



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:57 PM UTC

PDB ID : 9EI3 / pdb_00009ei3
EMDB ID : EMD-48075
Title : Cryo-EM structure of Human RNA polymerase II Elongation Complex bound to the RECQL5 helicase in the presence of AMPPNP
Authors : Florez Ariza, A.; Lue, N.; Nogales, E.
Deposited on : 2024-11-25
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

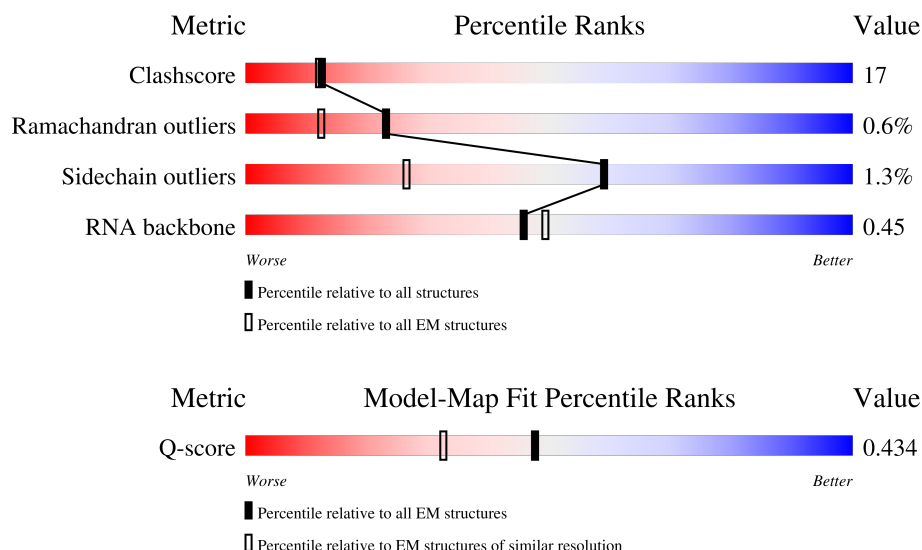
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1174	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	43	
14	P	20	
15	T	28	
16	U	991	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 36621 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1441	Total	C	N	O	S	0	0
			11426	7186	2041	2126	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2060	1296	351	407	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1711	1084	300	319	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	PHE	SER	conflict	UNP P19388

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			658	419	113	121	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a DNA chain called Non-template DNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	22	Total	C	N	O	P	0	0
			455	217	86	130	22		

- Molecule 14 is a RNA chain called RNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	11	Total	C	N	O	P	0	0
			239	107	49	72	11		

- Molecule 15 is a DNA chain called Template DNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	24	Total	C	N	O	P	0	0
			486	233	82	147	24		

- Molecule 16 is a protein called ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	538	Total	C	N	O	S	1	0
			4207	2646	756	778	27		

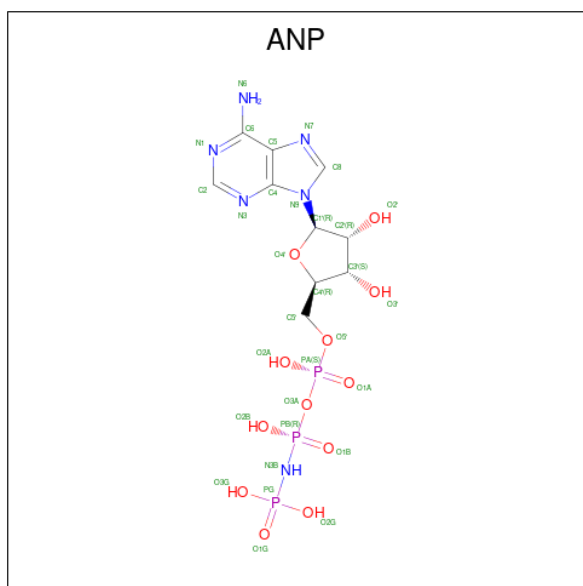
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	C	1	Total	Zn	0
			1	1	
17	I	2	Total	Zn	0
			2	2	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

- Molecule 19 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

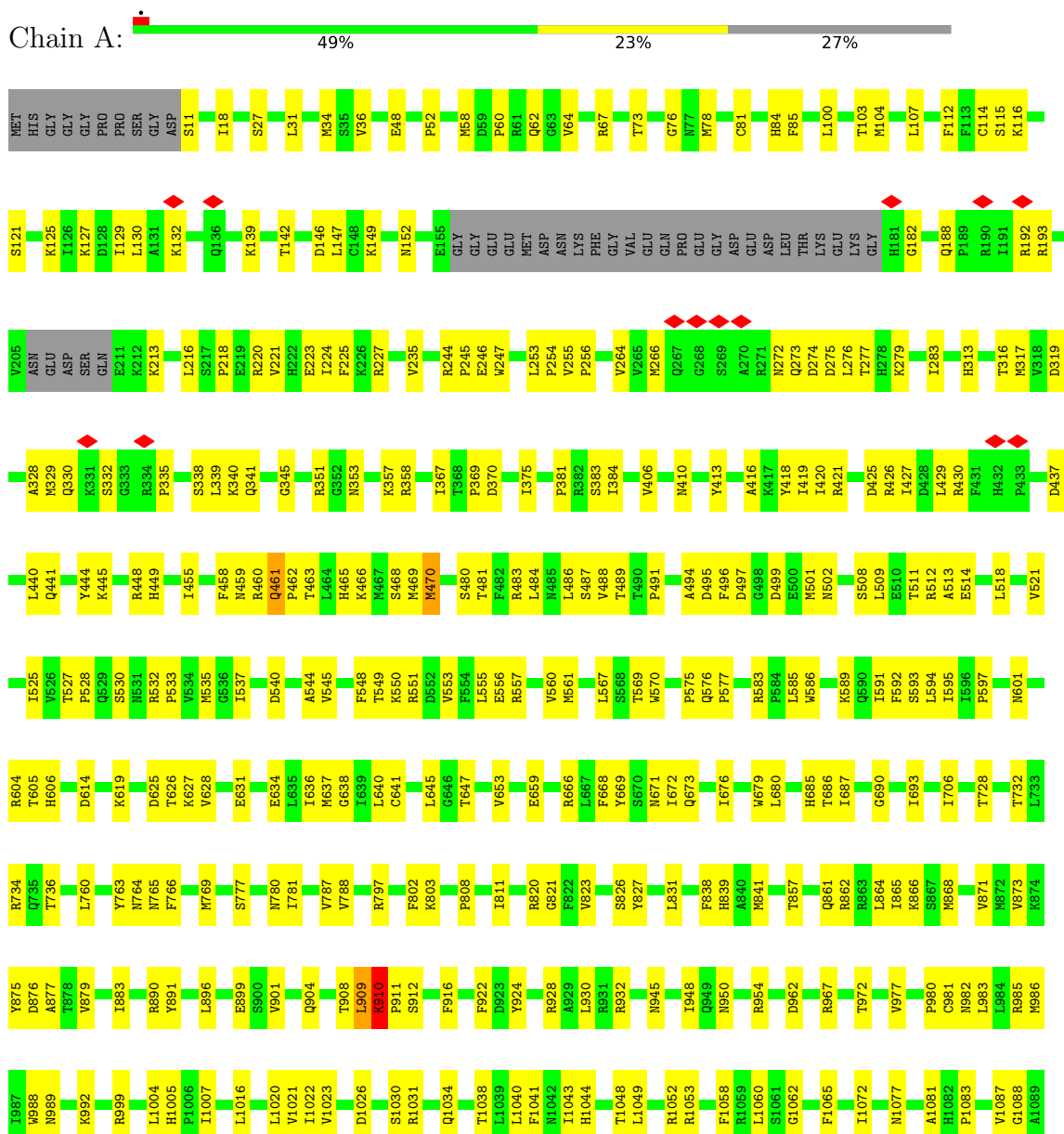


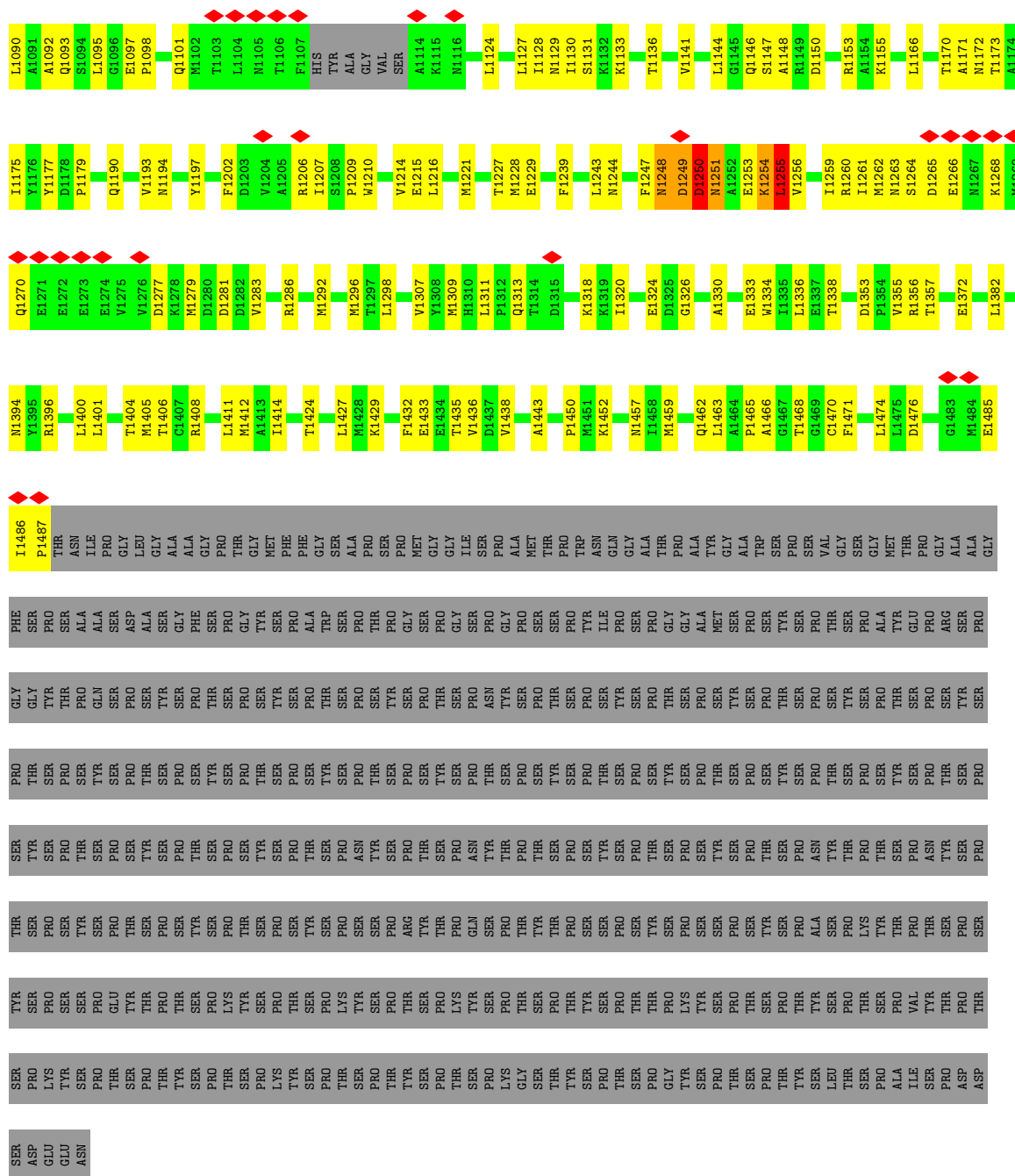
Mol	Chain	Residues	Atoms					AltConf
19	U	1	Total	C	N	O	P	0
			31	10	6	12	3	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

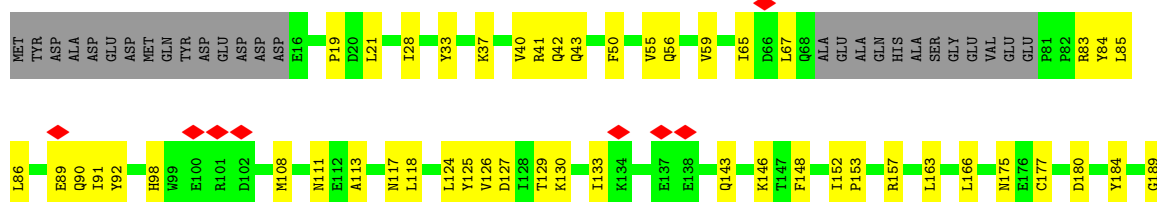
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

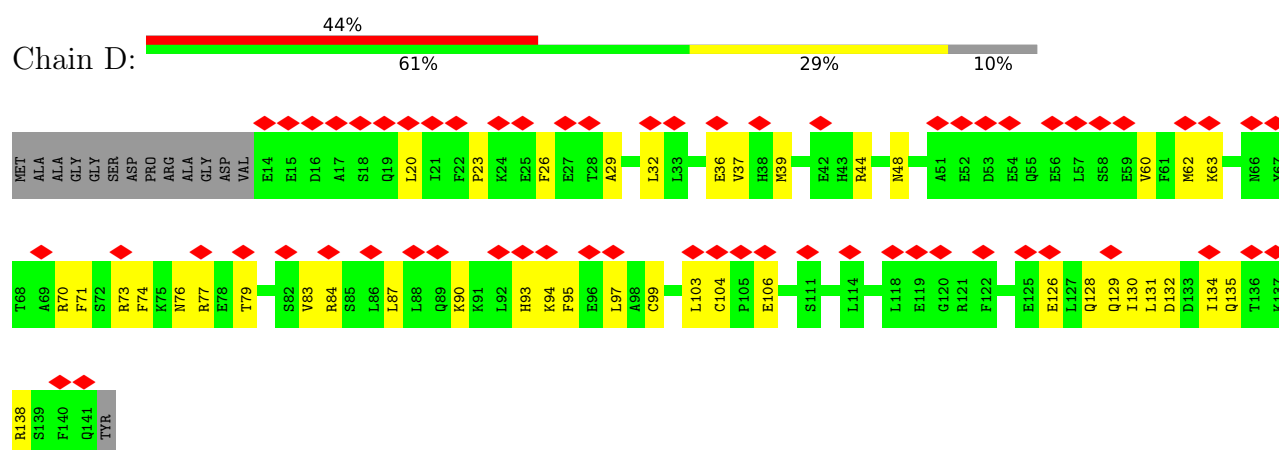




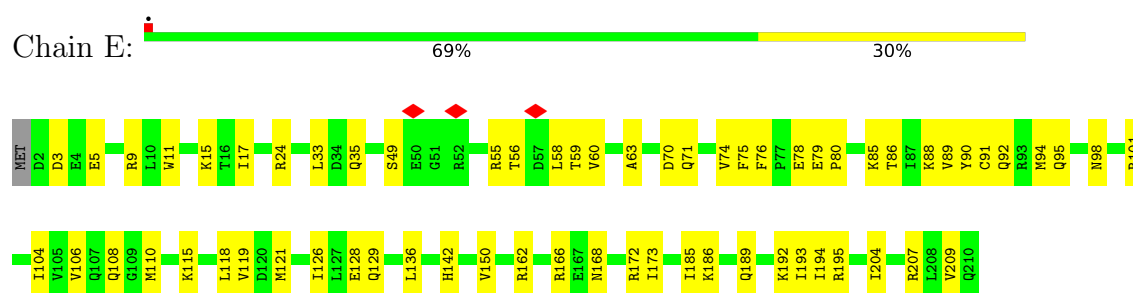
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B: 66% 31%

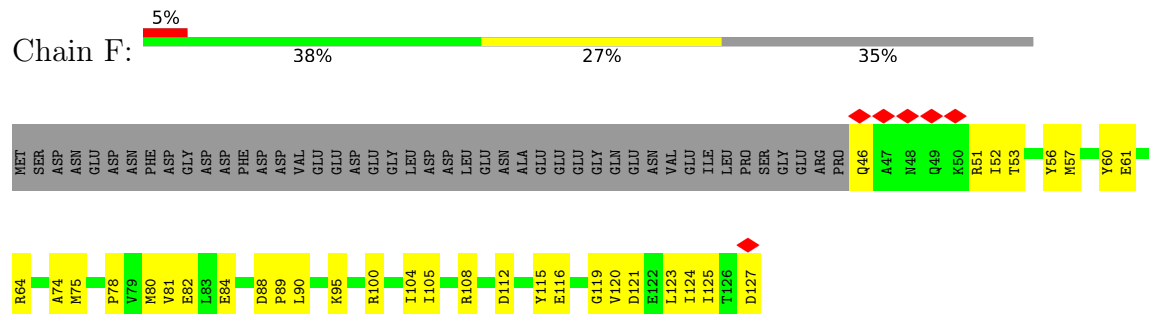




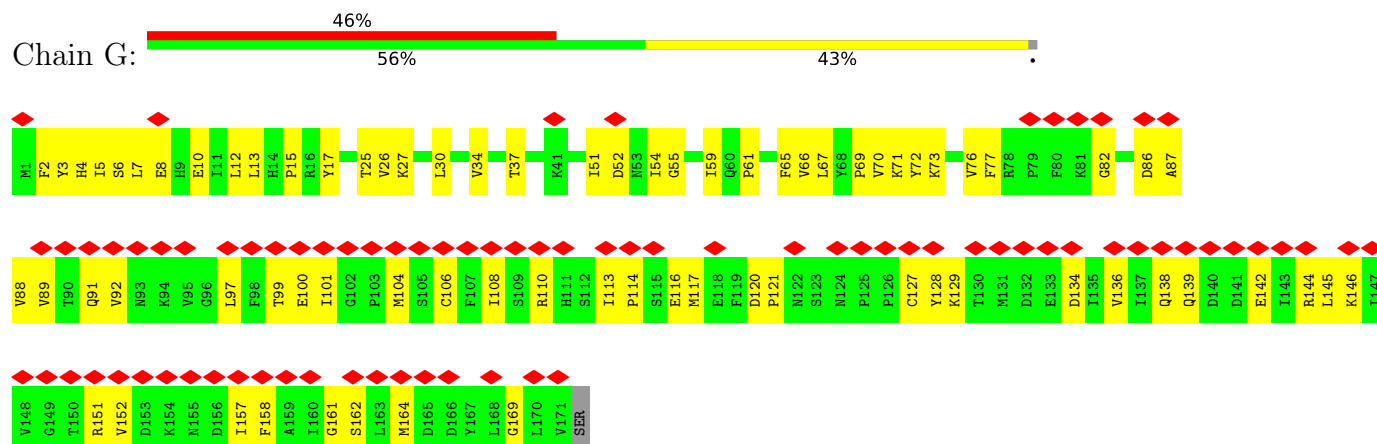
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



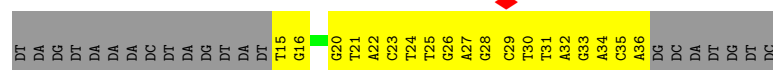
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



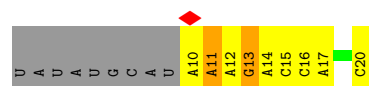
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



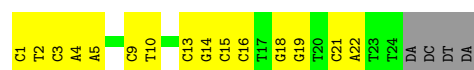
- Molecule 13: Non-template DNA, nucleic acid scaffold



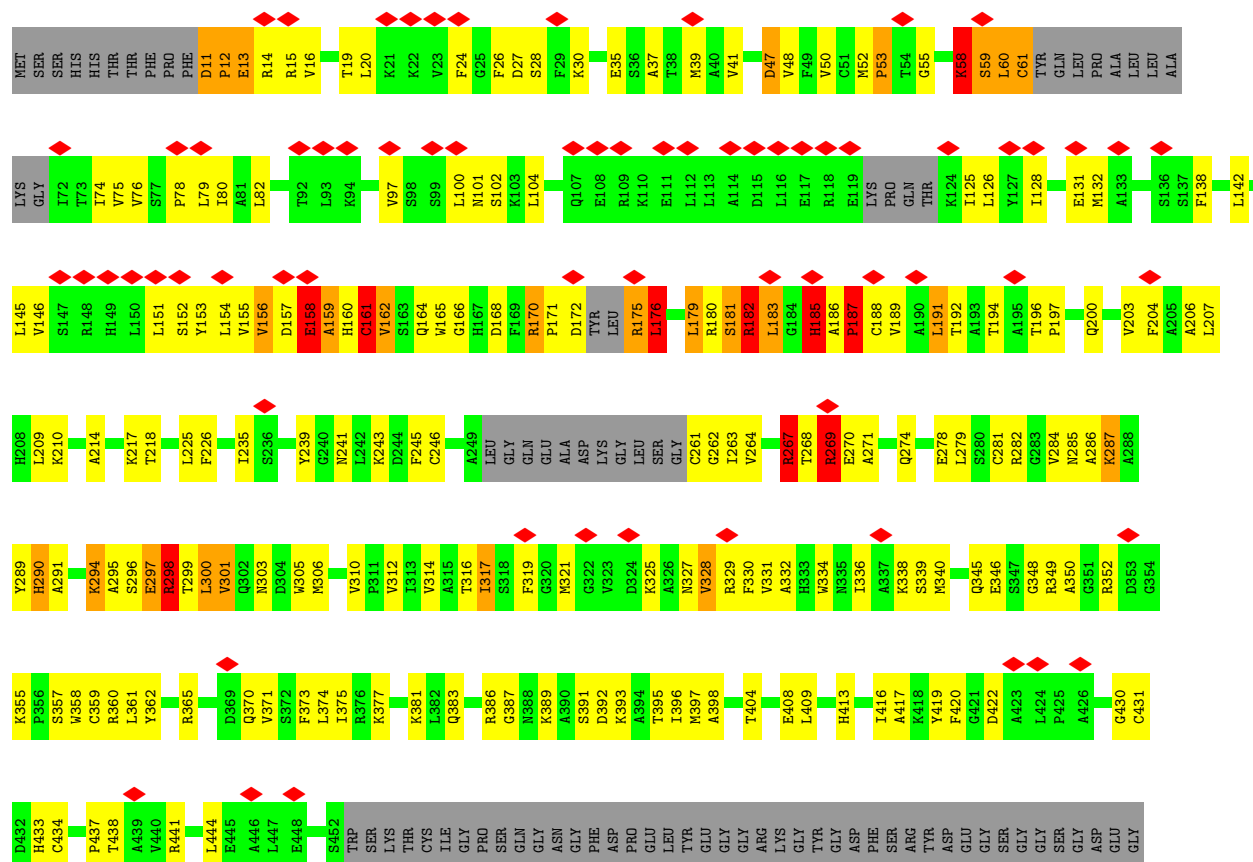
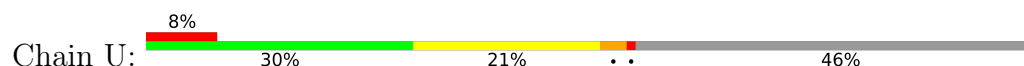
- Molecule 14: RNA, nucleic acid scaffold



