



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:40 PM BST

PDB ID : 2Y7H
EMDB ID: : EMD-1534
Title : Atomic model of the DNA-bound methylase complex from the Type I restrict ion-modification enzyme EcoKI (M2S1). Based on fitting into EM map 1534.
Authors : Kennaway, C.K.; Obarska-Kosinska, A.; White, J.H.; Tuszynska, I.; Cooper, L.P.; Bujnicki, J.M.; Trinick, J.; Dryden, D.T.F.
Deposited on : 2011-01-31
Resolution : 18.00 Å(reported)
Based on PDB ID : 1S7Z, 1YF2, 2AR0

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

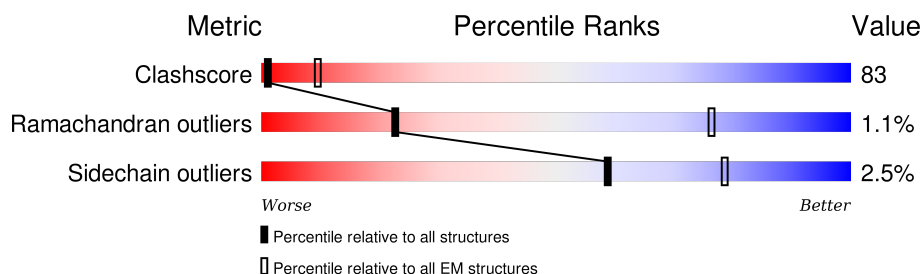
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 18.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	464	24% 71% 5%
2	B	529	38% 59% .
2	C	529	37% 61% .
3	D	20	25% 70% 5%
4	E	20	30% 70%

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
5	SAM	B	530	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SAM	C	530	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12846 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TYPE-1 RESTRICTION ENZYME ECOKI SPECIFICITY PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	464	Total	C	N	O	S	0	0
			3622	2298	644	671	9		

- Molecule 2 is a protein called TYPE I RESTRICTION ENZYME ECOKI M PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	529	Total	C	N	O	S	0	0
			4175	2612	730	816	17		
2	C	529	Total	C	N	O	S	0	0
			4175	2612	730	816	17		

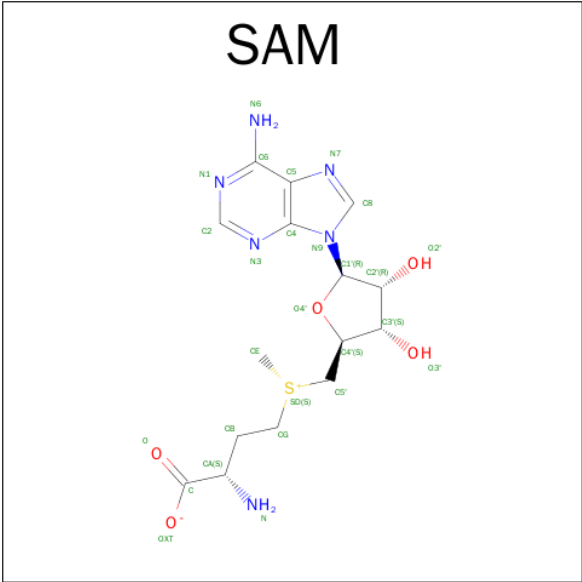
- Molecule 3 is a DNA chain called 5'-D(*GP*TP*TP*CP*AP*AP*CP*GP*TP*CP*GP*A P*CP*GP *TP*GP*CP*AP*AP*C)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	20	Total	C	N	O	P	0	0
			409	194	76	119	20		

- Molecule 4 is a DNA chain called 5'-D(*GP*TP*TP*GP*CP*AP*CP*GP*TP*CP*GP*A P*CP*GP *TP*TP*GP*AP*AP*C)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	20	Total	C	N	O	P	0	0
			411	195	75	121	20		

- Molecule 5 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).

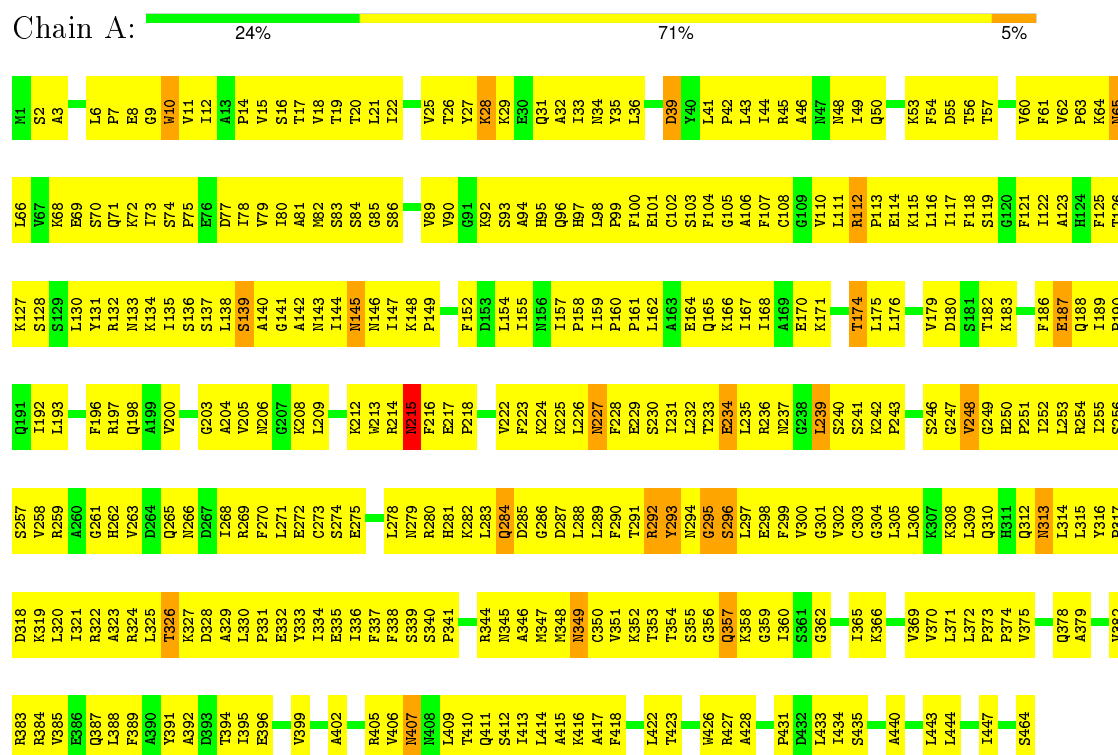


Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	S	0
			27	15	6	5	1	
5	C	1	Total	C	N	O	S	0
			27	15	6	5	1	

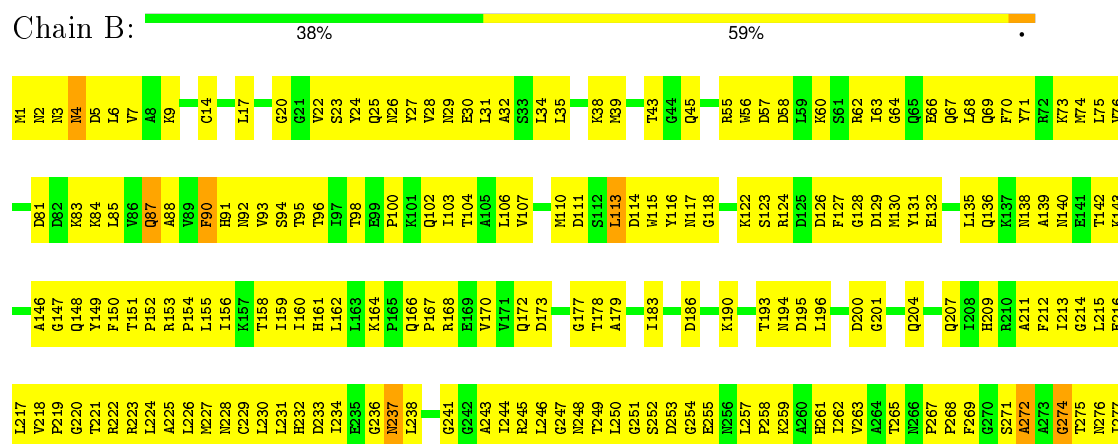
3 Residue-property plots

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

• Molecule 1: TYPE-1 RESTRICTION ENZYME ECOKI SPECIFICITY PROTEIN

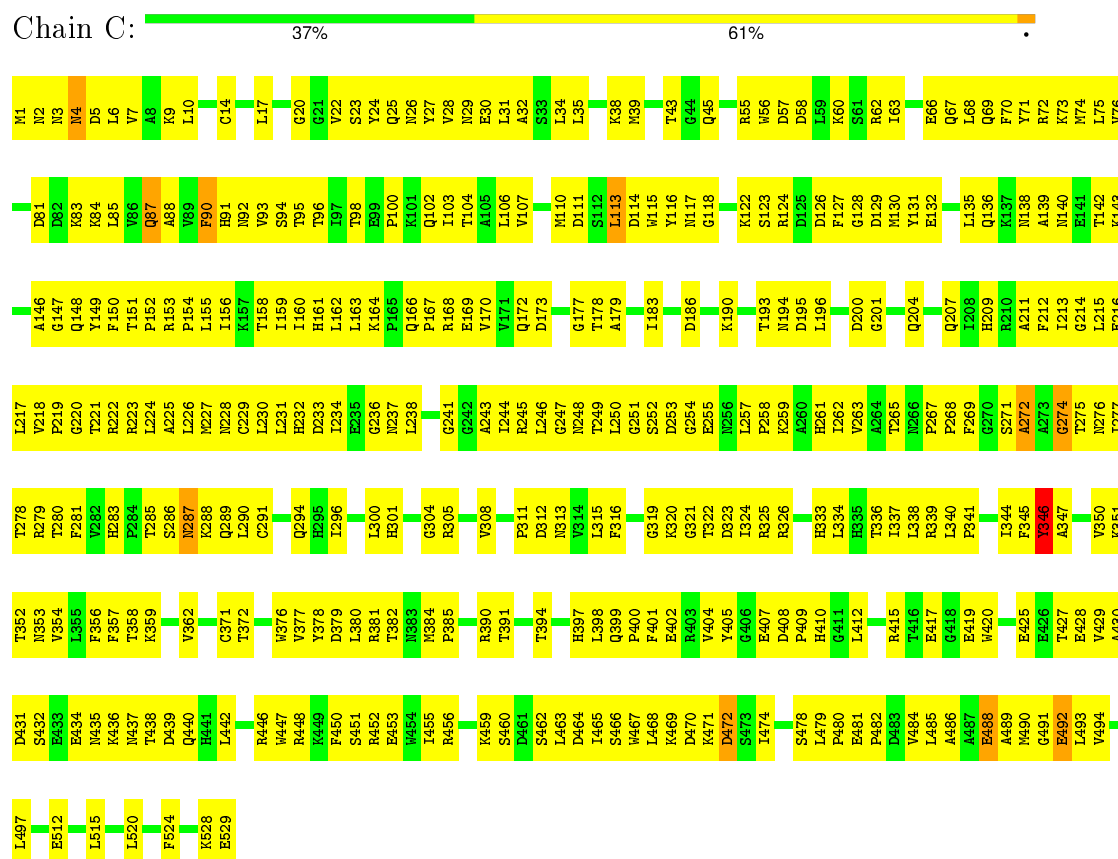


• Molecule 2: TYPE I RESTRICTION ENZYME ECOKI M PROTEIN





• Molecule 2: TYPE I RESTRICTION ENZYME ECOKI M PROTEIN



• Molecule 3: 5'-D(*GP*TP*TP*CP*AP*AP*CP*GP*TP*CP*GP*AP*CP*GP *TP*GP*CP*AP*AP*C)-3'



• Molecule 4: 5'-D(*GP*TP*TP*GP*CP*AP*CP*GP*TP*CP*GP*AP*CP*GP *TP*TP*GP*AP*AP*C)-3'



G1	T2	T3	C4	C5	A6	C7	C8	T9	C10	G11	A12	C13	G14	T15	T16	G17	A18	A19	C20
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FILTERED AT FIRST ZERO	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	80	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	275	Depositor
Maximum defocus (nm)	870	Depositor
Magnification	40000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.98	2/3685 (0.1%)	1.05	3/4968 (0.1%)
2	B	0.94	0/4262	1.05	3/5773 (0.1%)
2	C	0.94	0/4262	1.02	2/5773 (0.0%)
3	D	3.89	80/458 (17.5%)	5.67	167/704 (23.7%)
4	E	3.95	79/460 (17.2%)	5.69	171/708 (24.2%)
All	All	1.39	161/13127 (1.2%)	1.88	346/17926 (1.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
3	D	1	1
All	All	1	3

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	ARG	C-N	15.10	1.68	1.34
3	D	14	DG	N3-C4	13.28	1.44	1.35
3	D	11	DG	N3-C4	13.10	1.44	1.35
3	D	16	DG	N3-C4	13.07	1.44	1.35
4	E	1	DG	N3-C4	13.03	1.44	1.35
3	D	1	DG	N3-C4	13.01	1.44	1.35
4	E	11	DG	N3-C4	13.00	1.44	1.35
4	E	8	DG	N3-C4	12.91	1.44	1.35
4	E	14	DG	N3-C4	12.90	1.44	1.35
3	D	8	DG	N3-C4	12.87	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	17	DG	N3-C4	12.87	1.44	1.35
4	E	4	DG	N3-C4	12.85	1.44	1.35
3	D	13	DC	C2-N3	11.56	1.45	1.35
4	E	20	DC	C2-N3	11.47	1.45	1.35
4	E	7	DC	C2-N3	11.46	1.45	1.35
3	D	20	DC	C2-N3	11.45	1.45	1.35
3	D	7	DC	C2-N3	11.42	1.44	1.35
4	E	10	DC	C2-N3	11.38	1.44	1.35
3	D	17	DC	C2-N3	11.29	1.44	1.35
3	D	10	DC	C2-N3	11.24	1.44	1.35
4	E	5	DC	C2-N3	11.23	1.44	1.35
4	E	13	DC	C2-N3	11.18	1.44	1.35
3	D	4	DC	C2-N3	11.05	1.44	1.35
4	E	5	DC	O3'-P	10.91	1.74	1.61
4	E	4	DG	N9-C8	-10.62	1.30	1.37
4	E	17	DG	N9-C8	-10.35	1.30	1.37
4	E	14	DG	N9-C8	-10.14	1.30	1.37
3	D	8	DG	N9-C8	-10.11	1.30	1.37
4	E	1	DG	N9-C8	-10.05	1.30	1.37
3	D	11	DG	N9-C8	-9.97	1.30	1.37
4	E	11	DG	N9-C8	-9.93	1.30	1.37
4	E	8	DG	N9-C8	-9.87	1.30	1.37
3	D	1	DG	N9-C8	-9.86	1.30	1.37
3	D	16	DG	N9-C8	-9.75	1.31	1.37
3	D	5	DA	O3'-P	9.36	1.72	1.61
4	E	5	DC	N3-C4	-9.28	1.27	1.33
3	D	6	DA	N7-C5	-9.17	1.33	1.39
3	D	4	DC	N3-C4	-9.14	1.27	1.33
3	D	17	DC	N3-C4	-9.09	1.27	1.33
4	E	13	DC	N3-C4	-9.06	1.27	1.33
4	E	20	DC	N3-C4	-9.04	1.27	1.33
4	E	7	DC	N3-C4	-8.99	1.27	1.33
3	D	13	DC	N3-C4	-8.97	1.27	1.33
3	D	10	DC	N3-C4	-8.97	1.27	1.33
3	D	20	DC	N3-C4	-8.96	1.27	1.33
3	D	7	DC	N3-C4	-8.93	1.27	1.33
4	E	10	DC	N3-C4	-8.76	1.27	1.33
3	D	5	DA	N7-C5	-8.76	1.33	1.39
3	D	12	DA	N7-C5	-8.56	1.34	1.39
3	D	14	DG	N9-C8	-8.46	1.31	1.37
3	D	1	DG	N7-C5	8.45	1.44	1.39
4	E	12	DA	N9-C8	-8.44	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	8	DG	N9-C4	-8.39	1.31	1.38
4	E	1	DG	N7-C5	8.37	1.44	1.39
4	E	12	DA	N7-C5	-8.36	1.34	1.39
3	D	18	DA	N7-C5	-8.35	1.34	1.39
4	E	17	DG	N7-C5	8.33	1.44	1.39
4	E	17	DG	N9-C4	-8.33	1.31	1.38
3	D	8	DG	N9-C4	-8.32	1.31	1.38
4	E	4	DG	N7-C5	8.32	1.44	1.39
3	D	12	DA	N9-C8	-8.31	1.31	1.37
4	E	18	DA	N9-C8	-8.30	1.31	1.37
3	D	8	DG	N7-C5	8.29	1.44	1.39
4	E	11	DG	N9-C4	-8.28	1.31	1.38
4	E	19	DA	N9-C8	-8.28	1.31	1.37
3	D	19	DA	N7-C5	-8.27	1.34	1.39
4	E	11	DG	N7-C5	8.26	1.44	1.39
4	E	18	DA	N7-C5	-8.23	1.34	1.39
4	E	6	DA	N7-C5	-8.23	1.34	1.39
4	E	8	DG	N7-C5	8.22	1.44	1.39
4	E	19	DA	N7-C5	-8.22	1.34	1.39
3	D	19	DA	N9-C8	-8.20	1.31	1.37
4	E	1	DG	N9-C4	-8.20	1.31	1.38
4	E	4	DG	N9-C4	-8.20	1.31	1.38
3	D	1	DG	N9-C4	-8.17	1.31	1.38
3	D	18	DA	N9-C8	-8.16	1.31	1.37
3	D	6	DA	N9-C8	-8.12	1.31	1.37
3	D	11	DG	N7-C5	8.11	1.44	1.39
3	D	16	DG	N9-C4	-8.06	1.31	1.38
3	D	16	DG	N7-C5	8.05	1.44	1.39
4	E	14	DG	N9-C4	-8.02	1.31	1.38
4	E	14	DG	N7-C5	7.94	1.44	1.39
3	D	11	DG	N9-C4	-7.93	1.31	1.38
4	E	6	DA	N9-C8	-7.87	1.31	1.37
3	D	5	DA	N9-C8	-7.66	1.31	1.37
4	E	11	DG	O3'-P	7.63	1.70	1.61
3	D	14	DG	N9-C4	-7.55	1.31	1.38
3	D	16	DG	O3'-P	7.38	1.70	1.61
3	D	14	DG	N7-C5	7.22	1.43	1.39
3	D	11	DG	C8-N7	-7.22	1.26	1.30
4	E	14	DG	C8-N7	-7.19	1.26	1.30
3	D	8	DG	C8-N7	-7.11	1.26	1.30
4	E	4	DG	C8-N7	-7.03	1.26	1.30
4	E	11	DG	C8-N7	-7.02	1.26	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	16	DG	C8-N7	-6.98	1.26	1.30
1	A	295	GLY	C-N	-6.93	1.18	1.34
4	E	17	DG	C5-C4	-6.89	1.33	1.38
3	D	16	DG	C5-C4	-6.85	1.33	1.38
3	D	17	DC	O3'-P	6.82	1.69	1.61
4	E	8	DG	C8-N7	-6.81	1.26	1.30
3	D	1	DG	C8-N7	-6.80	1.26	1.30
3	D	11	DG	C5-C4	-6.80	1.33	1.38
4	E	17	DG	C8-N7	-6.76	1.26	1.30
3	D	15	DT	O3'-P	6.75	1.69	1.61
4	E	13	DC	C4-C5	6.72	1.48	1.43
4	E	1	DG	C8-N7	-6.71	1.26	1.30
3	D	1	DG	C5-C4	-6.70	1.33	1.38
4	E	11	DG	C5-C4	-6.70	1.33	1.38
4	E	4	DG	C5-C4	-6.68	1.33	1.38
4	E	8	DG	C5-C4	-6.67	1.33	1.38
4	E	1	DG	C5-C4	-6.66	1.33	1.38
3	D	8	DG	C5-C4	-6.65	1.33	1.38
4	E	16	DT	O3'-P	6.63	1.69	1.61
3	D	5	DA	C8-N7	-6.62	1.26	1.31
4	E	14	DG	C5-C4	-6.60	1.33	1.38
4	E	20	DC	C4-C5	6.55	1.48	1.43
3	D	7	DC	C4-C5	6.55	1.48	1.43
3	D	13	DC	C4-C5	6.54	1.48	1.43
4	E	7	DC	C4-C5	6.51	1.48	1.43
3	D	20	DC	C4-C5	6.49	1.48	1.43
4	E	5	DC	C4-C5	6.47	1.48	1.43
4	E	17	DG	O3'-P	6.45	1.68	1.61
3	D	17	DC	C4-C5	6.45	1.48	1.43
3	D	14	DG	C8-N7	-6.44	1.27	1.30
4	E	10	DC	C4-C5	6.38	1.48	1.43
3	D	10	DC	C4-C5	6.38	1.48	1.43
3	D	18	DA	C8-N7	-6.32	1.27	1.31
4	E	7	DC	O3'-P	6.32	1.68	1.61
4	E	18	DA	C8-N7	-6.29	1.27	1.31
4	E	19	DA	C8-N7	-6.20	1.27	1.31
4	E	17	DG	C2-N3	-6.20	1.27	1.32
3	D	12	DA	C8-N7	-6.16	1.27	1.31
3	D	19	DA	C8-N7	-6.10	1.27	1.31
4	E	12	DA	C8-N7	-6.07	1.27	1.31
3	D	14	DG	C2-N3	-6.06	1.27	1.32
3	D	3	DT	O3'-P	6.06	1.68	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	8	DG	C2-N3	-6.06	1.27	1.32
4	E	8	DG	C2-N3	-6.04	1.27	1.32
3	D	6	DA	O3'-P	6.02	1.68	1.61
4	E	11	DG	C2-N3	-5.95	1.27	1.32
4	E	1	DG	C2-N3	-5.90	1.28	1.32
3	D	16	DG	C2-N3	-5.87	1.28	1.32
3	D	4	DC	C4-C5	5.86	1.47	1.43
3	D	1	DG	C2-N3	-5.85	1.28	1.32
4	E	14	DG	C2-N3	-5.85	1.28	1.32
4	E	6	DA	C8-N7	-5.85	1.27	1.31
4	E	4	DG	C2-N3	-5.79	1.28	1.32
3	D	11	DG	C2-N3	-5.75	1.28	1.32
4	E	3	DT	O3'-P	5.69	1.68	1.61
3	D	4	DC	N1-C2	-5.67	1.34	1.40
3	D	6	DA	C8-N7	-5.65	1.27	1.31
4	E	15	DT	O3'-P	5.61	1.67	1.61
3	D	14	DG	C6-N1	-5.54	1.35	1.39
4	E	4	DG	O3'-P	5.49	1.67	1.61
4	E	6	DA	O3'-P	5.37	1.67	1.61
3	D	7	DC	O3'-P	5.36	1.67	1.61
3	D	11	DG	O3'-P	5.25	1.67	1.61
3	D	14	DG	C5-C4	-5.18	1.34	1.38
3	D	9	DT	O3'-P	-5.15	1.54	1.61
3	D	11	DG	C6-N1	-5.04	1.36	1.39
4	E	2	DT	O3'-P	5.03	1.67	1.61

