



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:04 AM UTC

PDB ID : 3EPL / pdb_00003epl
Title : Crystallographic snapshots of eukaryotic dimethylallyltransferase acting on tRNA: Insight into tRNA recognition and reaction mechanism
Authors : Huang, R.H.; Zhou, C.
Deposited on : 2008-09-29
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

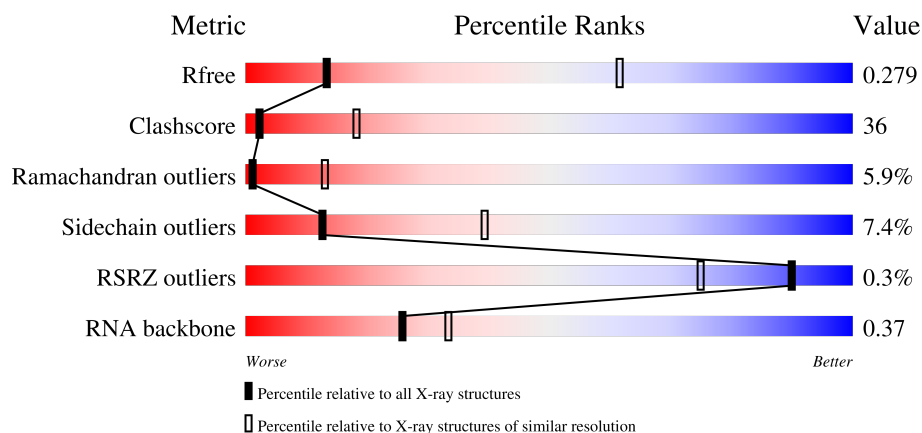
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	409	35% 55% 8%
1	B	409	32% 56% 9%
2	E	69	32% 54% 10%
3	F	69	4% 30% 43% 14% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9775 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 tRNA isopentenyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3339	2119	589	617	14			
1	B	402	Total	C	N	O	S	0	0	0
			3339	2119	589	617	14			

- Molecule 2 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	69	Total	C	N	O	P	0	0	0
			1478	661	258	490	69			

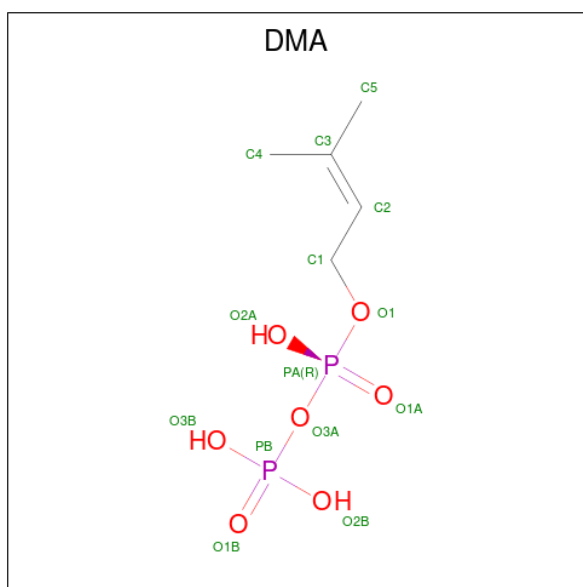
- Molecule 3 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	69	Total	C	N	O	P	0	0	0
			1473	656	258	490	69			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is DIMETHYLALLYL DIPHOSPHATE (CCD ID: DMA) (formula: C₅H₁₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			9	7	2		
5	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	F	2	Total	Mg	0	0
			2	2		

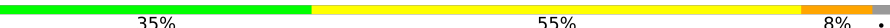
- Molecule 7 is water.

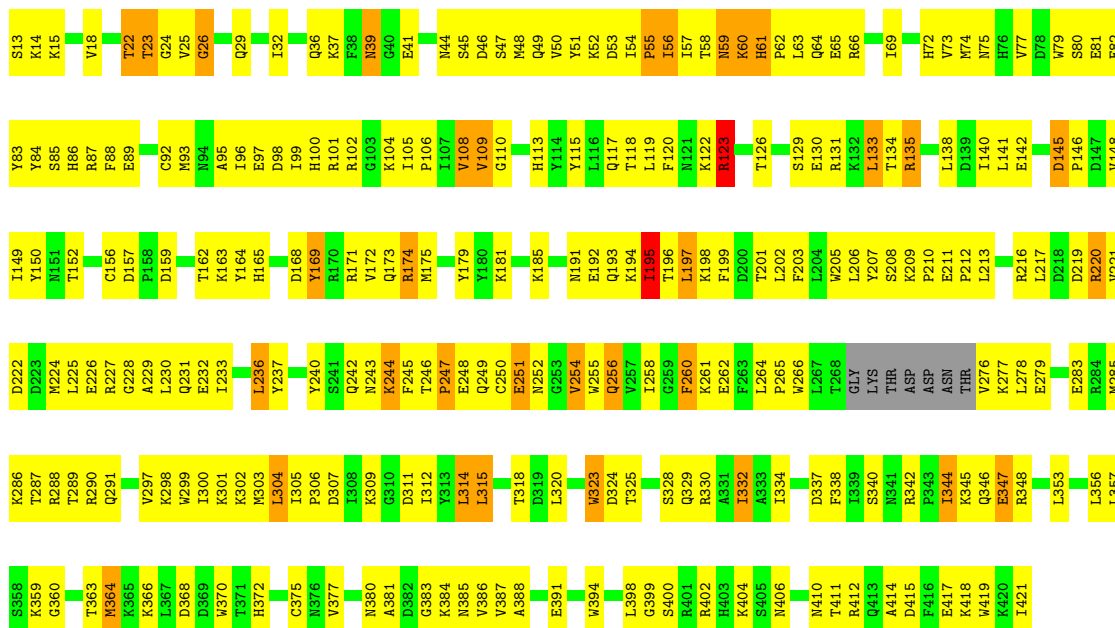
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	24	Total	O	0	0
			24	24		
7	E	22	Total	O	0	0
			22	22		
7	B	42	Total	O	0	0
			42	42		
7	F	34	Total	O	0	0
			34	34		

3 Residue-property plots

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

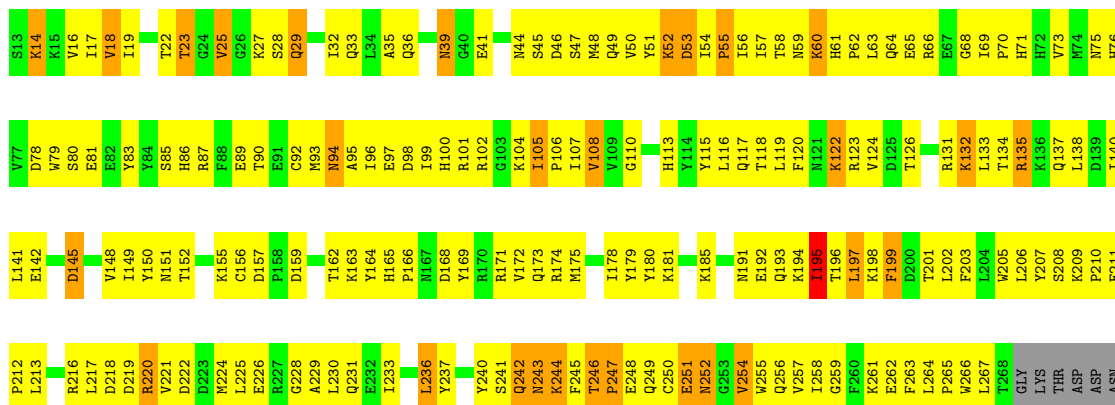
• Molecule 1: tRNA isopentenyltransferase

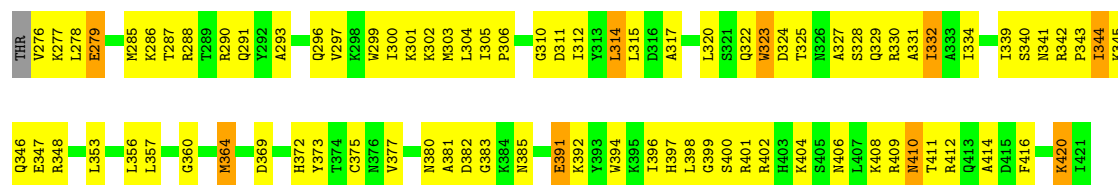
Chain A: 



• Molecule 1: tRNA isopentenyltransferase

Chain B: 

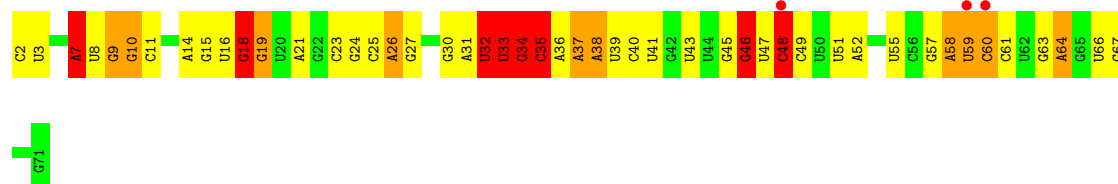




• Molecule 2: tRNA



• Molecule 3: tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	164.07Å 209.85Å 127.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	77.5 (50.00-3.60) 83.5 (50.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.91 (at 3.56Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.266 0.216 , 0.279	Depositor DCC
R_{free} test set	1759 reflections (7.88%)	wwPDB-VP
Wilson B-factor (Å ²)	103.1	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9775	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMA, MG, ZN, 6IA