- Molecule 15: Template DNA, nucleic acid scaffold



- Molecule 16: ATP-dependent DNA helicase Q5



LEU	SER	PRO	GLY	ALA	PRO	GLY	ASN	GLY	ALA	ASP	CYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80622	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.887	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	335.36, 335.36, 335.36	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.048, 1.048, 1.048	Depositor

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: MG, ZN, ANP

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	0.17	0/11635	0.43	2/15707 (0.0%)
2	B	0.15	0/9243	0.40	0/12475
3	C	0.19	0/2103	0.37	0/2858
4	D	0.12	0/1019	0.37	0/1374
5	E	0.16	0/1742	0.47	0/2353
6	F	0.17	0/668	0.56	0/903
7	G	0.17	0/1365	0.47	1/1853 (0.1%)
8	H	0.15	0/1207	0.38	0/1628
9	I	0.18	0/948	0.49	0/1284
10	J	0.16	0/542	0.43	0/730
11	K	0.18	0/939	0.41	0/1271
12	L	0.20	0/377	0.57	0/500
13	N	0.45	0/511	0.74	0/787
14	P	0.12	0/268	0.28	0/416
15	T	0.29	0/542	0.53	0/833
16	U	0.37	0/4282	0.66	4/5777 (0.1%)
All	All	0.21	0/37391	0.46	7/50749 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
16	U	0	7
All	All	0	8

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	U	12	PRO	N-CA-C	-7.42	103.05	113.81
1	A	1253	GLU	N-CA-C	-6.88	106.08	114.75
16	U	317	ILE	N-CA-C	-6.64	106.83	113.20
16	U	27	ASP	N-CA-C	-5.95	104.88	113.21
16	U	187	PRO	N-CA-CB	-5.47	97.51	103.25
7	G	121	PRO	CA-N-CD	-5.28	104.60	112.00
1	A	1248	ASN	CB-CA-C	-5.13	104.01	111.14

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	GLN	Peptide
16	U	170	ARG	Sidechain
16	U	175	ARG	Sidechain
16	U	182	ARG	Sidechain
16	U	267	ARG	Sidechain
16	U	269	ARG	Sidechain
16	U	298	ARG	Sidechain
16	U	610	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11426	0	11546	350	0
2	B	9062	0	9107	258	0
3	C	2060	0	2011	67	0
4	D	1005	0	964	29	0
5	E	1711	0	1729	48	0
6	F	658	0	686	35	0
7	G	1334	0	1333	59	0
8	H	1186	0	1147	47	0
9	I	927	0	859	39	0
10	J	533	0	553	25	0
11	K	920	0	942	33	0
12	L	372	0	378	19	0
13	N	455	0	249	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	P	239	0	121	10	0
15	T	486	0	273	27	0
16	U	4207	0	4204	276	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
19	U	31	0	13	8	0
All	All	36621	0	36115	1220	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 17.

