55
1:E:222:LEU:HD12	1:E:244:ARG:C	2.27	0.55
1:E:393:ARG:HB3	1:E:393:ARG:NH2	2.14	0.55
1:C:165:GLY:O	1:C:168:VAL:HG22	2.07	0.55
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: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: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:C:38:GLU:O	1:C:39:ASN:O	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ILE:N	1:C:322:ILE:CD1	2.70	0.54
2:D:14:A:O2'	2:D:15:G:H5'	2.07	0.54
1:E:7:ARG:C	1:E:8:THR:HG22	2.28	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:223:MET:HE1	1:A:238:ALA:O	2.08	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
1:A:333:GLY:HA3	1:A:361:MET:HE3	1.90	0.54
2:B:29:A:N6	2:B:41:U:H3	2.05	0.54
1:C:7:ARG:C	1:C:8:THR:HG22	2.28	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: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
1:A:149:LEU:HA	1:A:152:MET:CE	2.37	0.54
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:47:TYR:C	1:C:49:ASP:N	2.61	0.54
1:C:189:LYS:N	1:C:192:GLU:OE1	2.35	0.54
1:A:7:ARG:C	1:A:8:THR:HG22	2.28	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:149:LEU:HA	1:C:152:MET:CE	2.37	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:223:MET:HE2	1:E:304:LEU:HD12	1.88	0.54
1:E:265:THR:CG2	1:E:290:LEU:HD13	2.38	0.54
1:C:341:GLN:H	1:C:341:GLN:CD	2.11	0.54
1:E:229:PHE:CD1	1:E:237:VAL:HG13	2.42	0.54
1:E:381:GLU:O	1:E:384:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:251:ASP:HB2	1:A:267:VAL:HG21	1.89	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:149:LEU:HA	1:E:152:MET:CE	2.37	0.54
1:E:290:LEU:HB2	1:E:293:VAL:HG21	1.90	0.54
1:A:115:GLN:O	1:A:116:THR:C	2.45	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:E:341:GLN:CD	1:E:341:GLN:H	2.11	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
1:E:47:TYR:C	1:E:49:ASP:N	2.61	0.53
1:E:271:GLU:HB2	2:F:76:A:O2'	2.07	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:115:GLN:O	1:E:116:THR:C	2.45	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: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:187:LYS:HB3	1:A:189:LYS:HZ2	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ARG:HG2	1:C:394:THR:N	2.22	0.53
1:E:89:ILE:HG22	1:E:93:ILE:HG13	1.90	0.53
1:A:30:ALA:O	1:A:31:LEU:HD23	2.09	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:248:LYS:N	1:C:279:GLU:HG3	2.24	0.53
1:C:256:VAL:O	1:C:303:VAL:HG22	2.09	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:26:THR:C	1:A:28:THR:N	2.61	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: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
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:115:GLN:O	1:C:116:THR:C	2.45	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:47:TYR:C	1:A:49:ASP:N	2.61	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:CG1	1:A:267:VAL:O	2.57	0.52
1:A:341:GLN:H	1:A:341:GLN:CD	2.11	0.52
1:C:89:ILE:CG2	1:C:93:ILE:HG13	2.39	0.52
1:C:92:MET:HE2	1:C:92:MET:O	2.09	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: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
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:36:ALA:C	1:A:38:GLU:N	2.62	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:36:ALA:C	1:E:38:GLU:N	2.63	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:C:63:ILE:CG1	1:C:64:ASN:N	2.67	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: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
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: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:34:VAL:HA	1:A:182:MET:HE1	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:A:38:GLU:HB2	1:A:39:ASN:ND2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:187:LYS:HB3	1:E:189:LYS:HZ2	1.76	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: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:144:PRO:C	1:C:146:LEU:H	2.14	0.50
1:C:222:LEU:HD12	1:C:244:ARG:N	2.23	0.50
1:E:390:GLU:O	1:E:391:GLY:C	2.50	0.50
1:E:393:ARG:HG2	1:E:394:THR:N	2.22	0.50
1:A:144:PRO:C	1:A:146:LEU:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:LYS:HE2	1:E:327:GLU:OE1	2.11	0.50
1:E:333:GLY:HA3	1:E:361:MET:HE3	1.93	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:C:356:PRO:C	1:C:358:GLY:H	2.15	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:61:ILE:HD12	1:C:61:ILE:C	2.32	0.50
1:C:77:TYR:CZ	1:C:206:ILE:HG21	2.46	0.50
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:163:PHE:C	1:E:165:GLY:H	2.15	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:C:163:PHE:C	1:C:165:GLY:H	2.15	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:C:371:THR:HG22	1:C:372:VAL:H	1.75	0.50
1:E:248:LYS:O	1:E:249:VAL:C	2.50	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:390:GLU:O	1:A:391:GLY:C	2.50	0.50
1:C:223:MET:HE1	1:C:238:ALA:O	2.12	0.50
1:E:151:GLU:O	1:E:155:ARG:HG3	2.12	0.50
1:A:161:TYR:O	1:A:162:GLU:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:MET:HE3	1:C:101:GLY:O	2.11	0.50
1:C:161:TYR:O	1:C:162:GLU:C	2.50	0.50
1:C:328:GLY:O	1:C:393:ARG:HG3	2.12	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: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:223:MET:CE	1:C:238:ALA:O	2.60	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: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
1:A:163:PHE:C	1:A:165:GLY:H	2.15	0.49
1:A:223:MET:HE2	1:A:304:LEU:HD12	1.91	0.49
1:A:361:MET:HG2	1:A:361:MET:O	2.12	0.49
1:C:248:LYS:O	1:C:249:VAL:C	2.50	0.49
1:C:339:ARG:CD	1:C:352:VAL:HG22	2.27	0.49
1:C:390:GLU:O	1:C:391:GLY:C	2.50	0.49
1:E:34:VAL:HA	1:E:182:MET:HE1	1.94	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:E:161:TYR:O	1:E:162:GLU:C	2.50	0.49
1:A:328:GLY:O	1:A:393:ARG:HG3	2.12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:356:PRO:C	1:E:358:GLY:H	2.15	0.49
1:A:223:MET:CE	1:A:238:ALA:O	2.60	0.49
1:A:344:PHE:CE2	1:A:386:PHE:HB3	2.48	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
1:A:344:PHE:CE1	1:A:378:VAL:HG11	2.48	0.49
1:A:356:PRO:C	1:A:358:GLY:H	2.15	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:144:PRO:C	1:E:146:LEU:H	2.15	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:A:248:LYS:O	1:A:249:VAL:C	2.50	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:216:ASP:OD1	1:E:218:ASP:HB2	2.13	0.49
1:E:223:MET:HE1	1:E:238:ALA:O	2.12	0.49
1:E:281:ILE:HD12	1:E:282:ALA:H	1.77	0.49
1:C:36:ALA:C	1:C:38:GLU:N	2.62	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:61:ILE:HD12	1:E:61:ILE:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:ARG:CA	1:E:399:VAL:HG13	2.43	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: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:61:ILE:HD12	1:A:61:ILE:C	2.32	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: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: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:95:GLY:C	1:E:97:ALA:N	2.67	0.48
1:E:134:PHE:O	1:E:136:ASN:N	2.46	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
2:B:7:U:C4	2:B:49:5MC:HM52	2.49	0.48
1:C:12:VAL:CG2	1:C:75:ARG:HD2	2.40	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:295:ARG:C	1:E:297:GLU:H	2.17	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:50:ILE:C	1:A:52:LYS:H	2.17	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: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:50:ILE:HG22	1:E:51:ASP:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ILE:O	1:E:90:LYS:C	2.51	0.48
1:E:156:ASP:O	1:E:159:ASN:HB2	2.14	0.48
2:F:7:U:C4	2:F:49:5MC:HM52	2.48	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:89:ILE:O	1:C:90:LYS:C	2.51	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
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:A:82:CYS:HB3	1:A:92:MET:HG2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ARG:C	1:A:297:GLU:H	2.17	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:38:GLU:O	1:C:39:ASN:C	2.52	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: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:95:GLY:C	1:C:97:ALA:N	2.67	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
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:271:GLU:HG3	2:B:76:A:C2	2.49	0.47
1:A:403:ILE:CG2	1:A:404:LEU:N	2.77	0.47
1:C:190:ARG:NH1	1:C:200:TRP:CB	2.77	0.47
1:C:363:MET:HE3	1:C:364:PRO:HD2	1.96	0.47
2:D:7:U:C4	2:D:49:5MC:HM52	2.49	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: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: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:17:H2U:O2'	2:F:18:G:OP1	2.20	0.47
2:F:49:5MC:C2	2:F:50:U:C5	3.02	0.47
1:A:36:ALA:O	1:A:38:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:E:50:ILE:C	1:E:52:LYS:H	2.17	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: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:89:ILE:O	1:A:90:LYS:C	2.51	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: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: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: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:361:MET:O	1:E:361:MET:CG	2.62	0.47
1:A:38:GLU:O	1:A:39:ASN:C	2.52	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: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:112:PRO:HB3	1:A:116:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ALA:O	1:A:209:TYR:N	2.45	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: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: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:38:GLU:O	1:E:39:ASN:C	2.52	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:C:35:ALA:O	1:C:42:VAL:HG21	2.15	0.47
1:C:99:MET:HE1	1:C:102:ALA:HB2	1.90	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:242:ILE:HG13	1:E:286:VAL:HG13	1.97	0.47
1:A:340:PRO:O	1:A:340:PRO:HG2	2.15	0.47
1:A:363:MET:HB2	1:A:366:ASP:CG	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:363:MET:HB2	1:C:366:ASP:CG	2.35	0.47
1:E:92:MET:CE	1:E:92:MET:C	2.84	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: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:E:363:MET:HB2	1:E:366:ASP:CG	2.35	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:295:ARG:C	1:C:297:GLU:H	2.17	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:403:ILE:C	1:E:404:LEU:HD23	2.36	0.46
1:A:95:GLY:C	1:A:97:ALA:N	2.67	0.46
1:A:223:MET:HG2	1:A:242:ILE:HG12	1.97	0.46
1:A:402:LYS:CG	1:A:403:ILE:N	2.72	0.46
1:C:34:VAL:HA	1:C:182:MET:HE1	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: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: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:C:403:ILE:C	1:C:404:LEU:HD23	2.36	0.46
1:E:35:ALA:O	1:E:42:VAL:HG21	2.15	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
1:C:10:PRO:O	1:C:76:HIS:N	2.47	0.46
1:C:92:MET:C	1:C:92:MET:CE	2.84	0.46
1:C:138:VAL:HG23	1:C:139:ASP:N	2.31	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:26:THR:C	1:E:28:THR:N	2.61	0.46
1:E:258:LEU:CD1	1:E:301:GLY:HA3	2.38	0.46
1:E:369:THR:O	1:E:370:PHE:HB3	2.16	0.46
1:A:217:VAL:HG11	1:A:246:LYS:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:163:PHE:C	1:A:165:GLY:N	2.69	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:9:LYS:NZ	1:C:73:ALA:O	2.42	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:222:LEU:HD22	1:E:222:LEU:C	2.37	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:92:MET:C	1:A:92:MET:CE	2.84	0.45
1:C:26:THR:C	1:C:28:THR:N	2.61	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:222:LEU:HD22	1:A:222:LEU:C	2.37	0.45
1:A:331:HIS:NE2	2:B:54:5MU:OP1	2.38	0.45
1:C:231:ILE:HG12	1:C:237:VAL:HG12	1.97	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:386:PHE:CD1	1:A:386:PHE:C	2.90	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: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: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: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:92:MET:HE2	1:A:92:MET:O	2.16	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:A:403:ILE:C	1:A:404:LEU:HD23	2.36	0.45
2:B:39:PSU:H3'	2:B:40:5MC:HM51	1.99	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:144:PRO:C	1:E:146:LEU:N	2.70	0.45
1:E:266:VAL:HG12	1:E:268:THR:HG23	1.97	0.45
1:A:17:ILE:HG22	1:A:82:CYS:HG	1.81	0.45
1:A:24:LYS:CE	1:A:82:CYS:O	2.65	0.45
1:A:144:PRO:C	1:A:146:LEU:N	2.70	0.45
1:A:269:GLY:HA3	1:A:289:LEU:HB3	1.99	0.45
1:E:24:LYS:CE	1:E:82:CYS:O	2.65	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:LYS:HD3	1:C:45:LYS:HA	1.60	0.45
1:C:144:PRO:C	1:C:146:LEU:N	2.70	0.45
1:C:301:GLY:HA2	1:C:346:THR:CG2	2.45	0.45
1:E:163:PHE:C	1:E:165:GLY:N	2.69	0.45
1:E:187:LYS:HB3	1:E:189:LYS:HZ1	1.81	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
2:F:39:PSU:H3'	2:F:40:5MC:HM51	1.99	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: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:163:PHE:C	1:C:165:GLY:N	2.69	0.45
1:C:215:ARG:HD2	1:C:282:ALA:HB1	1.98	0.45
1:C:386:PHE:C	1:C:386:PHE:CD1	2.90	0.45
1:C:24:LYS:CE	1:C:82:CYS:O	2.65	0.45
1:C:50:ILE:C	1:C:52:LYS:H	2.17	0.45
1:E:43:GLU:CG	1:E:44:VAL:N	2.77	0.45
1:E:45:LYS:HA	1:E:45:LYS:HD3	1.60	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:139:ASP:OD1	1:A:174:SER:HB2	2.16	0.45
1:C:12:VAL:HG22	1:C:213:PRO:HG3	1.99	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:E:386:PHE:CD1	1:E:386:PHE:C	2.90	0.45
1:A:227:ASP:O	1:A:238:ALA:HA	2.17	0.45
1:A:344:PHE:C	1:A:345:ARG:HG2	2.38	0.45
1:C:77:TYR:OH	1:C:206:ILE:HG22	2.17	0.45
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:46:ASP:C	1:A:49:ASP:HB2	2.37	0.44
1:A:140:MET:HG2	3:A:1406:GNP:N2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:222:LEU:HD22	1:C:222:LEU:C	2.37	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: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
2:D:39:PSU:H3'	2:D:40:5MC:HM51	1.99	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
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: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:138:VAL:HG22	1:E:173:GLY:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:M2G:H5'	2:F:27:C:OP2	2.18	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
1:E:92:MET:HE2	1:E:92:MET:O	2.17	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
1:C:279:GLU:O	1:C:280:GLY:C	2.56	0.44
1:C:344:PHE:C	1:C:345:ARG:HG2	2.38	0.44
2:D:26:M2G:H5'	2:D:27:C:OP2	2.18	0.44
1:E:23:GLY:O	1:E:24:LYS:C	2.56	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:229:PHE:CD2	2:B:77(A):C:H4'	2.53	0.44
1:A:279:GLU:O	1:A:280:GLY:C	2.56	0.44
1:C:266:VAL:O	1:C:290:LEU:CA	2.50	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: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:335:PHE:CD2	1:A:361:MET:HB2	2.52	0.44
1:C:23:GLY:O	1:C:24:LYS:C	2.56	0.44
1:C:46:ASP:C	1:C:49:ASP:HB2	2.37	0.44
1:E:217:VAL:HB	1:E:246:LYS:HG3	2.00	0.44
1:E:229:PHE:CD2	2:F:77(A):C:H4'	2.53	0.44
1:E:279:GLU:O	1:E:280:GLY:C	2.56	0.44
1:E:382:GLU:CG	1:E:402:LYS:HA	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:275:LYS:O	1:A:276:THR:C	2.56	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:46:ASP:C	1:E:49:ASP:HB2	2.37	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:299:GLU:O	1:E:300:ARG:C	2.57	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:72:THR:HG21	1:C:207:ASP:OD1	2.18	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
1:C:229:PHE:HB2	2:D:77(A):C:H1'	2.00	0.43
1:A:104:LEU:HD23	1:A:133:VAL:HG22	1.99	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:92:MET:HE1	1:E:93:ILE:CA	2.47	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:138:VAL:HG22	1:A:173:GLY:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:MET:HE3	1:E:101:GLY:O	2.18	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:299:GLU:O	1:C:300:ARG:C	2.57	0.43
1:C:346:THR:CG2	1:C:347:THR:H	2.10	0.43
1:E:29:ALA:C	1:E:31:LEU:N	2.72	0.43
1:A:32:THR:C	1:A:36:ALA:HB2	2.39	0.43
1:A:137:LYS:HA	3:A:1406:GNP:N1	2.34	0.43
1:A:157:LEU:C	1:A:159:ASN:N	2.72	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:203:LEU:C	1:C:205:ALA:N	2.72	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:A:43:GLU:CG	1:A:44:VAL:N	2.77	0.43
1:A:132:VAL:O	1:A:132:VAL:HG23	2.19	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
1:A:363:MET:HE2	1:A:363:MET:HB3	1.83	0.43
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:E:32:THR:C	1:E:36:ALA:HB2	2.39	0.43
1:E:181:GLU:C	1:E:183:HIS:N	2.72	0.43
1:E:344:PHE:C	1:E:345:ARG:HG2	2.38	0.43
1:A:203:LEU:C	1:A:205:ALA:N	2.72	0.43
1:A:299:GLU:O	1:A:300:ARG:C	2.57	0.43
1:C:181:GLU:C	1:C:183:HIS:N	2.72	0.43
1:C:231:ILE:HB	1:C:234:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:GLY:O	1:A:24:LYS:C	2.56	0.43
1:A:50:ILE:O	1:A:52:LYS:N	2.42	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:138:VAL:HG22	1:C:173:GLY:C	2.38	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:91:ASN:O	1:E:92:MET:C	2.57	0.43
1:E:132:VAL:HG23	1:E:132:VAL:O	2.19	0.43
1:E:339:ARG:HA	1:E:351:GLY:O	2.19	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:203:LEU:C	1:E:205:ALA:N	2.72	0.42
1:E:255:ILE:HG23	1:E:304:LEU:CD2	2.49	0.42
1:E:275:LYS:O	1:E:276:THR:C	2.56	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:34:VAL:HA	1:C:182:MET:CE	2.49	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:E:281:ILE:CG1	1:E:282:ALA:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASN:O	1:A:92:MET:C	2.57	0.42
1:A:93:ILE:O	1:A:94:THR:C	2.58	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
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:91:ASN:O	1:C:92:MET:C	2.57	0.42
1:C:255:ILE:HG23	1:C:304:LEU:CD2	2.49	0.42
1:C:275:LYS:O	1:C:276:THR:C	2.56	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:34:VAL:HA	1:E:182:MET:CE	2.49	0.42
1:E:36:ALA:HA	1:E:42:VAL:CG1	2.48	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
1:A:181:GLU:C	1:A:183:HIS:N	2.72	0.42
2:B:19:G:H5"	2:B:20:G:C5'	2.47	0.42
1:C:32:THR:C	1:C:36:ALA:HB2	2.39	0.42
1:C:333:GLY:CA	1:C:361:MET:HE3	2.50	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:93:ILE:O	1:E:94:THR:C	2.58	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:ARG:C	1:E:241:ARG:CD	2.80	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
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: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:344:PHE:C	1:E:345:ARG:CG	2.88	0.42
1:A:53:ALA:HA	1:A:54:PRO:HD3	1.89	0.42
1:A:216:ASP:OD2	1:A:218:ASP:OD2	2.37	0.42
1:A:344:PHE:C	1:A:345:ARG:CG	2.88	0.42
1:C:18:GLY:O	1:C:19:HIS:O	2.38	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:157:LEU:C	1:E:159:ASN:N	2.72	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: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: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:C:132:VAL:HG23	1:C:132:VAL:O	2.19	0.42
1:C:157:LEU:C	1:C:159:ASN:N	2.72	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
1:C:344:PHE:C	1:C:345:ARG:CG	2.88	0.42
1:C:393:ARG:CG	1:C:394:THR:N	2.82	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:319:SER:H	1:E:401:THR:HG23	1.85	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
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:29:ALA:C	1:C:31:LEU:N	2.72	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: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:221:PHE:CE2	1:A:253:VAL:CG1	3.03	0.41
1:A:320:VAL:O	1:A:367:ASN:ND2	2.53	0.41
1:C:125:GLN:C	1:C:127:GLY:H	2.24	0.41
1:C:169:PRO:CB	1:C:171:ILE:HD11	2.49	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:117:ARG:O	1:E:118:GLU:C	2.59	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:277:LEU:HD23	1:E:280:GLY:HA2	2.03	0.41
2:F:1:G:O2'	2:F:2:C:H5'	2.21	0.41
1:A:34:VAL:HA	1:A:182:MET:CE	2.49	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:94:THR:O	1:E:95:GLY:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:386:PHE:C	5:E:1408:ENX:CL30	2.96	0.41
1:A:25:THR:O	1:A:28:THR:HB	2.20	0.41
1:A:92:MET:HE1	1:A:93:ILE:CA	2.48	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: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:94:THR:O	1:A:95:GLY:C	2.58	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
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
1:E:200:TRP:O	1:E:201:GLU:C	2.59	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
1:A:205:ALA:O	1:A:209:TYR:HB2	2.21	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
1:A:386:PHE:C	5:A:1408:ENX:CL30	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:93:ILE:O	1:C:94:THR:C	2.58	0.41
1:C:165:GLY:O	1:C:168:VAL:CG2	2.68	0.41
1:C:200:TRP:O	1:C:201:GLU:C	2.59	0.41
1:C:386:PHE:C	5:C:1408:ENX:CL30	2.96	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:C	1:A:33:TYR:H	2.25	0.40
1:A:99:MET:HE3	1:A:101:GLY:O	2.21	0.40
1:A:117:ARG:O	1:A:118:GLU:C	2.59	0.40
1:A:184:LYS:C	1:A:186:PRO:HD3	2.40	0.40
1:A:333:GLY:CA	1:A:361:MET:HE3	2.51	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
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:125:GLN:C	1:E:127:GLY:H	2.24	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: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: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:119:HIS:O	1:A:120:ILE:C	2.59	0.40
1:A:135:MET:HE2	1:A:150:VAL:O	2.21	0.40
1:A:187:LYS:HB3	1:A:189:LYS:HZ1	1.84	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:184:LYS:C	1:C:186:PRO:HD3	2.40	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:C:323:LEU:HD12	1:C:395:VAL:C	2.42	0.40
1:E:119:HIS:O	1:E:120:ILE:C	2.59	0.40
1:E:214:VAL:CG2	1:E:215:ARG:N	2.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LYS:HE3	1:A:84:GLY:N	2.36	0.40
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: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:79:HIS:CD2	1:E:79:HIS:C	2.95	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 1

