



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:08 PM GMT

PDB ID : 3W1K
Title : Crystal structure of the selenocysteine synthase SelA and tRNA^{Sec} complex
Authors : Itoh, Y.; Sekine, S.; Yokoyama, S.
Deposited on : 2012-11-15
Resolution : 7.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

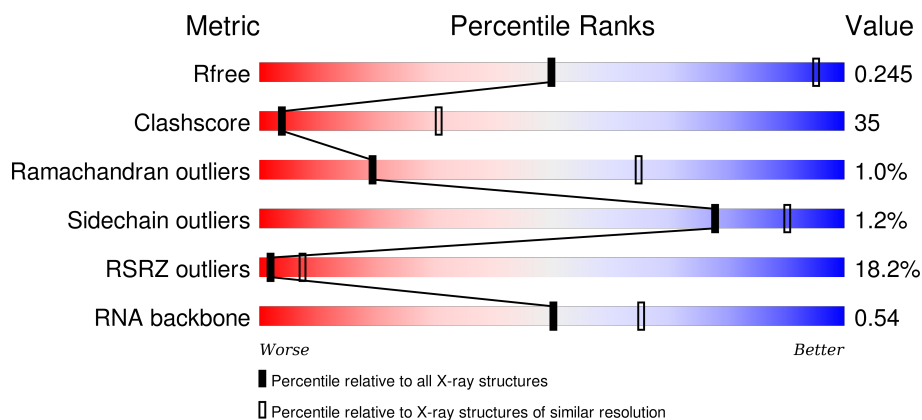
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)
RNA backbone	2183	1106 (11.50-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	452	<div> <div>20%</div> <div>44%</div> <div>54%</div> </div>
1	B	452	<div> <div>14%</div> <div>46%</div> <div>54%</div> </div>
1	C	452	<div> <div>14%</div> <div>48%</div> <div>51%</div> </div>
1	D	452	<div> <div>17%</div> <div>47%</div> <div>52%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	452	<div><div></div><div>23%46%53%.</div></div>
2	F	95	<div><div></div><div>6%16%78%. .</div></div>
2	G	95	<div><div></div><div>23%14%79%. .</div></div>
2	H	95	<div><div></div><div>41%17%77%. .</div></div>
2	I	95	<div><div></div><div>13%14%76%7%. .</div></div>
2	J	95	<div><div></div><div>19%14%78%5%. .</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27660 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called L-seryl-tRNA(Sec) selenium transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	B	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	C	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	D	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	E	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140

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Chain	Residue	Modelled	Actual	Comment	Reference
E	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140

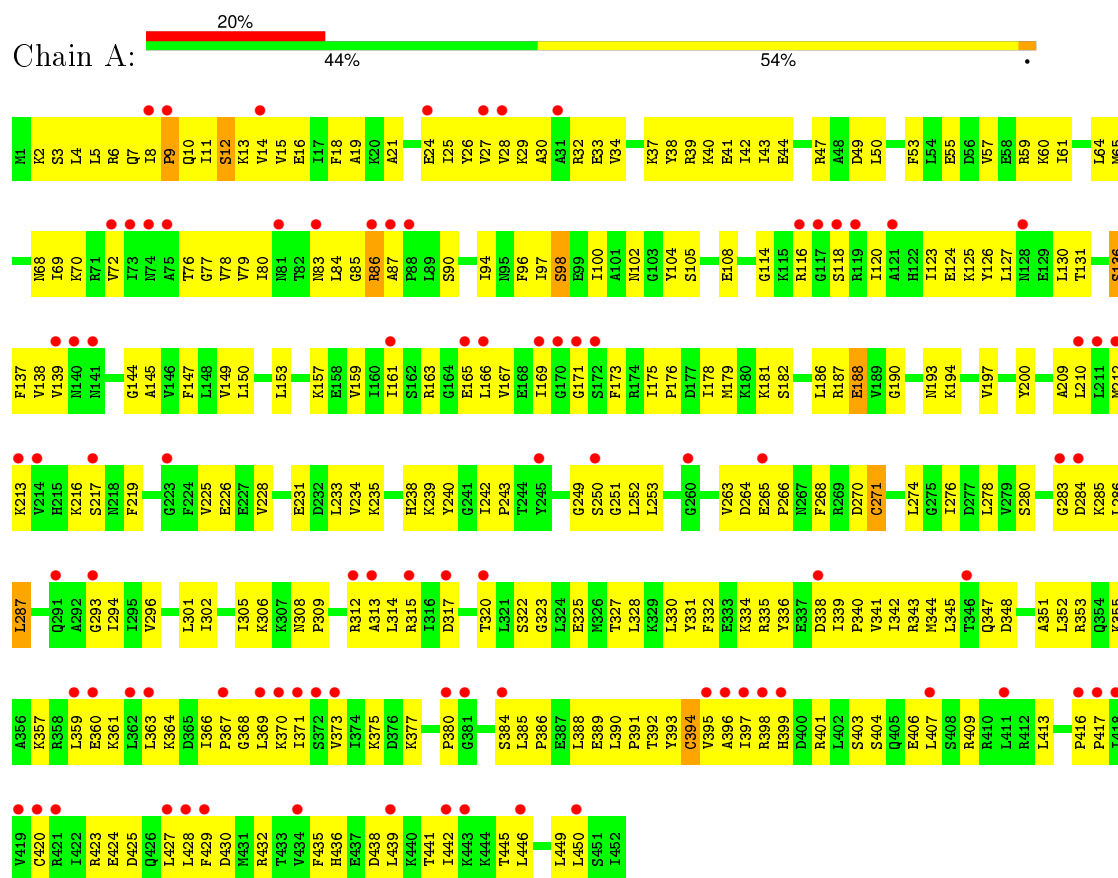
- Molecule 2 is a RNA chain called selenocysteine tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	G	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	H	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	I	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	J	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			

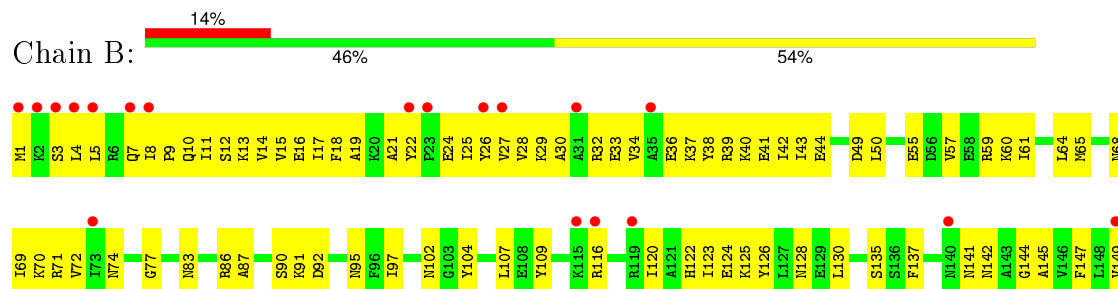
3 Residue-property plots [i](#)

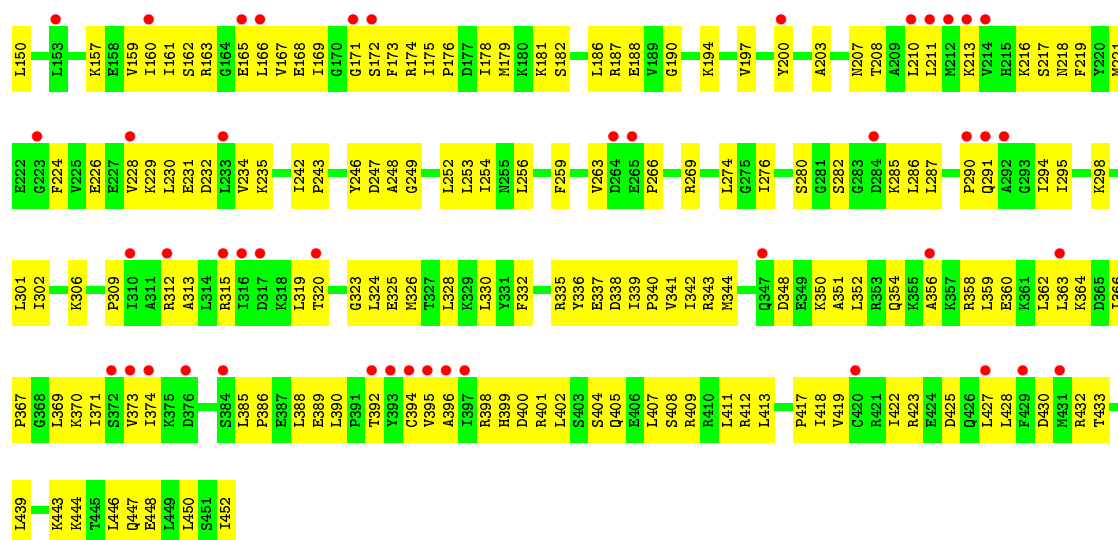
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: L-seryl-tRNA(Sec) selenium transferase

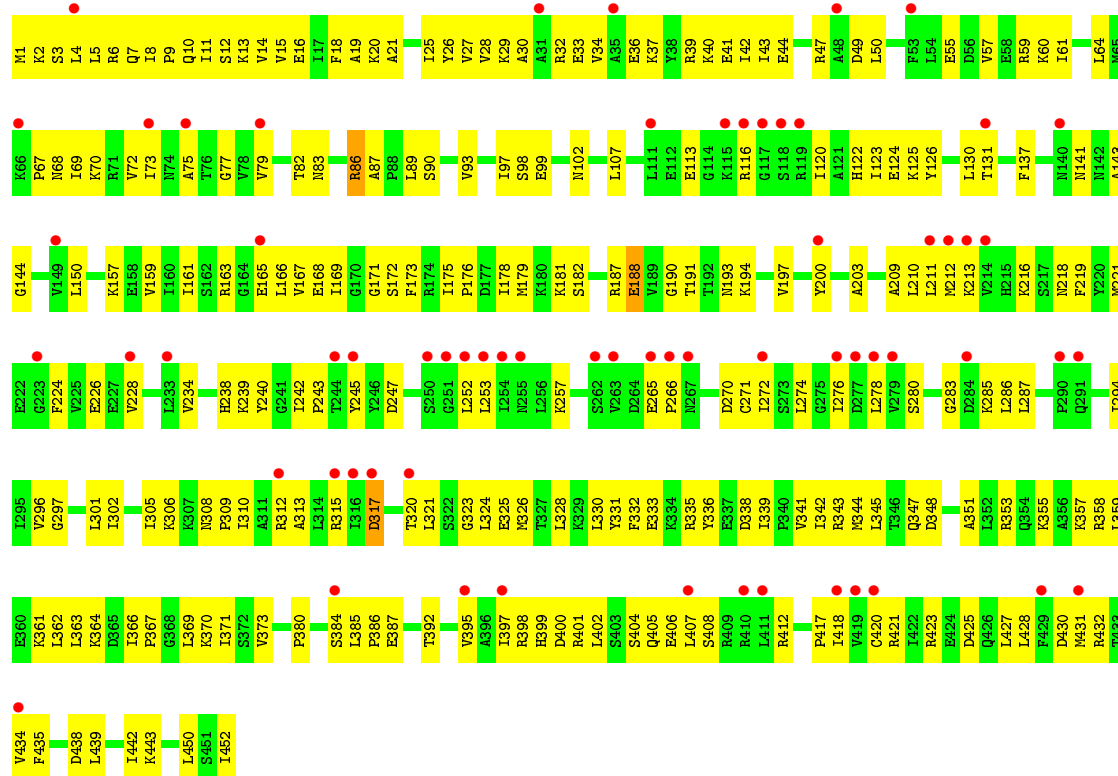


- Molecule 1: L-seryl-tRNA(Sec) selenium transferase

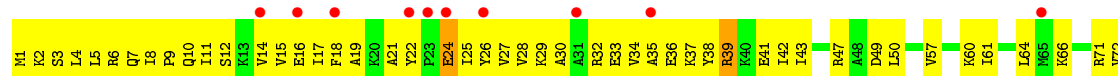


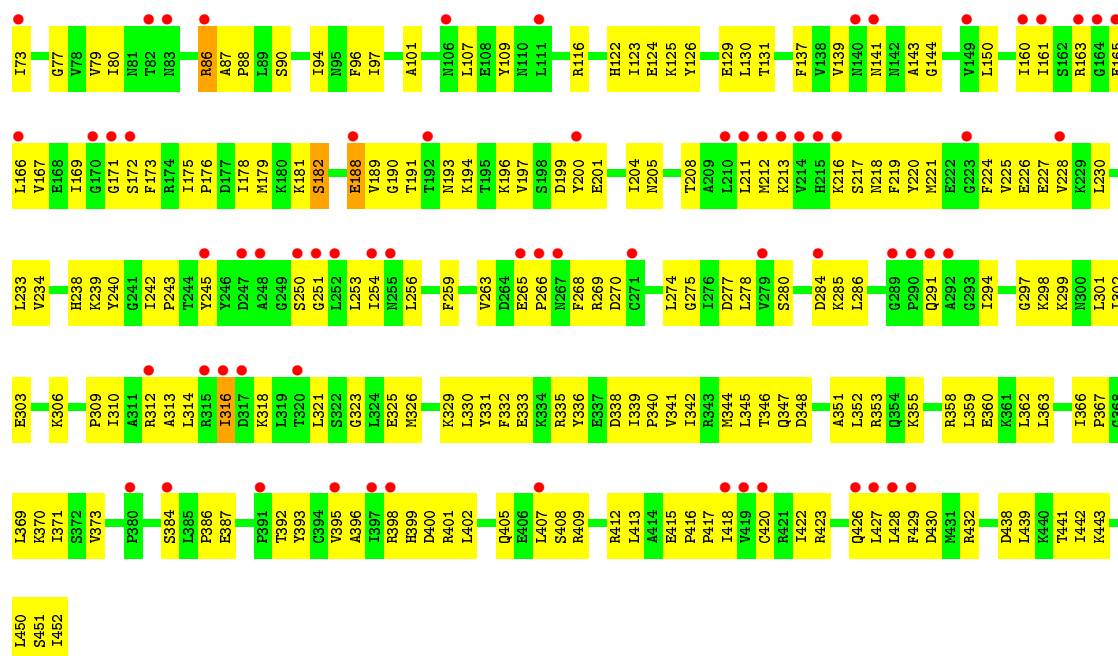


• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

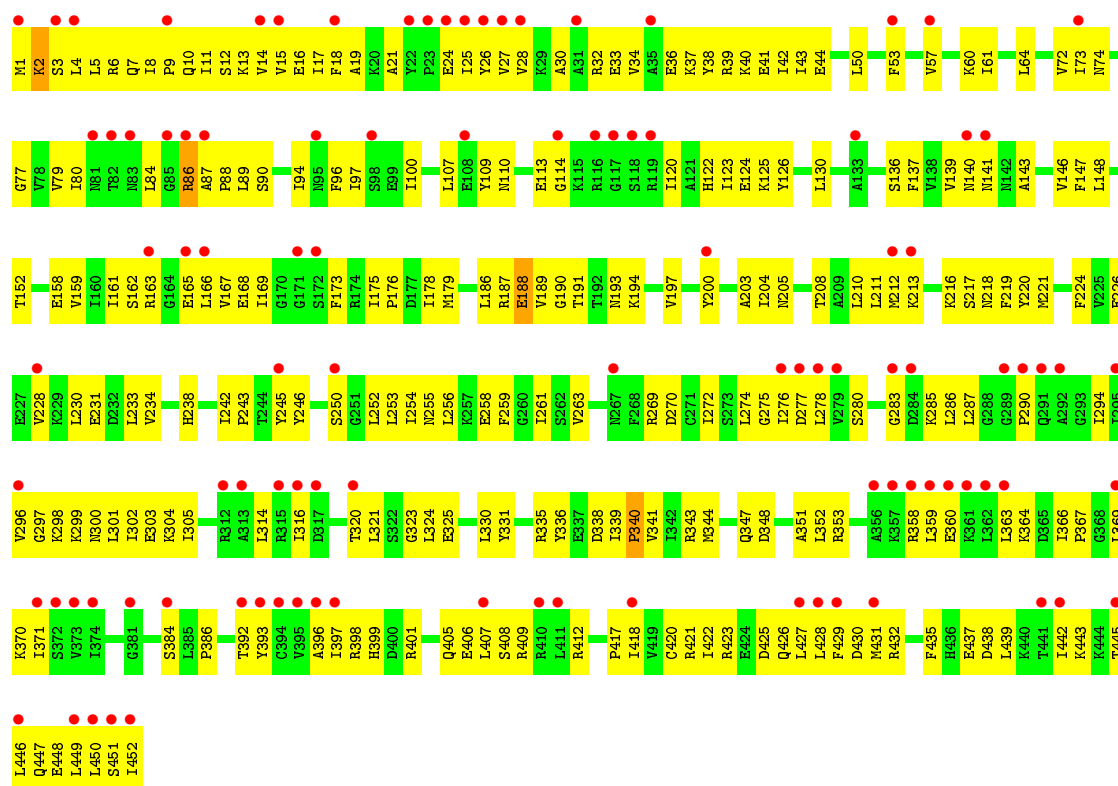


• Molecule 1: L-seryl-tRNA(Sec) selenium transferase



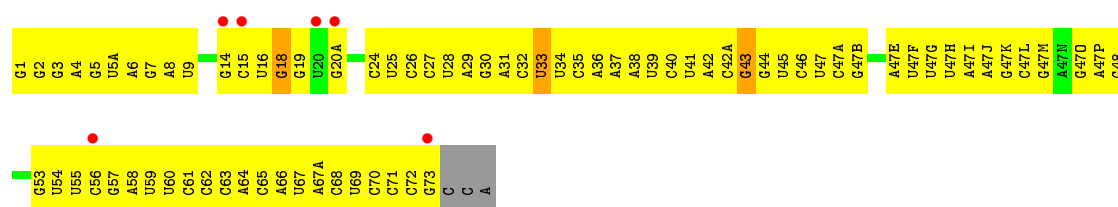


• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

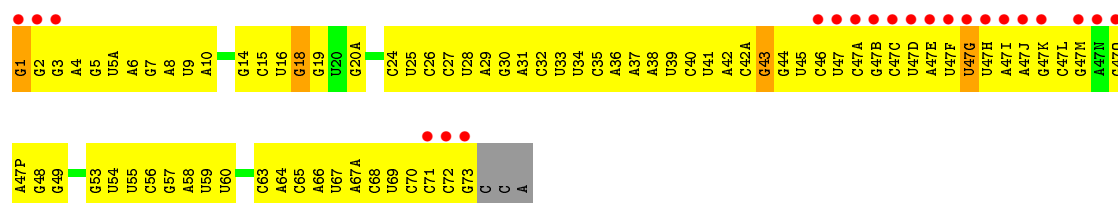


• Molecule 2: selenocysteine tRNA

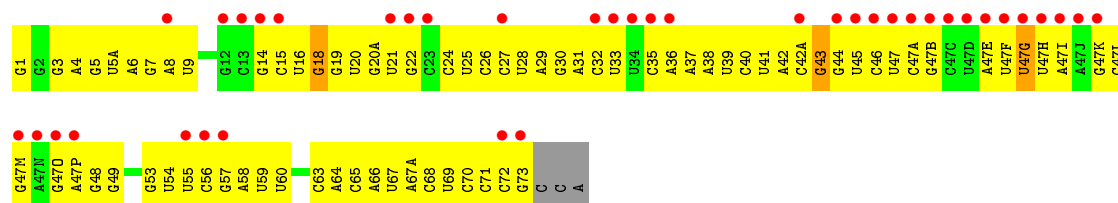
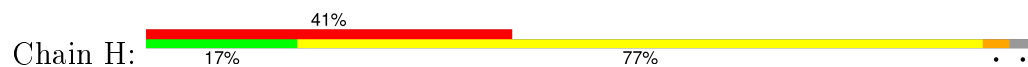




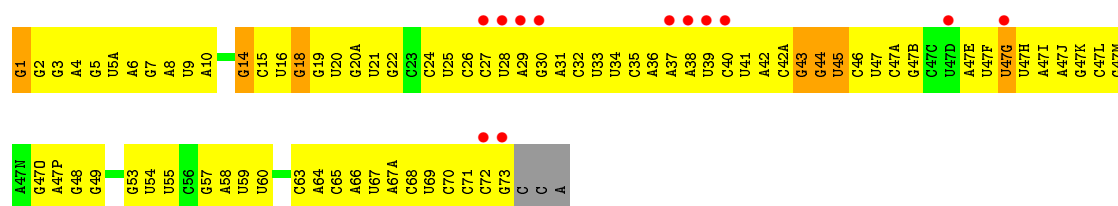
- Molecule 2: selenocysteine tRNA



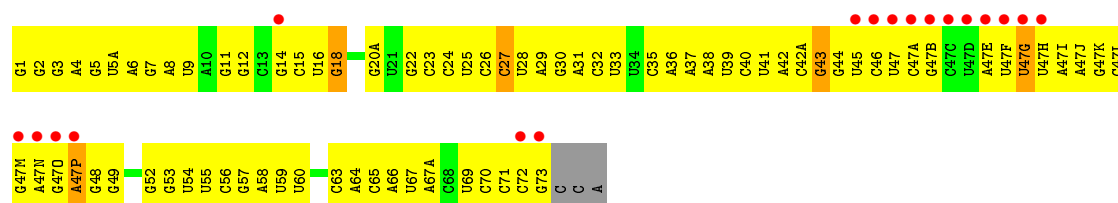
- Molecule 2: selenocysteine tRNA



- Molecule 2: selenocysteine tRNA



- Molecule 2: selenocysteine tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.55Å 355.97Å 165.50Å 90.00° 115.41° 90.00°	Depositor
Resolution (Å)	49.94 – 7.50 49.94 – 7.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.94-7.50) 98.0 (49.94-7.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 7.37Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.194 , 0.240 0.200 , 0.245	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	391.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 555.7	EDS
Estimated twinning fraction	0.085 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	1 of 9776 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	27660	wwPDB-VP
Average B, all atoms (Å ²)	525.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/3597	0.65	0/4831
1	B	0.39	0/3597	0.65	0/4831
1	C	0.39	0/3597	0.64	0/4831
1	D	0.41	0/3597	0.65	0/4831
1	E	0.40	0/3597	0.64	0/4831
2	F	0.49	1/2185 (0.0%)	0.75	0/3401
2	G	0.44	1/2185 (0.0%)	0.73	0/3401
2	H	0.42	1/2185 (0.0%)	0.73	0/3401
2	I	0.43	1/2185 (0.0%)	0.72	0/3401
2	J	0.43	1/2185 (0.0%)	0.72	2/3401 (0.1%)
All	All	0.42	5/28910 (0.0%)	0.68	2/41160 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	G	OP3-P	-7.24	1.52	1.61
2	I	1	G	OP3-P	-7.05	1.52	1.61
2	J	1	G	OP3-P	-7.05	1.52	1.61
2	H	1	G	OP3-P	-6.86	1.52	1.61
2	G	1	G	OP3-P	-6.77	1.53	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	47(P)	A	OP2-P-O3'	6.24	118.93	105.20
2	J	27	C	OP2-P-O3'	5.73	117.81	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3575	0	3760	295	0
1	B	3575	0	3760	291	0
1	C	3575	0	3760	282	0
1	D	3575	0	3760	298	0
1	E	3575	0	3760	255	0
2	F	1957	0	989	102	0
2	G	1957	0	989	124	0
2	H	1957	0	989	105	0
2	I	1957	0	989	112	0
2	J	1957	0	989	91	0
All	All	27660	0	23745	1783	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 35.