All (346) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	DG	C4-C5-N7	-24.73	100.91	110.80
3	D	1	DG	C4-C5-N7	-24.21	101.12	110.80
4	E	8	DG	C4-C5-N7	-24.19	101.12	110.80
4	E	17	DG	C4-C5-N7	-24.18	101.13	110.80
4	E	11	DG	C4-C5-N7	-24.05	101.18	110.80
3	D	8	DG	C4-C5-N7	-23.95	101.22	110.80
4	E	1	DG	C4-C5-N7	-23.87	101.25	110.80
4	E	14	DG	C4-C5-N7	-23.83	101.27	110.80
3	D	16	DG	C4-C5-N7	-23.73	101.31	110.80
3	D	11	DG	C4-C5-N7	-23.50	101.40	110.80
3	D	14	DG	C4-C5-N7	-22.48	101.81	110.80
3	D	11	DG	N3-C4-C5	-19.57	118.81	128.60
3	D	16	DG	N3-C4-C5	-19.24	118.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	14	DG	N3-C4-C5	-19.15	119.02	128.60
4	E	11	DG	N3-C4-C5	-18.91	119.14	128.60
4	E	4	DG	N3-C4-C5	-18.88	119.16	128.60
3	D	1	DG	N3-C4-C5	-18.77	119.21	128.60
4	E	8	DG	N3-C4-C5	-18.70	119.25	128.60
3	D	14	DG	N3-C4-C5	-18.57	119.31	128.60
4	E	1	DG	N3-C4-C5	-18.56	119.32	128.60
3	D	8	DG	N3-C4-C5	-18.48	119.36	128.60
3	D	14	DG	N9-C4-C5	18.47	112.79	105.40
4	E	17	DG	N3-C4-C5	-18.32	119.44	128.60
3	D	14	DG	C2-N3-C4	17.51	120.65	111.90
4	E	6	DA	C2-N3-C4	17.50	119.35	110.60
2	B	470	ASP	O-C-N	-17.15	95.26	122.70
4	E	14	DG	C2-N3-C4	16.93	120.36	111.90
3	D	1	DG	C2-N3-C4	16.89	120.34	111.90
3	D	16	DG	C2-N3-C4	16.89	120.34	111.90
4	E	11	DG	C2-N3-C4	16.84	120.32	111.90
4	E	8	DG	C2-N3-C4	16.72	120.26	111.90
3	D	11	DG	C2-N3-C4	16.72	120.26	111.90
4	E	17	DG	C2-N3-C4	16.71	120.25	111.90
3	D	6	DA	C2-N3-C4	16.68	118.94	110.60
4	E	1	DG	C2-N3-C4	16.67	120.24	111.90
4	E	4	DG	C2-N3-C4	16.56	120.18	111.90
3	D	8	DG	C2-N3-C4	16.54	120.17	111.90
3	D	6	DA	N1-C2-N3	-16.50	121.05	129.30
4	E	6	DA	N1-C2-N3	-16.34	121.13	129.30
3	D	18	DA	C2-N3-C4	15.98	118.59	110.60
3	D	19	DA	C2-N3-C4	15.95	118.57	110.60
4	E	18	DA	C2-N3-C4	15.91	118.56	110.60
4	E	19	DA	C2-N3-C4	15.75	118.47	110.60
3	D	5	DA	C2-N3-C4	15.67	118.44	110.60
3	D	1	DG	N9-C4-C5	15.52	111.61	105.40
4	E	8	DG	N9-C4-C5	15.51	111.60	105.40
3	D	16	DG	N9-C4-C5	15.32	111.53	105.40
3	D	12	DA	C2-N3-C4	15.30	118.25	110.60
4	E	17	DG	N9-C4-C5	15.29	111.52	105.40
3	D	5	DA	N1-C2-N3	-15.25	121.67	129.30
4	E	1	DG	N9-C4-C5	15.23	111.49	105.40
4	E	4	DG	N9-C4-C5	15.22	111.49	105.40
3	D	4	DC	N3-C4-C5	-15.21	115.82	121.90
3	D	14	DG	C5-C6-O6	-15.15	119.51	128.60
4	E	19	DA	N1-C2-N3	-15.11	121.75	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	19	DA	N1-C2-N3	-15.10	121.75	129.30
3	D	8	DG	N9-C4-C5	15.07	111.43	105.40
4	E	11	DG	N9-C4-C5	15.01	111.40	105.40
4	E	14	DG	N9-C4-C5	14.99	111.39	105.40
4	E	12	DA	C2-N3-C4	14.91	118.06	110.60
3	D	18	DA	N1-C2-N3	-14.86	121.87	129.30
4	E	18	DA	N1-C2-N3	-14.81	121.89	129.30
3	D	11	DG	N9-C4-C5	14.67	111.27	105.40
3	D	12	DA	N1-C2-N3	-13.87	122.37	129.30
4	E	17	DG	C6-C5-N7	13.86	138.71	130.40
3	D	1	DG	C6-C5-N7	13.58	138.55	130.40
4	E	4	DG	C6-C5-N7	13.55	138.53	130.40
4	E	12	DA	N1-C2-N3	-13.55	122.53	129.30
3	D	8	DG	C6-C5-N7	13.54	138.52	130.40
3	D	11	DG	C5-C6-O6	-13.50	120.50	128.60
3	D	14	DG	C6-C5-N7	13.50	138.50	130.40
4	E	8	DG	C6-C5-N7	13.49	138.49	130.40
4	E	1	DG	C6-C5-N7	13.45	138.47	130.40
4	E	11	DG	C6-C5-N7	13.39	138.44	130.40
3	D	8	DG	C5-C6-O6	-13.06	120.76	128.60
4	E	8	DG	C5-C6-O6	-12.97	120.82	128.60
4	E	11	DG	C5-C6-O6	-12.94	120.83	128.60
4	E	14	DG	C6-C5-N7	12.91	138.15	130.40
4	E	17	DG	C5-C6-O6	-12.90	120.86	128.60
3	D	16	DG	C6-C5-N7	12.87	138.12	130.40
4	E	14	DG	C5-C6-O6	-12.80	120.92	128.60
4	E	1	DG	C5-C6-O6	-12.76	120.95	128.60
4	E	4	DG	C5-C6-O6	-12.70	120.98	128.60
3	D	16	DG	C5-C6-O6	-12.69	120.99	128.60
3	D	1	DG	C5-C6-O6	-12.40	121.16	128.60
3	D	11	DG	C6-C5-N7	12.31	137.78	130.40
3	D	12	DA	C5-N7-C8	12.31	110.05	103.90
4	E	6	DA	C5-N7-C8	12.22	110.01	103.90
3	D	18	DA	C5-N7-C8	12.05	109.92	103.90
3	D	6	DA	C5-N7-C8	12.03	109.91	103.90
3	D	13	DC	N3-C4-C5	-11.95	117.12	121.90
4	E	12	DA	C5-N7-C8	11.88	109.84	103.90
4	E	18	DA	C5-N7-C8	11.87	109.83	103.90
4	E	6	DA	C4-C5-C6	11.80	122.90	117.00
3	D	19	DA	C5-N7-C8	11.66	109.73	103.90
3	D	5	DA	C4-C5-C6	11.64	122.82	117.00
3	D	20	DC	N3-C4-C5	-11.49	117.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	7	DC	N3-C4-C5	-11.46	117.32	121.90
4	E	19	DA	C5-N7-C8	11.45	109.63	103.90
4	E	6	DA	N3-C4-C5	-11.45	118.79	126.80
4	E	10	DC	N3-C4-C5	-11.42	117.33	121.90
4	E	20	DC	N3-C4-C5	-11.32	117.37	121.90
3	D	17	DC	N3-C4-C5	-11.32	117.37	121.90
3	D	6	DA	C4-C5-C6	11.31	122.66	117.00
4	E	7	DC	N3-C4-C5	-11.21	117.42	121.90
3	D	18	DA	C4-C5-C6	11.20	122.60	117.00
3	D	5	DA	C5-N7-C8	11.15	109.48	103.90
4	E	18	DA	C4-C5-C6	11.10	122.55	117.00
4	E	6	DA	C4-C5-N7	-11.07	105.16	110.70
4	E	13	DC	N3-C4-C5	-11.06	117.48	121.90
3	D	12	DA	C4-C5-C6	11.05	122.53	117.00
3	D	6	DA	C4-C5-N7	-11.00	105.20	110.70
3	D	6	DA	N3-C4-C5	-10.88	119.18	126.80
4	E	5	DC	N3-C4-C5	-10.87	117.55	121.90
4	E	19	DA	C4-C5-C6	10.85	122.42	117.00
3	D	12	DA	C4-C5-N7	-10.83	105.28	110.70
3	D	19	DA	C4-C5-C6	10.83	122.41	117.00
3	D	18	DA	C4-C5-N7	-10.82	105.29	110.70
3	D	18	DA	N3-C4-C5	-10.79	119.25	126.80
3	D	10	DC	N3-C4-C5	-10.71	117.61	121.90
4	E	18	DA	N3-C4-C5	-10.68	119.33	126.80
4	E	18	DA	C4-C5-N7	-10.66	105.37	110.70
3	D	19	DA	C4-C5-N7	-10.62	105.39	110.70
4	E	4	DG	C5-N7-C8	10.61	109.60	104.30
3	D	15	DT	O4'-C1'-N1	10.56	115.39	108.00
4	E	12	DA	C4-C5-N7	-10.56	105.42	110.70
3	D	19	DA	N3-C4-C5	-10.52	119.43	126.80
3	D	12	DA	N3-C4-C5	-10.50	119.45	126.80
4	E	12	DA	C4-C5-C6	10.47	122.24	117.00
3	D	5	DA	N3-C4-C5	-10.45	119.48	126.80
4	E	19	DA	C4-C5-N7	-10.38	105.51	110.70
4	E	19	DA	N3-C4-C5	-10.36	119.55	126.80
4	E	11	DG	C5-N7-C8	10.32	109.46	104.30
3	D	2	DT	O4'-C1'-N1	10.27	115.19	108.00
3	D	1	DG	C5-N7-C8	10.15	109.38	104.30
4	E	8	DG	C5-N7-C8	10.15	109.38	104.30
4	E	17	DG	C5-N7-C8	10.08	109.34	104.30
4	E	12	DA	N3-C4-C5	-10.08	119.74	126.80
4	E	14	DG	C5-N7-C8	10.02	109.31	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	11	DG	C5-N7-C8	9.96	109.28	104.30
3	D	16	DG	C5-N7-C8	9.96	109.28	104.30
3	D	8	DG	C5-N7-C8	9.94	109.27	104.30
4	E	1	DG	C5-N7-C8	9.80	109.20	104.30
3	D	5	DA	C4-C5-N7	-9.76	105.82	110.70
3	D	17	DC	OP1-P-OP2	-9.61	105.18	119.60
4	E	17	DG	OP1-P-OP2	-9.61	105.19	119.60
3	D	2	DT	C2-N3-C4	-9.46	121.52	127.20
3	D	3	DT	OP1-P-OP2	-9.30	105.64	119.60
4	E	9	DT	C2-N3-C4	-9.26	121.64	127.20
4	E	2	DT	C2-N3-C4	-9.25	121.65	127.20
3	D	3	DT	C2-N3-C4	-9.24	121.65	127.20
4	E	3	DT	OP1-P-OP2	-9.24	105.74	119.60
4	E	3	DT	C2-N3-C4	-9.18	121.69	127.20
1	A	174	THR	CA-CB-CG2	-9.17	99.56	112.40
4	E	15	DT	O4'-C1'-N1	9.17	114.42	108.00
3	D	9	DT	C2-N3-C4	-9.16	121.70	127.20
4	E	15	DT	C2-N3-C4	-9.07	121.76	127.20
4	E	6	DA	N3-C4-N9	8.99	134.59	127.40
4	E	16	DT	C2-N3-C4	-8.90	121.86	127.20
4	E	18	DA	OP1-P-OP2	-8.89	106.26	119.60
3	D	18	DA	OP1-P-OP2	-8.89	106.27	119.60
3	D	14	DG	N1-C6-O6	8.87	125.22	119.90
3	D	15	DT	C2-N3-C4	-8.79	121.93	127.20
4	E	18	DA	N3-C4-N9	8.64	134.31	127.40
3	D	18	DA	N3-C4-N9	8.64	134.31	127.40
3	D	5	DA	N1-C6-N6	8.61	123.77	118.60
3	D	4	DC	C4-C5-C6	8.56	121.68	117.40
3	D	5	DA	N3-C4-N9	8.53	134.22	127.40
3	D	17	DC	O4'-C1'-N1	8.48	113.94	108.00
3	D	12	DA	N3-C4-N9	8.43	134.15	127.40
3	D	14	DG	OP1-P-OP2	-8.42	106.97	119.60
3	D	5	DA	OP1-P-OP2	-8.40	107.01	119.60
3	D	19	DA	N3-C4-N9	8.35	134.08	127.40
4	E	19	DA	N3-C4-N9	8.32	134.06	127.40
3	D	6	DA	N3-C4-N9	8.17	133.93	127.40
3	D	7	DC	O4'-C1'-N1	8.15	113.71	108.00
4	E	12	DA	N3-C4-N9	8.13	133.91	127.40
3	D	1	DG	O4'-C1'-N9	8.08	113.66	108.00
4	E	14	DG	OP1-P-OP2	-7.89	107.76	119.60
4	E	7	DC	O4'-C1'-N1	7.79	113.45	108.00
3	D	2	DT	C5-C4-O4	-7.63	119.56	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	DT	C5-C6-N1	-7.58	119.15	123.70
3	D	14	DG	C5-C6-N1	7.53	115.27	111.50
3	D	4	DC	N1-C2-O2	7.52	123.41	118.90
3	D	3	DT	C5-C4-O4	-7.51	119.64	124.90
4	E	17	DG	C5-C6-N1	7.50	115.25	111.50
4	E	3	DT	N1-C2-N3	7.50	119.10	114.60
4	E	11	DG	C5-C6-N1	7.48	115.24	111.50
3	D	1	DG	C5-C6-N1	7.47	115.23	111.50
4	E	6	DA	N1-C6-N6	7.45	123.07	118.60
4	E	15	DT	N1-C2-N3	7.45	119.07	114.60
1	A	292	ARG	O-C-N	-7.42	110.82	122.70
3	D	9	DT	C5-C4-O4	-7.41	119.72	124.90
3	D	11	DG	N1-C6-O6	7.41	124.34	119.90
4	E	9	DT	C5-C4-O4	-7.41	119.72	124.90
3	D	16	DG	C5-C6-N1	7.39	115.20	111.50
3	D	8	DG	C5-C6-N1	7.38	115.19	111.50
4	E	16	DT	C5-C4-O4	-7.38	119.73	124.90
4	E	1	DG	C5-C6-N1	7.34	115.17	111.50
4	E	10	DC	N3-C4-N4	7.32	123.12	118.00
3	D	11	DG	C5-C6-N1	7.31	115.16	111.50
4	E	8	DG	C5-C6-N1	7.30	115.15	111.50
4	E	19	DA	N1-C6-N6	7.30	122.98	118.60
4	E	14	DG	C5-C6-N1	7.29	115.14	111.50
4	E	3	DT	C5-C4-O4	-7.28	119.80	124.90
3	D	13	DC	N3-C4-N4	7.28	123.09	118.00
4	E	2	DT	C5-C4-O4	-7.27	119.81	124.90
3	D	2	DT	N1-C2-N3	7.25	118.95	114.60
4	E	16	DT	N1-C2-N3	7.25	118.95	114.60
4	E	15	DT	C5-C4-O4	-7.23	119.84	124.90
3	D	13	DC	C4-C5-C6	7.21	121.01	117.40
3	D	15	DT	N1-C2-N3	7.21	118.93	114.60
3	D	7	DC	N3-C4-N4	7.20	123.04	118.00
4	E	9	DT	N1-C2-N3	7.18	118.91	114.60
3	D	17	DC	N3-C4-N4	7.18	123.02	118.00
3	D	4	DC	N3-C4-N4	7.17	123.02	118.00
4	E	4	DG	N7-C8-N9	-7.15	109.52	113.10
4	E	6	DA	C6-N1-C2	7.15	122.89	118.60
3	D	3	DT	N1-C2-N3	7.14	118.89	114.60
3	D	5	DA	C6-N1-C2	7.13	122.88	118.60
3	D	15	DT	C5-C4-O4	-7.13	119.91	124.90
4	E	11	DG	N7-C8-N9	-7.13	109.54	113.10
3	D	1	DG	OP1-P-OP2	-7.12	108.91	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	10	DC	N3-C4-N4	7.11	122.97	118.00
3	D	20	DC	N3-C4-N4	7.08	122.96	118.00
4	E	7	DC	N3-C4-N4	7.07	122.95	118.00
4	E	18	DA	N1-C6-N6	7.05	122.83	118.60
3	D	19	DA	N1-C6-N6	7.04	122.83	118.60
4	E	20	DC	N3-C4-N4	7.04	122.93	118.00
3	D	6	DA	C6-N1-C2	7.03	122.82	118.60
3	D	18	DA	N1-C6-N6	7.03	122.82	118.60
3	D	9	DT	N1-C2-N3	7.02	118.81	114.60
4	E	13	DC	N3-C4-N4	7.02	122.91	118.00
4	E	2	DT	N1-C2-N3	7.01	118.81	114.60
4	E	4	DG	C5-C6-N1	7.01	115.00	111.50
4	E	2	DT	O4'-C1'-N1	7.00	112.90	108.00
3	D	12	DA	N1-C6-N6	6.98	122.79	118.60
4	E	17	DG	N7-C8-N9	-6.95	109.63	113.10
4	E	5	DC	N3-C4-N4	6.93	122.85	118.00
3	D	8	DG	N1-C6-O6	6.91	124.05	119.90
4	E	8	DG	N1-C6-O6	6.88	124.03	119.90
4	E	8	DG	N7-C8-N9	-6.88	109.66	113.10
3	D	20	DC	C4-C5-C6	6.87	120.84	117.40
4	E	4	DG	N1-C6-O6	6.86	124.01	119.90
3	D	1	DG	N7-C8-N9	-6.82	109.69	113.10
3	D	17	DC	C4-C5-C6	6.82	120.81	117.40
4	E	12	DA	N1-C6-N6	6.80	122.68	118.60
4	E	14	DG	N1-C6-O6	6.72	123.93	119.90
3	D	6	DA	N1-C6-N6	6.71	122.63	118.60
4	E	11	DG	N1-C6-O6	6.71	123.93	119.90
4	E	13	DC	C4-C5-C6	6.71	120.76	117.40
3	D	7	DC	C4-C5-C6	6.68	120.74	117.40
3	D	13	DC	N3-C2-O2	-6.66	117.24	121.90
4	E	20	DC	C4-C5-C6	6.66	120.73	117.40
3	D	13	DC	N1-C2-O2	6.66	122.89	118.90
4	E	17	DG	N1-C6-O6	6.65	123.89	119.90
4	E	1	DG	N1-C6-O6	6.64	123.88	119.90
3	D	8	DG	N7-C8-N9	-6.63	109.79	113.10
3	D	11	DG	N7-C8-N9	-6.60	109.80	113.10
4	E	11	DG	O4'-C1'-N9	6.59	112.62	108.00
3	D	11	DG	OP1-P-OP2	-6.57	109.74	119.60
4	E	1	DG	N7-C8-N9	-6.57	109.81	113.10
3	D	16	DG	N7-C8-N9	-6.55	109.83	113.10
4	E	19	DA	C6-N1-C2	6.55	122.53	118.60
4	E	9	DT	O4'-C1'-N1	6.54	112.58	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	11	DG	N3-C4-N9	6.53	129.92	126.00
3	D	10	DC	C4-C5-C6	6.53	120.67	117.40
3	D	4	DC	N3-C2-O2	-6.53	117.33	121.90
3	D	16	DG	N1-C6-O6	6.52	123.81	119.90
4	E	2	DT	C5-C6-N1	-6.50	119.80	123.70
4	E	7	DC	N3-C2-O2	-6.43	117.40	121.90
4	E	10	DC	C4-C5-C6	6.43	120.61	117.40
3	D	19	DA	C6-N1-C2	6.41	122.45	118.60
4	E	14	DG	N7-C8-N9	-6.41	109.90	113.10
3	D	13	DC	O4'-C1'-N1	6.40	112.48	108.00
4	E	7	DC	N1-C2-O2	6.37	122.72	118.90
3	D	2	DT	P-O3'-C3'	6.31	127.27	119.70
4	E	10	DC	N1-C2-O2	6.31	122.69	118.90
4	E	20	DC	N1-C2-O2	6.30	122.68	118.90
4	E	9	DT	C5-C6-N1	-6.30	119.92	123.70
3	D	7	DC	N1-C2-O2	6.29	122.67	118.90
4	E	7	DC	C4-C5-C6	6.27	120.54	117.40
4	E	3	DT	C5-C6-N1	-6.26	119.94	123.70
3	D	9	DT	C5-C6-N1	-6.26	119.95	123.70
3	D	20	DC	N1-C2-O2	6.23	122.64	118.90
4	E	18	DA	C6-N1-C2	6.23	122.34	118.60
3	D	18	DA	C6-N1-C2	6.22	122.33	118.60
3	D	12	DA	OP1-P-OP2	-6.22	110.27	119.60
3	D	10	DC	N1-C2-O2	6.19	122.61	118.90
3	D	1	DG	N1-C6-O6	6.17	123.60	119.90
4	E	20	DC	N3-C2-O2	-6.16	117.59	121.90
4	E	5	DC	C4-C5-C6	6.15	120.48	117.40
3	D	7	DC	N3-C2-O2	-6.14	117.60	121.90
3	D	3	DT	C5-C6-N1	-6.12	120.03	123.70
3	D	17	DC	N3-C2-O2	-6.12	117.62	121.90
3	D	20	DC	N3-C2-O2	-6.12	117.62	121.90
4	E	13	DC	N3-C2-O2	-6.11	117.62	121.90
3	D	13	DC	P-O3'-C3'	6.09	127.00	119.70
3	D	15	DT	C5-C6-N1	-6.08	120.05	123.70
4	E	5	DC	N3-C2-O2	-6.06	117.66	121.90
4	E	15	DT	C5-C6-N1	-6.04	120.08	123.70
3	D	5	DA	C5-C6-N1	-6.01	114.69	117.70
3	D	14	DG	C5-N7-C8	6.01	107.31	104.30
3	D	17	DC	N1-C2-O2	6.01	122.50	118.90
3	D	10	DC	N3-C2-O2	-5.99	117.70	121.90
3	D	14	DG	N1-C2-N3	-5.97	120.32	123.90
4	E	14	DG	N3-C4-N9	5.97	129.58	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5	DC	N1-C2-O2	5.90	122.44	118.90
4	E	10	DC	N3-C2-O2	-5.86	117.80	121.90
2	B	346	TYR	CB-CG-CD2	-5.83	117.50	121.00
3	D	16	DG	N3-C4-N9	5.82	129.49	126.00
4	E	13	DC	N1-C2-O2	5.79	122.38	118.90
2	C	346	TYR	CB-CG-CD2	-5.77	117.54	121.00
3	D	4	DC	C2-N3-C4	5.76	122.78	119.90
4	E	11	DG	N3-C4-N9	5.75	129.45	126.00
4	E	1	DG	OP1-P-OP2	-5.71	111.04	119.60
3	D	15	DT	OP1-P-OP2	-5.69	111.06	119.60
4	E	15	DT	OP1-P-OP2	-5.67	111.09	119.60
4	E	1	DG	O4'-C1'-N9	5.67	111.97	108.00
4	E	4	DG	N3-C4-N9	5.59	129.35	126.00
2	B	90	PHE	CA-CB-CG	-5.57	100.53	113.90
2	C	90	PHE	CA-CB-CG	-5.56	100.56	113.90
3	D	12	DA	N7-C8-N9	-5.55	111.03	113.80
4	E	6	DA	C5-C6-N1	-5.54	114.93	117.70
4	E	17	DG	O4'-C1'-N9	5.52	111.86	108.00
4	E	16	DT	C5-C6-N1	-5.50	120.40	123.70
4	E	2	DT	P-O3'-C3'	5.49	126.29	119.70
4	E	12	DA	N7-C8-N9	-5.44	111.08	113.80
3	D	12	DA	C6-N1-C2	5.43	121.86	118.60
3	D	8	DG	N3-C4-N9	5.35	129.21	126.00
4	E	6	DA	N7-C8-N9	-5.32	111.14	113.80
4	E	4	DG	O4'-C1'-N9	-5.31	104.28	108.00
4	E	1	DG	N3-C4-N9	5.31	129.18	126.00
3	D	1	DG	N3-C4-N9	5.30	129.18	126.00
4	E	8	DG	N3-C4-N9	5.25	129.15	126.00
4	E	3	DT	O4'-C1'-N1	5.19	111.63	108.00
4	E	16	DT	O3'-P-O5'	5.18	113.84	104.00
4	E	4	DG	C8-N9-C4	5.17	108.47	106.40
3	D	18	DA	N7-C8-N9	-5.17	111.21	113.80
4	E	18	DA	N7-C8-N9	-5.12	111.24	113.80
4	E	13	DC	O4'-C1'-N1	5.08	111.55	108.00
3	D	6	DA	OP1-P-OP2	-5.07	111.99	119.60
4	E	17	DG	N3-C4-N9	5.07	129.04	126.00
4	E	12	DA	C6-N1-C2	5.06	121.64	118.60
1	A	39	ASP	CA-CB-CG	-5.06	102.26	113.40
4	E	11	DG	C8-N9-C4	5.05	108.42	106.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	15	DT	C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	TYR	Sidechain
2	B	470	ASP	Mainchain
3	D	18	DA	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3622	0	3738	1029	0
2	B	4175	0	4050	560	0
2	C	4175	0	4050	582	0
3	D	409	0	225	91	0
4	E	411	0	226	80	0
5	B	27	0	22	28	0
5	C	27	0	22	30	0
All	All	12846	0	12333	2091	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 83.