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

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

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Mol	Chain	Res	Type
1	C	246	LYS
1	C	249	VAL
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

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Mol	Chain	Res	Type
1	A	276	THR
1	A	345	ARG
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

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Mol	Chain	Res	Type
1	C	370	PHE
1	E	164	PRO
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

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Mol	Chain	Res	Type
1	A	306	LYS
1	C	298	VAL
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 (i)

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

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	21	ASP
1	A	28	THR
1	A	38	GLU
1	A	39	ASN
1	A	42	VAL
1	A	49	ASP

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Mol	Chain	Res	Type
1	A	51	ASP
1	A	63	ILE
1	A	64	ASN
1	A	65	THR
1	A	67	HIS
1	A	78	SER
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	209	TYR
1	A	219	LYS
1	A	220	PRO
1	A	221	PHE
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	239	THR
1	A	241	ARG
1	A	255	ILE
1	A	262	THR
1	A	272	MET
1	A	281	ILE
1	A	286	VAL
1	A	288	LEU
1	A	289	LEU
1	A	297	GLU
1	A	306	LYS
1	A	311	THR
1	A	316	PHE

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Mol	Chain	Res	Type
1	A	335	PHE
1	A	341	GLN
1	A	349	VAL
1	A	360	GLU
1	A	367	ASN
1	A	374	LEU
1	A	385	ARG
1	A	386	PHE
1	A	393	ARG
1	A	399	VAL
1	C	7	ARG
1	C	8	THR
1	C	21	ASP
1	C	28	THR
1	C	38	GLU
1	C	39	ASN
1	C	42	VAL
1	C	49	ASP
1	C	51	ASP
1	C	63	ILE
1	C	64	ASN
1	C	65	THR
1	C	67	HIS
1	C	78	SER
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	209	TYR
1	C	219	LYS
1	C	220	PRO
1	C	221	PHE
1	C	222	LEU
1	C	223	MET