All (1783) 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:C:157:LYS:HE2	1:C:209:ALA:HB2	1.27	1.14
1:B:1:MET:HG3	1:B:4:LEU:HD12	1.31	1.12
1:C:102:ASN:HB3	1:D:71:ARG:HH22	1.15	1.08
1:A:10:GLN:H	1:A:13:LYS:HD2	1.13	1.08
2:J:32:C:H2'	2:J:33:U:C6	1.93	1.02
1:B:10:GLN:H	1:B:13:LYS:HD2	1.20	1.02
1:C:353:ARG:HE	1:C:357:LYS:HD2	1.24	1.01
1:C:67:PRO:HD3	1:D:329:LYS:HE3	1.42	0.99
1:A:60:LYS:O	1:A:64:LEU:HG	1.63	0.98
1:B:374:ILE:HD11	1:B:428:LEU:HD21	1.42	0.97
1:D:221:MET:HG2	1:E:221:MET:HG2	1.47	0.97
2:G:47(H):U:H2'	2:G:47(I):A:O4'	1.65	0.97
1:D:4:LEU:O	1:D:42:ILE:HD13	1.65	0.95
1:B:423:ARG:HD2	1:B:428:LEU:HD12	1.49	0.95
1:B:373:VAL:HG22	1:B:395:VAL:HG22	1.49	0.94
1:A:157:LYS:HE2	1:A:209:ALA:HB2	1.50	0.94
1:A:442:ILE:O	1:A:446:LEU:HG	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:HD12	2:F:18:G:OP1	1.68	0.93
1:E:5:LEU:HD11	1:E:39:ARG:HA	1.47	0.93
1:C:163:ARG:HD2	1:C:190:GLY:O	1.67	0.93
1:A:181:LYS:HG3	1:B:309:PRO:HG2	1.49	0.93
2:F:36:A:H2'	2:F:37:A:O4'	1.67	0.93
1:C:10:GLN:H	1:C:13:LYS:HD2	1.31	0.92
1:C:399:HIS:HE1	1:C:401:ARG:HD3	1.35	0.91
1:C:83:ASN:HB3	1:D:109:TYR:HD2	1.36	0.91
1:B:10:GLN:HB3	1:B:13:LYS:HG3	1.51	0.91
1:E:187:ARG:HE	1:E:203:ALA:HB1	1.34	0.91
1:C:332:PHE:CZ	1:D:29:LYS:HD2	2.06	0.91
1:D:150:LEU:HD13	1:D:179:MET:HG3	1.52	0.91
2:J:7:G:H22	2:J:66:A:H2	1.18	0.90
1:A:97:ILE:HD11	1:A:323:GLY:HA3	1.52	0.90
1:E:254:ILE:HD11	1:E:259:PHE:CE2	2.08	0.89
2:I:33:U:H5'	2:I:34:U:OP2	1.70	0.89
1:B:366:ILE:HB	1:B:369:LEU:HD12	1.55	0.89
2:F:47(H):U:H2'	2:F:47(I):A:O4'	1.74	0.88
2:I:7:G:H22	2:I:66:A:H2	1.19	0.88
1:A:171:GLY:HA3	1:B:116:ARG:NH2	1.86	0.88
1:A:68:ASN:HD22	1:B:122:HIS:HA	1.37	0.88
2:G:29:A:H2'	2:G:30:G:O4'	1.74	0.87
2:F:7:G:H22	2:F:66:A:H2	1.23	0.87
2:G:7:G:H22	2:G:66:A:H2	1.20	0.87
1:D:29:LYS:HD3	1:D:64:LEU:HD13	1.55	0.86
1:B:221:MET:HG2	1:C:221:MET:HG2	1.56	0.86
1:E:254:ILE:HD11	1:E:259:PHE:HE2	1.39	0.86
1:B:358:ARG:HH21	1:B:439:LEU:HD12	1.39	0.86
1:B:231:GLU:HG3	1:B:274:LEU:HD11	1.58	0.85
1:E:330:LEU:HD23	1:E:335:ARG:HD3	1.58	0.85
2:G:65:C:H2'	2:G:66:A:C8	2.11	0.85
1:C:73:ILE:HB	1:C:418:ILE:HG12	1.57	0.85
1:B:10:GLN:HG2	1:B:12:SER:H	1.42	0.85
1:B:176:PRO:HG3	1:C:191:THR:HG22	1.59	0.84
1:A:136:SER:HB3	1:A:296:VAL:HG12	1.60	0.84
2:I:47(A):C:H2'	2:I:47(B):G:H8	1.40	0.84
1:E:1:MET:CG	1:E:4:LEU:HD12	2.07	0.84
1:C:29:LYS:HD2	1:D:332:PHE:CZ	2.11	0.84
1:E:252:LEU:HD21	1:E:256:LEU:HG	1.58	0.84
1:B:298:LYS:HB2	1:B:301:LEU:HD12	1.60	0.83
2:I:25:U:O2'	2:I:26:C:H5'	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:VAL:HG12	1:D:219:PHE:HE2	1.41	0.83
2:F:47(G):U:H6	2:F:47(G):U:O5'	1.62	0.83
1:A:90:SER:HB3	1:A:338:ASP:O	1.77	0.83
1:E:443:LYS:O	1:E:447:GLN:HG2	1.79	0.83
2:F:32:C:H2'	2:F:33:U:O4'	1.80	0.82
1:C:5:LEU:HD11	1:C:39:ARG:HA	1.60	0.82
2:I:47(H):U:H2'	2:I:47(I):A:O4'	1.80	0.82
1:B:263:VAL:HG11	1:B:388:LEU:HD13	1.62	0.82
2:H:7:G:H22	2:H:66:A:H2	1.24	0.81
1:A:10:GLN:HB2	1:A:13:LYS:HE3	1.61	0.81
1:A:29:LYS:HD2	1:B:332:PHE:CZ	2.16	0.81
1:B:97:ILE:HD11	1:B:323:GLY:HA3	1.61	0.81
1:D:362:LEU:HB3	1:D:443:LYS:HD2	1.62	0.81
2:G:25:U:H2'	2:G:26:C:H6	1.46	0.81
1:B:411:LEU:HD22	1:B:418:ILE:HD12	1.61	0.80
1:C:126:TYR:CB	1:C:328:LEU:HD13	2.12	0.80
1:A:171:GLY:HA3	1:B:116:ARG:HH22	1.44	0.80
2:G:25:U:H2'	2:G:26:C:C6	2.17	0.80
1:E:187:ARG:NE	1:E:203:ALA:HB1	1.97	0.80
2:J:47(L):C:H2'	2:J:47(M):G:C8	2.17	0.80
2:G:27:C:H2'	2:G:28:U:O4'	1.80	0.80
1:A:28:VAL:O	1:A:32:ARG:HG3	1.80	0.79
1:A:5:LEU:HD11	1:A:39:ARG:HG2	1.63	0.79
1:A:12:SER:O	1:A:16:GLU:HG3	1.82	0.79
1:D:5:LEU:HD12	1:D:8:ILE:HD12	1.62	0.79
1:B:60:LYS:O	1:B:64:LEU:HG	1.83	0.79
1:C:102:ASN:HB3	1:D:71:ARG:NH2	1.96	0.79
2:J:47(L):C:H2'	2:J:47(M):G:H8	1.48	0.79
1:D:176:PRO:HG3	1:E:191:THR:HG22	1.64	0.79
1:B:10:GLN:H	1:B:13:LYS:CD	1.95	0.79
1:A:366:ILE:HB	1:A:369:LEU:CD1	2.12	0.79
2:J:38:A:O2'	2:J:39:U:H5'	1.82	0.79
1:B:217:SER:O	1:B:386:PRO:HD3	1.83	0.79
2:H:67(A):A:H2'	2:H:68:C:C6	2.18	0.79
1:A:10:GLN:N	1:A:13:LYS:HD2	1.96	0.78
1:C:97:ILE:HD11	1:C:323:GLY:HA3	1.65	0.78
1:E:366:ILE:HB	1:E:369:LEU:HD12	1.66	0.78
1:C:234:VAL:CG2	1:C:276:ILE:HD13	2.14	0.78
1:D:344:MET:O	1:D:432:ARG:HD2	1.81	0.78
1:C:11:ILE:HB	2:I:16:U:H4'	1.65	0.78
2:I:55:U:H2'	2:I:57:G:OP2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:VAL:HG22	1:B:228:VAL:HG13	1.64	0.78
2:J:47(H):U:H2'	2:J:47(I):A:O4'	1.84	0.78
1:D:10:GLN:HG2	1:D:12:SER:H	1.49	0.78
1:E:1:MET:C	1:E:3:SER:H	1.86	0.78
1:C:126:TYR:HB2	1:C:328:LEU:HD13	1.64	0.78
1:B:405:GLN:HE22	1:B:422:ILE:HG21	1.49	0.78
1:C:253:LEU:HD23	1:C:331:TYR:CD1	2.19	0.78
1:E:343:ARG:O	1:E:347:GLN:HG3	1.83	0.77
1:D:39:ARG:O	1:D:43:ILE:HG13	1.85	0.77
1:A:332:PHE:CZ	1:B:29:LYS:HD2	2.20	0.77
1:D:42:ILE:HD11	1:D:50:LEU:HD21	1.66	0.77
1:A:366:ILE:HB	1:A:369:LEU:HD12	1.64	0.77
1:C:126:TYR:CE2	1:C:325:GLU:HG3	2.20	0.77
2:I:47(A):C:H2'	2:I:47(B):G:C8	2.18	0.76
1:B:37:LYS:O	1:B:41:GLU:HG3	1.85	0.76
1:C:397:ILE:HD11	1:C:427:LEU:HD23	1.67	0.76
1:A:399:HIS:HE1	1:A:401:ARG:HD3	1.50	0.76
1:E:5:LEU:CD1	1:E:39:ARG:HA	2.16	0.76
1:B:90:SER:HB3	1:B:338:ASP:O	1.84	0.76
1:A:163:ARG:HD2	1:A:190:GLY:O	1.85	0.76
1:D:10:GLN:HB2	2:H:19:G:H3'	1.66	0.76
1:B:5:LEU:HD11	1:B:39:ARG:HA	1.68	0.76
1:A:217:SER:O	1:A:386:PRO:HD3	1.86	0.76
2:G:65:C:H2'	2:G:66:A:H8	1.52	0.75
2:F:65:C:H2'	2:F:66:A:C8	2.20	0.75
1:C:130:LEU:HD13	1:C:253:LEU:HD21	1.69	0.75
2:H:15:C:H2'	2:H:16:U:C6	2.20	0.75
1:D:1:MET:HG3	1:D:2:LYS:N	2.00	0.75
1:E:37:LYS:O	1:E:41:GLU:HG3	1.87	0.75
1:D:399:HIS:CE1	1:D:450:LEU:HD22	2.21	0.75
2:F:37:A:H2'	2:F:38:A:O4'	1.87	0.75
1:E:163:ARG:HD2	1:E:190:GLY:O	1.87	0.75
1:A:216:LYS:HG2	1:A:219:PHE:CZ	2.22	0.74
1:A:60:LYS:HD2	1:A:64:LEU:HD21	1.67	0.74
1:E:363:LEU:CD2	1:E:446:LEU:HD12	2.16	0.74
1:E:72:VAL:HG22	1:E:417:PRO:HG2	1.69	0.74
1:C:181:LYS:HG3	1:D:309:PRO:HG2	1.68	0.74
2:I:8:A:N6	2:I:21:U:O4	2.20	0.74
1:C:29:LYS:HD3	1:C:64:LEU:HD13	1.69	0.74
2:J:65:C:H2'	2:J:66:A:C8	2.23	0.74
1:D:366:ILE:HB	1:D:369:LEU:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ALA:O	1:A:149:VAL:HG23	1.88	0.74
1:C:301:LEU:O	1:C:305:ILE:HG13	1.87	0.74
2:F:47:U:H2'	2:F:47(A):C:C6	2.22	0.74
1:B:399:HIS:CE1	1:B:450:LEU:HD22	2.22	0.74
1:A:28:VAL:HG12	1:A:32:ARG:NE	2.03	0.73
1:A:61:ILE:O	1:A:65:MET:HG3	1.88	0.73
1:E:73:ILE:HB	1:E:418:ILE:HG12	1.69	0.73
1:B:169:ILE:O	1:B:173:PHE:HB3	1.88	0.73
1:B:12:SER:O	1:B:16:GLU:HG3	1.88	0.73
2:H:46:C:C2'	2:H:47:U:H5'	2.18	0.73
1:E:363:LEU:HD21	1:E:446:LEU:HD12	1.69	0.73
2:G:58:A:H1'	2:G:60:U:OP2	1.88	0.73
2:G:28:U:O2'	2:G:29:A:H5'	1.88	0.73
1:A:147:PHE:HB2	1:A:178:ILE:HD11	1.69	0.73
1:C:39:ARG:HH22	2:I:18:G:H2'	1.54	0.73
1:A:68:ASN:ND2	1:B:122:HIS:HA	2.02	0.73
1:B:10:GLN:HB3	1:B:13:LYS:HE3	1.70	0.72
2:F:58:A:H1'	2:F:60:U:OP2	1.89	0.72
1:D:5:LEU:HD11	1:D:39:ARG:HG3	1.70	0.72
1:B:150:LEU:HD13	1:B:179:MET:HG3	1.70	0.72
1:B:39:ARG:O	1:B:43:ILE:HG13	1.88	0.72
2:J:55:U:H2'	2:J:57:G:OP2	1.89	0.72
1:C:359:LEU:HB2	1:C:439:LEU:HD22	1.70	0.72
2:F:47(A):C:H2'	2:F:47(B):G:H8	1.53	0.72
2:J:47(I):A:H2'	2:J:47(J):A:O4'	1.89	0.72
1:E:280:SER:HA	1:E:294:ILE:O	1.90	0.72
1:B:25:ILE:HG13	1:B:26:TYR:N	2.04	0.72
1:B:10:GLN:HB2	2:F:19:G:H3'	1.71	0.72
2:I:15:C:H2'	2:I:16:U:C6	2.24	0.72
1:B:163:ARG:NH1	1:C:188:GLU:OE1	2.22	0.72
2:F:47(A):C:H2'	2:F:47(B):G:C8	2.25	0.72
1:B:224:PHE:CD1	1:C:218:ASN:HB2	2.25	0.72
1:B:10:GLN:N	1:B:13:LYS:HD2	2.00	0.71
2:I:47:U:H2'	2:I:47(A):C:C6	2.26	0.71
1:B:336:TYR:O	1:B:339:ILE:HG12	1.90	0.71
1:E:30:ALA:O	1:E:34:VAL:HG23	1.91	0.71
2:H:37:A:H2'	2:H:38:A:O4'	1.91	0.71
2:G:47(J):A:O2'	2:G:47(K):G:H5'	1.91	0.71
2:G:63:C:H2'	2:G:64:A:C8	2.25	0.71
1:D:169:ILE:HG22	1:D:218:ASN:OD1	1.91	0.71
2:F:35:C:H2'	2:F:36:A:C8	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:C:H2'	2:F:64:A:C8	2.25	0.71
1:A:330:LEU:HD23	1:A:335:ARG:HD3	1.72	0.71
1:A:11:ILE:O	1:A:15:VAL:HG23	1.90	0.71
1:E:1:MET:SD	1:E:4:LEU:HD12	2.30	0.71
1:B:159:VAL:HG22	1:B:210:LEU:HB3	1.70	0.71
2:I:9:U:H4'	2:I:45:U:C2	2.26	0.71
1:D:280:SER:HA	1:D:294:ILE:O	1.90	0.71
1:B:28:VAL:HG12	1:B:32:ARG:NE	2.04	0.70
2:H:46:C:H2'	2:H:47:U:O4'	1.91	0.70
1:A:407:LEU:CD2	1:A:427:LEU:HD22	2.21	0.70
2:I:47(G):U:H2'	2:I:47(H):U:O4'	1.90	0.70
1:B:77:GLY:HA2	1:B:433:THR:HG23	1.73	0.70
2:J:37:A:H2'	2:J:38:A:O4'	1.92	0.70
1:E:90:SER:HB3	1:E:338:ASP:O	1.90	0.70
1:B:1:MET:HG3	1:B:4:LEU:CD1	2.18	0.70
1:C:12:SER:O	1:C:16:GLU:HG3	1.91	0.70
1:B:163:ARG:HD2	1:B:190:GLY:O	1.92	0.70
1:D:407:LEU:CD2	1:D:427:LEU:HD22	2.21	0.70
1:E:330:LEU:CD2	1:E:335:ARG:HD3	2.22	0.70
1:A:138:VAL:HG13	1:A:293:GLY:O	1.91	0.70
1:B:280:SER:HA	1:B:294:ILE:O	1.92	0.70
2:F:47(O):G:H2'	2:F:47(P):A:C8	2.27	0.70
1:D:5:LEU:CD1	1:D:8:ILE:HD12	2.22	0.70
1:A:301:LEU:O	1:A:305:ILE:HG13	1.91	0.70
1:E:77:GLY:HA3	1:E:430:ASP:CG	2.12	0.70
1:E:211:LEU:HG	1:E:242:ILE:CG2	2.21	0.70
1:E:1:MET:HG3	1:E:4:LEU:HD12	1.72	0.70
1:D:408:SER:O	1:D:412:ARG:HG3	1.91	0.69
2:G:47:U:H2'	2:G:47(A):C:C6	2.27	0.69
2:H:47:U:H2'	2:H:47(A):C:C6	2.27	0.69
1:E:217:SER:O	1:E:386:PRO:HD3	1.93	0.69
1:C:10:GLN:HG3	2:I:19:G:O5'	1.91	0.69
1:B:290:PRO:HB2	1:B:320:THR:HG22	1.75	0.69
1:E:435:PHE:HB3	1:E:437:GLU:OE1	1.93	0.69
1:E:230:LEU:HD23	1:E:233:LEU:HD12	1.74	0.69
1:C:280:SER:HA	1:C:294:ILE:O	1.93	0.69
1:B:1:MET:CG	1:B:4:LEU:HD12	2.18	0.69
1:A:280:SER:HA	1:A:294:ILE:O	1.93	0.69
2:J:47(A):C:H2'	2:J:47(B):G:H8	1.57	0.69
2:I:37:A:H2'	2:I:38:A:O4'	1.91	0.69
1:B:374:ILE:HD11	1:B:428:LEU:CD2	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:VAL:O	1:C:32:ARG:HG3	1.91	0.69
2:F:55:U:H2'	2:F:57:G:OP2	1.93	0.69
1:E:11:ILE:HG21	1:E:28:VAL:HG13	1.73	0.69
2:J:47:U:H2'	2:J:47(A):C:C6	2.28	0.69
1:A:253:LEU:HD23	1:A:331:TYR:CD1	2.28	0.69
2:G:37:A:H2'	2:G:38:A:O4'	1.93	0.69
1:D:200:TYR:CE2	1:D:228:VAL:HG21	2.28	0.69
1:E:10:GLN:HG2	1:E:12:SER:H	1.57	0.68
2:I:6:A:H2'	2:I:7:G:C8	2.29	0.68
2:F:47(I):A:H2'	2:F:47(J):A:O4'	1.93	0.68
1:B:187:ARG:HE	1:B:203:ALA:HB1	1.58	0.68
1:A:399:HIS:CE1	1:A:401:ARG:HD3	2.28	0.68
1:C:402:LEU:HD22	1:C:406:GLU:HG2	1.76	0.68
1:E:141:ASN:OD1	1:E:143:ALA:HB3	1.93	0.68
1:D:8:ILE:HD11	1:D:38:TYR:HB3	1.74	0.68
2:F:38:A:C2'	2:F:39:U:H5'	2.23	0.68
1:B:407:LEU:HD23	1:B:427:LEU:HD22	1.76	0.68
1:E:405:GLN:HE22	1:E:422:ILE:HG21	1.56	0.68
2:I:28:U:O2'	2:I:29:A:H5'	1.94	0.68
1:D:298:LYS:HB2	1:D:301:LEU:HD12	1.75	0.68
2:H:47(H):U:H2'	2:H:47(I):A:O4'	1.93	0.68
1:A:345:LEU:CD2	1:A:380:PRO:HB3	2.24	0.68
1:E:358:ARG:HH21	1:E:439:LEU:HD12	1.58	0.68
2:G:25:U:O2'	2:G:26:C:H5'	1.94	0.68
2:H:47(A):C:H2'	2:H:47(B):G:H8	1.59	0.68
1:C:366:ILE:HG23	1:C:367:PRO:HD2	1.75	0.68
1:B:390:LEU:HB2	1:B:432:ARG:NH2	2.09	0.68
1:E:234:VAL:HG22	1:E:276:ILE:HD13	1.74	0.68
1:A:320:THR:HG22	1:B:319:LEU:HD12	1.76	0.68
2:F:65:C:H2'	2:F:66:A:H8	1.56	0.67
2:J:47(A):C:H2'	2:J:47(B):G:C8	2.29	0.67
1:D:126:TYR:O	1:D:130:LEU:HG	1.94	0.67
1:E:197:VAL:HG22	1:E:228:VAL:HG13	1.77	0.67
1:E:162:SER:HB2	1:E:200:TYR:OH	1.94	0.67
2:I:47(L):C:H2'	2:I:47(M):G:C8	2.29	0.67
1:C:42:ILE:HD11	1:C:50:LEU:HD21	1.76	0.67
1:E:159:VAL:HG22	1:E:210:LEU:HB3	1.75	0.67
1:A:10:GLN:H	1:A:13:LYS:CD	2.00	0.67
1:A:2:LYS:O	1:A:6:ARG:HG3	1.94	0.67
2:J:47(O):G:H2'	2:J:47(P):A:C8	2.29	0.67
1:C:39:ARG:O	1:C:43:ILE:HG13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LEU:CB	1:B:432:ARG:HH22	2.08	0.67
1:B:194:LYS:HG2	1:B:226:GLU:HB2	1.76	0.67
1:E:420:CYS:SG	1:E:427:LEU:HD11	2.35	0.67
1:E:8:ILE:HD11	1:E:38:TYR:HB3	1.75	0.67
1:D:2:LYS:HE2	1:D:6:ARG:NH2	2.10	0.67
1:E:8:ILE:CD1	1:E:38:TYR:HB3	2.24	0.67
1:B:256:LEU:HD23	1:B:263:VAL:CG2	2.24	0.67
1:C:302:ILE:HD13	1:C:305:ILE:HD12	1.76	0.67
1:A:123:ILE:CD1	1:A:325:GLU:HB2	2.23	0.67
1:A:85:GLY:HA2	1:B:107:LEU:HD23	1.76	0.67
1:B:28:VAL:HG12	1:B:32:ARG:HE	1.59	0.67
1:E:407:LEU:HD23	1:E:427:LEU:HD22	1.77	0.67
2:I:47(O):G:H2'	2:I:47(P):A:C8	2.30	0.67
1:E:423:ARG:HD2	1:E:428:LEU:CD1	2.25	0.67
1:A:392:THR:HG21	1:A:430:ASP:OD2	1.95	0.66
1:A:10:GLN:HB2	1:A:13:LYS:CE	2.25	0.66
1:C:187:ARG:HE	1:C:203:ALA:HB1	1.59	0.66
1:A:39:ARG:O	1:A:43:ILE:HG13	1.95	0.66
1:C:5:LEU:HD12	1:C:42:ILE:HD12	1.76	0.66
2:H:36:A:O2'	2:H:37:A:H5'	1.95	0.66
2:I:38:A:C2'	2:I:39:U:H5'	2.25	0.66
2:J:58:A:H1'	2:J:60:U:OP2	1.95	0.66
1:B:145:ALA:O	1:B:149:VAL:HG23	1.95	0.66
1:D:97:ILE:HD11	1:D:323:GLY:HA3	1.76	0.66
1:A:165:GLU:OE1	1:A:213:LYS:HG3	1.96	0.66
1:A:42:ILE:HD11	1:A:50:LEU:HD21	1.77	0.66
1:C:399:HIS:CD2	1:C:450:LEU:HD13	2.30	0.66
1:A:343:ARG:O	1:A:347:GLN:HG3	1.95	0.66
2:I:63:C:H2'	2:I:64:A:C8	2.31	0.66
1:D:340:PRO:O	1:D:344:MET:HG3	1.95	0.66
1:C:167:VAL:HG12	1:C:219:PHE:HE2	1.61	0.66
1:C:90:SER:HB3	1:C:338:ASP:O	1.95	0.66
1:A:30:ALA:O	1:A:34:VAL:HG23	1.95	0.66
2:G:30:G:O2'	2:G:31:A:H5'	1.95	0.66
1:B:390:LEU:HB2	1:B:432:ARG:HH22	1.58	0.66
2:H:58:A:H1'	2:H:60:U:OP2	1.95	0.66
1:A:361:LYS:HA	1:A:364:LYS:HE3	1.77	0.66
1:E:12:SER:O	1:E:16:GLU:HG3	1.96	0.66
1:D:242:ILE:HG23	1:D:243:PRO:HD2	1.77	0.66
2:J:27:C:H2'	2:J:28:U:O4'	1.95	0.66
2:G:63:C:H2'	2:G:64:A:H8	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ARG:HD2	1:B:419:VAL:HG22	1.78	0.65
1:A:263:VAL:HG12	1:A:265:GLU:H	1.59	0.65
1:C:11:ILE:HG21	1:C:28:VAL:HG13	1.78	0.65
1:A:169:ILE:HG13	1:A:173:PHE:HD2	1.60	0.65
1:D:217:SER:O	1:D:386:PRO:HD3	1.96	0.65
1:C:37:LYS:O	1:C:41:GLU:HG3	1.96	0.65
2:G:47(O):G:H2'	2:G:47(P):A:C8	2.30	0.65
1:A:68:ASN:HD22	1:B:122:HIS:CA	2.07	0.65
1:E:211:LEU:HG	1:E:242:ILE:HG22	1.78	0.65
1:D:302:ILE:CG2	1:D:306:LYS:HE3	2.26	0.65
2:J:24:C:O2'	2:J:25:U:H5'	1.96	0.65
1:A:302:ILE:CG2	1:A:306:LYS:HE3	2.27	0.65
1:E:130:LEU:HD13	1:E:253:LEU:HD21	1.79	0.65
1:E:39:ARG:O	1:E:43:ILE:HG13	1.97	0.65
2:J:63:C:H2'	2:J:64:A:C8	2.32	0.65
1:A:401:ARG:NH1	1:A:450:LEU:O	2.28	0.65
1:C:72:VAL:HG13	1:C:417:PRO:HG2	1.79	0.65
1:D:39:ARG:HG2	2:H:56:C:N4	2.10	0.65
1:A:68:ASN:ND2	1:B:122:HIS:CD2	2.64	0.65
2:G:31:A:N7	2:G:32:C:C4	2.64	0.65
2:F:28:U:O2'	2:F:29:A:H5'	1.96	0.65
1:E:371:ILE:HG12	1:E:397:ILE:HG22	1.77	0.65
1:A:309:PRO:HG2	1:B:181:LYS:HG3	1.78	0.65
2:F:67(A):A:H2'	2:F:68:C:C6	2.32	0.65
1:A:123:ILE:HG23	1:A:328:LEU:HD12	1.77	0.65
2:F:69:U:H2'	2:F:70:C:C6	2.32	0.65
2:H:47(O):G:H2'	2:H:47(P):A:C8	2.32	0.65
1:B:32:ARG:HH22	2:F:18:G:P	2.19	0.65
1:A:83:ASN:HB3	1:B:109:TYR:HD2	1.62	0.65
1:A:13:LYS:HA	1:A:16:GLU:OE1	1.97	0.64
2:G:36:A:H2'	2:G:37:A:C8	2.31	0.64
2:J:25:U:O2'	2:J:26:C:H5'	1.96	0.64
1:D:250:SER:HB2	1:D:286:LEU:CD1	2.27	0.64
1:B:423:ARG:HD2	1:B:428:LEU:CD1	2.26	0.64
1:D:218:ASN:ND2	1:E:224:PHE:HB2	2.13	0.64
1:B:352:LEU:HD13	1:B:392:THR:HA	1.78	0.64
2:I:47(L):C:H2'	2:I:47(M):G:H8	1.60	0.64
1:C:333:GLU:HA	1:D:25:ILE:HD12	1.80	0.64
1:D:11:ILE:HG22	2:H:16:U:H4'	1.78	0.64
2:G:24:C:O2'	2:G:25:U:H5'	1.97	0.64
2:G:29:A:C2'	2:G:30:G:O4'	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:SER:OG	1:D:422:ILE:HD11	1.98	0.64
1:A:271:CYS:O	1:A:276:ILE:HG12	1.98	0.64
1:E:152:THR:HG21	1:E:305:ILE:HA	1.79	0.64
1:A:32:ARG:HH11	1:A:32:ARG:HG2	1.62	0.64
1:D:302:ILE:HG22	1:D:306:LYS:HE3	1.80	0.64
1:D:359:LEU:HB2	1:D:439:LEU:HD22	1.79	0.64
1:B:359:LEU:HB2	1:B:439:LEU:HD22	1.79	0.64
2:J:65:C:H2'	2:J:66:A:H8	1.62	0.64
1:D:353:ARG:HB2	1:D:393:TYR:CE2	2.31	0.64