All (2091) 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:292:ARG:C	1:A:293:TYR:N	1.68	1.43
1:A:209:LEU:HB2	1:A:216:PHE:CZ	1.60	1.36
1:A:3:ALA:O	2:B:488:GLU:HG3	1.22	1.28
1:A:412:SER:HB2	2:B:495:GLN:CG	1.68	1.23
2:C:512:GLU:HB2	2:C:515:LEU:HD23	1.20	1.17
2:B:1:MET:HE1	2:B:129:ASP:HA	1.23	1.16
1:A:3:ALA:O	2:B:488:GLU:CG	1.93	1.15
1:A:193:LEU:HG	1:A:388:LEU:HD13	1.19	1.14
1:A:234:GLU:HG3	4:E:2:DT:H3'	1.20	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:HB2	3:D:2:DT:C7	1.76	1.14
2:B:512:GLU:HB2	2:B:515:LEU:HD23	1.20	1.13
2:C:440:GLN:HB2	2:C:484:VAL:HG21	1.30	1.13
1:A:209:LEU:CB	1:A:216:PHE:CZ	2.32	1.12
1:A:415:ALA:HB2	2:B:492:GLU:CG	1.80	1.12
1:A:412:SER:HB2	2:B:495:GLN:HG3	1.21	1.11
1:A:6:LEU:HD21	1:A:10:TRP:HB2	1.26	1.10
1:A:325:LEU:HD13	1:A:329:ALA:HB3	1.32	1.10
1:A:189:ILE:HG23	1:A:190:PRO:HD3	1.33	1.10
2:B:269:PHE:HB2	3:D:6:DA:C8	1.88	1.09
2:C:139:ALA:HB1	2:C:150:PHE:HB2	1.29	1.09
1:A:412:SER:HB2	2:B:495:GLN:CD	1.73	1.08
2:C:269:PHE:HB2	4:E:6:DA:C8	1.87	1.08
1:A:265:GLN:HG3	1:A:269:ARG:HH21	1.12	1.08
1:A:234:GLU:HG3	4:E:2:DT:C3'	1.83	1.07
2:B:93:VAL:HG12	2:B:223:ARG:HD3	1.32	1.07
2:C:122:LYS:HD3	2:C:124:ARG:HE	1.13	1.07
1:A:279:ASN:O	4:E:1:DG:P	2.13	1.06
1:A:143:ASN:HB2	2:B:313:ASN:HA	1.11	1.06
2:B:139:ALA:HB1	2:B:150:PHE:HB2	1.29	1.06
2:B:122:LYS:HD3	2:B:124:ARG:HE	1.13	1.06
2:C:163:LEU:HD11	2:C:262:ILE:HD13	1.34	1.06
2:C:440:GLN:HB2	2:C:484:VAL:CG2	1.84	1.06
2:B:440:GLN:HB2	2:B:484:VAL:HG21	1.31	1.06
1:A:294:ASN:ND2	3:D:13:DC:H2''	1.69	1.05
1:A:75:PRO:HG2	1:A:111:LEU:HD21	1.38	1.05
1:A:289:LEU:HD11	1:A:320:LEU:HD11	1.37	1.05
2:C:93:VAL:HG12	2:C:223:ARG:HD3	1.33	1.05
1:A:175:LEU:HG	1:A:406:VAL:HG22	1.38	1.05
1:A:139:SER:HB2	2:B:466:SER:HB3	1.33	1.05
1:A:25:VAL:HG13	1:A:71:GLN:HA	1.37	1.05
1:A:355:SER:HB3	2:C:316:PHE:HE1	1.22	1.04
1:A:294:ASN:HD21	3:D:13:DC:H2''	0.88	1.04
2:B:440:GLN:HB2	2:B:484:VAL:CG2	1.85	1.04
5:C:530:SAM:CE	4:E:6:DA:N6	2.19	1.04
1:A:239:LEU:HD22	1:A:241:SER:H	1.18	1.03
1:A:160:PRO:HG2	1:A:165:GLN:HG2	1.35	1.03
2:B:350:VAL:CG1	3:D:6:DA:H4'	1.88	1.02
1:A:415:ALA:HB2	2:B:492:GLU:HG3	1.40	1.02
1:A:83:SER:HA	1:A:147:ILE:HG22	1.41	1.02
1:A:252:ILE:HG13	1:A:317:PRO:HD3	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:HE2	2:B:132:GLU:HG3	1.42	1.01
1:A:71:GLN:HG2	1:A:102:CYS:HB3	1.41	1.01
1:A:428:ALA:HB1	1:A:433:LEU:HD12	1.39	1.01
1:A:412:SER:CB	2:B:495:GLN:HG3	1.90	1.00
2:B:285:THR:HG22	2:B:287:ASN:H	1.22	1.00
5:B:530:SAM:CE	3:D:6:DA:N6	2.25	1.00
1:A:209:LEU:HB2	1:A:216:PHE:HZ	1.23	1.00
2:C:24:TYR:HA	2:C:27:TYR:CE2	1.97	1.00
2:B:24:TYR:HA	2:B:27:TYR:CE2	1.97	1.00
2:C:285:THR:HG22	2:C:287:ASN:H	1.22	0.99
1:A:28:LYS:H	1:A:28:LYS:HD3	1.27	0.99
1:A:196:PHE:CZ	1:A:384:ARG:HD2	1.97	0.99
1:A:209:LEU:HB2	1:A:216:PHE:CE2	1.98	0.99
5:C:530:SAM:HE3	4:E:6:DA:N6	1.78	0.99
2:C:276:ASN:HD22	2:C:278:THR:HG23	1.26	0.99
3:D:12:DA:H2''	3:D:13:DC:H5'	1.45	0.99
1:A:70:SER:HB2	3:D:2:DT:H72	1.43	0.98
1:A:85:GLY:HA2	4:E:14:DG:C8	1.99	0.98
1:A:62:VAL:HG12	1:A:64:LYS:H	1.28	0.98
1:A:355:SER:HB3	2:C:316:PHE:CE1	1.99	0.98
2:C:220:GLY:HA2	2:C:223:ARG:HE	1.27	0.98
2:B:220:GLY:HA2	2:B:223:ARG:HE	1.28	0.97
1:A:39:ASP:HB3	1:A:60:VAL:HG12	1.42	0.97
1:A:70:SER:HB2	3:D:2:DT:H71	1.45	0.97
2:C:430:ALA:HB2	2:C:469:LYS:HG3	1.46	0.97
2:B:276:ASN:HD22	2:B:278:THR:HG23	1.26	0.97
1:A:251:PRO:HA	1:A:269:ARG:HG2	1.45	0.97
1:A:283:LEU:HD22	1:A:322:ARG:HD2	1.46	0.97
1:A:234:GLU:CG	4:E:2:DT:H3'	1.95	0.97
2:B:448:ARG:HD3	2:B:467:TRP:CE2	2.01	0.96
1:A:283:LEU:HD11	1:A:316:TYR:CE1	2.00	0.96
2:C:128:GLY:HA3	2:C:231:LEU:HD22	1.46	0.96
1:A:293:TYR:HB2	1:A:319:LYS:HD2	1.47	0.96
1:A:215:ASN:HD21	2:C:492:GLU:CB	1.77	0.96
2:C:448:ARG:HD3	2:C:467:TRP:CE2	2.01	0.96
1:A:209:LEU:HD22	1:A:216:PHE:HE2	1.26	0.96
1:A:196:PHE:CZ	1:A:200:VAL:HG21	2.00	0.96
2:C:93:VAL:HG12	2:C:223:ARG:CD	1.96	0.95
1:A:143:ASN:CB	2:B:313:ASN:HA	1.95	0.95
2:C:28:VAL:HB	2:C:131:TYR:CZ	2.02	0.95
1:A:19:THR:HG21	1:A:22:ILE:HD11	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:PHE:CD1	4:E:6:DA:C5	2.54	0.95
1:A:334:ILE:HG12	1:A:338:PHE:CE2	2.01	0.95
2:C:84:LYS:HA	2:C:87:GLN:HG2	1.49	0.94
2:B:93:VAL:HG12	2:B:223:ARG:CD	1.96	0.94
5:B:530:SAM:HE3	3:D:6:DA:N6	1.81	0.94
1:A:142:ALA:CA	2:B:312:ASP:HB3	1.98	0.94
2:C:322:THR:HA	2:C:325:ARG:HE	1.33	0.94
1:A:271:LEU:HD22	1:A:273:CYS:H	1.30	0.94
2:B:128:GLY:HA3	2:B:231:LEU:HD22	1.46	0.94
1:A:209:LEU:CB	1:A:216:PHE:CE2	2.50	0.94
2:B:28:VAL:HB	2:B:131:TYR:CZ	2.02	0.94
2:C:257:LEU:HD12	2:C:258:PRO:HD2	1.47	0.94
1:A:292:ARG:HH12	4:E:3:DT:C7	1.81	0.94
2:B:257:LEU:HD12	2:B:258:PRO:HD2	1.47	0.94
1:A:223:PHE:CE1	1:A:369:VAL:HG13	2.04	0.93
1:A:46:ALA:HB1	1:A:82:MET:HE1	1.50	0.93
2:B:250:LEU:HD13	2:B:277:ILE:HG12	1.50	0.93
2:C:268:PRO:HG3	5:C:530:SAM:C8	1.97	0.93
1:A:427:ARG:HB3	1:A:447:ILE:HD12	1.50	0.93
2:B:268:PRO:HG3	5:B:530:SAM:C8	1.99	0.93
2:B:350:VAL:HG12	3:D:6:DA:H4'	1.46	0.93
1:A:142:ALA:HA	2:B:312:ASP:HB3	1.50	0.93
1:A:325:LEU:HD13	1:A:329:ALA:CB	1.98	0.93
2:C:440:GLN:CG	2:C:484:VAL:HB	1.98	0.92
1:A:319:LYS:HE3	3:D:15:DT:H4'	1.49	0.92
1:A:212:LYS:HE3	1:A:223:PHE:HB2	1.49	0.92
2:B:84:LYS:HA	2:B:87:GLN:HG2	1.49	0.92
1:A:215:ASN:OD1	2:C:489:ALA:HA	1.70	0.92
1:A:212:LYS:CE	1:A:223:PHE:HB2	1.99	0.92
1:A:290:PHE:HB3	1:A:321:ILE:CG2	1.98	0.92
2:B:20:GLY:HA2	2:B:102:GLN:HG3	1.51	0.92
2:B:440:GLN:CG	2:B:484:VAL:HB	1.99	0.92
1:A:428:ALA:CB	1:A:433:LEU:HD12	1.98	0.91
2:B:149:TYR:HD1	5:B:530:SAM:HO3'	0.92	0.91
1:A:168:ILE:CD1	1:A:417:ALA:HB1	2.00	0.91
1:A:90:VAL:HG13	1:A:132:ARG:HD2	1.49	0.91
1:A:232:LEU:CG	1:A:321:ILE:HD11	2.01	0.91
2:C:71:TYR:CE2	2:C:75:LEU:HD11	2.06	0.91
2:B:71:TYR:CE2	2:B:75:LEU:HD11	2.06	0.91
4:E:12:DA:H2''	4:E:13:DC:H5''	1.53	0.90
2:C:20:GLY:HA2	2:C:102:GLN:HG3	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:250:LEU:HD13	2:C:277:ILE:HG12	1.50	0.90
1:A:112:ARG:HB2	1:A:117:ILE:HG23	1.50	0.90
1:A:168:ILE:HG23	1:A:413:ILE:CD1	2.00	0.90
1:A:71:GLN:CG	1:A:102:CYS:HB3	2.01	0.90
1:A:280:ARG:HB2	1:A:315:LEU:HD11	1.51	0.90
2:B:1:MET:CE	2:B:129:ASP:HA	2.00	0.90
1:A:248:VAL:HG11	1:A:269:ARG:CB	2.01	0.90
1:A:348:MET:SD	2:C:469:LYS:HG2	2.12	0.90
2:B:84:LYS:HA	2:B:87:GLN:CG	2.01	0.89
1:A:209:LEU:HD22	1:A:216:PHE:CE2	2.07	0.89
1:A:285:ASP:HB3	1:A:308:LYS:HG2	1.55	0.89
1:A:294:ASN:HA	3:D:14:DG:C8	2.07	0.89
2:C:439:ASP:HA	2:C:485:LEU:CD2	2.02	0.89
2:B:269:PHE:CD1	3:D:6:DA:C5	2.61	0.89
2:C:84:LYS:HA	2:C:87:GLN:CG	2.01	0.89
2:B:6:LEU:HB3	2:B:130:MET:SD	2.13	0.89
2:C:394:THR:H	2:C:397:HIS:HD2	1.20	0.89
2:B:439:ASP:HA	2:B:485:LEU:CD2	2.02	0.89
1:A:168:ILE:HG23	1:A:413:ILE:HD11	1.52	0.89
2:B:394:THR:H	2:B:397:HIS:HD2	1.20	0.89
2:B:215:LEU:HD13	2:B:245:ARG:HE	1.38	0.88
2:B:217:LEU:HD22	2:B:275:THR:HG22	1.55	0.88
1:A:300:VAL:HG13	1:A:344:ARG:HD2	1.55	0.88
1:A:75:PRO:HA	1:A:100:PHE:CD2	2.08	0.88
1:A:32:ALA:HB3	1:A:35:TYR:CD2	2.08	0.88
1:A:426:TRP:CZ2	1:A:444:LEU:HG	2.08	0.88
2:B:115:TRP:HH2	2:B:122:LYS:HE2	1.39	0.88
1:A:196:PHE:CE1	1:A:384:ARG:HD2	2.09	0.88
1:A:352:LYS:HE2	2:C:468:LEU:H	1.39	0.88
2:C:217:LEU:HD22	2:C:275:THR:HG22	1.55	0.88
2:C:217:LEU:HD22	2:C:275:THR:CG2	2.03	0.87
2:C:149:TYR:HA	5:C:530:SAM:SD	2.14	0.87
2:C:6:LEU:HB3	2:C:130:MET:SD	2.13	0.87
1:A:215:ASN:ND2	1:A:216:PHE:H	1.71	0.87
1:A:215:ASN:HD21	2:C:492:GLU:HB2	1.40	0.87
2:B:217:LEU:HD22	2:B:275:THR:CG2	2.03	0.87
2:C:115:TRP:HH2	2:C:122:LYS:HE2	1.39	0.87
1:A:292:ARG:HH12	4:E:3:DT:H72	1.39	0.87
2:B:149:TYR:HA	5:B:530:SAM:SD	2.15	0.86
1:A:415:ALA:HB2	2:B:492:GLU:HG2	1.57	0.86
2:C:220:GLY:HA2	2:C:223:ARG:NE	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3:ASN:HD22	2:C:7:VAL:HG11	1.39	0.86
2:B:440:GLN:HG2	2:B:484:VAL:HB	1.57	0.86
1:A:326:THR:HG23	1:A:327:LYS:H	1.38	0.86
2:C:283:HIS:H	2:C:294:GLN:HE22	1.24	0.86
1:A:39:ASP:HB2	1:A:62:VAL:CG2	2.06	0.86
1:A:143:ASN:HB2	2:B:313:ASN:CA	2.02	0.86
1:A:320:LEU:HD23	1:A:321:ILE:N	1.90	0.86
2:C:440:GLN:HG2	2:C:484:VAL:HB	1.56	0.86
1:A:85:GLY:HA2	4:E:14:DG:H8	1.38	0.86
3:D:12:DA:H2''	3:D:13:DC:C5'	2.06	0.86
2:C:84:LYS:HD3	2:C:87:GLN:HG2	1.58	0.86
1:A:98:LEU:HB3	1:A:99:PRO:HD2	1.56	0.86
2:C:207:GLN:HA	2:C:211:ALA:HB2	1.58	0.86
2:B:24:TYR:HB3	2:B:138:ASN:HD21	1.41	0.86
1:A:232:LEU:HD23	1:A:233:THR:N	1.91	0.85
1:A:215:ASN:ND2	1:A:216:PHE:N	2.23	0.85
1:A:215:ASN:ND2	2:C:492:GLU:HB2	1.89	0.85
1:A:280:ARG:CB	1:A:315:LEU:HD11	2.06	0.85
1:A:46:ALA:HA	1:A:107:PHE:CZ	2.11	0.85
1:A:428:ALA:HB2	1:A:443:LEU:HD21	1.57	0.85
1:A:303:CYS:SG	1:A:335:GLU:HG3	2.16	0.85
2:B:220:GLY:HA2	2:B:223:ARG:NE	1.91	0.85
1:A:49:ILE:HG13	1:A:107:PHE:HE2	1.40	0.85
2:B:222:ARG:NH1	2:B:226:LEU:HD11	1.91	0.85
1:A:433:LEU:HD13	1:A:443:LEU:HD13	1.58	0.85
1:A:6:LEU:HD23	1:A:7:PRO:N	1.90	0.85
2:C:350:VAL:HG12	4:E:6:DA:H4'	1.59	0.85
1:A:252:ILE:CG2	1:A:268:ILE:HG23	2.06	0.85
1:A:299:PHE:CE2	1:A:347:MET:HG2	2.12	0.85
2:C:215:LEU:HD13	2:C:245:ARG:HE	1.38	0.84
1:A:118:PHE:CZ	1:A:166:LYS:HE3	2.12	0.84
2:B:207:GLN:HA	2:B:211:ALA:HB2	1.58	0.84
2:C:222:ARG:NH1	2:C:226:LEU:HD11	1.91	0.84
1:A:133:ASN:HD21	2:B:430:ALA:HA	1.39	0.84
2:C:122:LYS:HD3	2:C:124:ARG:NE	1.93	0.84
2:C:24:TYR:HB3	2:C:138:ASN:HD21	1.41	0.84
2:B:115:TRP:CH2	2:B:122:LYS:HE2	2.12	0.84
2:B:84:LYS:HD3	2:B:87:GLN:HG2	1.58	0.84
1:A:235:LEU:HD23	1:A:236:ARG:N	1.92	0.84
1:A:348:MET:HB3	2:C:469:LYS:HZ2	1.43	0.84
1:A:347:MET:HE1	1:A:360:ILE:HD12	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:LEU:CD1	2:C:262:ILE:HD13	2.06	0.84
2:B:481:GLU:HB2	2:B:482:PRO:HD3	1.60	0.84
5:C:530:SAM:HE3	4:E:6:DA:H62	1.38	0.84
1:A:77:ASP:HA	1:A:95:HIS:NE2	1.91	0.84
1:A:143:ASN:HD21	3:D:5:DA:P	2.01	0.84
1:A:290:PHE:HB3	1:A:321:ILE:HG23	1.58	0.84
2:B:339:ARG:HD3	2:B:381:ARG:NH2	1.93	0.84
1:A:75:PRO:HA	1:A:100:PHE:CE2	2.12	0.83
2:B:439:ASP:HA	2:B:485:LEU:HD22	1.60	0.83
2:C:115:TRP:CH2	2:C:122:LYS:HE2	2.12	0.83
1:A:289:LEU:HD11	1:A:320:LEU:CD1	2.08	0.83
1:A:73:ILE:CG2	1:A:100:PHE:HB3	2.07	0.83
2:C:149:TYR:HD1	5:C:530:SAM:O3'	1.60	0.83
1:A:39:ASP:OD1	1:A:62:VAL:HA	1.78	0.83
2:C:38:LYS:HD3	2:C:56:TRP:CZ2	2.13	0.83
1:A:254:ARG:NH2	1:A:256:SER:HB2	1.93	0.83
1:A:196:PHE:CE2	1:A:200:VAL:HG21	2.12	0.83
1:A:236:ARG:HA	1:A:318:ASP:OD2	1.78	0.83
2:B:38:LYS:HD3	2:B:56:TRP:CZ2	2.13	0.83
1:A:348:MET:HB3	2:C:469:LYS:NZ	1.94	0.83
1:A:248:VAL:HG13	1:A:270:PHE:C	1.98	0.83
2:B:122:LYS:HD3	2:B:124:ARG:NE	1.93	0.83
2:C:439:ASP:HA	2:C:485:LEU:HD22	1.58	0.83
2:B:3:ASN:HD22	2:B:7:VAL:HG11	1.41	0.83
2:C:319:GLY:O	2:C:322:THR:HG22	1.77	0.83
1:A:315:LEU:HD23	1:A:316:TYR:N	1.93	0.83
4:E:1:DG:C8	4:E:2:DT:H72	2.14	0.83
1:A:70:SER:OG	3:D:1:DG:H2'	1.79	0.83
2:B:1:MET:HE2	2:B:132:GLU:CG	2.08	0.83
1:A:415:ALA:CB	2:B:492:GLU:CG	2.57	0.82
2:B:431:ASP:OD2	2:B:488:GLU:HB3	1.79	0.82
1:A:391:TYR:O	1:A:394:THR:HG22	1.79	0.82
1:A:253:LEU:HD11	1:A:263:VAL:HG21	1.59	0.82
2:C:442:LEU:HG	2:C:448:ARG:NH1	1.94	0.82
1:A:10:TRP:CE2	1:A:418:PHE:HA	2.15	0.82
2:B:283:HIS:H	2:B:294:GLN:HE22	1.24	0.82
1:A:142:ALA:CB	2:B:312:ASP:HB3	2.09	0.82
1:A:75:PRO:HG3	1:A:111:LEU:HD11	1.60	0.82
1:A:83:SER:HA	1:A:147:ILE:CG2	2.08	0.82
1:A:10:TRP:CH2	1:A:161:PRO:HD2	2.15	0.82
2:C:480:PRO:HG3	2:C:520:LEU:HD21	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:481:GLU:HB2	2:C:482:PRO:HD3	1.60	0.82
1:A:25:VAL:CG1	1:A:71:GLN:HA	2.10	0.82
1:A:6:LEU:HD21	1:A:10:TRP:CB	2.10	0.81
1:A:270:PHE:HD2	1:A:274:SER:HB3	1.44	0.81
1:A:10:TRP:CZ2	1:A:161:PRO:HD2	2.15	0.81
2:B:442:LEU:HG	2:B:448:ARG:NH1	1.95	0.81
2:B:372:THR:O	2:B:452:ARG:HD2	1.81	0.81
2:C:431:ASP:OD2	2:C:488:GLU:HB3	1.79	0.81
1:A:25:VAL:HG11	1:A:71:GLN:HG3	1.62	0.81
2:C:372:THR:O	2:C:452:ARG:HD2	1.80	0.81
2:B:6:LEU:HB2	2:B:117:ASN:CG	2.01	0.81
1:A:45:ARG:HA	1:A:104:PHE:CE1	2.14	0.81
1:A:46:ALA:HB1	1:A:82:MET:CE	2.09	0.81
1:A:285:ASP:CB	1:A:308:LYS:HG2	2.11	0.81
1:A:270:PHE:CE2	1:A:275:GLU:HB3	2.15	0.81
1:A:319:LYS:HD2	3:D:15:DT:OP2	1.80	0.81
1:A:42:PRO:HB3	1:A:57:THR:HG21	1.63	0.81
2:C:3:ASN:ND2	2:C:7:VAL:HG11	1.96	0.81
1:A:235:LEU:HD23	1:A:236:ARG:H	1.45	0.80
1:A:39:ASP:HB2	1:A:62:VAL:HG23	1.61	0.80
1:A:6:LEU:HD13	1:A:12:ILE:HD11	1.62	0.80
1:A:179:VAL:O	1:A:182:THR:HG22	1.81	0.80
1:A:215:ASN:HD22	1:A:216:PHE:N	1.79	0.80
1:A:223:PHE:HE1	1:A:369:VAL:HG13	1.45	0.80
2:B:91:HIS:HB3	2:B:222:ARG:NH2	1.95	0.80
1:A:225:LYS:HB2	1:A:228:PHE:CE1	2.16	0.80
1:A:283:LEU:HD22	1:A:322:ARG:CD	2.10	0.80
2:C:91:HIS:HB3	2:C:222:ARG:NH2	1.95	0.80
2:C:32:ALA:HB1	2:C:227:MET:SD	2.22	0.80
1:A:352:LYS:CG	2:C:466:SER:HB3	2.12	0.80
1:A:294:ASN:HB2	3:D:14:DG:H5"	1.62	0.80
2:B:480:PRO:HG3	2:B:520:LEU:HD21	1.62	0.80
1:A:50:GLN:HG3	4:E:14:DG:OP1	1.82	0.80
2:C:350:VAL:CG1	4:E:6:DA:H4'	2.12	0.80
1:A:352:LYS:CD	2:C:466:SER:HB3	2.10	0.80
2:C:6:LEU:HB2	2:C:117:ASN:CG	2.01	0.80
1:A:250:HIS:HE1	1:A:282:LYS:HE3	1.47	0.80
1:A:281:HIS:O	1:A:315:LEU:HG	1.79	0.80
1:A:314:LEU:HD23	1:A:315:LEU:N	1.97	0.80
1:A:296:SER:OG	1:A:300:VAL:HB	1.82	0.80
2:B:32:ALA:HB1	2:B:227:MET:SD	2.22	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:LYS:NZ	2:C:124:ARG:HG2	1.97	0.79
1:A:282:LYS:C	1:A:283:LEU:HD23	2.02	0.79
2:C:471:LYS:HD2	2:C:472:ASP:H	1.47	0.79
1:A:188:GLN:HE22	1:A:192:ILE:HG13	1.47	0.79
1:A:112:ARG:HB2	1:A:117:ILE:CG2	2.11	0.79
2:B:471:LYS:HD2	2:B:472:ASP:H	1.47	0.79
1:A:208:LYS:C	1:A:209:LEU:HD12	2.03	0.79
1:A:319:LYS:CE	3:D:15:DT:H4'	2.12	0.79
2:C:480:PRO:O	2:C:484:VAL:HG13	1.83	0.79
1:A:189:ILE:CG2	1:A:190:PRO:HD3	2.13	0.79
1:A:209:LEU:CD2	1:A:216:PHE:CE2	2.66	0.79
1:A:239:LEU:CD2	1:A:241:SER:H	1.96	0.79
1:A:248:VAL:HG11	1:A:269:ARG:HB3	1.65	0.79
1:A:131:TYR:CZ	1:A:135:ILE:HD11	2.18	0.79
1:A:160:PRO:HG2	1:A:165:GLN:CG	2.13	0.79
1:A:248:VAL:HG12	1:A:250:HIS:H	1.49	0.78
2:C:149:TYR:HD1	5:C:530:SAM:HO3'	0.79	0.78
2:C:163:LEU:HD11	2:C:262:ILE:CD1	2.11	0.78
1:A:373:PRO:HG2	1:A:378:GLN:HG2	1.65	0.78
1:A:26:THR:CG2	1:A:70:SER:HB3	2.13	0.78
2:B:480:PRO:O	2:B:484:VAL:HG13	1.83	0.78
2:B:6:LEU:HB3	2:B:130:MET:HE3	1.64	0.78
2:B:122:LYS:NZ	2:B:124:ARG:HG2	1.97	0.78
2:C:322:THR:HB	2:C:325:ARG:HH21	1.49	0.78
1:A:374:PRO:O	1:A:378:GLN:HG3	1.83	0.78
1:A:49:ILE:HD12	1:A:82:MET:HG3	1.66	0.78
2:B:394:THR:H	2:B:397:HIS:CD2	2.01	0.78
1:A:283:LEU:HD11	1:A:316:TYR:CD1	2.19	0.78
2:C:3:ASN:HB2	2:C:7:VAL:HB	1.65	0.78
1:A:164:GLU:HG3	1:A:423:THR:HA	1.65	0.78
1:A:78:ILE:HA	1:A:112:ARG:HH12	1.47	0.78
5:C:530:SAM:HE2	4:E:6:DA:N6	1.98	0.78
2:B:146:ALA:O	2:B:149:TYR:HD2	1.65	0.78
2:C:394:THR:H	2:C:397:HIS:CD2	2.01	0.78
1:A:434:ILE:O	1:A:440:ALA:HB2	1.84	0.78
1:A:294:ASN:HD21	3:D:13:DC:C2'	1.84	0.78
1:A:3:ALA:O	2:B:488:GLU:CD	2.21	0.78
1:A:3:ALA:C	2:B:488:GLU:HG3	2.03	0.78
2:B:481:GLU:O	2:B:485:LEU:HG	1.84	0.78
1:A:247:GLY:O	1:A:271:LEU:HB2	1.83	0.78
1:A:148:LYS:CG	1:A:149:PRO:HD2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD23	1:A:42:PRO:N	1.98	0.77
2:B:3:ASN:ND2	2:B:7:VAL:HG11	1.98	0.77
2:C:481:GLU:O	2:C:485:LEU:HG	1.84	0.77
2:C:200:ASP:O	2:C:204:GLN:HG3	1.85	0.77
1:A:236:ARG:HD2	4:E:2:DT:O4	1.83	0.77
1:A:289:LEU:CD1	1:A:320:LEU:HD21	2.15	0.77
2:B:268:PRO:HG3	5:B:530:SAM:H8	1.64	0.77
2:C:83:LYS:HD3	2:C:83:LYS:H	1.50	0.77
1:A:46:ALA:HA	1:A:107:PHE:CE1	2.19	0.77
1:A:35:TYR:CD1	1:A:65:ASN:HA	2.20	0.77
4:E:16:DT:H2"	4:E:17:DG:C8	2.18	0.77
2:B:384:MET:HB3	2:B:385:PRO:HD2	1.67	0.77
2:B:149:TYR:HD1	5:B:530:SAM:O3'	1.66	0.77
2:B:334:LEU:HD12	2:B:356:PHE:O	1.85	0.77
2:B:200:ASP:O	2:B:204:GLN:HG3	1.84	0.77
1:A:271:LEU:HD23	1:A:272:GLU:N	1.99	0.77
5:B:530:SAM:HE2	3:D:6:DA:H61	1.47	0.77
2:C:6:LEU:HB3	2:C:130:MET:HE3	1.66	0.77
1:A:141:GLY:HA2	2:B:464:ASP:OD2	1.85	0.77
1:A:283:LEU:CD2	1:A:322:ARG:HD2	2.15	0.77
1:A:392:ALA:O	1:A:395:ILE:HG22	1.85	0.77
2:B:83:LYS:H	2:B:83:LYS:HD3	1.50	0.77
1:A:253:LEU:HD22	1:A:320:LEU:CD1	2.15	0.77
1:A:289:LEU:CD1	1:A:320:LEU:HD11	2.12	0.77
1:A:271:LEU:CD2	1:A:273:CYS:H	1.97	0.76
1:A:10:TRP:NE1	1:A:418:PHE:HA	2.00	0.76
1:A:70:SER:CB	3:D:2:DT:H72	2.14	0.76
2:C:490:MET:O	2:C:494:VAL:HG23	1.85	0.76
1:A:46:ALA:CB	4:E:14:DG:H5'	2.15	0.76
2:C:268:PRO:HG3	5:C:530:SAM:H8	1.66	0.76
2:C:9:LYS:NZ	2:C:113:LEU:HB2	2.01	0.76
2:B:179:ALA:O	2:B:183:ILE:HD13	1.85	0.76
1:A:39:ASP:HB3	1:A:60:VAL:CG1	2.15	0.76
5:B:530:SAM:CE	3:D:6:DA:H61	1.96	0.76
1:A:426:TRP:CE2	1:A:444:LEU:HG	2.21	0.76
2:B:490:MET:O	2:B:494:VAL:HG23	1.85	0.76
1:A:232:LEU:HG	1:A:321:ILE:HD11	1.68	0.76
2:B:113:LEU:O	2:B:113:LEU:HD23	1.86	0.76
2:B:350:VAL:HG11	3:D:6:DA:C4'	2.16	0.76
2:C:512:GLU:HB2	2:C:515:LEU:CD2	2.11	0.76
2:C:20:GLY:CA	2:C:102:GLN:HG3	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:384:MET:HB3	2:C:385:PRO:HD2	1.67	0.76
1:A:10:TRP:CE2	1:A:160:PRO:HA	2.21	0.76
1:A:168:ILE:HD13	1:A:417:ALA:HB1	1.66	0.76
2:B:271:SER:O	2:B:288:LYS:HG3	1.86	0.76
2:C:271:SER:O	2:C:288:LYS:HG3	1.86	0.76
2:C:478:SER:C	2:C:479:LEU:HD12	2.05	0.76
1:A:35:TYR:HB3	1:A:65:ASN:OD1	1.85	0.76
2:C:71:TYR:HE2	2:C:95:THR:HB	1.50	0.76
1:A:270:PHE:CZ	1:A:315:LEU:HD13	2.20	0.75
1:A:25:VAL:HG12	1:A:26:THR:H	1.48	0.75
1:A:225:LYS:HB2	1:A:228:PHE:CD1	2.20	0.75
2:B:478:SER:C	2:B:479:LEU:HD12	2.05	0.75
2:B:6:LEU:HB3	2:B:130:MET:CE	2.16	0.75
1:A:427:ARG:HB3	1:A:447:ILE:CD1	2.14	0.75
1:A:352:LYS:CE	2:C:468:LEU:H	1.99	0.75
1:A:78:ILE:HD12	1:A:111:LEU:HD21	1.68	0.75
1:A:133:ASN:ND2	2:B:430:ALA:HA	2.02	0.75
2:B:222:ARG:CD	2:B:246:LEU:HB2	2.17	0.75
2:C:113:LEU:O	2:C:113:LEU:HD23	1.86	0.75
1:A:294:ASN:O	1:A:358:LYS:HD2	1.86	0.75
2:C:131:TYR:OH	2:C:224:LEU:HG	1.87	0.75
2:B:71:TYR:HE2	2:B:95:THR:HB	1.52	0.75
1:A:90:VAL:HG13	1:A:132:ARG:CD	2.16	0.75
2:C:6:LEU:HB3	2:C:130:MET:CE	2.17	0.75
2:C:471:LYS:CD	2:C:472:ASP:H	2.00	0.75
2:C:100:PRO:O	2:C:103:ILE:HG22	1.86	0.75
1:A:333:TYR:O	1:A:336:ILE:HG22	1.87	0.75
1:A:42:PRO:HB2	1:A:101:GLU:OE2	1.87	0.75
2:B:305:ARG:HD3	2:B:410:HIS:CE1	2.22	0.75
2:C:1:MET:SD	2:C:132:GLU:HB2	2.26	0.75
5:C:530:SAM:HE2	4:E:6:DA:H61	1.49	0.75
1:A:139:SER:HB2	2:B:466:SER:CB	2.16	0.75
2:B:20:GLY:CA	2:B:102:GLN:HG3	2.15	0.75
2:B:128:GLY:HA3	2:B:231:LEU:CD2	2.18	0.74
1:A:137:SER:HB3	2:B:432:SER:HB3	1.69	0.74
2:B:9:LYS:NZ	2:B:113:LEU:HB2	2.01	0.74
1:A:239:LEU:HD22	1:A:241:SER:N	1.98	0.74
2:C:305:ARG:HD3	2:C:410:HIS:CE1	2.22	0.74