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Mol	Chain	Res	Type
1	C	226	GLU
1	C	229	PHE
1	C	231	ILE
1	C	234	ARG
1	C	236	THR
1	C	239	THR
1	C	241	ARG
1	C	255	ILE
1	C	262	THR
1	C	272	MET
1	C	281	ILE
1	C	286	VAL
1	C	288	LEU
1	C	289	LEU
1	C	297	GLU
1	C	306	LYS
1	C	311	THR
1	C	316	PHE
1	C	335	PHE
1	C	341	GLN
1	C	349	VAL
1	C	360	GLU
1	C	367	ASN
1	C	374	LEU
1	C	385	ARG
1	C	386	PHE
1	C	393	ARG
1	C	399	VAL
1	E	7	ARG
1	E	8	THR
1	E	21	ASP
1	E	28	THR
1	E	38	GLU
1	E	39	ASN
1	E	42	VAL
1	E	49	ASP
1	E	51	ASP
1	E	63	ILE
1	E	64	ASN
1	E	65	THR
1	E	67	HIS
1	E	78	SER

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Mol	Chain	Res	Type
1	E	89	ILE
1	E	92	MET
1	E	115	GLN
1	E	122	LEU
1	E	128	VAL
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	209	TYR
1	E	219	LYS
1	E	220	PRO
1	E	221	PHE
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	239	THR
1	E	241	ARG
1	E	255	ILE
1	E	262	THR
1	E	272	MET
1	E	281	ILE
1	E	286	VAL
1	E	288	LEU
1	E	289	LEU
1	E	297	GLU
1	E	306	LYS
1	E	311	THR
1	E	316	PHE
1	E	335	PHE
1	E	341	GLN
1	E	349	VAL
1	E	360	GLU
1	E	367	ASN
1	E	374	LEU

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Mol	Chain	Res	Type
1	E	385	ARG
1	E	386	PHE
1	E	393	ARG
1	E	399	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) 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	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	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 (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	73/78 (93%)	9 (12%)	2 (2%)
2	D	73/78 (93%)	9 (12%)	2 (2%)
2	F	73/78 (93%)	9 (12%)	2 (2%)
All	All	219/234 (93%)	27 (12%)	6 (2%)

All (27) 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	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
2	D	73	A

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Mol	Chain	Res	Type
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	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 (i)

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	M2G	D	26	2	20,27,28	1.16	3 (15%)	22,40,43	0.80	1 (4%)
2	7MG	F	46	2	22,26,27	3.30	2 (9%)	29,39,42	1.50	2 (6%)
2	PHA	F	77	2	10,11,11	0.65	0	10,13,13	0.17	0
2	YG	D	37	2	31,42,43	1.75	7 (22%)	33,62,65	2.77	15 (45%)
2	OMC	D	32	2	19,22,23	0.34	0	26,31,34	0.70	1 (3%)
2	5MU	F	54	2	19,22,23	0.66	0	28,32,35	0.45	0
2	YG	B	37	2	31,42,43	1.75	7 (22%)	33,62,65	2.78	15 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	H2U	F	17	2	18,21,22	0.72	0	21,30,33	1.11	2 (9%)
2	1MA	F	58	2	16,25,26	1.44	2 (12%)	18,37,40	1.13	3 (16%)
2	PHA	D	77	2	10,11,11	0.65	0	10,13,13	0.18	0
2	OMG	D	34	2	18,26,27	1.26	2 (11%)	19,38,41	1.00	2 (10%)
2	PSU	B	39	2	18,21,22	0.81	1 (5%)	22,30,33	0.97	2 (9%)
2	PSU	F	39	2	18,21,22	0.80	1 (5%)	22,30,33	0.96	2 (9%)
2	1MA	B	58	2	16,25,26	1.44	2 (12%)	18,37,40	1.12	3 (16%)
2	1MA	D	58	2	16,25,26	1.44	2 (12%)	18,37,40	1.12	3 (16%)
2	PSU	F	55	2	18,21,22	0.64	0	22,30,33	0.79	0
2	2MG	F	10	2	18,26,27	1.17	2 (11%)	16,38,41	0.75	1 (6%)
2	PSU	D	55	2	18,21,22	0.64	0	22,30,33	0.79	1 (4%)
2	M2G	F	26	2	20,27,28	1.16	3 (15%)	22,40,43	0.80	1 (4%)
2	PSU	B	55	2	18,21,22	0.63	0	22,30,33	0.79	0
2	2MG	B	10	2	18,26,27	1.17	2 (11%)	16,38,41	0.75	1 (6%)
2	5MC	F	49	2	18,22,23	0.43	0	26,32,35	0.77	1 (3%)
2	OMG	B	34	2	18,26,27	1.26	2 (11%)	19,38,41	1.00	2 (10%)
2	5MU	D	54	2	19,22,23	0.67	0	28,32,35	0.45	0
2	OMC	F	32	2	19,22,23	0.33	0	26,31,34	0.70	1 (3%)
2	OMG	F	34	2	18,26,27	1.27	2 (11%)	19,38,41	1.00	2 (10%)
2	H2U	B	16	2	18,21,22	0.59	0	21,30,33	0.74	0
2	PHA	B	77	2	10,11,11	0.65	0	10,13,13	0.18	0
2	5MC	B	49	2	18,22,23	0.43	0	26,32,35	0.76	1 (3%)
2	YG	F	37	2	31,42,43	1.75	7 (22%)	33,62,65	2.78	15 (45%)
2	H2U	B	17	2	18,21,22	0.72	0	21,30,33	1.11	2 (9%)
2	M2G	B	26	2	20,27,28	1.16	3 (15%)	22,40,43	0.80	1 (4%)
2	7MG	B	46	2	22,26,27	3.28	2 (9%)	29,39,42	1.50	2 (6%)
2	H2U	D	16	2	18,21,22	0.58	0	21,30,33	0.74	0
2	5MU	B	54	2	19,22,23	0.66	0	28,32,35	0.45	0
2	5MC	D	40	2	18,22,23	0.45	0	26,32,35	0.78	2 (7%)
2	5MC	D	49	2	18,22,23	0.43	0	26,32,35	0.76	1 (3%)
2	7MG	D	46	2	22,26,27	3.29	2 (9%)	29,39,42	1.50	2 (6%)
2	PSU	D	39	2	18,21,22	0.80	1 (5%)	22,30,33	0.97	2 (9%)
2	H2U	D	17	2	18,21,22	0.73	0	21,30,33	1.10	2 (9%)
2	H2U	F	16	2	18,21,22	0.59	0	21,30,33	0.73	0
2	5MC	F	40	2	18,22,23	0.46	0	26,32,35	0.78	2 (7%)
2	5MC	B	40	2	18,22,23	0.46	0	26,32,35	0.78	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	2MG	D	10	2	18,26,27	1.18	2 (11%)	16,38,41	0.75	1 (6%)
2	OMC	B	32	2	19,22,23	0.33	0	26,31,34	0.70	1 (3%)

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	M2G	D	26	2	-	1/7/29/30	0/3/3/3
2	7MG	F	46	2	-	0/7/37/38	0/3/3/3
2	PHA	F	77	2	-	0/5/6/6	0/1/1/1
2	YG	D	37	2	-	7/20/42/43	0/3/4/4
2	OMC	D	32	2	-	0/9/27/28	0/2/2/2
2	5MU	F	54	2	-	0/7/25/26	0/2/2/2
2	YG	B	37	2	-	7/20/42/43	0/3/4/4
2	H2U	F	17	2	-	3/7/38/39	0/2/2/2
2	1MA	F	58	2	-	0/3/25/26	0/3/3/3
2	PHA	D	77	2	-	0/5/6/6	0/1/1/1
2	OMG	D	34	2	-	1/5/27/28	0/3/3/3
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
2	PSU	F	39	2	-	0/7/25/26	0/2/2/2
2	1MA	B	58	2	-	0/3/25/26	0/3/3/3
2	1MA	D	58	2	-	0/3/25/26	0/3/3/3
2	PSU	F	55	2	-	1/7/25/26	0/2/2/2
2	2MG	F	10	2	-	0/5/27/28	0/3/3/3
2	PSU	D	55	2	-	1/7/25/26	0/2/2/2
2	M2G	F	26	2	-	1/7/29/30	0/3/3/3
2	PSU	B	55	2	-	1/7/25/26	0/2/2/2
2	2MG	B	10	2	-	0/5/27/28	0/3/3/3
2	5MC	F	49	2	-	1/7/25/26	0/2/2/2
2	OMG	B	34	2	-	1/5/27/28	0/3/3/3
2	5MU	D	54	2	-	0/7/25/26	0/2/2/2
2	OMC	F	32	2	-	0/9/27/28	0/2/2/2
2	OMG	F	34	2	-	1/5/27/28	0/3/3/3
2	H2U	B	16	2	-	1/7/38/39	0/2/2/2
2	PHA	B	77	2	-	0/5/6/6	0/1/1/1
2	5MC	B	49	2	-	1/7/25/26	0/2/2/2
2	YG	F	37	2	-	7/20/42/43	0/3/4/4
2	H2U	B	17	2	-	3/7/38/39	0/2/2/2
2	M2G	B	26	2	-	1/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	7MG	B	46	2	-	0/7/37/38	0/3/3/3
2	H2U	D	16	2	-	1/7/38/39	0/2/2/2
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
2	5MC	D	40	2	-	0/7/25/26	0/2/2/2
2	5MC	D	49	2	-	1/7/25/26	0/2/2/2
2	7MG	D	46	2	-	0/7/37/38	0/3/3/3
2	PSU	D	39	2	-	0/7/25/26	0/2/2/2
2	H2U	D	17	2	-	3/7/38/39	0/2/2/2
2	H2U	F	16	2	-	1/7/38/39	0/2/2/2
2	5MC	F	40	2	-	0/7/25/26	0/2/2/2
2	5MC	B	40	2	-	0/7/25/26	0/2/2/2
2	2MG	D	10	2	-	0/5/27/28	0/3/3/3
2	OMC	B	32	2	-	0/9/27/28	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	46	7MG	C8-N9	-15.04	1.37	1.46
2	D	46	7MG	C8-N9	-14.99	1.37	1.46
2	B	46	7MG	C8-N9	-14.96	1.37	1.46
2	D	37	YG	C15-N20	4.66	1.55	1.45
2	B	37	YG	C15-N20	4.63	1.55	1.45
2	F	37	YG	C15-N20	4.63	1.55	1.45
2	B	58	1MA	C2-N3	4.40	1.34	1.29
2	D	58	1MA	C2-N3	4.40	1.34	1.29
2	F	58	1MA	C2-N3	4.39	1.34	1.29
2	F	34	OMG	C5-C6	-3.49	1.40	1.47
2	B	34	OMG	C5-C6	-3.46	1.40	1.47
2	D	34	OMG	C5-C6	-3.45	1.40	1.47
2	F	37	YG	C21-N20	3.41	1.43	1.34
2	D	37	YG	C10-C11	-3.41	1.44	1.50
2	B	37	YG	C21-N20	3.40	1.43	1.34
2	D	37	YG	C21-N20	3.38	1.43	1.34
2	B	37	YG	C10-C11	-3.37	1.44	1.50
2	F	37	YG	C10-C11	-3.35	1.44	1.50
2	F	37	YG	O23-C21	-3.18	1.28	1.34
2	B	37	YG	O23-C21	-3.14	1.28	1.34
2	D	37	YG	O23-C21	-3.12	1.28	1.34
2	D	10	2MG	C5-C6	-2.88	1.41	1.47
2	B	10	2MG	C5-C6	-2.85	1.41	1.47
2	F	10	2MG	C5-C6	-2.84	1.41	1.47
2	F	37	YG	O18-C16	-2.79	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	37	YG	C4-N3	-2.78	1.35	1.40
2	B	37	YG	O18-C16	-2.77	1.26	1.33
2	D	37	YG	O18-C16	-2.76	1.26	1.33
2	D	37	YG	C4-N3	-2.76	1.35	1.40
2	B	37	YG	C4-N3	-2.76	1.35	1.40
2	D	46	7MG	C5-N7	2.73	1.38	1.35
2	B	46	7MG	C5-N7	2.69	1.38	1.35
2	F	46	7MG	C5-N7	2.69	1.38	1.35
2	D	58	1MA	C6-N6	2.61	1.34	1.27
2	B	58	1MA	C6-N6	2.60	1.34	1.27
2	F	58	1MA	C6-N6	2.60	1.34	1.27
2	F	26	M2G	C5-C6	-2.52	1.42	1.47
2	B	26	M2G	C5-C6	-2.49	1.42	1.47
2	D	26	M2G	C5-C6	-2.47	1.42	1.47
2	F	10	2MG	C8-N7	-2.34	1.31	1.35
2	D	10	2MG	C8-N7	-2.33	1.31	1.35
2	B	10	2MG	C8-N7	-2.33	1.31	1.35
2	D	26	M2G	C8-N7	-2.29	1.31	1.35
2	B	26	M2G	C8-N7	-2.28	1.31	1.35
2	F	26	M2G	C8-N7	-2.26	1.31	1.35
2	D	37	YG	C8-N7	-2.20	1.31	1.35
2	B	37	YG	C8-N7	-2.20	1.31	1.35
2	F	37	YG	C8-N7	-2.19	1.31	1.35
2	F	34	OMG	C8-N7	-2.19	1.31	1.35
2	D	34	OMG	C8-N7	-2.19	1.31	1.35
2	B	34	OMG	C8-N7	-2.15	1.31	1.35
2	D	26	M2G	C2-N3	2.11	1.33	1.30
2	B	39	PSU	C6-C5	-2.10	1.32	1.35
2	D	39	PSU	C6-C5	-2.09	1.32	1.35
2	B	26	M2G	C2-N3	2.09	1.33	1.30
2	F	26	M2G	C2-N3	2.08	1.33	1.30
2	F	39	PSU	C6-C5	-2.06	1.32	1.35