1:A:373:VAL:HG22	1:A:395:VAL:HG22	1.80	0.64
2:F:6:A:H2'	2:F:7:G:C8	2.33	0.64
1:D:218:ASN:HD22	1:E:224:PHE:HB2	1.63	0.64
1:D:250:SER:HB2	1:D:286:LEU:HD12	1.79	0.64
1:E:86:ARG:NH1	1:E:285:LLP:HE2	2.12	0.64
1:B:10:GLN:NE2	2:F:19:G:OP1	2.31	0.63
1:C:11:ILE:O	1:C:15:VAL:HG23	1.97	0.63
1:D:161:ILE:HG21	1:D:166:LEU:HD21	1.79	0.63
1:D:3:SER:O	1:D:7:GLN:HG2	1.98	0.63
2:I:10:A:H4'	2:I:45:U:O4'	1.98	0.63
1:A:309:PRO:CG	1:B:181:LYS:HG3	2.28	0.63
1:C:211:LEU:HG	1:C:242:ILE:HG21	1.80	0.63
1:C:339:ILE:HD11	1:C:342:ILE:HG13	1.80	0.63
1:A:28:VAL:HG12	1:A:32:ARG:HE	1.63	0.63
1:C:5:LEU:CD1	1:C:42:ILE:HD12	2.28	0.63
2:I:10:A:C5'	2:I:45:U:O4'	2.47	0.63
1:D:259:PHE:HB3	1:D:346:THR:HG21	1.80	0.63
1:A:270:ASP:O	1:A:274:LEU:HG	1.98	0.63
1:C:317:ASP:HA	1:D:291:GLN:OE1	1.98	0.63
1:C:431:MET:CE	1:C:434:VAL:HG21	2.28	0.63
1:B:12:SER:OG	2:F:16:U:H1'	1.99	0.63
2:H:21:U:H2'	2:H:22:G:C8	2.34	0.63
2:H:63:C:H2'	2:H:64:A:C8	2.34	0.63
2:I:35:C:H2'	2:I:36:A:O4'	1.98	0.63
2:G:47(E):A:H2	2:G:47(I):A:N7	1.96	0.63
1:E:4:LEU:O	1:E:42:ILE:HD13	1.99	0.63
1:B:25:ILE:HG13	1:B:26:TYR:H	1.60	0.63
2:I:30:G:O2'	2:I:31:A:H5'	1.98	0.63
1:A:161:ILE:HG23	1:A:166:LEU:HD21	1.80	0.63
1:E:423:ARG:HD2	1:E:428:LEU:HD12	1.81	0.63
2:F:24:C:O2'	2:F:25:U:H5'	1.99	0.63
1:B:32:ARG:HG2	1:B:32:ARG:HH11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:NH1	2:F:18:G:OP1	2.32	0.62
2:H:47(A):C:H2'	2:H:47(B):G:C8	2.34	0.62
1:D:224:PHE:HD1	1:E:218:ASN:HB2	1.62	0.62
1:B:128:ASN:HD21	1:B:135:SER:HA	1.64	0.62
1:B:178:ILE:HG23	1:B:179:MET:N	2.14	0.62
1:A:302:ILE:HG22	1:A:306:LYS:HE3	1.81	0.62
2:H:32:C:H2'	2:H:33:U:C6	2.34	0.62
1:C:25:ILE:HG13	1:C:26:TYR:N	2.14	0.62
2:F:63:C:H2'	2:F:64:A:H8	1.62	0.62
1:E:396:ALA:HB2	1:E:428:LEU:HD23	1.82	0.62
1:D:5:LEU:HD21	1:D:39:ARG:HG2	1.82	0.62
2:G:67(A):A:H2'	2:G:68:C:C6	2.34	0.62
2:G:47(H):U:O2'	2:G:47(I):A:H5'	1.99	0.62
1:B:33:GLU:OE1	1:B:60:LYS:HD2	2.00	0.62
1:A:37:LYS:O	1:A:41:GLU:HG3	1.99	0.62
2:G:32:C:H2'	2:G:33:U:C6	2.34	0.62
1:A:11:ILE:HD12	2:G:18:G:OP1	2.00	0.62
2:I:47(E):A:H2'	2:I:47(F):U:O4'	2.00	0.62
2:I:58:A:H1'	2:I:60:U:OP2	2.00	0.62
1:B:123:ILE:HD11	1:B:325:GLU:HB2	1.81	0.62
1:A:25:ILE:HG13	1:A:26:TYR:N	2.14	0.62
1:D:1:MET:CG	1:D:2:LYS:N	2.62	0.62
1:C:312:ARG:HG2	1:D:173:PHE:HB2	1.82	0.62
1:B:187:ARG:NE	1:B:203:ALA:HB1	2.14	0.62
1:C:57:VAL:O	1:C:61:ILE:HG13	2.00	0.62
1:C:32:ARG:HH11	1:C:32:ARG:HG2	1.64	0.61
1:A:425:ASP:CG	1:A:425:ASP:O	2.37	0.61
2:F:69:U:H2'	2:F:70:C:H6	1.64	0.61
1:C:67:PRO:HB2	1:D:96:PHE:CZ	2.34	0.61
2:F:47(G):U:C6	2:F:47(G):U:O5'	2.51	0.61
1:A:69:ILE:HG12	1:B:122:HIS:ND1	2.14	0.61
1:C:362:LEU:O	1:C:443:LYS:HG3	2.00	0.61
1:C:187:ARG:NE	1:C:203:ALA:HB1	2.15	0.61
1:C:348:ASP:HB2	1:C:351:ALA:HB2	1.82	0.61
1:C:99:GLU:O	1:D:71:ARG:NH2	2.33	0.61
1:E:33:GLU:OE1	1:E:60:LYS:HD2	2.01	0.61
1:D:79:VAL:HG21	1:D:345:LEU:HG	1.81	0.61
1:C:30:ALA:O	1:C:34:VAL:HG23	2.01	0.61
1:B:61:ILE:O	1:B:65:MET:HG3	1.99	0.61
1:E:363:LEU:HB2	1:E:371:ILE:CD1	2.31	0.61
1:C:405:GLN:HG3	2:G:1:G:O4'	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LEU:HD13	1:C:179:MET:HG3	1.83	0.61
1:A:445:THR:O	1:A:449:LEU:HG	2.01	0.61
2:G:54:U:H2'	2:G:55:U:O4'	2.01	0.61
2:J:30:G:O2'	2:J:31:A:H5'	2.01	0.61
2:H:6:A:H2'	2:H:7:G:C8	2.36	0.61
1:B:123:ILE:CD1	1:B:325:GLU:HB2	2.31	0.61
2:I:67(A):A:H2'	2:I:68:C:C6	2.36	0.61
2:G:29:A:O2'	2:G:30:G:H5'	2.01	0.61
1:C:355:LYS:HG3	1:C:439:LEU:HD11	1.83	0.61
2:G:69:U:H2'	2:G:70:C:C6	2.35	0.61
1:B:405:GLN:NE2	1:B:422:ILE:HG21	2.15	0.61
1:C:102:ASN:CB	1:D:71:ARG:HH22	2.04	0.60
1:D:125:LYS:O	1:D:129:GLU:HG3	2.00	0.60
1:D:347:GLN:NE2	1:D:352:LEU:HD21	2.16	0.60
1:C:75:ALA:HB3	1:C:420:CYS:HB3	1.83	0.60
1:E:11:ILE:O	1:E:15:VAL:HG23	2.01	0.60
1:E:10:GLN:OE1	1:E:13:LYS:HE3	2.01	0.60
1:D:347:GLN:HE21	1:D:352:LEU:HD21	1.66	0.60
2:G:71:C:H2'	2:G:72:C:C6	2.36	0.60
1:B:452:ILE:HG23	1:B:452:ILE:OXT	2.00	0.60
1:E:158:GLU:OE2	1:E:187:ARG:HD2	2.00	0.60
1:A:251:GLY:HA2	1:A:268:PHE:HE2	1.66	0.60
2:H:69:U:H2'	2:H:70:C:C6	2.36	0.60
1:A:130:LEU:HD13	1:A:253:LEU:HD21	1.83	0.60
2:F:30:G:O2'	2:F:31:A:H5'	2.01	0.60
2:H:53:G:O2'	2:H:54:U:H5'	2.00	0.60
2:G:47(A):C:H2'	2:G:47(B):G:H8	1.66	0.60
2:I:71:C:H2'	2:I:72:C:C6	2.36	0.60
1:A:420:CYS:SG	1:A:427:LEU:HD21	2.41	0.60
1:E:88:PRO:HG2	1:E:340:PRO:CB	2.31	0.60
1:B:10:GLN:HG2	1:B:12:SER:N	2.15	0.60
1:D:216:LYS:HG2	1:D:219:PHE:CZ	2.37	0.60
1:D:163:ARG:HH11	1:E:166:LEU:CD1	2.14	0.60
1:B:57:VAL:O	1:B:61:ILE:HG13	2.01	0.60
1:C:344:MET:O	1:C:432:ARG:HD2	2.01	0.60
1:B:28:VAL:O	1:B:32:ARG:HG3	2.02	0.60
1:E:57:VAL:O	1:E:61:ILE:HG13	2.01	0.60
2:J:6:A:H2'	2:J:7:G:C8	2.37	0.60
1:A:399:HIS:HE1	1:A:401:ARG:CD	2.14	0.60
1:D:123:ILE:CD1	1:D:325:GLU:HB2	2.32	0.60
2:I:69:U:H2'	2:I:70:C:C6	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:NH1	1:A:32:ARG:HG2	2.16	0.60
2:G:15:C:H2'	2:G:16:U:C6	2.37	0.60
1:B:11:ILE:O	1:B:15:VAL:HG23	2.02	0.60
1:B:178:ILE:CG2	1:B:179:MET:N	2.65	0.60
1:D:200:TYR:CD2	1:D:228:VAL:HG21	2.36	0.60
1:C:285:LLP:OP1	1:D:312:ARG:NH1	2.33	0.60
2:G:6:A:H2'	2:G:7:G:C8	2.37	0.60
1:C:423:ARG:HD2	1:C:428:LEU:CD1	2.32	0.60
1:A:363:LEU:O	1:A:371:ILE:HD11	2.02	0.60
1:C:14:VAL:HG13	1:C:18:PHE:HE2	1.66	0.60
1:A:10:GLN:HB3	1:A:13:LYS:HG3	1.84	0.59
1:C:11:ILE:CB	2:I:16:U:H4'	2.32	0.59
2:F:71:C:H2'	2:F:72:C:C6	2.36	0.59
1:D:336:TYR:O	1:D:339:ILE:HG12	2.02	0.59
2:J:69:U:H2'	2:J:70:C:C6	2.36	0.59
1:E:107:LEU:HD11	1:E:321:LEU:HD23	1.84	0.59
1:B:10:GLN:CB	1:B:13:LYS:HE3	2.31	0.59
1:C:399:HIS:CE1	1:C:401:ARG:HD3	2.27	0.59
2:J:38:A:HO2'	2:J:39:U:H5'	1.67	0.59
2:I:10:A:C2	2:I:26:C:O2	2.54	0.59
1:A:397:ILE:HD11	1:A:427:LEU:HD23	1.84	0.59
1:E:107:LEU:O	1:E:122:HIS:HE1	1.85	0.59
1:D:32:ARG:O	1:D:36:GLU:HG2	2.02	0.59
1:B:32:ARG:NH1	1:B:32:ARG:HG2	2.18	0.59
1:C:187:ARG:HD3	1:C:203:ALA:HB1	1.84	0.59
1:C:93:VAL:HA	1:C:326:MET:HG2	1.84	0.59
1:A:10:GLN:HG3	2:G:19:G:P	2.43	0.59
2:I:38:A:O2'	2:I:39:U:H5'	2.02	0.59
2:J:71:C:H2'	2:J:72:C:C6	2.37	0.59
1:D:2:LYS:O	1:D:2:LYS:HG2	2.03	0.59
1:A:150:LEU:HD13	1:A:179:MET:HG3	1.84	0.59
1:E:187:ARG:CD	1:E:203:ALA:HB1	2.32	0.59
1:D:208:THR:HG22	1:D:242:ILE:HD13	1.85	0.59
1:C:10:GLN:HG3	2:I:19:G:P	2.43	0.59
2:I:63:C:H2'	2:I:64:A:H8	1.67	0.59
1:C:366:ILE:HB	1:C:369:LEU:CD1	2.33	0.59
1:D:373:VAL:HG22	1:D:395:VAL:HG22	1.85	0.59
1:B:12:SER:HG	2:F:16:U:H1'	1.68	0.59
1:C:285:LLP:P	1:D:312:ARG:HH22	2.26	0.59
1:E:2:LYS:O	1:E:6:ARG:HG3	2.02	0.59
1:A:193:ASN:O	1:A:225:VAL:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:67(A):A:H2'	2:H:68:C:H6	1.68	0.58
1:B:30:ALA:O	1:B:34:VAL:HG23	2.02	0.58
2:G:4:A:H2'	2:G:5:G:C8	2.38	0.58
1:C:13:LYS:HA	1:C:16:GLU:OE1	2.03	0.58
1:C:32:ARG:NH1	1:C:32:ARG:HG2	2.18	0.58
1:C:83:ASN:HB3	1:D:109:TYR:CD2	2.27	0.58
2:G:39:U:H2'	2:G:40:C:O4'	2.04	0.58
1:B:242:ILE:HG23	1:B:243:PRO:HD2	1.85	0.58
1:D:420:CYS:SG	1:D:427:LEU:HD11	2.43	0.58
1:A:153:LEU:HD11	1:A:301:LEU:HD22	1.85	0.58
1:C:373:VAL:HG22	1:C:395:VAL:HG22	1.84	0.58
1:D:66:LYS:NZ	1:D:415:GLU:OE2	2.36	0.58
1:B:1:MET:C	1:B:3:SER:H	2.06	0.58
2:F:67:U:H2'	2:F:67(A):A:H8	1.68	0.58
2:H:24:C:O2'	2:H:25:U:H5'	2.03	0.58
2:I:10:A:C4'	2:I:45:U:O4'	2.51	0.58
1:E:396:ALA:HB1	1:E:426:GLN:CD	2.24	0.58
1:E:169:ILE:O	1:E:173:PHE:HB3	2.04	0.58
1:A:409:ARG:NH1	1:A:413:LEU:CD1	2.67	0.58
1:D:10:GLN:HG2	1:D:12:SER:N	2.16	0.58
1:A:181:LYS:HG3	1:B:309:PRO:CG	2.29	0.58
1:B:256:LEU:HD23	1:B:263:VAL:HG21	1.83	0.58
2:J:53:G:H2'	2:J:54:U:H6	1.68	0.58
2:H:35:C:N4	2:H:36:A:N6	2.50	0.58
1:A:126:TYR:CB	1:A:328:LEU:HD13	2.34	0.58
2:H:69:U:H2'	2:H:70:C:H6	1.68	0.58
1:E:7:GLN:HB2	1:E:50:LEU:CD1	2.33	0.58
1:C:332:PHE:HZ	1:D:29:LYS:HD2	1.61	0.58
1:C:344:MET:O	1:C:432:ARG:CD	2.52	0.58
1:E:399:HIS:CE1	1:E:450:LEU:HD22	2.38	0.58
2:F:4:A:H2'	2:F:5:G:H8	1.69	0.58
2:H:71:C:H2'	2:H:72:C:C6	2.39	0.58
1:C:55:GLU:O	1:C:59:ARG:HG3	2.03	0.58
1:B:358:ARG:NH2	1:B:439:LEU:HD12	2.16	0.58
2:H:21:U:H2'	2:H:22:G:H8	1.67	0.58
2:I:59:U:O2'	2:I:60:U:H5'	2.03	0.58
2:J:69:U:H2'	2:J:70:C:H6	1.69	0.58
1:C:272:ILE:HD11	1:C:296:VAL:HG23	1.86	0.58
2:F:38:A:O2'	2:F:39:U:H5'	2.03	0.58
1:B:298:LYS:O	1:B:302:ILE:HG12	2.03	0.58
1:D:33:GLU:OE1	1:D:60:LYS:HD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:MET:O	1:D:432:ARG:CD	2.52	0.58
2:J:54:U:H2'	2:J:55:U:O4'	2.04	0.58
1:C:69:ILE:HD11	1:D:321:LEU:HG	1.85	0.58
1:B:32:ARG:O	1:B:36:GLU:HG2	2.04	0.58
2:J:18:G:O2'	2:J:57:G:N2	2.35	0.58
1:C:363:LEU:HD22	1:C:366:ILE:HD12	1.86	0.58
1:D:37:LYS:O	1:D:41:GLU:HG3	2.04	0.58
2:J:63:C:H2'	2:J:64:A:H8	1.69	0.57
2:J:53:G:O2'	2:J:54:U:H5'	2.03	0.57
1:C:10:GLN:HB3	1:C:13:LYS:HG3	1.85	0.57
2:H:7:G:C2	2:H:49:G:C8	2.92	0.57
2:J:28:U:O2'	2:J:29:A:H5'	2.04	0.57
1:D:224:PHE:CD1	1:E:218:ASN:HB2	2.38	0.57
2:G:4:A:H2'	2:G:5:G:H8	1.69	0.57
1:A:409:ARG:HH12	1:A:413:LEU:CD1	2.17	0.57
1:E:353:ARG:HB2	1:E:393:TYR:CE2	2.39	0.57
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.70	0.57
2:G:53:G:H2'	2:G:54:U:H6	1.68	0.57
1:B:24:GLU:O	1:B:28:VAL:HG23	2.04	0.57
1:C:49:ASP:OD1	1:C:50:LEU:N	2.37	0.57
2:G:26:C:H2'	2:G:27:C:O4'	2.04	0.57
2:F:6:A:O2'	2:F:7:G:H5'	2.04	0.57
2:J:53:G:H2'	2:J:54:U:C6	2.39	0.57
1:A:85:GLY:HA2	1:B:107:LEU:CD2	2.35	0.57
1:A:435:PHE:HB2	1:A:438:ASP:OD2	2.04	0.57
1:E:120:ILE:HG21	1:E:137:PHE:CD1	2.39	0.57
1:B:3:SER:O	1:B:7:GLN:HG2	2.04	0.57
1:B:10:GLN:HB2	2:F:19:G:C3'	2.34	0.57
2:F:54:U:H2'	2:F:55:U:O4'	2.04	0.57
2:H:53:G:H2'	2:H:54:U:H6	1.70	0.57
2:H:30:G:O2'	2:H:31:A:H5'	2.05	0.57
1:C:157:LYS:HE2	1:C:209:ALA:CB	2.19	0.57
1:C:423:ARG:HD2	1:C:428:LEU:HD12	1.86	0.57
1:D:399:HIS:CE1	1:D:401:ARG:HB2	2.40	0.57
2:F:71:C:H2'	2:F:72:C:H6	1.70	0.57
2:G:25:U:C2	2:G:26:C:C5	2.93	0.57
2:H:48:G:H4'	2:H:49:G:H5''	1.86	0.57
1:B:224:PHE:HD1	1:C:218:ASN:HB2	1.69	0.57
2:F:4:A:H2'	2:F:5:G:C8	2.39	0.57
2:F:35:C:O2'	2:F:36:A:H5'	2.03	0.57
2:H:15:C:H2'	2:H:16:U:H6	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:LEU:HD23	1:D:427:LEU:HD22	1.86	0.57
1:A:359:LEU:HB2	1:A:439:LEU:HD22	1.87	0.57
1:A:251:GLY:HA2	1:A:268:PHE:CE2	2.40	0.57
1:C:386:PRO:HG2	1:C:387:GLU:H	1.70	0.57
1:B:175:ILE:N	1:B:176:PRO:HD2	2.19	0.57
1:E:169:ILE:HG22	1:E:218:ASN:OD1	2.05	0.57
1:C:339:ILE:CD1	1:C:342:ILE:HG13	2.34	0.57
1:E:408:SER:O	1:E:412:ARG:HG3	2.04	0.57
1:C:421:ARG:HH11	1:C:421:ARG:HG2	1.68	0.57
2:I:47(I):A:H2'	2:I:47(J):A:O4'	2.05	0.57
2:F:53:G:H2'	2:F:54:U:H6	1.69	0.57
1:C:187:ARG:CD	1:C:203:ALA:HB1	2.33	0.57
1:B:137:PHE:CE1	1:B:306:LYS:HG2	2.40	0.57
1:D:234:VAL:HG11	1:D:275:GLY:HA3	1.87	0.57
1:E:25:ILE:HG13	1:E:26:TYR:N	2.19	0.57
1:B:10:GLN:HB3	1:B:13:LYS:CG	2.30	0.57
2:I:54:U:H2'	2:I:55:U:O4'	2.03	0.57
2:G:26:C:O2'	2:G:27:C:H5'	2.04	0.57
1:A:161:ILE:CG2	1:A:166:LEU:HD21	2.35	0.57
2:H:4:A:H2'	2:H:5:G:H8	1.70	0.57
1:C:11:ILE:HD12	2:I:18:G:OP1	2.05	0.56
2:G:43:G:H5'	2:G:43:G:H8	1.70	0.56
2:F:53:G:O2'	2:F:54:U:H5'	2.05	0.56
1:A:360:GLU:O	1:A:364:LYS:HG3	2.05	0.56
1:A:169:ILE:O	1:A:173:PHE:HB3	2.05	0.56
1:A:137:PHE:CD1	1:A:306:LYS:HG2	2.40	0.56
1:E:299:LYS:O	1:E:303:GLU:HG2	2.05	0.56
1:D:87:ALA:CB	1:D:341:VAL:HG21	2.35	0.56
1:B:216:LYS:HG2	1:B:219:PHE:CZ	2.40	0.56
2:I:38:A:H2'	2:I:39:U:O4'	2.04	0.56
2:G:69:U:H2'	2:G:70:C:H6	1.69	0.56
1:B:443:LYS:O	1:B:447:GLN:HG2	2.05	0.56
1:A:194:LYS:HG2	1:A:226:GLU:HB2	1.87	0.56
2:J:14:G:O2'	2:J:15:C:H5'	2.05	0.56
2:G:53:G:H2'	2:G:54:U:C6	2.40	0.56
1:E:1:MET:HG3	1:E:4:LEU:CD1	2.35	0.56
1:C:6:ARG:NH1	2:I:20:U:O4	2.38	0.56
2:H:36:A:H2'	2:H:37:A:O4'	2.05	0.56
1:C:69:ILE:CD1	1:D:321:LEU:HG	2.36	0.56
1:E:200:TYR:CE2	1:E:228:VAL:HG21	2.41	0.56
1:C:14:VAL:HG13	1:C:18:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4:A:H2'	2:J:5:G:H8	1.70	0.56
1:C:141:ASN:OD1	1:C:143:ALA:HB3	2.05	0.56
1:E:336:TYR:O	1:E:339:ILE:HG12	2.04	0.56
1:D:360:GLU:HG3	1:D:371:ILE:HG21	1.87	0.56
2:H:47(E):A:H2'	2:H:47(F):U:H5'	1.88	0.56
1:C:169:ILE:O	1:C:173:PHE:HB3	2.05	0.56
2:H:41:U:O2'	2:H:42:A:H5'	2.05	0.56
2:J:35:C:H2'	2:J:36:A:O4'	2.06	0.56
1:B:15:VAL:HA	1:B:27:VAL:HG11	1.88	0.56
1:E:1:MET:C	1:E:3:SER:N	2.57	0.56
2:I:10:A:H5'	2:I:45:U:O4'	2.06	0.56
1:C:194:LYS:NZ	1:C:224:PHE:HB3	2.21	0.56
1:B:187:ARG:CD	1:B:203:ALA:HB1	2.36	0.56
1:D:107:LEU:HD11	1:D:321:LEU:HD23	1.88	0.56
1:C:211:LEU:HG	1:C:242:ILE:CG2	2.34	0.56
1:E:18:PHE:HB3	1:E:21:ALA:HB3	1.87	0.56
2:I:15:C:H2'	2:I:16:U:H6	1.70	0.56
2:G:47(K):G:O2'	2:G:47(L):C:H5'	2.06	0.56
2:H:47(E):A:C2'	2:H:47(F):U:H5'	2.35	0.56
2:H:32:C:C4	2:H:33:U:C4	2.93	0.56
1:E:401:ARG:NH1	1:E:450:LEU:O	2.39	0.56
1:D:22:TYR:CG	1:D:61:ILE:HG21	2.41	0.56
1:C:366:ILE:HB	1:C:369:LEU:HD12	1.88	0.56
2:H:4:A:H2'	2:H:5:G:C8	2.40	0.56
1:D:194:LYS:HB2	1:E:168:GLU:OE1	2.06	0.56
2:G:53:G:O2'	2:G:54:U:H5'	2.05	0.56
1:D:5:LEU:HD21	2:H:56:C:N4	2.21	0.56
1:E:161:ILE:HG13	1:E:212:MET:O	2.05	0.56
1:E:88:PRO:HG2	1:E:340:PRO:HB2	1.88	0.56
1:D:194:LYS:HG2	1:D:226:GLU:HB2	1.87	0.56
1:E:269:ARG:HG3	1:E:269:ARG:HH11	1.71	0.56
2:I:53:G:O2'	2:I:54:U:H5'	2.06	0.56
1:C:26:TYR:OH	1:D:333:GLU:CG	2.54	0.56
1:C:285:LLP:OP3	1:D:312:ARG:NH2	2.26	0.56
1:D:30:ALA:O	1:D:34:VAL:HG23	2.06	0.56
1:B:40:LYS:O	1:B:44:GLU:HG3	2.06	0.56
1:C:39:ARG:HH22	2:I:18:G:C2'	2.17	0.56
2:J:4:A:H2'	2:J:5:G:C8	2.41	0.56
1:A:57:VAL:O	1:A:61:ILE:HG13	2.05	0.55
1:B:402:LEU:HD12	1:B:450:LEU:CD2	2.36	0.55
1:E:213:LYS:HE3	1:E:246:TYR:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:39:U:H2'	2:I:40:C:O4'	2.05	0.55
2:F:27:C:H2'	2:F:28:U:O4'	2.06	0.55
2:I:69:U:H2'	2:I:70:C:H6	1.69	0.55
1:D:230:LEU:O	1:D:234:VAL:HG23	2.06	0.55
2:F:67:U:H2'	2:F:67(A):A:C8	2.42	0.55
1:A:366:ILE:HG23	1:A:367:PRO:HD2	1.89	0.55
1:E:399:HIS:CE1	1:E:401:ARG:HD3	2.41	0.55
1:D:201:GLU:OE2	1:D:239:LYS:NZ	2.37	0.55
1:B:282:SER:OG	1:B:285:LLP:H4'2	2.07	0.55
1:B:72:VAL:HG22	1:B:417:PRO:HG2	1.88	0.55
1:D:163:ARG:HG2	1:D:188:GLU:HB2	1.87	0.55
1:E:87:ALA:CB	1:E:341:VAL:HG21	2.37	0.55
1:D:123:ILE:HD11	1:D:325:GLU:HB2	1.89	0.55
1:D:27:VAL:HG22	1:D:61:ILE:HD13	1.88	0.55
1:D:220:TYR:CD2	1:D:387:GLU:HG2	2.41	0.55
1:A:39:ARG:NH2	2:G:18:G:O2'	2.40	0.55
2:I:53:G:H2'	2:I:54:U:H6	1.72	0.55
1:C:420:CYS:SG	1:C:427:LEU:HD11	2.47	0.55
1:E:169:ILE:HD11	1:E:285:LLP:H5'1	1.87	0.55
2:I:4:A:H2'	2:I:5:G:C8	2.42	0.55
1:C:107:LEU:O	1:C:122:HIS:HE1	1.90	0.55
2:G:47(A):C:H2'	2:G:47(B):G:C8	2.42	0.55
2:G:59:U:O2'	2:G:60:U:H5'	2.06	0.55
2:F:59:U:O2'	2:F:60:U:H5'	2.07	0.55
1:A:123:ILE:HD11	1:A:325:GLU:HB2	1.87	0.55
1:C:216:LYS:HG2	1:C:219:PHE:CZ	2.42	0.55
1:C:242:ILE:HG23	1:C:243:PRO:HD2	1.88	0.55
1:A:234:VAL:HG12	1:A:238:HIS:CD2	2.41	0.55
1:B:399:HIS:CD2	1:B:450:LEU:HD13	2.41	0.55
1:A:194:LYS:HG2	1:A:226:GLU:CB	2.36	0.55
1:D:326:MET:O	1:D:330:LEU:HG	2.06	0.55
1:A:157:LYS:CE	1:A:209:ALA:HB2	2.32	0.55
1:C:39:ARG:NH2	2:I:18:G:O2'	2.39	0.55
1:D:150:LEU:HB3	1:D:182:SER:OG	2.07	0.55
1:C:363:LEU:HD21	1:C:443:LYS:HA	1.88	0.55
1:A:169:ILE:HG13	1:A:173:PHE:CD2	2.41	0.55
2:H:47(L):C:H2'	2:H:47(M):G:C8	2.41	0.55
2:J:43:G:H8	2:J:43:G:H5'	1.72	0.55
1:D:10:GLN:HB2	2:H:19:G:C3'	2.37	0.55
2:G:41:U:O2'	2:G:42:A:H5'	2.07	0.55
2:H:63:C:H2'	2:H:64:A:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:47(G):U:H2'	2:J:47(H):U:O4'	2.07	0.55
1:C:26:TYR:OH	1:D:333:GLU:HG2	2.07	0.55
1:A:348:ASP:O	1:A:351:ALA:HB3	2.06	0.55