All (1220) 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)
13:N:29:DC:C6	16:U:269:ARG:HG3	1.34	1.60
13:N:26:DG:H1	15:T:3:DC:N4	1.26	1.32
13:N:33:DG:H4'	16:U:79:LEU:CD2	1.59	1.30
13:N:29:DC:C5	16:U:269:ARG:HB3	1.68	1.27
13:N:26:DG:N2	15:T:3:DC:C5	2.03	1.25
13:N:33:DG:H1'	13:N:34:DA:C5'	1.71	1.20
13:N:29:DC:C6	16:U:269:ARG:CG	2.24	1.20
13:N:31:DT:H2''	16:U:317:ILE:CD1	1.71	1.20
13:N:31:DT:OP1	16:U:290:HIS:HE1	1.26	1.17
13:N:29:DC:H6	16:U:269:ARG:CG	1.57	1.16
13:N:31:DT:H2''	16:U:317:ILE:HD13	1.21	1.16
13:N:33:DG:H1'	13:N:34:DA:H5'	1.26	1.15
13:N:33:DG:C4'	16:U:79:LEU:HD23	1.76	1.14
13:N:29:DC:H5	16:U:269:ARG:CB	1.68	1.06
16:U:278:GLU:OE2	16:U:282:ARG:NH1	1.90	1.04
13:N:29:DC:C5	16:U:269:ARG:CB	2.43	0.98
13:N:33:DG:C4'	16:U:79:LEU:CD2	2.37	0.97
13:N:31:DT:OP1	16:U:290:HIS:CE1	2.16	0.97
13:N:31:DT:C2'	16:U:317:ILE:CD1	2.44	0.96
16:U:172:ASP:HA	16:U:175:ARG:HB2	1.48	0.95
13:N:29:DC:H5	16:U:269:ARG:HB3	0.81	0.94
16:U:55:GLY:HA2	19:U:1000:ANP:H8	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:31:DT:C2'	16:U:317:ILE:HD13	2.01	0.90
16:U:239:TYR:CD2	16:U:278:GLU:OE2	2.25	0.90
16:U:172:ASP:HB3	16:U:207:LEU:HD22	1.53	0.89
13:N:26:DG:N2	15:T:3:DC:H5	1.68	0.88
16:U:431:CYS:HB2	16:U:434:CYS:H	1.36	0.88
13:N:33:DG:C1'	13:N:34:DA:H5'	2.03	0.88
13:N:33:DG:H4'	16:U:79:LEU:HD23	0.88	0.88
13:N:29:DC:C5	16:U:269:ARG:HG3	2.08	0.88
13:N:33:DG:H5''	16:U:79:LEU:CD2	2.04	0.88
13:N:33:DG:H5''	16:U:79:LEU:HD21	1.55	0.87
13:N:33:DG:H1'	13:N:34:DA:H5''	1.53	0.87
16:U:172:ASP:O	16:U:206:ALA:O	1.92	0.87
16:U:172:ASP:H	16:U:175:ARG:N	1.73	0.86
13:N:34:DA:OP1	16:U:80:ILE:HG13	1.76	0.86
16:U:41:VAL:HG21	16:U:61:CYS:SG	2.17	0.85
16:U:53:PRO:HB3	16:U:218:THR:HG21	1.57	0.84
13:N:29:DC:C5	16:U:269:ARG:CG	2.60	0.84
13:N:33:DG:C1'	13:N:34:DA:C5'	2.54	0.84
13:N:26:DG:C2	15:T:3:DC:C5	2.65	0.84
2:B:508:MET:HE3	2:B:621:ILE:HG12	1.57	0.83
2:B:718:GLN:HB2	2:B:976:MET:HB2	1.59	0.83
13:N:35:DC:P	16:U:102:SER:HB3	2.18	0.83
13:N:33:DG:H2''	13:N:34:DA:O5'	1.78	0.83
1:A:544:ALA:HB2	1:A:680:LEU:HD12	1.60	0.82
11:K:47:LYS:HG3	11:K:60:GLY:HA2	1.59	0.82
16:U:79:LEU:HB2	16:U:321:MET:HE1	1.61	0.82
13:N:26:DG:N1	15:T:3:DC:N4	2.05	0.82
16:U:160:HIS:C	16:U:162:VAL:H	1.85	0.81
13:N:33:DG:C5'	16:U:79:LEU:CD2	2.60	0.80
16:U:172:ASP:C	16:U:206:ALA:O	2.23	0.80
3:C:56:SER:HB2	3:C:158:GLU:H	1.46	0.80
13:N:26:DG:C2	15:T:3:DC:H5	1.99	0.80
16:U:160:HIS:C	16:U:162:VAL:N	2.36	0.79
1:A:11:SER:N	2:B:1135:TYR:HH	1.79	0.79
1:A:1244:ASN:HB2	1:A:1262:MET:HG2	1.64	0.79
1:A:605:THR:HA	1:A:627:LYS:HA	1.64	0.78
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.65	0.78
13:N:30:DT:H72	16:U:338:LYS:NZ	1.99	0.78
3:C:173:HIS:HD2	3:C:175:LYS:H	1.30	0.78
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.66	0.77
13:N:28:DG:C6	16:U:274:GLN:OE1	2.37	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1457:ASN:HD22	1:A:1465:PRO:HD3	1.49	0.77
16:U:55:GLY:CA	19:U:1000:ANP:H8	2.15	0.76
16:U:20:LEU:HA	16:U:24:PHE:HB2	1.68	0.76
16:U:78:PRO:HG3	16:U:162:VAL:HG11	1.67	0.76
1:A:130:LEU:HD21	1:A:235:VAL:HG23	1.68	0.76
2:B:216:ALA:HB2	2:B:241:ALA:HA	1.69	0.75
5:E:104:ILE:HB	5:E:129:GLN:HA	1.69	0.75
5:E:121:MET:H	5:E:121:MET:HE3	1.51	0.75
13:N:34:DA:C8	16:U:131:GLU:OE1	2.39	0.75
8:H:90:TYR:HB3	8:H:145:MET:HB2	1.68	0.75
16:U:175:ARG:HA	16:U:179:LEU:HB2	1.68	0.75
2:B:299:GLU:HA	2:B:302:LYS:HE3	1.68	0.74
1:A:1254:LYS:HB3	1:A:1256:VAL:HG23	1.68	0.74
13:N:26:DG:H1	15:T:3:DC:H41	0.76	0.74
13:N:30:DT:C7	16:U:338:LYS:NZ	2.49	0.74
1:A:631:GLU:HB2	1:A:636:ILE:HD12	1.69	0.74
3:C:90:CYS:SG	3:C:94:CYS:HB3	2.27	0.74
2:B:192:LYS:HE2	2:B:469:VAL:HG22	1.69	0.74
13:N:26:DG:N1	15:T:3:DC:C5	2.56	0.74
13:N:35:DC:OP1	16:U:102:SER:HB3	1.87	0.74
13:N:31:DT:C2'	16:U:317:ILE:HD11	2.18	0.73
1:A:948:ILE:HD12	1:A:1007:ILE:HG13	1.70	0.72
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.70	0.72
10:J:5:VAL:HG22	10:J:6:ARG:HG2	1.71	0.72
1:A:129:ILE:HD12	1:A:132:LYS:HZ1	1.55	0.72
1:A:152:ASN:ND2	16:U:281:CYS:SG	2.62	0.72
13:N:33:DG:C5'	16:U:79:LEU:HD21	2.18	0.72
5:E:91:CYS:HA	5:E:94:MET:HB2	1.72	0.71
1:A:461:GLN:HA	1:A:463:THR:HG23	1.70	0.71
7:G:110:ARG:HH12	7:G:117:MET:HG3	1.53	0.71
4:D:73:ARG:HD2	4:D:138:ARG:HH11	1.55	0.71
1:A:606:HIS:HD1	1:A:641:CYS:HG	1.39	0.71
1:A:876:ASP:O	1:A:890:ARG:NH1	2.24	0.71
6:F:100:ARG:HH22	6:F:124:ILE:HA	1.56	0.70
2:B:1139:GLY:H	2:B:1141:ARG:HH22	1.36	0.70
1:A:62:GLN:HE22	1:A:255:VAL:HG12	1.55	0.70
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.24	0.69
16:U:172:ASP:HB3	16:U:207:LEU:CD2	2.23	0.69
16:U:245:PHE:HE2	16:U:360:ARG:HB2	1.56	0.69
2:B:866:ILE:HD11	2:B:896:LEU:HG	1.74	0.69
1:A:576:GLN:HA	8:H:75:TYR:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:13:DC:H2'	15:T:14:DG:H8	1.58	0.68
16:U:348:GLY:O	16:U:352:ARG:NH1	2.25	0.68
9:I:66:THR:OG1	9:I:67:GLN:OE1	2.10	0.68
13:N:35:DC:O5'	16:U:102:SER:HB3	1.92	0.68
4:D:44:ARG:O	4:D:48:ASN:ND2	2.26	0.68
2:B:37:LYS:HD3	2:B:41:ARG:HG2	1.75	0.68
2:B:636:LYS:H	2:B:639:HIS:HD2	1.41	0.68
2:B:929:PRO:O	2:B:948:GLN:NE2	2.27	0.68
16:U:175:ARG:O	16:U:176:LEU:C	2.38	0.67
2:B:674:MET:HE2	9:I:77:THR:HA	1.76	0.67
1:A:1486:ILE:HG13	1:A:1487:PRO:HD3	1.76	0.67
3:C:27:ASP:OD1	3:C:28:LEU:N	2.28	0.67
10:J:35:LEU:HD13	10:J:46:ARG:HB3	1.76	0.67
1:A:583:ARG:NH1	3:C:222:PRO:O	2.27	0.67
13:N:34:DA:H8	16:U:131:GLU:CD	2.02	0.67
11:K:27:VAL:HG21	11:K:74:ARG:HH22	1.60	0.67
1:A:1128:ILE:HG23	1:A:1414:ILE:HB	1.75	0.67
1:A:1022:ILE:H	1:A:1034:GLN:HE22	1.44	0.66
1:A:419:ILE:HG13	1:A:429:LEU:HD11	1.78	0.66
2:B:707:CYS:SG	2:B:730:LYS:NZ	2.69	0.66
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.26	0.66
13:N:32:DA:P	16:U:291:ALA:HB2	2.36	0.66
16:U:28:SER:HA	19:U:1000:ANP:N6	2.10	0.66
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.28	0.66
2:B:1120:ASN:HD22	2:B:1145:GLN:HB2	1.61	0.66
5:E:59:THR:OG1	5:E:74:VAL:O	2.14	0.66
3:C:190:ASN:ND2	3:C:195:THR:O	2.28	0.66
7:G:55:GLY:HA3	7:G:69:PRO:HG2	1.76	0.65
2:B:721:ARG:HD2	2:B:975:ARG:HB2	1.78	0.65
5:E:185:ILE:HG21	5:E:209:VAL:HG21	1.77	0.65
1:A:112:PHE:H	1:A:188:GLN:HE22	1.45	0.65
1:A:686:THR:O	1:A:765:ASN:ND2	2.29	0.65
2:B:747:LEU:HD23	15:T:19:DG:H5''	1.78	0.65
1:A:1355:VAL:HG23	1:A:1356:ARG:HG3	1.78	0.65
9:I:59:THR:OG1	9:I:61:GLU:OE1	2.14	0.65
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.60	0.65
1:A:78:MET:O	2:B:1072:ARG:NH2	2.29	0.65
13:N:28:DG:N1	16:U:274:GLN:OE1	2.30	0.64
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.78	0.64
8:H:32:SER:HB3	8:H:37:MET:H	1.61	0.64
1:A:922:PHE:HA	1:A:1052:ARG:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:VAL:HG11	3:C:127:VAL:HG21	1.80	0.64
9:I:82:GLU:OE1	9:I:82:GLU:N	2.31	0.64
16:U:329:ARG:HH22	16:U:355:LYS:HB2	1.60	0.64
8:H:130:ASN:OD1	8:H:131:ASN:N	2.30	0.64
3:C:36:ARG:NH1	11:K:41:THR:OG1	2.30	0.64
9:I:86:CYS:HB2	9:I:114:CYS:SG	2.37	0.64
16:U:151:LEU:HD12	16:U:183:LEU:HD11	1.78	0.64
1:A:427:ILE:HD13	1:A:437:ASP:HB3	1.79	0.64
1:A:114:CYS:SG	1:A:116:LYS:NZ	2.68	0.64
5:E:150:VAL:HG22	5:E:185:ILE:HD11	1.79	0.64
2:B:222:ARG:HG2	2:B:232:THR:HG21	1.79	0.64
3:C:30:VAL:HA	11:K:45:ILE:HD11	1.79	0.64
5:E:75:PHE:CE2	5:E:90:TYR:HD2	2.16	0.64
12:L:44:MET:HE3	12:L:44:MET:HA	1.80	0.64
1:A:413:TYR:O	1:A:449:HIS:ND1	2.32	0.63
1:A:548:PHE:HE1	1:A:555:LEU:HD11	1.63	0.63
1:A:1279:MET:O	16:U:515:ARG:NH2	2.30	0.63
1:A:1427:LEU:HD22	1:A:1459:MET:HE1	1.78	0.63
2:B:905:ASP:HB2	2:B:924:ARG:HG2	1.80	0.63
2:B:927:ARG:HD3	2:B:1054:MET:HE1	1.80	0.63
16:U:145:LEU:HD23	16:U:151:LEU:HD21	1.81	0.63
1:A:1127:LEU:HD13	1:A:1382:LEU:HD22	1.78	0.63
11:K:38:GLU:OE1	11:K:42:LEU:HB2	1.99	0.63
2:B:930:GLN:N	2:B:933:ASP:OD2	2.32	0.63
2:B:1115:GLN:HE21	2:B:1150:ARG:HH11	1.46	0.63
13:N:31:DT:H2'	16:U:317:ILE:HD11	1.80	0.63
16:U:541:ARG:NH2	16:U:588:PHE:O	2.31	0.63
1:A:811:ILE:HD12	9:I:79:PRO:HB3	1.80	0.63
16:U:243:LYS:HG3	16:U:282:ARG:HB3	1.80	0.62
1:A:569:THR:HG23	1:A:671:ASN:HD21	1.63	0.62
13:N:33:DG:C2'	13:N:34:DA:C5'	2.77	0.62
5:E:186:LYS:HG2	5:E:189:GLN:HE21	1.63	0.62
11:K:45:ILE:HG22	11:K:46:ILE:HD12	1.80	0.62
2:B:1105:GLU:HA	2:B:1109:GLU:HB2	1.81	0.62
13:N:30:DT:C7	16:U:338:LYS:HZ3	2.13	0.62
13:N:31:DT:H2''	16:U:317:ILE:CG1	2.29	0.62
6:F:53:THR:OG1	6:F:108:ARG:NH1	2.33	0.62
13:N:30:DT:H72	16:U:338:LYS:HZ3	1.61	0.62
1:A:1030:SER:OG	5:E:162:ARG:NE	2.33	0.62
3:C:154:ARG:HD3	10:J:64:PRO:HD3	1.82	0.62
15:T:18:DG:H2'	15:T:19:DG:C8	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:76:VAL:HB	16:U:156:VAL:HA	1.82	0.62
2:B:626:LEU:HG	2:B:698:ILE:HD13	1.81	0.62
8:H:59:VAL:HB	8:H:144:LEU:HB2	1.82	0.62
1:A:924:TYR:HA	1:A:930:LEU:HD11	1.81	0.62
5:E:192:LYS:HE2	5:E:194:ILE:HD11	1.82	0.62
1:A:862:ARG:HH12	1:A:1433:GLU:HG3	1.65	0.62
16:U:536:GLU:HG2	16:U:585:HIS:HE1	1.65	0.62
1:A:329:MET:HE3	1:A:329:MET:HA	1.82	0.61
2:B:241:ALA:O	2:B:249:LYS:NZ	2.33	0.61
3:C:7:PRO:HD2	11:K:100:LEU:HD23	1.82	0.61
3:C:110:ASP:OD1	3:C:111:GLN:N	2.33	0.61
13:N:33:DG:H4'	16:U:79:LEU:HD21	1.75	0.61
16:U:269:ARG:C	16:U:271:ALA:H	2.09	0.61
13:N:30:DT:C7	16:U:338:LYS:HZ1	2.14	0.61
15:T:2:DT:H2''	15:T:3:DC:C2	2.36	0.61
1:A:868:MET:HE3	1:A:1404:THR:HG21	1.82	0.61
5:E:9:ARG:HG2	5:E:136:LEU:HD21	1.83	0.61
6:F:82:GLU:OE2	6:F:82:GLU:N	2.30	0.61
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.83	0.61
13:N:33:DG:H2''	13:N:34:DA:C5'	2.31	0.61
16:U:11:ASP:C	16:U:13:GLU:N	2.56	0.61
16:U:154:LEU:O	16:U:188:CYS:HA	2.01	0.61
16:U:175:ARG:HG3	16:U:179:LEU:HB3	1.83	0.61
1:A:866:LYS:HG2	1:A:1432:PHE:HB2	1.83	0.61
5:E:55:ARG:HA	5:E:58:LEU:HD12	1.83	0.61
16:U:185:HIS:O	16:U:186:ALA:C	2.44	0.61
7:G:89:VAL:HA	7:G:99:THR:HA	1.83	0.60
10:J:66:GLU:N	10:J:66:GLU:OE1	2.33	0.60
14:P:11:A:H2'	14:P:12:A:C8	2.36	0.60
15:T:18:DG:H2'	15:T:19:DG:H8	1.66	0.60
1:A:909:LEU:O	1:A:910:LYS:HB2	2.00	0.60
1:A:1170:THR:HA	1:A:1216:LEU:HA	1.83	0.60
7:G:89:VAL:O	7:G:139:GLN:NE2	2.34	0.60
11:K:42:LEU:O	11:K:46:ILE:HD12	2.01	0.60
2:B:709:SER:HB2	2:B:767:LEU:HD11	1.83	0.60
13:N:27:DA:N1	15:T:2:DT:O2	2.35	0.60
2:B:111:ASN:ND2	2:B:175:ASN:O	2.34	0.60
7:G:92:VAL:HG11	7:G:127:CYS:HA	1.84	0.60
9:I:109:ARG:NH1	9:I:124:THR:OG1	2.33	0.60
1:A:1372:GLU:OE2	5:E:207:ARG:NH1	2.35	0.60
2:B:474:THR:OG1	2:B:732:ALA:O	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:159:ALA:HB3	16:U:191:LEU:H	1.67	0.60
16:U:298:ARG:HA	16:U:301:VAL:HB	1.84	0.60
9:I:73:SER:HA	9:I:95:VAL:HG11	1.83	0.60
1:A:11:SER:N	2:B:1135:TYR:OH	2.35	0.60
1:A:1202:PHE:HE2	1:A:1264:SER:HB3	1.67	0.60
2:B:89:GLU:HB2	2:B:127:ASP:HB2	1.84	0.60
2:B:699:HIS:HD2	2:B:701:SER:HB3	1.64	0.60
1:A:982:ASN:O	1:A:986:MET:HG3	2.01	0.60
2:B:197:GLN:HE21	2:B:466:VAL:HB	1.67	0.60
1:A:560:VAL:HG22	1:A:591:ILE:HD11	1.83	0.59
6:F:84:GLU:N	6:F:84:GLU:OE1	2.35	0.59
2:B:930:GLN:NE2	2:B:1056:ASP:OD2	2.34	0.59
7:G:99:THR:HG23	7:G:106:CYS:HB3	1.83	0.59
13:N:22:DA:H2''	13:N:23:DC:H5''	1.83	0.59
14:P:13:G:H2'	14:P:14:A:C8	2.36	0.59
16:U:37:ALA:O	16:U:41:VAL:HG23	2.02	0.59
9:I:92:LYS:HE3	9:I:92:LYS:HA	1.84	0.59
1:A:687:ILE:HG22	2:B:782:ILE:HG21	1.84	0.59
4:D:71:PHE:CZ	7:G:86:ASP:HB3	2.38	0.59
1:A:514:GLU:OE2	2:B:1101:GLN:HG3	2.01	0.59
1:A:728:THR:H	1:A:736:THR:HG21	1.68	0.59
8:H:105:SER:OG	8:H:106:THR:N	2.31	0.59
10:J:66:GLU:HA	12:L:23:HIS:HB3	1.83	0.59
13:N:34:DA:OP1	16:U:80:ILE:CG1	2.50	0.59
1:A:706:ILE:HD11	1:A:787:VAL:HG21	1.85	0.59
3:C:27:ASP:OD1	3:C:29:ALA:N	2.34	0.59
16:U:164:GLN:HE22	16:U:203:VAL:HA	1.67	0.59
1:A:614:ASP:HA	1:A:619:LYS:HG3	1.85	0.59
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.84	0.59
1:A:1227:THR:OG1	1:A:1229:GLU:OE1	2.16	0.59
2:B:124:LEU:HD22	2:B:152:ILE:HD11	1.85	0.59
1:A:1254:LYS:O	1:A:1256:VAL:N	2.36	0.59
2:B:253:GLY:N	2:B:254:GLN:OE1	2.36	0.59
7:G:88:VAL:O	7:G:100:GLU:N	2.36	0.59
1:A:1406:THR:O	5:E:207:ARG:NH2	2.34	0.58
2:B:1142:ASN:HD21	2:B:1145:GLN:HG3	1.68	0.58
16:U:289:TYR:CZ	16:U:298:ARG:HB3	2.38	0.58
3:C:173:HIS:CD2	3:C:175:LYS:H	2.16	0.58
16:U:319:PHE:O	16:U:349:ARG:NH1	2.36	0.58
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.37	0.58
16:U:179:LEU:HD13	16:U:182:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:VAL:O	2:B:304:SER:OG	2.19	0.58
16:U:41:VAL:O	16:U:153:TYR:OH	2.17	0.58
16:U:619:ASP:OD1	16:U:619:ASP:N	2.35	0.58
1:A:31:LEU:HD11	1:A:254:PRO:HG3	1.86	0.58
1:A:358:ARG:NH2	15:T:16:DC:OP2	2.35	0.58
1:A:896:LEU:HA	1:A:1081:ALA:H	1.68	0.58
1:A:1221:MET:HG3	1:A:1255:LEU:HD23	1.85	0.58
1:A:1166:LEU:HD23	1:A:1292:MET:HB3	1.85	0.58
1:A:1210:TRP:CD1	1:A:1281:ASP:HB2	2.38	0.58
1:A:1248:ASN:O	1:A:1249:ASP:C	2.46	0.58
2:B:1085:ARG:HD3	15:T:15:DC:H5'	1.85	0.58
16:U:328:VAL:HB	16:U:350:ALA:HA	1.86	0.58
1:A:857:THR:O	1:A:861:GLN:HG3	2.03	0.58
15:T:13:DC:H2'	15:T:14:DG:C8	2.37	0.58
16:U:217:LYS:NZ	16:U:420:PHE:O	2.37	0.58
2:B:1060:HIS:NE2	2:B:1082:GLY:O	2.32	0.58
16:U:371:VAL:O	16:U:375:ILE:HG12	2.03	0.58
1:A:659:GLU:OE1	1:A:985:ARG:NH1	2.26	0.58
1:A:928:ARG:HE	8:H:106:THR:HB	1.69	0.57
2:B:65:ILE:HB	2:B:86:LEU:HB2	1.85	0.57
5:E:79:GLU:OE2	5:E:86:THR:OG1	2.21	0.57
6:F:46:GLN:N	6:F:115:TYR:O	2.37	0.57
6:F:57:MET:HB2	6:F:123:LEU:HD13	1.86	0.57
1:A:470:MET:HE3	1:A:521:VAL:HG22	1.86	0.57
1:A:631:GLU:OE1	1:A:992:LYS:NZ	2.37	0.57
1:A:1190:GLN:O	1:A:1194:ASN:ND2	2.37	0.57
2:B:992:ASN:O	10:J:46:ARG:NH1	2.37	0.57
9:I:20:CYS:SG	9:I:41:ASN:ND2	2.76	0.57
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.37	0.57
1:A:1171:ALA:N	1:A:1215:GLU:O	2.35	0.57
2:B:757:PRO:HG2	2:B:764:MET:HE1	1.84	0.57
8:H:90:TYR:HE2	8:H:92:MET:HE2	1.68	0.57
8:H:92:MET:HB2	8:H:143:LEU:HB3	1.86	0.57
5:E:63:ALA:HA	5:E:71:GLN:HA	1.86	0.57
12:L:35:ARG:NH2	12:L:36:CYS:O	2.37	0.57
8:H:96:VAL:HA	8:H:116:VAL:HA	1.87	0.57
2:B:706:VAL:HG13	2:B:767:LEU:HD22	1.87	0.57
9:I:54:TYR:CE1	9:I:56:ASN:HB2	2.39	0.57
2:B:474:THR:HG22	2:B:476:ALA:H	1.69	0.57
2:B:854:ILE:HD12	2:B:904:VAL:HG21	1.86	0.57
5:E:88:LYS:NZ	5:E:88:LYS:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:32:DA:OP2	16:U:291:ALA:HB3	2.05	0.57
16:U:172:ASP:N	16:U:175:ARG:N	2.50	0.57
2:B:678:THR:H	2:B:682:LEU:HD13	1.70	0.57
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.87	0.56
5:E:5:GLU:OE1	5:E:9:ARG:NH2	2.38	0.56
16:U:82:LEU:HB2	16:U:321:MET:HE3	1.86	0.56
16:U:263:ILE:HD11	16:U:305:TRP:HZ2	1.70	0.56
1:A:583:ARG:HG3	1:A:585:LEU:HD13	1.87	0.56
4:D:36:GLU:OE2	4:D:84:ARG:NH1	2.38	0.56
10:J:43:TYR:HA	10:J:46:ARG:HG3	1.87	0.56
16:U:160:HIS:O	16:U:162:VAL:N	2.38	0.56
16:U:339:SER:HB2	16:U:398:ALA:HB1	1.88	0.56
1:A:330:GLN:NE2	1:A:332:SER:OG	2.30	0.56
2:B:42:GLN:HG2	2:B:43:GLN:N	2.18	0.56
2:B:329:GLY:O	2:B:335:ARG:NH1	2.38	0.56
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.86	0.56
7:G:101:ILE:HB	7:G:104:MET:HB3	1.86	0.56
7:G:117:MET:SD	7:G:128:TYR:HB3	2.45	0.56
8:H:98:ARG:HH21	8:H:100:GLU:HG3	1.70	0.56
13:N:32:DA:O4'	16:U:317:ILE:HD11	2.05	0.56
16:U:171:PRO:O	16:U:172:ASP:HB2	2.04	0.56
5:E:80:PRO:HB3	5:E:108:GLN:HE22	1.71	0.56
1:A:1179:PRO:O	9:I:33:ARG:NH2	2.38	0.56
2:B:395:LEU:HD13	2:B:532:ILE:HG21	1.87	0.56
13:N:30:DT:H72	16:U:338:LYS:HZ1	1.69	0.56
1:A:465:HIS:O	1:A:468:SER:OG	2.23	0.56
2:B:855:ALA:HB3	12:L:49:THR:HB	1.87	0.56
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.36	0.56
16:U:157:ASP:O	16:U:158:GLU:C	2.49	0.56
2:B:668:LEU:HD23	2:B:668:LEU:H	1.71	0.56
2:B:311:ILE:HG23	2:B:316:VAL:HG23	1.88	0.56
2:B:1139:GLY:H	2:B:1141:ARG:NH2	2.03	0.56
8:H:8:ASP:OD2	8:H:32:SER:OG	2.21	0.56
12:L:34:ILE:HG23	12:L:44:MET:HG2	1.87	0.56
1:A:1147:SER:HA	1:A:1153:ARG:HB2	1.88	0.56
2:B:713:PHE:HB3	2:B:716:HIS:HD2	1.71	0.56
1:A:1266:GLU:HB2	1:A:1268:LYS:HE2	1.87	0.55
1:A:865:ILE:HD11	1:A:1093:GLN:HG3	1.88	0.55
2:B:277:GLY:HA2	2:B:314:GLN:HG3	1.86	0.55
16:U:39:MET:SD	16:U:39:MET:N	2.80	0.55
1:A:64:VAL:HG11	1:A:78:MET:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:HIS:HE2	1:A:769:MET:HE3	1.71	0.55
9:I:61:GLU:OE1	9:I:61:GLU:N	2.37	0.55
1:A:34:MET:HE1	2:B:1124:ILE:HG21	1.89	0.55
9:I:69:ILE:HG13	9:I:72:VAL:HG23	1.88	0.55
1:A:909:LEU:C	1:A:911:PRO:HD2	2.32	0.55
1:A:977:VAL:HG21	1:A:1040:LEU:HD21	1.87	0.55
4:D:130:ILE:O	4:D:134:ILE:HG23	2.06	0.55
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.89	0.55
16:U:20:LEU:O	16:U:26:PHE:N	2.38	0.55
1:A:1250:ASP:O	1:A:1251:ASN:C	2.50	0.55
2:B:807:ARG:NH1	12:L:58:ARG:O	2.29	0.55
1:A:18:ILE:H	1:A:1462:GLN:HE22	1.53	0.55
1:A:1450:PRO:HB2	1:A:1452:LYS:HG2	1.88	0.55
14:P:10:A:H2'	14:P:11:A:C8	2.42	0.55
1:A:606:HIS:ND1	1:A:641:CYS:SG	2.69	0.55
2:B:561:ILE:HG13	2:B:576:ILE:HG21	1.89	0.55
2:B:1060:HIS:HB2	2:B:1078:ARG:HG3	1.87	0.55
2:B:265:GLN:HE22	2:B:324:ARG:HG2	1.72	0.54
2:B:487:SER:OG	2:B:524:LYS:NZ	2.40	0.54
2:B:627:ILE:HD11	2:B:663:GLU:HB2	1.87	0.54
3:C:190:ASN:O	3:C:193:ARG:NH1	2.39	0.54
8:H:104:THR:N	8:H:107:GLU:OE2	2.36	0.54
16:U:161:CYS:O	16:U:162:VAL:C	2.50	0.54
1:A:528:PRO:HG2	1:A:1090:LEU:HD11	1.88	0.54
5:E:121:MET:HE3	5:E:121:MET:N	2.21	0.54
1:A:551:ARG:NE	1:A:625:ASP:OD1	2.32	0.54
5:E:17:ILE:HG21	5:E:74:VAL:HG11	1.88	0.54
8:H:37:MET:SD	8:H:127:GLY:HA3	2.47	0.54
16:U:294:LYS:HB3	16:U:297:GLU:H	1.73	0.54
9:I:63:ASP:OD1	9:I:65:LEU:HD12	2.07	0.54
1:A:604:ARG:O	1:A:628:VAL:N	2.39	0.54
1:A:1372:GLU:HG3	5:E:193:ILE:HD13	1.89	0.54
2:B:789:ASN:HB3	2:B:795:ILE:HG13	1.90	0.54
2:B:861:SER:HA	2:B:901:THR:HA	1.90	0.54
7:G:162:SER:HB3	7:G:164:MET:HE1	1.88	0.54
13:N:35:DC:O5'	16:U:102:SER:CB	2.55	0.54
16:U:53:PRO:CB	16:U:218:THR:HG21	2.33	0.54
16:U:28:SER:HA	19:U:1000:ANP:HN62	1.72	0.54
16:U:158:GLU:O	16:U:160:HIS:N	2.31	0.54
2:B:506:TRP:NE1	2:B:697:GLU:OE2	2.36	0.54
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PRO:HA	1:A:221:VAL:HG12	1.90	0.54
1:A:551:ARG:NH1	8:H:42:ASP:OD2	2.41	0.54
2:B:486:ASN:OD1	2:B:491:ARG:NH2	2.41	0.54
2:B:285:LEU:HD21	2:B:305:LEU:HD11	1.90	0.53
16:U:82:LEU:H	16:U:321:MET:HE3	1.72	0.53
16:U:197:PRO:HA	16:U:200:GLN:HE21	1.73	0.53
16:U:267:ARG:O	16:U:268:THR:HG23	2.08	0.53
1:A:460:ARG:HG2	1:A:462:PRO:HD2	1.90	0.53
1:A:514:GLU:HG3	1:A:518:LEU:HD12	1.88	0.53
16:U:152:SER:C	16:U:186:ALA:HA	2.33	0.53
1:A:1049:LEU:HD12	1:A:1065:PHE:HE1	1.74	0.53
16:U:306:MET:HE3	16:U:306:MET:HA	1.91	0.53
1:A:1263:ASN:ND2	1:A:1264:SER:O	2.40	0.53
2:B:331:THR:HG22	2:B:334:LYS:HE2	1.89	0.53
2:B:516:GLU:OE1	2:B:516:GLU:HA	2.09	0.53
2:B:1119:CYS:HB2	2:B:1137:CYS:SG	2.49	0.53
6:F:52:ILE:HD12	6:F:52:ILE:O	2.08	0.53
6:F:80:MET:HE3	6:F:80:MET:HA	1.90	0.53
7:G:52:ASP:N	7:G:71:LYS:O	2.41	0.53
16:U:601:VAL:O	16:U:605:VAL:HG13	2.09	0.53
2:B:380:ARG:NH1	2:B:611:GLU:OE2	2.42	0.53
8:H:128:ASP:N	8:H:128:ASP:OD1	2.41	0.53
16:U:289:TYR:CE1	16:U:298:ARG:HB3	2.44	0.53
1:A:469:MET:HB3	2:B:1093:CYS:SG	2.49	0.53
3:C:40:ALA:O	3:C:169:PHE:HB2	2.09	0.53
3:C:70:LEU:HB3	10:J:6:ARG:HG3	1.89	0.53
3:C:70:LEU:HD12	10:J:6:ARG:HG3	1.90	0.53
1:A:593:SER:HB2	1:A:634:GLU:HA	1.90	0.53
1:A:1264:SER:OG	1:A:1265:ASP:N	2.42	0.53
5:E:115:LYS:O	5:E:119:VAL:HG12	2.09	0.53
9:I:117:PRO:HB2	9:I:118:HIS:ND1	2.24	0.53
10:J:65:LEU:HG	12:L:18:ILE:HD11	1.89	0.53
16:U:340:MET:SD	16:U:340:MET:N	2.82	0.53
1:A:406:VAL:HG13	1:A:429:LEU:HD21	1.90	0.53
1:A:1401:LEU:O	1:A:1405:MET:HG3	2.09	0.53
2:B:588:ARG:O	2:B:592:ARG:HD3	2.08	0.53
3:C:154:ARG:HB3	10:J:60:LEU:HD22	1.91	0.53
4:D:29:ALA:O	4:D:94:LYS:NZ	2.38	0.53
4:D:126:GLU:O	4:D:129:GLN:HG3	2.09	0.53
1:A:1263:ASN:ND2	16:U:515:ARG:HB3	2.24	0.52
3:C:238:SER:OG	3:C:239:LEU:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:610:ARG:NH1	9:I:71:ASP:OD2	2.42	0.52
4:D:39:MET:HB2	4:D:77:ARG:HH11	1.75	0.52
7:G:97:LEU:HB3	7:G:108:ILE:HB	1.91	0.52
7:G:145:LEU:HD13	7:G:161:GLY:HA3	1.91	0.52
13:N:28:DG:H4'	13:N:29:DC:C2	2.44	0.52
16:U:12:PRO:C	16:U:14:ARG:N	2.68	0.52
16:U:295:ALA:O	16:U:299:THR:N	2.38	0.52
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.91	0.52
1:A:76:GLY:HA2	1:A:81:CYS:HB2	1.90	0.52
1:A:107:LEU:HD21	1:A:221:VAL:HG23	1.92	0.52
13:N:30:DT:H71	16:U:338:LYS:NZ	2.25	0.52
13:N:31:DT:P	16:U:268:THR:HB	2.50	0.52
16:U:585:HIS:CD2	16:U:589:ARG:HE	2.27	0.52
2:B:910:THR:OG1	2:B:911:LEU:N	2.41	0.52
7:G:34:VAL:O	7:G:37:THR:OG1	2.26	0.52
1:A:369:PRO:HB3	1:A:486:LEU:HD21	1.92	0.52
2:B:713:PHE:HB3	2:B:716:HIS:CD2	2.45	0.52
2:B:908:MET:HE2	2:B:920:LYS:HB2	1.92	0.52
3:C:52:ILE:HG21	3:C:55:ASN:HB2	1.90	0.52
11:K:31:CYS:SG	11:K:84:GLN:NE2	2.82	0.52
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.34	0.52
3:C:24:GLU:OE2	3:C:228:ARG:NE	2.39	0.52
4:D:29:ALA:HB2	7:G:5:ILE:HG13	1.92	0.52
10:J:30:THR:OG1	10:J:33:ASP:OD2	2.24	0.52
2:B:906:GLN:OE1	2:B:922:ARG:NH2	2.43	0.52
3:C:31:ALA:O	3:C:231:TYR:OH	2.28	0.52
4:D:20:LEU:HD11	4:D:93:HIS:CD2	2.45	0.52
7:G:106:CYS:SG	7:G:161:GLY:N	2.79	0.52
7:G:117:MET:HA	7:G:117:MET:HE2	1.92	0.52
6:F:121:ASP:OD1	6:F:121:ASP:N	2.39	0.52
12:L:19:CYS:SG	12:L:20:GLY:N	2.83	0.52
1:A:533:PRO:O	1:A:647:THR:OG1	2.19	0.52
1:A:803:LYS:NZ	2:B:381:GLU:OE1	2.43	0.52
1:A:873:VAL:HG22	1:A:879:VAL:HG22	1.91	0.52
3:C:48:ASP:OD1	12:L:58:ARG:NH1	2.43	0.52
11:K:19:ILE:HG13	11:K:35:ILE:HG12	1.92	0.52
13:N:34:DA:H8	16:U:131:GLU:OE1	1.86	0.52
16:U:100:LEU:HB3	16:U:128:ILE:HG13	1.92	0.52
1:A:865:ILE:HD13	1:A:1092:ALA:HB3	1.90	0.51
2:B:223:SER:OG	2:B:233:SER:O	2.28	0.51
7:G:87:ALA:HB2	7:G:101:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:16:C:H2'	14:P:17:A:C8	2.45	0.51
16:U:433:HIS:CE1	16:U:437:PRO:HB3	2.44	0.51
1:A:67:ARG:HA	1:A:78:MET:HE3	1.90	0.51
1:A:1136:THR:O	1:A:1136:THR:OG1	2.26	0.51
2:B:194:LEU:HD23	2:B:396:ALA:HA	1.91	0.51
3:C:39:ILE:HG23	3:C:177:ASN:HD21	1.75	0.51
4:D:37:VAL:HG21	7:G:2:PHE:CD2	2.45	0.51
1:A:875:TYR:HA	1:A:1083:PRO:HB3	1.92	0.51
1:A:1239:PHE:O	16:U:508:TYR:OH	2.28	0.51
16:U:269:ARG:C	16:U:271:ALA:N	2.69	0.51
1:A:877:ALA:HB3	1:A:890:ARG:HH11	1.75	0.51
2:B:924:ARG:NH1	3:C:62:GLU:OE1	2.43	0.51
15:T:21:DC:H2''	15:T:22:DA:C8	2.45	0.51
16:U:268:THR:HG22	16:U:316:THR:HB	1.93	0.51
16:U:383:GLN:NE2	16:U:386:ARG:O	2.43	0.51
2:B:177:CYS:SG	2:B:738:THR:OG1	2.60	0.51
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.92	0.51
5:E:173:ILE:HG23	5:E:209:VAL:HG22	1.92	0.51
7:G:104:MET:HE1	7:G:157:ILE:HG13	1.92	0.51
1:A:358:ARG:NH1	15:T:16:DC:OP1	2.41	0.51
1:A:549:THR:HG21	1:A:640:LEU:HG	1.92	0.51
4:D:129:GLN:HA	4:D:132:ASP:OD2	2.11	0.51
7:G:12:LEU:HD23	7:G:65:PHE:HD2	1.75	0.51
16:U:152:SER:O	16:U:187:PRO:HD2	2.11	0.51
16:U:155:VAL:HG12	16:U:189:VAL:HB	1.91	0.51
5:E:110:MET:HE1	5:E:118:LEU:HD12	1.91	0.51
16:U:387:GLY:O	16:U:389:LYS:NZ	2.43	0.51
13:N:32:DA:P	16:U:291:ALA:CB	2.99	0.51
1:A:732:THR:O	1:A:736:THR:HG23	2.11	0.51
1:A:1311:LEU:O	1:A:1313:GLN:NE2	2.44	0.51
2:B:225:LEU:HD23	2:B:225:LEU:H	1.76	0.51
16:U:19:THR:O	16:U:24:PHE:N	2.43	0.51
1:A:537:ILE:HG13	1:A:672:ILE:HG21	1.93	0.51
1:A:890:ARG:HH21	1:A:1023:VAL:HG13	1.75	0.51
7:G:30:LEU:O	7:G:34:VAL:HG12	2.11	0.51
16:U:160:HIS:HA	16:U:192:THR:OG1	2.11	0.51
2:B:452:ASN:HD21	2:B:462:ALA:HB3	1.76	0.50
10:J:10:CYS:SG	10:J:42:ARG:NH1	2.83	0.50
1:A:62:GLN:NE2	1:A:256:PRO:O	2.43	0.50
7:G:17:TYR:HB3	7:G:25:THR:HG21	1.93	0.50
9:I:71:ASP:OD1	9:I:71:ASP:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:32:DA:H5'	13:N:33:DG:OP2	2.11	0.50
1:A:1166:LEU:O	1:A:1170:THR:HG23	2.12	0.50
9:I:23:MET:HE2	9:I:25:TYR:CE1	2.47	0.50
16:U:175:ARG:HA	16:U:179:LEU:CB	2.39	0.50
1:A:1020:LEU:HD13	1:A:1041:PHE:HE2	1.76	0.50
2:B:846:ASP:OD1	2:B:846:ASP:N	2.43	0.50
2:B:934:LYS:HZ1	2:B:942:LYS:HD3	1.76	0.50
6:F:104:ILE:O	6:F:120:VAL:HG23	2.11	0.50
8:H:64:LEU:HD13	8:H:84:ARG:HD3	1.91	0.50
9:I:65:LEU:HD11	9:I:124:THR:HG22	1.94	0.50
16:U:48:VAL:HA	16:U:214:ALA:HB3	1.93	0.50
1:A:1307:VAL:HG13	1:A:1338:THR:HG22	1.92	0.50
2:B:911:LEU:HD12	12:L:42:ARG:HD2	1.92	0.50
3:C:263:LEU:HD22	11:K:87:PHE:HD1	1.77	0.50
16:U:392:ASP:O	16:U:395:THR:OG1	2.25	0.50
3:C:69:GLY:HA3	12:L:57:ALA:HB1	1.93	0.50
3:C:88:CYS:SG	3:C:97:CYS:HB3	2.51	0.50
3:C:159:LEU:HD11	3:C:161:LEU:HD23	1.93	0.50
9:I:44:TYR:CE2	9:I:46:GLN:HB3	2.46	0.50
1:A:653:VAL:HG11	1:A:669:TYR:CZ	2.46	0.50
1:A:1058:PHE:HB3	1:A:1060:LEU:HD13	1.92	0.50
2:B:228:SER:O	2:B:405:ARG:NH1	2.43	0.50
3:C:205:LYS:HE3	3:C:213:GLU:HA	1.92	0.50
9:I:54:TYR:CZ	9:I:56:ASN:HB2	2.47	0.50
2:B:759:VAL:HG12	2:B:999:ALA:HB2	1.94	0.50
3:C:44:ILE:HG23	3:C:176:TRP:HD1	1.76	0.50
16:U:158:GLU:C	16:U:160:HIS:H	2.17	0.50
16:U:172:ASP:C	16:U:206:ALA:C	2.80	0.50
1:A:345:GLY:HA2	1:A:351:ARG:HD3	1.92	0.50
1:A:797:ARG:HG2	1:A:820:ARG:HB3	1.93	0.50
1:A:1263:ASN:ND2	16:U:515:ARG:O	2.45	0.50
2:B:794:VAL:HG12	2:B:967:ILE:HG22	1.94	0.50
4:D:70:ARG:HH21	7:G:142:GLU:HB3	1.76	0.50
9:I:61:GLU:H	9:I:61:GLU:CD	2.20	0.50
10:J:25:LEU:HD21	10:J:31:GLU:HA	1.94	0.50
13:N:26:DG:N2	15:T:3:DC:C6	2.65	0.50
16:U:226:PHE:HB3	16:U:358:TRP:HA	1.94	0.50
16:U:263:ILE:HD11	16:U:305:TRP:CZ2	2.47	0.50
16:U:360:ARG:HG2	16:U:361:LEU:H	1.77	0.50
13:N:31:DT:O3'	16:U:317:ILE:HG12	2.11	0.49
1:A:223:GLU:HG3	1:A:227:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HB	1:A:272:ASN:HD21	1.78	0.49
1:A:1277:ASP:O	16:U:511:GLN:NE2	2.32	0.49
11:K:77:THR:OG1	11:K:81:TYR:O	2.23	0.49
16:U:267:ARG:C	16:U:268:THR:HG23	2.37	0.49
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.23	0.49
7:G:7:LEU:HB2	7:G:72:TYR:CZ	2.48	0.49
7:G:59:ILE:HG12	7:G:66:VAL:HG22	1.95	0.49
8:H:6:PHE:CZ	8:H:37:MET:HG3	2.47	0.49
16:U:47:ASP:OD2	16:U:210:LYS:N	2.43	0.49
16:U:179:LEU:O	16:U:180:ARG:C	2.54	0.49
1:A:220:ARG:HH21	1:A:224:ILE:HD11	1.77	0.49
1:A:316:THR:HG21	1:A:328:ALA:HB2	1.93	0.49
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.94	0.49
2:B:937:SER:OG	2:B:938:ARG:N	2.45	0.49
1:A:891:TYR:CZ	1:A:1396:ARG:HD3	2.47	0.49
2:B:249:LYS:HE3	2:B:254:GLN:H	1.77	0.49
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.94	0.49
13:N:31:DT:H4'	16:U:268:THR:HG21	1.93	0.49
13:N:34:DA:OP1	16:U:80:ILE:CD1	2.60	0.49
15:T:4:DA:H2''	15:T:5:DA:C8	2.47	0.49
16:U:325:LYS:HD2	16:U:327:ASN:HD21	1.77	0.49
1:A:358:ARG:NE	2:B:1076:GLU:HG3	2.28	0.49
1:A:1485:GLU:HB3	6:F:78:PRO:HB3	1.94	0.49
1:A:1487:PRO:HG2	6:F:78:PRO:HA	1.95	0.49
8:H:6:PHE:HB3	8:H:60:ILE:HB	1.95	0.49
1:A:410:ASN:OD1	1:A:449:HIS:NE2	2.43	0.49
1:A:1124:LEU:HD23	1:A:1128:ILE:HG12	1.95	0.49
2:B:242:ARG:HD2	2:B:242:ARG:O	2.13	0.49
8:H:64:LEU:HB3	8:H:84:ARG:HG2	1.94	0.49
10:J:3:ILE:HD12	10:J:4:PRO:HD2	1.93	0.49
16:U:393:LYS:HA	16:U:396:ILE:HG22	1.95	0.49
1:A:1210:TRP:HD1	1:A:1281:ASP:HB2	1.77	0.49
13:N:24:DT:H2''	13:N:25:DT:C6	2.48	0.49
1:A:18:ILE:H	1:A:1462:GLN:NE2	2.11	0.49
1:A:418:TYR:HD2	1:A:426:ARG:HG2	1.77	0.49
1:A:545:VAL:HG11	1:A:645:LEU:HD12	1.94	0.49
1:A:589:LYS:HZ1	1:A:638:GLY:H	1.59	0.49
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.46	0.49
1:A:877:ALA:HB3	1:A:890:ARG:NH1	2.27	0.49
1:A:972:THR:HA	1:A:1320:ILE:HG21	1.94	0.49
1:A:1408:ARG:NH1	5:E:172:ARG:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:HA	2:B:1085:ARG:HA	1.95	0.48
1:A:530:SER:O	1:A:532:ARG:HG3	2.12	0.48
1:A:1022:ILE:N	1:A:1034:GLN:HE22	2.10	0.48
5:E:166:ARG:HH12	5:E:168:ASN:ND2	2.09	0.48
8:H:71:ASP:OD2	8:H:142:TYR:OH	2.23	0.48
1:A:481:THR:HG22	2:B:1055:VAL:HG21	1.95	0.48
3:C:40:ALA:O	3:C:170:GLY:N	2.45	0.48
7:G:152:VAL:HA	7:G:157:ILE:HA	1.94	0.48
16:U:269:ARG:HD2	16:U:269:ARG:HA	1.51	0.48
1:A:253:LEU:HD21	1:A:317:MET:HE1	1.95	0.48
1:A:528:PRO:HB3	1:A:899:GLU:HG3	1.95	0.48
2:B:1038:THR:HA	3:C:195:THR:HA	1.95	0.48
1:A:734:ARG:NH2	9:I:107:ALA:O	2.45	0.48
7:G:127:CYS:HB2	7:G:138:GLN:HA	1.95	0.48
16:U:269:ARG:O	16:U:271:ALA:N	2.46	0.48
16:U:602:LEU:O	16:U:605:VAL:HG22	2.13	0.48
16:U:12:PRO:O	16:U:15:ARG:N	2.47	0.48
16:U:541:ARG:HH22	16:U:589:ARG:HA	1.78	0.48
1:A:48:GLU:OE1	1:A:48:GLU:N	2.47	0.48
2:B:587:LEU:HB3	2:B:603:MET:SD	2.53	0.48