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	37	YG	C11-C12-N1	-7.61	102.24	106.53
2	B	37	YG	C11-C12-N1	-7.60	102.24	106.53
2	D	37	YG	C11-C12-N1	-7.57	102.26	106.53
2	F	46	7MG	N9-C8-N7	6.42	112.55	103.38
2	B	46	7MG	N9-C8-N7	6.41	112.54	103.38
2	D	46	7MG	N9-C8-N7	6.40	112.54	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	37	YG	O23-C21-N20	5.64	120.71	110.80
2	B	37	YG	O23-C21-N20	5.64	120.71	110.80
2	D	37	YG	O23-C21-N20	5.62	120.66	110.80
2	B	37	YG	C3-N3-C4	4.86	125.34	116.71
2	D	37	YG	C3-N3-C4	4.85	125.33	116.71
2	F	37	YG	C3-N3-C4	4.84	125.31	116.71
2	D	37	YG	O23-C21-O22	-4.53	117.91	124.58
2	B	37	YG	O23-C21-O22	-4.53	117.91	124.58
2	F	37	YG	O23-C21-O22	-4.52	117.93	124.58
2	D	37	YG	O18-C16-C15	4.38	122.73	111.52
2	F	37	YG	O18-C16-C15	4.38	122.73	111.52
2	B	37	YG	O18-C16-C15	4.38	122.73	111.52
2	B	37	YG	C14-C15-C16	-4.20	98.05	110.30
2	F	37	YG	C14-C15-C16	-4.19	98.06	110.30
2	D	37	YG	C14-C15-C16	-4.19	98.06	110.30
2	F	37	YG	C24-O23-C21	4.12	120.52	115.66
2	B	37	YG	C24-O23-C21	4.09	120.50	115.66
2	D	37	YG	C24-O23-C21	4.08	120.48	115.66
2	B	37	YG	C14-C13-C12	-3.51	104.71	112.66
2	F	37	YG	C14-C13-C12	-3.51	104.72	112.66
2	D	37	YG	C14-C13-C12	-3.50	104.73	112.66
2	F	46	7MG	C4-C5-N7	3.44	110.31	105.53
2	B	46	7MG	C4-C5-N7	3.44	110.30	105.53
2	D	46	7MG	C4-C5-N7	3.40	110.26	105.53
2	B	37	YG	C4-N3-C2	-3.25	112.30	122.15
2	D	37	YG	C4-N3-C2	-3.24	112.33	122.15
2	F	37	YG	C4-N3-C2	-3.22	112.38	122.15
2	D	40	5MC	CM5-C5-C6	-2.69	119.25	122.85
2	B	40	5MC	CM5-C5-C6	-2.68	119.26	122.85
2	D	37	YG	O6-C6-C5	2.68	128.92	124.17
2	F	40	5MC	CM5-C5-C6	-2.67	119.28	122.85
2	B	37	YG	O6-C6-C5	2.67	128.91	124.17
2	F	37	YG	O6-C6-C5	2.66	128.88	124.17
2	F	58	1MA	N1-C2-N3	2.61	129.07	126.02
2	B	49	5MC	C5-C6-N1	-2.57	120.69	123.34
2	F	49	5MC	C5-C6-N1	-2.57	120.70	123.34
2	D	58	1MA	N1-C2-N3	2.56	129.00	126.02
2	B	58	1MA	N1-C2-N3	2.55	128.99	126.02
2	D	49	5MC	C5-C6-N1	-2.52	120.74	123.34
2	F	58	1MA	C5-C6-N1	2.49	117.61	113.90
2	D	58	1MA	C5-C6-N1	2.48	117.59	113.90
2	B	58	1MA	C5-C6-N1	2.45	117.55	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	34	OMG	O2'-C2'-C1'	2.38	113.81	109.09
2	B	34	OMG	O2'-C2'-C1'	2.38	113.80	109.09
2	F	34	OMG	O2'-C2'-C1'	2.37	113.78	109.09
2	D	58	1MA	O3'-C3'-C4'	-2.34	104.29	111.05
2	B	58	1MA	O3'-C3'-C4'	-2.33	104.31	111.05
2	F	58	1MA	O3'-C3'-C4'	-2.33	104.31	111.05
2	B	37	YG	C3-N3-C2	2.31	122.30	120.13
2	D	37	YG	O18-C16-O17	-2.30	119.33	123.84
2	B	37	YG	O18-C16-O17	-2.30	119.34	123.84
2	D	37	YG	C3-N3-C2	2.30	122.28	120.13
2	F	37	YG	O18-C16-O17	-2.29	119.37	123.84
2	F	37	YG	C3-N3-C2	2.27	122.25	120.13
2	B	39	PSU	C6-C5-C4	2.23	119.75	118.20
2	D	39	PSU	C6-C5-C4	2.22	119.75	118.20
2	F	39	PSU	C6-C5-C4	2.20	119.73	118.20
2	B	39	PSU	O4'-C1'-C2'	2.15	108.18	105.14
2	F	39	PSU	O4'-C1'-C2'	2.13	108.15	105.14
2	F	37	YG	C15-N20-C21	2.13	126.11	120.90
2	F	37	YG	O22-C21-N20	-2.13	121.36	124.85
2	D	39	PSU	O4'-C1'-C2'	2.12	108.14	105.14
2	B	37	YG	C15-N20-C21	2.12	126.08	120.90
2	B	37	YG	O22-C21-N20	-2.12	121.38	124.85
2	D	37	YG	C15-N20-C21	2.11	126.06	120.90
2	B	40	5MC	C5-C6-N1	-2.10	121.18	123.34
2	D	37	YG	O22-C21-N20	-2.09	121.42	124.85
2	F	40	5MC	C5-C6-N1	-2.09	121.19	123.34
2	D	40	5MC	C5-C6-N1	-2.07	121.20	123.34
2	F	32	OMC	C2'-C1'-N1	-2.07	110.20	114.22
2	D	17	H2U	O3'-C3'-C2'	2.07	118.51	111.82
2	D	10	2MG	O6-C6-C5	2.07	128.41	124.37
2	B	32	OMC	C2'-C1'-N1	-2.07	110.21	114.22
2	F	17	H2U	O3'-C3'-C2'	2.06	118.50	111.82
2	B	17	H2U	O3'-C3'-C2'	2.06	118.48	111.82
2	D	32	OMC	C2'-C1'-N1	-2.06	110.23	114.22
2	B	26	M2G	O6-C6-C5	2.06	128.39	124.37
2	D	26	M2G	O6-C6-C5	2.06	128.39	124.37
2	B	10	2MG	O6-C6-C5	2.05	128.38	124.37
2	F	10	2MG	O6-C6-C5	2.05	128.37	124.37
2	F	26	M2G	O6-C6-C5	2.04	128.36	124.37
2	B	34	OMG	CM2-O2'-C2'	-2.03	109.19	114.52
2	D	55	PSU	C6-C5-C4	2.03	119.62	118.20
2	D	34	OMG	CM2-O2'-C2'	-2.03	109.20	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	34	OMG	CM2-O2'-C2'	-2.03	109.20	114.52
2	F	17	H2U	N3-C2-N1	-2.03	114.51	116.65
2	F	37	YG	O17-C16-C15	-2.02	117.90	123.92
2	B	17	H2U	N3-C2-N1	-2.01	114.52	116.65
2	B	37	YG	O17-C16-C15	-2.01	117.93	123.92
2	D	17	H2U	N3-C2-N1	-2.01	114.53	116.65
2	D	37	YG	O17-C16-C15	-2.01	117.93	123.92

There are no chirality outliers.

All (45) 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	F	34	OMG	C1'-C2'-O2'-CM2
2	F	37	YG	C15-C16-O18-C19
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	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	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	D	17	H2U	C4'-C5'-O5'-P
2	F	17	H2U	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
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	26	M2G	C4'-C5'-O5'-P
2	D	26	M2G	C4'-C5'-O5'-P
2	F	26	M2G	C4'-C5'-O5'-P
2	F	16	H2U	C2'-C1'-N1-C6
2	B	16	H2U	C2'-C1'-N1-C6
2	D	16	H2U	C2'-C1'-N1-C6
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	37	YG	C12-C13-C14-C15
2	D	37	YG	C12-C13-C14-C15
2	F	37	YG	C12-C13-C14-C15

There are no ring outliers.

45 monomers are involved in 152 short contacts:

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	29,34,34	1.87	8 (27%)	33,54,54	2.43	9 (27%)
5	ENX	A	1408	-	44,47,47	1.30	7 (15%)	47,62,62	1.35	9 (19%)
3	GNP	E	1406	4	29,34,34	1.88	7 (24%)	33,54,54	2.42	8 (24%)
5	ENX	C	1408	-	44,47,47	1.30	7 (15%)	47,62,62	1.35	9 (19%)
3	GNP	C	1406	4	29,34,34	1.88	7 (24%)	33,54,54	2.43	8 (24%)
5	ENX	E	1408	-	44,47,47	1.30	7 (15%)	47,62,62	1.35	9 (19%)