2:H:28:U:O2'	2:H:29:A:H5'	2.06	0.55
1:C:270:ASP:O	1:C:274:LEU:HG	2.06	0.55
1:B:10:GLN:CB	1:B:13:LYS:HG3	2.33	0.55
1:D:163:ARG:HD2	1:D:190:GLY:O	2.07	0.55
1:E:80:ILE:HG22	1:E:80:ILE:O	2.07	0.55
2:F:47(K):G:O2'	2:F:47(L):C:H5'	2.07	0.54
1:B:208:THR:HG22	1:B:242:ILE:HD13	1.90	0.54
1:E:430:ASP:OD1	1:E:432:ARG:HB3	2.06	0.54
2:J:3:G:H2'	2:J:4:A:O4'	2.08	0.54
1:C:313:ALA:HB1	1:D:144:GLY:CA	2.37	0.54
1:E:278:LEU:HD23	1:E:297:GLY:HA3	1.89	0.54
1:E:74:ASN:HB2	1:E:84:LEU:HD13	1.89	0.54
2:F:38:A:H2'	2:F:39:U:H5'	1.90	0.54
1:A:436:HIS:CD2	1:A:439:LEU:HD12	2.42	0.54
1:C:435:PHE:HB2	1:C:438:ASP:OD2	2.07	0.54
2:J:39:U:H2'	2:J:40:C:O4'	2.07	0.54
1:D:402:LEU:HD12	1:D:450:LEU:CD2	2.38	0.54
2:H:47(F):U:O2'	2:H:47(G):U:H5''	2.08	0.54
2:J:26:C:O2'	2:J:27:C:H5'	2.08	0.54
1:A:239:LYS:HD3	1:A:240:TYR:CE2	2.42	0.54
1:C:171:GLY:HA3	1:D:116:ARG:NH2	2.22	0.54
1:B:169:ILE:HG22	1:B:218:ASN:OD1	2.08	0.54
1:A:265:GLU:HB2	1:A:385:LEU:HD21	1.90	0.54
1:C:317:ASP:HB3	1:D:291:GLN:HB3	1.90	0.54
2:I:4:A:H2'	2:I:5:G:H8	1.72	0.54
2:I:3:G:H2'	2:I:4:A:O4'	2.08	0.54
1:D:392:THR:HG21	1:D:430:ASP:OD2	2.07	0.54
1:A:396:ALA:HB2	1:A:428:LEU:CD2	2.37	0.54
1:D:57:VAL:O	1:D:61:ILE:HG13	2.07	0.54
1:C:302:ILE:CG2	1:C:306:LYS:HE3	2.38	0.54
1:D:405:GLN:HE22	1:D:422:ILE:HG21	1.72	0.54
2:I:47(K):G:O2'	2:I:47(L):C:H5'	2.07	0.54
1:D:438:ASP:O	1:D:442:ILE:HG13	2.08	0.54
1:C:278:LEU:HD23	1:C:297:GLY:HA3	1.89	0.54
1:C:10:GLN:N	1:C:13:LYS:HD2	2.13	0.54
1:C:420:CYS:HB2	1:C:428:LEU:O	2.06	0.54
1:A:388:LEU:HD21	1:A:390:LEU:HD11	1.90	0.54
2:I:71:C:H2'	2:I:72:C:H6	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:GLY:O	1:C:287:LEU:HB3	2.08	0.54
1:A:40:LYS:O	1:A:44:GLU:HG3	2.08	0.54
1:C:234:VAL:HG22	1:C:276:ILE:HD13	1.88	0.54
1:E:347:GLN:NE2	1:E:352:LEU:HD21	2.22	0.54
2:J:71:C:H2'	2:J:72:C:H6	1.73	0.54
1:C:421:ARG:NH1	1:C:421:ARG:HG2	2.22	0.54
1:A:100:ILE:HD12	1:B:69:ILE:HG22	1.90	0.54
1:D:86:ARG:HD2	1:D:284:ASP:OD2	2.08	0.54
1:D:14:VAL:CG1	1:D:18:PHE:HE2	2.21	0.54
1:C:407:LEU:CD2	1:C:427:LEU:HD22	2.38	0.54
1:A:25:ILE:HG13	1:A:26:TYR:H	1.71	0.54
2:H:53:G:H2'	2:H:54:U:C6	2.43	0.54
1:A:96:PHE:O	1:A:100:ILE:HG12	2.08	0.54
1:D:139:VAL:HB	1:D:314:LEU:HB3	1.89	0.54
1:C:28:VAL:HG11	2:I:16:U:OP1	2.08	0.54
1:D:176:PRO:HG3	1:E:191:THR:CG2	2.36	0.54
1:E:28:VAL:HG12	1:E:32:ARG:HE	1.71	0.54
1:A:263:VAL:HG12	1:A:264:ASP:N	2.22	0.54
1:D:423:ARG:HD2	1:D:428:LEU:CD1	2.38	0.54
1:D:256:LEU:HD23	1:D:263:VAL:CG2	2.37	0.54
2:G:55:U:H2'	2:G:57:G:OP2	2.08	0.53
2:G:64:A:H2'	2:G:65:C:C6	2.43	0.53
1:E:220:TYR:HD2	1:E:386:PRO:HB2	1.74	0.53
1:A:171:GLY:CA	1:B:116:ARG:NH2	2.67	0.53
2:G:5(A):U:C2'	2:G:6:A:H5'	2.38	0.53
1:D:191:THR:HG22	1:E:176:PRO:HG3	1.90	0.53
2:I:39:U:H2'	2:I:40:C:C6	2.43	0.53
2:F:53:G:H2'	2:F:54:U:C6	2.42	0.53
2:H:59:U:O2'	2:H:60:U:H5'	2.08	0.53
1:C:194:LYS:HG2	1:C:226:GLU:HB2	1.90	0.53
2:G:71:C:H2'	2:G:72:C:H6	1.72	0.53
1:A:102:ASN:HB3	1:B:71:ARG:HH12	1.72	0.53
1:D:239:LYS:HD3	1:D:240:TYR:CE2	2.43	0.53
1:E:136:SER:HB3	1:E:296:VAL:HG12	1.89	0.53
2:G:10:A:C6	2:G:44:G:N1	2.76	0.53
1:A:420:CYS:SG	1:A:427:LEU:HD11	2.49	0.53
1:E:32:ARG:O	1:E:36:GLU:HG2	2.08	0.53
1:D:348:ASP:HB2	1:D:351:ALA:HB2	1.90	0.53
1:D:47:ARG:HD3	1:D:49:ASP:O	2.08	0.53
1:C:10:GLN:OE1	2:I:20:U:OP1	2.26	0.53
1:D:179:MET:HA	1:D:182:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:HIS:CE1	1:B:401:ARG:HB2	2.44	0.53
1:A:340:PRO:HA	1:A:343:ARG:NH1	2.23	0.53
1:C:179:MET:O	1:C:182:SER:HB3	2.09	0.53
1:B:351:ALA:O	1:B:354:GLN:HB3	2.09	0.53
1:C:343:ARG:O	1:C:347:GLN:HG3	2.09	0.53
1:E:178:ILE:HG23	1:E:179:MET:N	2.23	0.53
2:J:47(K):G:O2'	2:J:47(L):C:H5'	2.07	0.53
2:G:35:C:N4	2:G:36:A:N6	2.56	0.53
1:A:10:GLN:CB	1:A:13:LYS:HE3	2.35	0.53
1:D:39:ARG:NE	2:H:19:G:O6	2.42	0.53
1:D:7:GLN:HB2	1:D:50:LEU:CD1	2.39	0.53
1:E:79:VAL:HG12	1:E:341:VAL:HG13	1.91	0.53
1:D:197:VAL:HG22	1:D:228:VAL:HG13	1.91	0.53
1:D:107:LEU:O	1:D:122:HIS:HE1	1.92	0.53
1:C:159:VAL:HG13	1:C:210:LEU:HB3	1.90	0.53
1:B:10:GLN:HG3	2:F:19:G:P	2.48	0.53
1:C:29:LYS:CD	1:D:332:PHE:CZ	2.89	0.53
1:E:161:ILE:HG21	1:E:166:LEU:HD21	1.90	0.53
1:E:234:VAL:HG12	1:E:238:HIS:CD2	2.44	0.53
2:J:46:C:C4	2:J:47:U:C4	2.97	0.53
1:E:200:TYR:CD2	1:E:228:VAL:HG21	2.44	0.53
2:F:39:U:H2'	2:F:40:C:O4'	2.08	0.53
1:E:79:VAL:HG13	1:E:344:MET:SD	2.48	0.53
1:B:187:ARG:HD3	1:B:203:ALA:HB1	1.91	0.53
2:J:15:C:H2'	2:J:16:U:C6	2.43	0.53
1:D:270:ASP:O	1:D:274:LEU:HG	2.08	0.53
1:A:97:ILE:HD11	1:A:323:GLY:CA	2.34	0.53
1:B:194:LYS:HD3	1:C:168:GLU:OE2	2.09	0.53
2:H:3:G:H2'	2:H:4:A:O4'	2.09	0.53
1:B:179:MET:O	1:B:182:SER:HB3	2.09	0.52
1:A:347:GLN:NE2	1:A:352:LEU:HD21	2.24	0.52
1:A:231:GLU:O	1:A:235:LYS:HG3	2.09	0.52
1:A:11:ILE:HG21	1:A:28:VAL:HG13	1.90	0.52
2:I:18:G:O2'	2:I:57:G:N2	2.38	0.52
1:B:263:VAL:CG1	1:B:388:LEU:HD13	2.35	0.52
1:D:363:LEU:HB2	1:D:371:ILE:HD13	1.90	0.52
1:B:142:ASN:HB3	1:B:285:LLP:OP4	2.08	0.52
1:A:334:LYS:HD2	1:A:336:TYR:OH	2.09	0.52
1:C:11:ILE:CG2	2:I:16:U:H4'	2.39	0.52
1:A:399:HIS:CE1	1:A:401:ARG:HB2	2.44	0.52
1:B:162:SER:HB2	1:B:200:TYR:OH	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HG13	1:A:212:MET:O	2.09	0.52
1:C:86:ARG:NH1	1:C:285:LLP:HE2	2.24	0.52
1:B:425:ASP:O	1:B:425:ASP:CG	2.48	0.52
1:D:396:ALA:HB1	1:D:426:GLN:CD	2.30	0.52
1:C:131:THR:HG21	1:C:296:VAL:HG11	1.92	0.52
1:D:77:GLY:HA3	1:D:430:ASP:CG	2.30	0.52
1:C:165:GLU:OE2	1:C:213:LYS:NZ	2.38	0.52
2:G:39:U:H2'	2:G:40:C:C6	2.45	0.52
2:G:10:A:C6	2:G:44:G:C6	2.97	0.52
2:I:31:A:H2'	2:I:32:C:O4'	2.09	0.52
2:I:41:U:O2'	2:I:42:A:H5'	2.08	0.52
2:I:53:G:H2'	2:I:54:U:C6	2.44	0.52
1:B:200:TYR:CE2	1:B:228:VAL:HG21	2.44	0.52
1:C:407:LEU:HD23	1:C:427:LEU:HD22	1.90	0.52
1:B:210:LEU:HD12	1:B:243:PRO:HG2	1.92	0.52
1:E:211:LEU:HG	1:E:242:ILE:HG21	1.91	0.52
1:C:25:ILE:HG13	1:C:26:TYR:H	1.72	0.52
2:G:3:G:H2'	2:G:4:A:O4'	2.10	0.52
2:H:71:C:H2'	2:H:72:C:H6	1.74	0.52
1:D:165:GLU:OE1	1:D:213:LYS:HG3	2.10	0.52
2:J:5(A):U:C2'	2:J:6:A:H5'	2.39	0.52
1:B:234:VAL:CG2	1:B:276:ILE:HD13	2.39	0.52
1:D:169:ILE:O	1:D:169:ILE:HD12	2.09	0.52
1:E:194:LYS:HG2	1:E:226:GLU:HB2	1.91	0.52
1:C:212:MET:HE3	1:C:245:TYR:HE1	1.75	0.52
1:C:28:VAL:HG12	1:C:32:ARG:NE	2.25	0.52
1:E:208:THR:HG22	1:E:242:ILE:HD13	1.92	0.52
1:B:252:LEU:HD12	1:B:253:LEU:N	2.25	0.52
1:A:370:LYS:HB2	1:A:398:ARG:O	2.10	0.52
2:G:47(E):A:C2	2:G:47(I):A:N7	2.77	0.52
1:D:35:ALA:HB1	1:D:39:ARG:NH2	2.25	0.52
1:C:47:ARG:HD3	1:C:49:ASP:O	2.09	0.52
2:H:6:A:O2'	2:H:7:G:H5'	2.10	0.52
1:B:169:ILE:O	1:B:169:ILE:HG13	2.08	0.52
1:D:254:ILE:HD13	1:D:336:TYR:HE1	1.74	0.52
1:E:25:ILE:HG13	1:E:26:TYR:H	1.73	0.52
1:B:230:LEU:HB3	1:B:274:LEU:CD2	2.39	0.51
1:A:427:LEU:HD23	1:A:429:PHE:HE1	1.75	0.51
1:E:147:PHE:HB2	1:E:178:ILE:HD11	1.92	0.51
1:B:38:TYR:O	1:B:42:ILE:HG13	2.10	0.51
1:C:29:LYS:HD2	1:D:332:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASN:ND2	1:C:224:PHE:HB2	2.25	0.51
1:B:224:PHE:HB2	1:C:218:ASN:ND2	2.25	0.51
1:B:142:ASN:HD22	1:B:285:LLP:C5	2.23	0.51
1:B:91:LYS:HE2	1:B:95:ASN:HD21	1.75	0.51
1:B:360:GLU:HG3	1:B:371:ILE:CG2	2.41	0.51
1:B:5:LEU:HD12	1:B:8:ILE:CD1	2.41	0.51
1:A:15:VAL:HA	1:A:27:VAL:HG11	1.91	0.51
2:F:39:U:H2'	2:F:40:C:C6	2.45	0.51
2:F:47(E):A:O2'	2:F:47(I):A:N6	2.41	0.51
2:G:27:C:O2'	2:G:28:U:H5'	2.10	0.51
2:G:6:A:O2'	2:G:7:G:H5'	2.11	0.51
1:E:234:VAL:HG11	1:E:275:GLY:HA3	1.92	0.51
1:E:123:ILE:HD13	1:E:324:LEU:HD23	1.92	0.51
2:G:47(G):U:H2'	2:G:47(H):U:O4'	2.11	0.51
1:C:2:LYS:O	1:C:6:ARG:HG3	2.09	0.51
2:I:6:A:O2'	2:I:7:G:H5'	2.09	0.51
2:F:67(A):A:H2'	2:F:68:C:H6	1.76	0.51
2:F:47:U:H2'	2:F:47(A):C:H6	1.72	0.51
1:A:278:LEU:HD11	1:A:305:ILE:HD11	1.93	0.51
1:D:227:GLU:HG2	1:D:228:VAL:N	2.26	0.51
2:H:39:U:H2'	2:H:40:C:O4'	2.10	0.51
2:F:43:G:H5'	2:F:43:G:H8	1.75	0.51
1:A:33:GLU:CD	1:A:60:LYS:HE3	2.30	0.51
2:J:6:A:O2'	2:J:7:G:H5'	2.10	0.51
1:E:363:LEU:HD22	1:E:446:LEU:HD12	1.91	0.51
1:D:208:THR:CG2	1:D:242:ILE:HD13	2.39	0.51
1:B:396:ALA:HB2	1:B:428:LEU:HD23	1.93	0.51
2:F:64:A:H2'	2:F:65:C:C6	2.46	0.51
2:J:59:U:O2'	2:J:60:U:H5'	2.10	0.51
1:B:147:PHE:CD2	1:B:147:PHE:C	2.83	0.51
2:I:14:G:O2'	2:I:15:C:H5'	2.10	0.51
2:J:64:A:H2'	2:J:65:C:C6	2.45	0.51
2:F:47(G):U:H2'	2:F:47(H):U:O4'	2.11	0.51
2:H:7:G:O2'	2:H:8:A:H5'	2.11	0.51
2:H:54:U:H2'	2:H:55:U:O4'	2.09	0.51
2:F:3:G:H2'	2:F:4:A:O4'	2.10	0.51
2:I:43:G:H5'	2:I:43:G:H8	1.75	0.51
1:C:361:LYS:HA	1:C:364:LYS:HE3	1.93	0.51
2:J:41:U:O2'	2:J:42:A:H5'	2.11	0.51
2:H:14:G:O2'	2:H:15:C:H5'	2.11	0.51
2:J:52:G:O2'	2:J:53:G:H5'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:O	1:B:18:PHE:HD2	1.93	0.51
2:I:64:A:H2'	2:I:65:C:C6	2.46	0.51
2:I:67:U:H2'	2:I:67(A):A:H8	1.76	0.51
1:B:5:LEU:CD1	1:B:42:ILE:HD12	2.41	0.51
1:B:11:ILE:HG22	2:F:16:U:H4'	1.93	0.51
1:B:10:GLN:NE2	1:B:12:SER:OG	2.44	0.51
1:E:1:MET:O	1:E:3:SER:N	2.44	0.51
2:F:36:A:O2'	2:F:37:A:H5'	2.11	0.51
1:E:242:ILE:HG23	1:E:243:PRO:HD2	1.93	0.51
1:B:404:SER:OG	1:B:425:ASP:HA	2.11	0.51
1:C:392:THR:HG21	1:C:430:ASP:OD2	2.10	0.51
1:A:187:ARG:HG3	1:A:187:ARG:HH11	1.76	0.51
1:E:261:ILE:HG22	1:E:263:VAL:HG13	1.92	0.51
2:G:31:A:N7	2:G:32:C:C5	2.80	0.50
1:A:179:MET:O	1:A:182:SER:HB3	2.11	0.50
1:A:87:ALA:CB	1:A:341:VAL:HG21	2.41	0.50
1:A:3:SER:O	1:A:7:GLN:HG2	2.10	0.50
1:B:5:LEU:HD12	1:B:8:ILE:HD12	1.93	0.50
2:G:25:U:N3	2:G:26:C:C4	2.80	0.50
2:H:64:A:H2'	2:H:65:C:C6	2.45	0.50
2:H:47(K):G:O2'	2:H:47(L):C:H5'	2.11	0.50
2:H:47(L):C:H2'	2:H:47(M):G:H8	1.75	0.50
1:C:252:LEU:HD13	1:C:286:LEU:HB3	1.94	0.50
1:B:337:GLU:N	1:B:337:GLU:OE1	2.43	0.50
2:J:32:C:H2'	2:J:33:U:C5	2.41	0.50
1:A:153:LEU:CD1	1:A:301:LEU:HD22	2.42	0.50
1:A:126:TYR:HB2	1:A:328:LEU:HD13	1.92	0.50
1:D:25:ILE:HG13	1:D:26:TYR:N	2.27	0.50
1:C:173:PHE:HB2	1:D:312:ARG:HG2	1.93	0.50
1:C:4:LEU:O	1:C:42:ILE:HD13	2.12	0.50
1:C:12:SER:OG	2:I:16:U:H1'	2.11	0.50
2:H:45:U:H2'	2:H:46:C:O4'	2.12	0.50
1:E:363:LEU:CB	1:E:371:ILE:CD1	2.89	0.50
1:C:79:VAL:HG21	1:C:345:LEU:CD2	2.42	0.50
1:D:452:ILE:OXT	1:D:452:ILE:HG23	2.12	0.50
1:C:157:LYS:CE	1:C:209:ALA:HB2	2.20	0.50
1:A:34:VAL:HG12	1:A:53:PHE:CE1	2.46	0.50
2:G:5(A):U:H2'	2:G:6:A:H5'	1.93	0.50
1:B:230:LEU:HB3	1:B:274:LEU:HD21	1.94	0.50
1:D:369:LEU:HD21	1:D:450:LEU:CD1	2.42	0.50
1:C:358:ARG:NH2	1:C:439:LEU:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:ND2	1:D:122:HIS:CD2	2.79	0.50
1:A:357:LYS:O	1:A:361:LYS:HG3	2.11	0.50
1:D:278:LEU:HD23	1:D:297:GLY:HA3	1.94	0.50
1:A:396:ALA:HB2	1:A:428:LEU:HD21	1.94	0.50
1:C:168:GLU:O	1:C:168:GLU:HG2	2.12	0.50
1:D:299:LYS:O	1:D:303:GLU:HG2	2.11	0.50
1:D:6:ARG:NH1	2:H:20:U:O4	2.45	0.50
1:E:34:VAL:HG21	1:E:57:VAL:HA	1.94	0.50
2:H:46:C:H2'	2:H:47:U:H5'	1.93	0.50
1:B:123:ILE:O	1:B:125:LYS:N	2.44	0.50
1:D:18:PHE:HB3	1:D:21:ALA:HB3	1.92	0.50
1:A:72:VAL:HG22	1:A:417:PRO:HG2	1.94	0.50
1:E:34:VAL:O	1:E:38:TYR:HD1	1.95	0.50
2:I:24:C:O2'	2:I:25:U:H5'	2.11	0.50
2:I:26:C:H2'	2:I:27:C:O4'	2.11	0.50
2:H:46:C:O2'	2:H:47:U:H5'	2.12	0.50
1:A:161:ILE:HG22	1:A:186:LEU:HD11	1.93	0.50
1:D:90:SER:HB3	1:D:338:ASP:O	2.12	0.50
2:H:25:U:O2'	2:H:26:C:H5'	2.11	0.50
1:C:161:ILE:CG2	1:C:166:LEU:HD21	2.41	0.50
1:B:55:GLU:O	1:B:59:ARG:HG3	2.11	0.50
1:E:7:GLN:HB2	1:E:50:LEU:HD11	1.92	0.50
1:B:186:LEU:HD12	1:B:187:ARG:N	2.27	0.50
1:B:22:TYR:CG	1:B:61:ILE:HG21	2.46	0.50
1:C:161:ILE:HD13	1:C:166:LEU:CD2	2.42	0.50
1:E:97:ILE:HD11	1:E:323:GLY:HA3	1.94	0.50
1:B:396:ALA:HB2	1:B:428:LEU:CD2	2.41	0.49
2:G:9:U:C4	2:G:48:G:C8	2.99	0.49
1:E:435:PHE:HB2	1:E:438:ASP:OD2	2.12	0.49
1:E:79:VAL:CG1	1:E:341:VAL:HG13	2.41	0.49
2:J:47(N):A:C6	2:J:47(O):G:C6	3.00	0.49
1:E:396:ALA:HB2	1:E:428:LEU:CD2	2.41	0.49
1:D:396:ALA:HB1	1:D:426:GLN:HG2	1.94	0.49
1:B:174:ARG:C	1:B:176:PRO:HD2	2.33	0.49
2:I:47:U:H2'	2:I:47(A):C:H6	1.76	0.49
1:A:340:PRO:O	1:A:344:MET:HG3	2.12	0.49
1:D:363:LEU:HB2	1:D:371:ILE:CD1	2.42	0.49
1:D:72:VAL:HG22	1:D:417:PRO:HG2	1.94	0.49
1:D:163:ARG:HG3	1:D:189:VAL:O	2.13	0.49
1:E:28:VAL:HG12	1:E:32:ARG:NE	2.28	0.49
1:D:200:TYR:HE2	1:D:228:VAL:HG21	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:43:G:H8	2:H:43:G:H5'	1.77	0.49
2:F:5(A):U:C2'	2:F:6:A:H5'	2.42	0.49
2:I:25:U:C2'	2:I:26:C:H5'	2.42	0.49
2:I:47(I):A:C2'	2:I:47(J):A:H5'	2.43	0.49
1:A:409:ARG:NH1	1:A:413:LEU:HD11	2.27	0.49
1:B:18:PHE:HB3	1:B:21:ALA:HB3	1.93	0.49
2:J:31:A:H2'	2:J:32:C:O4'	2.13	0.49
2:H:67:U:H2'	2:H:67(A):A:H8	1.77	0.49
1:C:194:LYS:HG2	1:C:226:GLU:N	2.27	0.49
2:H:47(F):U:C2'	2:H:47(G):U:H5''	2.42	0.49
2:H:39:U:H2'	2:H:40:C:C6	2.47	0.49
1:A:8:ILE:CD1	1:A:38:TYR:HB3	2.42	0.49
2:F:47(L):C:H2'	2:F:47(M):G:C8	2.48	0.49
1:C:312:ARG:HD2	1:C:315:ARG:NH1	2.28	0.49
1:E:347:GLN:NE2	1:E:352:LEU:CD2	2.75	0.49
1:E:77:GLY:HA3	1:E:430:ASP:CB	2.42	0.49
1:C:1:MET:HG3	1:C:4:LEU:HD12	1.94	0.49
2:J:5(A):U:H2'	2:J:6:A:H5'	1.95	0.49
1:C:123:ILE:HG23	1:C:328:LEU:HD12	1.95	0.49
2:J:47(E):A:H2	2:J:47(I):A:N7	2.11	0.49
1:D:358:ARG:HH21	1:D:439:LEU:HD12	1.76	0.49
1:E:399:HIS:HE1	1:E:401:ARG:HD3	1.77	0.49
1:C:257:LYS:HD2	2:H:5:G:H4'	1.94	0.49
1:D:360:GLU:HG3	1:D:371:ILE:CG2	2.42	0.49
1:A:313:ALA:HB1	1:B:144:GLY:CA	2.43	0.49
2:G:47(G):U:O5'	2:G:47(G):U:H6	1.95	0.49
1:D:178:ILE:CG2	1:D:179:MET:N	2.76	0.49
1:E:366:ILE:HG23	1:E:367:PRO:HD2	1.95	0.49
1:D:163:ARG:NH1	1:E:188:GLU:OE1	2.46	0.49
1:C:330:LEU:HD22	1:C:335:ARG:HD3	1.95	0.49
1:C:172:SER:OG	1:D:312:ARG:HB2	2.13	0.49
1:A:250:SER:HB2	1:A:286:LEU:HD12	1.94	0.49
1:A:200:TYR:CD2	1:A:233:LEU:HD21	2.48	0.49
1:A:5:LEU:HD12	1:A:8:ILE:HD12	1.94	0.49
2:G:67:U:H2'	2:G:67(A):A:H8	1.78	0.49
2:I:26:C:O2'	2:I:27:C:H5'	2.13	0.49
2:I:46:C:C4	2:I:47:U:C4	3.00	0.49
1:B:408:SER:O	1:B:412:ARG:HG3	2.12	0.49
1:D:161:ILE:HD13	1:D:166:LEU:HD23	1.94	0.49
1:B:145:ALA:HB1	1:B:295:ILE:HD11	1.95	0.49
1:D:196:LYS:N	1:D:199:ASP:OD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:G:O2'	2:G:15:C:H5'	2.13	0.48
1:E:363:LEU:HD22	1:E:366:ILE:HD12	1.95	0.48
1:D:123:ILE:O	1:D:125:LYS:N	2.46	0.48
2:F:28:U:H2'	2:F:29:A:C8	2.48	0.48
1:E:370:LYS:HG3	1:E:398:ARG:O	2.13	0.48
1:C:266:PRO:HB2	1:C:271:CYS:SG	2.53	0.48
1:B:324:LEU:O	1:B:324:LEU:HD12	2.12	0.48
2:G:49:G:O5'	2:G:49:G:C8	2.66	0.48
1:E:421:ARG:HG2	1:E:421:ARG:NH1	2.27	0.48
2:G:46:C:O2'	2:G:47:U:H5'	2.13	0.48
1:B:231:GLU:O	1:B:235:LYS:HG3	2.12	0.48
1:B:335:ARG:NH1	1:B:338:ASP:OD2	2.45	0.48
1:D:11:ILE:O	1:D:15:VAL:HG23	2.13	0.48
1:B:339:ILE:HG13	1:B:342:ILE:HB	1.95	0.48
1:A:6:ARG:HH11	1:A:6:ARG:HG2	1.78	0.48
1:A:344:MET:O	1:A:432:ARG:CD	2.60	0.48
1:D:439:LEU:HD23	1:D:442:ILE:HD12	1.96	0.48
1:B:229:LYS:HB2	1:B:232:ASP:OD2	2.13	0.48
1:C:89:LEU:HD12	1:D:101:ALA:HB1	1.95	0.48
1:A:377:LYS:HE2	1:A:389:GLU:OE2	2.14	0.48
1:E:406:GLU:HA	1:E:406:GLU:OE1	2.11	0.48
1:A:197:VAL:HG22	1:A:228:VAL:HG13	1.95	0.48
1:A:163:ARG:HG2	1:A:188:GLU:HB2	1.94	0.48
1:E:72:VAL:HG22	1:E:417:PRO:CG	2.42	0.48
1:C:194:LYS:HZ1	1:C:224:PHE:HB3	1.78	0.48
2:I:35:C:O2'	2:I:36:A:H5'	2.14	0.48
1:E:353:ARG:HB2	1:E:393:TYR:CD2	2.47	0.48
1:C:408:SER:O	1:C:412:ARG:HG3	2.13	0.48
1:A:442:ILE:O	1:A:446:LEU:CG	2.53	0.48
2:I:47(E):A:C2'	2:I:47(F):U:H5'	2.43	0.48
2:H:5(A):U:C2'	2:H:6:A:H5'	2.42	0.48
1:B:219:PHE:CD2	1:C:193:ASN:HB3	2.48	0.48
1:B:211:LEU:HG	1:B:242:ILE:HG21	1.94	0.48