5:E:15:LYS:NZ	5:E:33:LEU:O	2.46	0.48
11:K:46:ILE:HG21	11:K:87:PHE:CE2	2.49	0.48
12:L:22:CYS:SG	12:L:24:THR:HG23	2.54	0.48
16:U:158:GLU:C	16:U:160:HIS:N	2.71	0.48
1:A:104:MET:SD	1:A:193:ARG:HB2	2.54	0.48
1:A:508:SER:HB3	1:A:511:THR:HG22	1.96	0.48
2:B:1118:VAL:HA	2:B:1125:MET:HA	1.95	0.48
3:C:9:VAL:HG12	3:C:23:ILE:HG12	1.96	0.48
7:G:134:ASP:OD1	7:G:134:ASP:N	2.47	0.48
1:A:276:LEU:HD11	1:A:339:LEU:HD21	1.96	0.48
1:A:811:ILE:HG22	2:B:674:MET:HE1	1.96	0.48
1:A:871:VAL:HB	1:A:1088:GLY:HA3	1.95	0.48
1:A:1016:LEU:HD21	1:A:1072:ILE:HG21	1.94	0.48
2:B:300:MET:HE1	2:B:377:LEU:HD13	1.96	0.48
2:B:1028:LEU:HD11	2:B:1043:ILE:HD11	1.96	0.48
13:N:21:DT:H2"	13:N:22:DA:C8	2.49	0.48
1:A:527:THR:HG22	1:A:532:ARG:O	2.14	0.48
2:B:534:VAL:N	2:B:600:GLU:OE2	2.46	0.48
16:U:16:VAL:HG22	16:U:60:LEU:HD13	1.95	0.48
2:B:566:LYS:HG2	2:B:573:TRP:CZ2	2.49	0.48
3:C:103:LEU:HD23	3:C:161:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:100:GLU:HG3	7:G:104:MET:O	2.14	0.48
11:K:16:GLU:OE1	11:K:16:GLU:N	2.45	0.48
13:N:29:DC:O5'	16:U:370:GLN:OE1	2.32	0.48
13:N:26:DG:H2''	13:N:27:DA:C8	2.49	0.47
16:U:172:ASP:CA	16:U:175:ARG:HB2	2.32	0.47
1:A:769:MET:HE1	2:B:969:PRO:HB2	1.96	0.47
1:A:922:PHE:HD2	1:A:1052:ARG:HA	1.79	0.47
2:B:263:ILE:HD13	2:B:325:GLY:HA2	1.95	0.47
1:A:116:LYS:HE3	1:A:182:GLY:HA3	1.96	0.47
1:A:864:LEU:O	1:A:868:MET:HG3	2.14	0.47
2:B:1111:SER:OG	2:B:1112:ASP:N	2.46	0.47
16:U:30:LYS:HB2	19:U:1000:ANP:C6	2.44	0.47
16:U:181:SER:O	16:U:182:ARG:C	2.57	0.47
1:A:589:LYS:HZ3	1:A:637:MET:HA	1.79	0.47
2:B:794:VAL:O	2:B:946:GLY:N	2.34	0.47
2:B:912:ASN:HD21	2:B:916:TYR:HB2	1.79	0.47
2:B:1119:CYS:SG	2:B:1120:ASN:N	2.87	0.47
16:U:377:LYS:O	16:U:381:LYS:HG3	2.15	0.47
1:A:369:PRO:HD3	1:A:496:PHE:CG	2.49	0.47
1:A:410:ASN:HD22	1:A:430:ARG:HG2	1.79	0.47
1:A:890:ARG:NE	1:A:1023:VAL:HG22	2.28	0.47
1:A:1177:TYR:CE1	1:A:1209:PRO:HB2	2.50	0.47
5:E:166:ARG:HH12	5:E:168:ASN:HD21	1.62	0.47
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.50	0.47
1:A:52:PRO:HB2	1:A:60:PRO:HD3	1.96	0.47
1:A:192:ARG:HH22	1:A:213:LYS:HE3	1.79	0.47
1:A:466:LYS:HB2	2:B:1097:HIS:CE1	2.49	0.47
1:A:983:LEU:HB3	1:A:1048:THR:HG21	1.96	0.47
1:A:1095:LEU:HD13	1:A:1401:LEU:HD22	1.96	0.47
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.94	0.47
2:B:567:ILE:HD13	2:B:612:ILE:HB	1.97	0.47
2:B:1115:GLN:HE21	2:B:1150:ARG:NH1	2.11	0.47
3:C:37:VAL:HG21	3:C:252:LEU:HD12	1.95	0.47
4:D:99:CYS:O	4:D:103:LEU:HB2	2.15	0.47
5:E:70:ASP:OD1	5:E:71:GLN:N	2.47	0.47
8:H:103:GLU:HB3	8:H:109:ALA:HB2	1.95	0.47
16:U:431:CYS:HB2	16:U:434:CYS:N	2.18	0.47
1:A:545:VAL:HG23	1:A:676:ILE:HG21	1.96	0.47
2:B:859:ARG:NH2	12:L:54:VAL:O	2.47	0.47
7:G:114:PRO:HB2	7:G:116:GLU:OE2	2.15	0.47
9:I:18:GLN:OE1	9:I:18:GLN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:9:DC:H2'	15:T:10:DT:H71	1.97	0.47
16:U:28:SER:OG	16:U:35:GLU:OE1	2.27	0.47
16:U:157:ASP:C	16:U:159:ALA:N	2.69	0.47
16:U:160:HIS:CE1	16:U:194:THR:HG23	2.50	0.47
16:U:181:SER:C	16:U:183:LEU:N	2.72	0.47
1:A:121:SER:O	1:A:127:LYS:NZ	2.47	0.47
1:A:513:ALA:HB2	6:F:90:LEU:HD11	1.97	0.47
1:A:680:LEU:HD23	1:A:680:LEU:O	2.14	0.47
1:A:932:ARG:NH1	8:H:107:GLU:O	2.47	0.47
8:H:84:ARG:NH1	8:H:85:ALA:O	2.48	0.47
14:P:12:A:O2'	14:P:13:G:H8	1.98	0.47
16:U:417:ALA:HB1	16:U:422:ASP:HB2	1.97	0.47
1:A:540:ASP:HB3	2:B:790:GLN:CD	2.40	0.47
1:A:555:LEU:HD21	1:A:679:TRP:HE1	1.79	0.47
2:B:245:GLN:HE22	2:B:249:LYS:HG3	1.80	0.47
9:I:24:LEU:HD23	9:I:39:CYS:HB2	1.97	0.47
13:N:35:DC:OP1	16:U:102:SER:CB	2.60	0.47
16:U:11:ASP:O	16:U:12:PRO:C	2.58	0.47
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.50	0.47
1:A:1243:LEU:HD12	1:A:1261:ILE:HA	1.96	0.47
7:G:3:TYR:HB3	7:G:76:VAL:HG23	1.96	0.47
11:K:106:ARG:O	11:K:109:ILE:HG22	2.15	0.47
1:A:1005:HIS:CD2	1:A:1007:ILE:HB	2.50	0.46
2:B:677:MET:H	2:B:682:LEU:HD22	1.79	0.46
2:B:1156:LYS:NZ	2:B:1160:GLN:OE1	2.48	0.46
13:N:31:DT:O5'	16:U:268:THR:HG21	2.15	0.46
16:U:294:LYS:O	16:U:298:ARG:HG2	2.15	0.46
16:U:551:GLU:O	16:U:555:ARG:HG3	2.15	0.46
1:A:375:ILE:HB	1:A:666:ARG:HG3	1.97	0.46
1:A:567:LEU:HB3	1:A:570:TRP:HB2	1.97	0.46
1:A:1279:MET:SD	1:A:1283:VAL:HG23	2.55	0.46
2:B:91:ILE:HG22	2:B:126:VAL:HG12	1.97	0.46
4:D:74:PHE:CE2	4:D:83:VAL:HG11	2.50	0.46
11:K:12:LEU:HD11	11:K:18:LYS:HD3	1.96	0.46
16:U:373:PHE:HE1	16:U:510:LYS:HA	1.79	0.46
16:U:613:LYS:HA	16:U:613:LYS:HD3	1.76	0.46
1:A:1357:THR:O	5:E:142:HIS:NE2	2.40	0.46
8:H:23:ASP:N	8:H:23:ASP:OD1	2.46	0.46
2:B:548:TRP:CZ2	2:B:586:THR:HG21	2.50	0.46
3:C:154:ARG:HH11	10:J:64:PRO:HD3	1.80	0.46
12:L:39:CYS:SG	12:L:41:TYR:HB2	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:15:DT:H2"	13:N:16:DG:C8	2.50	0.46
13:N:32:DA:OP2	16:U:291:ALA:CB	2.63	0.46
16:U:179:LEU:HD13	16:U:179:LEU:HA	1.72	0.46
1:A:1476:ASP:HB2	6:F:105:ILE:HG23	1.98	0.46
2:B:83:ARG:HB2	2:B:133:ILE:HB	1.97	0.46
2:B:645:GLU:O	2:B:649:ASN:HB2	2.16	0.46
5:E:55:ARG:HG2	5:E:76:PHE:HB3	1.97	0.46
7:G:10:GLU:HB3	7:G:67:LEU:HD11	1.97	0.46
8:H:57:ARG:HG3	8:H:148:LEU:HD11	1.97	0.46
1:A:273:GLN:HB3	1:A:277:THR:HB	1.97	0.46
1:A:763:TYR:OH	8:H:23:ASP:OD2	2.25	0.46
2:B:92:TYR:N	2:B:125:TYR:O	2.47	0.46
8:H:79:ASP:O	8:H:82:PRO:HD2	2.16	0.46
1:A:525:ILE:HA	1:A:535:MET:HE3	1.97	0.46
8:H:115:TYR:CE1	8:H:124:ARG:HD3	2.50	0.46
14:P:14:A:H2'	14:P:15:C:C6	2.49	0.46
16:U:146:VAL:HG22	16:U:183:LEU:HD13	1.97	0.46
16:U:360:ARG:NH1	16:U:362:TYR:OH	2.49	0.46
1:A:1229:GLU:OE1	1:A:1229:GLU:N	2.35	0.46
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	1.97	0.46
7:G:82:GLY:O	7:G:146:LYS:NZ	2.41	0.46
7:G:120:ASP:N	7:G:120:ASP:OD1	2.46	0.46
16:U:550:ARG:NE	16:U:584:GLU:OE2	2.47	0.46
1:A:1292:MET:O	1:A:1296:MET:HB2	2.16	0.46
4:D:90:LYS:HA	4:D:90:LYS:HD2	1.80	0.46
16:U:300:LEU:O	16:U:301:VAL:C	2.58	0.46
1:A:266:MET:HE3	1:A:266:MET:HA	1.97	0.46
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.98	0.46
1:A:540:ASP:HB3	2:B:790:GLN:OE1	2.16	0.46
1:A:1172:ASN:ND2	1:A:1215:GLU:OE1	2.45	0.46
3:C:260:GLN:HE22	11:K:88:THR:HG23	1.81	0.46
8:H:36:LYS:HA	8:H:36:LYS:HD3	1.64	0.46
1:A:274:ASP:OD1	1:A:275:ASP:N	2.49	0.45
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.50	0.45
2:B:59:VAL:HG21	2:B:91:ILE:HG23	1.97	0.45
2:B:1162:LEU:HD22	2:B:1167:ILE:HD12	1.98	0.45
3:C:110:ASP:HA	3:C:155:LYS:HB2	1.98	0.45
8:H:28:LEU:N	8:H:41:LEU:O	2.45	0.45
13:N:25:DT:H2"	13:N:26:DG:C8	2.51	0.45
1:A:73:THR:OG1	1:A:84:HIS:NE2	2.45	0.45
1:A:338:SER:H	1:A:341:GLN:NE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:THR:HA	2:B:143:GLN:HA	1.98	0.45
2:B:269:ILE:HD12	2:B:269:ILE:HA	1.85	0.45
2:B:817:GLN:OE1	2:B:912:ASN:ND2	2.46	0.45
7:G:3:TYR:HD1	7:G:4:HIS:H	1.63	0.45
8:H:34:SER:OG	8:H:35:PHE:N	2.48	0.45
16:U:79:LEU:HB2	16:U:321:MET:CE	2.39	0.45
16:U:535:LYS:HB3	16:U:585:HIS:ND1	2.31	0.45
1:A:381:PRO:HB3	1:A:480:SER:HA	1.98	0.45
1:A:489:THR:HG23	1:A:494:ALA:O	2.16	0.45
1:A:945:ASN:HB3	1:A:948:ILE:HG12	1.99	0.45
1:A:1207:ILE:HD11	1:A:1260:ARG:HD2	1.97	0.45
1:A:1471:PHE:CE2	6:F:64:ARG:HD3	2.52	0.45
2:B:861:SER:N	2:B:864:ASP:OD2	2.39	0.45
9:I:35:LEU:HD12	9:I:36:LEU:N	2.31	0.45
9:I:106:ASP:OD1	9:I:106:ASP:N	2.43	0.45
16:U:373:PHE:HZ	16:U:509:GLN:HB3	1.81	0.45
1:A:353:ASN:O	1:A:357:LYS:HE2	2.16	0.45
1:A:685:HIS:NE2	1:A:769:MET:HE3	2.32	0.45
1:A:1405:MET:HA	1:A:1412:MET:HE2	1.97	0.45
2:B:540:PRO:HB2	2:B:596:ILE:HG23	1.97	0.45
2:B:783:ALA:HB2	2:B:1041:ILE:HG23	1.97	0.45
5:E:60:VAL:O	5:E:74:VAL:N	2.35	0.45
13:N:26:DG:N1	15:T:3:DC:C4	2.61	0.45
13:N:30:DT:C6	16:U:374:LEU:HD21	2.52	0.45
1:A:910:LYS:H	1:A:967:ARG:HH12	1.62	0.45
2:B:125:TYR:HB3	2:B:146:LYS:HA	1.98	0.45
3:C:18:ASN:OD1	3:C:19:VAL:N	2.49	0.45
3:C:74:ILE:O	3:C:127:VAL:HG12	2.16	0.45
4:D:32:LEU:HD22	7:G:4:HIS:HB2	1.97	0.45
4:D:37:VAL:HG21	7:G:2:PHE:HD2	1.81	0.45
8:H:84:ARG:HD2	8:H:85:ALA:N	2.32	0.45
16:U:156:VAL:HG22	16:U:159:ALA:HB2	1.97	0.45
16:U:285:ASN:ND2	16:U:310:VAL:HG12	2.31	0.45
16:U:499:ALA:HA	16:U:502:ARG:HE	1.80	0.45
16:U:553:CYS:HB3	16:U:601:VAL:HG11	1.98	0.45
1:A:597:PRO:HD3	1:A:668:PHE:CD1	2.52	0.45
2:B:761:THR:HG23	2:B:1000:THR:HA	1.99	0.45
16:U:391:SER:O	16:U:395:THR:HG23	2.17	0.45
2:B:1117:HIS:NE2	2:B:1148:LEU:HD12	2.32	0.45
3:C:78:ILE:HD11	3:C:127:VAL:HG13	1.99	0.45
7:G:77:PHE:CE2	7:G:104:MET:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:152:VAL:HG13	7:G:157:ILE:HG22	1.98	0.45
8:H:114:ALA:HB3	8:H:125:LEU:HB3	1.97	0.45
9:I:117:PRO:HB2	9:I:118:HIS:CE1	2.52	0.45
13:N:33:DG:C2'	13:N:34:DA:O5'	2.55	0.45
1:A:950:ASN:HB3	1:A:954:ARG:HH21	1.82	0.45
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.98	0.45
1:A:1166:LEU:HD13	1:A:1298:LEU:HD11	1.98	0.45
2:B:33:TYR:HD1	2:B:653:TRP:CE2	2.34	0.45
2:B:197:GLN:NE2	2:B:466:VAL:HB	2.32	0.45
2:B:297:MET:O	2:B:301:VAL:HG12	2.17	0.45
2:B:451:GLY:HA2	2:B:467:SER:OG	2.17	0.45
7:G:151:ARG:O	7:G:158:PHE:N	2.35	0.45
16:U:55:GLY:CA	19:U:1000:ANP:C8	2.91	0.45
16:U:74:ILE:HD11	16:U:151:LEU:HD13	1.99	0.45
16:U:604:LYS:HE3	16:U:604:LYS:HB3	1.30	0.45
1:A:487:SER:OG	1:A:673:GLN:NE2	2.50	0.45
2:B:83:ARG:HH21	2:B:85:LEU:HD21	1.82	0.45
2:B:1101:GLN:HE22	6:F:64:ARG:HG3	1.81	0.45
11:K:100:LEU:HG	11:K:104:ARG:HD2	1.99	0.45
16:U:300:LEU:HA	16:U:303:ASN:ND2	2.32	0.45
1:A:64:VAL:HG13	1:A:78:MET:HE2	1.99	0.45
1:A:383:SER:HG	11:K:2:ASN:HD21	1.62	0.45
2:B:251:ALA:HB3	2:B:254:GLN:NE2	2.31	0.45
2:B:721:ARG:HH11	2:B:975:ARG:HB2	1.82	0.45
2:B:1021:HIS:CD2	2:B:1025:ASN:HB2	2.51	0.45
13:N:31:DT:O5'	16:U:268:THR:CG2	2.65	0.45
16:U:239:TYR:CE2	16:U:278:GLU:OE2	2.69	0.45
16:U:279:LEU:HD13	16:U:284:VAL:HG11	1.99	0.45
16:U:511:GLN:O	16:U:515:ARG:NH1	2.50	0.45
16:U:548:LYS:HZ3	16:U:548:LYS:H	1.64	0.45
1:A:827:TYR:OH	1:A:839:HIS:NE2	2.30	0.44
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	1.97	0.44
1:A:1146:GLN:HE21	1:A:1150:ASP:HB2	1.82	0.44
2:B:192:LYS:NZ	2:B:449:ALA:O	2.50	0.44
4:D:60:VAL:HA	4:D:63:LYS:HZ1	1.81	0.44
16:U:172:ASP:O	16:U:176:LEU:HD12	2.17	0.44
16:U:264:VAL:HG13	16:U:314:VAL:HG13	1.99	0.44
1:A:27:SER:HB3	1:A:247:TRP:CE2	2.52	0.44
1:A:631:GLU:HG2	1:A:988:TRP:CZ2	2.52	0.44
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.99	0.44
1:A:777:SER:N	1:A:780:ASN:HD22	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	1.98	0.44
7:G:73:LYS:HZ3	7:G:73:LYS:HB3	1.81	0.44
7:G:104:MET:HA	7:G:104:MET:HE2	1.99	0.44
13:N:34:DA:H2''	13:N:35:DC:H5''	1.99	0.44
16:U:41:VAL:CG2	16:U:61:CYS:SG	2.99	0.44
16:U:58:LYS:O	16:U:60:LEU:N	2.51	0.44
1:A:370:ASP:HB2	1:A:483:ARG:HB3	1.99	0.44
1:A:1133:LYS:HE2	1:A:1133:LYS:HB3	1.75	0.44
2:B:55:VAL:HG12	2:B:91:ILE:HG21	1.98	0.44
8:H:10:PHE:CE2	8:H:32:SER:HB2	2.53	0.44
15:T:1:DC:H2''	15:T:2:DT:C5	2.53	0.44
1:A:499:ASP:OD1	14:P:20:C:O2'	2.21	0.44
1:A:1175:ILE:HD12	1:A:1286:ARG:HE	1.82	0.44
2:B:452:ASN:ND2	2:B:462:ALA:HB3	2.32	0.44
2:B:626:LEU:HD23	2:B:662:VAL:HG22	1.99	0.44
2:B:674:MET:HE3	2:B:690:CYS:SG	2.57	0.44
2:B:757:PRO:HA	2:B:777:ASN:HD21	1.82	0.44
6:F:75:MET:HE3	7:G:15:PRO:HG2	2.00	0.44
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	2.00	0.44
6:F:105:ILE:HA	6:F:119:GLY:HA2	1.99	0.44
16:U:30:LYS:HG3	19:U:1000:ANP:C2	2.47	0.44
16:U:393:LYS:O	16:U:397:MET:SD	2.75	0.44
1:A:146:ASP:HA	1:A:149:LYS:HE3	2.00	0.44
1:A:1394:ASN:OD1	1:A:1396:ARG:NH1	2.37	0.44
2:B:98:HIS:HB2	2:B:108:MET:HE2	2.00	0.44
2:B:388:TYR:H	2:B:504:THR:HG21	1.83	0.44
2:B:735:VAL:HG23	2:B:754:PRO:HG2	2.00	0.44
3:C:154:ARG:NE	10:J:60:LEU:O	2.43	0.44
13:N:35:DC:H3'	13:N:36:DA:H3'	1.99	0.44
16:U:197:PRO:O	16:U:200:GLN:NE2	2.51	0.44
1:A:1210:TRP:CZ3	9:I:53:ILE:HD11	2.53	0.44
2:B:371:ARG:HE	2:B:371:ARG:HB3	1.70	0.44
2:B:759:VAL:HG13	2:B:986:GLN:HG2	1.98	0.44
3:C:92:GLU:HB3	3:C:93:PHE:H	1.64	0.44
8:H:60:ILE:HG23	8:H:141:VAL:HG13	2.00	0.44
13:N:26:DG:C6	15:T:3:DC:N4	2.71	0.44
16:U:393:LYS:O	16:U:396:ILE:HG22	2.17	0.44
1:A:139:LYS:HA	1:A:142:THR:HG22	1.98	0.44
1:A:406:VAL:HG21	1:A:440:LEU:HD11	1.99	0.44
3:C:43:PRO:HB3	3:C:167:LYS:HE3	2.00	0.44
3:C:47:ILE:HA	3:C:165:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.99	0.44
14:P:16:C:H2'	14:P:17:A:H8	1.81	0.44
1:A:550:LYS:HB3	1:A:550:LYS:HE3	1.82	0.44
2:B:201:ALA:HB3	2:B:206:TYR:OH	2.17	0.44
3:C:263:LEU:HD22	11:K:87:PHE:CD1	2.53	0.44
9:I:89:CYS:SG	9:I:91:HIS:HB2	2.58	0.44
11:K:45:ILE:HD12	11:K:45:ILE:HA	1.86	0.44
12:L:56:ASP:OD1	12:L:56:ASP:C	2.60	0.44
16:U:101:ASN:HD21	16:U:104:LEU:HD13	1.83	0.44
16:U:243:LYS:HA	16:U:246:CYS:SG	2.57	0.44
16:U:334:TRP:HA	16:U:362:TYR:HB2	2.00	0.44
16:U:350:ALA:HB1	16:U:357:SER:HB3	1.99	0.44
1:A:459:ASN:ND2	2:B:1090:GLU:OE1	2.32	0.43
2:B:40:VAL:HG11	2:B:482:LEU:HD13	1.99	0.43
2:B:236:TRP:HB2	2:B:259:THR:HB	1.99	0.43
2:B:344:GLN:NE2	2:B:355:ASP:H	2.15	0.43
5:E:3:ASP:OD2	5:E:49:SER:OG	2.21	0.43
5:E:106:VAL:HG21	5:E:110:MET:HG3	2.00	0.43
16:U:60:LEU:HG	16:U:61:CYS:N	2.33	0.43
1:A:254:PRO:HB2	2:B:1164:SER:HA	2.00	0.43
1:A:266:MET:HE1	14:P:10:A:C2	2.54	0.43
1:A:484:LEU:HD12	1:A:488:VAL:HG12	2.00	0.43
2:B:153:PRO:HG2	2:B:448:LEU:HD12	2.00	0.43
2:B:294:ASP:O	2:B:298:MET:HG3	2.17	0.43
2:B:653:TRP:CH2	2:B:662:VAL:HG11	2.53	0.43
2:B:901:THR:O	2:B:901:THR:OG1	2.35	0.43
16:U:327:ASN:O	16:U:328:VAL:C	2.61	0.43
1:A:416:ALA:HA	1:A:448:ARG:HA	2.01	0.43
1:A:548:PHE:HB2	1:A:679:TRP:CZ3	2.53	0.43
1:A:556:GLU:OE1	1:A:583:ARG:NH2	2.47	0.43
1:A:764:ASN:HD21	1:A:766:PHE:HB2	1.83	0.43
2:B:403:LEU:HD21	2:B:447:SER:CB	2.48	0.43
3:C:38:PHE:CE1	3:C:245:VAL:HG23	2.53	0.43
4:D:37:VAL:HG11	7:G:2:PHE:HD2	1.83	0.43
8:H:81:ARG:HG3	8:H:82:PRO:HD3	2.01	0.43
11:K:56:VAL:HG11	11:K:59:ALA:HB2	2.01	0.43
16:U:159:ALA:N	16:U:191:LEU:O	2.51	0.43
1:A:335:PRO:HD3	2:B:460:HIS:CE1	2.54	0.43
1:A:1155:LYS:HE2	1:A:1155:LYS:HB2	1.82	0.43
1:A:1411:LEU:HD12	1:A:1411:LEU:HA	1.70	0.43
2:B:28:ILE:HD13	2:B:644:LYS:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:ALA:O	2:B:500:GLN:HG3	2.18	0.43
3:C:103:LEU:HB3	3:C:161:LEU:HG	1.99	0.43
4:D:106:GLU:HA	4:D:135:GLN:NE2	2.33	0.43
5:E:192:LYS:HE3	5:E:204:ILE:HD13	2.01	0.43
7:G:54:ILE:HD13	7:G:70:VAL:HG12	1.99	0.43
10:J:65:LEU:O	12:L:23:HIS:ND1	2.51	0.43
13:N:20:DG:C8	13:N:21:DT:H72	2.54	0.43
2:B:214:LYS:HE2	2:B:215:TYR:CE1	2.53	0.43
4:D:93:HIS:CD2	4:D:95:PHE:HB3	2.53	0.43
5:E:98:ASN:OD1	5:E:98:ASN:C	2.61	0.43
9:I:111:TYR:HD1	9:I:124:THR:HB	1.83	0.43
16:U:246:CYS:SG	16:U:284:VAL:HG21	2.58	0.43
16:U:331:VAL:HG23	16:U:350:ALA:HB2	2.00	0.43
16:U:565:ARG:HG3	16:U:566:GLN:HE22	1.83	0.43
1:A:85:PHE:CZ	2:B:1163:MET:HB2	2.53	0.43
1:A:488:VAL:O	1:A:491:PRO:HD2	2.19	0.43
1:A:589:LYS:HE2	1:A:638:GLY:O	2.18	0.43
1:A:637:MET:HB3	8:H:122:LEU:HD21	1.99	0.43
2:B:148:PHE:CD2	2:B:437:THR:HG21	2.53	0.43
5:E:92:GLN:OE1	5:E:95:GLN:NE2	2.48	0.43
7:G:3:TYR:N	7:G:76:VAL:O	2.41	0.43
8:H:106:THR:OG1	8:H:107:GLU:N	2.51	0.43
1:A:1283:VAL:HA	1:A:1286:ARG:HB2	1.99	0.43
1:A:1309:MET:HE3	1:A:1334:TRP:CD2	2.54	0.43
2:B:180:ASP:OD2	2:B:184:TYR:OH	2.34	0.43
2:B:556:ILE:HD12	2:B:556:ILE:HA	1.82	0.43
2:B:907:VAL:HG22	2:B:921:ILE:HG12	2.01	0.43
16:U:154:LEU:N	16:U:186:ALA:HB1	2.33	0.43
16:U:172:ASP:C	16:U:207:LEU:HA	2.43	0.43
16:U:286:ALA:HA	16:U:312:VAL:O	2.19	0.43
1:A:244:ARG:HE	1:A:246:GLU:CD	2.27	0.43
1:A:421:ARG:HB2	1:A:425:ASP:OD1	2.19	0.43
1:A:626:THR:OG1	1:A:627:LYS:N	2.49	0.43
1:A:983:LEU:HD23	1:A:1044:HIS:CD2	2.53	0.43
3:C:37:VAL:O	3:C:42:VAL:HG23	2.19	0.43
11:K:70:LYS:HB2	11:K:70:LYS:HE2	1.79	0.43
16:U:157:ASP:O	16:U:159:ALA:N	2.51	0.43
1:A:592:PHE:HA	1:A:595:ILE:HD12	1.99	0.43
1:A:1144:LEU:HG	1:A:1353:ASP:HA	1.99	0.43
1:A:1206:ARG:NH2	1:A:1265:ASP:OD2	2.52	0.43
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:242:GLU:HG2	3:C:243:THR:N	2.34	0.43
5:E:92:GLN:O	5:E:95:GLN:HG3	2.18	0.43
8:H:97:TYR:CD2	8:H:98:ARG:HG2	2.53	0.43
16:U:138:PHE:O	16:U:142:LEU:N	2.40	0.43
16:U:336:ILE:HA	16:U:361:LEU:HD11	2.01	0.43
1:A:575:PRO:HG3	1:A:594:LEU:HD11	2.01	0.43
1:A:823:VAL:HG11	1:A:831:LEU:HD22	2.00	0.43
2:B:251:ALA:HB3	2:B:254:GLN:HE22	1.84	0.43
2:B:414:GLU:OE1	2:B:436:LYS:HD2	2.19	0.43
2:B:528:LEU:HD23	2:B:528:LEU:HA	1.83	0.43
2:B:820:LYS:HD2	2:B:826:GLU:HB2	2.00	0.43
2:B:1062:ARG:NE	2:B:1065:GLY:H	2.17	0.43
6:F:51:ARG:HA	6:F:116:GLU:OE1	2.18	0.43
6:F:90:LEU:HD12	6:F:90:LEU:HA	1.80	0.43
16:U:196:THR:HG21	16:U:419:TYR:CE1	2.54	0.43
16:U:536:GLU:HG2	16:U:585:HIS:CE1	2.49	0.43
2:B:67:LEU:HD12	2:B:84:TYR:HB2	2.01	0.42
2:B:240:LEU:O	2:B:249:LYS:NZ	2.40	0.42
2:B:589:LYS:O	2:B:593:GLN:HG2	2.20	0.42
7:G:10:GLU:OE1	7:G:10:GLU:HA	2.19	0.42
11:K:60:GLY:O	11:K:73:ILE:HG23	2.19	0.42
16:U:75:VAL:N	16:U:126:LEU:O	2.42	0.42
16:U:183:LEU:HD13	16:U:183:LEU:HA	1.76	0.42
16:U:332:ALA:HA	16:U:360:ARG:H	1.83	0.42
16:U:535:LYS:HE3	16:U:535:LYS:HB2	1.71	0.42
16:U:606:ALA:O	16:U:607:ASP:C	2.61	0.42
1:A:73:THR:HG1	1:A:84:HIS:CE1	2.37	0.42
2:B:896:LEU:HD23	2:B:896:LEU:HA	1.86	0.42
13:N:26:DG:N1	15:T:3:DC:H5	2.05	0.42
16:U:331:VAL:HG11	16:U:346:GLU:O	2.19	0.42
16:U:565:ARG:HG3	16:U:566:GLN:NE2	2.35	0.42
1:A:509:LEU:HD21	6:F:89:PRO:HG2	2.01	0.42
1:A:1173:THR:OG1	1:A:1214:VAL:HG12	2.19	0.42
3:C:106:ARG:HB2	3:C:158:GLU:HG3	2.01	0.42
3:C:189:ASP:OD1	3:C:189:ASP:N	2.41	0.42
4:D:76:ASN:HB3	4:D:79:THR:HB	2.01	0.42
6:F:61:GLU:OE2	6:F:108:ARG:NE	2.35	0.42
16:U:161:CYS:O	16:U:164:GLN:N	2.52	0.42
1:A:908:THR:HG23	1:A:916:PHE:HE1	1.83	0.42
1:A:1021:VAL:HA	1:A:1034:GLN:HE22	1.83	0.42
1:A:1026:ASP:O	1:A:1031:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1468:THR:H	6:F:60:TYR:HB3	1.84	0.42
2:B:56:GLN:HE22	2:B:90:GLN:HA	1.85	0.42
2:B:230:ARG:NE	2:B:231:PRO:HD2	2.35	0.42
2:B:856:PRO:HG2	12:L:48:ARG:HA	2.01	0.42
2:B:941:GLN:NE2	2:B:977:THR:OG1	2.51	0.42
3:C:234:GLU:OE1	10:J:42:ARG:NH2	2.48	0.42
6:F:88:ASP:C	6:F:88:ASP:OD1	2.61	0.42
7:G:8:GLU:OE1	7:G:8:GLU:HA	2.19	0.42
11:K:14:GLU:OE1	11:K:14:GLU:HA	2.19	0.42
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.54	0.42
13:N:27:DA:H2''	13:N:28:DG:C8	2.54	0.42
16:U:191:LEU:HD13	16:U:191:LEU:HA	1.85	0.42
1:A:112:PHE:H	1:A:188:GLN:NE2	2.13	0.42
1:A:319:ASP:OD1	1:A:319:ASP:C	2.62	0.42
1:A:788:VAL:HG23	1:A:826:SER:HA	2.00	0.42
4:D:135:GLN:HG2	4:D:138:ARG:NH2	2.34	0.42
5:E:85:LYS:O	5:E:89:VAL:HG13	2.19	0.42
6:F:112:ASP:OD1	6:F:112:ASP:C	2.62	0.42
14:P:13:G:H2'	14:P:14:A:H8	1.81	0.42
16:U:235:ILE:HD13	16:U:241:ASN:HD22	1.85	0.42
16:U:383:GLN:NE2	16:U:383:GLN:O	2.47	0.42
1:A:548:PHE:O	1:A:553:VAL:HG11	2.20	0.42
1:A:1097:GLU:OE2	1:A:1101:GLN:NE2	2.49	0.42
1:A:1463:LEU:HD22	7:G:61:PRO:HB3	2.02	0.42
2:B:242:ARG:HH12	2:B:250:SER:HA	1.84	0.42
9:I:59:THR:O	9:I:60:HIS:ND1	2.53	0.42
16:U:261:CYS:O	16:U:329:ARG:N	2.41	0.42
1:A:497:ASP:N	1:A:497:ASP:OD1	2.51	0.42
1:A:576:GLN:NE2	8:H:142:TYR:OH	2.37	0.42
1:A:992:LYS:HA	1:A:992:LYS:HD3	1.71	0.42
1:A:1250:ASP:HB2	1:A:1251:ASN:H	1.51	0.42
2:B:163:LEU:HA	2:B:166:LEU:HD12	2.01	0.42
2:B:403:LEU:HD22	2:B:453:TRP:CZ2	2.55	0.42
7:G:52:ASP:OD1	7:G:52:ASP:C	2.62	0.42
11:K:39:ASP:O	11:K:71:ILE:HD11	2.20	0.42
16:U:97:VAL:HG23	16:U:125:ILE:HB	2.01	0.42
16:U:160:HIS:O	16:U:161:CYS:C	2.63	0.42
16:U:585:HIS:HD2	16:U:589:ARG:HH21	1.68	0.42
2:B:193:VAL:O	2:B:467:SER:HA	2.19	0.42
2:B:1075:MET:HE3	2:B:1075:MET:HB3	1.89	0.42
9:I:83:ASP:OD1	9:I:83:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:12:PRO:O	16:U:14:ARG:N	2.53	0.42
16:U:55:GLY:HA2	19:U:1000:ANP:C8	2.33	0.42
1:A:486:LEU:HD13	2:B:790:GLN:NE2	2.35	0.42
1:A:1048:THR:HA	1:A:1053:ARG:HH21	1.85	0.42
1:A:1216:LEU:HB2	1:A:1255:LEU:HB3	2.01	0.42
2:B:789:ASN:O	2:B:968:ASN:HB2	2.18	0.42
2:B:863:ASP:OD1	2:B:863:ASP:C	2.63	0.42
2:B:957:THR:HG22	2:B:958:CYS:H	1.85	0.42
5:E:104:ILE:HD13	5:E:104:ILE:HA	1.90	0.42
7:G:129:LYS:HD3	7:G:136:VAL:HG13	2.02	0.42
9:I:17:CYS:O	9:I:21:ASN:HA	2.20	0.42
16:U:413:HIS:HA	16:U:416:ILE:HG22	2.02	0.42
16:U:594:ALA:O	16:U:598:LYS:HG3	2.20	0.42
1:A:883:ILE:HD11	1:A:1424:THR:HG22	2.01	0.42
1:A:999:ARG:NH2	8:H:103:GLU:OE2	2.51	0.42
2:B:725:GLN:HE22	2:B:1049:GLN:HE22	1.68	0.42
5:E:11:TRP:NE1	5:E:35:GLN:O	2.44	0.42
5:E:118:LEU:HD23	5:E:118:LEU:HA	1.82	0.42
16:U:204:PHE:CD1	16:U:209:LEU:HD12	2.55	0.42
1:A:557:ARG:O	1:A:561:MET:HG2	2.20	0.41
1:A:1463:LEU:HD12	1:A:1463:LEU:HA	1.80	0.41
2:B:427:LYS:HG3	2:B:428:ASP:H	1.85	0.41
2:B:628:VAL:HG22	2:B:633:LEU:HD23	2.01	0.41
8:H:59:VAL:HG21	8:H:88:PHE:CZ	2.54	0.41
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.55	0.41
1:A:780:ASN:HA	2:B:976:MET:HE1	2.02	0.41
2:B:19:PRO:C	2:B:21:LEU:H	2.29	0.41
2:B:526:LEU:HD23	2:B:526:LEU:HA	1.93	0.41
16:U:365:ARG:H	16:U:365:ARG:HG2	1.67	0.41
16:U:404:THR:O	16:U:408:GLU:HB3	2.20	0.41
1:A:114:CYS:O	1:A:115:SER:OG	2.36	0.41
1:A:147:LEU:HD23	1:A:147:LEU:C	2.45	0.41
1:A:1202:PHE:HZ	1:A:1266:GLU:HA	1.85	0.41
1:A:1474:LEU:HB2	6:F:105:ILE:HG13	2.02	0.41
2:B:445:LYS:HE3	2:B:445:LYS:HB2	1.77	0.41
2:B:509:VAL:HG11	2:B:524:LYS:HB3	2.03	0.41
2:B:556:ILE:HD11	2:B:576:ILE:HD11	2.03	0.41
11:K:57:LEU:N	11:K:76:GLN:O	2.51	0.41
15:T:18:DG:H2''	15:T:19:DG:H5'	2.01	0.41
16:U:262:GLY:HA3	16:U:330:PHE:CE1	2.54	0.41
16:U:593:VAL:HG23	16:U:596:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:PHE:CE2	1:A:808:PRO:HD3	2.56	0.41
1:A:904:GLN:NE2	1:A:981:CYS:O	2.53	0.41
1:A:948:ILE:HG23	1:A:1007:ILE:CG1	2.51	0.41
1:A:1228:MET:HE1	1:A:1255:LEU:CA	2.50	0.41
2:B:113:ALA:HA	2:B:118:LEU:HB2	2.02	0.41
2:B:117:ASN:HA	2:B:189:GLY:HA3	2.02	0.41
2:B:157:ARG:NH1	2:B:180:ASP:O	2.53	0.41
2:B:276:LEU:HD21	2:B:343:LEU:HD12	2.01	0.41
2:B:485:LEU:N	2:B:524:LYS:O	2.42	0.41
2:B:956:PHE:CE2	3:C:184:PHE:HB3	2.56	0.41
3:C:60:HIS:CD2	3:C:60:HIS:H	2.38	0.41
5:E:101:ARG:NE	5:E:126:ILE:HD11	2.35	0.41
16:U:296:SER:O	16:U:297:GLU:C	2.63	0.41
16:U:298:ARG:O	16:U:299:THR:C	2.62	0.41
16:U:602:LEU:HD13	16:U:602:LEU:HA	1.87	0.41
1:A:225:PHE:HB3	1:A:245:PRO:HB2	2.02	0.41
1:A:455:ILE:HB	1:A:512:ARG:HG3	2.02	0.41
1:A:690:GLY:HA2	1:A:693:ILE:HD11	2.03	0.41
1:A:1318:LYS:HD2	1:A:1330:ALA:HB1	2.02	0.41
1:A:1468:THR:O	6:F:64:ARG:HD2	2.21	0.41
2:B:309:PHE:CD1	2:B:309:PHE:C	2.98	0.41
4:D:20:LEU:HD12	4:D:20:LEU:HA	1.79	0.41
4:D:23:PRO:HG2	4:D:26:PHE:CE2	2.55	0.41
7:G:6:SER:HB2	7:G:73:LYS:HD2	2.01	0.41
7:G:13:LEU:HD11	7:G:26:VAL:HG22	2.03	0.41
7:G:110:ARG:NH2	7:G:113:ILE:HG21	2.36	0.41
12:L:17:TYR:HB3	12:L:44:MET:HE2	2.02	0.41
1:A:112:PHE:HZ	1:A:216:LEU:HD13	1.85	0.41
1:A:367:ILE:HG21	1:A:501:MET:HG3	2.01	0.41
1:A:369:PRO:CB	1:A:486:LEU:HD21	2.50	0.41
1:A:1466:ALA:O	1:A:1470:CYS:N	2.53	0.41
2:B:782:ILE:HG12	2:B:967:ILE:HD11	2.02	0.41
6:F:84:GLU:OE1	6:F:95:LYS:NZ	2.51	0.41
16:U:102:SER:N	16:U:132:MET:HE1	2.36	0.41
16:U:204:PHE:HD1	16:U:209:LEU:HD12	1.85	0.41
16:U:438:THR:HG22	16:U:441:ARG:HH22	1.86	0.41
1:A:36:VAL:HG21	1:A:73:THR:HG21	2.02	0.41
1:A:458:PHE:HE2	1:A:484:LEU:HD13	1.86	0.41
1:A:495:ASP:OD1	1:A:495:ASP:N	2.53	0.41
6:F:81:VAL:HG22	6:F:82:GLU:OE2	2.21	0.41
16:U:409:LEU:HG	16:U:444:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ASP:HA	2:B:970:HIS:CE1	2.56	0.41
1:A:604:ARG:HB2	1:A:628:VAL:HB	2.02	0.41
2:B:130:LYS:NZ	2:B:429:PHE:O	2.54	0.41
2:B:515:PRO:HG3	2:B:523:VAL:HB	2.02	0.41
2:B:737:ILE:HD12	2:B:737:ILE:HA	1.93	0.41
9:I:43:ASP:C	9:I:43:ASP:OD1	2.63	0.41
10:J:56:ILE:HD12	10:J:56:ILE:HA	1.79	0.41
16:U:187:PRO:O	16:U:188:CYS:HB3	2.19	0.41
16:U:287:LYS:HD3	16:U:287:LYS:HA	1.75	0.41
1:A:279:LYS:HD2	1:A:279:LYS:HA	1.96	0.41
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.61	0.41
1:A:1038:THR:O	1:A:1038:THR:HG22	2.20	0.41
1:A:1097:GLU:HB3	1:A:1098:PRO:HD3	2.02	0.41
1:A:1324:GLU:OE2	1:A:1324:GLU:HA	2.21	0.41
1:A:1435:THR:OG1	1:A:1436:VAL:N	2.50	0.41
2:B:92:TYR:HB2	2:B:125:TYR:HB2	2.03	0.41
2:B:108:MET:HE2	2:B:108:MET:HB2	1.93	0.41
2:B:484:ARG:HG3	2:B:525:ASN:HD22	1.84	0.41
2:B:897:ARG:O	2:B:900:GLU:HG2	2.20	0.41
4:D:87:LEU:HB3	4:D:97:LEU:HD11	2.03	0.41
5:E:185:ILE:HG22	5:E:209:VAL:HG11	2.02	0.41
6:F:74:ALA:HB2	6:F:89:PRO:HG3	2.01	0.41
7:G:144:ARG:HB2	7:G:169:GLY:H	1.86	0.41
8:H:75:TYR:CZ	8:H:77:PRO:HG3	2.56	0.41
8:H:98:ARG:HG3	8:H:115:TYR:CD2	2.56	0.41
9:I:23:MET:HE2	9:I:25:TYR:CD1	2.54	0.41
11:K:110:LYS:HB2	11:K:110:LYS:HE2	1.90	0.41
16:U:289:TYR:CD1	16:U:319:PHE:HE1	2.39	0.41
1:A:220:ARG:HA	1:A:220:ARG:HD2	1.70	0.41
1:A:384:ILE:HG12	2:B:1061:SER:HB3	2.03	0.41
1:A:410:ASN:ND2	1:A:430:ARG:HG2	2.36	0.41
1:A:686:THR:HG21	2:B:1040:GLN:O	2.21	0.41
1:A:901:VAL:HG12	1:A:980:PRO:HA	2.03	0.41
2:B:1144:THR:OG1	2:B:1145:GLN:N	2.54	0.41
4:D:104:CYS:HB2	4:D:138:ARG:HH12	1.86	0.41
6:F:57:MET:HE1	6:F:125:ILE:HD12	2.02	0.41
9:I:18:GLN:NE2	9:I:44:TYR:OH	2.51	0.41
16:U:12:PRO:O	16:U:13:GLU:C	2.61	0.41
16:U:506:LEU:O	16:U:510:LYS:HG2	2.21	0.41
1:A:1131:SER:OG	13:N:20:DG:OP1	2.23	0.40
1:A:1193:VAL:HG13	1:A:1197:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:LYS:HD3	2:B:394:ASP:OD2	2.21	0.40
2:B:393:LEU:HD13	2:B:485:LEU:HD22	2.03	0.40
3:C:82:LEU:HD23	3:C:82:LEU:HA	1.86	0.40
4:D:128:GLN:O	4:D:131:LEU:HG	2.22	0.40
10:J:48:MET:O	10:J:52:HIS:HB2	2.21	0.40
10:J:53:VAL:HG13	10:J:55:LEU:HD12	2.02	0.40
11:K:13:PHE:N	11:K:16:GLU:OE2	2.54	0.40
16:U:345:GLN:HE21	16:U:349:ARG:NH2	2.19	0.40
16:U:373:PHE:CE1	16:U:510:LYS:HA	2.55	0.40
1:A:577:PRO:HB3	1:A:586:TRP:CD2	2.56	0.40
1:A:1372:GLU:OE1	5:E:195:ARG:NH1	2.54	0.40
2:B:249:LYS:HD2	2:B:255:ARG:HB3	2.03	0.40
2:B:399:LEU:HB3	2:B:453:TRP:CZ2	2.57	0.40
2:B:715:ASP:OD1	2:B:715:ASP:N	2.54	0.40
1:A:58:MET:HE3	1:A:58:MET:HB2	1.88	0.40
1:A:502:ASN:ND2	2:B:1084:LEU:HD13	2.37	0.40
1:A:841:MET:HE1	2:B:503:ASN:CG	2.46	0.40
2:B:412:LEU:HD23	2:B:412:LEU:HA	1.83	0.40
2:B:588:ARG:HA	2:B:603:MET:HE1	2.03	0.40
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.55	0.40
2:B:772:LEU:HD23	10:J:55:LEU:HD21	2.03	0.40
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.57	0.40
3:C:93:PHE:HE1	3:C:166:LYS:HD2	1.86	0.40
5:E:24:ARG:HH22	5:E:128:GLU:CD	2.29	0.40
10:J:44:CYS:O	10:J:47:ARG:HG2	2.21	0.40
10:J:65:LEU:HD11	12:L:45:TYR:CD2	2.56	0.40
13:N:29:DC:H2'	16:U:269:ARG:HG3	2.03	0.40
16:U:613:LYS:C	16:U:615:GLY:H	2.29	0.40
1:A:100:LEU:O	1:A:103:THR:OG1	2.32	0.40
1:A:283:ILE:HG12	1:A:313:HIS:HB3	2.03	0.40
1:A:486:LEU:HD13	2:B:790:GLN:CD	2.45	0.40
1:A:732:THR:HB	9:I:106:ASP:HB3	2.03	0.40
1:A:802:PHE:HE2	1:A:808:PRO:HD3	1.85	0.40
1:A:831:LEU:HG	2:B:715:ASP:O	2.22	0.40
2:B:470:LEU:HD11	2:B:478:THR:HG23	2.03	0.40
7:G:27:LYS:HD3	7:G:51:ILE:HD12	2.03	0.40
7:G:91:GLN:OE1	7:G:91:GLN:HA	2.21	0.40
8:H:81:ARG:CG	8:H:82:PRO:HD3	2.51	0.40
16:U:166:GLY:C	16:U:168:ASP:N	2.79	0.40
16:U:225:LEU:HD23	16:U:225:LEU:HA	1.88	0.40
16:U:226:PHE:HA	16:U:430:GLY:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:294:LYS:O	16:U:295:ALA:C	2.64	0.40
1:A:125:LYS:HB3	1:A:125:LYS:HE2	1.96	0.40
1:A:1077:ASN:ND2	6:F:56:TYR:OH	2.55	0.40
1:A:1129:ASN:C	1:A:1130:ILE:HD12	2.47	0.40
2:B:1101:GLN:NE2	6:F:64:ARG:HG3	2.36	0.40
6:F:125:ILE:HG22	6:F:127:ASP:H	1.85	0.40
16:U:58:LYS:HA	16:U:61:CYS:C	2.47	0.40
16:U:76:VAL:O	16:U:157:ASP:N	2.53	0.40
16:U:279:LEU:HB3	16:U:284:VAL:HB	2.03	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1433/1970 (73%)	1357 (95%)	71 (5%)	5 (0%)	36	68
2	B	1128/1174 (96%)	1057 (94%)	69 (6%)	2 (0%)	43	73
3	C	253/275 (92%)	243 (96%)	10 (4%)	0	100	100
4	D	126/142 (89%)	123 (98%)	3 (2%)	0	100	100
5	E	207/210 (99%)	192 (93%)	15 (7%)	0	100	100
6	F	80/127 (63%)	80 (100%)	0	0	100	100
7	G	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
8	H	146/150 (97%)	137 (94%)	8 (6%)	1 (1%)	18	52
9	I	112/125 (90%)	100 (89%)	11 (10%)	1 (1%)	14	47
10	J	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
16	U	527/991 (53%)	450 (85%)	61 (12%)	16 (3%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4401/5578 (79%)	4108 (93%)	268 (6%)	25 (1%)	23	56