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	-	6/14/38/38	0/3/3/3
5	ENX	A	1408	-	-	11/54/71/71	0/1/1/1
3	GNP	E	1406	4	-	6/14/38/38	0/3/3/3
5	ENX	C	1408	-	-	11/54/71/71	0/1/1/1
3	GNP	C	1406	4	-	6/14/38/38	0/3/3/3
5	ENX	E	1408	-	-	11/54/71/71	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1406	GNP	C6-N1	6.13	1.43	1.33
3	C	1406	GNP	C6-N1	6.12	1.43	1.33
3	A	1406	GNP	C6-N1	6.10	1.43	1.33
3	C	1406	GNP	PG-O2G	-3.62	1.47	1.56
3	E	1406	GNP	PG-O2G	-3.61	1.47	1.56
3	A	1406	GNP	PG-O2G	-3.60	1.47	1.56
5	E	1408	ENX	C38-C25	3.27	1.57	1.52
5	A	1408	ENX	C38-C25	3.25	1.57	1.52
5	C	1408	ENX	C38-C25	3.23	1.57	1.52
5	A	1408	ENX	O24-C23	3.08	1.41	1.34
5	C	1408	ENX	O24-C23	3.07	1.41	1.34
5	E	1408	ENX	O24-C23	3.06	1.41	1.34
3	C	1406	GNP	PG-O1G	2.90	1.50	1.46
3	A	1406	GNP	PG-O1G	2.89	1.50	1.46
3	E	1406	GNP	PG-O1G	2.89	1.50	1.46
5	E	1408	ENX	O44-C42	2.63	1.25	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1408	ENX	O44-C42	2.60	1.25	1.21
3	C	1406	GNP	C2-N1	2.59	1.40	1.35
3	E	1406	GNP	C2-N1	2.59	1.40	1.35
3	A	1406	GNP	C2-N1	2.59	1.40	1.35
5	C	1408	ENX	O44-C42	2.53	1.25	1.21
3	E	1406	GNP	C4-N3	2.37	1.39	1.35
3	A	1406	GNP	C4-N3	2.37	1.39	1.35
3	C	1406	GNP	C4-N3	2.34	1.39	1.35
3	C	1406	GNP	C8-N7	-2.24	1.30	1.34
3	A	1406	GNP	C8-N7	-2.24	1.30	1.34
3	E	1406	GNP	C8-N7	-2.22	1.30	1.34
5	C	1408	ENX	C39-C38	2.14	1.55	1.52
5	A	1408	ENX	C39-C38	2.10	1.55	1.52
5	C	1408	ENX	O29-C42	2.10	1.40	1.35
5	E	1408	ENX	C39-C38	2.09	1.55	1.52
5	E	1408	ENX	C8-C7	-2.08	1.50	1.53
5	A	1408	ENX	O29-C42	2.07	1.40	1.35
5	E	1408	ENX	O47-C28	2.07	1.37	1.30
5	A	1408	ENX	C8-C7	-2.06	1.50	1.53
3	E	1406	GNP	PG-O3G	-2.05	1.51	1.56
5	E	1408	ENX	O29-C42	2.05	1.40	1.35
3	A	1406	GNP	PG-O3G	-2.05	1.51	1.56
5	C	1408	ENX	C8-C7	-2.05	1.50	1.53
5	A	1408	ENX	O47-C28	2.04	1.37	1.30
5	C	1408	ENX	O47-C28	2.04	1.37	1.30
3	C	1406	GNP	PG-O3G	-2.03	1.51	1.56
3	A	1406	GNP	O4'-C1'	2.01	1.43	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1406	GNP	C5-C6-N1	-7.60	113.04	123.43
3	A	1406	GNP	C5-C6-N1	-7.56	113.08	123.43
3	E	1406	GNP	C5-C6-N1	-7.55	113.10	123.43
3	C	1406	GNP	C2-N1-C6	5.36	124.44	115.93
3	A	1406	GNP	C2-N1-C6	5.33	124.40	115.93
3	E	1406	GNP	C2-N1-C6	5.29	124.34	115.93
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	4.10	118.56	107.64
3	A	1406	GNP	O2G-PG-O3G	4.10	118.56	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1406	GNP	O2G-PG-O3G	4.10	118.55	107.64
5	E	1408	ENX	O47-C28-O46	-3.47	116.20	124.09
5	A	1408	ENX	O47-C28-O46	-3.47	116.22	124.09
5	C	1408	ENX	O47-C28-O46	-3.46	116.24	124.09
3	C	1406	GNP	N3-C2-N1	-3.42	122.66	127.22
3	A	1406	GNP	N3-C2-N1	-3.39	122.70	127.22
3	E	1406	GNP	N3-C2-N1	-3.36	122.74	127.22
3	E	1406	GNP	O2G-PG-O1G	-3.06	105.75	113.45
3	A	1406	GNP	O2G-PG-O1G	-3.06	105.76	113.45
3	C	1406	GNP	O2G-PG-O1G	-3.05	105.79	113.45
5	C	1408	ENX	O29-C42-O44	-2.63	121.03	123.69
5	A	1408	ENX	O29-C42-O44	-2.61	121.05	123.69
5	E	1408	ENX	O29-C42-O44	-2.60	121.06	123.69
5	E	1408	ENX	O24-C23-O37	-2.57	119.17	123.35
5	A	1408	ENX	O24-C23-O37	-2.56	119.17	123.35
5	C	1408	ENX	O24-C23-O37	-2.55	119.19	123.35
3	C	1406	GNP	O3G-PG-O1G	-2.50	107.17	113.45
3	A	1406	GNP	O3G-PG-O1G	-2.47	107.25	113.45
3	E	1406	GNP	O3G-PG-O1G	-2.45	107.29	113.45
5	E	1408	ENX	O46-C28-C27	2.45	128.91	122.93
5	A	1408	ENX	O46-C28-C27	2.43	128.89	122.93
5	C	1408	ENX	O46-C28-C27	2.43	128.87	122.93
5	E	1408	ENX	O33-C11-C10	-2.39	104.84	109.21
5	C	1408	ENX	O33-C11-C10	-2.39	104.85	109.21
5	A	1408	ENX	O33-C11-C10	-2.39	104.86	109.21
5	A	1408	ENX	C7-C8-C9	-2.27	109.03	114.19
3	A	1406	GNP	C4-C5-C6	-2.26	118.64	120.80
5	C	1408	ENX	C7-C8-C9	-2.26	109.05	114.19
5	E	1408	ENX	C7-C8-C9	-2.25	109.08	114.19
3	C	1406	GNP	C4-C5-C6	-2.23	118.67	120.80
3	E	1406	GNP	C4-C5-C6	-2.21	118.69	120.80
5	E	1408	ENX	C25-O24-C23	2.17	120.67	117.45
5	C	1408	ENX	C25-O24-C23	2.16	120.67	117.45
5	A	1408	ENX	C25-O24-C23	2.16	120.66	117.45
5	A	1408	ENX	C26-C25-C38	-2.04	108.84	111.00
5	E	1408	ENX	C26-C25-C38	-2.03	108.84	111.00
5	E	1408	ENX	C5-O29-C42	2.03	119.89	116.53
5	A	1408	ENX	C5-O29-C42	2.02	119.87	116.53
5	C	1408	ENX	C26-C25-C38	-2.01	108.87	111.00
3	A	1406	GNP	C2-N3-C4	-2.00	113.07	115.36
5	C	1408	ENX	C5-O29-C42	2.00	119.85	116.53

There are no chirality outliers.

All (51) 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-O1A
3	A	1406	GNP	C5'-O5'-PA-O2A
3	C	1406	GNP	PG-N3B-PB-O1B
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-O1A
3	E	1406	GNP	C5'-O5'-PA-O2A
5	A	1408	ENX	C1-C2-C3-C4
5	A	1408	ENX	C17-C18-C19-C20
5	A	1408	ENX	C36-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	C1-C2-C3-C4
5	C	1408	ENX	C17-C18-C19-C20
5	C	1408	ENX	C36-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	C1-C2-C3-C4
5	E	1408	ENX	C17-C18-C19-C20
5	E	1408	ENX	C36-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	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	C3-C4-C5-C6
5	C	1408	ENX	C3-C4-C5-C6
5	E	1408	ENX	C3-C4-C5-C6
5	A	1408	ENX	C9-C10-C11-O33
5	C	1408	ENX	C9-C10-C11-O33
5	E	1408	ENX	C9-C10-C11-O33

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Mol	Chain	Res	Type	Atoms
3	A	1406	GNP	C3'-C4'-C5'-O5'
3	C	1406	GNP	C3'-C4'-C5'-O5'
3	E	1406	GNP	C3'-C4'-C5'-O5'
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	C5'-O5'-PA-O3A
3	C	1406	GNP	C5'-O5'-PA-O3A
3	E	1406	GNP	C5'-O5'-PA-O3A

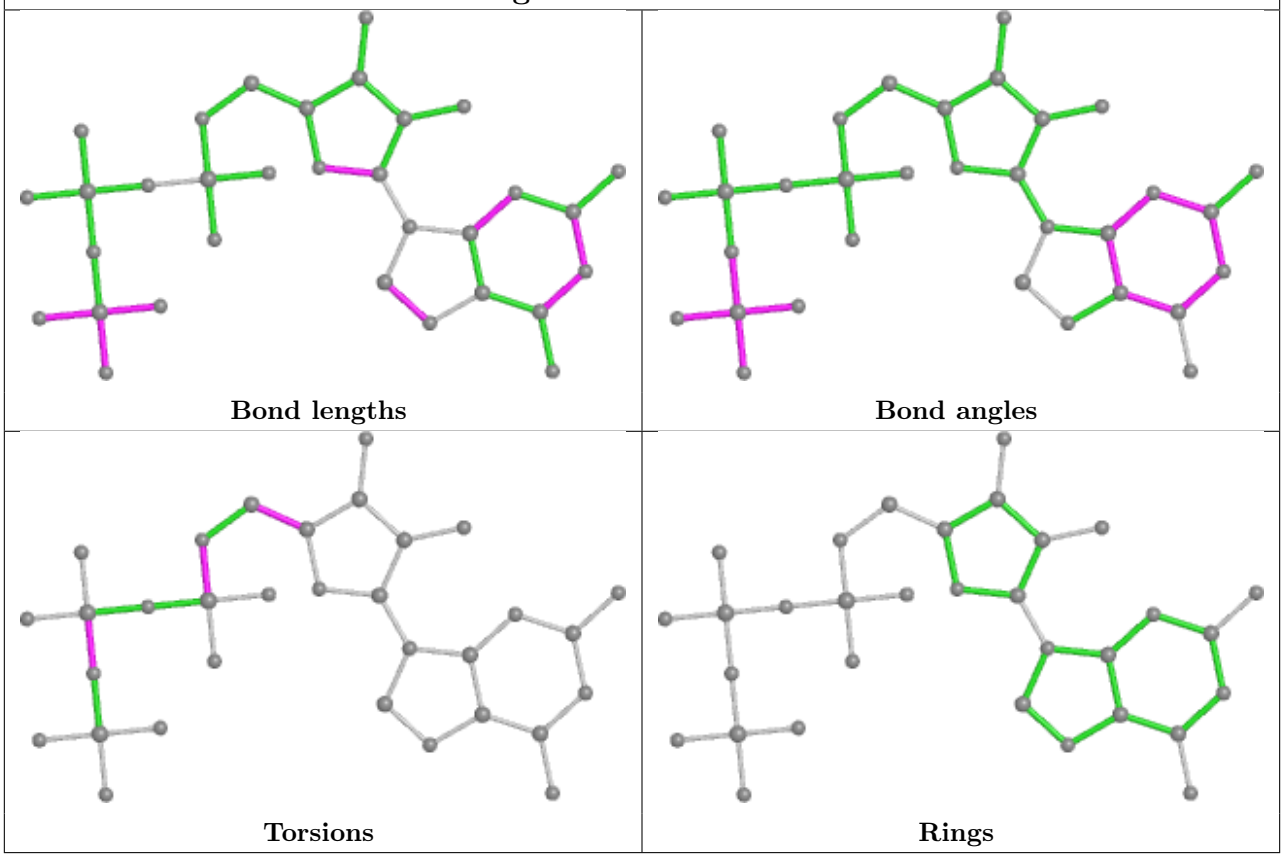
There are no ring outliers.

6 monomers are involved in 37 short contacts:

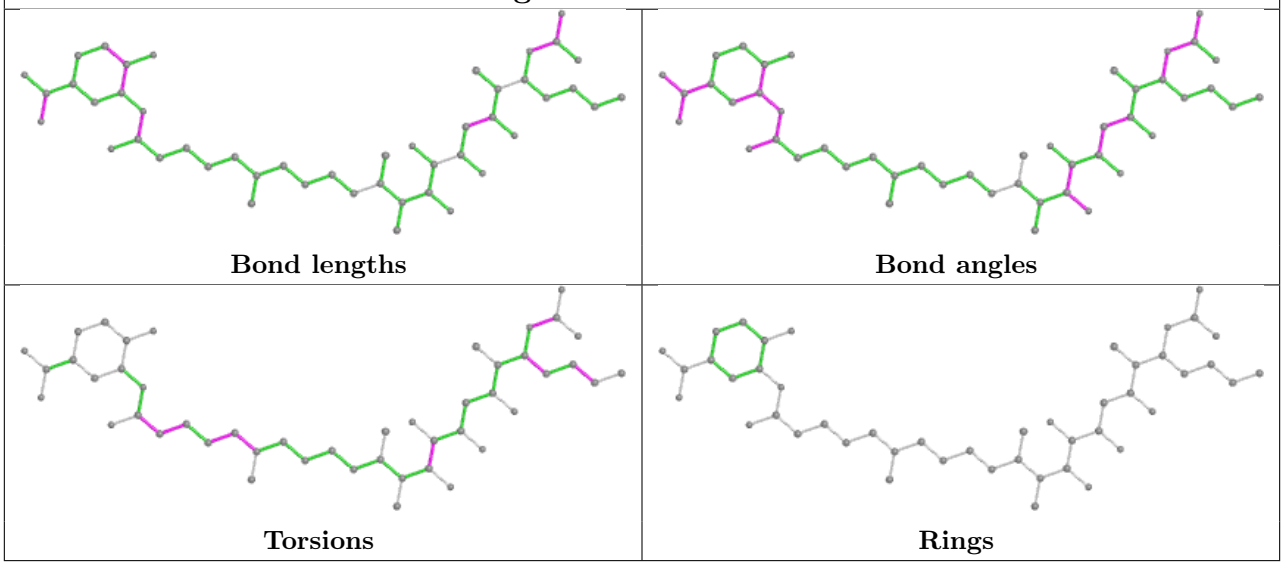
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1406	GNP	7	0
5	A	1408	ENX	5	0
3	E	1406	GNP	8	0
5	C	1408	ENX	5	0
3	C	1406	GNP	7	0
5	E	1408	ENX	5	0

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 then 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.