2:H:47(E):A:H2'	2:H:47(F):U:O4'	2.13	0.48
1:D:254:ILE:HD12	1:D:259:PHE:CE2	2.49	0.48
2:I:67:U:H2'	2:I:67(A):A:C8	2.49	0.48
1:A:286:LEU:HG	1:A:384:SER:HB2	1.95	0.48
1:C:370:LYS:HB2	1:C:398:ARG:O	2.14	0.48
1:E:96:PHE:O	1:E:100:ILE:HG12	2.13	0.48
2:G:34:U:H6	2:G:34:U:O5'	1.96	0.48
1:D:11:ILE:HG21	1:D:28:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:ARG:CD	1:E:190:GLY:O	2.61	0.48
1:A:268:PHE:HD2	1:A:268:PHE:H	1.62	0.48
1:A:250:SER:O	1:A:286:LEU:HB2	2.13	0.48
1:E:204:ILE:HG22	1:E:205:ASN:N	2.28	0.48
2:F:14:G:O2'	2:F:15:C:H5'	2.14	0.48
1:D:5:LEU:CD1	1:D:39:ARG:HA	2.44	0.48
1:A:442:ILE:CG2	1:A:446:LEU:HD11	2.43	0.48
2:I:45:U:H2'	2:I:46:C:O4'	2.13	0.48
1:B:411:LEU:CD2	1:B:418:ILE:HD12	2.37	0.48
1:D:163:ARG:NH1	1:E:166:LEU:HD13	2.28	0.48
1:B:400:ASP:OD1	1:B:401:ARG:N	2.47	0.48
1:A:126:TYR:HB3	1:A:328:LEU:HD13	1.95	0.48
2:I:48:G:H4'	2:I:49:G:H5''	1.96	0.48
1:C:169:ILE:HG13	1:C:173:PHE:HD2	1.77	0.48
2:J:3:G:O2'	2:J:4:A:H5'	2.13	0.48
1:C:212:MET:CE	1:C:245:TYR:HE1	2.26	0.48
1:E:421:ARG:HG2	1:E:421:ARG:HH11	1.77	0.48
1:D:39:ARG:HG2	2:H:56:C:H42	1.78	0.48
1:C:5:LEU:HD13	1:C:42:ILE:HB	1.95	0.48
2:G:10:A:H4'	2:G:45:U:O4'	2.14	0.48
2:I:10:A:C2	2:I:26:C:C2	3.00	0.48
1:C:123:ILE:HD13	1:C:325:GLU:HB2	1.96	0.48
1:C:197:VAL:CG2	1:C:228:VAL:HG13	2.43	0.48
1:B:254:ILE:CD1	1:B:259:PHE:HE2	2.27	0.48
2:F:9:U:H5	2:F:48:G:H5'	1.78	0.48
1:A:366:ILE:HB	1:A:369:LEU:HD11	1.92	0.48
1:A:432:ARG:O	1:A:432:ARG:HG3	2.12	0.48
1:A:231:GLU:H	1:A:231:GLU:CD	2.16	0.48
1:C:200:TYR:CE2	1:C:228:VAL:HG21	2.48	0.48
1:B:165:GLU:OE1	1:B:213:LYS:HG3	2.13	0.48
1:A:210:LEU:HD12	1:A:243:PRO:HG2	1.96	0.48
1:C:40:LYS:O	1:C:44:GLU:HG3	2.14	0.48
1:D:10:GLN:CG	1:D:12:SER:H	2.22	0.48
1:D:176:PRO:CG	1:E:191:THR:HG22	2.39	0.48
1:C:363:LEU:O	1:C:371:ILE:HD11	2.13	0.48
1:C:68:ASN:HD22	1:D:122:HIS:CB	2.26	0.48
1:A:165:GLU:OE2	1:A:213:LYS:NZ	2.47	0.48
1:A:108:GLU:HB2	1:B:83:ASN:HA	1.96	0.48
1:D:131:THR:O	1:D:269:ARG:HA	2.13	0.48
1:E:146:VAL:HG22	1:E:245:TYR:OH	2.13	0.48
1:E:425:ASP:O	1:E:425:ASP:CG	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:35:C:H2'	2:J:36:A:C8	2.49	0.48
2:F:37:A:O2'	2:F:38:A:H5'	2.14	0.48
2:G:36:A:O2'	2:G:37:A:H5'	2.14	0.48
2:F:26:C:H2'	2:F:27:C:O4'	2.13	0.48
1:A:34:VAL:O	1:A:38:TYR:HD1	1.97	0.47
1:B:150:LEU:HB3	1:B:182:SER:OG	2.14	0.47
1:A:87:ALA:HB2	1:A:341:VAL:HG21	1.96	0.47
1:D:335:ARG:NH1	1:D:338:ASP:OD2	2.47	0.47
2:I:3:G:O2'	2:I:4:A:H5'	2.14	0.47
1:C:313:ALA:HB1	1:D:144:GLY:HA2	1.95	0.47
1:A:242:ILE:HG23	1:A:243:PRO:HD2	1.95	0.47
1:E:452:ILE:OXT	1:E:452:ILE:HG23	2.14	0.47
1:B:5:LEU:CD1	1:B:39:ARG:HA	2.42	0.47
2:I:5(A):U:C2'	2:I:6:A:H5'	2.44	0.47
2:G:31:A:C8	2:G:32:C:C5	3.02	0.47
2:H:5(A):U:H2'	2:H:6:A:H5'	1.96	0.47
1:D:191:THR:HB	1:E:166:LEU:O	2.14	0.47
2:I:37:A:O2'	2:I:38:A:H5'	2.14	0.47
1:B:128:ASN:ND2	1:B:135:SER:HA	2.29	0.47
2:F:41:U:O2'	2:F:42:A:H5'	2.14	0.47
1:B:409:ARG:HH12	1:B:413:LEU:HD11	1.79	0.47
2:G:27:C:C2'	2:G:28:U:O4'	2.58	0.47
1:E:344:MET:O	1:E:432:ARG:CD	2.63	0.47
1:B:42:ILE:HD11	1:B:50:LEU:HD21	1.96	0.47
1:E:187:ARG:HD3	1:E:203:ALA:HB1	1.95	0.47
2:G:10:A:C4	2:G:44:G:C2	3.02	0.47
1:C:302:ILE:HA	1:C:305:ILE:HD12	1.94	0.47
1:C:358:ARG:HH21	1:C:439:LEU:HD12	1.79	0.47
1:A:116:ARG:HD3	1:B:83:ASN:OD1	2.15	0.47
2:J:67:U:H2'	2:J:67(A):A:H8	1.78	0.47
1:E:298:LYS:O	1:E:302:ILE:HG12	2.14	0.47
2:F:61:C:H2'	2:F:62:C:C6	2.49	0.47
1:A:33:GLU:OE1	1:A:60:LYS:HD2	2.14	0.47
2:I:47(E):A:H2'	2:I:47(F):U:H5'	1.95	0.47
1:C:363:LEU:HB2	1:C:371:ILE:HD13	1.97	0.47
1:A:138:VAL:HG22	1:A:294:ILE:HA	1.96	0.47
1:D:228:VAL:CG1	1:D:233:LEU:HG	2.45	0.47
1:E:10:GLN:HG2	1:E:12:SER:N	2.25	0.47
1:D:339:ILE:HG13	1:D:339:ILE:O	2.15	0.47
1:D:24:GLU:O	1:D:24:GLU:HG3	2.14	0.47
2:J:39:U:H2'	2:J:40:C:C6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LEU:O	1:C:191:THR:HB	2.15	0.47
2:I:47(I):A:H2'	2:I:47(J):A:H5'	1.96	0.47
1:C:68:ASN:HD22	1:D:122:HIS:HB3	1.80	0.47
1:D:87:ALA:HB2	1:D:341:VAL:HG21	1.97	0.47
1:E:216:LYS:HG2	1:E:219:PHE:CE2	2.49	0.47
2:J:36:A:H2'	2:J:37:A:O4'	2.14	0.47
1:B:10:GLN:HB3	1:B:13:LYS:CE	2.43	0.47
1:B:423:ARG:NH1	1:B:423:ARG:HG2	2.30	0.47
2:G:31:A:C5	2:G:32:C:C4	3.01	0.47
1:C:60:LYS:HA	1:C:60:LYS:HD3	1.70	0.47
1:C:33:GLU:OE1	1:C:60:LYS:HD2	2.14	0.47
1:E:194:LYS:HE3	1:E:224:PHE:HB3	1.95	0.47
1:E:37:LYS:O	1:E:41:GLU:CG	2.59	0.47
1:D:163:ARG:NH1	1:E:166:LEU:CD1	2.78	0.47
1:E:188:GLU:H	1:E:188:GLU:HG2	1.47	0.47
1:E:161:ILE:CG2	1:E:166:LEU:HD21	2.45	0.47
1:A:178:ILE:HG23	1:A:179:MET:N	2.29	0.47
1:C:366:ILE:CG2	1:C:367:PRO:HD2	2.43	0.47
1:A:407:LEU:HD21	1:A:427:LEU:HD22	1.94	0.47
2:J:8:A:HO2'	2:J:9:U:P	2.37	0.47
2:I:47(P):A:H2'	2:I:48:G:H5'	1.96	0.47
1:C:18:PHE:HB3	1:C:21:ALA:HB3	1.96	0.47
1:E:123:ILE:O	1:E:126:TYR:N	2.41	0.47
2:H:26:C:H2'	2:H:27:C:O4'	2.14	0.47
1:D:131:THR:HG22	1:D:268:PHE:HB3	1.97	0.47
1:E:283:GLY:O	1:E:287:LEU:HB3	2.14	0.47
1:A:55:GLU:O	1:A:59:ARG:HG3	2.14	0.47
1:A:406:GLU:OE1	1:A:406:GLU:HA	2.13	0.47
1:E:8:ILE:HD13	1:E:38:TYR:HB3	1.96	0.47
2:F:47(E):A:H2'	2:F:47(F):U:H5'	1.97	0.47
2:H:65:C:H2'	2:H:66:A:H8	1.79	0.47
1:C:181:LYS:HB3	1:D:310:ILE:HD11	1.96	0.47
1:B:402:LEU:HD12	1:B:450:LEU:HD21	1.97	0.47
1:E:139:VAL:HB	1:E:314:LEU:HB3	1.97	0.47
1:E:348:ASP:O	1:E:351:ALA:HB3	2.14	0.47
1:D:175:ILE:N	1:D:176:PRO:HD2	2.29	0.47
2:G:37:A:O2'	2:G:38:A:H5'	2.15	0.47
1:D:161:ILE:CG2	1:D:166:LEU:HD21	2.45	0.47
1:E:107:LEU:O	1:E:122:HIS:CE1	2.66	0.47
1:A:72:VAL:HG22	1:A:417:PRO:CG	2.45	0.47
1:D:251:GLY:HA2	1:D:268:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:PRO:HG2	1:D:181:LYS:HG3	1.96	0.47
1:D:318:LYS:HB3	1:D:318:LYS:HE2	1.73	0.47
1:D:7:GLN:CB	1:D:50:LEU:CD1	2.93	0.47
2:G:10:A:N6	2:G:44:G:C6	2.83	0.47
2:G:40:C:H2'	2:G:41:U:C6	2.51	0.47
1:D:335:ARG:O	1:D:338:ASP:HB2	2.15	0.47
2:I:59:U:C2'	2:I:60:U:H5'	2.45	0.47
1:B:123:ILE:O	1:B:126:TYR:N	2.43	0.47
2:H:43:G:O2'	2:H:44:G:H5'	2.15	0.47
2:F:42:A:O2'	2:F:43:G:C8	2.68	0.47
2:G:47(F):U:O2'	2:G:47(H):U:OP2	2.21	0.46
1:A:366:ILE:CG2	1:A:367:PRO:HD2	2.45	0.46
1:C:348:ASP:HB2	1:C:351:ALA:CB	2.44	0.46
1:B:444:LYS:O	1:B:448:GLU:HG3	2.15	0.46
1:A:18:PHE:HB3	1:A:21:ALA:HB3	1.97	0.46
1:E:429:PHE:HB3	1:E:431:MET:CE	2.46	0.46
1:E:255:ASN:HB3	1:E:258:GLU:OE2	2.15	0.46
2:G:25:U:C2	2:G:26:C:C6	3.04	0.46
1:A:399:HIS:ND1	1:A:401:ARG:HB2	2.30	0.46
1:E:230:LEU:O	1:E:234:VAL:HG23	2.15	0.46
1:B:161:ILE:HG22	1:B:186:LEU:HD11	1.97	0.46
1:D:107:LEU:CD1	1:D:321:LEU:HD23	2.45	0.46
1:E:123:ILE:O	1:E:125:LYS:N	2.48	0.46
1:A:72:VAL:HG13	1:A:417:PRO:HG2	1.97	0.46
1:A:175:ILE:N	1:A:176:PRO:HD2	2.30	0.46
1:A:68:ASN:HD22	1:B:122:HIS:CB	2.27	0.46
2:I:47(H):U:O2'	2:I:47(I):A:H5'	2.16	0.46
2:J:47:U:H2'	2:J:47(A):C:H6	1.76	0.46
1:A:345:LEU:CD2	1:A:380:PRO:CB	2.91	0.46
1:A:80:ILE:HD12	1:A:285:LLP:HA	1.97	0.46
1:D:7:GLN:HB2	1:D:50:LEU:HD13	1.95	0.46
2:I:65:C:H2'	2:I:66:A:C8	2.50	0.46
1:C:302:ILE:HG22	1:C:306:LYS:HE3	1.97	0.46
1:B:344:MET:O	1:B:432:ARG:HD2	2.15	0.46
1:A:2:LYS:O	1:A:6:ARG:NE	2.48	0.46
1:D:234:VAL:HG12	1:D:238:HIS:CD2	2.50	0.46
1:B:11:ILE:HG21	1:B:28:VAL:HG13	1.98	0.46
1:E:254:ILE:HD11	1:E:259:PHE:CZ	2.50	0.46
2:H:9:U:H4'	2:H:45:U:C2	2.50	0.46
1:C:123:ILE:O	1:C:125:LYS:N	2.48	0.46
1:A:369:LEU:HD21	1:A:450:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:46:C:C4	2:J:47:U:O4	2.69	0.46
1:C:68:ASN:HD21	1:D:122:HIS:HD2	1.63	0.46
1:C:317:ASP:HA	1:D:291:GLN:CD	2.36	0.46
1:B:130:LEU:O	1:B:269:ARG:NH2	2.49	0.46
1:C:169:ILE:HD11	1:C:285:LLP:H5'1	1.98	0.46
1:D:34:VAL:HG21	1:D:57:VAL:HA	1.97	0.46
1:E:270:ASP:O	1:E:274:LEU:HG	2.15	0.46
1:D:2:LYS:CE	2:H:56:C:O2'	2.63	0.46
1:C:123:ILE:HG23	1:C:328:LEU:CD1	2.45	0.46
1:D:228:VAL:HG11	1:D:233:LEU:HG	1.98	0.46
1:D:339:ILE:HG13	1:D:342:ILE:HB	1.97	0.46
1:D:316:ILE:H	1:D:316:ILE:HG12	1.48	0.46
1:D:2:LYS:HE2	1:D:6:ARG:CZ	2.45	0.46
2:F:36:A:C2'	2:F:37:A:H5'	2.46	0.46
2:F:47(J):A:N6	2:F:47(K):G:O6	2.48	0.46
2:G:25:U:O2'	2:G:26:C:C5'	2.64	0.46
2:G:9:U:O4	2:G:48:G:C8	2.68	0.46
1:E:442:ILE:O	1:E:446:LEU:HG	2.15	0.46
1:B:160:ILE:HD12	1:B:211:LEU:CD2	2.45	0.46
1:B:285:LLP:C4'	1:B:285:LLP:OP4	2.63	0.46
1:B:285:LLP:H4'2	1:B:285:LLP:OP4	2.16	0.46
1:A:334:LYS:CD	1:A:336:TYR:OH	2.64	0.46
1:C:308:ASN:OD1	1:C:310:ILE:HG13	2.16	0.46
1:C:320:THR:O	1:C:324:LEU:HB2	2.15	0.46
1:C:87:ALA:HB2	1:C:341:VAL:HG21	1.97	0.46
1:C:67:PRO:HB2	1:D:96:PHE:CE1	2.51	0.46
1:A:68:ASN:O	1:A:70:LYS:HE3	2.15	0.46
2:G:10:A:C5	2:G:44:G:C2	3.04	0.46
1:A:427:LEU:HD23	1:A:429:PHE:CE1	2.50	0.46
1:A:436:HIS:HD2	1:A:439:LEU:HD12	1.81	0.46
1:D:60:LYS:HA	1:D:60:LYS:HD3	1.77	0.46
1:A:348:ASP:HB2	1:A:351:ALA:HB2	1.97	0.46
1:B:326:MET:O	1:B:330:LEU:HG	2.15	0.46
1:B:246:TYR:OH	1:B:266:PRO:HG3	2.16	0.46
1:C:60:LYS:O	1:C:64:LEU:HG	2.16	0.46
1:D:169:ILE:O	1:D:173:PHE:HB3	2.15	0.46
2:I:47(E):A:C2	2:I:47(J):A:C6	3.04	0.46
2:H:8:A:O2'	2:H:9:U:P	2.74	0.46
2:H:67:U:H2'	2:H:67(A):A:C8	2.50	0.46
2:J:59:U:C2'	2:J:60:U:H5'	2.46	0.46
2:F:26:C:O2'	2:F:27:C:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TYR:O	1:B:130:LEU:HG	2.15	0.46
1:A:24:GLU:O	1:A:28:VAL:HG23	2.16	0.46
1:A:60:LYS:HA	1:A:60:LYS:HD3	1.73	0.46
1:A:320:THR:CG2	1:B:319:LEU:HD12	2.45	0.46
1:A:309:PRO:HG3	1:B:181:LYS:HG3	1.97	0.46
1:A:116:ARG:HH22	1:B:171:GLY:HA3	1.81	0.46
1:E:40:LYS:O	1:E:44:GLU:HG3	2.16	0.46
1:E:109:TYR:OH	1:E:114:GLY:O	2.32	0.46
1:A:120:ILE:HD11	1:A:315:ARG:HG3	1.97	0.46
1:B:370:LYS:HB2	1:B:398:ARG:O	2.16	0.46
1:D:167:VAL:HG12	1:D:219:PHE:CE2	2.34	0.45
1:E:73:ILE:HD13	1:E:438:ASP:HB3	1.97	0.45
1:C:234:VAL:HG12	1:C:238:HIS:CD2	2.51	0.45
1:B:14:VAL:CG1	1:B:18:PHE:HE2	2.29	0.45
1:A:181:LYS:HE3	1:B:309:PRO:HD2	1.99	0.45
1:A:68:ASN:ND2	1:B:122:HIS:HD2	2.11	0.45
2:G:40:C:H2'	2:G:41:U:O4'	2.16	0.45
2:G:67:U:H2'	2:G:67(A):A:C8	2.51	0.45
2:I:36:A:H2'	2:I:37:A:O4'	2.16	0.45
1:D:347:GLN:NE2	1:D:352:LEU:CD2	2.80	0.45
1:C:67:PRO:CG	1:D:96:PHE:CE1	2.99	0.45
2:J:65:C:H2'	2:J:66:A:O4'	2.17	0.45
2:G:31:A:C6	2:G:32:C:N3	2.84	0.45
1:E:432:ARG:HG3	1:E:432:ARG:O	2.16	0.45
1:A:123:ILE:O	1:A:126:TYR:N	2.45	0.45
1:C:431:MET:HE2	1:C:434:VAL:HG21	1.98	0.45
1:C:14:VAL:O	1:C:18:PHE:HD2	1.98	0.45
1:D:212:MET:HG2	1:D:213:LYS:N	2.29	0.45
1:A:375:LYS:NZ	1:A:391:PRO:HB2	2.32	0.45
2:F:38:A:H2'	2:F:39:U:C5'	2.46	0.45
1:A:420:CYS:HB2	1:A:428:LEU:O	2.16	0.45
1:D:123:ILE:HG12	1:D:321:LEU:HD11	1.99	0.45
1:D:409:ARG:NH1	1:D:413:LEU:HD11	2.30	0.45
2:G:18:G:O2'	2:G:57:G:N2	2.50	0.45
2:G:28:U:H2'	2:G:29:A:C8	2.52	0.45
1:B:92:ASP:CG	1:B:335:ARG:HH12	2.19	0.45
1:C:181:LYS:HG3	1:D:309:PRO:CG	2.44	0.45
1:E:234:VAL:HG12	1:E:238:HIS:HD2	1.80	0.45
2:H:55:U:H2'	2:H:57:G:OP2	2.17	0.45
1:E:14:VAL:CG1	1:E:18:PHE:HE2	2.29	0.45
1:D:1:MET:CG	1:D:2:LYS:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ARG:HE	1:E:203:ALA:CB	2.15	0.45
2:F:8:A:HO2'	2:F:9:U:P	2.39	0.45
1:C:73:ILE:CB	1:C:418:ILE:HG12	2.40	0.45
2:I:25:U:HO2'	2:I:26:C:H5'	1.78	0.45
1:D:169:ILE:HG13	1:D:173:PHE:HD2	1.82	0.45
1:E:15:VAL:HA	1:E:27:VAL:HG11	1.98	0.45
2:F:25:U:O2'	2:F:26:C:H5'	2.16	0.45
1:C:107:LEU:O	1:C:122:HIS:CE1	2.68	0.45
1:E:360:GLU:O	1:E:364:LYS:HG3	2.16	0.45
2:G:47(C):C:O2'	2:G:47(D):U:H5'	2.16	0.45
1:E:445:THR:O	1:E:449:LEU:HG	2.16	0.45
2:I:5(A):U:H2'	2:I:6:A:H5'	1.99	0.45
2:G:25:U:C4	2:G:26:C:N4	2.85	0.45
2:I:28:U:H2'	2:I:29:A:C8	2.52	0.45
2:I:47(I):A:H2'	2:I:47(J):A:C5'	2.47	0.45
2:I:21:U:H2'	2:I:22:G:H8	1.81	0.45
2:H:47(E):A:H2'	2:H:47(F):U:C5'	2.45	0.45
1:D:33:GLU:CD	1:D:60:LYS:HE3	2.37	0.45
2:J:67:U:H2'	2:J:67(A):A:C8	2.50	0.45
1:D:188:GLU:OE1	1:E:163:ARG:NH1	2.38	0.45
1:E:88:PRO:HD2	1:E:341:VAL:HG22	1.98	0.45
1:C:70:LYS:O	1:C:72:VAL:HG23	2.17	0.45
1:B:34:VAL:HG21	1:B:57:VAL:HA	1.99	0.45
2:H:42:A:O2'	2:H:43:G:C8	2.64	0.45
1:B:360:GLU:O	1:B:364:LYS:HG3	2.17	0.45
2:F:43:G:O2'	2:F:44:G:H5'	2.17	0.45
1:A:283:GLY:O	1:A:287:LEU:HB3	2.17	0.45
1:E:193:ASN:HB2	1:E:224:PHE:O	2.17	0.45
1:E:344:MET:O	1:E:432:ARG:HD2	2.17	0.45
1:B:363:LEU:O	1:B:371:ILE:HD11	2.17	0.45
1:E:89:LEU:HB2	1:E:94:ILE:HD11	1.99	0.45
1:A:34:VAL:HG21	1:A:57:VAL:HA	1.98	0.45
1:D:10:GLN:HA	2:H:19:G:H2'	1.98	0.45
1:D:219:PHE:CD2	1:E:193:ASN:HB3	2.52	0.45
2:H:46:C:H2'	2:H:47:U:C5'	2.46	0.45
1:B:60:LYS:HD3	1:B:60:LYS:HA	1.58	0.45
2:J:28:U:H2'	2:J:29:A:C8	2.52	0.45
1:A:353:ARG:HB2	1:A:393:TYR:CE2	2.52	0.45
1:D:5:LEU:HD13	1:D:39:ARG:HA	1.98	0.44
1:A:322:SER:OG	1:A:323:GLY:N	2.50	0.44
1:C:358:ARG:O	1:C:362:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:HD13	1:A:325:GLU:HB2	1.99	0.44
1:C:335:ARG:O	1:C:338:ASP:HB2	2.17	0.44
1:D:396:ALA:HB1	1:D:426:GLN:CG	2.47	0.44
1:C:5:LEU:CD1	1:C:39:ARG:HA	2.40	0.44
2:H:47:U:H2'	2:H:47(A):C:H6	1.78	0.44
1:E:438:ASP:O	1:E:442:ILE:HG13	2.18	0.44
1:E:165:GLU:OE1	1:E:213:LYS:HG3	2.17	0.44
2:H:28:U:H2'	2:H:29:A:C8	2.53	0.44
1:C:77:GLY:CA	1:C:430:ASP:HB3	2.46	0.44
1:C:120:ILE:HG21	1:C:137:PHE:CD1	2.52	0.44
1:E:7:GLN:CB	1:E:50:LEU:CD1	2.95	0.44
2:H:49:G:C8	2:H:49:G:O5'	2.70	0.44
1:C:423:ARG:HD2	1:C:428:LEU:HD11	2.00	0.44
2:H:37:A:O2'	2:H:38:A:H5'	2.17	0.44
1:A:359:LEU:HD11	1:A:363:LEU:HD11	2.00	0.44
1:A:263:VAL:CG2	1:A:388:LEU:HD13	2.48	0.44
2:H:26:C:O2'	2:H:27:C:H5'	2.17	0.44
1:C:5:LEU:HD12	1:C:8:ILE:CD1	2.48	0.44
1:E:347:GLN:HE21	1:E:352:LEU:CD2	2.31	0.44
1:D:11:ILE:HD13	2:H:18:G:OP1	2.16	0.44
1:E:316:ILE:HD11	1:E:321:LEU:HD13	1.99	0.44
1:B:348:ASP:O	1:B:351:ALA:HB3	2.17	0.44
2:F:43:G:H2'	2:F:44:G:C8	2.53	0.44
1:C:123:ILE:O	1:C:126:TYR:N	2.43	0.44
1:E:367:PRO:HG3	1:E:451:SER:OG	2.17	0.44
2:J:26:C:H2'	2:J:27:C:O4'	2.17	0.44
1:C:197:VAL:HG22	1:C:228:VAL:HG13	1.98	0.44
1:A:14:VAL:HG13	1:A:18:PHE:HE2	1.82	0.44
1:A:94:ILE:HD11	1:B:102:ASN:HA	1.99	0.44
1:A:423:ARG:O	1:A:424:GLU:HB3	2.18	0.44
1:B:87:ALA:HB2	1:B:341:VAL:HG21	2.00	0.44
2:F:5(A):U:H2'	2:F:6:A:H5'	1.99	0.44
1:C:423:ARG:HH11	1:C:423:ARG:HG2	1.82	0.44
1:D:400:ASP:OD1	1:D:401:ARG:N	2.51	0.44
1:E:359:LEU:HB2	1:E:439:LEU:HD22	1.98	0.44
1:A:77:GLY:CA	1:A:430:ASP:HB3	2.47	0.44
1:D:286:LEU:HD21	1:D:384:SER:OG	2.17	0.44
1:B:141:ASN:HB2	1:B:285:LLP:OP1	2.18	0.44
1:C:77:GLY:HA3	1:C:430:ASP:HB3	1.99	0.44
1:C:161:ILE:HG21	1:C:166:LEU:HD21	1.98	0.44
1:A:317:ASP:HB2	1:B:291:GLN:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ILE:HD11	1:E:50:LEU:HD21	2.00	0.44
2:G:47:U:H2'	2:G:47(A):C:H6	1.77	0.44
1:A:131:THR:HG21	1:A:296:VAL:HG11	1.99	0.44
1:D:254:ILE:HD13	1:D:336:TYR:CE1	2.53	0.44
1:D:254:ILE:HD12	1:D:259:PHE:HE2	1.82	0.44
1:A:200:TYR:CE2	1:A:233:LEU:HD21	2.53	0.44
1:A:159:VAL:HG13	1:A:210:LEU:HB3	2.00	0.44
1:C:404:SER:OG	1:C:425:ASP:HA	2.18	0.44
1:E:110:ASN:ND2	1:E:113:GLU:OE1	2.51	0.44
1:D:2:LYS:NZ	2:H:56:C:O2'	2.49	0.44
2:G:29:A:C2'	2:G:30:G:H5'	2.47	0.44
1:E:213:LYS:HD3	1:E:230:LEU:HD21	2.00	0.44
1:E:148:LEU:HG	1:E:305:ILE:HG23	1.99	0.44
1:C:178:ILE:CG2	1:C:179:MET:N	2.81	0.44
1:C:169:ILE:HG13	1:C:169:ILE:O	2.17	0.44
1:E:123:ILE:CD1	1:E:321:LEU:HD12	2.48	0.44
1:D:14:VAL:HG12	1:D:18:PHE:CE2	2.52	0.44
1:E:17:ILE:HG22	1:E:17:ILE:O	2.18	0.44
1:B:366:ILE:HG23	1:B:367:PRO:HD2	2.00	0.44
2:I:65:C:H2'	2:I:66:A:H8	1.83	0.44
2:I:47(E):A:H2'	2:I:47(F):U:C5'	2.48	0.44
2:J:47(E):A:C2	2:J:47(I):A:N7	2.85	0.44
1:E:77:GLY:CA	1:E:430:ASP:HB3	2.48	0.44