1:A:253:LEU:O	1:A:317:PRO:HD2	1.87	0.74
3:D:16:DG:H2"	3:D:17:DC:C5	2.22	0.74
2:B:6:LEU:HB2	2:B:117:ASN:CB	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:HIS:HB3	2:B:222:ARG:HH21	1.51	0.74
1:A:118:PHE:HZ	1:A:166:LYS:HE3	1.52	0.74
2:C:179:ALA:O	2:C:183:ILE:HD13	1.85	0.74
1:A:148:LYS:HG3	1:A:149:PRO:HD2	1.69	0.74
2:C:334:LEU:HD12	2:C:356:PHE:O	1.86	0.74
1:A:371:LEU:HD23	1:A:371:LEU:H	1.52	0.74
1:A:19:THR:HG21	1:A:22:ILE:CD1	2.17	0.74
4:E:12:DA:H2''	4:E:13:DC:C5'	2.17	0.74
1:A:176:LEU:O	1:A:179:VAL:HG22	1.86	0.74
1:A:272:GLU:O	1:A:275:GLU:HG2	1.87	0.74
1:A:309:LEU:CD2	1:A:310:GLN:H	2.01	0.74
1:A:234:GLU:O	4:E:2:DT:OP2	2.06	0.74
1:A:49:ILE:HG23	1:A:94:ALA:HB2	1.69	0.74
2:C:222:ARG:CD	2:C:246:LEU:HB2	2.17	0.74
1:A:334:ILE:HG12	1:A:338:PHE:HE2	1.53	0.73
1:A:255:ILE:HD13	3:D:14:DG:H5'	1.69	0.73
1:A:319:LYS:HG3	3:D:15:DT:OP1	1.88	0.73
2:B:131:TYR:OH	2:B:224:LEU:HG	1.87	0.73
2:C:91:HIS:HB3	2:C:222:ARG:HH21	1.51	0.73
1:A:253:LEU:CD1	1:A:263:VAL:HG21	2.18	0.73
1:A:252:ILE:CD1	1:A:315:LEU:HD22	2.18	0.73
2:C:24:TYR:CD2	2:C:27:TYR:HE2	2.06	0.73
1:A:112:ARG:HD2	1:A:119:SER:OG	1.88	0.73
1:A:142:ALA:HB1	2:B:312:ASP:HB3	1.70	0.73
1:A:285:ASP:HB3	1:A:308:LYS:CG	2.17	0.73
1:A:133:ASN:OD1	2:B:431:ASP:HB2	1.89	0.73
1:A:250:HIS:O	1:A:269:ARG:HB3	1.88	0.73
1:A:415:ALA:CB	2:B:492:GLU:HG3	2.17	0.73
1:A:62:VAL:HG12	1:A:64:LYS:N	2.04	0.73
1:A:26:THR:CG2	1:A:69:GLU:HG2	2.18	0.73
2:B:6:LEU:HB2	2:B:117:ASN:HB2	1.70	0.73
2:B:24:TYR:CD2	2:B:27:TYR:HE2	2.06	0.73
2:B:350:VAL:CG1	3:D:6:DA:C4'	2.65	0.73
2:B:471:LYS:CD	2:B:472:ASP:H	2.00	0.73
2:B:100:PRO:O	2:B:103:ILE:HG22	1.86	0.73
1:A:123:ALA:O	1:A:126:THR:HG22	1.89	0.73
2:B:435:ASN:HD21	2:B:467:TRP:HB2	1.52	0.73
1:A:84:SER:HA	1:A:146:ASN:HD22	1.52	0.73
1:A:32:ALA:HB3	1:A:35:TYR:CE2	2.22	0.73
1:A:407:ASN:O	1:A:410:THR:HG22	1.88	0.73
1:A:175:LEU:CG	1:A:406:VAL:HG22	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HA	1:A:104:PHE:HE1	1.53	0.73
1:A:186:PHE:HD1	1:A:395:ILE:HG21	1.53	0.73
2:B:512:GLU:HB2	2:B:515:LEU:CD2	2.10	0.73
2:C:275:THR:HG21	5:C:530:SAM:N6	2.04	0.73
2:C:263:VAL:HG23	2:C:300:LEU:HD21	1.71	0.73
1:A:271:LEU:HD23	1:A:272:GLU:H	1.53	0.72
2:C:6:LEU:HB2	2:C:117:ASN:CB	2.19	0.72
1:A:154:LEU:HD23	1:A:154:LEU:O	1.89	0.72
2:B:275:THR:HG21	5:B:530:SAM:N6	2.05	0.72
2:C:128:GLY:HA3	2:C:231:LEU:CD2	2.17	0.72
2:C:220:GLY:O	2:C:224:LEU:HD13	1.89	0.72
1:A:196:PHE:CE1	1:A:200:VAL:HG21	2.23	0.72
1:A:349:ASN:HD21	2:C:467:TRP:HA	1.53	0.72
1:A:6:LEU:HD13	1:A:12:ILE:CD1	2.18	0.72
2:B:220:GLY:O	2:B:224:LEU:HD13	1.89	0.72
2:C:149:TYR:CD1	5:C:530:SAM:O3'	2.38	0.72
2:C:69:GLN:O	2:C:72:ARG:HG2	1.88	0.72
1:A:285:ASP:CG	1:A:308:LYS:HG2	2.10	0.72
2:B:433:GLU:HA	2:B:436:LYS:HB2	1.72	0.72
2:B:1:MET:HE3	2:B:132:GLU:HB2	1.70	0.72
5:B:530:SAM:HE2	3:D:6:DA:N6	2.04	0.72
2:B:263:VAL:HG23	2:B:300:LEU:HD21	1.71	0.72
1:A:231:ILE:O	1:A:323:ALA:HA	1.90	0.72
1:A:111:LEU:HD22	1:A:112:ARG:HH22	1.55	0.72
2:C:146:ALA:O	2:C:149:TYR:HD2	1.71	0.72
2:B:362:VAL:HG21	2:B:412:LEU:HD11	1.71	0.72
1:A:253:LEU:HD22	1:A:320:LEU:HD12	1.72	0.72
1:A:78:ILE:HG13	1:A:111:LEU:HD23	1.70	0.72
1:A:257:SER:HB2	1:A:266:ASN:ND2	2.05	0.71
1:A:330:LEU:HD22	1:A:333:TYR:H	1.54	0.71
1:A:339:SER:HA	1:A:344:ARG:NH2	2.05	0.71
2:B:92:ASN:CB	2:B:219:PRO:HB3	2.20	0.71
2:C:276:ASN:ND2	2:C:278:THR:HG23	2.04	0.71
1:A:331:PRO:O	1:A:334:ILE:HG22	1.90	0.71
1:A:293:TYR:CB	1:A:319:LYS:HD2	2.20	0.71
1:A:315:LEU:HD23	1:A:316:TYR:H	1.53	0.71
1:A:330:LEU:CD1	1:A:379:ALA:HA	2.20	0.71
2:C:92:ASN:CB	2:C:219:PRO:HB3	2.20	0.71
2:C:362:VAL:HG21	2:C:412:LEU:HD11	1.72	0.71
1:A:288:LEU:HD11	1:A:303:CYS:SG	2.31	0.71
1:A:137:SER:CB	2:B:432:SER:HB3	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:VAL:HG11	3:D:6:DA:H4'	1.71	0.71
2:C:90:PHE:HA	2:C:93:VAL:HG11	1.73	0.71
1:A:388:LEU:O	1:A:388:LEU:HD23	1.90	0.71
1:A:119:SER:O	1:A:122:ILE:HG22	1.91	0.71
2:C:322:THR:HA	2:C:325:ARG:NE	2.03	0.71
1:A:353:THR:HG23	2:C:351:LYS:CE	2.20	0.71
1:A:197:ARG:HD3	1:A:341:PRO:HD2	1.71	0.71
1:A:29:LYS:HE3	1:A:31:GLN:HB3	1.72	0.71
1:A:253:LEU:HB2	1:A:314:LEU:HD11	1.73	0.71
1:A:289:LEU:HD12	1:A:320:LEU:HD21	1.73	0.71
1:A:28:LYS:HG3	1:A:65:ASN:OD1	1.90	0.71
2:B:439:ASP:HA	2:B:485:LEU:HD23	1.73	0.71
2:B:399:GLN:O	2:B:402:GLU:HG2	1.90	0.71
2:C:399:GLN:HB2	2:C:400:PRO:HD3	1.72	0.71
1:A:357:GLN:OE1	1:A:358:LYS:HG2	1.91	0.71
1:A:295:GLY:HA3	1:A:358:LYS:HA	1.71	0.71
1:A:111:LEU:HD22	1:A:112:ARG:NH2	2.05	0.71
1:A:15:VAL:HG23	1:A:155:ILE:HG23	1.71	0.71
2:B:245:ARG:NH2	2:B:253:ASP:HB3	2.06	0.71
2:B:39:MET:HA	2:B:39:MET:HE2	1.73	0.71
1:A:212:LYS:HB3	1:A:215:ASN:O	1.91	0.70
1:A:319:LYS:CD	3:D:15:DT:OP2	2.39	0.70
1:A:35:TYR:HD1	1:A:65:ASN:HA	1.53	0.70
2:C:170:VAL:H	2:C:261:HIS:HD2	1.39	0.70
2:B:3:ASN:HB2	2:B:7:VAL:HB	1.73	0.70
5:B:530:SAM:HE3	3:D:6:DA:H62	1.52	0.70
2:C:6:LEU:HB2	2:C:117:ASN:HB2	1.72	0.70
1:A:270:PHE:CZ	1:A:275:GLU:HB3	2.26	0.70
1:A:319:LYS:HG3	3:D:15:DT:P	2.31	0.70
2:B:90:PHE:HA	2:B:93:VAL:HG11	1.73	0.70
2:C:5:ASP:CB	2:C:116:TYR:HE2	2.05	0.70
1:A:294:ASN:ND2	3:D:14:DG:H8	1.88	0.70
2:B:350:VAL:HG11	3:D:6:DA:C1'	2.22	0.70
1:A:232:LEU:CD2	1:A:321:ILE:HD11	2.22	0.70
1:A:78:ILE:HG22	1:A:96:GLN:HG2	1.74	0.70
2:B:6:LEU:CB	2:B:130:MET:HE3	2.20	0.70
1:A:193:LEU:HG	1:A:388:LEU:CD1	2.11	0.70
1:A:144:ILE:CG2	1:A:146:ASN:H	2.05	0.70
2:C:321:GLY:O	2:C:325:ARG:HG3	1.91	0.70
2:B:69:GLN:OE1	2:C:76:VAL:HG13	1.92	0.70
1:A:197:ARG:NE	1:A:340:SER:HA	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:TYR:CD1	1:A:319:LYS:HD3	2.26	0.70
2:C:6:LEU:CB	2:C:130:MET:HE3	2.22	0.70
2:B:399:GLN:HB2	2:B:400:PRO:HD3	1.72	0.70
2:B:5:ASP:CB	2:B:116:TYR:HE2	2.05	0.70
1:A:252:ILE:HA	1:A:315:LEU:O	1.92	0.69
2:C:245:ARG:NH2	2:C:253:ASP:HB3	2.06	0.69
2:C:399:GLN:O	2:C:402:GLU:HG2	1.90	0.69
2:B:147:GLY:HA3	2:B:346:TYR:CG	2.28	0.69
1:A:282:LYS:O	1:A:283:LEU:HD23	1.92	0.69
2:B:28:VAL:HB	2:B:131:TYR:CE1	2.27	0.69
1:A:20:THR:CG2	1:A:111:LEU:HB2	2.23	0.69
2:B:339:ARG:HD3	2:B:381:ARG:CZ	2.23	0.69
1:A:28:LYS:HD3	1:A:28:LYS:N	2.04	0.69
1:A:144:ILE:HG12	2:B:316:PHE:CZ	2.26	0.69
1:A:175:LEU:O	1:A:175:LEU:HD13	1.92	0.69
1:A:209:LEU:HB3	1:A:216:PHE:CZ	2.27	0.69
2:C:222:ARG:HD3	2:C:246:LEU:HB2	1.75	0.69
2:C:149:TYR:O	5:C:530:SAM:HB2	1.93	0.69
2:C:269:PHE:CB	4:E:6:DA:C8	2.73	0.69
1:A:345:ASN:HA	2:C:469:LYS:CE	2.22	0.69
1:A:270:PHE:CE1	1:A:315:LEU:HD13	2.28	0.69
1:A:362:GLY:O	1:A:365:ILE:HG22	1.93	0.69
2:C:257:LEU:CD1	2:C:258:PRO:HD2	2.21	0.69
1:A:352:LYS:HE3	2:C:466:SER:HB3	1.75	0.69
2:B:170:VAL:H	2:B:261:HIS:HD2	1.39	0.69
1:A:341:PRO:HA	1:A:344:ARG:HG2	1.75	0.69
2:B:146:ALA:O	2:B:149:TYR:CD2	2.45	0.69
1:A:349:ASN:HB2	2:C:431:ASP:N	2.08	0.69
1:A:70:SER:OG	3:D:1:DG:H3'	1.93	0.69
2:B:222:ARG:HD3	2:B:246:LEU:HB2	1.74	0.69
2:C:110:MET:O	2:C:113:LEU:HD22	1.93	0.69
1:A:39:ASP:CB	1:A:60:VAL:HG12	2.20	0.68
2:C:147:GLY:HA3	2:C:346:TYR:CG	2.27	0.68
1:A:250:HIS:CE1	1:A:282:LYS:HE3	2.28	0.68
1:A:14:PRO:O	1:A:17:THR:HG22	1.93	0.68
1:A:193:LEU:O	1:A:193:LEU:HD23	1.92	0.68
1:A:44:ILE:HG12	1:A:102:CYS:O	1.93	0.68
1:A:80:ILE:CD1	1:A:107:PHE:HD2	2.06	0.68
2:C:135:LEU:O	2:C:135:LEU:HD23	1.93	0.68
1:A:270:PHE:CD2	1:A:274:SER:HB3	2.27	0.68
1:A:345:ASN:HA	2:C:469:LYS:HE2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG13	1:A:107:PHE:CE2	2.27	0.68
1:A:75:PRO:CG	1:A:111:LEU:HD11	2.24	0.68
2:B:28:VAL:HG23	2:B:224:LEU:HD21	1.75	0.68
1:A:118:PHE:HZ	1:A:162:LEU:HD11	1.57	0.68
2:C:440:GLN:OE1	2:C:440:GLN:O	2.12	0.68
1:A:255:ILE:HG21	3:D:14:DG:H5'	1.76	0.68
1:A:75:PRO:HG2	1:A:111:LEU:CD2	2.21	0.68
2:B:110:MET:O	2:B:113:LEU:HD22	1.93	0.68
2:C:28:VAL:HB	2:C:131:TYR:CE1	2.27	0.68
1:A:198:GLN:O	1:A:198:GLN:OE1	2.12	0.68
2:B:135:LEU:HD23	2:B:135:LEU:O	1.93	0.68
2:C:28:VAL:HG23	2:C:224:LEU:HD21	1.75	0.68
1:A:232:LEU:HD21	1:A:321:ILE:HD11	1.76	0.68
1:A:283:LEU:HD11	1:A:316:TYR:HE1	1.55	0.68
1:A:73:ILE:HG23	1:A:100:PHE:HB3	1.75	0.68
1:A:79:VAL:HB	1:A:110:VAL:CG1	2.24	0.68
2:B:276:ASN:ND2	2:B:278:THR:HG23	2.04	0.68
1:A:236:ARG:HG2	1:A:237:ASN:N	2.09	0.67
1:A:25:VAL:O	1:A:105:GLY:HA2	1.93	0.67
1:A:292:ARG:HB3	1:A:319:LYS:O	1.93	0.67
2:B:1:MET:CE	2:B:132:GLU:HB2	2.24	0.67
1:A:35:TYR:HB3	1:A:65:ASN:CG	2.14	0.67
1:A:252:ILE:HG22	1:A:268:ILE:O	1.95	0.67
1:A:164:GLU:O	1:A:167:ILE:HG22	1.94	0.67
2:B:149:TYR:O	5:B:530:SAM:HB2	1.94	0.67
1:A:130:LEU:O	1:A:130:LEU:HD23	1.95	0.67
1:A:293:TYR:O	1:A:294:ASN:HB3	1.95	0.67
2:C:439:ASP:HA	2:C:485:LEU:HD23	1.75	0.67
2:C:269:PHE:HB3	4:E:6:DA:H5''	1.76	0.67
1:A:209:LEU:CD2	1:A:216:PHE:HE2	2.00	0.67
2:B:218:VAL:HG12	2:B:220:GLY:H	1.60	0.67
2:C:9:LYS:HZ1	2:C:113:LEU:HB2	1.60	0.67
2:C:322:THR:CB	2:C:325:ARG:HH21	2.07	0.67
1:A:292:ARG:NH1	4:E:3:DT:H72	2.09	0.67
1:A:25:VAL:HG12	1:A:26:THR:N	2.10	0.67
2:B:481:GLU:O	2:B:484:VAL:HG22	1.95	0.67
1:A:193:LEU:CG	1:A:388:LEU:HD13	2.12	0.67
2:B:380:LEU:O	2:B:384:MET:HG3	1.95	0.67
1:A:292:ARG:HH12	4:E:3:DT:H71	1.59	0.66
3:D:17:DC:H2''	3:D:18:DA:N7	2.10	0.66
2:B:440:GLN:O	2:B:440:GLN:OE1	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:22:VAL:HG22	2:C:96:THR:OG1	1.95	0.66
1:A:232:LEU:CD1	1:A:321:ILE:HD11	2.25	0.66
1:A:349:ASN:HB3	2:C:432:SER:HB3	1.76	0.66
3:D:16:DG:H2''	3:D:17:DC:C6	2.31	0.66
1:A:152:PHE:O	1:A:155:ILE:HG22	1.94	0.66
1:A:316:TYR:CD2	1:A:320:LEU:HB3	2.30	0.66
2:C:486:ALA:HB3	2:C:489:ALA:CB	2.26	0.66
1:A:25:VAL:CG1	1:A:71:GLN:HG3	2.24	0.66
2:C:486:ALA:HB1	2:C:488:GLU:OE2	1.95	0.66
1:A:77:ASP:HA	1:A:95:HIS:CE1	2.30	0.66
2:C:380:LEU:O	2:C:384:MET:HG3	1.94	0.66
2:B:486:ALA:HB1	2:B:488:GLU:OE2	1.95	0.66
2:C:39:MET:HE2	2:C:39:MET:HA	1.76	0.66
2:B:339:ARG:HA	2:B:353:ASN:HD22	1.59	0.66
1:A:204:ALA:HB3	1:A:218:PRO:HG3	1.76	0.66
1:A:248:VAL:HG12	1:A:249:GLY:N	2.11	0.66
1:A:112:ARG:CB	1:A:117:ILE:HG23	2.24	0.66
2:B:257:LEU:CD1	2:B:258:PRO:HD2	2.21	0.66
1:A:352:LYS:CE	2:C:466:SER:HB3	2.25	0.66
1:A:142:ALA:HB1	2:B:312:ASP:O	1.96	0.66
1:A:233:THR:CG2	1:A:322:ARG:HB3	2.26	0.66
1:A:28:LYS:HZ1	1:A:43:LEU:HD21	1.61	0.66
2:B:148:GLN:O	5:B:530:SAM:HE3	1.96	0.66
2:B:350:VAL:HG11	3:D:6:DA:H1'	1.78	0.66
1:A:372:LEU:HD13	1:A:373:PRO:O	1.96	0.65
2:C:481:GLU:O	2:C:484:VAL:HG22	1.95	0.65
2:C:344:ILE:HG13	2:C:345:PHE:CD1	2.31	0.65
1:A:198:GLN:OE1	1:A:198:GLN:C	2.33	0.65
1:A:289:LEU:HD21	1:A:320:LEU:HD11	1.78	0.65
1:A:345:ASN:HA	2:C:469:LYS:NZ	2.11	0.65
1:A:196:PHE:O	1:A:200:VAL:HG23	1.95	0.65
1:A:250:HIS:CD2	1:A:270:PHE:HE1	2.14	0.65
1:A:282:LYS:HE2	1:A:313:ASN:OD1	1.96	0.65
2:C:163:LEU:HG	2:C:262:ILE:HG21	1.79	0.65
2:C:6:LEU:HG	2:C:10:LEU:CD1	2.26	0.65
1:A:230:SER:OG	1:A:323:ALA:HB1	1.96	0.65
2:B:344:ILE:HG13	2:B:345:PHE:CD1	2.32	0.65
2:C:24:TYR:HB3	2:C:138:ASN:ND2	2.10	0.65
1:A:352:LYS:HG3	2:C:466:SER:HB3	1.77	0.65
1:A:305:LEU:HD23	1:A:306:LEU:N	2.11	0.65
1:A:46:ALA:HB1	4:E:14:DG:H5'	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:339:ARG:HA	2:C:353:ASN:HD22	1.62	0.65
2:B:269:PHE:CD2	2:B:311:PRO:HB3	2.31	0.65
2:B:22:VAL:HG22	2:B:96:THR:OG1	1.95	0.65
2:C:269:PHE:HB2	4:E:6:DA:N9	2.10	0.65
2:C:71:TYR:CE2	2:C:95:THR:HB	2.31	0.65
2:C:5:ASP:HB3	2:C:116:TYR:HE2	1.61	0.65
1:A:265:GLN:HG3	1:A:269:ARG:NH2	1.98	0.65
1:A:10:TRP:HE3	1:A:10:TRP:N	1.93	0.65
1:A:44:ILE:HD11	1:A:103:SER:HB2	1.79	0.65
2:C:218:VAL:HG12	2:C:220:GLY:H	1.60	0.65
1:A:410:THR:O	1:A:413:ILE:HG22	1.96	0.65
1:A:355:SER:H	2:C:312:ASP:CB	2.10	0.65
1:A:20:THR:O	1:A:21:LEU:HD23	1.97	0.65
2:B:448:ARG:HD3	2:B:467:TRP:CD2	2.32	0.65
2:B:90:PHE:C	2:B:93:VAL:HG13	2.17	0.65
1:A:39:ASP:HB2	1:A:62:VAL:HG22	1.78	0.64
1:A:61:PHE:CZ	1:A:66:LEU:HA	2.32	0.64
2:B:24:TYR:HB3	2:B:138:ASN:ND2	2.10	0.64
2:C:28:VAL:CG2	2:C:224:LEU:HD21	2.27	0.64
1:A:300:VAL:HG12	1:A:301:GLY:N	2.12	0.64
1:A:164:GLU:HG3	1:A:423:THR:CA	2.27	0.64
1:A:70:SER:OG	3:D:1:DG:C2'	2.45	0.64
2:C:90:PHE:C	2:C:93:VAL:HG13	2.17	0.64
2:B:5:ASP:HB3	2:B:116:TYR:HE2	1.61	0.64
1:A:140:ALA:HB1	2:B:351:LYS:NZ	2.13	0.64
2:C:442:LEU:HG	2:C:448:ARG:HH12	1.62	0.64
2:B:29:ASN:HD22	2:B:224:LEU:CD1	2.11	0.64
2:C:269:PHE:CE1	4:E:6:DA:C6	2.85	0.64
1:A:282:LYS:HE2	1:A:313:ASN:CG	2.18	0.64
2:B:440:GLN:C	2:B:440:GLN:OE1	2.36	0.64
1:A:261:GLY:O	1:A:263:VAL:HG13	1.98	0.64
1:A:330:LEU:HD23	1:A:332:GLU:H	1.62	0.64
2:B:106:LEU:CD2	2:B:110:MET:HE3	2.28	0.64
2:B:269:PHE:CE1	3:D:6:DA:C6	2.85	0.64
2:C:216:GLU:O	2:C:246:LEU:HD22	1.98	0.64
2:B:229:CYS:HB3	2:B:234:ILE:HB	1.80	0.64
1:A:214:ARG:HD2	1:A:369:VAL:CG1	2.28	0.64
1:A:248:VAL:HG11	1:A:269:ARG:HB2	1.79	0.64
2:B:269:PHE:CB	3:D:6:DA:C8	2.76	0.64
2:C:6:LEU:HD23	2:C:130:MET:CB	2.27	0.64
2:C:229:CYS:HB3	2:C:234:ILE:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:263:VAL:HG23	2:C:300:LEU:CD2	2.28	0.64
1:A:286:GLY:HA2	1:A:305:LEU:HD21	1.79	0.64
1:A:28:LYS:HB2	1:A:65:ASN:HD21	1.63	0.63
1:A:413:ILE:HG12	1:A:417:ALA:HB2	1.80	0.63
1:A:35:TYR:HE1	1:A:68:LYS:HD2	1.63	0.63
1:A:44:ILE:HG22	1:A:54:PHE:CZ	2.33	0.63
1:A:300:VAL:HG12	1:A:301:GLY:H	1.63	0.63
2:C:448:ARG:HD3	2:C:467:TRP:CD2	2.33	0.63
1:A:70:SER:CB	3:D:2:DT:C7	2.66	0.63
2:B:6:LEU:HD23	2:B:130:MET:CB	2.28	0.63
2:B:216:GLU:O	2:B:246:LEU:HD22	1.98	0.63
1:A:426:TRP:CE3	1:A:447:ILE:HB	2.33	0.63
2:C:29:ASN:HD22	2:C:224:LEU:CD1	2.11	0.63
1:A:232:LEU:HD12	1:A:365:ILE:HG21	1.80	0.63
1:A:265:GLN:HG2	1:A:266:ASN:N	2.13	0.63
1:A:15:VAL:O	1:A:19:THR:HG22	1.99	0.63
1:A:175:LEU:HG	1:A:406:VAL:CG2	2.24	0.63
2:B:304:GLY:O	2:B:358:THR:HG23	1.99	0.63
2:C:486:ALA:HB3	2:C:489:ALA:HB3	1.80	0.63
2:B:92:ASN:HB3	2:B:219:PRO:HB3	1.81	0.63
2:C:304:GLY:O	2:C:358:THR:HG23	1.99	0.63
1:A:253:LEU:HD23	1:A:254:ARG:O	1.99	0.63
2:B:28:VAL:CG2	2:B:224:LEU:HD21	2.28	0.63
1:A:115:LYS:O	1:A:162:LEU:HD23	1.99	0.63
2:C:440:GLN:OE1	2:C:440:GLN:C	2.36	0.63
2:B:24:TYR:HA	2:B:27:TYR:CD2	2.34	0.63
2:C:68:LEU:HD23	2:C:68:LEU:O	1.99	0.63
2:B:71:TYR:CE2	2:B:95:THR:HB	2.33	0.62
2:C:263:VAL:CG2	2:C:300:LEU:HD21	2.30	0.62
2:B:68:LEU:HD23	2:B:68:LEU:O	1.99	0.62
1:A:41:LEU:HD23	1:A:42:PRO:CD	2.28	0.62
2:C:84:LYS:HA	2:C:87:GLN:HG3	1.82	0.62
2:B:84:LYS:HA	2:B:87:GLN:HG3	1.81	0.62
1:A:188:GLN:NE2	1:A:192:ILE:HG13	2.14	0.62
2:C:146:ALA:O	2:C:149:TYR:CD2	2.52	0.62
1:A:371:LEU:CD2	1:A:371:LEU:H	2.12	0.62
1:A:9:GLY:C	1:A:10:TRP:HE3	2.02	0.62
3:D:2:DT:H2"	3:D:3:DT:H72	1.80	0.62
1:A:326:THR:HG23	1:A:327:LYS:N	2.13	0.62
1:A:232:LEU:HD11	1:A:321:ILE:HD11	1.81	0.62
1:A:299:PHE:CZ	1:A:347:MET:HE2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HA	1:A:112:ARG:NH1	2.13	0.62
2:B:263:VAL:HG23	2:B:300:LEU:CD2	2.28	0.62
2:B:83:LYS:N	2:B:83:LYS:HD3	2.14	0.62
2:C:55:ARG:NE	2:C:57:ASP:HB2	2.15	0.62
1:A:294:ASN:CB	3:D:14:DG:H5"	2.29	0.62
1:A:284:GLN:CD	1:A:322:ARG:HH22	2.03	0.62
1:A:28:LYS:NZ	1:A:43:LEU:HD21	2.15	0.62
1:A:383:ARG:O	1:A:387:GLN:HG2	2.00	0.62
1:A:131:TYR:CE2	1:A:135:ILE:HD11	2.33	0.62
2:B:149:TYR:O	5:B:530:SAM:CB	2.47	0.62
1:A:333:TYR:HA	1:A:382:VAL:HG22	1.81	0.61
1:A:125:PHE:HE1	1:A:418:PHE:HZ	1.47	0.61
2:C:24:TYR:HA	2:C:27:TYR:CD2	2.34	0.61
2:C:83:LYS:N	2:C:83:LYS:HD3	2.14	0.61
2:B:263:VAL:CG2	2:B:300:LEU:HD21	2.30	0.61
2:C:70:PHE:HE2	2:C:74:MET:HE1	1.65	0.61
1:A:214:ARG:HD2	1:A:369:VAL:HG11	1.82	0.61
1:A:12:ILE:HD12	1:A:12:ILE:N	2.15	0.61
2:C:92:ASN:HB2	2:C:219:PRO:HB3	1.82	0.61
1:A:157:ILE:O	1:A:157:ILE:HD12	1.99	0.61
2:B:322:THR:HA	2:B:325:ARG:NH2	2.16	0.61
1:A:248:VAL:HG13	1:A:270:PHE:O	2.00	0.61
1:A:274:SER:O	1:A:278:LEU:HD23	2.00	0.61
1:A:319:LYS:HE3	3:D:15:DT:C4'	2.27	0.61
2:C:92:ASN:HB3	2:C:219:PRO:HB3	1.81	0.61
2:C:38:LYS:HB2	2:C:56:TRP:CZ3	2.35	0.61
2:B:249:THR:O	2:B:254:GLY:HA3	2.01	0.61
1:A:330:LEU:HD23	1:A:331:PRO:HD2	1.81	0.61
1:A:234:GLU:CB	4:E:2:DT:H3'	2.30	0.61
1:A:35:TYR:HD1	1:A:65:ASN:CA	2.13	0.61
2:C:227:MET:O	2:C:231:LEU:HD13	2.01	0.61
1:A:186:PHE:CD1	1:A:395:ILE:HG21	2.35	0.61
1:A:85:GLY:CA	4:E:14:DG:C8	2.80	0.61
1:A:427:ARG:O	1:A:447:ILE:HD11	2.00	0.61
1:A:217:GLU:CG	1:A:218:PRO:HD2	2.30	0.61
2:B:92:ASN:HB2	2:B:219:PRO:HB3	1.82	0.61
2:C:215:LEU:CD1	2:C:245:ARG:HE	2.13	0.61
1:A:353:THR:C	2:C:351:LYS:HE2	2.21	0.61
1:A:270:PHE:HE2	1:A:275:GLU:HB3	1.63	0.61
1:A:118:PHE:CE2	1:A:162:LEU:HD22	2.35	0.61
2:B:5:ASP:HB3	2:B:116:TYR:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:339:ARG:HH22	2:C:464:ASP:HA	1.66	0.61
1:A:128:SER:O	1:A:131:TYR:HB3	2.01	0.61
2:B:486:ALA:HB3	2:B:489:ALA:CB	2.31	0.61
2:C:149:TYR:O	5:C:530:SAM:CB	2.49	0.61
2:C:71:TYR:HE2	2:C:75:LEU:HD11	1.66	0.61
2:B:38:LYS:HB2	2:B:56:TRP:CZ3	2.35	0.61
1:A:347:MET:CE	1:A:360:ILE:HD12	2.29	0.61
1:A:74:SER:OG	1:A:78:ILE:HD13	2.01	0.61
1:A:78:ILE:HD12	1:A:111:LEU:CD2	2.30	0.61
2:B:215:LEU:CD1	2:B:245:ARG:HE	2.13	0.61
1:A:209:LEU:N	1:A:209:LEU:HD12	2.16	0.61
1:A:15:VAL:HA	1:A:18:VAL:HG22	1.83	0.61
2:B:315:LEU:O	2:B:325:ARG:HD3	2.01	0.61
2:C:249:THR:O	2:C:254:GLY:HA3	2.01	0.61
2:B:55:ARG:NE	2:B:57:ASP:HB2	2.15	0.61
1:A:39:ASP:O	1:A:60:VAL:HG11	2.00	0.60
2:C:287:ASN:HB3	2:C:290:LEU:HB2	1.84	0.60
2:C:456:ARG:O	2:C:460:SER:HA	2.00	0.60
1:A:294:ASN:HB2	3:D:14:DG:C5'	2.31	0.60
2:C:93:VAL:CG1	2:C:223:ARG:HD3	2.21	0.60
2:B:35:LEU:O	2:B:39:MET:HG2	2.02	0.60
1:A:209:LEU:HG	1:A:218:PRO:HA	1.83	0.60
1:A:248:VAL:HG12	1:A:249:GLY:H	1.66	0.60
1:A:164:GLU:O	1:A:168:ILE:HG13	2.02	0.60
2:B:90:PHE:O	2:B:93:VAL:HG13	2.01	0.60
1:A:297:LEU:O	1:A:298:GLU:HG2	2.01	0.60
1:A:328:ASP:OD1	1:A:375:VAL:HG22	2.02	0.60
2:C:90:PHE:O	2:C:93:VAL:HG13	2.01	0.60
2:B:287:ASN:HB3	2:B:290:LEU:HB2	1.84	0.60
1:A:233:THR:HG22	1:A:322:ARG:HB3	1.81	0.60
2:C:106:LEU:HD23	2:C:106:LEU:O	2.01	0.60
2:B:118:GLY:HA2	2:B:123:SER:HB2	1.83	0.60
2:B:106:LEU:O	2:B:106:LEU:HD23	2.02	0.60
2:B:227:MET:O	2:B:231:LEU:HD13	2.00	0.60
1:A:101:GLU:HG2	1:A:102:CYS:H	1.65	0.60
2:C:163:LEU:HD13	2:C:163:LEU:O	2.01	0.60
1:A:160:PRO:CG	1:A:165:GLN:HG2	2.21	0.60
1:A:143:ASN:ND2	3:D:5:DA:P	2.74	0.60
1:A:236:ARG:HA	1:A:318:ASP:CG	2.22	0.60
1:A:319:LYS:HE2	3:D:16:DG:N7	2.16	0.60
1:A:25:VAL:HB	1:A:104:PHE:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:275:THR:HG21	5:C:530:SAM:HN61	1.67	0.60
1:A:83:SER:CA	1:A:147:ILE:HG22	2.24	0.60
1:A:162:LEU:HD13	1:A:162:LEU:O	2.02	0.60
2:C:244:ILE:N	2:C:244:ILE:HD12	2.17	0.60
1:A:209:LEU:HB3	1:A:216:PHE:CE2	2.33	0.59