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	0.56	2/3411 (0.1%)	0.85	3/4598 (0.1%)
1	B	0.56	1/3411 (0.0%)	0.86	5/4598 (0.1%)
2	E	0.41	0/1619	0.94	12/2518 (0.5%)
3	F	0.42	0/1645	1.07	21/2561 (0.8%)
All	All	0.52	3/10086 (0.0%)	0.91	41/14275 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	MET	SD-CE	6.38	1.95	1.79
1	A	108	VAL	CA-CB	5.69	1.60	1.54
1	B	364	MET	SD-CE	5.49	1.93	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	32	U	C2'-C3'-O3'	13.28	129.41	109.50
3	F	32	U	C2'-C3'-O3'	13.23	129.35	109.50
3	F	18	G	C2'-C3'-O3'	11.83	127.25	109.50
3	F	37	A	C2'-C3'-O3'	11.36	126.53	109.50
2	E	33	U	C2'-C3'-O3'	11.19	126.28	109.50
3	F	33	U	C2'-C3'-O3'	11.12	126.17	109.50
3	F	34	G	C2'-C3'-O3'	10.79	125.68	109.50
2	E	34	G	C2'-C3'-O3'	9.95	124.42	109.50
3	F	34	G	C4'-C3'-O3'	8.54	122.22	109.40
3	F	46	G	C4'-C3'-O3'	-8.51	100.24	113.00
3	F	46	G	N9-C1'-C2'	8.32	124.48	112.00
3	F	7	A	N9-C1'-C2'	8.30	124.44	112.00
3	F	18	G	C4'-C3'-O3'	7.66	120.88	109.40
2	E	34	G	C4'-C3'-O3'	7.61	120.81	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	32	U	C4'-C3'-O3'	7.43	120.55	109.40
2	E	48	C	C2'-C3'-O3'	7.37	120.55	109.50
3	F	48	C	C2'-C3'-O3'	7.15	120.23	109.50
2	E	33	U	C4'-C3'-O3'	6.84	119.66	109.40
3	F	32	U	C4'-C3'-O3'	6.76	119.53	109.40
2	E	36	A	C4'-C3'-O3'	6.39	118.98	109.40
1	B	219	ASP	N-CA-C	-6.13	105.65	113.01
1	A	219	ASP	N-CA-C	-6.08	105.13	112.54
3	F	7	A	C4'-C3'-O3'	-6.06	103.92	113.00
3	F	60	C	N1-C1'-C2'	5.83	120.75	112.00
3	F	33	U	C4'-C3'-O3'	5.82	118.12	109.40
3	F	60	C	C2'-C3'-O3'	-5.75	105.08	113.70
3	F	26	A	C4'-C3'-O3'	-5.60	104.60	113.00
3	F	35	C	C2'-C3'-O3'	5.55	117.82	109.50
1	A	145	ASP	CA-C-N	5.53	125.05	119.19
1	A	145	ASP	C-N-CA	5.53	125.05	119.19
2	E	33	U	C4'-C3'-C2'	5.50	108.10	102.60
2	E	18	G	C2'-C3'-O3'	5.47	121.90	113.70
3	F	32	U	C4'-C3'-C2'	5.34	107.94	102.60
1	B	105	ILE	N-CA-C	5.31	113.72	107.77
2	E	32	U	C4'-C3'-C2'	5.17	107.77	102.60
3	F	33	U	C4'-C3'-C2'	5.15	107.75	102.60
3	F	18	G	C4'-C3'-C2'	5.14	107.74	102.60
1	B	410	ASN	N-CA-C	-5.11	105.17	111.40
1	B	145	ASP	CA-C-N	5.11	124.61	119.19
1	B	145	ASP	C-N-CA	5.11	124.61	119.19
2	E	34	G	C4'-C3'-C2'	5.07	107.67	102.60