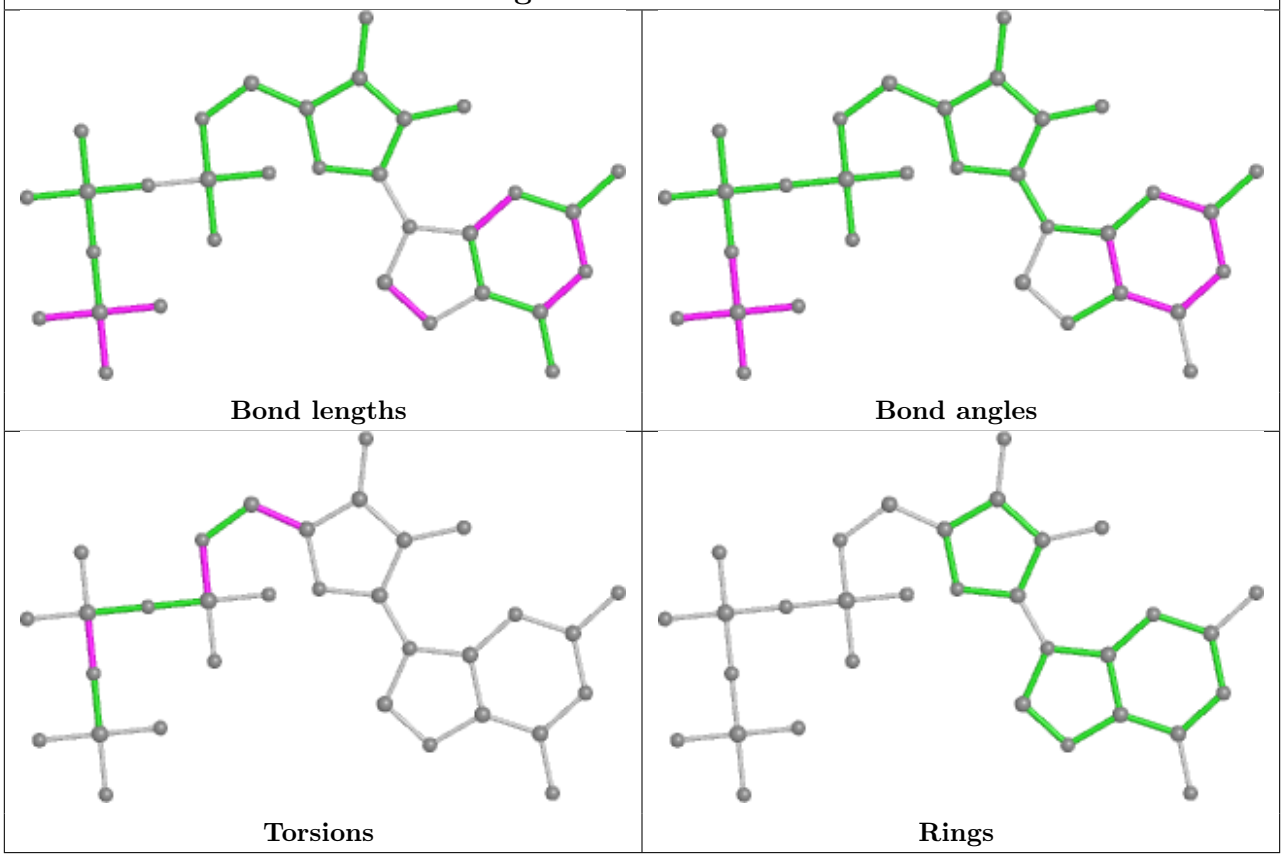
Ligand GNP A 1406



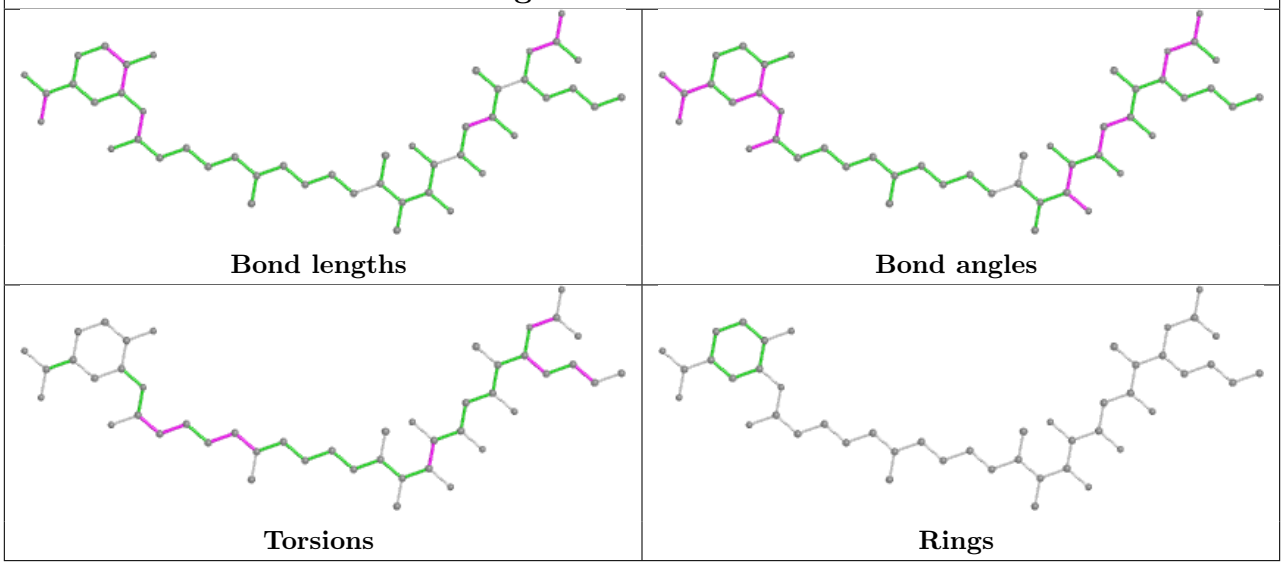
Ligand ENX A 1408



Ligand GNP E 1406



Ligand ENX C 1408



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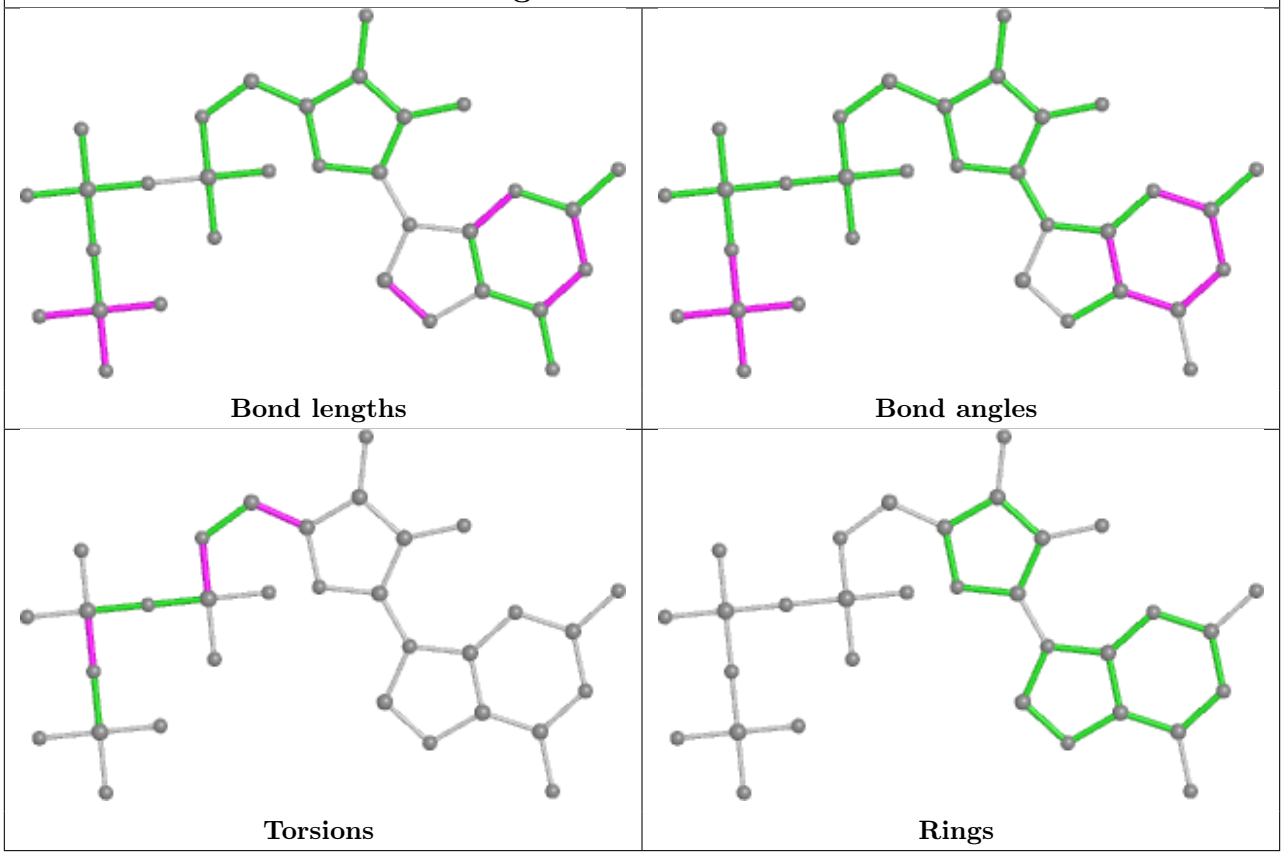
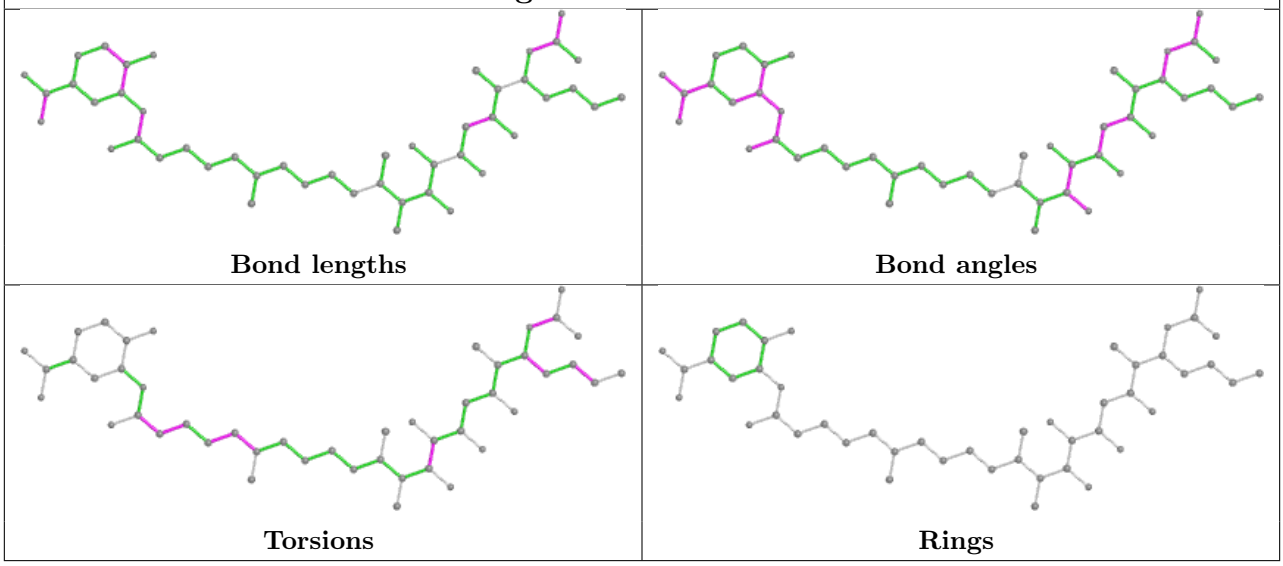