1:A:232:LEU:HD12	1:A:365:ILE:CG2	2.32	0.59
1:A:357:GLN:CD	1:A:358:LYS:HG2	2.23	0.59
2:B:149:TYR:CD1	5:B:530:SAM:O3'	2.46	0.59
2:C:5:ASP:HB3	2:C:116:TYR:CE2	2.35	0.59
1:A:46:ALA:HA	1:A:107:PHE:HZ	1.65	0.59
2:C:90:PHE:O	2:C:93:VAL:HG22	2.03	0.59
1:A:309:LEU:HD22	1:A:310:GLN:H	1.65	0.59
2:B:90:PHE:O	2:B:93:VAL:HG22	2.03	0.59
2:C:35:LEU:O	2:C:39:MET:HG2	2.02	0.59
2:C:334:LEU:HA	2:C:357:PHE:HB3	1.84	0.59
1:A:263:VAL:O	1:A:263:VAL:HG23	2.03	0.59
1:A:280:ARG:HB3	1:A:315:LEU:HD11	1.85	0.59
2:C:489:ALA:O	2:C:493:LEU:HD23	2.02	0.59
2:B:55:ARG:HE	2:B:57:ASP:HB2	1.67	0.59
2:B:269:PHE:CD1	3:D:6:DA:C6	2.90	0.59
2:C:269:PHE:CD1	4:E:6:DA:C4	2.90	0.59
2:B:524:PHE:CE2	2:B:528:LYS:HD2	2.37	0.59
1:A:349:ASN:HB2	2:C:430:ALA:CB	2.32	0.59
1:A:70:SER:OG	3:D:1:DG:C3'	2.51	0.59
2:B:70:PHE:HE2	2:B:74:MET:HE3	1.67	0.59
1:A:353:THR:HG23	2:C:351:LYS:HE2	1.85	0.59
1:A:319:LYS:HZ1	3:D:15:DT:H4'	1.68	0.59
4:E:16:DT:H2''	4:E:17:DG:N7	2.18	0.59
1:A:32:ALA:HB3	1:A:35:TYR:HD2	1.62	0.59
2:C:269:PHE:CB	4:E:6:DA:O4'	2.50	0.59
2:C:524:PHE:CE2	2:C:528:LYS:HD2	2.37	0.59
1:A:215:ASN:HD21	2:C:492:GLU:CG	2.14	0.59
1:A:226:LEU:CD2	1:A:365:ILE:HG12	2.32	0.59
1:A:131:TYR:HE1	1:A:155:ILE:CD1	2.16	0.59
1:A:20:THR:HG23	1:A:21:LEU:N	2.17	0.59
2:C:269:PHE:CD1	4:E:6:DA:C6	2.91	0.59
2:B:290:LEU:HD13	2:B:324:ILE:HD12	1.85	0.59
1:A:6:LEU:CD2	1:A:10:TRP:HB2	2.17	0.58
1:A:412:SER:CB	2:B:495:GLN:CD	2.62	0.58
1:A:83:SER:OG	1:A:146:ASN:HB3	2.02	0.58
2:B:76:VAL:HG13	2:C:69:GLN:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLN:H	1:A:322:ARG:NH2	2.00	0.58
2:B:489:ALA:O	2:B:493:LEU:HD23	2.02	0.58
2:B:269:PHE:CE2	2:B:311:PRO:HB3	2.37	0.58
1:A:143:ASN:OD1	3:D:5:DA:OP2	2.20	0.58
1:A:144:ILE:N	2:B:316:PHE:HZ	2.00	0.58
2:B:334:LEU:HA	2:B:357:PHE:HB3	1.85	0.58
2:C:72:ARG:HG3	2:C:73:LYS:N	2.18	0.58
1:A:3:ALA:O	2:B:488:GLU:OE1	2.21	0.58
2:C:123:SER:HB3	2:C:126:ASP:CG	2.23	0.58
1:A:143:ASN:ND2	3:D:5:DA:OP1	2.36	0.58
1:A:351:VAL:HG12	1:A:352:LYS:O	2.04	0.58
2:C:6:LEU:HG	2:C:10:LEU:HD13	1.85	0.58
1:A:253:LEU:H	1:A:316:TYR:HA	1.68	0.58
1:A:49:ILE:CG1	1:A:107:PHE:HE2	2.13	0.58
1:A:186:PHE:HD1	1:A:395:ILE:CG2	2.15	0.58
1:A:312:GLN:HG2	1:A:313:ASN:N	2.19	0.58
4:E:2:DT:H2''	4:E:3:DT:H71	1.84	0.58
2:B:275:THR:HG21	5:B:530:SAM:HN61	1.68	0.58
2:C:6:LEU:O	2:C:10:LEU:HD13	2.02	0.58
2:C:494:VAL:HA	2:C:497:LEU:HD13	1.85	0.58
2:B:268:PRO:HD3	5:B:530:SAM:C5'	2.33	0.58
2:C:106:LEU:CD2	2:C:110:MET:HE2	2.33	0.58
1:A:139:SER:CB	2:B:466:SER:HB3	2.22	0.58
1:A:225:LYS:HB2	1:A:228:PHE:HE1	1.66	0.58
2:B:244:ILE:N	2:B:244:ILE:HD12	2.17	0.58
1:A:36:LEU:HD22	1:A:36:LEU:N	2.18	0.58
1:A:209:LEU:HB3	1:A:217:GLU:O	2.03	0.58
1:A:345:ASN:HD22	2:C:469:LYS:HE2	1.67	0.58
4:E:1:DG:H2'	4:E:2:DT:C7	2.34	0.58
2:B:6:LEU:HD23	2:B:130:MET:HB2	1.86	0.58
2:B:218:VAL:HG12	2:B:220:GLY:N	2.19	0.58
2:C:118:GLY:HA2	2:C:123:SER:HB2	1.83	0.58
2:B:156:ILE:O	2:B:160:ILE:HD13	2.03	0.58
2:C:268:PRO:HD3	5:C:530:SAM:C5'	2.34	0.58
2:C:55:ARG:HE	2:C:57:ASP:HB2	1.67	0.58
2:C:156:ILE:O	2:C:160:ILE:HD13	2.03	0.58
1:A:265:GLN:CG	1:A:269:ARG:HH21	2.03	0.58
1:A:231:ILE:HG22	1:A:324:ARG:HB3	1.84	0.58
1:A:345:ASN:HA	2:C:469:LYS:HZ1	1.67	0.58
1:A:348:MET:HE2	2:C:469:LYS:HA	1.85	0.58
1:A:412:SER:CA	2:B:495:GLN:HG3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:SER:HB3	2:B:126:ASP:CG	2.23	0.58
1:A:349:ASN:HB2	2:C:430:ALA:HB1	1.85	0.58
1:A:11:VAL:HG12	1:A:12:ILE:N	2.19	0.58
1:A:26:THR:HG23	1:A:69:GLU:HG2	1.84	0.58
2:C:17:LEU:HB2	2:C:27:TYR:CD1	2.39	0.58
1:A:306:LEU:N	1:A:306:LEU:HD12	2.19	0.58
1:A:279:ASN:HB3	4:E:1:DG:OP1	2.04	0.57
1:A:294:ASN:ND2	3:D:14:DG:H5''	2.18	0.57
1:A:46:ALA:HB3	4:E:14:DG:H5'	1.86	0.57
2:C:275:THR:CG2	5:C:530:SAM:N6	2.67	0.57
2:C:222:ARG:CZ	2:C:226:LEU:HD11	2.34	0.57
2:B:153:ARG:HB3	2:B:154:PRO:HD3	1.86	0.57
2:B:93:VAL:CG1	2:B:223:ARG:HD3	2.20	0.57
2:C:39:MET:HA	2:C:39:MET:CE	2.33	0.57
2:B:39:MET:CE	2:B:39:MET:HA	2.33	0.57
1:A:182:THR:HG21	1:A:399:VAL:HG22	1.85	0.57
2:B:494:VAL:HA	2:B:497:LEU:HD13	1.85	0.57
1:A:305:LEU:HD22	1:A:306:LEU:O	2.04	0.57
1:A:241:SER:O	1:A:243:PRO:HD3	2.04	0.57
1:A:293:TYR:HE2	4:E:5:DC:H41	1.52	0.57
2:B:222:ARG:CZ	2:B:226:LEU:HD11	2.34	0.57
2:C:148:GLN:O	5:C:530:SAM:CE	2.52	0.57
2:B:401:PHE:O	2:B:404:VAL:HG22	2.05	0.57
1:A:85:GLY:CA	4:E:14:DG:H8	2.15	0.57
1:A:188:GLN:HE22	1:A:192:ILE:CG1	2.16	0.57
1:A:270:PHE:HE2	1:A:275:GLU:CA	2.17	0.57
1:A:355:SER:H	2:C:312:ASP:HB3	1.69	0.57
2:C:122:LYS:HZ1	2:C:124:ARG:HG2	1.69	0.57
1:A:53:LYS:CE	1:A:97:HIS:HE1	2.17	0.57
1:A:234:GLU:OE2	4:E:3:DT:H71	2.03	0.57
1:A:274:SER:O	1:A:278:LEU:HB2	2.04	0.57
2:C:38:LYS:HB2	2:C:56:TRP:CH2	2.40	0.57
2:C:218:VAL:HG12	2:C:220:GLY:N	2.19	0.57
1:A:233:THR:HG23	1:A:316:TYR:OH	2.04	0.57
2:B:9:LYS:HZ1	2:B:113:LEU:HB2	1.68	0.57
3:D:10:DC:O2	3:D:11:DG:H1'	2.04	0.57
1:A:74:SER:O	1:A:100:PHE:HA	2.05	0.57
2:B:432:SER:O	2:B:436:LYS:HB2	2.05	0.57
2:B:106:LEU:HD21	2:B:110:MET:HE3	1.87	0.57
2:B:148:GLN:O	5:B:530:SAM:CE	2.53	0.57
2:C:28:VAL:HG23	2:C:29:ASN:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:LEU:HD13	2:C:324:ILE:HD12	1.87	0.57
1:A:86:SER:OG	1:A:90:VAL:HB	2.05	0.57
1:A:251:PRO:HG3	1:A:269:ARG:CZ	2.35	0.56
2:C:153:ARG:HB3	2:C:154:PRO:HD3	1.86	0.56
2:B:17:LEU:HB2	2:B:27:TYR:CD1	2.39	0.56
1:A:314:LEU:HD23	1:A:314:LEU:C	2.25	0.56
1:A:346:ALA:HA	2:C:431:ASP:O	2.04	0.56
1:A:222:VAL:HG12	1:A:223:PHE:N	2.18	0.56
2:C:350:VAL:CG1	4:E:6:DA:C4'	2.83	0.56
1:A:305:LEU:HD23	1:A:306:LEU:H	1.68	0.56
4:E:1:DG:H2'	4:E:2:DT:H73	1.88	0.56
1:A:45:ARG:CA	1:A:104:PHE:HE1	2.18	0.56
1:A:61:PHE:HE2	1:A:66:LEU:HB2	1.71	0.56
1:A:26:THR:HG22	1:A:70:SER:HB3	1.86	0.56
1:A:412:SER:HB2	2:B:495:GLN:NE2	2.18	0.56
2:C:34:LEU:HB3	2:C:110:MET:SD	2.44	0.56
2:C:94:SER:H	2:C:223:ARG:NH1	2.04	0.56
2:C:153:ARG:HB3	2:C:154:PRO:CD	2.36	0.56
1:A:168:ILE:HD11	1:A:417:ALA:HB1	1.86	0.56
2:B:28:VAL:HG23	2:B:29:ASN:N	2.19	0.56
2:B:34:LEU:HB3	2:B:110:MET:SD	2.44	0.56
1:A:433:LEU:HD13	1:A:443:LEU:CD1	2.34	0.56
2:C:279:ARG:HH21	2:C:281:PHE:HZ	1.54	0.56
2:B:358:THR:HG22	2:B:359:LYS:N	2.21	0.56
1:A:33:ILE:HG23	1:A:34:ASN:N	2.20	0.56
1:A:259:ARG:HD3	3:D:14:DG:OP1	2.05	0.56
1:A:274:SER:HA	1:A:278:LEU:HD23	1.87	0.56
1:A:302:VAL:HG12	1:A:303:CYS:N	2.20	0.56
2:B:248:ASN:O	2:B:253:ASP:HB2	2.06	0.56
2:C:142:THR:HG23	2:C:143:LYS:N	2.21	0.56
1:A:248:VAL:HG11	1:A:269:ARG:C	2.26	0.56
1:A:378:GLN:O	1:A:382:VAL:HG23	2.05	0.56
1:A:319:LYS:NZ	3:D:15:DT:H4'	2.20	0.56
1:A:104:PHE:CE1	1:A:107:PHE:CE1	2.94	0.56
1:A:239:LEU:HD23	1:A:240:SER:N	2.21	0.56
2:B:71:TYR:HE2	2:B:75:LEU:HD11	1.64	0.56
1:A:444:LEU:O	1:A:444:LEU:HD23	2.06	0.56
1:A:348:MET:CE	2:C:470:ASP:H	2.19	0.56
2:C:401:PHE:O	2:C:404:VAL:HG22	2.05	0.55
1:A:26:THR:HG23	1:A:69:GLU:CG	2.35	0.55
1:A:365:ILE:HG23	1:A:366:LYS:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:450:PHE:CZ	2:C:467:TRP:CZ3	2.94	0.55
2:C:440:GLN:CB	2:C:484:VAL:CG2	2.74	0.55
2:C:38:LYS:HD3	2:C:56:TRP:CE2	2.41	0.55
2:C:103:ILE:HG23	2:C:104:THR:N	2.21	0.55
1:A:205:VAL:HG23	1:A:205:VAL:O	2.06	0.55
2:B:62:ARG:HD2	2:B:70:PHE:CG	2.41	0.55
1:A:217:GLU:HG3	1:A:218:PRO:HD2	1.89	0.55
1:A:17:THR:HG23	1:A:18:VAL:N	2.21	0.55
1:A:61:PHE:CE2	1:A:66:LEU:HA	2.41	0.55
2:B:38:LYS:HD3	2:B:56:TRP:CE2	2.41	0.55
2:B:63:ILE:N	2:B:67:GLN:HB2	2.21	0.55
1:A:236:ARG:HG2	1:A:237:ASN:H	1.72	0.55
1:A:253:LEU:HD23	1:A:253:LEU:C	2.27	0.55
1:A:255:ILE:HG23	1:A:256:SER:N	2.21	0.55
1:A:291:THR:O	1:A:291:THR:HG23	2.05	0.55
2:B:153:ARG:HB3	2:B:154:PRO:CD	2.36	0.55
1:A:164:GLU:CG	1:A:423:THR:HA	2.36	0.55
2:B:275:THR:CG2	5:B:530:SAM:N6	2.68	0.55
2:C:94:SER:H	2:C:223:ARG:HH12	1.55	0.55
2:B:316:PHE:HB3	2:B:462:SER:OG	2.06	0.55
2:B:338:LEU:HD13	2:B:401:PHE:CD1	2.42	0.55
2:B:38:LYS:HB2	2:B:56:TRP:CH2	2.40	0.55
2:C:81:ASP:HB2	2:C:83:LYS:NZ	2.22	0.55
2:B:193:THR:O	2:B:194:ASN:HB2	2.06	0.55
2:B:43:THR:CG2	2:B:45:GLN:HB2	2.37	0.55
1:A:20:THR:HG22	1:A:111:LEU:O	2.07	0.55
2:B:215:LEU:HD13	2:B:245:ARG:NE	2.17	0.55
1:A:144:ILE:HG12	2:B:316:PHE:CE1	2.41	0.55
2:C:353:ASN:HD21	2:C:381:ARG:NH2	2.05	0.55
1:A:25:VAL:HG11	1:A:103:SER:O	2.07	0.55
1:A:103:SER:HG	1:A:107:PHE:CB	2.19	0.55
1:A:78:ILE:HG13	1:A:110:VAL:O	2.06	0.55
2:C:248:ASN:O	2:C:253:ASP:HB2	2.06	0.55
1:A:431:PRO:O	1:A:434:ILE:HG12	2.05	0.55
1:A:330:LEU:CD2	1:A:332:GLU:H	2.19	0.55
1:A:354:THR:OG1	2:C:312:ASP:HB3	2.07	0.55
1:A:345:ASN:HD22	2:C:469:LYS:CE	2.20	0.55
1:A:57:THR:O	1:A:57:THR:HG23	2.07	0.55
2:B:442:LEU:HG	2:B:448:ARG:HH12	1.69	0.55
1:A:144:ILE:HG23	1:A:146:ASN:H	1.72	0.55
2:B:259:LYS:HB2	2:B:301:HIS:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:390:ARG:HG3	2:C:391:THR:N	2.22	0.55
1:A:254:ARG:HG2	1:A:255:ILE:H	1.72	0.54
2:B:94:SER:H	2:B:223:ARG:NH1	2.05	0.54
2:C:222:ARG:HD3	2:C:246:LEU:CB	2.37	0.54
1:A:142:ALA:HB1	2:B:312:ASP:CB	2.36	0.54
2:C:193:THR:O	2:C:194:ASN:HB2	2.06	0.54
2:C:269:PHE:HB3	4:E:6:DA:C5'	2.37	0.54
4:E:17:DG:H2"	4:E:18:DA:N7	2.21	0.54
2:C:265:THR:HG23	2:C:267:PRO:HD3	1.89	0.54
2:B:427:THR:HG22	2:B:428:GLU:N	2.21	0.54
1:A:15:VAL:CG2	1:A:155:ILE:HG23	2.36	0.54
1:A:144:ILE:HB	2:B:316:PHE:CZ	2.42	0.54
1:A:143:ASN:CG	3:D:5:DA:OP2	2.46	0.54
2:B:103:ILE:HG23	2:B:104:THR:N	2.21	0.54
2:C:358:THR:HG22	2:C:359:LYS:N	2.21	0.54
2:C:436:LYS:HG2	2:C:437:ASN:ND2	2.22	0.54
1:A:409:LEU:C	1:A:409:LEU:HD23	2.27	0.54
1:A:289:LEU:CG	1:A:320:LEU:HD11	2.37	0.54
1:A:319:LYS:HE3	3:D:15:DT:O5'	2.07	0.54
1:A:357:GLN:HG2	1:A:358:LYS:H	1.73	0.54
1:A:7:PRO:HG2	1:A:418:PHE:O	2.07	0.54
1:A:157:ILE:C	1:A:157:ILE:HD12	2.28	0.54
1:A:251:PRO:HA	1:A:269:ARG:CG	2.30	0.54
2:C:338:LEU:HD13	2:C:401:PHE:CD1	2.41	0.54
1:A:104:PHE:CE2	1:A:106:ALA:HB3	2.43	0.54
2:B:450:PHE:CZ	2:B:467:TRP:CZ3	2.95	0.54
2:B:17:LEU:HB2	2:B:27:TYR:CE1	2.43	0.54
2:C:6:LEU:HD23	2:C:130:MET:HB2	1.89	0.54
2:B:336:THR:HG22	2:B:337:ILE:N	2.23	0.54
2:B:1:MET:HB3	2:B:129:ASP:OD1	2.08	0.54
2:B:71:TYR:CZ	2:B:75:LEU:HD21	2.43	0.54
2:C:269:PHE:CE2	2:C:311:PRO:HD3	2.43	0.54
1:A:144:ILE:CG1	2:B:316:PHE:CZ	2.91	0.54
2:C:63:ILE:N	2:C:67:GLN:HB2	2.23	0.54
2:C:43:THR:CG2	2:C:45:GLN:HB2	2.37	0.54
2:B:390:ARG:HG3	2:B:391:THR:N	2.23	0.54
2:B:230:LEU:HD13	2:B:230:LEU:C	2.28	0.54
1:A:290:PHE:CE2	1:A:360:ILE:HG21	2.43	0.54
1:A:355:SER:HB2	2:C:312:ASP:HB2	1.88	0.54
1:A:168:ILE:HG23	1:A:413:ILE:HD13	1.88	0.54
2:C:350:VAL:HG11	4:E:6:DA:C4'	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:71:TYR:CZ	2:C:75:LEU:HD21	2.43	0.54
2:C:62:ARG:HD2	2:C:70:PHE:CB	2.37	0.54
2:C:60:LYS:HE3	2:C:111:ASP:OD2	2.07	0.54
1:A:270:PHE:HE2	1:A:275:GLU:N	2.06	0.54
2:B:6:LEU:HB3	2:B:130:MET:CG	2.37	0.54
2:C:275:THR:HG21	5:C:530:SAM:C6	2.38	0.54
2:B:142:THR:HG23	2:B:143:LYS:N	2.21	0.54
1:A:345:ASN:HD21	2:C:430:ALA:HA	1.73	0.54
1:A:92:LYS:HG3	1:A:93:SER:N	2.23	0.54
2:B:94:SER:H	2:B:223:ARG:HH12	1.56	0.54
2:B:60:LYS:HE3	2:B:111:ASP:OD2	2.07	0.54
2:B:246:LEU:C	2:B:246:LEU:HD13	2.28	0.54
2:C:246:LEU:C	2:C:246:LEU:HD13	2.28	0.54
1:A:428:ALA:HB2	1:A:443:LEU:CD2	2.35	0.54
2:C:427:THR:HG22	2:C:428:GLU:N	2.21	0.54
2:B:434:GLU:OE1	2:B:465:ILE:HG23	2.08	0.54
1:A:212:LYS:HD3	1:A:217:GLU:OE1	2.08	0.53
1:A:246:SER:O	1:A:248:VAL:HG23	2.08	0.53
2:C:313:ASN:ND2	4:E:5:DC:H5"	2.22	0.53
1:A:255:ILE:HD13	3:D:14:DG:C5'	2.35	0.53
1:A:138:LEU:N	1:A:138:LEU:HD22	2.23	0.53
1:A:272:GLU:HG3	1:A:275:GLU:OE2	2.08	0.53
1:A:293:TYR:HE2	4:E:5:DC:N4	2.05	0.53
1:A:299:PHE:HE2	1:A:347:MET:HG2	1.69	0.53
2:B:222:ARG:HD3	2:B:246:LEU:CB	2.37	0.53
2:C:17:LEU:HB2	2:C:27:TYR:CE1	2.42	0.53
2:C:322:THR:CA	2:C:325:ARG:HH21	2.21	0.53
2:B:279:ARG:HH21	2:B:281:PHE:HZ	1.54	0.53
1:A:254:ARG:HG2	1:A:255:ILE:N	2.22	0.53
1:A:252:ILE:CG1	1:A:317:PRO:HD3	2.29	0.53
1:A:332:GLU:CB	1:A:382:VAL:HG11	2.39	0.53
2:C:92:ASN:HB3	2:C:219:PRO:CB	2.38	0.53
2:C:2:ASN:ND2	2:C:3:ASN:H	2.07	0.53
1:A:77:ASP:HA	1:A:95:HIS:HE2	1.72	0.53
2:C:62:ARG:HD2	2:C:70:PHE:CG	2.43	0.53
2:C:336:THR:HG22	2:C:337:ILE:N	2.23	0.53
2:C:259:LYS:HB2	2:C:301:HIS:CE1	2.43	0.53
4:E:1:DG:N9	4:E:2:DT:H72	2.23	0.53
1:A:35:TYR:O	1:A:62:VAL:HB	2.09	0.53
1:A:196:PHE:CD2	1:A:200:VAL:HG21	2.43	0.53
1:A:395:ILE:HG23	1:A:396:GLU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ALA:HA	1:A:405:ARG:HD3	1.90	0.53
1:A:293:TYR:CD1	1:A:319:LYS:CD	2.91	0.53
2:C:350:VAL:HG11	4:E:6:DA:C1'	2.38	0.53
1:A:144:ILE:HG22	1:A:146:ASN:H	1.71	0.53
2:B:81:ASP:HB2	2:B:83:LYS:NZ	2.22	0.53
1:A:223:PHE:HE1	1:A:369:VAL:CG1	2.20	0.53
1:A:332:GLU:HB3	1:A:382:VAL:HG11	1.91	0.53
2:C:481:GLU:CB	2:C:482:PRO:HD3	2.37	0.53
1:A:215:ASN:CG	2:C:492:GLU:HB2	2.28	0.53
1:A:35:TYR:OH	1:A:68:LYS:HD3	2.09	0.53
1:A:134:LYS:HA	2:B:431:ASP:O	2.08	0.53
2:B:440:GLN:HG3	2:B:484:VAL:HB	1.89	0.53
2:B:2:ASN:H	2:B:129:ASP:CG	2.11	0.53
2:B:92:ASN:HB3	2:B:219:PRO:CB	2.38	0.53
2:C:222:ARG:NE	2:C:246:LEU:HB2	2.23	0.53
2:C:344:ILE:HD11	2:C:345:PHE:CE1	2.44	0.53
1:A:143:ASN:ND2	3:D:5:DA:OP2	2.41	0.53
1:A:243:PRO:O	1:A:246:SER:HB3	2.09	0.53
1:A:370:VAL:HG22	1:A:371:LEU:N	2.24	0.53
2:B:438:THR:O	2:B:485:LEU:HA	2.08	0.53
1:A:433:LEU:CB	1:A:443:LEU:HD22	2.38	0.53
2:C:6:LEU:HB3	2:C:130:MET:CG	2.39	0.53
2:B:114:ASP:C	2:B:116:TYR:H	2.12	0.53
2:C:163:LEU:HD13	2:C:163:LEU:C	2.29	0.53
1:A:316:TYR:HD2	1:A:320:LEU:HB3	1.74	0.53
1:A:35:TYR:CE1	1:A:68:LYS:HD2	2.43	0.53
2:B:440:GLN:CB	2:B:484:VAL:CG2	2.75	0.53
2:B:222:ARG:NE	2:B:246:LEU:HB2	2.23	0.53
1:A:196:PHE:HZ	1:A:384:ARG:HD2	1.68	0.53
2:B:431:ASP:OD2	2:B:488:GLU:CB	2.56	0.53
2:B:6:LEU:HB3	2:B:130:MET:HG2	1.91	0.53
1:A:193:LEU:HD12	1:A:388:LEU:HD22	1.90	0.53
2:B:122:LYS:HZ1	2:B:124:ARG:HG2	1.73	0.53
2:C:230:LEU:C	2:C:230:LEU:HD13	2.29	0.53
2:C:232:HIS:O	2:C:233:ASP:HB2	2.09	0.53
1:A:410:THR:O	1:A:414:LEU:HG	2.09	0.52
1:A:327:LYS:HG3	1:A:328:ASP:N	2.25	0.52
2:B:305:ARG:NH1	2:B:409:PRO:HG2	2.24	0.52
2:B:232:HIS:O	2:B:233:ASP:HB2	2.09	0.52
1:A:354:THR:HG23	1:A:356:GLY:N	2.24	0.52
1:A:372:LEU:HD13	1:A:372:LEU:C	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:O	1:A:159:ILE:HG23	2.08	0.52
2:C:106:LEU:HD21	2:C:110:MET:HE2	1.91	0.52
2:C:438:THR:O	2:C:485:LEU:HA	2.09	0.52
1:A:136:SER:HB2	2:B:469:LYS:HE3	1.90	0.52
2:B:85:LEU:HD21	2:B:238:LEU:HD21	1.92	0.52
1:A:309:LEU:HD23	1:A:310:GLN:H	1.72	0.52
2:B:4:ASN:O	2:B:7:VAL:HG12	2.10	0.52
2:B:275:THR:HG21	5:B:530:SAM:C6	2.39	0.52
2:C:3:ASN:HA	2:C:130:MET:SD	2.49	0.52
2:C:62:ARG:CD	2:C:70:PHE:HB2	2.39	0.52
1:A:252:ILE:HD11	1:A:316:TYR:C	2.29	0.52
1:A:147:ILE:HG23	1:A:147:ILE:O	2.08	0.52
2:C:304:GLY:H	2:C:359:LYS:HB3	1.75	0.52
2:B:213:ILE:HG22	2:B:214:GLY:N	2.24	0.52
1:A:80:ILE:O	1:A:93:SER:HA	2.09	0.52
2:C:285:THR:HG22	2:C:286:SER:N	2.23	0.52
1:A:98:LEU:CB	1:A:99:PRO:HD2	2.32	0.52
1:A:10:TRP:CE3	1:A:10:TRP:N	2.77	0.52
1:A:10:TRP:NE1	1:A:418:PHE:CD1	2.77	0.52
1:A:158:PRO:HG2	1:A:418:PHE:CE2	2.45	0.52
2:B:344:ILE:HD11	2:B:345:PHE:CE1	2.44	0.52
1:A:84:SER:CA	1:A:146:ASN:HD22	2.22	0.52
1:A:308:LYS:HB2	1:A:312:GLN:O	2.10	0.52
1:A:348:MET:HE1	2:C:470:ASP:H	1.74	0.52
1:A:80:ILE:CG2	1:A:94:ALA:HB3	2.40	0.52
2:C:268:PRO:HD3	5:C:530:SAM:O4'	2.10	0.52
2:B:285:THR:HG22	2:B:286:SER:N	2.23	0.52
1:A:394:THR:HG23	1:A:395:ILE:N	2.24	0.52
1:A:235:LEU:HD11	1:A:315:LEU:CD2	2.40	0.52
1:A:347:MET:HE1	1:A:360:ILE:CD1	2.36	0.52
2:B:6:LEU:HD22	2:B:117:ASN:HB2	1.92	0.52
1:A:352:LYS:HD3	2:C:382:THR:HG21	1.91	0.52
1:A:55:ASP:O	1:A:98:LEU:HD12	2.10	0.52
4:E:15:DT:H3'	4:E:16:DT:C6	2.45	0.52
2:C:114:ASP:C	2:C:116:TYR:H	2.12	0.52
1:A:341:PRO:HA	1:A:344:ARG:CG	2.39	0.52
1:A:101:GLU:HG2	1:A:102:CYS:N	2.25	0.52
1:A:118:PHE:CZ	1:A:162:LEU:HD11	2.42	0.52
4:E:15:DT:H5'	4:E:16:DT:C7	2.40	0.52
2:B:376:TRP:CZ3	2:B:447:TRP:NE1	2.78	0.52
2:C:313:ASN:HB3	4:E:5:DC:OP1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:429:VAL:HG11	2:B:443:ALA:HB1	1.91	0.51
1:A:412:SER:N	2:B:495:GLN:HG3	2.24	0.51
1:A:179:VAL:HG23	1:A:180:ASP:N	2.24	0.51
2:C:305:ARG:NH1	2:C:409:PRO:HG2	2.24	0.51
2:C:339:ARG:NH2	2:C:465:ILE:H	2.08	0.51
2:B:229:CYS:SG	2:B:244:ILE:HD11	2.50	0.51
2:C:229:CYS:SG	2:C:244:ILE:HD11	2.50	0.51
1:A:78:ILE:CG1	1:A:111:LEU:HD23	2.39	0.51
1:A:39:ASP:CG	1:A:62:VAL:HA	2.29	0.51
2:B:62:ARG:HD2	2:B:70:PHE:CB	2.40	0.51
2:C:213:ILE:HG22	2:C:214:GLY:N	2.24	0.51
1:A:252:ILE:HG21	1:A:268:ILE:HG23	1.89	0.51
1:A:143:ASN:HB3	2:B:316:PHE:CE1	2.45	0.51
2:C:172:GLN:HG2	2:C:173:ASP:N	2.26	0.51
2:C:313:ASN:HA	2:C:316:PHE:CE1	2.46	0.51
1:A:28:LYS:CB	1:A:65:ASN:HD21	2.22	0.51
1:A:80:ILE:HD11	1:A:107:PHE:HB3	1.92	0.51
2:B:98:THR:HG23	2:C:94:SER:OG	2.11	0.51
1:A:293:TYR:HB2	3:D:15:DT:OP2	2.10	0.51
2:B:486:ALA:HB3	2:B:489:ALA:HB3	1.91	0.51
2:C:138:ASN:OD1	2:C:146:ALA:HB2	2.10	0.51
2:B:455:ILE:O	2:B:459:LYS:HB2	2.10	0.51
2:B:304:GLY:H	2:B:359:LYS:HB3	1.76	0.51
1:A:312:GLN:HG2	1:A:313:ASN:H	1.76	0.51
1:A:289:LEU:CD2	1:A:320:LEU:HD11	2.40	0.51
1:A:322:ARG:HG2	1:A:323:ALA:N	2.26	0.51
1:A:61:PHE:CE2	1:A:66:LEU:CA	2.94	0.51
2:B:456:ARG:O	2:B:460:SER:HA	2.10	0.51
2:C:85:LEU:HD21	2:C:238:LEU:HD21	1.91	0.51
1:A:170:GLU:O	1:A:174:THR:HG23	2.11	0.51
1:A:285:ASP:HB3	1:A:308:LYS:CB	2.40	0.51
1:A:18:VAL:O	1:A:116:LEU:HD23	2.11	0.51
1:A:96:GLN:O	1:A:96:GLN:HG3	2.09	0.51
1:A:175:LEU:C	1:A:175:LEU:HD13	2.31	0.51
1:A:118:PHE:CE2	1:A:166:LYS:HG3	2.45	0.51
1:A:270:PHE:HE2	1:A:275:GLU:CB	2.23	0.51
2:C:431:ASP:OD2	2:C:488:GLU:CB	2.57	0.51
1:A:10:TRP:NE1	1:A:160:PRO:HB3	2.26	0.51
1:A:167:ILE:HG23	1:A:168:ILE:N	2.24	0.51
1:A:41:LEU:HD21	1:A:101:GLU:HA	1.93	0.51
1:A:44:ILE:HG23	1:A:101:GLU:CD	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:ASN:OD1	2:B:146:ALA:HB2	2.10	0.51
2:B:268:PRO:HD3	5:B:530:SAM:O4'	2.10	0.51
2:C:217:LEU:O	2:C:219:PRO:HD3	2.11	0.51
2:C:287:ASN:ND2	2:C:290:LEU:H	2.08	0.51
1:A:215:ASN:OD1	2:C:489:ALA:CA	2.52	0.51
1:A:248:VAL:HG13	1:A:270:PHE:CA	2.40	0.51
1:A:131:TYR:CE2	1:A:135:ILE:CD1	2.94	0.51
1:A:135:ILE:O	1:A:138:LEU:HD23	2.11	0.51
1:A:137:SER:CB	2:B:432:SER:CB	2.88	0.51
2:B:172:GLN:HG2	2:B:173:ASP:N	2.26	0.51
2:C:283:HIS:H	2:C:294:GLN:NE2	2.02	0.51
1:A:118:PHE:HZ	1:A:162:LEU:CD1	2.24	0.51
2:B:70:PHE:CE2	2:B:74:MET:HE3	2.46	0.51
1:A:122:ILE:HG23	1:A:123:ALA:N	2.25	0.50
2:B:515:LEU:N	2:B:515:LEU:HD22	2.26	0.50
2:C:6:LEU:HB3	2:C:130:MET:HG2	1.93	0.50