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	3339	0	3346	294	0
1	B	3339	0	3346	277	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1478	0	750	40	0
3	F	1473	0	741	49	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	9	0	0	2	0
5	B	9	0	0	2	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	0	0
7	A	24	0	0	7	0
7	B	42	0	0	9	0
7	E	22	0	0	0	0
7	F	34	0	0	8	0
All	All	9775	0	8183	640	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (640) 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:B:266:TRP:HE1	1:B:277:LYS:HG3	1.09	1.16
1:A:122:LYS:HD3	1:A:193:GLN:HE22	1.18	1.06
1:B:45:SER:HB3	1:B:110:GLY:HA3	1.33	1.05
1:B:303:MET:HE3	7:F:104:HOH:O	1.56	1.02
1:A:45:SER:HB3	1:A:110:GLY:HA3	1.40	1.00
1:A:211:GLU:HB2	1:A:212:PRO:HD3	1.44	0.98
1:B:258:ILE:HD11	1:B:285:MET:HA	1.41	0.98
1:A:334:ILE:HG12	1:A:346:GLN:HG3	1.49	0.95
1:B:334:ILE:HG12	1:B:346:GLN:HG3	1.47	0.94
1:B:211:GLU:HB2	1:B:212:PRO:HD3	1.51	0.92
1:B:113:HIS:HA	1:B:116:LEU:HD23	1.52	0.92
1:A:133:LEU:HD22	1:A:133:LEU:H	1.32	0.91
3:F:9:G:H3'	7:F:107:HOH:O	1.74	0.88
1:B:108:VAL:HG11	1:B:119:LEU:HD11	1.57	0.85
3:F:31:A:O2'	3:F:32:U:H5'	1.78	0.84
1:B:14:LYS:H	1:B:14:LYS:HD2	1.42	0.84
2:E:6:U:H3	2:E:67:G:H1	1.26	0.83
3:F:7:A:H3'	7:F:101:HOH:O	1.80	0.82
1:A:122:LYS:HD3	1:A:193:GLN:NE2	1.95	0.81
1:B:353:LEU:HB3	1:B:356:LEU:HD12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:HB2	1:A:185:LYS:HD2	1.62	0.81
2:E:16:U:H3	2:E:59:U:H3	1.24	0.81
1:A:277:LYS:O	1:A:277:LYS:HD3	1.81	0.81
1:A:79:TRP:CD1	1:A:79:TRP:H	1.98	0.79
1:A:63:LEU:HA	1:A:66:ARG:HB2	1.65	0.78
1:A:14:LYS:H	1:A:14:LYS:HD2	1.48	0.78
1:A:96:ILE:HA	1:A:99:ILE:HD12	1.66	0.78
1:B:79:TRP:H	1:B:79:TRP:CD1	2.01	0.78
1:B:266:TRP:HE1	1:B:277:LYS:CG	1.93	0.78
3:F:36:A:H5'	7:F:95:HOH:O	1.84	0.78
2:E:51:U:H3	2:E:63:G:H1	1.30	0.78
1:A:55:PRO:HA	1:A:58:THR:HG22	1.67	0.77
1:A:120:PHE:HB3	1:A:197:LEU:HA	1.65	0.76
1:A:109:VAL:HG12	1:A:110:GLY:H	1.49	0.76
1:B:266:TRP:NE1	1:B:277:LYS:HG3	1.95	0.75
1:B:45:SER:CB	1:B:110:GLY:HA3	2.15	0.75
2:E:56:C:H2'	2:E:57:G:H8	1.52	0.74
1:A:246:THR:HB	1:A:247:PRO:HD2	1.69	0.74
1:A:394:TRP:CE2	1:A:398:LEU:HD11	2.21	0.74
1:A:133:LEU:HD23	1:A:138:LEU:HD21	1.69	0.74
1:B:14:LYS:HD2	1:B:14:LYS:N	2.02	0.74
1:A:276:VAL:HG12	1:A:278:LEU:H	1.53	0.73
1:B:122:LYS:HD3	1:B:193:GLN:HE22	1.53	0.72
1:B:394:TRP:CE2	1:B:398:LEU:HD11	2.23	0.72
1:B:157:ASP:HB2	1:B:185:LYS:HD2	1.71	0.72
1:B:79:TRP:H	1:B:79:TRP:HD1	1.36	0.72
1:B:225:LEU:HA	1:B:229:ALA:HB3	1.69	0.71
1:B:159:ASP:O	1:B:162:THR:HG22	1.90	0.71
1:A:15:LYS:HB2	1:A:105:ILE:HD11	1.72	0.70
1:A:96:ILE:HG23	1:A:106:PRO:HG2	1.74	0.70
1:A:353:LEU:HB3	1:A:356:LEU:HD12	1.71	0.70
1:A:415:ASP:OD2	1:A:418:LYS:HD2	1.91	0.70
1:B:246:THR:HB	1:B:247:PRO:HD2	1.72	0.70
1:A:82:GLU:HG3	1:A:252:ASN:HB3	1.72	0.69
1:A:258:ILE:HD11	1:A:285:MET:HA	1.74	0.69
1:B:79:TRP:HZ3	1:B:236:LEU:HA	1.56	0.69
1:A:406:ASN:O	1:A:410:ASN:HB2	1.92	0.69
1:B:78:ASP:HB3	1:B:81:GLU:CD	2.17	0.69
1:B:33:GLN:HA	1:B:36:GLN:HE22	1.58	0.69
1:A:400:SER:HB3	2:E:43:U:H5''	1.75	0.69
1:A:174:ARG:HH11	2:E:34:G:H5''	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:TYR:HB2	7:A:442:HOH:O	1.93	0.68
1:B:25:VAL:HB	1:B:206:LEU:HG	1.76	0.68
1:A:25:VAL:HG23	1:A:26:GLY:H	1.59	0.67
1:B:406:ASN:O	1:B:410:ASN:HB2	1.95	0.67
1:A:159:ASP:O	1:A:162:THR:HG22	1.95	0.67
2:E:29:A:H2'	2:E:30:G:H8	1.60	0.67
1:B:39:ASN:HD21	1:B:104:LYS:HG2	1.59	0.67
1:A:122:LYS:HA	1:A:193:GLN:NE2	2.09	0.66
1:A:18:VAL:HG13	1:A:203:PHE:HA	1.77	0.66
1:A:394:TRP:CH2	1:A:398:LEU:HD21	2.30	0.66
1:A:264:LEU:N	1:A:265:PRO:HD2	2.11	0.66
1:B:18:VAL:HG13	1:B:203:PHE:HA	1.75	0.66
1:A:229:ALA:O	1:A:233:ILE:HG12	1.96	0.66
1:B:55:PRO:HA	1:B:60:LYS:HD3	1.78	0.66
1:A:39:ASN:HD21	1:A:104:LYS:HG2	1.59	0.65
1:A:51:TYR:CD1	1:A:254:VAL:HG22	2.31	0.65
1:A:297:VAL:HG12	1:A:301:LYS:HD3	1.79	0.65
1:A:117:GLN:OE1	1:A:122:LYS:HG2	1.98	0.64
1:A:39:ASN:ND2	1:A:104:LYS:HG2	2.13	0.64
1:A:168:ASP:CG	1:A:171:ARG:HG3	2.23	0.64
1:A:92:CYS:O	1:A:96:ILE:HG13	1.98	0.64
1:B:305:ILE:HB	1:B:306:PRO:HD3	1.80	0.64
1:A:225:LEU:HA	1:A:229:ALA:HB3	1.79	0.63
1:B:408:LYS:O	1:B:412:ARG:HB2	1.97	0.63
2:E:5:G:H2'	2:E:6:U:O4'	1.98	0.63
1:B:251:GLU:HB3	1:B:261:LYS:HZ3	1.63	0.63
1:A:51:TYR:CE1	1:A:254:VAL:HG22	2.33	0.63
1:A:109:VAL:HG12	1:A:110:GLY:N	2.13	0.63
1:A:344:ILE:HG22	1:A:346:GLN:HG2	1.79	0.63
1:A:324:ASP:O	1:A:328:SER:HB3	1.98	0.63
1:B:123:ARG:HH21	1:B:198:LYS:HE2	1.63	0.63
1:A:83:TYR:CE2	1:A:87:ARG:HB3	2.34	0.63
2:E:56:C:H2'	2:E:57:G:C8	2.33	0.63
1:A:120:PHE:C	1:A:198:LYS:HE3	2.24	0.62
3:F:60:C:H5''	3:F:61:C:OP2	2.00	0.62
1:A:305:ILE:HB	1:A:306:PRO:HD3	1.82	0.62
1:A:36:GLN:HG3	1:A:37:LYS:H	1.64	0.62
1:A:98:ASP:HA	1:A:101:ARG:NH1	2.14	0.62
1:B:347:GLU:O	1:B:348:ARG:HB3	1.99	0.62
2:E:57:G:O2'	2:E:58:A:H5'	2.00	0.61
1:B:224:MET:O	1:B:229:ALA:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:HB3	1:A:338:PHE:CZ	2.35	0.61
1:A:39:ASN:O	1:A:105:ILE:HG22	1.99	0.61
1:B:52:LYS:O	1:B:54:ILE:HG22	2.00	0.61
1:A:13:SER:OG	1:A:14:LYS:HD2	2.00	0.61
1:B:237:TYR:O	1:B:240:TYR:HB3	2.01	0.61
1:B:297:VAL:HG12	1:B:301:LYS:HD3	1.82	0.61
3:F:30:G:O2'	3:F:31:A:H5'	2.00	0.61
1:B:39:ASN:O	1:B:105:ILE:HG22	2.00	0.61
1:A:93:MET:O	1:A:97:GLU:HG2	2.01	0.61
1:A:240:TYR:O	1:A:244:LYS:HA	2.01	0.61
1:A:340:SER:O	1:A:342:ARG:HG3	2.01	0.61
1:B:344:ILE:HG22	1:B:346:GLN:HG2	1.81	0.61
1:B:207:TYR:HD2	1:B:353:LEU:HD13	1.66	0.60
1:B:287:THR:O	1:B:291:GLN:HG3	2.01	0.60
1:B:41:GLU:OE1	1:B:70:PRO:HB2	2.01	0.60
1:A:79:TRP:HA	1:A:254:VAL:HG21	1.83	0.60
1:A:133:LEU:HD22	1:A:133:LEU:N	2.11	0.60
1:A:168:ASP:OD1	1:A:171:ARG:HG3	2.02	0.60
1:B:394:TRP:CH2	1:B:398:LEU:HD21	2.37	0.60
1:A:85:SER:HA	1:A:115:TYR:CE1	2.36	0.60
1:A:120:PHE:HA	1:A:198:LYS:HG3	1.83	0.59
3:F:24:G:O2'	3:F:25:C:H5'	2.02	0.59
1:A:162:THR:O	1:A:372:HIS:HE1	1.85	0.59
1:A:325:THR:HG22	1:A:329:GLN:NE2	2.16	0.59
1:B:80:SER:HB3	7:B:437:HOH:O	2.02	0.59
1:B:258:ILE:HD11	1:B:285:MET:CA	2.25	0.59
3:F:66:U:H2'	3:F:67:G:C8	2.37	0.59
1:A:56:ILE:HG23	1:A:227:ARG:HB3	1.85	0.59
2:E:11:C:H2'	2:E:12:G:H8	1.67	0.59
1:B:162:THR:O	1:B:372:HIS:HE1	1.86	0.59
1:A:62:PRO:HG2	1:A:65:GLU:OE1	2.01	0.59
1:A:380:ASN:CG	1:A:402:ARG:HH22	2.10	0.59
1:B:220:ARG:O	1:B:224:MET:HB2	2.02	0.59
1:A:231:GLN:H	1:A:231:GLN:CD	2.11	0.59
2:E:30:G:O2'	2:E:31:A:H5'	2.01	0.59
2:E:31:A:O2'	2:E:32:U:H5'	2.03	0.59
1:B:138:LEU:O	1:B:142:GLU:HG2	2.02	0.59
1:A:47:SER:O	1:A:48:MET:HE2	2.03	0.59
1:B:115:TYR:O	1:B:118:THR:HG22	2.03	0.59
1:B:168:ASP:CG	1:B:171:ARG:HG3	2.27	0.59
1:A:120:PHE:CB	1:A:197:LEU:HA	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:TRP:H	1:A:79:TRP:HD1	1.51	0.58
1:A:138:LEU:O	1:A:142:GLU:HG2	2.03	0.58
3:F:9:G:C3'	7:F:107:HOH:O	2.41	0.58
1:B:194:LYS:O	1:B:195:ILE:HG22	2.03	0.58
1:A:237:TYR:O	1:A:240:TYR:HB3	2.02	0.58
1:B:93:MET:HE3	1:B:96:ILE:HD12	1.84	0.58
1:B:400:SER:HB3	3:F:43:U:H5''	1.85	0.58
1:A:220:ARG:HH11	1:A:220:ARG:CG	2.16	0.58