2:J:47(N):A:H2'	2:J:47(O):G:C8	2.52	0.44
1:A:347:GLN:HE21	1:A:352:LEU:HD21	1.80	0.44
1:E:448:GLU:O	1:E:452:ILE:CG2	2.65	0.44
1:B:409:ARG:NH1	1:B:413:LEU:HD11	2.32	0.44
1:A:375:LYS:HB2	1:A:393:TYR:CE1	2.52	0.44
2:F:15:C:H2'	2:F:16:U:C6	2.53	0.43
1:C:11:ILE:HD12	2:I:18:G:P	2.58	0.43
1:E:443:LYS:HE2	1:E:447:GLN:OE1	2.18	0.43
1:B:37:LYS:O	1:B:41:GLU:CG	2.59	0.43
2:G:47(J):A:H2'	2:G:47(K):G:O4'	2.18	0.43
2:F:56:C:H2'	2:F:57:G:C8	2.53	0.43
1:D:123:ILE:O	1:D:126:TYR:N	2.44	0.43
1:C:167:VAL:HG12	1:C:219:PHE:CE2	2.48	0.43
1:A:363:LEU:HB2	1:A:371:ILE:HD13	2.00	0.43
1:C:431:MET:HE1	1:C:434:VAL:HG21	2.00	0.43
2:F:2:G:O2'	2:F:3:G:H5'	2.18	0.43
1:D:194:LYS:CB	1:E:168:GLU:OE1	2.66	0.43
1:B:157:LYS:HB3	1:B:207:ASN:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ILE:N	1:C:176:PRO:HD2	2.33	0.43
1:D:17:ILE:HG22	1:D:17:ILE:O	2.18	0.43
1:A:127:LEU:O	1:A:131:THR:HG23	2.18	0.43
2:F:59:U:C2'	2:F:60:U:H5'	2.48	0.43
1:B:392:THR:HG21	1:B:430:ASP:OD2	2.19	0.43
2:J:46:C:H2'	2:J:47:U:C6	2.53	0.43
1:E:159:VAL:HG13	1:E:210:LEU:HB3	2.00	0.43
1:A:360:GLU:HG3	1:A:371:ILE:HG21	1.99	0.43
1:E:269:ARG:HG3	1:E:269:ARG:NH1	2.32	0.43
1:C:98:SER:HA	1:D:94:ILE:CG2	2.48	0.43
1:A:8:ILE:HD11	1:A:38:TYR:HB3	2.00	0.43
2:G:10:A:C2	2:G:26:C:O2	2.71	0.43
2:G:31:A:H2'	2:G:32:C:O4'	2.18	0.43
2:I:27:C:C4	2:I:28:U:C4	3.06	0.43
1:A:252:LEU:HD12	1:A:253:LEU:N	2.33	0.43
2:F:28:U:H2'	2:F:29:A:H8	1.83	0.43
1:A:271:CYS:HA	1:A:274:LEU:HD12	2.00	0.43
1:D:367:PRO:HG3	1:D:451:SER:OG	2.18	0.43
2:G:29:A:H2'	2:G:30:G:C8	2.53	0.43
1:A:339:ILE:HG13	1:A:342:ILE:HB	2.01	0.43
1:A:344:MET:O	1:A:432:ARG:HD2	2.17	0.43
1:D:259:PHE:HB3	1:D:346:THR:CG2	2.48	0.43
1:D:259:PHE:CB	1:D:346:THR:HG21	2.48	0.43
1:C:107:LEU:HD11	1:C:321:LEU:HD23	2.00	0.43
1:E:348:ASP:HB2	1:E:351:ALA:HB2	2.00	0.43
1:B:312:ARG:HD2	1:B:315:ARG:NH1	2.33	0.43
2:F:45:U:H2'	2:F:46:C:O4'	2.19	0.43
1:C:265:GLU:OE1	1:C:385:LEU:CD2	2.66	0.43
2:G:28:U:C2'	2:G:29:A:H5'	2.48	0.43
1:C:312:ARG:CD	1:C:315:ARG:NH1	2.82	0.43
1:A:450:LEU:HA	1:A:450:LEU:HD23	1.80	0.43
1:B:200:TYR:HE2	1:B:228:VAL:HG21	1.83	0.43
1:D:366:ILE:HB	1:D:369:LEU:CD1	2.44	0.43
2:G:47(L):C:H2'	2:G:47(M):G:C8	2.53	0.43
2:J:45:U:H2'	2:J:46:C:O4'	2.18	0.43
1:A:123:ILE:CG2	1:A:328:LEU:HD12	2.48	0.43
2:J:47(P):A:H2'	2:J:48:G:H5'	1.99	0.43
1:E:253:LEU:HD23	1:E:331:TYR:CG	2.54	0.43
1:B:120:ILE:HG21	1:B:137:PHE:CD1	2.54	0.43
1:D:86:ARG:CD	1:D:284:ASP:OD2	2.66	0.43
1:B:254:ILE:HD12	1:B:259:PHE:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:11:G:C2	2:J:12:G:N7	2.86	0.43
1:A:104:TYR:CD1	1:A:104:TYR:N	2.86	0.43
1:B:287:LEU:HD23	1:B:287:LEU:C	2.39	0.43
1:D:1:MET:HG3	1:D:2:LYS:H	1.81	0.43
1:E:5:LEU:HD13	1:E:42:ILE:HB	2.00	0.43
2:F:8:A:C5	2:F:48:G:N2	2.86	0.43
1:B:25:ILE:CG1	1:B:26:TYR:N	2.80	0.43
1:B:343:ARG:HH21	1:B:343:ARG:HG2	1.84	0.43
1:A:76:THR:OG1	1:A:78:VAL:HG23	2.17	0.43
1:A:442:ILE:HG23	1:A:446:LEU:HD11	1.99	0.43
1:E:8:ILE:HD13	1:E:38:TYR:CB	2.49	0.43
2:G:26:C:C4	2:G:27:C:C4	3.06	0.43
2:J:47(E):A:H2'	2:J:47(F):U:H5'	2.00	0.43
1:D:11:ILE:HB	2:H:16:U:O2'	2.19	0.43
1:D:399:HIS:CD2	1:D:450:LEU:HD13	2.54	0.43
1:E:28:VAL:O	1:E:32:ARG:HG3	2.17	0.43
1:E:405:GLN:HE22	1:E:422:ILE:CG2	2.29	0.43
1:A:271:CYS:O	1:A:274:LEU:HB2	2.19	0.43
1:B:360:GLU:HG3	1:B:371:ILE:HG22	1.99	0.43
1:B:77:GLY:CA	1:B:433:THR:HG23	2.47	0.43
1:A:312:ARG:HB2	1:B:172:SER:OG	2.19	0.43
1:B:286:LEU:HA	1:B:286:LEU:HD23	1.76	0.43
1:D:370:LYS:HB2	1:D:398:ARG:O	2.18	0.43
2:J:38:A:C2'	2:J:39:U:H5'	2.49	0.43
2:G:47(E):A:H2'	2:G:47(F):U:O4'	2.19	0.43
1:D:169:ILE:HG13	1:D:173:PHE:CD2	2.54	0.43
1:E:88:PRO:HD2	1:E:341:VAL:CG2	2.49	0.43
1:C:336:TYR:O	1:C:339:ILE:HG12	2.18	0.43
1:D:14:VAL:O	1:D:18:PHE:HD2	2.01	0.43
1:A:313:ALA:HB1	1:B:144:GLY:HA2	2.00	0.43
1:B:179:MET:HA	1:B:182:SER:HB3	2.01	0.43
1:A:169:ILE:CG1	1:A:173:PHE:HD2	2.30	0.43
1:C:179:MET:HA	1:C:182:SER:HB3	2.00	0.43
1:E:14:VAL:HG21	1:E:53:PHE:HE2	1.84	0.43
1:B:348:ASP:HB2	1:B:351:ALA:HB2	2.00	0.43
1:C:345:LEU:CD2	1:C:380:PRO:HB3	2.49	0.43
2:G:15:C:H2'	2:G:16:U:H6	1.81	0.42
1:C:126:TYR:HB3	1:C:328:LEU:HD13	1.96	0.42
1:A:325:GLU:OE2	1:B:68:ASN:HB2	2.19	0.42
1:A:345:LEU:HD21	1:A:380:PRO:HB3	2.01	0.42
2:H:3:G:O2'	2:H:4:A:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2:G:O2'	2:J:3:G:H5'	2.18	0.42
1:A:94:ILE:O	1:A:98:SER:HB2	2.19	0.42
1:B:87:ALA:CB	1:B:341:VAL:HG21	2.48	0.42
1:D:73:ILE:HB	1:D:418:ILE:HG12	2.00	0.42
1:B:10:GLN:HB2	2:F:19:G:C2'	2.49	0.42
2:G:8:A:O2'	2:G:9:U:P	2.77	0.42
1:B:230:LEU:HD22	1:B:276:ILE:HD11	2.00	0.42
1:D:11:ILE:CD1	2:H:18:G:OP1	2.67	0.42
2:G:59:U:C2'	2:G:60:U:H5'	2.49	0.42
1:A:79:VAL:HG12	1:A:341:VAL:HG13	2.00	0.42
1:D:212:MET:HG3	1:D:245:TYR:CD1	2.54	0.42
1:D:80:ILE:HD12	1:D:285:LLP:HA	2.01	0.42
1:A:8:ILE:HA	1:A:9:PRO:HD2	1.82	0.42
1:D:88:PRO:HG2	1:D:340:PRO:CB	2.49	0.42
2:I:21:U:H2'	2:I:22:G:C8	2.55	0.42
2:H:47(G):U:H2'	2:H:47(H):U:O4'	2.18	0.42
1:A:169:ILE:CG1	1:A:173:PHE:CD2	3.03	0.42
1:C:386:PRO:HG2	1:C:387:GLU:N	2.32	0.42
1:E:277:ASP:O	1:E:297:GLY:HA3	2.19	0.42
1:D:193:ASN:O	1:D:225:VAL:HG13	2.19	0.42
1:D:5:LEU:HD21	1:D:39:ARG:CG	2.48	0.42
1:C:5:LEU:HD21	1:C:39:ARG:HG2	2.00	0.42
2:G:45:U:H2'	2:G:46:C:O4'	2.18	0.42
1:D:218:ASN:HD22	1:E:224:PHE:CB	2.29	0.42
1:E:347:GLN:HE21	1:E:352:LEU:HD21	1.82	0.42
1:B:168:GLU:OE2	1:C:194:LYS:HD2	2.20	0.42
1:D:427:LEU:HD23	1:D:429:PHE:HE1	1.84	0.42
1:A:123:ILE:O	1:A:125:LYS:N	2.52	0.42
2:G:36:A:H2'	2:G:37:A:H8	1.81	0.42
2:J:22:G:H2'	2:J:23:C:H6	1.83	0.42
1:A:114:GLY:HA3	1:B:412:ARG:NH2	2.35	0.42
1:A:161:ILE:CG2	1:A:186:LEU:HD11	2.49	0.42
1:B:70:LYS:O	1:B:72:VAL:HG23	2.18	0.42
1:D:14:VAL:HG12	1:D:18:PHE:HE2	1.84	0.42
1:E:216:LYS:HG2	1:E:219:PHE:CZ	2.55	0.42
1:B:350:LYS:HG3	1:B:350:LYS:H	1.51	0.42
1:A:5:LEU:HD11	1:A:39:ARG:CG	2.44	0.42
2:G:27:C:C4	2:G:28:U:C4	3.08	0.42
2:I:38:A:H2'	2:I:39:U:H5'	2.00	0.42
1:D:137:PHE:CD1	1:D:306:LYS:HG2	2.54	0.42
1:E:358:ARG:NH2	1:E:439:LEU:HD12	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LYS:HG3	1:A:439:LEU:HD11	2.01	0.42
1:A:114:GLY:CA	1:B:412:ARG:HH21	2.33	0.42
1:D:25:ILE:HG13	1:D:26:TYR:H	1.84	0.42
1:C:343:ARG:HH21	1:C:343:ARG:HG2	1.85	0.42
1:C:425:ASP:O	1:C:425:ASP:CG	2.57	0.42
1:E:250:SER:O	1:E:286:LEU:HB2	2.20	0.42
1:C:239:LYS:HD3	1:C:240:TYR:CE2	2.54	0.42
1:B:49:ASP:OD1	1:B:50:LEU:N	2.53	0.42
1:D:7:GLN:O	1:D:8:ILE:C	2.58	0.42
1:A:169:ILE:HD11	1:A:285:LLP:H5'1	2.02	0.42
1:E:167:VAL:HG12	1:E:219:PHE:HE2	1.85	0.42
1:C:116:ARG:HH22	1:D:171:GLY:HA3	1.84	0.42
1:B:394:CYS:HB3	1:B:428:LEU:HD22	2.00	0.42
1:D:16:GLU:OE2	2:H:22:G:H5'	2.20	0.42
2:F:3:G:O2'	2:F:4:A:H5'	2.20	0.42
1:B:287:LEU:HD23	1:B:287:LEU:O	2.20	0.42
1:E:300:ASN:O	1:E:304:LYS:HG3	2.20	0.42
1:D:160:ILE:HB	1:D:211:LEU:HD23	2.01	0.42
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.85	0.42
1:B:13:LYS:O	1:B:17:ILE:HG13	2.20	0.42
1:B:167:VAL:HG12	1:B:219:PHE:HE2	1.85	0.42
1:C:68:ASN:HD22	1:D:122:HIS:HA	1.85	0.42
1:C:82:THR:HG22	1:C:86:ARG:HE	1.85	0.42
1:E:126:TYR:CE2	1:E:325:GLU:HG3	2.54	0.42
1:C:144:GLY:CA	1:D:313:ALA:HB1	2.50	0.42
1:D:141:ASN:OD1	1:D:143:ALA:HB3	2.19	0.42
1:B:5:LEU:HD12	1:B:42:ILE:HD12	2.01	0.42
2:F:34:U:O2'	2:F:35:C:H5'	2.20	0.42
1:A:97:ILE:HG12	1:A:322:SER:OG	2.20	0.42
2:H:46:C:C2'	2:H:47:U:C5'	2.96	0.42
1:C:423:ARG:NH1	1:C:423:ARG:HG2	2.35	0.42
1:B:77:GLY:HA3	1:B:430:ASP:CG	2.40	0.42
1:D:194:LYS:HD2	1:E:168:GLU:CD	2.39	0.42
1:B:363:LEU:HD21	1:B:446:LEU:HD12	2.02	0.42
1:C:452:ILE:OXT	1:C:452:ILE:HG23	2.20	0.42
2:G:47(E):A:H2'	2:G:47(F):U:H5'	2.01	0.42
1:C:6:ARG:HG2	1:C:6:ARG:HH11	1.85	0.42
2:J:47(E):A:O2'	2:J:47(I):A:N6	2.53	0.42
1:B:33:GLU:CD	1:B:60:LYS:HE3	2.40	0.42
1:A:4:LEU:O	1:A:42:ILE:HD13	2.19	0.42
2:G:3:G:O2'	2:G:4:A:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:15:C:H2'	2:J:16:U:H6	1.84	0.42
1:D:77:GLY:CA	1:D:430:ASP:HB3	2.49	0.42
1:B:363:LEU:CD2	1:B:446:LEU:HD12	2.50	0.42
1:D:2:LYS:HE3	2:H:56:C:O2'	2.19	0.41
1:A:394:CYS:HB2	1:A:428:LEU:HD22	2.01	0.41
1:E:392:THR:HG21	1:E:430:ASP:OD2	2.20	0.41
2:H:59:U:C2'	2:H:60:U:H5'	2.50	0.41
1:C:20:LYS:HG2	1:C:20:LYS:O	2.20	0.41
1:A:11:ILE:HB	2:G:16:U:H4'	2.02	0.41
2:J:38:A:H2'	2:J:39:U:O4'	2.20	0.41
1:D:42:ILE:HD11	1:D:50:LEU:CD2	2.44	0.41
1:D:49:ASP:OD1	1:D:50:LEU:N	2.53	0.41
1:E:7:GLN:O	1:E:8:ILE:C	2.56	0.41
1:C:7:GLN:O	1:C:8:ILE:C	2.58	0.41
2:F:47(E):A:C2'	2:F:47(F):U:H5'	2.49	0.41
1:A:368:GLY:O	1:A:399:HIS:HA	2.20	0.41
1:A:363:LEU:C	1:A:371:ILE:HD11	2.40	0.41
1:A:249:GLY:O	1:A:285:LLP:HD3	2.20	0.41
2:F:26:C:C4	2:F:27:C:C4	3.07	0.41
1:C:344:MET:O	1:C:432:ARG:HD3	2.19	0.41
1:B:444:LYS:HA	1:B:447:GLN:HG2	2.03	0.41
2:G:56:C:H2'	2:G:57:G:C8	2.55	0.41
1:C:67:PRO:CG	1:D:96:PHE:HE1	2.33	0.41
2:F:9:U:C4	2:F:48:G:C8	3.07	0.41
2:G:7:G:O2'	2:G:8:A:H5'	2.20	0.41
1:C:328:LEU:HA	1:C:328:LEU:HD23	1.89	0.41
1:D:432:ARG:HG3	1:D:432:ARG:O	2.20	0.41
1:C:362:LEU:HB3	1:C:443:LYS:HD2	2.03	0.41
1:E:189:VAL:HG21	1:E:200:TYR:CD1	2.55	0.41
2:H:32:C:C4	2:H:33:U:O4	2.74	0.41
1:A:268:PHE:N	1:A:268:PHE:CD2	2.88	0.41
1:B:249:GLY:O	1:B:285:LLP:HD3	2.19	0.41
1:D:38:TYR:CE2	1:D:47:ARG:NE	2.88	0.41
2:F:7:G:O2'	2:F:8:A:H5'	2.19	0.41
1:B:97:ILE:HD11	1:B:323:GLY:CA	2.41	0.41
1:E:88:PRO:HG2	1:E:340:PRO:HB3	2.00	0.41
1:D:227:GLU:CG	1:D:228:VAL:N	2.83	0.41
1:E:140:ASN:ND2	1:E:141:ASN:ND2	2.69	0.41
1:A:114:GLY:CA	1:B:412:ARG:NH2	2.84	0.41
1:E:14:VAL:O	1:E:18:PHE:HD2	2.03	0.41
1:A:250:SER:HB2	1:A:286:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASN:OD1	1:A:308:ASN:C	2.58	0.41
1:C:113:GLU:H	1:C:113:GLU:HG3	1.71	0.41
1:C:15:VAL:HA	1:C:27:VAL:HG11	2.01	0.41
2:F:66:A:H2'	2:F:67:U:C6	2.56	0.41
1:B:175:ILE:N	1:B:176:PRO:CD	2.83	0.41
1:D:191:THR:HG22	1:E:176:PRO:CG	2.51	0.41
1:C:355:LYS:CG	1:C:439:LEU:HD11	2.48	0.41
1:D:298:LYS:O	1:D:302:ILE:HG12	2.19	0.41
1:A:339:ILE:HA	1:A:340:PRO:HD3	1.88	0.41
1:A:388:LEU:HD21	1:A:390:LEU:CD1	2.50	0.41
1:B:452:ILE:CG2	1:B:452:ILE:OXT	2.68	0.41
1:E:409:ARG:HG3	1:E:412:ARG:NH2	2.34	0.41
1:E:286:LEU:HG	1:E:384:SER:HB2	2.03	0.41
1:A:144:GLY:HA2	1:B:313:ALA:HB1	2.03	0.41
1:E:290:PRO:HB2	1:E:320:THR:HG22	2.03	0.41
1:B:247:ASP:C	1:B:247:ASP:OD1	2.59	0.41
1:A:60:LYS:C	1:A:64:LEU:HG	2.37	0.41
2:F:35:C:H2'	2:F:36:A:O4'	2.21	0.41
1:B:366:ILE:CG2	1:B:367:PRO:HD2	2.51	0.41
2:G:43:G:N1	2:G:44:G:C6	2.88	0.41
2:H:46:C:C3'	2:H:47:U:H5'	2.49	0.41
1:D:333:GLU:OE1	1:D:335:ARG:HD2	2.21	0.41
1:A:102:ASN:HB3	1:B:71:ARG:HH22	1.85	0.41
1:A:144:GLY:CA	1:B:313:ALA:HB1	2.50	0.41
1:D:253:LEU:HD23	1:D:331:TYR:CD2	2.55	0.41
1:B:7:GLN:O	1:B:8:ILE:C	2.58	0.41
1:C:67:PRO:CB	1:D:96:PHE:CE1	3.04	0.41
2:G:10:A:N6	2:G:44:G:O6	2.54	0.41
1:D:369:LEU:HD21	1:D:450:LEU:HD11	2.03	0.41
1:A:216:LYS:HG2	1:A:219:PHE:CE2	2.55	0.41
1:B:167:VAL:HG12	1:B:219:PHE:CE2	2.55	0.41
1:A:404:SER:O	1:A:407:LEU:HB3	2.20	0.41
1:A:407:LEU:HD23	1:A:427:LEU:HD22	2.00	0.41
1:A:359:LEU:CD1	1:A:363:LEU:HD11	2.50	0.41
1:E:60:LYS:O	1:E:64:LEU:HG	2.20	0.41
1:C:178:ILE:HG23	1:C:179:MET:N	2.36	0.41
2:I:67(A):A:H2'	2:I:68:C:H6	1.83	0.41
2:J:43:G:H2'	2:J:44:G:C8	2.56	0.41
1:E:178:ILE:CG2	1:E:179:MET:N	2.83	0.41
1:D:277:ASP:O	1:D:278:LEU:HD23	2.20	0.41
2:J:32:C:C4	2:J:33:U:O4	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ALA:O	1:B:395:VAL:HG21	2.20	0.41
1:C:32:ARG:O	1:C:36:GLU:HG2	2.21	0.41
1:B:160:ILE:HB	1:B:211:LEU:HD23	2.03	0.41
1:A:77:GLY:HA3	1:A:430:ASP:HB3	2.03	0.41
1:D:355:LYS:HG3	1:D:439:LEU:HD11	2.03	0.41
1:B:362:LEU:HD22	1:B:443:LYS:HD2	2.01	0.41
1:E:179:MET:SD	1:E:186:LEU:HB2	2.61	0.41
1:C:79:VAL:HG21	1:C:345:LEU:HG	2.03	0.41
1:B:246:TYR:CE2	1:B:248:ALA:HA	2.56	0.41
1:A:12:SER:HG	2:G:16:U:H1'	1.86	0.41
2:J:7:G:O2'	2:J:49:G:OP2	2.37	0.41
2:I:10:A:C5'	2:I:45:U:C1'	2.99	0.41
2:J:47(J):A:H2'	2:J:47(K):G:C8	2.56	0.41
1:D:399:HIS:ND1	1:D:450:LEU:HD22	2.35	0.41
1:B:339:ILE:HG13	1:B:342:ILE:CG1	2.51	0.41
1:E:90:SER:CB	1:E:338:ASP:O	2.66	0.41
1:E:211:LEU:CD2	1:E:242:ILE:HG21	2.51	0.41
1:A:79:VAL:HG21	1:A:345:LEU:CD2	2.51	0.41
1:B:389:GLU:O	1:B:390:LEU:HD23	2.21	0.41
1:C:72:VAL:HG22	1:C:417:PRO:CG	2.51	0.41
2:H:26:C:C4	2:H:27:C:C4	3.09	0.41
1:B:137:PHE:CD1	1:B:306:LYS:HG2	2.55	0.41
1:D:256:LEU:HD23	1:D:263:VAL:HG21	2.03	0.41
1:B:74:ASN:OD1	1:B:74:ASN:C	2.59	0.41
1:D:265:GLU:HG3	1:D:266:PRO:HD2	2.03	0.41
1:D:204:ILE:HG22	1:D:205:ASN:N	2.35	0.41
1:A:139:VAL:HB	1:A:314:LEU:HB3	2.02	0.41
1:B:1:MET:C	1:B:3:SER:N	2.74	0.41
1:C:33:GLU:CD	1:C:60:LYS:HE3	2.42	0.41
1:B:385:LEU:HD13	1:B:388:LEU:HD22	2.03	0.41
1:E:88:PRO:HG3	1:E:344:MET:CE	2.51	0.41
1:A:126:TYR:O	1:A:130:LEU:HG	2.21	0.41
1:A:265:GLU:CD	1:A:266:PRO:HD2	2.40	0.41
1:D:254:ILE:CD1	1:D:336:TYR:CE1	3.04	0.41
1:C:432:ARG:HG3	1:C:432:ARG:O	2.20	0.41
2:I:43:G:H2'	2:I:44:G:C8	2.56	0.41
2:G:47(H):U:H2'	2:G:47(I):A:C4'	2.51	0.40
1:E:30:ALA:O	1:E:34:VAL:CG2	2.66	0.40
2:G:66:A:H2'	2:G:67:U:C6	2.56	0.40
1:A:29:LYS:HD2	1:B:332:PHE:CE1	2.56	0.40
2:I:30:G:N2	2:I:40:C:O2	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:ARG:HA	1:E:412:ARG:CZ	2.52	0.40
1:C:438:ASP:O	1:C:442:ILE:HG13	2.20	0.40
1:E:272:ILE:HD11	1:E:296:VAL:HG23	2.03	0.40
1:A:84:LEU:HB3	1:B:104:TYR:HB3	2.02	0.40
1:E:301:LEU:HA	1:E:301:LEU:HD23	1.75	0.40
1:C:99:GLU:O	1:D:71:ARG:CZ	2.69	0.40
2:H:65:C:H2'	2:H:66:A:C8	2.56	0.40
1:D:163:ARG:HH11	1:E:166:LEU:HD13	1.83	0.40
1:A:396:ALA:HB2	1:A:428:LEU:HD23	2.03	0.40
1:E:15:VAL:HG11	1:E:24:GLU:OE2	2.21	0.40
1:A:327:THR:O	1:A:331:TYR:HD2	2.05	0.40
1:A:79:VAL:CG1	1:A:341:VAL:HG13	2.51	0.40
2:J:23:C:N4	2:J:24:C:N4	2.69	0.40
1:D:86:ARG:HB3	1:D:284:ASP:O	2.21	0.40
1:E:231:GLU:H	1:E:231:GLU:CD	2.23	0.40
1:B:7:GLN:HB2	1:B:50:LEU:CD1	2.51	0.40
1:B:10:GLN:HB2	2:F:19:G:H2'	2.02	0.40
2:F:38:A:H2'	2:F:39:U:O4'	2.20	0.40
2:J:47(E):A:C2'	2:J:47(F):U:H5'	2.51	0.40
1:C:193:ASN:HB2	1:C:224:PHE:O	2.21	0.40
2:J:56:C:H2'	2:J:57:G:C8	2.56	0.40
1:A:263:VAL:CG1	1:A:264:ASP:N	2.85	0.40
1:A:169:ILE:HG13	1:A:169:ILE:O	2.21	0.40
1:B:137:PHE:HD1	1:B:306:LYS:HE2	1.86	0.40
1:A:47:ARG:HD3	1:A:49:ASP:O	2.22	0.40
1:A:86:ARG:HD2	1:A:284:ASP:OD2	2.22	0.40
2:I:1:G:H2'	2:I:2:G:C8	2.56	0.40
2:J:35:C:C2'	2:J:36:A:O4'	2.69	0.40
2:G:29:A:O2'	2:G:30:G:O4'	2.39	0.40
2:I:28:U:H2'	2:I:29:A:H8	1.86	0.40
1:E:175:ILE:N	1:E:176:PRO:HD2	2.36	0.40
1:C:70:LYS:HE2	1:C:70:LYS:HB3	1.88	0.40
2:G:2:G:H2'	2:G:3:G:C8	2.56	0.40
1:D:363:LEU:O	1:D:371:ILE:HD11	2.22	0.40
1:D:220:TYR:CD1	1:D:220:TYR:C	2.95	0.40
1:D:348:ASP:O	1:D:351:ALA:HB3	2.21	0.40
1:C:87:ALA:CB	1:C:341:VAL:HG21	2.52	0.40
1:C:247:ASP:OD1	1:C:247:ASP:C	2.60	0.40
1:A:335:ARG:NE	1:A:338:ASP:OD2	2.54	0.40
2:H:8:A:HO2'	2:H:9:U:P	2.44	0.40
1:A:167:VAL:HG12	1:A:219:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:SER:CB	1:E:296:VAL:HG12	2.49	0.40
1:A:416:PRO:HG3	1:A:441:THR:HG21	2.04	0.40
1:D:416:PRO:CG	1:D:441:THR:HG21	2.51	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/452 (99%)	423 (94%)	22 (5%)	4 (1%)	21	67
1	B	449/452 (99%)	419 (93%)	25 (6%)	5 (1%)	17	63
1	C	449/452 (99%)	421 (94%)	24 (5%)	4 (1%)	21	67
1	D	449/452 (99%)	421 (94%)	24 (5%)	4 (1%)	21	67
1	E	449/452 (99%)	420 (94%)	23 (5%)	6 (1%)	15	60
All	All	2245/2260 (99%)	2104 (94%)	118 (5%)	23 (1%)	19	65