2:B:243:ALA:HB3	2:B:244:ILE:HD12	1.93	0.50
2:C:376:TRP:CZ3	2:C:447:TRP:NE1	2.78	0.50
2:C:315:LEU:HD22	2:C:463:LEU:CB	2.41	0.50
2:B:24:TYR:CD2	2:B:27:TYR:CE2	2.95	0.50
2:C:322:THR:HG23	2:C:323:ASP:N	2.26	0.50
2:C:1:MET:CE	2:C:132:GLU:HG3	2.41	0.50
2:B:265:THR:HG23	2:B:267:PRO:HD3	1.92	0.50
1:A:336:ILE:HG23	1:A:337:PHE:N	2.26	0.50
1:A:7:PRO:HG2	1:A:418:PHE:CB	2.41	0.50
1:A:61:PHE:HZ	1:A:66:LEU:HA	1.76	0.50
2:B:287:ASN:ND2	2:B:290:LEU:H	2.08	0.50
2:C:305:ARG:HD3	2:C:410:HIS:ND1	2.26	0.50
1:A:104:PHE:CE2	1:A:106:ALA:CB	2.95	0.50
2:C:515:LEU:N	2:C:515:LEU:HD22	2.26	0.50
2:B:3:ASN:HA	2:B:130:MET:SD	2.52	0.50
2:C:268:PRO:HD3	5:C:530:SAM:H5'2	1.93	0.50
2:B:122:LYS:HZ2	2:B:124:ARG:HG2	1.76	0.50
2:C:63:ILE:HG13	2:C:104:THR:HG21	1.94	0.50
2:B:73:LYS:HA	2:C:72:ARG:HH12	1.76	0.50
2:C:243:ALA:HB3	2:C:244:ILE:HD12	1.94	0.50
1:A:164:GLU:HA	1:A:167:ILE:HG22	1.93	0.50
2:B:436:LYS:HG2	2:B:437:ASN:ND2	2.27	0.50
2:B:28:VAL:HB	2:B:131:TYR:OH	2.12	0.50
1:A:162:LEU:C	1:A:162:LEU:HD13	2.32	0.50
2:C:70:PHE:CE2	2:C:74:MET:HE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ALA:HB2	2:C:241:GLY:CA	2.42	0.50
1:A:49:ILE:CD1	1:A:107:PHE:CE2	2.94	0.50
2:B:3:ASN:HB2	2:B:130:MET:SD	2.52	0.50
2:C:90:PHE:HA	2:C:93:VAL:CG1	2.41	0.50
2:B:287:ASN:HD22	2:B:289:GLN:N	2.10	0.50
1:A:118:PHE:CZ	1:A:162:LEU:CD1	2.95	0.50
1:A:118:PHE:CE2	1:A:162:LEU:CD2	2.95	0.50
1:A:22:ILE:HG23	1:A:108:CYS:SG	2.51	0.50
2:B:486:ALA:HB3	2:B:489:ALA:HB2	1.93	0.50
2:B:217:LEU:O	2:B:219:PRO:HD3	2.11	0.50
2:B:220:GLY:HA2	2:B:223:ARG:CZ	2.41	0.50
2:C:29:ASN:HB2	2:C:224:LEU:HD11	1.94	0.50
2:C:322:THR:O	2:C:326:ARG:HG3	2.11	0.50
2:C:340:LEU:HD12	2:C:352:THR:OG1	2.12	0.50
2:C:26:ASN:O	2:C:30:GLU:HG2	2.12	0.50
3:D:17:DC:H2"	3:D:18:DA:C8	2.46	0.50
1:A:131:TYR:CE1	1:A:155:ILE:CD1	2.94	0.50
1:A:15:VAL:O	1:A:18:VAL:HG22	2.12	0.50
1:A:48:ASN:HB3	1:A:54:PHE:CE1	2.47	0.50
2:C:28:VAL:HB	2:C:131:TYR:OH	2.12	0.50
2:C:177:GLY:O	2:C:225:ALA:HB2	2.12	0.50
1:A:316:TYR:HE2	1:A:320:LEU:O	1.95	0.50
2:C:113:LEU:C	2:C:113:LEU:HD23	2.32	0.50
2:C:6:LEU:HD22	2:C:117:ASN:HB2	1.94	0.50
2:C:55:ARG:HG2	2:C:58:ASP:OD2	2.11	0.50
2:C:474:ILE:HG23	2:C:474:ILE:O	2.10	0.50
2:B:88:ALA:HB2	2:B:241:GLY:CA	2.42	0.50
1:A:290:PHE:HE2	1:A:360:ILE:HG21	1.77	0.49
1:A:299:PHE:CZ	1:A:347:MET:CE	2.95	0.49
1:A:44:ILE:HG22	1:A:54:PHE:CE1	2.46	0.49
2:C:280:THR:HG22	2:C:281:PHE:N	2.26	0.49
2:B:178:THR:O	2:B:179:ALA:HB3	2.12	0.49
1:A:140:ALA:HB1	2:B:351:LYS:HZ1	1.77	0.49
2:B:474:ILE:O	2:B:474:ILE:HG23	2.10	0.49
1:A:44:ILE:HG13	1:A:103:SER:OG	2.12	0.49
1:A:44:ILE:CG2	1:A:54:PHE:CZ	2.95	0.49
2:C:70:PHE:CE2	2:C:74:MET:CE	2.95	0.49
2:B:55:ARG:HG2	2:B:58:ASP:OD2	2.12	0.49
1:A:308:LYS:HE3	1:A:312:GLN:O	2.12	0.49
1:A:334:ILE:HG23	1:A:335:GLU:N	2.26	0.49
1:A:103:SER:HG	1:A:107:PHE:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:THR:HG23	1:A:411:GLN:N	2.27	0.49
1:A:7:PRO:HG2	1:A:418:PHE:HB3	1.93	0.49
2:B:29:ASN:HB2	2:B:224:LEU:HD11	1.94	0.49
2:C:350:VAL:HG11	4:E:6:DA:H1'	1.92	0.49
1:A:433:LEU:HB2	1:A:443:LEU:HD22	1.94	0.49
2:C:287:ASN:HD22	2:C:289:GLN:N	2.09	0.49
1:A:171:LYS:HE2	1:A:409:LEU:HD11	1.95	0.49
1:A:320:LEU:HD23	1:A:321:ILE:O	2.12	0.49
1:A:330:LEU:HD23	1:A:331:PRO:CD	2.41	0.49
2:B:220:GLY:CA	2:B:223:ARG:HH21	2.25	0.49
2:C:220:GLY:CA	2:C:223:ARG:HH21	2.26	0.49
2:B:280:THR:HG22	2:B:281:PHE:N	2.26	0.49
2:B:305:ARG:HD3	2:B:410:HIS:ND1	2.26	0.49
2:B:5:ASP:HB2	2:B:116:TYR:HE2	1.76	0.49
2:C:376:TRP:CZ2	2:C:415:ARG:HB2	2.47	0.49
2:B:162:LEU:HD22	2:B:405:TYR:CD2	2.47	0.49
1:A:354:THR:O	1:A:357:GLN:HB2	2.12	0.49
1:A:371:LEU:HG	1:A:373:PRO:HD3	1.93	0.49
1:A:215:ASN:ND2	2:C:492:GLU:CB	2.52	0.49
2:B:417:GLU:HA	2:B:447:TRP:HD1	1.77	0.49
2:C:417:GLU:HA	2:C:447:TRP:HD1	1.77	0.49
1:A:126:THR:HG23	1:A:127:LYS:N	2.27	0.49
1:A:161:PRO:O	1:A:165:GLN:HG3	2.12	0.49
2:B:113:LEU:C	2:B:113:LEU:HD23	2.32	0.49
2:C:28:VAL:O	2:C:131:TYR:HE1	1.96	0.49
1:A:112:ARG:NE	1:A:112:ARG:H	2.11	0.49
1:A:443:LEU:O	1:A:447:ILE:HG12	2.13	0.49
2:C:285:THR:HG22	2:C:287:ASN:N	2.07	0.49
2:C:63:ILE:HG13	2:C:104:THR:CG2	2.43	0.49
2:C:315:LEU:HD22	2:C:463:LEU:HB3	1.94	0.49
1:A:371:LEU:HD23	1:A:371:LEU:N	2.24	0.49
2:B:268:PRO:CG	5:B:530:SAM:C8	2.83	0.49
1:A:144:ILE:CB	2:B:316:PHE:HZ	2.25	0.49
2:B:26:ASN:O	2:B:30:GLU:HG2	2.12	0.49
1:A:415:ALA:O	1:A:418:PHE:HB2	2.12	0.49
1:A:49:ILE:HD12	1:A:82:MET:CG	2.38	0.49
2:B:9:LYS:HZ2	2:B:113:LEU:HB2	1.76	0.49
1:A:212:LYS:HG2	1:A:214:ARG:H	1.77	0.49
1:A:232:LEU:C	1:A:232:LEU:HD23	2.32	0.49
3:D:15:DT:H5"	3:D:16:DG:P	2.53	0.49
1:A:71:GLN:HG2	1:A:102:CYS:CB	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:ILE:HG13	2:B:345:PHE:N	2.28	0.49
2:C:6:LEU:HD23	2:C:130:MET:CG	2.42	0.49
1:A:225:LYS:HB2	1:A:228:PHE:HD1	1.75	0.49
2:B:376:TRP:CZ2	2:B:415:ARG:HB2	2.48	0.49
2:B:177:GLY:O	2:B:225:ALA:HB2	2.12	0.49
2:B:529:GLU:OXT	2:B:529:GLU:HG2	2.12	0.49
2:C:333:HIS:HD2	2:C:371:CYS:O	1.96	0.49
2:B:155:LEU:O	2:B:159:ILE:HG13	2.13	0.49
1:A:43:LEU:HB2	1:A:61:PHE:HB2	1.95	0.48
3:D:1:DG:C5	3:D:2:DT:C7	2.95	0.48
2:B:268:PRO:HD3	5:B:530:SAM:H5'2	1.94	0.48
2:C:106:LEU:HD21	2:C:110:MET:CE	2.43	0.48
2:C:178:THR:O	2:C:179:ALA:HB3	2.12	0.48
1:A:252:ILE:HD11	1:A:316:TYR:O	2.12	0.48
1:A:197:ARG:CZ	1:A:341:PRO:HD3	2.43	0.48
2:C:488:GLU:H	2:C:488:GLU:CD	2.17	0.48
1:A:32:ALA:CB	1:A:35:TYR:CE2	2.94	0.48
2:B:448:ARG:HD3	2:B:467:TRP:CZ2	2.44	0.48
2:B:283:HIS:H	2:B:294:GLN:NE2	2.02	0.48
2:C:162:LEU:HD22	2:C:405:TYR:CD2	2.48	0.48
1:A:235:LEU:HD23	1:A:236:ARG:O	2.14	0.48
1:A:248:VAL:CG1	1:A:269:ARG:HB3	2.38	0.48
1:A:89:VAL:HG21	1:A:135:ILE:HG22	1.95	0.48
1:A:22:ILE:HG12	1:A:110:VAL:HG23	1.95	0.48
2:B:219:PRO:O	2:B:223:ARG:HG3	2.14	0.48
2:C:344:ILE:HG13	2:C:345:PHE:N	2.28	0.48
2:C:6:LEU:HD23	2:C:130:MET:HG2	1.96	0.48
2:B:63:ILE:HG13	2:B:104:THR:CG2	2.43	0.48
2:C:167:PRO:O	2:C:168:ARG:HB2	2.14	0.48
2:B:488:GLU:H	2:B:488:GLU:CD	2.17	0.48
2:C:128:GLY:O	2:C:131:TYR:HB3	2.14	0.48
2:B:338:LEU:HD12	2:B:378:TYR:HB3	1.95	0.48
2:B:167:PRO:O	2:B:168:ARG:HB2	2.13	0.48
2:B:379:ASP:O	2:B:446:ARG:HD3	2.14	0.48
2:C:529:GLU:HG2	2:C:529:GLU:OXT	2.12	0.48
1:A:235:LEU:HD11	1:A:315:LEU:HD21	1.94	0.48
1:A:248:VAL:CG1	1:A:249:GLY:H	2.25	0.48
1:A:274:SER:CA	1:A:278:LEU:HD23	2.43	0.48
1:A:349:ASN:HB2	2:C:430:ALA:C	2.33	0.48
1:A:110:VAL:O	1:A:110:VAL:HG13	2.13	0.48
2:B:2:ASN:ND2	2:B:3:ASN:H	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:PHE:CB	3:D:6:DA:O4'	2.61	0.48
2:C:268:PRO:CG	5:C:530:SAM:C8	2.81	0.48
2:B:262:ILE:HG22	2:B:263:VAL:N	2.28	0.48
1:A:387:GLN:OE1	1:A:387:GLN:HA	2.13	0.48
1:A:234:GLU:CD	1:A:235:LEU:H	2.17	0.48
1:A:299:PHE:CE2	1:A:347:MET:HE2	2.48	0.48
2:B:433:GLU:CA	2:B:436:LYS:HB2	2.42	0.48
2:C:29:ASN:HD22	2:C:224:LEU:HD11	1.78	0.48
2:C:4:ASN:O	2:C:7:VAL:HG12	2.12	0.48
1:A:235:LEU:HD22	1:A:316:TYR:O	2.14	0.48
2:C:122:LYS:CE	2:C:124:ARG:HG2	2.44	0.48
4:E:15:DT:H5'	4:E:16:DT:H73	1.95	0.48
2:B:63:ILE:HG13	2:B:104:THR:HG21	1.94	0.48
1:A:281:HIS:HE1	4:E:1:DG:H3'	1.77	0.48
2:B:217:LEU:HD21	2:B:274:GLY:O	2.14	0.48
2:C:217:LEU:HD22	2:C:275:THR:HG23	1.93	0.48
1:A:142:ALA:HA	2:B:312:ASP:CB	2.35	0.48
2:C:163:LEU:HG	2:C:262:ILE:CG2	2.43	0.48
1:A:234:GLU:HB3	4:E:2:DT:O5'	2.14	0.48
1:A:333:TYR:HB2	1:A:382:VAL:CG2	2.44	0.48
2:C:220:GLY:HA2	2:C:223:ARG:CZ	2.41	0.48
2:C:346:TYR:CD1	2:C:347:ALA:N	2.82	0.48
2:B:153:ARG:N	2:B:154:PRO:HD2	2.29	0.48
1:A:270:PHE:HD2	1:A:274:SER:CB	2.22	0.48
1:A:278:LEU:N	1:A:278:LEU:HD22	2.29	0.48
2:C:486:ALA:HB3	2:C:489:ALA:HB2	1.95	0.48
1:A:413:ILE:CG1	1:A:417:ALA:HB2	2.42	0.48
1:A:41:LEU:HD22	1:A:42:PRO:O	2.13	0.48
1:A:39:ASP:OD1	1:A:63:PRO:HD3	2.13	0.48
2:B:90:PHE:HA	2:B:93:VAL:CG1	2.41	0.48
2:C:219:PRO:O	2:C:223:ARG:HG3	2.13	0.48
2:C:6:LEU:HG	2:C:10:LEU:HD11	1.96	0.48
2:B:346:TYR:CD1	2:B:347:ALA:N	2.82	0.48
1:A:253:LEU:HD11	1:A:263:VAL:CG2	2.38	0.47
1:A:280:ARG:HB3	1:A:315:LEU:HD21	1.96	0.47
1:A:316:TYR:HB2	1:A:317:PRO:HD2	1.95	0.47
2:C:338:LEU:HD12	2:C:378:TYR:HB3	1.95	0.47
2:C:207:GLN:HA	2:C:211:ALA:CB	2.39	0.47
2:B:63:ILE:CA	2:B:67:GLN:HB2	2.44	0.47
1:A:8:GLU:OE2	1:A:464:SER:HB3	2.14	0.47
1:A:270:PHE:CZ	1:A:315:LEU:CD1	2.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LYS:HG3	3:D:14:DG:O6	2.14	0.47
1:A:62:VAL:CG1	1:A:63:PRO:N	2.77	0.47
2:B:28:VAL:O	2:B:131:TYR:HE1	1.97	0.47
1:A:148:LYS:HG2	1:A:149:PRO:HD2	1.92	0.47
2:C:339:ARG:HH21	2:C:465:ILE:H	1.62	0.47
2:B:160:ILE:N	2:B:160:ILE:HD12	2.29	0.47
2:C:153:ARG:N	2:C:154:PRO:HD2	2.29	0.47
2:B:195:ASP:O	2:B:196:LEU:HB2	2.14	0.47
1:A:250:HIS:CD2	1:A:270:PHE:CE1	2.99	0.47
1:A:270:PHE:HB3	1:A:280:ARG:NH1	2.29	0.47
2:B:94:SER:OG	2:C:98:THR:HG23	2.13	0.47
2:B:39:MET:SD	2:B:115:TRP:CH2	3.07	0.47
1:A:409:LEU:HD23	1:A:409:LEU:O	2.13	0.47
2:B:230:LEU:HD13	2:B:230:LEU:O	2.14	0.47
2:B:333:HIS:HD2	2:B:371:CYS:O	1.96	0.47
1:A:330:LEU:HD21	1:A:332:GLU:HB2	1.96	0.47
1:A:236:ARG:HB2	4:E:2:DT:C7	2.45	0.47
2:B:435:ASN:ND2	2:B:467:TRP:HB2	2.25	0.47
3:D:18:DA:C6	3:D:19:DA:C6	3.03	0.47
1:A:39:ASP:OD2	1:A:60:VAL:HG12	2.14	0.47
2:B:93:VAL:HG23	2:B:93:VAL:O	2.15	0.47
2:C:24:TYR:CD2	2:C:27:TYR:CE2	2.95	0.47
2:C:6:LEU:CG	2:C:130:MET:HG2	2.45	0.47
1:A:308:LYS:HG3	1:A:309:LEU:O	2.13	0.47
2:C:440:GLN:HG3	2:C:484:VAL:HB	1.88	0.47
1:A:62:VAL:HG12	1:A:63:PRO:N	2.29	0.47
1:A:62:VAL:HG13	1:A:63:PRO:HD2	1.94	0.47
2:C:269:PHE:HB2	4:E:6:DA:O4'	2.13	0.47
2:B:118:GLY:HA2	2:B:123:SER:CB	2.45	0.47
1:A:225:LYS:HB2	1:A:227:ASN:HD21	1.80	0.47
2:B:305:ARG:HH11	2:B:410:HIS:CD2	2.32	0.47
2:C:230:LEU:O	2:C:230:LEU:HD13	2.14	0.47
1:A:232:LEU:HD13	1:A:366:LYS:HE3	1.97	0.47
3:D:15:DT:H5''	3:D:16:DG:OP2	2.14	0.47
1:A:265:GLN:HG2	1:A:266:ASN:H	1.79	0.47
2:C:438:THR:HG23	2:C:442:LEU:HD23	1.97	0.47
1:A:10:TRP:HE1	1:A:160:PRO:HB3	1.79	0.47
1:A:103:SER:OG	1:A:107:PHE:HB2	2.13	0.47
1:A:10:TRP:CD2	1:A:418:PHE:O	2.67	0.47
2:B:1:MET:HE2	2:B:132:GLU:CB	2.44	0.47
2:B:6:LEU:CG	2:B:130:MET:HG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:PHE:CD1	2:B:269:PHE:N	2.83	0.47
2:B:128:GLY:CA	2:B:231:LEU:HD22	2.33	0.47
2:C:245:ARG:HG2	2:C:246:LEU:N	2.30	0.47
2:C:39:MET:SD	2:C:115:TRP:CH2	3.07	0.47
1:A:353:THR:O	1:A:353:THR:HG23	2.14	0.47
2:B:43:THR:HG22	2:B:45:GLN:HB2	1.97	0.47
1:A:145:ASN:ND2	1:A:145:ASN:H	2.13	0.47
2:C:209:HIS:O	2:C:236:GLY:HA2	2.14	0.47
2:C:379:ASP:O	2:C:446:ARG:HD3	2.15	0.47
2:C:195:ASP:O	2:C:196:LEU:HB2	2.15	0.47
1:A:223:PHE:O	1:A:224:LYS:HG3	2.15	0.47
1:A:250:HIS:HD2	1:A:251:PRO:O	1.98	0.47
1:A:186:PHE:CD1	1:A:395:ILE:CG2	2.95	0.47
1:A:215:ASN:HD21	2:C:492:GLU:HG3	1.79	0.47
1:A:235:LEU:HD13	1:A:316:TYR:O	2.14	0.47
1:A:239:LEU:HD23	1:A:240:SER:H	1.79	0.47
2:B:440:GLN:HB2	2:B:484:VAL:CB	2.44	0.47
2:B:106:LEU:HD21	2:B:110:MET:CE	2.43	0.47
2:C:275:THR:CG2	5:C:530:SAM:HN61	2.28	0.47
2:C:155:LEU:O	2:C:159:ILE:HG13	2.14	0.47
1:A:235:LEU:O	1:A:318:ASP:HA	2.15	0.47
1:A:252:ILE:O	1:A:252:ILE:HG23	2.15	0.47
2:C:313:ASN:HA	2:C:316:PHE:CZ	2.49	0.47
2:C:377:VAL:HB	2:C:467:TRP:HH2	1.78	0.47
2:B:25:GLN:HA	2:B:138:ASN:OD1	2.15	0.47
1:A:144:ILE:CB	2:B:316:PHE:CZ	2.97	0.47
1:A:352:LYS:HE2	2:C:468:LEU:N	2.18	0.47
2:B:70:PHE:CE2	2:B:74:MET:CE	2.97	0.47
2:B:62:ARG:CD	2:B:70:PHE:HB2	2.45	0.47
2:B:209:HIS:O	2:B:236:GLY:HA2	2.14	0.47
1:A:355:SER:H	2:C:312:ASP:HB2	1.80	0.46
1:A:39:ASP:CB	1:A:62:VAL:HG22	2.44	0.46
2:B:450:PHE:HZ	2:B:467:TRP:CZ3	2.31	0.46
2:B:439:ASP:CA	2:B:485:LEU:HD22	2.39	0.46
2:C:217:LEU:HD21	2:C:274:GLY:O	2.14	0.46
2:C:93:VAL:HG23	2:C:93:VAL:O	2.14	0.46
1:A:98:LEU:HB3	1:A:99:PRO:CD	2.37	0.46
2:C:271:SER:O	2:C:272:ALA:HB3	2.16	0.46
2:C:455:ILE:O	2:C:459:LYS:HB2	2.15	0.46
2:C:43:THR:HG22	2:C:45:GLN:HB2	1.97	0.46
1:A:80:ILE:HD11	1:A:107:PHE:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:HE2	1:A:66:LEU:CB	2.28	0.46
2:B:245:ARG:HG2	2:B:246:LEU:N	2.30	0.46
2:C:22:VAL:HG12	2:C:23:SER:O	2.15	0.46
1:A:144:ILE:HG23	1:A:146:ASN:N	2.31	0.46
2:B:122:LYS:CE	2:B:124:ARG:HG2	2.44	0.46
2:B:201:GLY:HA2	2:B:204:GLN:OE1	2.15	0.46
2:B:524:PHE:HE2	2:B:528:LYS:HD2	1.81	0.46
1:A:145:ASN:HD22	1:A:145:ASN:H	1.62	0.46
1:A:234:GLU:HG3	4:E:2:DT:C2'	2.43	0.46
1:A:313:ASN:HD22	1:A:313:ASN:C	2.19	0.46
1:A:46:ALA:CA	1:A:107:PHE:CE1	2.95	0.46
2:C:3:ASN:HB2	2:C:130:MET:SD	2.55	0.46
2:C:201:GLY:HA2	2:C:204:GLN:OE1	2.15	0.46
2:C:296:ILE:HD13	2:C:308:VAL:HG21	1.96	0.46
1:A:357:GLN:HG2	1:A:358:LYS:N	2.28	0.46
1:A:117:ILE:HD13	1:A:159:ILE:CD1	2.45	0.46
2:B:459:LYS:O	2:B:460:SER:HB2	2.16	0.46
1:A:271:LEU:O	1:A:274:SER:HB3	2.15	0.46
2:C:378:TYR:HE1	2:C:419:GLU:HG2	1.81	0.46
1:A:164:GLU:OE2	1:A:422:LEU:HB2	2.16	0.46
1:A:89:VAL:CG2	1:A:135:ILE:CG2	2.93	0.46
2:C:148:GLN:O	5:C:530:SAM:HE3	2.14	0.46
1:A:444:LEU:C	1:A:444:LEU:HD23	2.36	0.46
1:A:255:ILE:O	1:A:258:VAL:HB	2.16	0.46
1:A:290:PHE:CD2	1:A:291:THR:N	2.83	0.46
1:A:349:ASN:CB	2:C:430:ALA:CB	2.94	0.46
2:B:231:LEU:HD12	2:B:231:LEU:N	2.30	0.46
2:B:22:VAL:HG12	2:B:23:SER:O	2.15	0.46
2:B:459:LYS:HB3	2:B:462:SER:H	1.80	0.46
2:B:408:ASP:OD2	2:B:410:HIS:HB2	2.16	0.46
2:C:305:ARG:HH11	2:C:410:HIS:CD2	2.32	0.46
1:A:355:SER:HB3	2:C:316:PHE:CZ	2.50	0.46
1:A:6:LEU:HD23	1:A:7:PRO:CD	2.44	0.46
2:B:29:ASN:HD22	2:B:224:LEU:HD11	1.78	0.46
2:C:215:LEU:HD13	2:C:245:ARG:NE	2.17	0.46
2:C:25:GLN:HA	2:C:138:ASN:OD1	2.15	0.46
2:C:75:LEU:HB3	2:C:93:VAL:HG23	1.97	0.46
1:A:196:PHE:CE1	1:A:200:VAL:CG2	2.95	0.46
2:C:322:THR:HB	2:C:325:ARG:NH2	2.25	0.46
1:A:53:LYS:HE2	1:A:97:HIS:CE1	2.51	0.46
2:C:228:ASN:O	2:C:232:HIS:HD2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LYS:HA	1:A:243:PRO:HD2	1.82	0.46
1:A:252:ILE:HG22	1:A:269:ARG:HA	1.96	0.46
1:A:197:ARG:HE	1:A:340:SER:HA	1.80	0.46
2:C:231:LEU:N	2:C:231:LEU:HD12	2.30	0.46
2:C:344:ILE:HD11	2:C:345:PHE:HE1	1.81	0.46
2:B:287:ASN:HD21	2:B:289:GLN:HB2	1.81	0.46
1:A:182:THR:HG23	1:A:183:LYS:N	2.29	0.46
2:C:85:LEU:CD2	2:C:238:LEU:CD2	2.94	0.46
1:A:27:TYR:CE1	1:A:28:LYS:HE2	2.51	0.46
2:B:431:ASP:O	2:B:432:SER:HB3	2.15	0.46
3:D:1:DG:C4	3:D:2:DT:H71	2.51	0.46
2:B:269:PHE:CD1	3:D:6:DA:C4	3.02	0.46
2:C:118:GLY:HA2	2:C:123:SER:CB	2.45	0.46
1:A:225:LYS:HD2	1:A:228:PHE:HE1	1.81	0.46
4:E:16:DT:C2	4:E:17:DG:C6	3.04	0.46
2:C:160:ILE:HD12	2:C:160:ILE:N	2.29	0.46
2:C:222:ARG:O	2:C:226:LEU:HG	2.16	0.46
2:C:148:GLN:O	5:C:530:SAM:HE1	2.15	0.46
2:B:296:ILE:HD13	2:B:308:VAL:HG21	1.98	0.46
1:A:252:ILE:HD13	1:A:315:LEU:HD22	1.96	0.45
2:C:430:ALA:HB1	2:C:469:LYS:HZ3	1.81	0.45
2:B:3:ASN:HD22	2:B:7:VAL:CG1	2.22	0.45
1:A:325:LEU:CD1	1:A:329:ALA:HB3	2.24	0.45
1:A:175:LEU:CD1	1:A:406:VAL:HG21	2.46	0.45
2:B:271:SER:O	2:B:272:ALA:HB3	2.15	0.45
2:C:1:MET:HE1	2:C:132:GLU:HG3	1.97	0.45
1:A:355:SER:N	2:C:312:ASP:HB2	2.31	0.45
2:C:482:PRO:HA	2:C:485:LEU:HG	1.99	0.45
1:A:44:ILE:HD11	1:A:103:SER:CB	2.45	0.45
2:B:275:THR:CG2	5:B:530:SAM:HN61	2.29	0.45
2:C:29:ASN:HD22	2:C:224:LEU:HD12	1.80	0.45
2:C:130:MET:HE2	2:C:130:MET:HB2	1.80	0.45
2:C:6:LEU:CD2	2:C:130:MET:HE3	2.46	0.45
1:A:227:ASN:HD22	1:A:227:ASN:H	1.63	0.45
2:C:63:ILE:CA	2:C:67:GLN:HB2	2.45	0.45
2:C:305:ARG:HH12	2:C:409:PRO:HG2	1.82	0.45
2:B:62:ARG:CD	2:B:70:PHE:CB	2.95	0.45
2:B:73:LYS:HA	2:C:72:ARG:NH1	2.30	0.45
2:C:341:PRO:HA	2:C:381:ARG:HG3	1.99	0.45
2:C:85:LEU:CD2	2:C:238:LEU:HD22	2.46	0.45
1:A:215:ASN:ND2	2:C:492:GLU:HG3	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TYR:HE1	1:A:155:ILE:HD12	1.80	0.45
1:A:79:VAL:HG12	1:A:80:ILE:N	2.31	0.45
2:B:481:GLU:CB	2:B:482:PRO:HD3	2.37	0.45
2:B:75:LEU:HB3	2:B:93:VAL:HG23	1.97	0.45
1:A:427:ARG:CB	1:A:447:ILE:HD12	2.36	0.45
2:C:408:ASP:OD2	2:C:410:HIS:HB2	2.16	0.45
2:C:5:ASP:HB2	2:C:116:TYR:HE2	1.76	0.45
2:B:430:ALA:HB3	2:B:467:TRP:O	2.16	0.45
1:A:70:SER:O	3:D:1:DG:P	2.75	0.45
2:B:17:LEU:HB3	2:B:22:VAL:HB	1.99	0.45
2:C:106:LEU:CD2	2:C:110:MET:CE	2.95	0.45
1:A:118:PHE:CZ	1:A:166:LYS:HG3	2.51	0.45
2:C:524:PHE:HE2	2:C:528:LYS:HD2	1.80	0.45
2:B:228:ASN:O	2:B:232:HIS:HD2	1.99	0.45
2:B:186:ASP:HA	2:B:212:PHE:CZ	2.51	0.45
1:A:248:VAL:HG13	1:A:270:PHE:N	2.32	0.45
2:B:32:ALA:HB2	2:B:131:TYR:CE1	2.52	0.45
2:B:275:THR:HG21	5:B:530:SAM:C5	2.47	0.45
1:A:175:LEU:CD1	1:A:406:VAL:CG2	2.94	0.45
1:A:434:ILE:HG13	1:A:435:SER:N	2.32	0.45
2:C:186:ASP:HA	2:C:212:PHE:CZ	2.51	0.45
1:A:253:LEU:C	1:A:317:PRO:HD2	2.37	0.45
1:A:293:TYR:CE2	4:E:5:DC:N4	2.84	0.45
1:A:10:TRP:NE1	1:A:160:PRO:HA	2.31	0.45
1:A:18:VAL:O	1:A:113:PRO:HG2	2.17	0.45
1:A:19:THR:O	1:A:19:THR:HG23	2.15	0.45
1:A:26:THR:HG21	1:A:70:SER:HB3	1.95	0.45
2:B:222:ARG:O	2:B:226:LEU:HG	2.16	0.45
2:C:128:GLY:CA	2:C:231:LEU:HD22	2.33	0.45
2:C:122:LYS:HD3	2:C:124:ARG:CG	2.47	0.45
2:B:85:LEU:CD2	2:B:238:LEU:CD2	2.94	0.45
2:B:85:LEU:CD2	2:B:238:LEU:HD22	2.47	0.45
1:A:214:ARG:HD2	1:A:369:VAL:HG12	1.97	0.45
1:A:349:ASN:HB3	2:C:431:ASP:C	2.37	0.45
1:A:81:ALA:HA	1:A:92:LYS:O	2.17	0.45
2:B:345:PHE:CD2	3:D:6:DA:C2	3.05	0.45
2:C:28:VAL:CG2	2:C:224:LEU:CD2	2.95	0.45
2:B:420:TRP:HB2	2:B:425:GLU:OE1	2.17	0.45
1:A:314:LEU:HD23	1:A:315:LEU:CA	2.46	0.45
1:A:236:ARG:HB2	4:E:2:DT:H71	1.99	0.45
1:A:10:TRP:NE1	1:A:160:PRO:CA	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PRO:O	1:A:66:LEU:HB3	2.17	0.45
2:B:429:VAL:HG12	2:B:430:ALA:N	2.31	0.45
2:C:269:PHE:N	2:C:269:PHE:CD1	2.83	0.45
2:C:275:THR:HG21	5:C:530:SAM:C5	2.47	0.45
2:C:287:ASN:HD21	2:C:289:GLN:HB2	1.81	0.45
1:A:352:LYS:HD3	2:C:382:THR:CG2	2.46	0.45
1:A:293:TYR:O	1:A:294:ASN:CB	2.64	0.45
1:A:355:SER:CB	2:C:312:ASP:HB2	2.47	0.45
2:C:448:ARG:HD3	2:C:467:TRP:NE1	2.30	0.45
2:B:85:LEU:HD23	2:B:238:LEU:HD22	1.98	0.45
2:C:85:LEU:HD23	2:C:238:LEU:HD22	1.99	0.45
2:B:164:LYS:HE3	2:B:407:GLU:O	2.17	0.45
1:A:212:LYS:HG2	1:A:213:TRP:N	2.32	0.45
1:A:292:ARG:HD3	1:A:293:TYR:HE1	1.82	0.45
1:A:10:TRP:CH2	1:A:164:GLU:OE1	2.70	0.45
2:B:28:VAL:CG2	2:B:224:LEU:CD2	2.95	0.45
2:B:29:ASN:HD22	2:B:224:LEU:HD12	1.80	0.45
2:C:115:TRP:CH2	2:C:122:LYS:CE	2.94	0.45
2:B:170:VAL:H	2:B:261:HIS:CD2	2.26	0.45
1:A:248:VAL:HG12	1:A:250:HIS:N	2.26	0.44
1:A:331:PRO:HG2	1:A:332:GLU:OE1	2.17	0.44
2:C:338:LEU:HD13	2:C:401:PHE:CE1	2.52	0.44
2:C:430:ALA:HB1	2:C:469:LYS:NZ	2.32	0.44
1:A:294:ASN:CG	3:D:14:DG:H5"	2.38	0.44
2:B:17:LEU:HD21	2:B:106:LEU:CD1	2.48	0.44
2:C:17:LEU:HD21	2:C:106:LEU:CD1	2.47	0.44