2:E:60:C:H5''	2:E:61:C:OP2	2.03	0.58
1:B:100:HIS:C	1:B:102:ARG:H	2.11	0.58
1:B:57:ILE:HD12	1:B:257:VAL:HG21	1.85	0.58
1:A:220:ARG:O	1:A:224:MET:HB2	2.04	0.58
1:A:220:ARG:HH11	1:A:220:ARG:HG2	1.69	0.58
1:B:79:TRP:CD1	1:B:79:TRP:N	2.72	0.58
1:A:207:TYR:HD2	1:A:353:LEU:HD13	1.68	0.57
1:A:216:ARG:HD3	1:A:320:LEU:HD11	1.86	0.57
1:A:236:LEU:HD22	1:A:260:PHE:CE1	2.39	0.57
1:B:135:ARG:HE	1:B:135:ARG:HA	1.69	0.57
1:B:46:ASP:C	1:B:48:MET:H	2.12	0.57
1:A:122:LYS:H	1:A:123:ARG:NH1	2.02	0.57
1:A:328:SER:O	1:A:332:ILE:HG13	2.04	0.57
1:B:50:VAL:HG21	1:B:83:TYR:CD1	2.39	0.57
1:B:86:HIS:O	1:B:89:GLU:HB3	2.05	0.57
1:A:135:ARG:HE	1:A:135:ARG:HA	1.70	0.57
1:B:122:LYS:HA	1:B:193:GLN:NE2	2.19	0.57
1:B:229:ALA:O	1:B:233:ILE:HG12	2.04	0.57
3:F:38:A:H5'	3:F:39:U:OP2	2.05	0.57
1:A:55:PRO:HG2	1:A:56:ILE:H	1.70	0.57
1:A:205:TRP:HB2	1:A:312:ILE:CD1	2.35	0.57
1:B:324:ASP:O	1:B:328:SER:HB3	2.05	0.57
1:B:394:TRP:CZ2	1:B:398:LEU:HD21	2.40	0.57
2:E:23:C:H2'	2:E:24:G:H8	1.70	0.57
1:B:251:GLU:HB3	1:B:261:LYS:NZ	2.20	0.57
1:B:164:TYR:CD2	1:B:171:ARG:HB3	2.40	0.56
1:B:205:TRP:HE1	1:B:300:ILE:HD12	1.70	0.56
1:B:399:GLY:O	1:B:404:LYS:HE3	2.05	0.56
1:A:57:ILE:HG23	1:A:232:GLU:HG3	1.86	0.56
1:A:205:TRP:HB2	1:A:312:ILE:HD11	1.87	0.56
1:B:85:SER:HA	1:B:115:TYR:HE1	1.69	0.56
1:A:246:THR:C	1:A:248:GLU:H	2.13	0.56
1:B:302:LYS:O	1:B:303:MET:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLN:CD	1:B:231:GLN:H	2.13	0.56
1:B:286:LYS:O	1:B:290:ARG:HG3	2.06	0.56
1:A:48:MET:HB3	1:A:58:THR:OG1	2.06	0.56
1:B:264:LEU:HB3	1:B:265:PRO:CD	2.35	0.55
1:B:51:TYR:CD1	1:B:254:VAL:HG22	2.41	0.55
1:B:60:LYS:HA	7:B:460:HOH:O	2.04	0.55
1:B:241:SER:HB2	7:B:446:HOH:O	2.06	0.55
1:B:258:ILE:HG23	1:B:258:ILE:O	2.06	0.55
1:B:205:TRP:HB2	1:B:312:ILE:HD11	1.88	0.55
1:B:54:ILE:HD11	1:B:57:ILE:HD11	1.88	0.55
1:B:168:ASP:OD1	1:B:171:ARG:HG3	2.06	0.55
1:B:22:THR:O	1:B:25:VAL:HG22	2.06	0.55
1:B:51:TYR:HD1	1:B:254:VAL:HG13	1.71	0.55
1:A:24:GLY:O	1:A:216:ARG:NH1	2.40	0.55
1:A:41:GLU:HG3	1:A:99:ILE:HG12	1.88	0.55
2:E:19:G:H5'	2:E:60:C:H42	1.71	0.55
1:B:264:LEU:HB3	1:B:265:PRO:HD3	1.89	0.55
1:B:334:ILE:HG12	1:B:346:GLN:CG	2.28	0.55
3:F:51:U:H2'	3:F:52:A:C8	2.42	0.55
3:F:10:G:N2	3:F:26:A:H1'	2.22	0.55
3:F:34:G:H4'	3:F:35:C:OP1	2.07	0.55
1:A:207:TYR:CG	1:A:208:SER:N	2.75	0.54
2:E:8:U:H3	2:E:14:A:H62	1.53	0.54
1:A:22:THR:HG21	1:A:213:LEU:HD21	1.89	0.54
1:A:347:GLU:O	1:A:348:ARG:HB3	2.07	0.54
1:B:117:GLN:CD	1:B:122:LYS:HG2	2.33	0.54
1:B:246:THR:C	1:B:248:GLU:H	2.16	0.54
1:A:133:LEU:H	1:A:133:LEU:CD2	2.12	0.54
2:E:31:A:C2'	2:E:32:U:H5'	2.38	0.54
1:A:411:THR:O	1:A:415:ASP:HB2	2.08	0.54
2:E:70:A:H2'	2:E:70:A:N3	2.23	0.54
1:B:22:THR:OG1	1:B:213:LEU:HD21	2.07	0.54
1:B:325:THR:HG22	1:B:329:GLN:NE2	2.22	0.54
1:A:32:ILE:HG23	1:A:69:ILE:HG13	1.89	0.53
1:B:258:ILE:HD11	1:B:285:MET:HG2	1.90	0.53
1:A:334:ILE:HG12	1:A:346:GLN:CG	2.30	0.53
1:A:83:TYR:HD2	1:A:84:TYR:H	1.56	0.53
1:A:83:TYR:HE2	1:A:87:ARG:HB3	1.74	0.53
1:B:205:TRP:HE1	1:B:300:ILE:CD1	2.21	0.53
1:B:302:LYS:C	1:B:303:MET:HE2	2.33	0.53
1:A:171:ARG:HH11	1:A:171:ARG:CG	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:O	1:A:195:ILE:HG22	2.09	0.53
1:A:262:GLU:HG2	1:A:285:MET:CG	2.39	0.53
1:A:25:VAL:HG23	1:A:26:GLY:N	2.24	0.53
1:A:205:TRP:NE1	7:A:442:HOH:O	2.42	0.53
3:F:38:A:N3	3:F:38:A:H2'	2.23	0.53
1:A:220:ARG:CG	1:A:220:ARG:NH1	2.71	0.52
1:B:14:LYS:O	1:B:199:PHE:HB3	2.08	0.52
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.74	0.52
1:B:151:ASN:O	1:B:155:LYS:HD3	2.08	0.52
1:B:408:LYS:HD3	1:B:412:ARG:HD2	1.91	0.52
3:F:31:A:C2'	3:F:32:U:H5'	2.39	0.52
1:B:68:GLY:O	1:B:70:PRO:HD3	2.10	0.52
1:B:63:LEU:C	1:B:65:GLU:H	2.18	0.52
1:A:208:SER:OG	1:A:318:THR:HA	2.09	0.52
2:E:15:G:H2'	2:E:16:U:C5	2.45	0.52
1:B:299:TRP:CD2	1:B:303:MET:HG3	2.45	0.52
1:B:392:LYS:O	1:B:396:ILE:HG13	2.10	0.52
3:F:63:G:H2'	3:F:64:A:C8	2.44	0.52
1:B:63:LEU:H	1:B:63:LEU:HD12	1.75	0.52
1:A:249:GLN:HE22	1:A:252:ASN:HB2	1.74	0.52
1:B:165:HIS:CG	1:B:166:PRO:HD2	2.45	0.52
1:B:171:ARG:HH11	1:B:171:ARG:CG	2.21	0.52
1:B:241:SER:HB3	1:B:242:GLN:NE2	2.25	0.52
1:A:201:THR:HG22	1:A:202:LEU:N	2.25	0.52
1:A:149:ILE:HD11	1:A:173:GLN:HA	1.92	0.52
1:B:54:ILE:O	1:B:54:ILE:HG12	2.10	0.52
1:A:359:LYS:HG3	1:B:346:GLN:O	2.09	0.51
1:B:278:LEU:HD23	7:B:468:HOH:O	2.09	0.51
3:F:9:G:C2'	7:F:107:HOH:O	2.57	0.51
1:A:334:ILE:HG23	1:A:344:ILE:HG21	1.92	0.51
1:A:89:GLU:OE2	1:A:123:ARG:HG2	2.10	0.51
1:A:287:THR:O	1:A:291:GLN:HG3	2.11	0.51
1:A:302:LYS:C	1:A:303:MET:HE2	2.35	0.51
2:E:22:G:N3	2:E:22:G:H2'	2.24	0.51
1:A:14:LYS:H	1:A:14:LYS:CD	2.18	0.51
1:A:85:SER:HA	1:A:115:TYR:HE1	1.76	0.51
1:A:205:TRP:HE1	1:A:300:ILE:CD1	2.23	0.51
1:A:45:SER:CB	1:A:110:GLY:HA3	2.27	0.51
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.74	0.51
1:A:230:LEU:HD12	1:A:230:LEU:H	1.75	0.51
1:A:286:LYS:O	1:A:290:ARG:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:SER:O	1:B:332:ILE:HG13	2.11	0.51
1:B:408:LYS:HD2	1:B:408:LYS:C	2.36	0.51
1:A:205:TRP:HE3	1:A:314:LEU:HG	1.73	0.51
1:A:264:LEU:N	1:A:265:PRO:CD	2.74	0.51
1:B:256:GLN:O	1:B:257:VAL:C	2.54	0.51
1:A:298:LYS:NZ	7:A:430:HOH:O	2.40	0.51
1:B:221:VAL:O	1:B:224:MET:HB3	2.11	0.51
1:A:340:SER:HB3	1:A:342:ARG:HD2	1.93	0.50
1:A:375:CYS:O	1:A:385:ASN:HB3	2.10	0.50
1:A:394:TRP:CZ2	1:A:398:LEU:HD21	2.46	0.50
1:B:197:LEU:N	1:B:197:LEU:HD23	2.26	0.50
1:B:210:PRO:HG2	1:B:211:GLU:H	1.76	0.50
1:B:288:ARG:HD2	1:B:291:GLN:OE1	2.11	0.50
1:A:236:LEU:HD22	1:A:260:PHE:CD1	2.47	0.50
1:A:414:ALA:O	1:A:418:LYS:HE3	2.11	0.50
1:A:415:ASP:HA	1:A:418:LYS:CD	2.41	0.50
1:A:50:VAL:HG21	1:A:83:TYR:CD1	2.47	0.50
1:A:164:TYR:CD2	1:A:171:ARG:HB3	2.47	0.50
2:E:22:G:N7	2:E:46:G:N2	2.59	0.50
1:A:145:ASP:O	1:A:148:VAL:HG12	2.12	0.50
1:A:256:GLN:HE21	1:A:261:LYS:CE	2.25	0.50
3:F:18:G:O2'	3:F:57:G:N2	2.45	0.50
1:A:242:GLN:C	1:A:244:LYS:H	2.19	0.50
3:F:19:G:H5'	3:F:60:C:N4	2.26	0.50
1:A:174:ARG:HD3	2:E:34:G:H5'	1.94	0.50
1:B:90:THR:O	1:B:94:ASN:HB2	2.12	0.50
1:A:205:TRP:CD1	7:A:442:HOH:O	2.65	0.50
1:A:230:LEU:HD12	1:A:230:LEU:N	2.27	0.50
1:B:55:PRO:HA	1:B:58:THR:HG22	1.94	0.50
1:A:98:ASP:CG	1:A:102:ARG:HD3	2.37	0.49
1:A:93:MET:HE1	1:A:198:LYS:HZ2	1.76	0.49
1:A:224:MET:O	1:A:229:ALA:HB2	2.13	0.49
2:E:59:U:H2'	2:E:60:C:O4'	2.12	0.49
3:F:9:G:H1'	3:F:46:G:H1'	1.95	0.49
2:E:23:C:H2'	2:E:24:G:C8	2.46	0.49
1:B:324:ASP:HB3	7:B:438:HOH:O	2.12	0.49
3:F:27:G:H1	3:F:43:U:H3	1.60	0.49
1:A:174:ARG:NH1	2:E:34:G:H5''	2.27	0.49
1:A:118:THR:C	1:A:120:PHE:H	2.20	0.49
1:A:344:ILE:HD11	7:A:444:HOH:O	2.12	0.49
1:B:94:ASN:HA	1:B:97:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:TRP:NE1	1:B:398:LEU:HD11	2.28	0.49
1:A:39:ASN:OD1	1:A:104:LYS:HE2	2.12	0.49
1:A:80:SER:O	1:A:81:GLU:HG3	2.12	0.49
1:A:130:GLU:O	1:A:131:ARG:C	2.56	0.49
1:B:276:VAL:HG11	1:B:279:GLU:OE2	2.13	0.49
1:A:174:ARG:HH11	2:E:34:G:C5'	2.24	0.49
1:A:206:LEU:HD21	1:A:323:TRP:HZ3	1.77	0.49
1:B:50:VAL:HG11	1:B:83:TYR:CE1	2.48	0.49