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	9	PRO
1	E	9	PRO
1	B	124	GLU
1	C	124	GLU
1	D	124	GLU
1	E	2	LYS
1	E	124	GLU
1	A	86	ARG
1	A	124	GLU
1	B	19	ALA
1	C	86	ARG

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Mol	Chain	Res	Type
1	D	19	ALA
1	A	19	ALA
1	B	86	ARG
1	C	19	ALA
1	D	86	ARG
1	E	19	ALA
1	E	86	ARG
1	A	9	PRO
1	C	9	PRO
1	E	340	PRO
1	B	9	PRO
1	B	340	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/390 (100%)	380 (97%)	10 (3%)	54	80
1	B	390/390 (100%)	389 (100%)	1 (0%)	94	96
1	C	390/390 (100%)	385 (99%)	5 (1%)	76	89
1	D	390/390 (100%)	384 (98%)	6 (2%)	72	88
1	E	390/390 (100%)	389 (100%)	1 (0%)	94	96
All	All	1950/1950 (100%)	1927 (99%)	23 (1%)	78	90

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	98	SER
1	A	105	SER
1	A	118	SER
1	A	136	SER
1	A	188	GLU
1	A	271	CYS

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Mol	Chain	Res	Type
1	A	287	LEU
1	A	394	CYS
1	A	403	SER
1	B	188	GLU
1	C	3	SER
1	C	188	GLU
1	C	317	ASP
1	C	384	SER
1	C	400	ASP
1	D	24	GLU
1	D	39	ARG
1	D	172	SER
1	D	182	SER
1	D	188	GLU
1	D	316	ILE
1	E	188	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	140	ASN
1	A	347	GLN
1	A	399	HIS
1	A	436	HIS
1	B	10	GLN
1	B	95	ASN
1	B	122	HIS
1	B	142	ASN
1	B	399	HIS
1	B	405	GLN
1	C	10	GLN
1	C	68	ASN
1	C	95	ASN
1	C	122	HIS
1	C	291	GLN
1	C	347	GLN
1	C	405	GLN
1	D	122	HIS
1	D	347	GLN
1	D	399	HIS
1	D	436	HIS