Ligand ENX E 1408



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%)	1.03	83 (20%)	1	0	24, 83, 127, 155	0
1	C	400/405 (98%)	0.90	79 (19%)	1	0	24, 83, 127, 155	0
1	E	400/405 (98%)	0.92	82 (20%)	1	0	24, 83, 127, 155	0
2	B	62/78 (79%)	0.03	0	100	100	22, 62, 102, 111	0
2	D	62/78 (79%)	-0.17	0	100	100	22, 62, 102, 111	0
2	F	62/78 (79%)	-0.04	0	100	100	22, 62, 102, 111	0
All	All	1386/1449 (95%)	0.82	244 (17%)	1	0	22, 80, 126, 155	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	GLY	13.4
1	E	235	GLY	10.6
1	A	247	VAL	9.5
1	A	278	GLN	8.1
1	A	280	GLY	6.7
1	E	245	GLY	6.6
1	A	217	VAL	6.5
1	E	108	ALA	6.4
1	E	134	PHE	6.3
1	A	193	ASN	6.0
1	A	246	LYS	5.9
1	A	288	LEU	5.8
1	C	79	HIS	5.8
1	C	198	LYS	5.5
1	E	217	VAL	5.5
1	C	68	VAL	5.4
1	A	245	GLY	5.3
1	E	68	VAL	5.2
1	C	235	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	135	MET	5.1
1	A	357	GLN	5.1
1	C	245	GLY	5.0
1	C	397	ALA	4.9
1	A	30	ALA	4.9
1	C	28	THR	4.8
1	A	27	LEU	4.8
1	C	263	ARG	4.8
1	C	262	THR	4.8
1	A	17	ILE	4.7
1	A	9	LYS	4.7
1	E	66	ALA	4.7
1	E	106	VAL	4.7
1	A	291	ARG	4.6
1	A	221	PHE	4.6
1	E	27	LEU	4.6
1	C	217	VAL	4.6
1	C	130	TYR	4.5
1	A	66	ALA	4.5
1	E	397	ALA	4.4
1	E	130	TYR	4.4
1	C	256	VAL	4.3
1	C	246	LYS	4.3
1	E	263	ARG	4.2
1	E	246	LYS	4.2
1	C	172	ARG	4.2
1	A	173	GLY	4.2
1	C	255	ILE	4.1
1	E	133	VAL	4.1
1	C	152	MET	4.1
1	E	171	ILE	4.1
1	E	387	ALA	4.0
1	C	71	GLU	4.0
1	C	30	ALA	4.0
1	E	70	TYR	4.0
1	E	104	LEU	4.0
1	A	223	MET	4.0
1	E	247	VAL	3.9
1	C	221	PHE	3.9
1	C	67	HIS	3.9
1	A	263	ARG	3.9
1	C	131	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	344	PHE	3.9
1	A	79	HIS	3.9
1	C	9	LYS	3.9
1	E	264	LYS	3.9
1	E	278	GLN	3.8
1	A	256	VAL	3.8
1	C	31	LEU	3.8
1	E	345	ARG	3.8
1	A	268	THR	3.8
1	E	12	VAL	3.8
1	A	171	ILE	3.7
1	A	281	ILE	3.7
1	A	22	HIS	3.7
1	A	279	GLU	3.7
1	A	198	LYS	3.7
1	C	108	ALA	3.7
1	A	136	ASN	3.6
1	E	67	HIS	3.6
1	C	74	LYS	3.6
1	C	345	ARG	3.5
1	A	71	GLU	3.5
1	E	22	HIS	3.5
1	A	128	VAL	3.5
1	A	134	PHE	3.5
1	A	70	TYR	3.5
1	E	82	CYS	3.5
1	C	149	LEU	3.4
1	C	382	GLU	3.4
1	E	223	MET	3.4
1	A	387	ALA	3.4
1	E	230	THR	3.4
1	A	172	ARG	3.4
1	A	28	THR	3.4
1	E	78	SER	3.3
1	E	107	SER	3.3
1	C	344	PHE	3.3
1	A	231	ILE	3.3
1	C	78	SER	3.3
1	C	195	TRP	3.3
1	E	166	ASP	3.3
1	E	231	ILE	3.3
1	C	280	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	292	GLY	3.2
1	C	264	LYS	3.2
1	C	247	VAL	3.1
1	E	202	LEU	3.1
1	E	26	THR	3.1
1	E	98	GLN	3.1
1	A	166	ASP	3.0
1	A	388	ILE	3.0
1	C	202	LEU	3.0
1	E	28	THR	3.0
1	E	243	GLU	3.0
1	E	170	VAL	3.0
1	A	80	VAL	3.0
1	A	72	THR	3.0
1	A	230	THR	3.0
1	A	74	LYS	2.9
1	E	135	MET	2.9
1	C	258	LEU	2.9
1	A	135	MET	2.9
1	E	47	TYR	2.9
1	C	80	VAL	2.9
1	E	343	TYR	2.8
1	E	176	LEU	2.8
1	A	106	VAL	2.8
1	C	175	ALA	2.8
1	E	30	ALA	2.8
1	E	173	GLY	2.8
1	C	171	ILE	2.8
1	C	211	PRO	2.8
1	C	278	GLN	2.7
1	C	136	ASN	2.7
1	A	307	PRO	2.7
1	A	68	VAL	2.7
1	C	17	ILE	2.7
1	A	289	LEU	2.7
1	A	200	TRP	2.7
1	A	262	THR	2.7
1	A	131	ILE	2.7
1	E	71	GLU	2.7
1	C	186	PRO	2.7
1	C	109	ALA	2.7
1	E	261	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	349	VAL	2.7
1	E	254	GLU	2.7
1	E	376	LYS	2.6
1	C	359	VAL	2.6
1	A	160	GLN	2.6
1	C	254	GLU	2.6
1	E	187	LYS	2.6
1	E	386	PHE	2.6
1	E	304	LEU	2.6
1	A	380	LEU	2.6
1	E	232	THR	2.6
1	C	134	PHE	2.6
1	A	14	VAL	2.6
1	E	359	VAL	2.6
1	E	388	ILE	2.6
1	C	55	GLU	2.6
1	E	72	THR	2.6
1	E	80	VAL	2.5
1	A	313	HIS	2.5
1	E	69	GLU	2.5
1	E	218	ASP	2.5
1	C	111	GLY	2.5
1	C	65	THR	2.5
1	C	210	ILE	2.5
1	E	160	GLN	2.5
1	A	242	ILE	2.5
1	C	231	ILE	2.5
1	C	103	ILE	2.5
1	E	242	ILE	2.5
1	A	277	LEU	2.5
1	C	288	LEU	2.5
1	E	105	VAL	2.5
1	E	356	PRO	2.5
1	C	197	ASP	2.4
1	E	237	VAL	2.4
1	C	70	TYR	2.4
1	C	307	PRO	2.4
1	C	72	THR	2.4
1	A	65	THR	2.4
1	A	309	SER	2.4
1	C	147	LEU	2.4
1	A	282	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	2.4
1	A	32	THR	2.4
1	C	32	THR	2.4
1	E	172	ARG	2.4
1	A	304	LEU	2.4
1	C	148	ASP	2.4
1	A	31	LEU	2.4
1	E	23	GLY	2.3
1	A	161	TYR	2.3
1	A	195	TRP	2.3
1	E	236	THR	2.3
1	E	17	ILE	2.3
1	A	237	VAL	2.3
1	C	313	HIS	2.3
1	E	279	GLU	2.3
1	C	27	LEU	2.3
1	C	29	ALA	2.3
1	C	128	VAL	2.3
1	C	304	LEU	2.3
1	A	47	TYR	2.3
1	A	158	LEU	2.3
1	E	141	VAL	2.3
1	C	106	VAL	2.2
1	E	313	HIS	2.2
1	A	176	LEU	2.2
1	E	31	LEU	2.2
1	A	132	VAL	2.2
1	E	224	PRO	2.2
1	E	37	ALA	2.2
1	A	397	ALA	2.2
1	E	334	PHE	2.2
1	C	362	VAL	2.2
1	E	244	ARG	2.2
1	C	133	VAL	2.1
1	E	10	PRO	2.1
1	A	111	GLY	2.1
1	C	200	TRP	2.1
1	E	109	ALA	2.1
1	E	161	TYR	2.1
1	A	105	VAL	2.1
1	A	343	TYR	2.1
1	E	344	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	133	VAL	2.1
1	C	190	ARG	2.1
1	A	98	GLN	2.1
1	E	347	THR	2.1
1	E	131	ILE	2.1
1	C	287	GLY	2.0
1	C	342	PHE	2.0
1	A	264	LYS	2.0
1	C	290	LEU	2.0
1	E	175	ALA	2.0
1	A	157	LEU	2.0
1	A	290	LEU	2.0
1	C	97	ALA	2.0
1	C	230	THR	2.0
1	C	343	TYR	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	PHA	F	77	11/11	0.72	0.95	98,114,124,126	0
2	PHA	B	77	11/11	0.73	0.53	98,114,124,126	0
2	PHA	D	77	11/11	0.81	0.53	98,114,124,126	0
2	2MG	F	10	24/25	0.82	0.17	76,85,97,103	0
2	2MG	B	10	24/25	0.84	0.17	76,85,97,103	0
2	5MU	B	54	21/22	0.84	0.24	3,28,45,54	0
2	H2U	F	17	20/21	0.85	0.17	91,123,146,146	0
2	H2U	D	17	20/21	0.85	0.18	91,123,146,146	0
2	2MG	D	10	24/25	0.86	0.14	76,85,97,103	0
2	PSU	B	55	20/21	0.86	0.21	18,38,54,57	0
2	OMG	D	34	24/25	0.87	0.21	2,29,39,50	0
2	H2U	B	17	20/21	0.87	0.17	91,123,146,146	0
2	H2U	D	16	20/21	0.87	0.15	50,92,109,111	0
2	H2U	F	16	20/21	0.87	0.18	50,92,109,111	0
2	H2U	B	16	20/21	0.87	0.15	50,92,109,111	0
2	M2G	D	26	25/26	0.87	0.12	67,87,114,121	0
2	OMC	B	32	21/22	0.88	0.22	44,63,73,89	0
2	PSU	B	39	20/21	0.88	0.19	16,36,50,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	M2G	B	26	25/26	0.88	0.20	67,87,114,121	0
2	OMG	B	34	24/25	0.89	0.20	2,29,39,50	0
2	YG	D	37	39/40	0.89	0.20	13,44,86,93	0
2	5MU	D	54	21/22	0.89	0.22	3,28,45,54	0
2	OMC	F	32	21/22	0.89	0.20	44,63,73,89	0
2	PSU	F	55	20/21	0.89	0.20	18,38,54,57	0
2	OMC	D	32	21/22	0.89	0.21	44,63,73,89	0
2	PSU	F	39	20/21	0.90	0.18	16,36,50,54	0
2	M2G	F	26	25/26	0.90	0.16	67,87,114,121	0
2	PSU	D	55	20/21	0.90	0.18	18,38,54,57	0
2	YG	B	37	39/40	0.91	0.20	13,44,86,93	0
2	7MG	D	46	24/25	0.91	0.18	25,53,93,99	0
2	5MC	D	49	21/22	0.91	0.20	19,28,35,50	0
2	5MC	B	40	21/22	0.91	0.15	23,42,56,65	0
2	OMG	F	34	24/25	0.91	0.19	2,29,39,50	0
2	1MA	B	58	23/24	0.91	0.21	6,25,34,37	0
2	7MG	F	46	24/25	0.91	0.17	25,53,93,99	0
2	7MG	B	46	24/25	0.91	0.17	25,53,93,99	0
2	5MC	B	49	21/22	0.91	0.18	19,28,35,50	0
2	1MA	D	58	23/24	0.92	0.20	6,25,34,37	0
2	1MA	F	58	23/24	0.92	0.25	6,25,34,37	0
2	YG	F	37	39/40	0.92	0.19	13,44,86,93	0
2	5MC	F	49	21/22	0.93	0.17	19,28,35,50	0
2	5MU	F	54	21/22	0.93	0.17	3,28,45,54	0
2	5MC	D	40	21/22	0.93	0.16	23,42,56,65	0
2	5MC	F	40	21/22	0.93	0.15	23,42,56,65	0
2	PSU	D	39	20/21	0.93	0.16	16,36,50,54	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ENX	A	1408	47/47	0.63	0.53	45,74,86,109	0