1:B:409:ARG:HA	1:B:412:ARG:HB3	1.94	0.49
3:F:10:G:OP2	3:F:10:G:H3'	2.13	0.49
1:A:207:TYR:CD2	1:A:353:LEU:HD13	2.48	0.49
1:A:302:LYS:O	1:A:303:MET:HE2	2.13	0.49
1:B:258:ILE:HD12	1:B:262:GLU:OE1	2.12	0.49
1:B:322:GLN:C	7:B:447:HOH:O	2.56	0.49
1:A:95:ALA:O	1:A:99:ILE:HG13	2.12	0.48
1:B:140:ILE:HG21	1:B:152:THR:HG21	1.94	0.48
1:B:230:LEU:N	1:B:230:LEU:HD12	2.27	0.48
1:B:314:LEU:HD12	1:B:357:LEU:HD21	1.94	0.48
1:A:55:PRO:HA	1:A:60:LYS:HE2	1.94	0.48
1:A:205:TRP:CE3	1:A:314:LEU:HG	2.49	0.48
1:B:222:ASP:C	1:B:224:MET:H	2.20	0.48
1:B:230:LEU:HD12	1:B:230:LEU:H	1.78	0.48
1:B:414:ALA:C	1:B:416:PHE:H	2.19	0.48
2:E:29:A:H2'	2:E:30:G:C8	2.45	0.48
1:B:55:PRO:O	1:B:57:ILE:N	2.46	0.48
1:B:39:ASN:ND2	1:B:104:LYS:HG2	2.28	0.48
1:A:237:TYR:CE1	1:A:264:LEU:HD12	2.49	0.48
1:B:28:SER:HB3	1:B:61:HIS:CE1	2.47	0.48
1:B:108:VAL:HG11	1:B:119:LEU:CD1	2.38	0.48
1:B:211:GLU:HB2	1:B:212:PRO:CD	2.34	0.48
1:A:47:SER:OG	1:A:115:TYR:HE2	1.97	0.48
1:A:56:ILE:HB	1:A:232:GLU:HG3	1.96	0.48
1:B:334:ILE:HG23	1:B:344:ILE:HG21	1.95	0.48
1:A:50:VAL:O	1:A:77:VAL:HB	2.14	0.48
1:B:23:THR:HB	5:B:422:DMA:O2B	2.13	0.48
1:A:88:PHE:CE2	1:A:115:TYR:HB3	2.48	0.48
1:A:222:ASP:C	1:A:224:MET:H	2.21	0.48
1:A:399:GLY:O	1:A:404:LYS:HE3	2.14	0.48
1:B:149:ILE:HD11	1:B:173:GLN:HA	1.95	0.48
1:A:14:LYS:HB3	1:A:100:HIS:NE2	2.29	0.47
1:A:56:ILE:CG2	1:A:227:ARG:HB3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:THR:HG22	1:B:202:LEU:N	2.29	0.47
1:A:203:PHE:HE2	1:A:304:LEU:HD11	1.79	0.47
2:E:63:G:H2'	2:E:64:A:O4'	2.13	0.47
3:F:55:U:H2'	3:F:57:G:N7	2.29	0.47
1:A:52:LYS:O	1:A:54:ILE:HG22	2.13	0.47
1:A:206:LEU:HD21	1:A:323:TRP:CZ3	2.49	0.47
1:B:98:ASP:O	1:B:102:ARG:HD3	2.14	0.47
1:B:131:ARG:HG2	1:B:180:TYR:O	2.14	0.47
1:B:205:TRP:NE1	1:B:300:ILE:HG21	2.28	0.47
1:B:207:TYR:CD2	1:B:353:LEU:HD13	2.46	0.47
1:B:258:ILE:CD1	1:B:285:MET:HG2	2.44	0.47
1:B:266:TRP:CD1	1:B:277:LYS:HZ2	2.32	0.47
1:A:14:LYS:HB3	1:A:100:HIS:CD2	2.50	0.47
1:A:221:VAL:O	1:A:224:MET:HB3	2.15	0.47
1:B:305:ILE:CB	1:B:306:PRO:HD3	2.44	0.47
1:A:156:CYS:HB2	1:A:179:TYR:CZ	2.50	0.47
1:B:61:HIS:HD1	1:B:61:HIS:N	2.12	0.47
1:B:205:TRP:HB2	1:B:312:ILE:CD1	2.44	0.47
1:A:18:VAL:HA	1:A:108:VAL:O	2.14	0.47
1:A:55:PRO:O	1:A:57:ILE:N	2.48	0.47
1:B:150:TYR:HA	1:B:172:VAL:HG11	1.96	0.47
1:B:156:CYS:O	1:B:157:ASP:HB3	2.15	0.47
1:B:327:ALA:O	1:B:331:ALA:HB2	2.15	0.47
3:F:23:C:H2'	3:F:24:G:C8	2.50	0.47
1:A:258:ILE:HD12	1:A:262:GLU:OE1	2.15	0.47
1:A:23:THR:HG22	5:A:422:DMA:O3B	2.15	0.47
1:A:55:PRO:HG2	1:A:56:ILE:N	2.30	0.47
1:A:163:LYS:NZ	1:A:370:TRP:CH2	2.83	0.47
1:B:50:VAL:HA	1:B:75:ASN:H	1.80	0.47
1:B:93:MET:O	1:B:97:GLU:HG2	2.15	0.47
1:B:171:ARG:NH2	3:F:38:A:N1	2.63	0.47
1:A:47:SER:HG	1:A:115:TYR:HE2	1.61	0.46
1:A:205:TRP:NE1	1:A:300:ILE:HG21	2.30	0.46
1:B:85:SER:HA	1:B:115:TYR:CE1	2.50	0.46
1:B:225:LEU:HA	1:B:229:ALA:CB	2.43	0.46
1:A:205:TRP:HE1	1:A:300:ILE:HD12	1.80	0.46
1:A:217:LEU:O	1:A:221:VAL:HG23	2.14	0.46
1:A:291:GLN:HE21	2:E:27:G:P	2.38	0.46
1:B:73:VAL:HG21	1:B:92:CYS:HA	1.96	0.46
1:B:171:ARG:CG	1:B:171:ARG:NH1	2.78	0.46
1:B:324:ASP:HA	1:B:328:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:SER:O	1:B:342:ARG:HG3	2.16	0.46
1:B:315:LEU:CD2	1:B:327:ALA:HA	2.45	0.46
1:B:344:ILE:HA	7:B:449:HOH:O	2.16	0.46
1:A:50:VAL:HG12	1:A:74:MET:HA	1.97	0.46
1:A:129:SER:C	1:A:131:ARG:H	2.22	0.46
1:A:314:LEU:O	1:A:315:LEU:HG	2.16	0.46
1:A:194:LYS:C	1:A:196:THR:H	2.24	0.46
1:B:175:MET:HA	1:B:175:MET:HE2	1.97	0.46
1:B:375:CYS:O	1:B:385:ASN:HB3	2.15	0.46
3:F:10:G:H2'	3:F:11:C:H6	1.80	0.46
1:A:216:ARG:O	1:A:220:ARG:HB2	2.15	0.46
1:A:330:ARG:HG2	1:A:330:ARG:HH11	1.80	0.46
1:A:171:ARG:CG	1:A:171:ARG:NH1	2.78	0.46
1:A:363:THR:O	1:A:366:LYS:HB2	2.16	0.46
1:B:18:VAL:HB	1:B:108:VAL:HG13	1.96	0.46
1:A:146:PRO:HG2	1:A:384:LYS:NZ	2.31	0.46
1:A:325:THR:HG22	1:A:329:GLN:HE22	1.81	0.46
1:B:19:ILE:HG22	1:B:27:LYS:HD2	1.97	0.46
1:B:27:LYS:C	1:B:29:GLN:H	2.24	0.46
1:B:120:PHE:CB	1:B:197:LEU:HA	2.46	0.46
3:F:51:U:H2'	3:F:52:A:H8	1.80	0.46
1:A:311:ASP:OD1	1:A:348:ARG:NH2	2.49	0.46
3:F:58:A:O2'	3:F:59:U:P	2.74	0.46
1:A:113:HIS:NE2	1:A:300:ILE:HD11	2.31	0.45
1:A:39:ASN:ND2	1:A:104:LYS:HA	2.31	0.45
1:A:175:MET:HE2	1:A:175:MET:HA	1.97	0.45
1:B:60:LYS:O	1:B:61:HIS:C	2.60	0.45
1:A:380:ASN:OD1	1:A:402:ARG:NH2	2.49	0.45
1:B:145:ASP:O	1:B:148:VAL:HG12	2.16	0.45
1:B:315:LEU:HD23	1:B:327:ALA:HA	1.98	0.45
1:A:394:TRP:CZ2	1:A:398:LEU:HD11	2.50	0.45
1:A:419:TRP:HA	1:A:419:TRP:CE3	2.51	0.45
1:A:54:ILE:HA	1:A:232:GLU:OE1	2.17	0.45
1:A:54:ILE:HG13	1:A:232:GLU:OE1	2.16	0.45
1:A:156:CYS:O	1:A:157:ASP:HB3	2.16	0.45
1:B:216:ARG:O	1:B:220:ARG:HB3	2.17	0.45
3:F:15:G:H2'	3:F:16:U:C5	2.52	0.45
1:B:57:ILE:HG13	1:B:58:THR:N	2.31	0.45
1:B:174:ARG:HH11	3:F:34:G:H5''	1.82	0.45
1:B:323:TRP:N	7:B:447:HOH:O	2.50	0.45
1:A:36:GLN:HG3	1:A:37:LYS:N	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PHE:CD2	1:A:115:TYR:HB3	2.51	0.45
1:A:242:GLN:O	1:A:243:ASN:HB3	2.15	0.45
1:A:288:ARG:HD2	1:A:291:GLN:OE1	2.17	0.45
1:A:415:ASP:HA	1:A:418:LYS:HE3	1.99	0.45
2:E:24:G:O2'	2:E:25:C:H5'	2.17	0.45
1:B:33:GLN:C	1:B:35:ALA:H	2.24	0.45
1:B:206:LEU:HD21	1:B:323:TRP:HZ3	1.82	0.45
1:B:207:TYR:CG	1:B:208:SER:N	2.84	0.45
1:B:360:GLY:HA2	1:B:364:MET:HB2	1.98	0.45
1:A:262:GLU:HG2	1:A:285:MET:HG2	1.98	0.45
1:B:181:LYS:HE2	1:B:181:LYS:HB3	1.83	0.45
1:B:259:GLY:O	1:B:263:PHE:HD1	2.00	0.45
1:A:15:LYS:HB2	1:A:105:ILE:CD1	2.46	0.45
1:A:32:ILE:O	1:A:36:GLN:HG2	2.17	0.45
1:A:197:LEU:HD23	1:A:197:LEU:N	2.32	0.45
1:A:299:TRP:CD2	1:A:303:MET:HG3	2.52	0.45
1:B:45:SER:HB3	1:B:110:GLY:CA	2.24	0.45
3:F:2:C:H2'	3:F:3:U:C6	2.52	0.45
3:F:14:A:H3'	3:F:15:G:H8	1.82	0.45
1:A:205:TRP:CH2	1:A:356:LEU:HD22	2.52	0.44
1:A:210:PRO:HG2	1:A:211:GLU:H	1.82	0.44
1:B:206:LEU:HD21	1:B:323:TRP:CZ3	2.52	0.44
1:B:381:ALA:C	1:B:383:GLY:H	2.24	0.44
2:E:57:G:N2	2:E:58:A:N3	2.65	0.44
1:B:347:GLU:O	1:B:348:ARG:CB	2.64	0.44
3:F:31:A:H2'	3:F:32:U:C6	2.53	0.44
1:A:174:ARG:HD3	2:E:34:G:C5'	2.47	0.44
1:A:211:GLU:HB2	1:A:212:PRO:CD	2.29	0.44
1:A:283:GLU:HA	1:A:283:GLU:OE1	2.16	0.44
1:B:330:ARG:O	1:B:334:ILE:HG13	2.17	0.44
2:E:11:C:H2'	2:E:12:G:C8	2.51	0.44
1:B:95:ALA:O	1:B:99:ILE:HG13	2.16	0.44
1:A:381:ALA:C	1:A:383:GLY:H	2.26	0.44
1:A:72:HIS:HB3	7:A:423:HOH:O	2.18	0.44
1:A:72:HIS:N	1:A:72:HIS:CD2	2.86	0.44
1:B:408:LYS:CD	1:B:412:ARG:HD2	2.47	0.44
1:A:46:ASP:OD2	2:E:37:6IA:H121	2.18	0.44
1:A:54:ILE:HG23	1:A:54:ILE:O	2.17	0.44
1:A:181:LYS:HE2	1:A:181:LYS:HB3	1.82	0.44
1:A:344:ILE:CG2	1:A:346:GLN:HG2	2.47	0.44
1:B:122:LYS:O	3:F:33:U:H1'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:TYR:HB3	1:B:394:TRP:CE3	2.52	0.44
3:F:58:A:H4'	3:F:59:U:OP1	2.18	0.44
1:B:16:VAL:O	1:B:201:THR:HG23	2.18	0.44
1:B:123:ARG:HA	3:F:34:G:OP2	2.17	0.44
1:A:249:GLN:NE2	1:A:252:ASN:HB2	2.31	0.43
1:A:388:ALA:HA	7:A:436:HOH:O	2.18	0.43
1:A:230:LEU:H	1:A:230:LEU:CD1	2.31	0.43
1:B:343:PRO:HG2	7:B:448:HOH:O	2.17	0.43