2:C:32:ALA:HB2	2:C:131:TYR:CE1	2.51	0.44
2:C:39:MET:CA	2:C:39:MET:CE	2.95	0.44
2:B:122:LYS:HD3	2:B:124:ARG:CG	2.47	0.44
2:B:250:LEU:HA	2:B:279:ARG:NH2	2.33	0.44
1:A:55:ASP:OD1	1:A:98:LEU:HG	2.17	0.44
2:C:334:LEU:HA	2:C:357:PHE:CB	2.46	0.44
2:C:459:LYS:O	2:C:460:SER:HB2	2.17	0.44
1:A:254:ARG:HG2	1:A:255:ILE:HG22	1.98	0.44
1:A:290:PHE:HB3	1:A:321:ILE:HG22	1.92	0.44
1:A:330:LEU:CD2	1:A:332:GLU:HB2	2.47	0.44
1:A:360:ILE:O	1:A:360:ILE:HG23	2.17	0.44
1:A:215:ASN:ND2	2:C:492:GLU:CG	2.79	0.44
1:A:15:VAL:CA	1:A:18:VAL:HG22	2.46	0.44
2:B:3:ASN:CB	2:B:130:MET:SD	3.06	0.44
2:B:344:ILE:HD11	2:B:345:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:THR:HG21	2:B:45:GLN:HB2	2.00	0.44
2:C:420:TRP:HB2	2:C:425:GLU:OE1	2.17	0.44
1:A:416:LYS:O	1:A:422:LEU:HG	2.16	0.44
3:D:1:DG:C5	3:D:2:DT:H73	2.52	0.44
2:B:106:LEU:CD2	2:B:110:MET:CE	2.95	0.44
2:C:149:TYR:CD1	5:C:530:SAM:C3'	2.99	0.44
4:E:18:DA:C6	4:E:19:DA:C6	3.06	0.44
2:C:451:SER:O	2:C:455:ILE:HG13	2.17	0.44
1:A:42:PRO:HB3	1:A:57:THR:CG2	2.42	0.44
2:C:17:LEU:HD22	2:C:22:VAL:HG21	2.00	0.44
2:B:277:ILE:HD13	2:B:291:CYS:SG	2.57	0.44
1:A:352:LYS:HB2	2:C:466:SER:CB	2.47	0.44
2:C:3:ASN:CB	2:C:130:MET:SD	3.05	0.44
2:B:384:MET:CB	2:B:385:PRO:HD2	2.37	0.44
2:C:62:ARG:CD	2:C:70:PHE:CB	2.95	0.44
1:A:257:SER:HB2	1:A:266:ASN:HD21	1.81	0.44
1:A:294:ASN:HD22	3:D:14:DG:H8	1.64	0.44
1:A:78:ILE:CD1	1:A:111:LEU:CD2	2.95	0.44
2:B:438:THR:HG23	2:B:442:LEU:HD23	1.98	0.44
2:C:279:ARG:NE	2:C:281:PHE:CZ	2.86	0.44
2:C:164:LYS:HE3	2:C:407:GLU:O	2.17	0.44
1:A:325:LEU:HD13	1:A:329:ALA:HB1	1.95	0.44
5:C:530:SAM:CE	4:E:6:DA:H61	2.05	0.44
2:B:39:MET:CE	2:B:39:MET:CA	2.95	0.44
2:C:287:ASN:HD22	2:C:290:LEU:H	1.66	0.44
1:A:53:LYS:HE2	1:A:97:HIS:HE1	1.82	0.44
2:B:252:SER:O	2:B:255:GLU:HG2	2.18	0.44
1:A:385:VAL:HG12	1:A:389:PHE:HE1	1.82	0.44
1:A:253:LEU:CD1	1:A:263:VAL:CG2	2.93	0.44
1:A:73:ILE:HG22	1:A:100:PHE:HB3	1.94	0.44
1:A:15:VAL:CG2	1:A:155:ILE:CG2	2.95	0.44
2:B:482:PRO:HA	2:B:485:LEU:HG	1.99	0.44
2:B:488:GLU:HG2	2:B:489:ALA:N	2.33	0.44
2:B:128:GLY:O	2:B:131:TYR:HB3	2.18	0.44
2:B:149:TYR:O	5:B:530:SAM:HB1	2.18	0.44
2:B:115:TRP:CH2	2:B:122:LYS:CE	2.94	0.44
2:B:287:ASN:HD22	2:B:290:LEU:H	1.66	0.44
2:C:277:ILE:HD13	2:C:291:CYS:SG	2.57	0.44
2:C:158:THR:OG1	2:C:398:LEU:HD13	2.18	0.44
1:A:234:GLU:C	4:E:2:DT:OP2	2.56	0.44
1:A:271:LEU:HD22	1:A:273:CYS:N	2.13	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:THR:HA	1:A:413:ILE:HG22	1.99	0.44
2:C:250:LEU:HA	2:C:279:ARG:NH2	2.33	0.44
2:B:158:THR:OG1	2:B:398:LEU:HD13	2.18	0.44
1:A:223:PHE:CG	1:A:224:LYS:N	2.85	0.44
1:A:254:ARG:HH21	1:A:256:SER:HB2	1.74	0.44
2:B:17:LEU:HD22	2:B:22:VAL:HG21	2.00	0.44
2:B:215:LEU:HD22	2:B:245:ARG:HH21	1.83	0.44
1:A:118:PHE:CZ	1:A:166:LYS:CE	2.95	0.44
2:C:252:SER:O	2:C:255:GLU:HG2	2.18	0.44
1:A:262:HIS:HD2	1:A:263:VAL:H	1.66	0.43
1:A:288:LEU:HG	1:A:289:LEU:N	2.32	0.43
2:C:488:GLU:HG2	2:C:489:ALA:N	2.32	0.43
1:A:187:GLU:O	1:A:190:PRO:HD2	2.18	0.43
2:C:459:LYS:HA	2:C:459:LYS:HD3	1.80	0.43
1:A:203:GLY:O	1:A:204:ALA:HB3	2.18	0.43
1:A:10:TRP:CZ2	1:A:417:ALA:O	2.71	0.43
2:B:6:LEU:HD23	2:B:130:MET:CG	2.48	0.43
2:C:17:LEU:HB3	2:C:22:VAL:HB	1.99	0.43
1:A:225:LYS:HB2	1:A:227:ASN:ND2	2.33	0.43
1:A:286:GLY:CA	1:A:305:LEU:HD21	2.48	0.43
2:B:6:LEU:CB	2:B:130:MET:HG2	2.47	0.43
2:B:459:LYS:HA	2:B:459:LYS:HD3	1.81	0.43
1:A:426:TRP:HE3	1:A:447:ILE:CB	2.31	0.43
1:A:196:PHE:CD1	1:A:200:VAL:HG21	2.54	0.43
1:A:232:LEU:HD21	1:A:321:ILE:CD1	2.45	0.43
2:C:439:ASP:CA	2:C:485:LEU:HD22	2.38	0.43
1:A:16:SER:HA	1:A:19:THR:HG22	2.01	0.43
1:A:45:ARG:HA	1:A:104:PHE:CD1	2.51	0.43
2:C:17:LEU:CB	2:C:27:TYR:CD1	3.01	0.43
2:C:275:THR:CB	5:C:530:SAM:HN61	2.31	0.43
2:B:207:GLN:HA	2:B:211:ALA:CB	2.39	0.43
1:A:291:THR:CG2	1:A:302:VAL:HB	2.48	0.43
1:A:291:THR:HG22	1:A:302:VAL:HB	1.99	0.43
2:B:220:GLY:HA2	2:B:223:ARG:NH2	2.34	0.43
2:C:169:GLU:OE1	2:C:262:ILE:HD11	2.18	0.43
2:B:283:HIS:HB3	2:B:320:LYS:HE3	2.00	0.43
2:B:315:LEU:HD22	2:B:463:LEU:HB3	2.00	0.43
2:B:338:LEU:HD13	2:B:401:PHE:CE1	2.53	0.43
1:A:248:VAL:CG1	1:A:270:PHE:N	2.82	0.43
1:A:300:VAL:CG1	1:A:301:GLY:N	2.80	0.43
1:A:314:LEU:HD23	1:A:315:LEU:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1:DG:H2"	4:E:2:DT:H6	1.84	0.43
1:A:44:ILE:CG1	1:A:103:SER:CB	2.96	0.43
1:A:89:VAL:CG2	1:A:135:ILE:HG22	2.47	0.43
2:C:269:PHE:CZ	2:C:311:PRO:HD3	2.53	0.43
2:B:279:ARG:NE	2:B:281:PHE:CZ	2.86	0.43
2:C:20:GLY:HA2	2:C:102:GLN:CG	2.37	0.43
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.82	0.43
2:B:322:THR:O	2:B:326:ARG:HG3	2.18	0.43
2:C:43:THR:HG21	2:C:45:GLN:HB2	2.00	0.43
2:B:376:TRP:CE3	2:B:447:TRP:NE1	2.87	0.43
1:A:252:ILE:HG23	1:A:268:ILE:HG23	1.92	0.43
1:A:80:ILE:HD11	1:A:107:PHE:CD2	2.53	0.43
1:A:131:TYR:CE1	1:A:155:ILE:HD12	2.54	0.43
1:A:48:ASN:HB3	1:A:54:PHE:CD1	2.54	0.43
1:A:411:GLN:HB3	2:B:491:GLY:O	2.19	0.43
2:B:166:GLN:HB3	2:B:167:PRO:HD2	2.01	0.43
1:A:254:ARG:CG	1:A:255:ILE:H	2.30	0.43
1:A:133:ASN:HA	2:B:469:LYS:NZ	2.34	0.43
2:B:17:LEU:CB	2:B:27:TYR:CD1	3.01	0.43
2:C:497:LEU:N	2:C:497:LEU:HD12	2.34	0.43
2:B:497:LEU:N	2:B:497:LEU:HD12	2.34	0.43
2:C:1:MET:SD	2:C:129:ASP:HA	2.58	0.43
2:B:14:CYS:SG	2:B:31:LEU:HD11	2.59	0.43
1:A:17:THR:CG2	1:A:18:VAL:N	2.82	0.43
1:A:20:THR:CG2	1:A:21:LEU:N	2.82	0.43
1:A:26:THR:HG21	1:A:70:SER:H	1.84	0.43
1:A:78:ILE:HG22	1:A:96:GLN:CG	2.44	0.43
2:C:322:THR:CG2	2:C:323:ASP:N	2.82	0.43
2:B:380:LEU:HD23	2:B:380:LEU:O	2.19	0.43
1:A:197:ARG:CZ	1:A:340:SER:HA	2.48	0.43
1:A:222:VAL:CG1	1:A:223:PHE:N	2.82	0.43
1:A:254:ARG:HA	1:A:317:PRO:HG2	2.01	0.43
1:A:112:ARG:H	1:A:112:ARG:CD	2.32	0.43
1:A:155:ILE:O	1:A:155:ILE:HG23	2.19	0.43
2:B:275:THR:CB	5:B:530:SAM:HN61	2.32	0.43
2:C:115:TRP:CE3	2:C:127:PHE:CE1	3.07	0.43
1:A:426:TRP:CE3	1:A:447:ILE:CB	3.00	0.43
2:B:62:ARG:HH11	2:B:66:GLU:HG2	1.84	0.43
2:B:378:TYR:HE1	2:B:419:GLU:HG2	1.84	0.43
1:A:365:ILE:CG2	1:A:366:LYS:N	2.82	0.42
1:A:89:VAL:O	1:A:89:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:C	1:A:388:LEU:HD23	2.39	0.42
2:B:224:LEU:N	2:B:224:LEU:HD12	2.34	0.42
2:B:269:PHE:CZ	2:B:311:PRO:HD3	2.54	0.42
2:C:122:LYS:HZ2	2:C:124:ARG:HG2	1.81	0.42
1:A:142:ALA:O	2:B:316:PHE:CZ	2.72	0.42
2:C:6:LEU:CB	2:C:117:ASN:HB2	2.47	0.42
2:B:334:LEU:HA	2:B:357:PHE:CB	2.46	0.42
2:B:305:ARG:HH12	2:B:409:PRO:HG2	1.82	0.42
1:A:154:LEU:HD23	1:A:154:LEU:C	2.39	0.42
2:B:151:THR:HG22	2:B:152:PRO:N	2.34	0.42
1:A:284:GLN:HE21	1:A:284:GLN:HB3	1.47	0.42
1:A:287:ASP:HB2	1:A:322:ARG:HH21	1.84	0.42
2:C:450:PHE:CE1	2:C:467:TRP:CZ3	3.07	0.42
2:C:493:LEU:N	2:C:493:LEU:HD22	2.34	0.42
1:A:10:TRP:CE2	1:A:418:PHE:CA	2.94	0.42
1:A:35:TYR:CD1	1:A:65:ASN:ND2	2.87	0.42
1:A:72:LYS:HB3	3:D:1:DG:OP2	2.19	0.42
2:B:130:MET:HB2	2:B:130:MET:HE2	1.75	0.42
2:C:34:LEU:CB	2:C:110:MET:SD	3.07	0.42
2:B:251:GLY:HA2	2:B:278:THR:OG1	2.19	0.42
2:C:103:ILE:CG2	2:C:104:THR:N	2.82	0.42
2:C:213:ILE:CG2	2:C:214:GLY:N	2.82	0.42
2:B:161:HIS:O	2:B:164:LYS:HG3	2.19	0.42
1:A:385:VAL:CG1	1:A:389:PHE:HE1	2.32	0.42
1:A:212:LYS:CG	1:A:213:TRP:N	2.83	0.42
1:A:224:LYS:O	1:A:370:VAL:HG12	2.20	0.42
1:A:233:THR:O	1:A:321:ILE:HG13	2.19	0.42
1:A:255:ILE:CG2	1:A:256:SER:N	2.83	0.42
1:A:265:GLN:CG	1:A:266:ASN:N	2.82	0.42
1:A:347:MET:CE	1:A:360:ILE:CD1	2.96	0.42
1:A:104:PHE:CZ	1:A:106:ALA:HB3	2.54	0.42
1:A:117:ILE:HD12	1:A:165:GLN:OE1	2.19	0.42
1:A:10:TRP:CE3	1:A:418:PHE:O	2.72	0.42
2:C:215:LEU:HD22	2:C:245:ARG:HH21	1.83	0.42
2:C:269:PHE:CG	4:E:6:DA:C4	3.07	0.42
1:A:118:PHE:CZ	1:A:162:LEU:HD21	2.53	0.42
2:C:62:ARG:HH11	2:C:66:GLU:HG2	1.84	0.42
1:A:254:ARG:CG	1:A:255:ILE:N	2.83	0.42
1:A:315:LEU:HD23	1:A:316:TYR:O	2.19	0.42
4:E:1:DG:C4	4:E:2:DT:H72	2.55	0.42
1:A:121:PHE:CZ	1:A:160:PRO:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD23	1:A:42:PRO:HD2	1.98	0.42
1:A:46:ALA:HB1	1:A:82:MET:HE3	1.97	0.42
3:D:1:DG:C4	3:D:2:DT:C7	3.03	0.42
1:A:142:ALA:O	2:B:316:PHE:CE2	2.72	0.42
2:B:277:ILE:O	2:B:277:ILE:HG22	2.20	0.42
1:A:198:GLN:NE2	2:C:491:GLY:HA3	2.34	0.42
2:C:358:THR:CG2	2:C:359:LYS:N	2.83	0.42
2:B:377:VAL:HG12	2:B:378:TYR:N	2.34	0.42
1:A:239:LEU:CD2	1:A:240:SER:N	2.82	0.42
1:A:333:TYR:CA	1:A:382:VAL:HG22	2.46	0.42
1:A:22:ILE:CG2	1:A:108:CYS:SG	3.07	0.42
1:A:126:THR:CG2	1:A:127:LYS:N	2.83	0.42
1:A:410:THR:CG2	1:A:411:GLN:N	2.83	0.42
1:A:417:ALA:HA	1:A:422:LEU:HG	2.00	0.42
2:B:245:ARG:HH22	2:B:253:ASP:C	2.23	0.42
2:C:220:GLY:HA3	2:C:223:ARG:HH21	1.85	0.42
1:A:395:ILE:CG2	1:A:396:GLU:N	2.83	0.42
2:B:478:SER:N	2:B:479:LEU:HD12	2.35	0.42
2:C:170:VAL:H	2:C:261:HIS:CD2	2.27	0.42
2:C:14:CYS:SG	2:C:31:LEU:HD11	2.59	0.42
1:A:334:ILE:CG2	1:A:335:GLU:N	2.83	0.42
1:A:15:VAL:HA	1:A:18:VAL:CG2	2.49	0.42
1:A:167:ILE:CG2	1:A:168:ILE:N	2.83	0.42
1:A:61:PHE:CE2	1:A:66:LEU:HB2	2.54	0.42
2:B:269:PHE:HB2	3:D:6:DA:N9	2.28	0.42
2:C:220:GLY:HA2	2:C:223:ARG:NH2	2.34	0.42
1:A:144:ILE:HG12	2:B:316:PHE:HZ	1.81	0.42
2:B:115:TRP:CE3	2:B:127:PHE:CE1	3.07	0.42
2:C:262:ILE:HG22	2:C:263:VAL:N	2.34	0.42
2:C:142:THR:CG2	2:C:143:LYS:N	2.83	0.42
2:C:336:THR:CG2	2:C:337:ILE:N	2.83	0.42
1:A:232:LEU:HG	1:A:321:ILE:CD1	2.46	0.42
1:A:223:PHE:CZ	1:A:369:VAL:HG13	2.49	0.42
1:A:229:GLU:OE2	1:A:329:ALA:HB2	2.20	0.42
2:C:224:LEU:N	2:C:224:LEU:HD12	2.34	0.42
2:C:222:ARG:HH12	2:C:226:LEU:HD11	1.81	0.42
1:A:144:ILE:N	2:B:316:PHE:CZ	2.83	0.42
2:B:285:THR:HG22	2:B:287:ASN:N	2.07	0.42
1:A:182:THR:CG2	1:A:183:LYS:N	2.83	0.42
2:C:478:SER:N	2:C:479:LEU:HD12	2.35	0.42
2:C:354:VAL:CG1	2:C:356:PHE:CZ	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:ILE:CG2	2:B:214:GLY:N	2.83	0.42
2:C:85:LEU:HD21	2:C:238:LEU:CD2	2.50	0.42
2:C:166:GLN:HB3	2:C:167:PRO:HD2	2.00	0.42
2:C:151:THR:HG22	2:C:152:PRO:N	2.34	0.42
2:B:136:GLN:HG2	2:B:140:ASN:HD21	1.85	0.42
1:A:330:LEU:HD22	1:A:333:TYR:N	2.30	0.42
1:A:330:LEU:C	1:A:330:LEU:HD23	2.39	0.42
1:A:332:GLU:HB3	1:A:382:VAL:CG1	2.50	0.42
2:C:435:ASN:HD21	2:C:467:TRP:HB2	1.84	0.42
1:A:255:ILE:CG2	3:D:14:DG:H5'	2.47	0.42
1:A:104:PHE:CE1	1:A:107:PHE:CD1	3.08	0.42
1:A:164:GLU:CG	1:A:423:THR:CA	2.95	0.42
1:A:54:PHE:O	1:A:54:PHE:CD2	2.73	0.42
2:B:22:VAL:HG13	2:B:96:THR:OG1	2.20	0.42
2:C:269:PHE:CD1	4:E:6:DA:N7	2.86	0.42
2:B:123:SER:O	2:B:127:PHE:HD1	2.03	0.42
2:B:479:LEU:HD12	2:B:479:LEU:N	2.33	0.42
1:A:6:LEU:CD1	1:A:12:ILE:CD1	2.95	0.42
1:A:414:LEU:O	1:A:418:PHE:CD2	2.73	0.42
2:B:493:LEU:N	2:B:493:LEU:HD22	2.34	0.42
2:B:216:GLU:HG2	2:B:221:THR:HB	2.01	0.42
1:A:142:ALA:HB1	2:B:312:ASP:CA	2.50	0.42
2:C:20:GLY:N	2:C:102:GLN:HG3	2.34	0.42
2:C:3:ASN:HB2	2:C:7:VAL:CB	2.44	0.42
2:B:305:ARG:HD3	2:B:410:HIS:CG	2.55	0.42
1:A:230:SER:HA	1:A:324:ARG:O	2.19	0.42
1:A:253:LEU:O	1:A:316:TYR:HB2	2.19	0.42
1:A:302:VAL:CG1	1:A:303:CYS:N	2.83	0.42
1:A:312:GLN:CG	1:A:313:ASN:N	2.82	0.42
1:A:289:LEU:HD11	1:A:320:LEU:HD21	1.97	0.42
1:A:122:ILE:CG2	1:A:123:ALA:N	2.83	0.42
2:B:481:GLU:HB2	2:B:482:PRO:CD	2.41	0.42
2:C:123:SER:O	2:C:127:PHE:HD1	2.03	0.42
2:C:72:ARG:CG	2:C:73:LYS:N	2.82	0.42
2:C:459:LYS:HB3	2:C:462:SER:H	1.85	0.42
2:C:427:THR:CG2	2:C:428:GLU:N	2.83	0.42
2:C:376:TRP:CE3	2:C:447:TRP:NE1	2.87	0.42
2:C:161:HIS:O	2:C:164:LYS:HG3	2.19	0.42
1:A:270:PHE:CD2	1:A:271:LEU:O	2.73	0.41
1:A:61:PHE:CE1	1:A:69:GLU:OE1	2.74	0.41
1:A:415:ALA:CB	2:B:492:GLU:HG2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:CE	2:B:132:GLU:CB	2.95	0.41
2:C:149:TYR:CD1	5:C:530:SAM:H3'	2.55	0.41
2:B:451:SER:O	2:B:455:ILE:HG13	2.19	0.41
2:C:172:GLN:CD	2:C:257:LEU:HD23	2.40	0.41
2:C:305:ARG:HD3	2:C:410:HIS:CG	2.55	0.41
1:A:293:TYR:C	1:A:295:GLY:H	2.23	0.41
1:A:336:ILE:CG2	1:A:337:PHE:N	2.83	0.41
2:C:484:VAL:CG2	2:C:485:LEU:N	2.83	0.41
4:E:1:DG:C4	4:E:2:DT:C5	3.07	0.41
1:A:80:ILE:HD13	1:A:107:PHE:HD2	1.81	0.41
1:A:20:THR:HG23	1:A:111:LEU:HB2	1.99	0.41
1:A:25:VAL:HB	1:A:104:PHE:C	2.40	0.41
1:A:7:PRO:HG3	1:A:415:ALA:O	2.20	0.41
2:C:22:VAL:HG13	2:C:96:THR:OG1	2.20	0.41
2:B:122:LYS:CD	2:B:124:ARG:HG2	2.50	0.41
2:C:263:VAL:CG2	2:C:300:LEU:CD2	2.95	0.41
2:B:172:GLN:CD	2:B:257:LEU:HD23	2.41	0.41
2:B:20:GLY:N	2:B:102:GLN:HG3	2.34	0.41
4:E:16:DT:C2'	4:E:17:DG:C8	2.99	0.41
2:C:479:LEU:HD12	2:C:479:LEU:N	2.33	0.41
2:B:103:ILE:CG2	2:B:104:THR:N	2.83	0.41
1:A:10:TRP:CE2	1:A:160:PRO:CA	3.00	0.41
1:A:159:ILE:HA	1:A:160:PRO:HD2	1.83	0.41
1:A:70:SER:HA	3:D:1:DG:H5'	2.03	0.41
1:A:328:ASP:O	1:A:329:ALA:HB2	2.20	0.41
2:B:217:LEU:HD22	2:B:275:THR:HG23	1.94	0.41
2:B:269:PHE:CE2	2:B:311:PRO:CB	3.02	0.41
2:C:122:LYS:CD	2:C:124:ARG:HG2	2.49	0.41
2:C:6:LEU:CB	2:C:130:MET:HG2	2.50	0.41
1:A:33:ILE:CG2	1:A:34:ASN:N	2.82	0.41
2:B:142:THR:CG2	2:B:143:LYS:N	2.83	0.41
2:B:85:LEU:HD21	2:B:238:LEU:CD2	2.50	0.41
1:A:44:ILE:HG12	1:A:103:SER:HA	2.02	0.41
2:B:344:ILE:CD1	2:B:345:PHE:CE1	3.03	0.41
2:B:345:PHE:CD2	3:D:6:DA:H2	2.38	0.41
2:C:277:ILE:O	2:C:277:ILE:HG22	2.20	0.41
2:B:336:THR:CG2	2:B:337:ILE:N	2.83	0.41
2:B:293:MET:HE3	2:B:310:VAL:HG11	2.02	0.41
1:A:158:PRO:CG	1:A:418:PHE:CE2	3.03	0.41
1:A:416:LYS:O	1:A:422:LEU:HD23	2.20	0.41
1:A:71:GLN:HG3	1:A:103:SER:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:LEU:CD2	2:B:130:MET:HE3	2.50	0.41
1:A:193:LEU:C	1:A:193:LEU:HD23	2.40	0.41
1:A:142:ALA:HB1	2:B:312:ASP:C	2.41	0.41
1:A:26:THR:HG21	3:D:2:DT:H72	2.03	0.41
1:A:41:LEU:HD11	1:A:73:ILE:HG12	2.02	0.41
1:A:61:PHE:CZ	1:A:66:LEU:CA	3.00	0.41
2:B:220:GLY:HA2	2:B:223:ARG:HH21	1.85	0.41
2:C:251:GLY:HA2	2:C:278:THR:OG1	2.19	0.41
2:B:62:ARG:HB3	2:B:67:GLN:HA	2.03	0.41
2:B:358:THR:CG2	2:B:359:LYS:N	2.83	0.41
2:C:420:TRP:O	2:C:420:TRP:CD1	2.73	0.41
1:A:209:LEU:N	1:A:209:LEU:CD1	2.83	0.41
1:A:316:TYR:CE2	1:A:320:LEU:O	2.74	0.41
1:A:42:PRO:HG2	1:A:101:GLU:HG3	2.03	0.41
1:A:422:LEU:N	1:A:422:LEU:CD2	2.83	0.41
1:A:6:LEU:HA	1:A:7:PRO:HD2	1.79	0.41
2:B:484:VAL:CG2	2:B:485:LEU:N	2.83	0.41
2:B:38:LYS:HA	2:B:56:TRP:CE3	2.56	0.41
2:B:283:HIS:N	2:B:294:GLN:HE22	2.05	0.41
2:C:384:MET:HE3	2:C:385:PRO:HD2	2.03	0.41
2:B:63:ILE:HG12	2:B:64:GLY:N	2.36	0.41
2:C:88:ALA:HB2	2:C:241:GLY:HA2	2.02	0.41
1:A:126:THR:O	1:A:131:TYR:CD2	2.74	0.41
1:A:12:ILE:N	1:A:12:ILE:CD1	2.83	0.41
1:A:136:SER:HB2	2:B:469:LYS:CE	2.51	0.41
2:B:440:GLN:CB	2:B:484:VAL:HB	2.50	0.41
2:C:216:GLU:HG2	2:C:221:THR:HB	2.01	0.41
2:C:269:PHE:HD1	4:E:6:DA:C5	2.25	0.41
1:A:426:TRP:HE3	1:A:447:ILE:HG21	1.84	0.41
1:A:394:THR:CG2	1:A:395:ILE:N	2.82	0.41
2:C:334:LEU:HD12	2:C:357:PHE:HB3	2.03	0.41
1:A:353:THR:CG2	2:C:351:LYS:CE	2.95	0.41
2:B:190:LYS:HA	2:B:193:THR:OG1	2.21	0.41
1:A:316:TYR:CD2	1:A:317:PRO:O	2.74	0.41
2:C:377:VAL:HG12	2:C:378:TYR:N	2.35	0.41
1:A:27:TYR:CE2	1:A:28:LYS:O	2.74	0.41
1:A:45:ARG:O	1:A:107:PHE:CZ	2.74	0.41
1:A:133:ASN:CG	2:B:431:ASP:HB2	2.41	0.41
1:A:138:LEU:HD22	1:A:138:LEU:H	1.83	0.41
1:A:41:LEU:CD2	1:A:42:PRO:N	2.78	0.41
1:A:61:PHE:CE1	1:A:65:ASN:CG	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:GLY:HA3	2:B:223:ARG:HH21	1.84	0.41
2:C:216:GLU:HG3	2:C:218:VAL:O	2.21	0.41
2:C:246:LEU:HD13	2:C:247:GLY:N	2.36	0.41
2:C:245:ARG:HH22	2:C:253:ASP:C	2.23	0.41
2:C:344:ILE:CD1	2:C:345:PHE:CE1	3.04	0.41
2:C:148:GLN:OE1	4:E:6:DA:C8	2.74	0.41
2:C:163:LEU:CG	2:C:262:ILE:HG21	2.48	0.41
2:C:408:ASP:OD1	2:C:409:PRO:HD2	2.21	0.41
2:B:103:ILE:O	2:B:107:VAL:HG23	2.21	0.41
2:C:244:ILE:N	2:C:244:ILE:CD1	2.84	0.41
2:B:427:THR:CG2	2:B:428:GLU:N	2.83	0.41
1:A:299:PHE:CD2	1:A:347:MET:HG2	2.54	0.41
1:A:356:GLY:N	2:C:316:PHE:CZ	2.89	0.41
2:C:450:PHE:HZ	2:C:467:TRP:CZ3	2.38	0.41
1:A:11:VAL:CG1	1:A:12:ILE:N	2.83	0.41
1:A:414:LEU:O	1:A:418:PHE:CG	2.74	0.41
1:A:411:GLN:OE1	2:B:491:GLY:HA3	2.20	0.41
2:C:515:LEU:HD22	2:C:515:LEU:H	1.86	0.41
1:A:36:LEU:CD2	1:A:36:LEU:N	2.83	0.41
2:B:88:ALA:HB2	2:B:241:GLY:HA2	2.02	0.41
1:A:252:ILE:HG22	1:A:268:ILE:C	2.42	0.40
1:A:268:ILE:HG12	1:A:269:ARG:N	2.36	0.40
1:A:294:ASN:ND2	3:D:13:DC:C2'	2.60	0.40
1:A:74:SER:O	1:A:100:PHE:CD2	2.74	0.40
1:A:27:TYR:CD2	1:A:28:LYS:O	2.74	0.40
2:B:28:VAL:CG2	2:B:29:ASN:N	2.85	0.40
2:B:279:ARG:NH2	2:B:281:PHE:HZ	2.19	0.40
2:C:283:HIS:HB3	2:C:320:LYS:HE3	2.03	0.40
2:B:390:ARG:CG	2:B:391:THR:N	2.85	0.40
2:B:420:TRP:CD1	2:B:420:TRP:O	2.73	0.40
2:C:136:GLN:HG2	2:C:140:ASN:HD21	1.86	0.40
1:A:236:ARG:CG	1:A:237:ASN:N	2.82	0.40
1:A:89:VAL:HG22	1:A:135:ILE:HG21	2.03	0.40
2:B:432:SER:HB2	2:B:433:GLU:H	1.62	0.40
2:B:216:GLU:HG3	2:B:218:VAL:O	2.21	0.40
2:C:115:TRP:CZ3	2:C:127:PHE:CE1	3.09	0.40
2:C:38:LYS:HA	2:C:56:TRP:CE3	2.56	0.40
2:C:62:ARG:HD3	2:C:70:PHE:HB2	2.02	0.40
2:C:390:ARG:CG	2:C:391:THR:N	2.84	0.40
2:B:237:ASN:HD22	2:B:238:LEU:N	2.19	0.40
1:A:232:LEU:HD11	1:A:321:ILE:CD1	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:CD1	1:A:302:VAL:O	2.74	0.40
1:A:299:PHE:C	1:A:300:VAL:HG23	2.42	0.40
1:A:303:CYS:SG	1:A:304:GLY:N	2.95	0.40
2:C:440:GLN:HB2	2:C:484:VAL:CB	2.45	0.40
3:D:18:DA:C2	4:E:4:DG:N2	2.89	0.40
1:A:114:GLU:C	1:A:116:LEU:H	2.25	0.40
1:A:49:ILE:CG1	1:A:107:PHE:CE2	2.98	0.40
3:D:10:DC:H2"	3:D:11:DG:O5'	2.21	0.40
2:C:190:LYS:HA	2:C:193:THR:OG1	2.21	0.40
1:A:292:ARG:O	1:A:359:GLY:HA2	2.22	0.40
2:C:429:VAL:HG12	2:C:430:ALA:N	2.37	0.40
1:A:350:CYS:N	2:C:432:SER:HB3	2.37	0.40
1:A:54:PHE:CE2	1:A:101:GLU:OE1	2.74	0.40
1:A:137:SER:OG	1:A:138:LEU:HD22	2.21	0.40
1:A:125:PHE:CE1	1:A:418:PHE:HZ	2.32	0.40
1:A:54:PHE:CE1	1:A:56:THR:O	2.75	0.40
3:D:1:DG:C8	3:D:2:DT:H71	2.56	0.40
2:B:34:LEU:CB	2:B:110:MET:SD	3.07	0.40
2:B:246:LEU:HD13	2:B:247:GLY:N	2.36	0.40
2:B:148:GLN:OE1	3:D:6:DA:C8	2.74	0.40
2:C:345:PHE:CD2	4:E:6:DA:C2	3.10	0.40
2:B:334:LEU:HD12	2:B:357:PHE:HB3	2.03	0.40
2:C:103:ILE:O	2:C:107:VAL:HG23	2.21	0.40
1:A:305:LEU:CD2	1:A:306:LEU:N	2.82	0.40
1:A:223:PHE:CD1	1:A:370:VAL:O	2.74	0.40
1:A:54:PHE:CZ	1:A:56:THR:O	2.74	0.40
1:A:75:PRO:HG3	1:A:111:LEU:CD1	2.41	0.40
2:B:6:LEU:CB	2:B:117:ASN:HB2	2.45	0.40
2:B:269:PHE:HD1	2:B:269:PHE:N	2.18	0.40
2:B:350:VAL:HG23	2:B:350:VAL:O	2.20	0.40
1:A:98:LEU:CB	1:A:99:PRO:CD	2.99	0.40
2:C:38:LYS:CD	2:C:56:TRP:CE2	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/464 (100%)	433 (94%)	22 (5%)	7 (2%)	13	57
2	B	527/529 (100%)	503 (95%)	18 (3%)	6 (1%)	17	63
2	C	527/529 (100%)	503 (95%)	20 (4%)	4 (1%)	24	69
All	All	1516/1522 (100%)	1439 (95%)	60 (4%)	17 (1%)	23	63