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	910	LYS
1	A	1270	GLN
16	U	53	PRO
16	U	176	LEU
16	U	328	VAL
2	B	241	ALA
16	U	13	GLU
16	U	158	GLU
16	U	159	ALA
16	U	185	HIS
16	U	187	PRO
16	U	267	ARG
16	U	522	ILE
1	A	1249	ASP
1	A	1250	ASP
1	A	1255	LEU
16	U	59	SER
16	U	161	CYS
16	U	270	GLU
8	H	34	SER
16	U	47	ASP
16	U	359	CYS
16	U	58	LYS
2	B	230	ARG
9	I	116	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1271/1748 (73%)	1261 (99%)	10 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	993/1028 (97%)	993 (100%)	0	100	100
3	C	234/252 (93%)	233 (100%)	1 (0%)	84	86
4	D	106/126 (84%)	105 (99%)	1 (1%)	70	81
5	E	189/192 (98%)	189 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	147/153 (96%)	147 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	101 (98%)	2 (2%)	50	73
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	103 (99%)	1 (1%)	68	80
12	L	41/55 (74%)	41 (100%)	0	100	100
16	U	450/820 (55%)	416 (92%)	34 (8%)	12	42
All	All	3894/4890 (80%)	3845 (99%)	49 (1%)	59	78