1:A:57:ILE:HG12	1:A:232:GLU:HB3	2.00	0.43
1:A:62:PRO:HB2	1:A:64:GLN:NE2	2.33	0.43
1:A:117:GLN:HA	1:A:120:PHE:CZ	2.53	0.43
1:A:262:GLU:HG2	1:A:285:MET:HG3	1.99	0.43
1:B:17:ILE:O	1:B:107:ILE:HA	2.19	0.43
1:B:78:ASP:HB3	1:B:81:GLU:OE1	2.19	0.43
1:A:44:ASN:ND2	1:A:49:GLN:HB2	2.33	0.43
1:A:165:HIS:NE2	1:A:387:VAL:HB	2.34	0.43
1:B:87:ARG:HG2	1:B:87:ARG:HH11	1.82	0.43
1:A:314:LEU:HD12	1:A:357:LEU:HD21	2.01	0.43
2:E:62:U:H2'	2:E:63:G:C8	2.54	0.43
1:B:217:LEU:O	1:B:221:VAL:HG23	2.19	0.43
1:B:241:SER:O	1:B:242:GLN:C	2.61	0.43
1:A:140:ILE:HG21	1:A:152:THR:HG21	2.01	0.43
1:A:217:LEU:HD22	1:A:289:THR:HG22	2.01	0.43
1:B:243:ASN:O	1:B:244:LYS:O	2.36	0.43
1:A:23:THR:HA	5:A:422:DMA:O2B	2.19	0.43
1:A:56:ILE:HD13	1:A:227:ARG:O	2.18	0.43
1:A:83:TYR:HD2	1:A:84:TYR:N	2.16	0.43
1:A:209:LYS:HG2	1:A:318:THR:OG1	2.19	0.43
1:A:412:ARG:C	1:A:414:ALA:H	2.27	0.43
1:B:118:THR:C	1:B:120:PHE:H	2.26	0.43
1:B:323:TRP:CD1	1:B:323:TRP:C	2.97	0.43
1:B:380:ASN:CG	1:B:402:ARG:HH22	2.26	0.43
1:B:205:TRP:HE3	1:B:314:LEU:HG	1.83	0.43
1:B:293:ALA:O	1:B:296:GLN:HB2	2.18	0.43
1:A:22:THR:OG1	1:A:213:LEU:HD21	2.19	0.43
1:A:299:TRP:O	1:A:303:MET:HB2	2.19	0.43
1:B:411:THR:O	1:B:411:THR:HG22	2.18	0.43
1:A:256:GLN:HE21	1:A:261:LYS:NZ	2.17	0.42
1:B:80:SER:C	1:B:81:GLU:HG3	2.44	0.42
1:B:164:TYR:CE2	1:B:171:ARG:HB3	2.54	0.42
1:B:369:ASP:OD2	1:B:391:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:C	1:A:224:MET:N	2.76	0.42
1:B:194:LYS:C	1:B:196:THR:H	2.28	0.42
1:B:134:THR:OG1	1:B:137:GLN:HG3	2.20	0.42
1:A:52:LYS:HA	1:A:75:ASN:OD1	2.18	0.42
1:A:251:GLU:HG3	1:A:252:ASN:OD1	2.19	0.42
1:B:53:ASP:HB3	1:B:54:ILE:H	1.52	0.42
1:A:44:ASN:CG	1:A:45:SER:N	2.76	0.42
1:A:122:LYS:HA	1:A:193:GLN:HE21	1.82	0.42
1:B:213:LEU:HD12	1:B:213:LEU:O	2.19	0.42
3:F:66:U:H2'	3:F:67:G:H8	1.80	0.42
1:A:49:GLN:HG2	1:A:59:ASN:O	2.19	0.42
1:A:226:GLU:C	1:A:228:GLY:N	2.78	0.42
1:B:51:TYR:CD1	1:B:254:VAL:HG13	2.54	0.42
1:B:69:ILE:O	1:B:71:HIS:ND1	2.52	0.42
1:B:250:CYS:HA	1:B:255:TRP:CD1	2.55	0.42
1:B:380:ASN:HB2	1:B:382:ASP:OD2	2.20	0.42
1:B:44:ASN:HD21	1:B:49:GLN:NE2	2.16	0.42
1:B:94:ASN:HA	1:B:97:GLU:CG	2.50	0.42
1:B:251:GLU:CB	1:B:261:LYS:HZ3	2.30	0.42
1:B:330:ARG:HG2	1:B:330:ARG:HH11	1.85	0.42
3:F:9:G:N2	3:F:45:G:C2	2.88	0.42
3:F:40:C:H2'	3:F:41:U:H6	1.84	0.42
1:A:126:THR:HG22	1:A:126:THR:O	2.20	0.42
1:A:211:GLU:CB	1:A:212:PRO:HD3	2.28	0.42
1:B:226:GLU:C	1:B:228:GLY:H	2.27	0.42
3:F:9:G:C8	7:F:107:HOH:O	2.57	0.42
1:B:179:TYR:CE1	1:B:185:LYS:HG2	2.55	0.42
1:B:208:SER:O	1:B:209:LYS:C	2.61	0.42
1:B:222:ASP:C	1:B:224:MET:N	2.77	0.42
1:B:263:PHE:O	1:B:267:LEU:HG	2.20	0.42
1:B:420:LYS:HD2	1:B:420:LYS:O	2.19	0.42
3:F:39:U:O2'	3:F:40:C:H5'	2.20	0.42
1:A:56:ILE:O	1:A:56:ILE:HG22	2.20	0.42
1:A:63:LEU:HD12	1:A:63:LEU:H	1.83	0.42
1:B:62:PRO:HG2	1:B:65:GLU:OE2	2.20	0.42
1:B:117:GLN:HA	1:B:120:PHE:CE1	2.55	0.42
1:B:226:GLU:C	1:B:228:GLY:N	2.77	0.42
1:A:150:TYR:HA	1:A:172:VAL:HG11	2.02	0.41
1:B:123:ARG:HH21	1:B:198:LYS:CE	2.31	0.41
1:B:175:MET:HE2	1:B:178:ILE:HD12	2.02	0.41
1:B:205:TRP:CE3	1:B:314:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ILE:C	1:B:341:ASN:H	2.27	0.41
3:F:33:U:H6	3:F:33:U:H5'	1.85	0.41
1:A:324:ASP:HA	1:A:328:SER:HB3	2.01	0.41
1:A:364:MET:SD	1:B:345:LYS:HD3	2.60	0.41
1:B:25:VAL:HG12	1:B:317:ALA:HB3	2.03	0.41
3:F:10:G:H2'	3:F:11:C:C6	2.55	0.41
1:A:134:THR:O	1:A:135:ARG:C	2.63	0.41
1:A:157:ASP:CB	1:A:185:LYS:HD2	2.41	0.41
2:E:57:G:N3	2:E:57:G:H2'	2.36	0.41
1:B:66:ARG:HD3	1:B:71:HIS:CE1	2.56	0.41
1:A:46:ASP:HB2	1:A:49:GLN:HE21	1.84	0.41
1:A:246:THR:O	1:A:248:GLU:N	2.53	0.41
1:A:345:LYS:HB3	1:B:364:MET:SD	2.60	0.41
1:B:25:VAL:O	1:B:323:TRP:CZ3	2.74	0.41
1:B:132:LYS:O	1:B:134:THR:N	2.53	0.41
3:F:39:U:H2'	3:F:40:C:C6	2.55	0.41
1:A:55:PRO:HB3	1:A:60:LYS:CE	2.50	0.41
1:A:206:LEU:HA	1:A:315:LEU:HB2	2.02	0.41
1:A:307:ASP:C	1:A:309:LYS:H	2.29	0.41
2:E:8:U:O4	2:E:14:A:N7	2.52	0.41
2:E:58:A:O2'	2:E:59:U:P	2.78	0.41
1:B:196:THR:HG22	1:B:197:LEU:N	2.35	0.41
1:B:230:LEU:H	1:B:230:LEU:CD1	2.32	0.41
1:B:397:HIS:C	1:B:399:GLY:H	2.28	0.41
1:A:226:GLU:C	1:A:228:GLY:H	2.28	0.41
1:B:216:ARG:HD3	1:B:320:LEU:HD11	2.03	0.41
1:A:14:LYS:HB3	1:A:100:HIS:CE1	2.55	0.41
1:A:46:ASP:CB	1:A:49:GLN:HE21	2.33	0.41
1:A:115:TYR:C	1:A:117:GLN:N	2.79	0.41
1:A:243:ASN:O	1:A:244:LYS:C	2.63	0.41
1:A:330:ARG:O	1:A:334:ILE:HG13	2.21	0.41
1:A:337:ASP:HB3	1:A:342:ARG:O	2.21	0.41
1:A:363:THR:HG21	1:B:344:ILE:O	2.21	0.41
1:A:394:TRP:O	1:A:398:LEU:HG	2.21	0.41
1:A:421:ILE:HG13	1:A:421:ILE:O	2.21	0.41
1:B:27:LYS:HB2	5:B:422:DMA:O1B	2.20	0.41
1:B:311:ASP:OD1	1:B:348:ARG:NH2	2.54	0.41
3:F:48:C:C2	3:F:59:U:H1'	2.55	0.41
1:A:49:GLN:HG2	1:A:60:LYS:HB3	2.02	0.41
1:A:50:VAL:HG21	1:A:83:TYR:HD1	1.85	0.41
1:A:53:ASP:C	1:A:54:ILE:HG22	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TYR:CE1	1:A:86:HIS:HB3	2.55	0.41
1:A:122:LYS:H	1:A:123:ARG:HH12	1.69	0.41
1:A:421:ILE:O	1:A:421:ILE:HG23	2.20	0.41
1:B:32:ILE:O	1:B:35:ALA:HB3	2.21	0.41
1:B:254:VAL:O	1:B:257:VAL:HG12	2.20	0.41
1:B:255:TRP:O	1:B:261:LYS:HG3	2.20	0.41
1:B:401:ARG:O	1:B:402:ARG:C	2.64	0.41
1:B:100:HIS:C	1:B:102:ARG:N	2.75	0.41
1:B:122:LYS:O	1:B:122:LYS:HG3	2.20	0.41
1:A:105:ILE:HA	1:A:106:PRO:HD3	1.88	0.40
1:A:231:GLN:CD	1:A:231:GLN:N	2.77	0.40
1:A:250:CYS:HA	1:A:255:TRP:CD1	2.57	0.40
1:A:394:TRP:NE1	1:A:398:LEU:HD11	2.36	0.40
2:E:6:U:H2'	2:E:7:A:O4'	2.21	0.40
1:B:124:VAL:HG12	1:B:126:THR:HG23	2.03	0.40
1:B:218:ASP:C	1:B:220:ARG:N	2.79	0.40
1:A:56:ILE:HB	1:A:232:GLU:CG	2.51	0.40
1:A:364:MET:HA	1:B:345:LYS:HE3	2.02	0.40
1:B:41:GLU:CG	1:B:99:ILE:HG23	2.51	0.40
1:B:105:ILE:HA	1:B:106:PRO:HD3	1.94	0.40
1:B:120:PHE:HB3	1:B:197:LEU:HA	2.03	0.40
1:B:175:MET:CE	1:B:178:ILE:HD12	2.51	0.40
3:F:39:U:H2'	3:F:40:C:H6	1.87	0.40
1:A:60:LYS:O	1:A:61:HIS:C	2.63	0.40
1:A:246:THR:C	1:A:248:GLU:N	2.78	0.40
1:A:345:LYS:HD3	1:B:364:MET:SD	2.61	0.40
1:A:360:GLY:HA2	1:A:364:MET:HB2	2.01	0.40
1:B:66:ARG:HB3	1:B:71:HIS:HE1	1.86	0.40
1:B:79:TRP:CZ3	1:B:236:LEU:HA	2.47	0.40
1:B:83:TYR:CE2	1:B:87:ARG:HB3	2.57	0.40
1:B:102:ARG:O	1:B:104:LYS:HG3	2.22	0.40
1:B:196:THR:HG22	1:B:197:LEU:H	1.86	0.40
1:B:225:LEU:HD23	1:B:229:ALA:HB3	2.03	0.40
1:B:382:ASP:OD2	1:B:382:ASP:N	2.55	0.40
1:B:394:TRP:O	1:B:398:LEU:HG	2.21	0.40
1:B:80:SER:O	1:B:81:GLU:HG3	2.22	0.40
1:B:116:LEU:HD13	1:B:116:LEU:HA	1.94	0.40
1:B:174:ARG:O	1:B:174:ARG:HD2	2.22	0.40
1:B:231:GLN:CD	1:B:231:GLN:N	2.79	0.40
1:B:266:TRP:O	1:B:267:LEU:HD23	2.21	0.40
1:B:381:ALA:C	1:B:383:GLY:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PRO:HB3	1:A:169:TYR:CE1	2.56	0.40
1:A:156:CYS:HB2	1:A:179:TYR:CE2	2.57	0.40
1:B:163:LYS:NZ	3:F:32:U:OP1	2.48	0.40
1:B:276:VAL:HG12	1:B:279:GLU:H	1.85	0.40
3:F:38:A:H1'	7:F:95:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/409 (97%)	312 (78%)	67 (17%)	19 (5%)	2	16
1	B	398/409 (97%)	303 (76%)	67 (17%)	28 (7%)	1	10
All	All	796/818 (97%)	615 (77%)	134 (17%)	47 (6%)	1	13