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Mol	Chain	Res	Type
1	E	122	HIS
1	E	140	ASN
1	E	238	HIS
1	E	347	GLN
1	E	399	HIS
1	E	405	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	91/95 (95%)	6 (6%)	0
2	G	91/95 (95%)	6 (6%)	0
2	H	91/95 (95%)	6 (6%)	0
2	I	91/95 (95%)	9 (9%)	1 (1%)
2	J	91/95 (95%)	6 (6%)	0
All	All	455/475 (95%)	33 (7%)	1 (0%)

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	18	G
2	F	20(A)	G
2	F	33	U
2	F	42(A)	C
2	F	43	G
2	F	73	G
2	G	18	G
2	G	20(A)	G
2	G	42(A)	C
2	G	43	G
2	G	47(G)	U
2	G	73	G
2	H	18	G
2	H	20(A)	G
2	H	42(A)	C
2	H	43	G
2	H	47(G)	U
2	H	73	G
2	I	14	G
2	I	18	G
2	I	20(A)	G

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Mol	Chain	Res	Type
2	I	42(A)	C
2	I	43	G
2	I	44	G
2	I	45	U
2	I	47(G)	U
2	I	73	G
2	J	18	G
2	J	20(A)	G
2	J	42(A)	C
2	J	43	G
2	J	47(G)	U
2	J	73	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	I	44	G

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LLP	A	285	1	23,24,25	1.17	1 (4%)	28,32,34	1.01	1 (3%)
1	LLP	B	285	1	23,24,25	1.29	2 (8%)	28,32,34	1.10	2 (7%)
1	LLP	C	285	1	23,24,25	1.14	2 (8%)	28,32,34	1.01	2 (7%)
1	LLP	D	285	1	23,24,25	1.15	1 (4%)	28,32,34	0.99	2 (7%)
1	LLP	E	285	1	23,24,25	1.18	1 (4%)	28,32,34	1.13	3 (10%)

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
1	LLP	A	285	1	-	0/15/17/19	0/1/1/1
1	LLP	B	285	1	-	0/15/17/19	0/1/1/1
1	LLP	C	285	1	-	0/15/17/19	0/1/1/1
1	LLP	D	285	1	-	0/15/17/19	0/1/1/1
1	LLP	E	285	1	-	0/15/17/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	LLP	C4-C4'	-3.45	1.40	1.46
1	E	285	LLP	C4-C4'	-3.18	1.41	1.46
1	A	285	LLP	C4-C4'	-3.05	1.41	1.46
1	C	285	LLP	C4-C4'	-2.77	1.41	1.46
1	D	285	LLP	C4-C4'	-2.68	1.42	1.46
1	B	285	LLP	C3-C2	-2.22	1.39	1.40
1	C	285	LLP	C4'-NZ	2.02	1.33	1.27

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	LLP	O-C-CA	-2.24	119.66	125.49
1	E	285	LLP	O-C-CA	-2.13	119.94	125.49
1	D	285	LLP	O-C-CA	-2.10	120.03	125.49
1	E	285	LLP	OP4-C5'-C5	2.14	112.54	108.99
1	C	285	LLP	OP4-P-OP1	2.18	112.69	107.14
1	D	285	LLP	OP4-P-OP1	2.20	112.73	107.14
1	B	285	LLP	OP4-C5'-C5	2.22	112.67	108.99
1	A	285	LLP	OP4-P-OP1	2.30	113.00	107.14
1	B	285	LLP	OP4-P-OP1	2.53	113.59	107.14
1	E	285	LLP	OP4-P-OP1	2.69	114.00	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	285	LLP	3	0
1	B	285	LLP	7	0
1	C	285	LLP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	285	LLP	1	0
1	E	285	LLP	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	451/452 (99%)	1.06	89 (19%) 1 7	363, 478, 546, 629	0
1	B	451/452 (99%)	0.95	64 (14%) 4 9	371, 474, 554, 648	0
1	C	451/452 (99%)	0.78	65 (14%) 3 9	364, 474, 549, 625	0
1	D	451/452 (99%)	0.98	77 (17%) 2 8	356, 463, 536, 601	0
1	E	451/452 (99%)	1.17	103 (22%) 1 6	330, 466, 539, 617	0
2	F	92/95 (96%)	0.31	6 (6%) 22 23	505, 594, 716, 786	0
2	G	92/95 (96%)	0.92	22 (23%) 1 6	505, 594, 744, 870	0
2	H	92/95 (96%)	1.69	39 (42%) 0 4	506, 596, 753, 853	0
2	I	92/95 (96%)	0.60	12 (13%) 5 10	506, 596, 746, 774	0
2	J	92/95 (96%)	0.88	18 (19%) 1 7	506, 595, 744, 791	0
All	All	2715/2735 (99%)	0.97	495 (18%) 2 7	330, 482, 656, 870	0

All (495) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	47(O)	G	6.9
1	E	291	GLN	6.9
2	G	47(O)	G	6.1
1	E	228	VAL	6.0
2	J	47(O)	G	6.0
1	A	420	CYS	5.8
2	G	47(N)	A	5.7
1	D	291	GLN	5.5
1	C	116	ARG	5.5
1	E	395	VAL	5.4
1	D	165	GLU	5.4
1	A	317	ASP	5.3
1	E	397	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
2	H	22	G	5.2
1	D	23	PRO	5.2
1	E	396	ALA	5.2
1	E	373	VAL	5.1
1	B	373	VAL	5.1
1	E	317	ASP	5.1
1	B	397	ILE	5.1
1	B	317	ASP	5.0
1	E	315	ARG	5.0
1	D	211	LEU	4.9
1	D	212	MET	4.9
1	C	317	ASP	4.8
1	D	397	ILE	4.8
1	E	171	GLY	4.7
1	D	429	PHE	4.7
1	E	371	ILE	4.7
1	D	171	GLY	4.6
1	A	291	GLN	4.6
1	B	395	VAL	4.6
1	D	213	LYS	4.5
2	G	73	G	4.5
2	J	47(N)	A	4.5
2	H	14	G	4.4
2	H	47(A)	C	4.4
1	D	284	ASP	4.4
1	E	360	GLU	4.3
2	G	47	U	4.3
1	A	73	ILE	4.3
1	C	73	ILE	4.3
1	A	165	GLU	4.3
1	B	394	CYS	4.2
1	D	251	GLY	4.2
2	J	73	G	4.2
1	D	317	ASP	4.2
2	H	34	U	4.1
2	H	47(I)	A	4.1
1	E	140	ASN	4.1
1	A	284	ASP	4.1
2	H	42(A)	C	4.1
2	J	47(F)	U	4.0
1	D	170	GLY	4.0
1	C	418	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	73	G	4.0
1	A	8	ILE	4.0
1	A	140	ASN	4.0
1	B	372	SER	4.0
1	A	87	ALA	4.0
1	E	372	SER	4.0
1	C	315	ARG	4.0
1	E	172	SER	3.9
1	E	23	PRO	3.9
2	H	47	U	3.9
2	J	47(E)	A	3.9
1	D	214	VAL	3.9
1	A	427	LEU	3.9
1	E	31	ALA	3.9
2	J	46	C	3.8
1	C	291	GLN	3.8
1	A	418	ILE	3.8
1	C	212	MET	3.7
1	D	267	ASN	3.7
1	D	250	SER	3.7
1	B	396	ALA	3.7
1	E	27	VAL	3.7
2	H	35	C	3.7
1	D	172	SER	3.7
1	E	284	ASP	3.6
2	H	47(N)	A	3.6
1	A	397	ILE	3.6
2	G	72	C	3.6
2	H	46	C	3.6
1	E	24	GLU	3.6
1	E	1	MET	3.6
1	B	140	ASN	3.6
1	B	291	GLN	3.6
1	E	26	TYR	3.5
1	A	211	LEU	3.5
2	J	47(D)	U	3.5
1	E	14	VAL	3.5
1	E	3	SER	3.5
1	C	31	ALA	3.5
1	B	429	PHE	3.5
1	A	212	MET	3.5
2	H	21	U	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	320	THR	3.5
1	E	312	ARG	3.5
1	B	393	TYR	3.4
1	B	2	LYS	3.4
2	G	46	C	3.4
1	C	119	ARG	3.4
2	H	47(P)	A	3.4
1	A	369	LEU	3.4
1	C	265	GLU	3.4
1	A	395	VAL	3.4
1	E	429	PHE	3.4
1	B	165	GLU	3.4
2	J	47	U	3.4
1	D	266	PRO	3.4
1	E	119	ARG	3.4
2	G	47(E)	A	3.4
2	H	47(C)	C	3.3
1	D	82	THR	3.3
1	C	165	GLU	3.3
1	C	228	VAL	3.3
1	D	420	CYS	3.3
2	G	47(A)	C	3.3
1	D	255	ASN	3.3
1	B	214	VAL	3.3
1	D	14	VAL	3.3
1	E	250	SER	3.2
2	H	47(H)	U	3.2
1	B	212	MET	3.2
1	A	428	LEU	3.2
2	H	47(B)	G	3.2
1	B	376	ASP	3.2
1	E	277	ASP	3.2
1	E	212	MET	3.2
1	A	429	PHE	3.2
1	B	265	GLU	3.2
2	F	14	G	3.2
1	C	429	PHE	3.2
1	C	266	PRO	3.2
1	E	316	ILE	3.2
1	E	116	ARG	3.2
1	E	445	THR	3.2
1	B	431	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	31	ALA	3.1
1	D	247	ASP	3.1
1	D	200	TYR	3.1
1	C	200	TYR	3.1
1	D	86	ARG	3.1
1	E	28	VAL	3.1
1	D	140	ASN	3.1
1	A	315	ARG	3.1
1	B	22	TYR	3.1
1	E	83	ASN	3.1
1	A	166	LEU	3.1
1	A	442	ILE	3.1
1	E	320	THR	3.1
2	F	15	C	3.1
1	D	192	THR	3.1
2	G	47(M)	G	3.1
1	E	394	CYS	3.1
1	D	22	TYR	3.1
2	G	2	G	3.1
1	A	213	LYS	3.0
2	J	47(C)	C	3.0
1	B	172	SER	3.0
1	B	316	ILE	3.0
1	E	200	TYR	3.0
2	J	47(M)	G	3.0
1	A	371	ILE	3.0
1	E	442	ILE	3.0
1	D	215	HIS	3.0
1	D	427	LEU	3.0
1	E	118	SER	3.0
1	C	118	SER	3.0
1	B	374	ILE	2.9
1	C	410	ARG	2.9
2	J	14	G	2.9
1	E	441	THR	2.9
1	E	290	PRO	2.9
1	B	315	ARG	2.9
2	G	47(K)	G	2.9
1	A	320	THR	2.9
1	B	356	ALA	2.9
1	B	211	LEU	2.9
1	C	279	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	419	VAL	2.9
1	A	172	SER	2.9
1	D	24	GLU	2.9
1	E	418	ILE	2.9
1	A	312	ARG	2.9
2	G	3	G	2.9
1	E	357	LYS	2.9
1	C	245	TYR	2.9
1	C	211	LEU	2.9
1	E	359	LEU	2.9
2	G	47(F)	U	2.8
1	D	419	VAL	2.8
1	B	8	ILE	2.8
2	H	47(J)	A	2.8
2	H	27	C	2.8
1	C	48	ALA	2.8
1	D	248	ALA	2.8
1	D	265	GLU	2.8
1	B	228	VAL	2.8
2	G	1	G	2.8
2	H	55	U	2.8
2	I	29	A	2.8
1	B	3	SER	2.8
1	E	114	GLY	2.8
1	E	278	LEU	2.8
1	C	214	VAL	2.8
1	C	384	SER	2.8
1	C	411	LEU	2.8
1	E	95	ASN	2.8
1	B	31	ALA	2.8
1	D	407	LEU	2.8
1	C	434	VAL	2.8
2	J	47(A)	C	2.8
1	A	421	ARG	2.8
1	C	312	ARG	2.8
1	E	15	VAL	2.8
1	E	82	THR	2.8
1	D	418	ILE	2.8
1	C	263	VAL	2.8
1	D	31	ALA	2.8
1	E	87	ALA	2.8
1	E	289	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	G	47(B)	G	2.8
1	D	228	VAL	2.8
1	E	369	LEU	2.8
1	C	419	VAL	2.8
1	E	279	VAL	2.7
1	E	25	ILE	2.7
1	E	449	LEU	2.7
1	C	420	CYS	2.7
1	B	320	THR	2.7
1	D	245	TYR	2.7
2	H	15	C	2.7
1	E	141	ASN	2.7
1	C	276	ILE	2.7
1	A	74	ASN	2.7
1	A	338	ASP	2.7
1	E	431	MET	2.7
2	I	38	A	2.7
1	A	88	PRO	2.7
1	A	363	LEU	2.7
1	C	252	LEU	2.7
1	A	370	LYS	2.7
1	C	53	PHE	2.7
2	H	47(G)	U	2.7
1	A	83	ASN	2.7
1	C	4	LEU	2.7
1	C	213	LYS	2.7
1	C	253	LEU	2.7
1	C	320	THR	2.7
2	G	47(C)	C	2.7
2	G	47(D)	U	2.7
1	D	26	TYR	2.7
1	B	347	GLN	2.7
1	A	373	VAL	2.7
1	B	153	LEU	2.7
2	J	45	U	2.7
1	B	160	ILE	2.7
1	C	284	ASP	2.7
1	D	384	SER	2.7
1	B	115	LYS	2.6
1	C	254	ILE	2.6
1	A	118	SER	2.6
1	E	245	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	161	ILE	2.6
2	I	72	C	2.6
1	A	381	GLY	2.6
1	B	26	TYR	2.6
2	H	56	C	2.6
1	B	171	GLY	2.6
1	A	170	GLY	2.6
2	H	36	A	2.6
1	E	276	ILE	2.6
1	D	428	LEU	2.6
1	B	223	GLY	2.6
1	B	23	PRO	2.6
2	H	44	G	2.6
1	A	362	LEU	2.6
1	A	86	ARG	2.6
1	A	214	VAL	2.6
1	C	117	GLY	2.6
1	A	14	VAL	2.6
2	H	13	C	2.6
1	A	141	ASN	2.6
1	A	360	GLU	2.6
1	A	28	VAL	2.6
2	G	47(J)	A	2.6
1	C	223	GLY	2.6
1	D	210	LEU	2.6
1	E	356	ALA	2.6
1	A	171	GLY	2.5
1	E	267	ASN	2.5
1	D	316	ILE	2.5
1	E	9	PRO	2.5
1	A	250	SER	2.5
1	A	446	LEU	2.5
1	E	166	LEU	2.5
1	D	391	PRO	2.5
1	C	251	GLY	2.5
1	E	4	LEU	2.5
1	A	417	PRO	2.5
1	B	310	ILE	2.5
2	H	47(M)	G	2.5
1	D	380	PRO	2.5
2	H	33	U	2.5
1	C	233	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	2.5
1	B	7	GLN	2.5
1	B	427	LEU	2.5
1	D	188	GLU	2.5
2	H	73	G	2.5
1	A	411	LEU	2.5
2	H	23	C	2.5
2	I	28	U	2.5
1	E	86	ARG	2.5
1	C	35	ALA	2.5
2	F	56	C	2.5
1	D	163	ARG	2.5
1	D	279	VAL	2.5
1	C	262	SER	2.5
1	D	160	ILE	2.5
1	A	359	LEU	2.5
1	A	434	VAL	2.5
1	B	384	SER	2.4
1	C	267	ASN	2.4
1	D	315	ARG	2.4
1	A	372	SER	2.4
1	B	233	LEU	2.4
1	E	296	VAL	2.4
1	A	398	ARG	2.4
1	B	392	THR	2.4
2	G	47(I)	A	2.4
1	B	213	LYS	2.4
1	D	166	LEU	2.4
1	E	410	ARG	2.4
1	D	141	ASN	2.4
1	E	108	GLU	2.4
1	E	428	LEU	2.4
2	H	47(K)	G	2.4
1	D	35	ALA	2.4
1	E	85	GLY	2.4
1	A	260	GLY	2.4
2	H	47(D)	U	2.4
1	A	245	TYR	2.4
1	C	407	LEU	2.4
1	C	79	VAL	2.4
2	I	47(G)	U	2.4
1	D	223	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	166	LEU	2.4
1	C	290	PRO	2.4
1	C	395	VAL	2.4
1	A	346	THR	2.4
1	E	450	LEU	2.4
2	G	47(H)	U	2.4
1	B	116	ARG	2.4
1	D	83	ASN	2.4
1	E	165	GLU	2.4
1	B	312	ARG	2.4
1	C	431	MET	2.4
1	D	73	ILE	2.4
1	D	254	ILE	2.4
1	D	426	GLN	2.4
1	D	65	MET	2.4
1	E	213	LYS	2.3
1	D	289	GLY	2.3
1	E	117	GLY	2.3
1	A	161	ILE	2.3
1	A	75	ALA	2.3
2	F	20	U	2.3
1	D	216	LYS	2.3
1	E	22	TYR	2.3
1	B	149	VAL	2.3
2	I	73	G	2.3
1	C	272	ILE	2.3
1	B	420	CYS	2.3
1	A	416	PRO	2.3
1	C	140	ASN	2.3
1	E	381	GLY	2.3
1	A	450	LEU	2.3
1	C	278	LEU	2.3
1	E	57	VAL	2.3
2	H	47(E)	A	2.3
1	A	128	ASN	2.3
1	E	363	LEU	2.3
2	I	27	C	2.3
1	A	119	ARG	2.3
1	A	380	PRO	2.3
2	G	47(G)	U	2.3
1	C	111	LEU	2.3
1	D	252	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	200	TYR	2.3
1	E	35	ALA	2.3
2	I	37	A	2.2
1	A	265	GLU	2.2
1	E	384	SER	2.2
1	C	115	LYS	2.2
1	D	164	GLY	2.2
1	E	295	ILE	2.2
1	A	121	ALA	2.2
1	E	393	TYR	2.2
2	H	32	C	2.2
1	A	9	PRO	2.2
1	B	4	LEU	2.2
1	B	292	ALA	2.2
1	B	27	VAL	2.2
1	D	312	ARG	2.2
1	E	283	GLY	2.2
1	E	18	PHE	2.2
1	E	362	LEU	2.2
1	E	411	LEU	2.2
1	E	452	ILE	2.2
1	A	217	SER	2.2
1	B	35	ALA	2.2
1	A	24	GLU	2.2
1	B	363	LEU	2.2
1	A	293	GLY	2.2
1	B	264	ASP	2.2
1	D	395	VAL	2.2
1	D	398	ARG	2.2
1	C	255	ASN	2.2
1	E	98	SER	2.2
1	E	374	ILE	2.2
1	A	396	ALA	2.2
1	A	283	GLY	2.2
1	A	81	ASN	2.2
1	B	119	ARG	2.2
1	E	446	LEU	2.2
1	E	292	ALA	2.2
1	C	66	LYS	2.2
2	F	20(A)	G	2.2
2	J	47(G)	U	2.2
1	D	290	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	2.1
2	H	12	G	2.1
2	H	45	U	2.1
1	E	407	LEU	2.1
2	I	40	C	2.1
1	C	397	ILE	2.1
1	A	223	GLY	2.1
1	B	284	ASP	2.1
1	A	116	ARG	2.1
1	A	367	PRO	2.1
2	I	47(D)	U	2.1
1	A	169	ILE	2.1
1	D	292	ALA	2.1
1	E	73	ILE	2.1
1	B	210	LEU	2.1
1	C	316	ILE	2.1
1	E	53	PHE	2.1
1	A	313	ALA	2.1
1	E	427	LEU	2.1
1	C	131	THR	2.1
1	C	244	THR	2.1
2	J	72	C	2.1
1	D	18	PHE	2.1
1	C	250	SER	2.1
1	A	27	VAL	2.1
1	E	358	ARG	2.1
2	J	47(H)	U	2.1
1	D	16	GLU	2.1
1	D	271	CYS	2.1
2	J	47(P)	A	2.1
1	E	313	ALA	2.1
1	A	72	VAL	2.1
2	H	47(F)	U	2.1
2	I	39	U	2.1
1	A	117	GLY	2.1
1	E	451	SER	2.1
1	B	73	ILE	2.1
1	A	407	LEU	2.1
1	D	111	LEU	2.1
1	C	149	VAL	2.1
1	C	277	ASP	2.1
1	E	392	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	71	C	2.1
1	C	75	ALA	2.1
1	E	163	ARG	2.1
1	B	290	PRO	2.0
1	A	384	SER	2.0
1	A	443	LYS	2.0
1	E	133	ALA	2.0
1	D	106	ASN	2.0
1	E	361	LYS	2.0
2	H	72	C	2.0
2	I	30	G	2.0
2	J	47(B)	G	2.0
1	D	149	VAL	2.0
1	E	81	ASN	2.0
1	A	139	VAL	2.0
2	H	8	A	2.0
2	H	57	G	2.0
1	A	439	LEU	2.0
1	A	399	HIS	2.0
1	A	210	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	LLP	B	285	24/25	0.75	0.61	-	429,446,491,495	0
1	LLP	E	285	24/25	0.70	0.67	-	290,384,467,493	0
1	LLP	D	285	24/25	0.57	0.70	-	310,432,455,471	0
1	LLP	A	285	24/25	0.65	0.69	-	384,433,449,452	0
1	LLP	C	285	24/25	0.64	0.65	-	416,449,487,497	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.