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	470	MET
1	A	909	LEU
1	A	910	LYS
1	A	912	SER
1	A	1247	PHE
1	A	1250	ASP
1	A	1251	ASN
1	A	1254	LYS
1	A	1255	LEU
1	A	1259	ILE
3	C	75	SER
4	D	62	MET
9	I	57	LYS
9	I	65	LEU
11	K	50	LEU
16	U	11	ASP
16	U	50	VAL
16	U	52	MET
16	U	58	LYS
16	U	59	SER
16	U	60	LEU

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Mol	Chain	Res	Type
16	U	61	CYS
16	U	156	VAL
16	U	158	GLU
16	U	161	CYS
16	U	162	VAL
16	U	165	TRP
16	U	170	ARG
16	U	176	LEU
16	U	179	LEU
16	U	181	SER
16	U	182	ARG
16	U	183	LEU
16	U	185	HIS
16	U	187	PRO
16	U	191	LEU
16	U	267	ARG
16	U	269	ARG
16	U	287	LYS
16	U	290	HIS
16	U	294	LYS
16	U	297	GLU
16	U	298	ARG
16	U	300	LEU
16	U	301	VAL
16	U	604	LYS
16	U	612	SER
16	U	613	LYS
16	U	620	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	72	GLN
1	A	77	ASN
1	A	152	ASN
1	A	188	GLN
1	A	272	ASN
1	A	293	ASN
1	A	330	GLN
1	A	341	GLN
1	A	403	GLN

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Mol	Chain	Res	Type
1	A	461	GLN
1	A	620	HIS
1	A	673	GLN
1	A	700	GLN
1	A	764	ASN
1	A	792	ASN
1	A	825	ASN
1	A	1032	GLN
1	A	1034	GLN
1	A	1077	ASN
1	A	1082	HIS
1	A	1116	ASN
1	A	1129	ASN
1	A	1146	GLN
1	A	1190	GLN
1	A	1263	ASN
1	A	1291	ASN
1	A	1445	HIS
1	A	1457	ASN
1	A	1462	GLN
2	B	56	GLN
2	B	145	GLN
2	B	312	GLN
2	B	452	ASN
2	B	456	GLN
2	B	460	HIS
2	B	503	ASN
2	B	639	HIS
2	B	699	HIS
2	B	717	ASN
2	B	725	GLN
2	B	731	GLN
2	B	749	HIS
2	B	790	GLN
2	B	842	HIS
2	B	941	GLN
2	B	1021	HIS
2	B	1025	ASN
2	B	1101	GLN
2	B	1115	GLN
2	B	1120	ASN
2	B	1145	GLN

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Mol	Chain	Res	Type
3	C	66	HIS
3	C	260	GLN
4	D	34	ASN
4	D	38	HIS
4	D	135	GLN
5	E	43	GLN
5	E	189	GLN
7	G	21	ASN
7	G	24	ASN
7	G	60	GLN
9	I	46	GLN
9	I	56	ASN
9	I	91	HIS
10	J	61	ASN
11	K	29	ASN
11	K	36	ASN
11	K	84	GLN
16	U	101	ASN
16	U	164	GLN
16	U	241	ASN
16	U	290	HIS
16	U	303	ASN
16	U	345	GLN
16	U	370	GLN
16	U	433	HIS
16	U	564	ASN
16	U	566	GLN
16	U	585	HIS
16	U	595	ASN
16	U	616	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	10/20 (50%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	11	A
14	P	13	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	$\# Z > 2$
19	ANP	U	1000	-	33,33,33	1.07	5 (15%)	45,52,52	1.00	4 (8%)