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	195	ILE
1	A	260	PHE
1	B	59	ASN
1	B	60	LYS
1	B	195	ILE
1	B	244	LYS
1	A	39	ASN
1	A	56	ILE
1	A	60	LYS
1	A	123	ARG
1	A	199	PHE
1	B	14	LYS

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Mol	Chain	Res	Type
1	B	39	ASN
1	B	132	LYS
1	B	199	PHE
1	B	242	GLN
1	B	304	LEU
1	B	420	LYS
1	A	169	TYR
1	A	245	PHE
1	A	304	LEU
1	B	55	PRO
1	B	56	ILE
1	B	101	ARG
1	B	122	LYS
1	B	133	LEU
1	B	169	TYR
1	B	243	ASN
1	B	249	GLN
1	B	252	ASN
1	B	310	GLY
1	A	22	THR
1	A	55	PRO
1	B	47	SER
1	B	76	HIS
1	A	73	VAL
1	A	109	VAL
1	A	347	GLU
1	B	52	LYS
1	B	247	PRO
1	A	26	GLY
1	A	119	LEU
1	B	53	ASP
1	B	64	GLN
1	A	247	PRO
1	B	246	THR

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	370/376 (98%)	340 (92%)	30 (8%)	11	36
1	B	370/376 (98%)	345 (93%)	25 (7%)	14	42
All	All	740/752 (98%)	685 (93%)	55 (7%)	13	39