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	SER
1	A	296	SER
1	A	326	THR
1	A	248	VAL
2	B	472	ASP
2	C	472	ASP
1	A	2	SER
2	B	4	ASN
2	B	272	ALA
2	B	432	SER
2	C	4	ASN
2	C	272	ALA
1	A	206	ASN
1	A	215	ASN
2	B	464	ASP
2	B	274	GLY
2	C	274	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	398/398 (100%)	383 (96%)	15 (4%)	40 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	452/452 (100%)	443 (98%)	9 (2%)	63	85
2	C	452/452 (100%)	443 (98%)	9 (2%)	63	85
All	All	1302/1302 (100%)	1269 (98%)	33 (2%)	59	81

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

Mol	Chain	Res	Type
1	A	10	TRP
1	A	28	LYS
1	A	65	ASN
1	A	112	ARG
1	A	145	ASN
1	A	187	GLU
1	A	215	ASN
1	A	227	ASN
1	A	234	GLU
1	A	239	LEU
1	A	284	GLN
1	A	313	ASN
1	A	349	ASN
1	A	357	GLN
1	A	407	ASN
2	B	87	GLN
2	B	113	LEU
2	B	237	ASN
2	B	287	ASN
2	B	316	PHE
2	B	346	TYR
2	B	453	GLU
2	B	488	GLU
2	B	492	GLU
2	C	87	GLN
2	C	113	LEU
2	C	237	ASN
2	C	287	ASN
2	C	346	TYR
2	C	434	GLU
2	C	453	GLU
2	C	488	GLU
2	C	492	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	34	ASN
1	A	96	GLN
1	A	97	HIS
1	A	133	ASN
1	A	143	ASN
1	A	146	ASN
1	A	156	ASN
1	A	191	GLN
1	A	215	ASN
1	A	227	ASN
1	A	250	HIS
1	A	262	HIS
1	A	265	GLN
1	A	281	HIS
1	A	294	ASN
1	A	313	ASN
1	A	345	ASN
1	A	349	ASN
1	A	368	GLN
1	A	398	GLN
1	A	407	ASN
2	B	2	ASN
2	B	3	ASN
2	B	4	ASN
2	B	29	ASN
2	B	69	GLN
2	B	91	HIS
2	B	92	ASN
2	B	140	ASN
2	B	232	HIS
2	B	237	ASN
2	B	240	HIS
2	B	261	HIS
2	B	276	ASN
2	B	287	ASN
2	B	294	GLN
2	B	301	HIS
2	B	348	GLN
2	B	397	HIS
2	B	399	GLN

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Mol	Chain	Res	Type
2	B	410	HIS
2	B	435	ASN
2	B	437	ASN
2	C	2	ASN
2	C	3	ASN
2	C	4	ASN
2	C	29	ASN
2	C	91	HIS
2	C	92	ASN
2	C	140	ASN
2	C	232	HIS
2	C	237	ASN
2	C	240	HIS
2	C	261	HIS
2	C	276	ASN
2	C	287	ASN
2	C	294	GLN
2	C	301	HIS
2	C	353	ASN
2	C	397	HIS
2	C	399	GLN
2	C	410	HIS
2	C	435	ASN
2	C	437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SAM	B	530	-	23,29,29	1.18	2 (8%)	15,42,42	2.86	2 (13%)
5	SAM	C	530	-	23,29,29	1.17	2 (8%)	15,42,42	2.88	2 (13%)

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
5	SAM	B	530	-	-	0/8/33/33	0/3/3/3
5	SAM	C	530	-	-	0/8/33/33	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	530	SAM	C2-N1	2.67	1.39	1.33
5	B	530	SAM	C2-N1	2.70	1.39	1.33
5	B	530	SAM	C2-N3	3.73	1.38	1.32
5	C	530	SAM	C2-N3	3.74	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	530	SAM	N3-C2-N1	-10.47	120.65	128.87
5	B	530	SAM	N3-C2-N1	-10.42	120.69	128.87
5	B	530	SAM	O2'-C2'-C3'	2.11	118.67	111.86
5	C	530	SAM	O2'-C2'-C3'	2.13	118.75	111.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	530	SAM	28	0
5	C	530	SAM	30	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.