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
19	ANP	U	1000	-	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	U	1000	ANP	PB-O1B	3.06	1.50	1.46
19	U	1000	ANP	PG-O1G	2.99	1.50	1.46
19	U	1000	ANP	PB-O2B	-2.26	1.50	1.56
19	U	1000	ANP	PG-O2G	-2.16	1.51	1.56
19	U	1000	ANP	PG-O3G	-2.11	1.51	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	U	1000	ANP	O2B-PB-O1B	4.00	118.45	109.87
19	U	1000	ANP	O3G-PG-O1G	-2.37	107.51	113.45
19	U	1000	ANP	O2G-PG-O1G	-2.08	108.22	113.45
19	U	1000	ANP	O3A-PB-N3B	-2.07	100.85	106.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

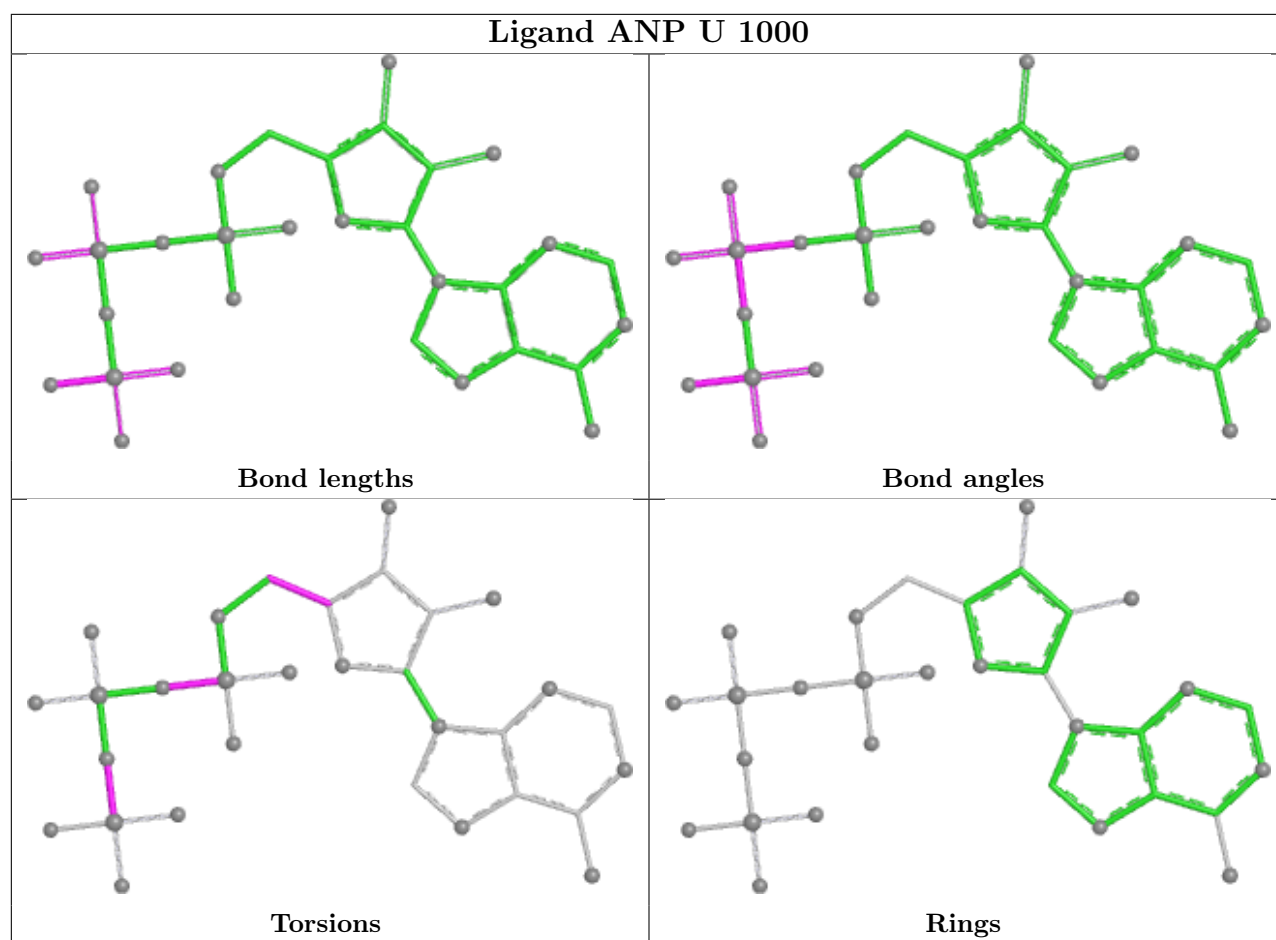
Mol	Chain	Res	Type	Atoms
19	U	1000	ANP	PB-N3B-PG-O1G
19	U	1000	ANP	O4'-C4'-C5'-O5'
19	U	1000	ANP	C3'-C4'-C5'-O5'
19	U	1000	ANP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	U	1000	ANP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

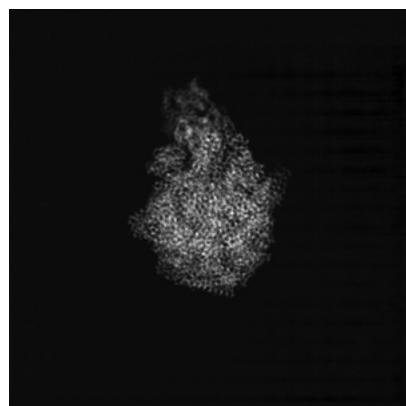
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48075. These allow visual inspection of the internal detail of the map and identification of artifacts.

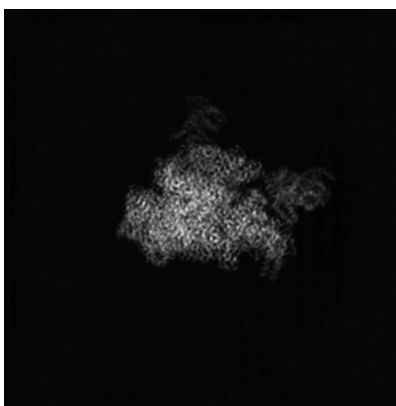
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

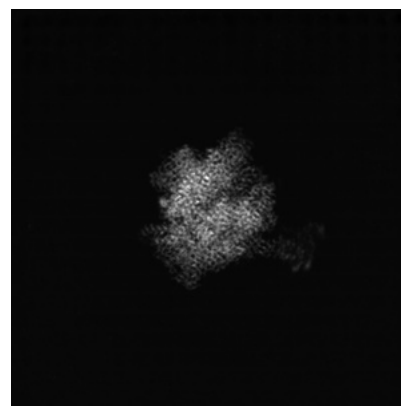
6.1.1 Primary map



X

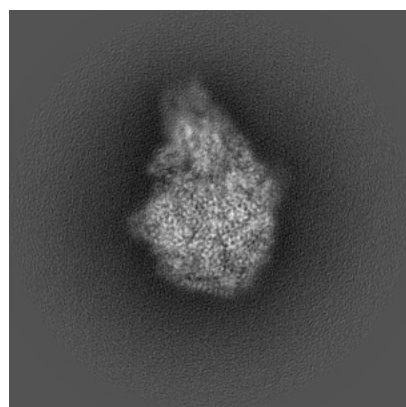


Y

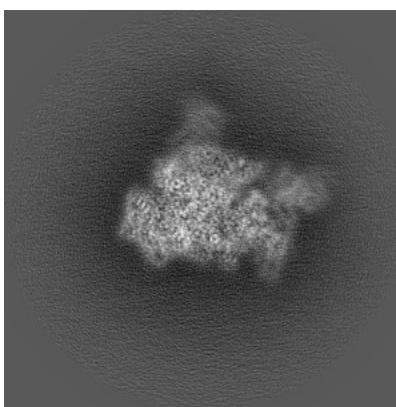


Z

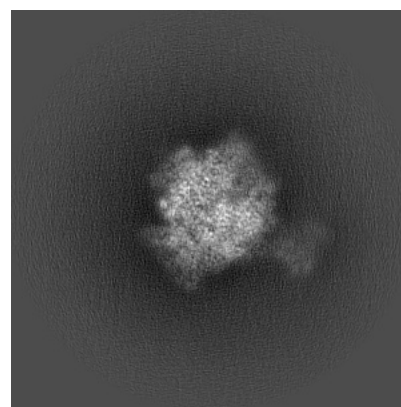
6.1.2 Raw map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

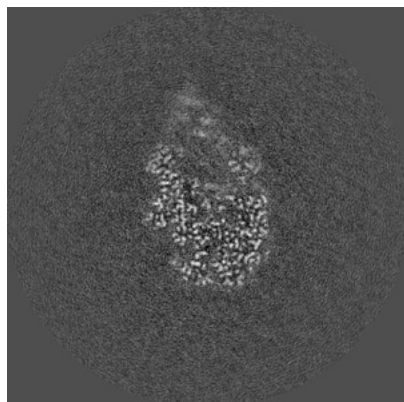


Y Index: 160

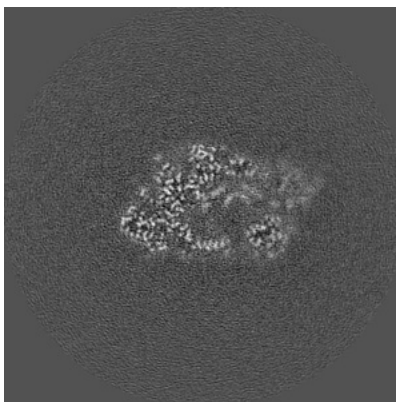


Z Index: 160

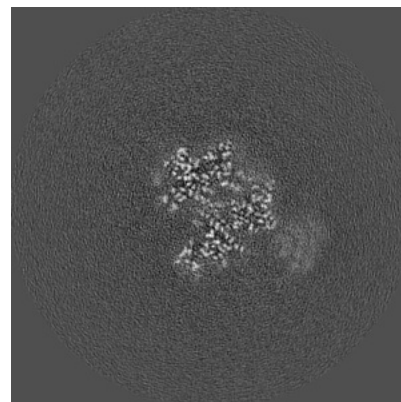
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 140

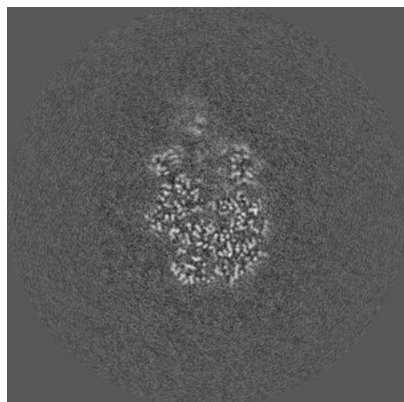


Y Index: 157

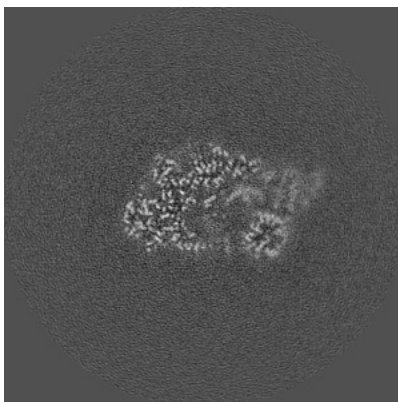


Z Index: 150

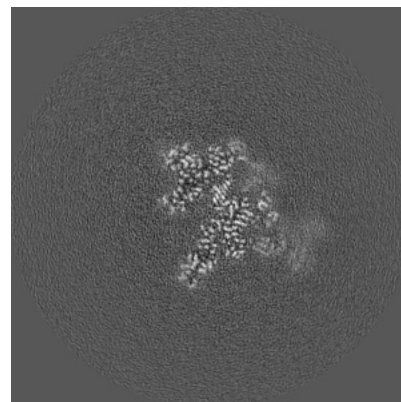
6.3.2 Raw map



X Index: 157



Y Index: 157

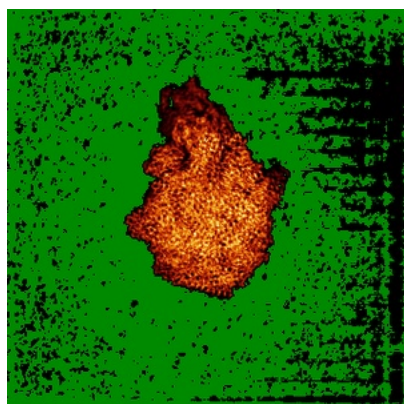


Z Index: 150

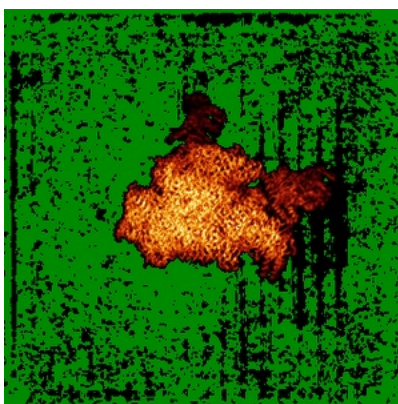
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

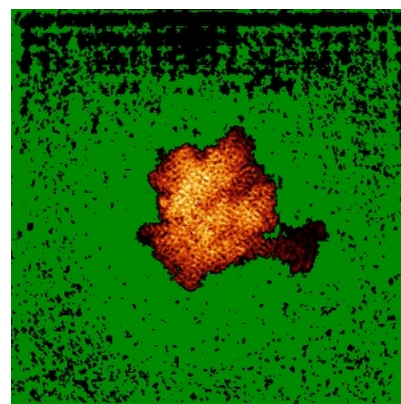
6.4.1 Primary map



X

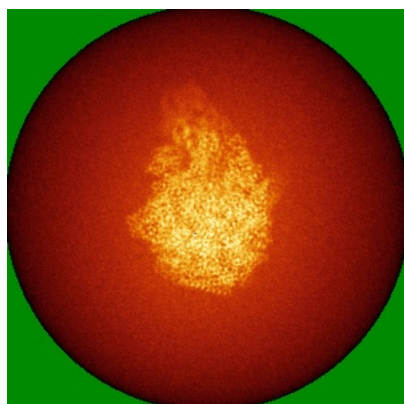


Y

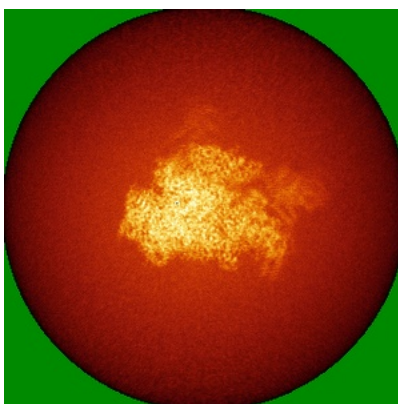


Z

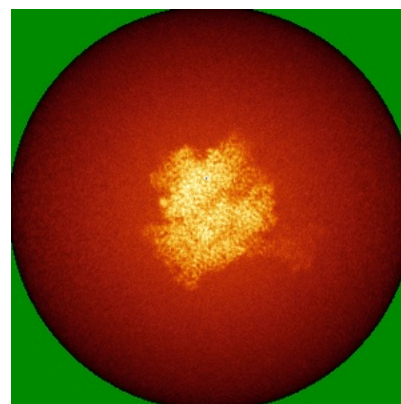
6.4.2 Raw map



X



Y

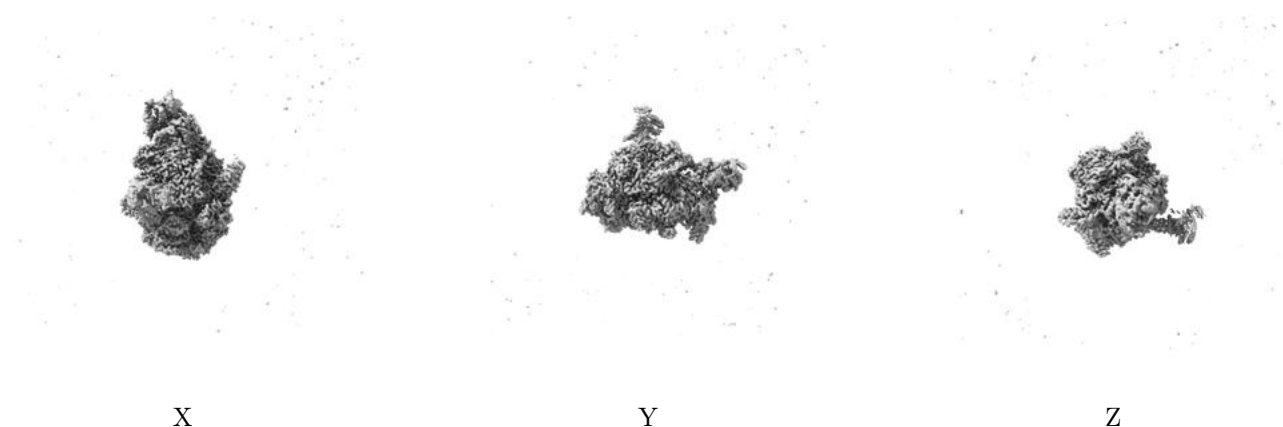


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

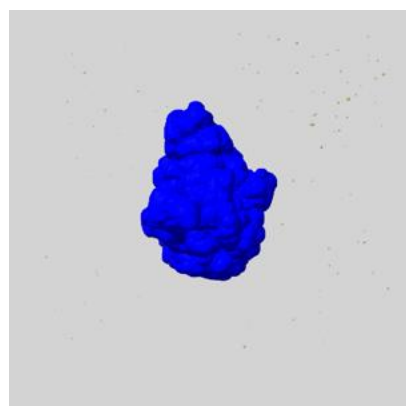
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

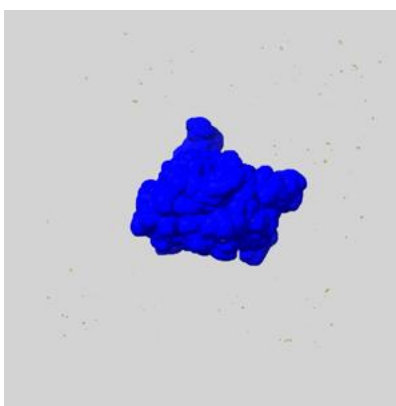
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

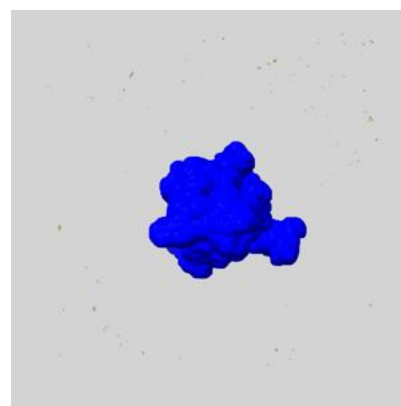
6.6.1 emd_48075_msk_1.map [i](#)