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	29	GLN
1	A	61	HIS
1	A	123	ARG
1	A	133	LEU
1	A	135	ARG
1	A	141	LEU
1	A	174	ARG
1	A	191	ASN
1	A	192	GLU
1	A	195	ILE
1	A	197	LEU
1	A	220	ARG
1	A	236	LEU
1	A	244	LYS
1	A	251	GLU
1	A	254	VAL
1	A	256	GLN
1	A	266	TRP
1	A	279	GLU
1	A	314	LEU
1	A	315	LEU
1	A	323	TRP
1	A	332	ILE
1	A	344	ILE
1	A	368	ASP
1	A	377	VAL
1	A	386	VAL
1	A	391	GLU
1	A	417	GLU
1	B	18	VAL
1	B	23	THR
1	B	25	VAL
1	B	29	GLN
1	B	94	ASN

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Mol	Chain	Res	Type
1	B	108	VAL
1	B	135	ARG
1	B	141	LEU
1	B	191	ASN
1	B	192	GLU
1	B	195	ILE
1	B	197	LEU
1	B	220	ARG
1	B	236	LEU
1	B	245	PHE
1	B	251	GLU
1	B	252	ASN
1	B	254	VAL
1	B	279	GLU
1	B	314	LEU
1	B	323	TRP
1	B	332	ILE
1	B	344	ILE
1	B	377	VAL
1	B	391	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	39	ASN
1	A	49	GLN
1	A	64	GLN
1	A	121	ASN
1	A	137	GLN
1	A	167	ASN
1	A	193	GLN
1	A	215	GLN
1	A	242	GLN
1	A	249	GLN
1	A	256	GLN
1	A	291	GLN
1	A	296	GLN
1	A	326	ASN
1	A	329	GLN
1	A	336	ASN
1	A	372	HIS

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Mol	Chain	Res	Type
1	B	36	GLN
1	B	39	ASN
1	B	49	GLN
1	B	64	GLN
1	B	137	GLN
1	B	151	ASN
1	B	193	GLN
1	B	215	GLN
1	B	242	GLN
1	B	243	ASN
1	B	252	ASN
1	B	296	GLN
1	B	326	ASN
1	B	329	GLN
1	B	372	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	68/69 (98%)	16 (23%)	7 (10%)
3	F	68/69 (98%)	18 (26%)	7 (10%)
All	All	136/138 (98%)	34 (25%)	14 (10%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	7	A
2	E	9	G
2	E	10	G
2	E	18	G
2	E	19	G
2	E	21	A
2	E	33	U
2	E	34	G
2	E	35	C
2	E	37	6IA
2	E	38	A
2	E	45	G
2	E	47	U
2	E	48	C
2	E	49	C

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Mol	Chain	Res	Type
2	E	59	U
3	F	7	A
3	F	8	U
3	F	9	G
3	F	10	G
3	F	18	G
3	F	19	G
3	F	21	A
3	F	33	U
3	F	34	G
3	F	35	C
3	F	37	A
3	F	38	A
3	F	46	G
3	F	47	U
3	F	48	C
3	F	49	C
3	F	59	U
3	F	64	A

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	9	G
2	E	18	G
2	E	32	U
2	E	33	U
2	E	34	G
2	E	48	C
2	E	58	A
3	F	18	G
3	F	32	U
3	F	33	U
3	F	34	G
3	F	37	A
3	F	48	C
3	F	58	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	6IA	E	37	2	26,29,30	0.87	1 (3%)	36,41,44	1.24	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6IA	E	37	2	-	10/13/31/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	37	6IA	C13-C12	-3.60	1.40	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	37	6IA	O3'-C3'-C2'	4.48	126.17	111.82
2	E	37	6IA	C2'-C3'-C4'	2.60	107.63	102.61
2	E	37	6IA	O3'-C3'-C4'	2.34	117.82	111.08
2	E	37	6IA	C16-C14-C15	2.09	119.84	110.53

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	37	6IA	N6-C12-C13-C14
2	E	37	6IA	O4'-C4'-C5'-O5'
2	E	37	6IA	C3'-C4'-C5'-O5'
2	E	37	6IA	C12-C13-C14-C15
2	E	37	6IA	C5-C6-N6-C12
2	E	37	6IA	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
2	E	37	6IA	N1-C6-N6-C12
2	E	37	6IA	C2'-C1'-N9-C4
2	E	37	6IA	O4'-C1'-N9-C8
2	E	37	6IA	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	37	6IA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DMA	A	422	-	6,8,13	2.52	2 (33%)	12,13,19	1.27	2 (16%)
5	DMA	B	422	-	6,8,13	2.46	2 (33%)	12,13,19	2.05	5 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMA	A	422	-	-	1/6/6/13	-
5	DMA	B	422	-	-	0/6/6/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	422	DMA	PB-O1B	3.60	1.61	1.50
5	A	422	DMA	PB-O1B	3.60	1.61	1.50
5	A	422	DMA	PA-O1A	3.52	1.61	1.50
5	B	422	DMA	PA-O1A	3.39	1.61	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	422	DMA	O2A-PA-O1	3.74	121.83	107.80
5	B	422	DMA	O3A-PA-O1A	-3.08	94.85	111.04
5	B	422	DMA	O1-PA-O1A	2.93	122.25	110.83
5	B	422	DMA	O2A-PA-O3A	-2.53	96.16	104.64
5	B	422	DMA	O3B-PB-O3A	2.48	112.94	104.64
5	A	422	DMA	O1-PA-O3A	2.45	112.84	104.64
5	A	422	DMA	O3B-PB-O3A	2.42	112.75	104.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	422	DMA	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	422	DMA	2	0
5	B	422	DMA	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	402/409 (98%)	-0.31	0	100	100	68, 121, 172, 193	0
1	B	402/409 (98%)	-0.35	0	100	100	66, 122, 169, 187	0
2	E	68/69 (98%)	0.05	0	100	100	80, 186, 212, 219	0
3	F	69/69 (100%)	0.01	3 (4%)	40	22	81, 155, 199, 206	0
All	All	941/956 (98%)	-0.28	3 (0%)	90	75	66, 126, 189, 219	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	59	U	2.7
3	F	48	C	2.3
3	F	60	C	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	6IA	E	37	27/28	0.96	0.08	109,112,120,122	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	E	72	1/1	0.59	0.15	132,132,132,132	0
6	MG	F	73	1/1	0.66	0.30	102,102,102,102	0
6	MG	F	72	1/1	0.87	0.20	106,106,106,106	0
5	DMA	A	422	9/14	0.89	0.07	175,175,177,177	0
5	DMA	B	422	9/14	0.92	0.07	163,164,166,167	0
6	MG	B	2	1/1	0.94	0.05	112,112,112,112	0
4	ZN	B	1	1/1	0.99	0.05	98,98,98,98	0
4	ZN	A	1	1/1	1.00	0.02	96,96,96,96	0

6.5 Other polymers

There are no such residues in this entry.