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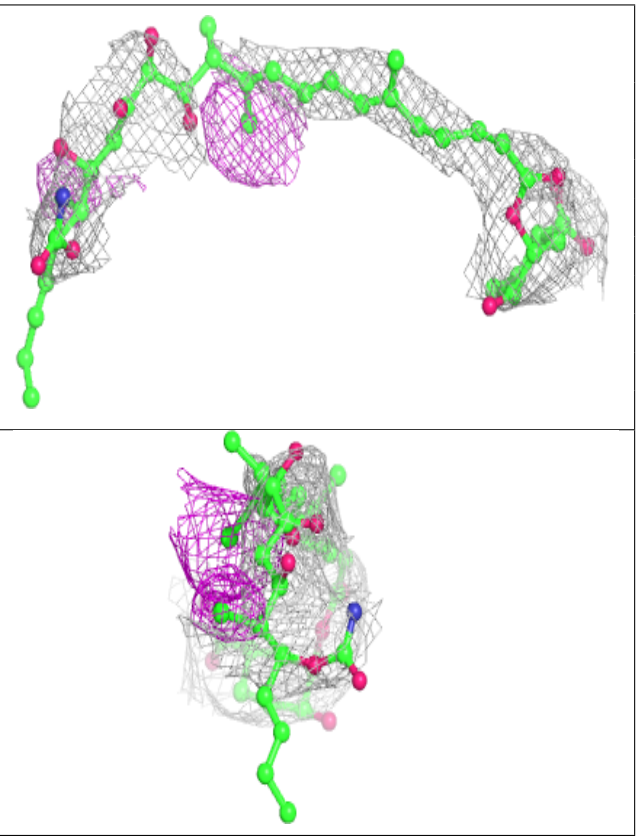
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ENX	E	1408	47/47	0.63	0.52	45,74,86,109	0
5	ENX	C	1408	47/47	0.71	0.43	45,74,86,109	0
4	MG	E	1407	1/1	0.88	0.20	57,57,57,57	0
3	GNP	A	1406	32/32	0.90	0.18	47,70,85,90	0
3	GNP	E	1406	32/32	0.91	0.18	47,70,85,90	0
3	GNP	C	1406	32/32	0.93	0.18	47,70,85,90	0
4	MG	C	1407	1/1	0.95	0.26	57,57,57,57	0
4	MG	A	1407	1/1	0.98	0.23	57,57,57,57	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.

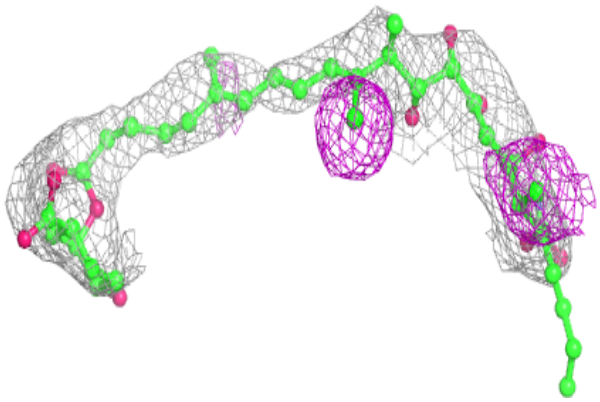
Electron density around ENX A 1408:

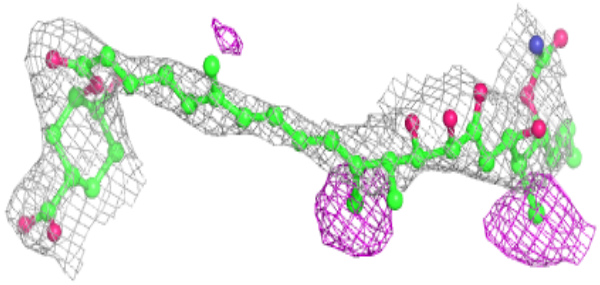
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

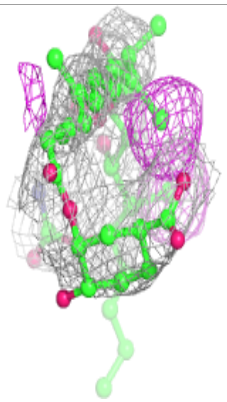


Electron density around ENX E 1408:

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

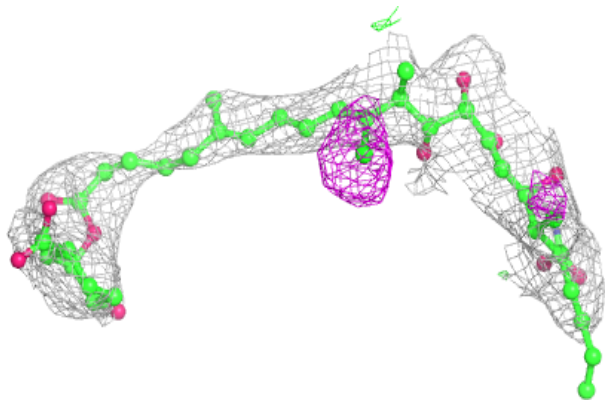


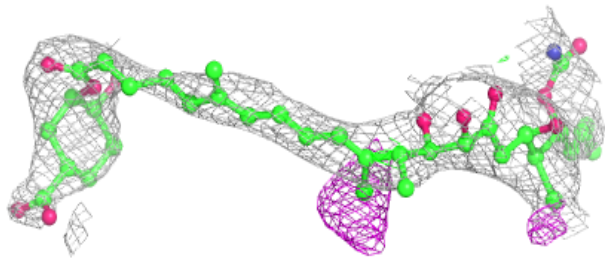


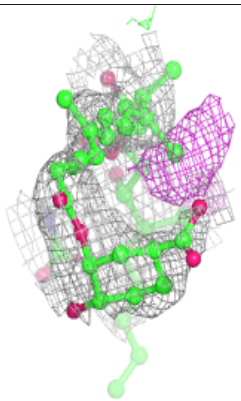


Electron density around ENX C 1408:

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

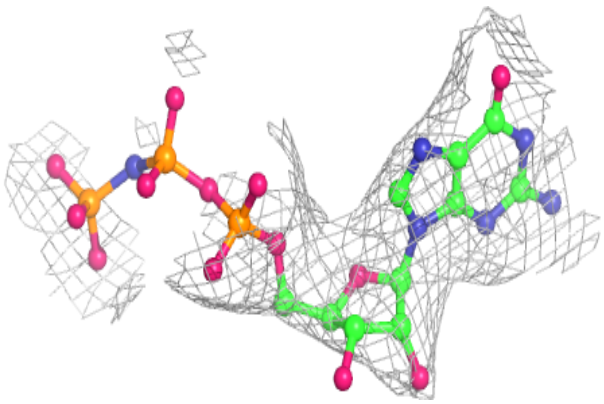


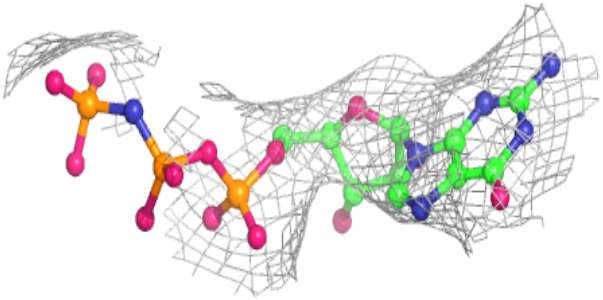


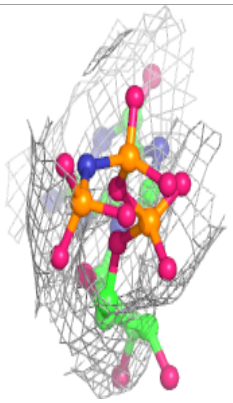


Electron density around GNP A 1406:

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

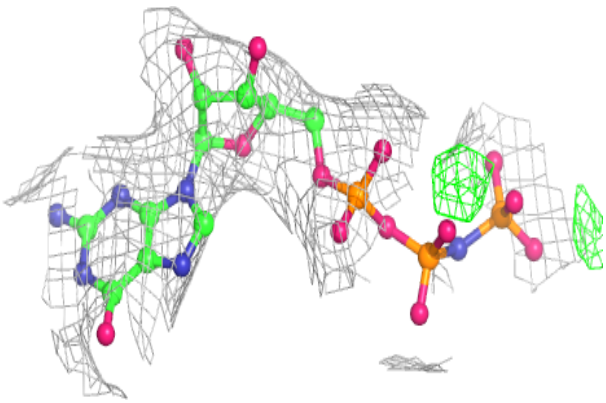


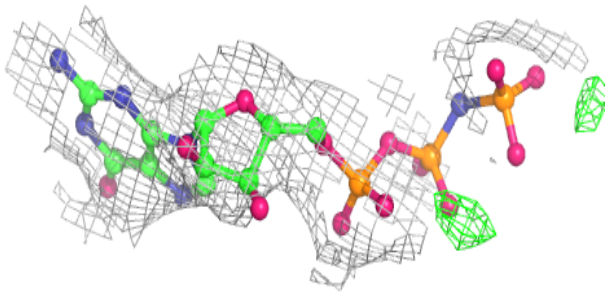


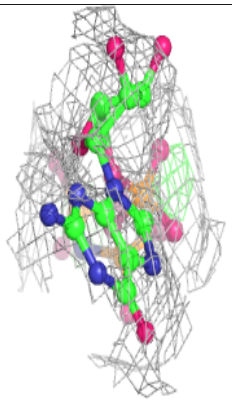


Electron density around GNP E 1406:

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

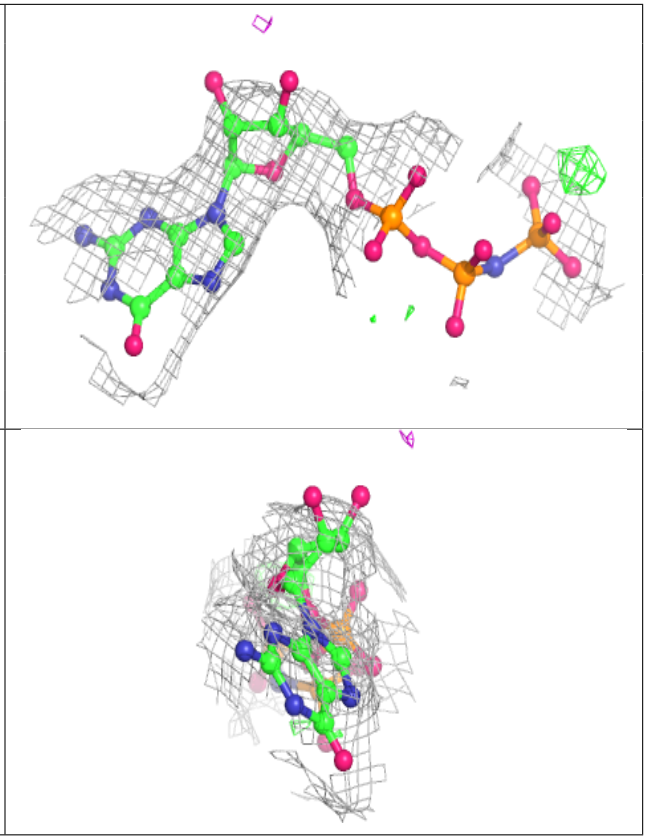






Electron density around GNP C 1406:

$2mF_o$-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.