X



Y

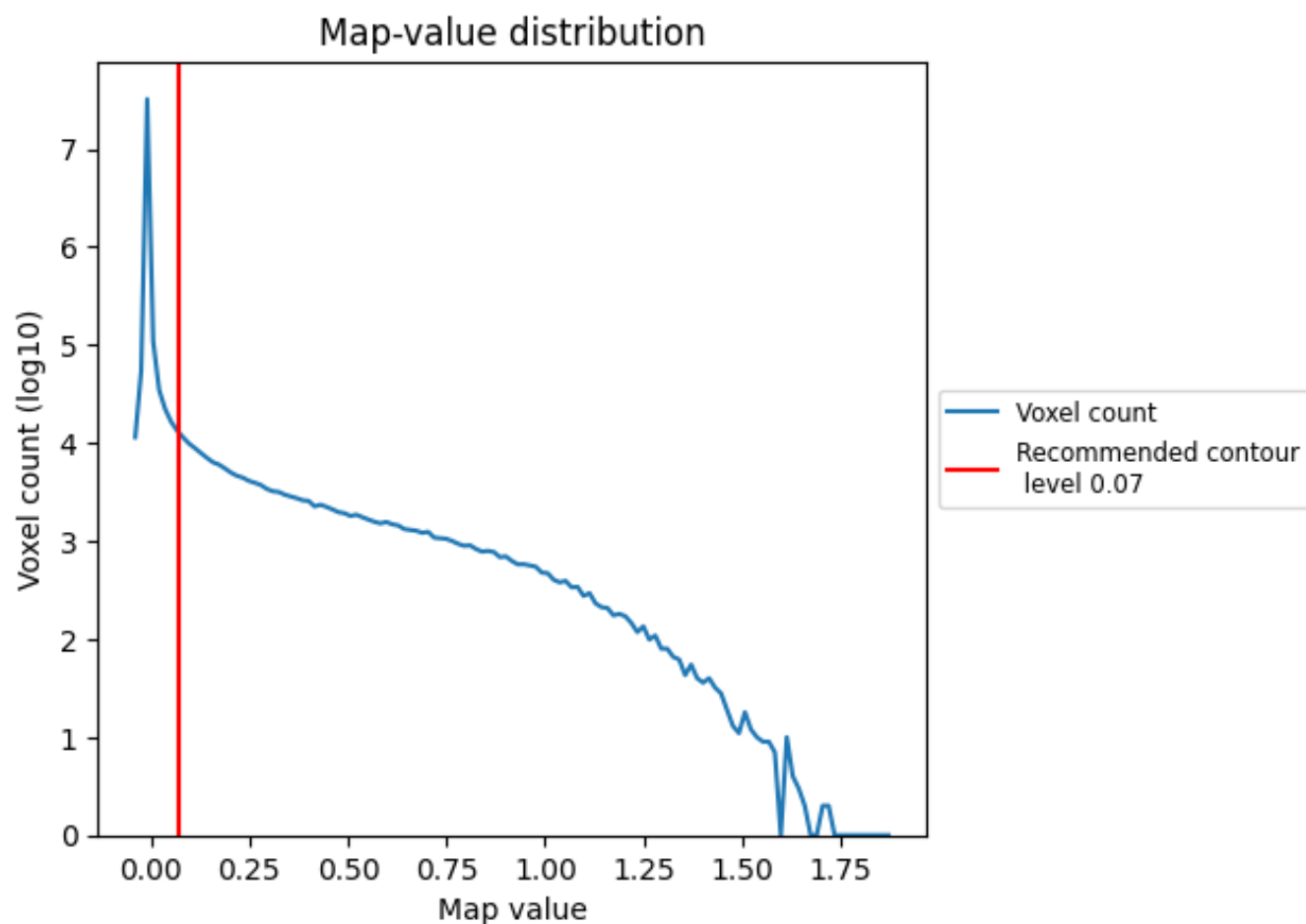


Z

7 Map analysis [i](#)

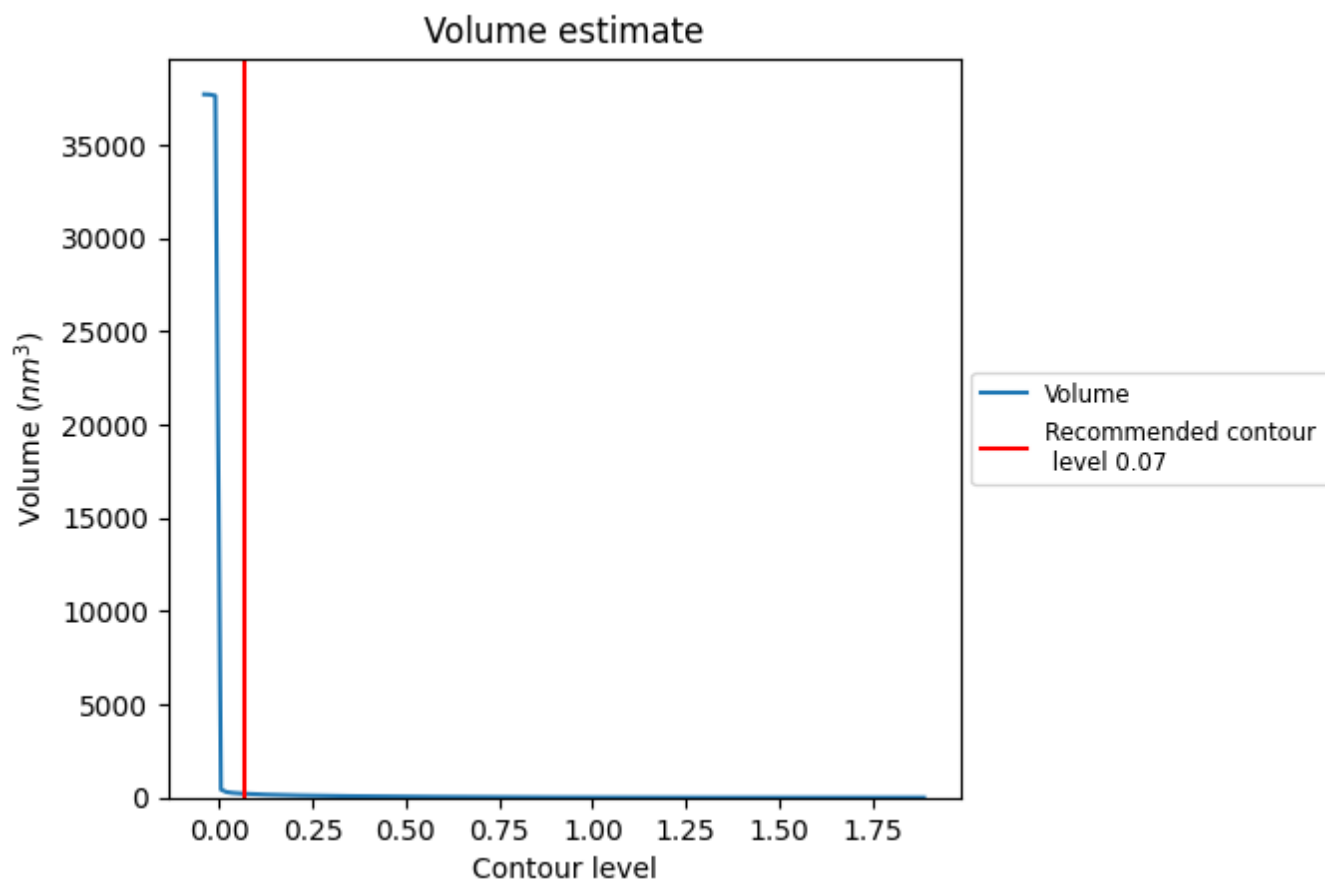
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

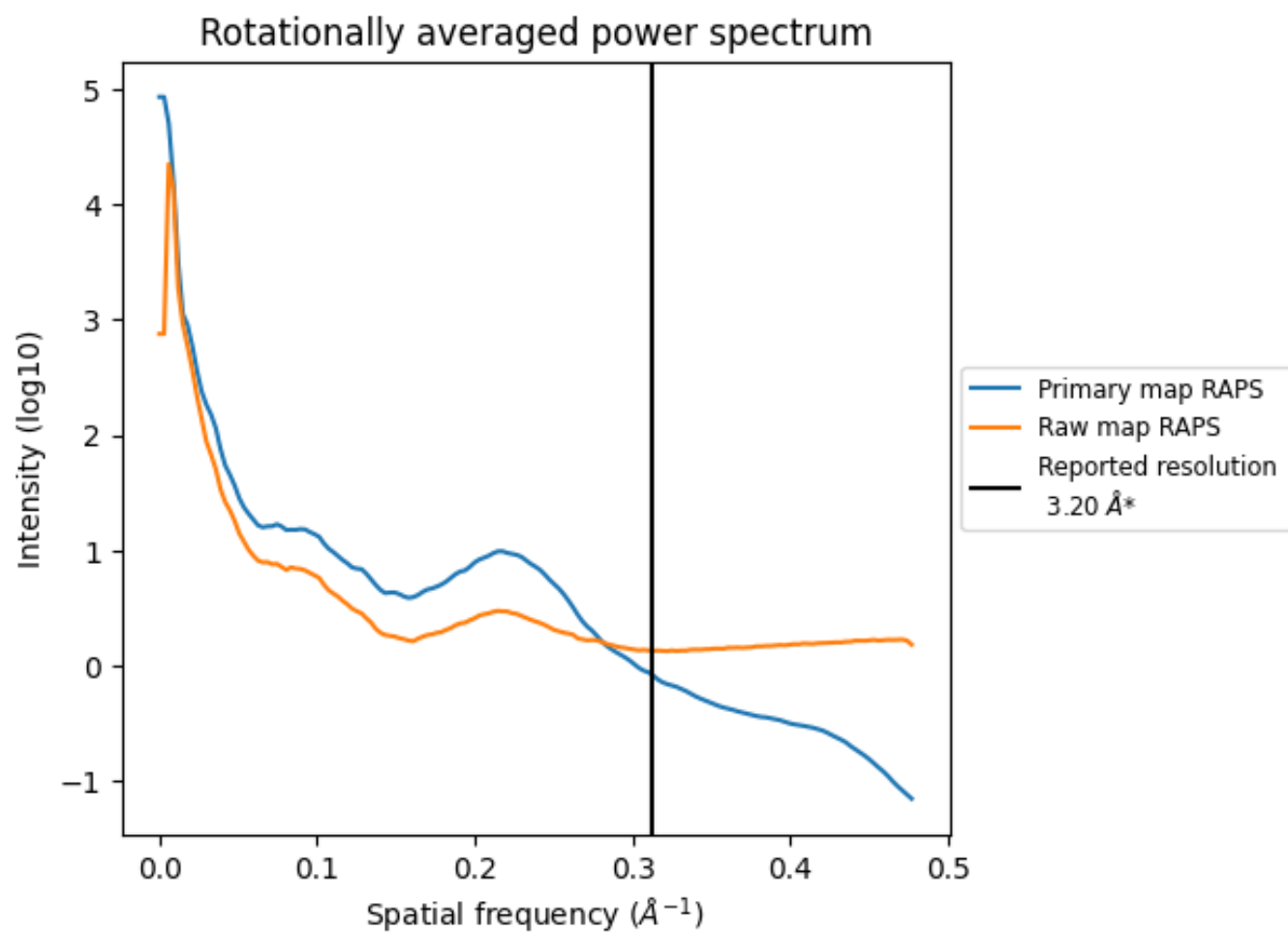
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm^3 ; this corresponds to an approximate mass of 185 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

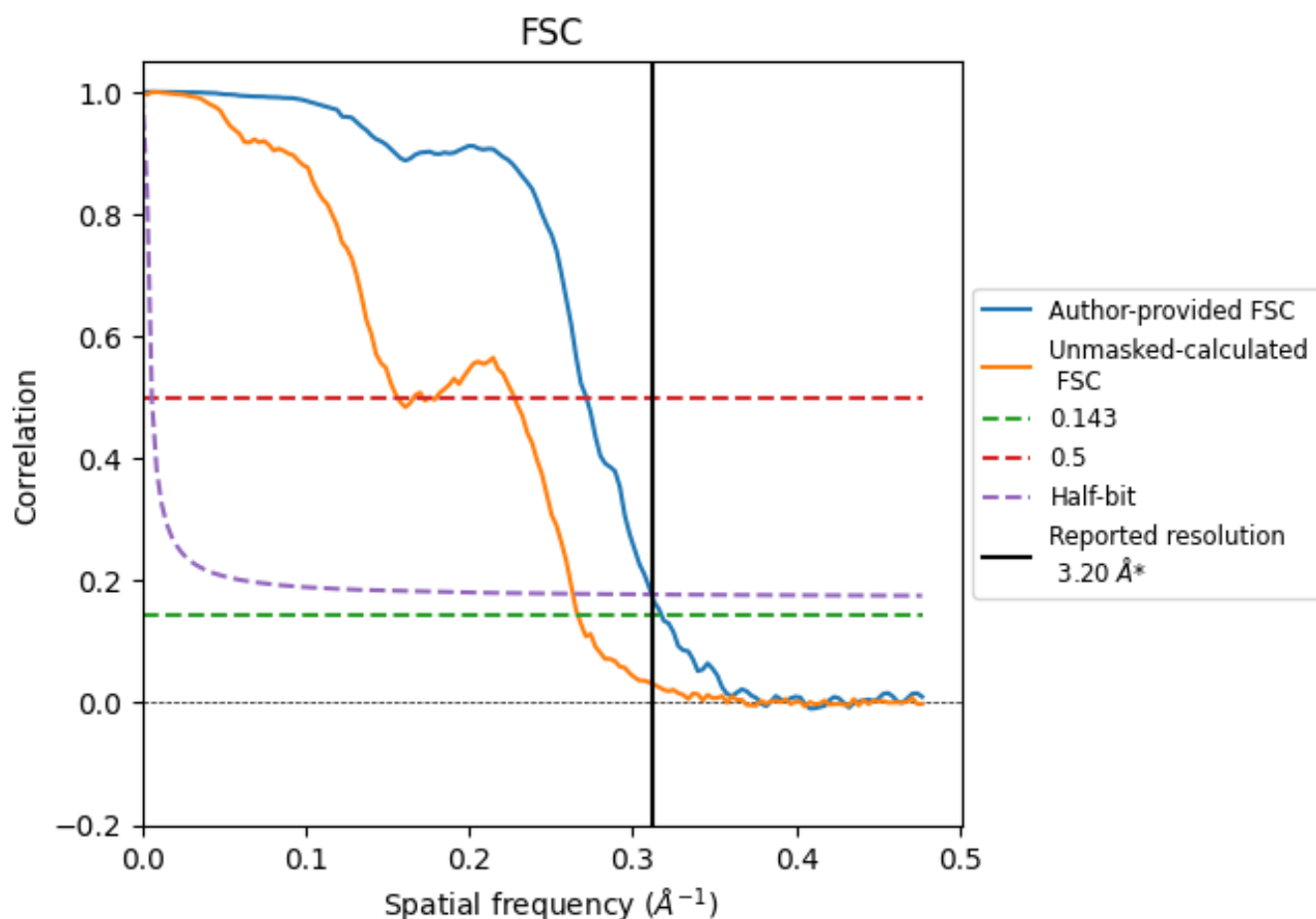


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

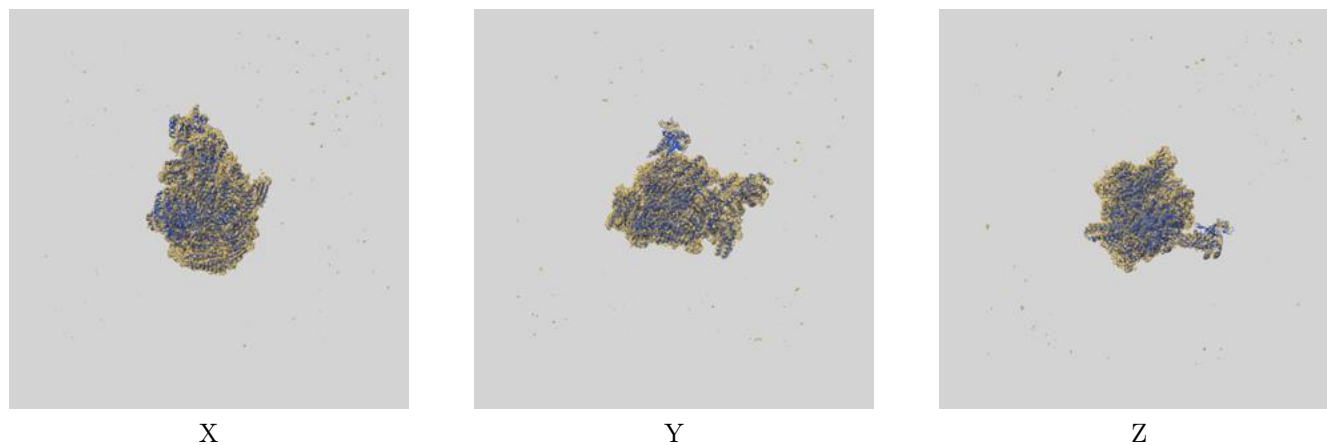
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.68	3.21
Unmasked-calculated*	3.75	6.41	3.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

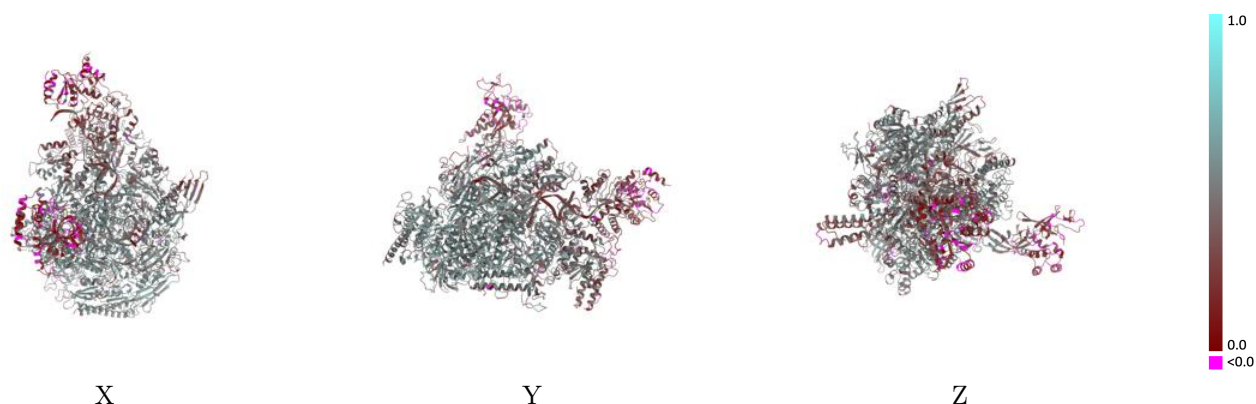
This section contains information regarding the fit between EMDB map EMD-48075 and PDB model 9EI3. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



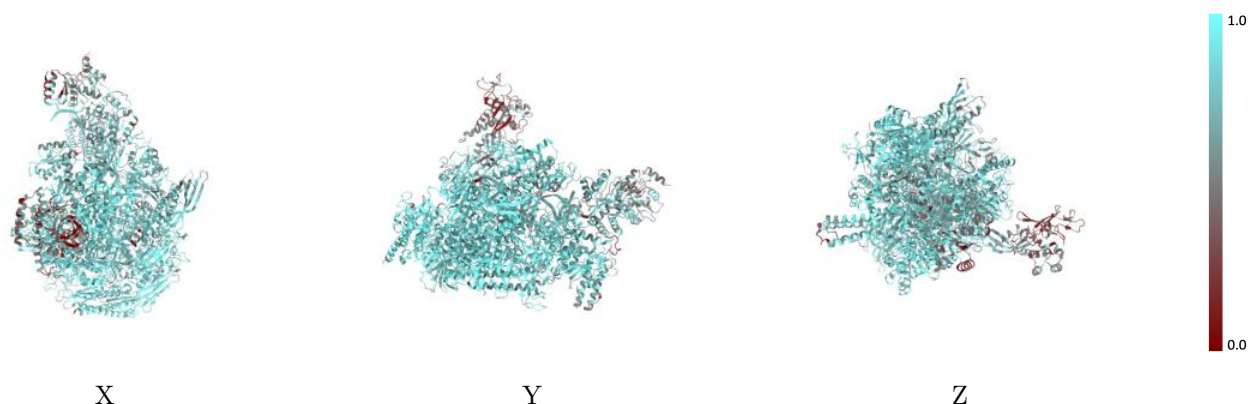
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



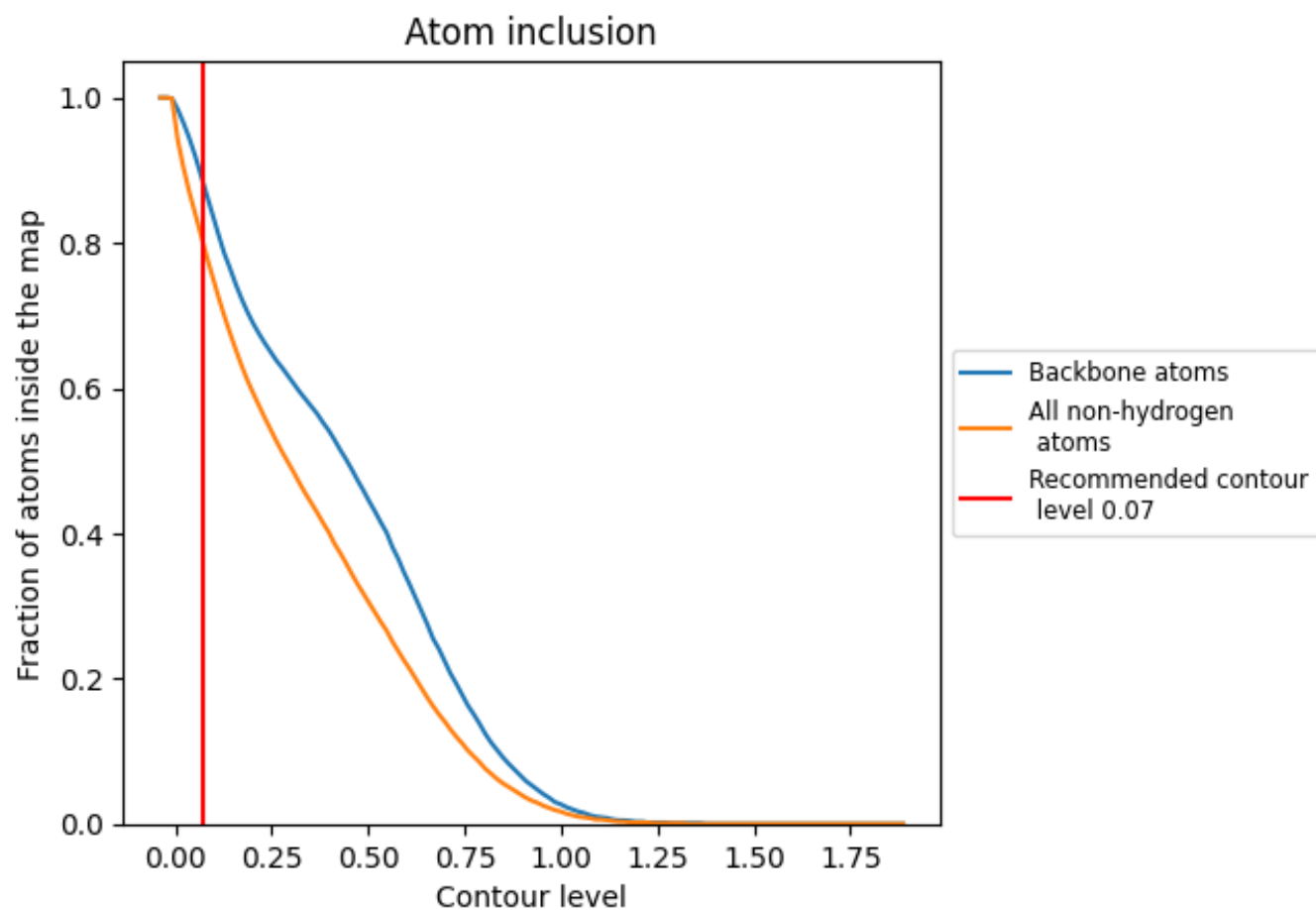
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.4340
A	 0.8600	 0.4850
B	 0.8590	 0.4870
C	 0.8760	 0.5070
D	 0.4150	 0.1410
E	 0.8260	 0.4360
F	 0.8480	 0.4930
G	 0.4470	 0.2600
H	 0.8180	 0.4590
I	 0.8040	 0.4090
J	 0.8580	 0.5080
K	 0.8870	 0.4940
L	 0.8010	 0.4250
N	 0.8000	 0.3140
P	 0.8030	 0.3880
T	 0.8290	 0.3730
U	 0.6390	 0.2600

