



## Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 08:10 AM EST

PDB ID : 6D6V  
EMDB ID : EMD-7821  
Title : CryoEM structure of Tetrahymena telomerase with telomeric DNA at 4.8 Angstrom resolution  
Authors : Jiang, J.; Wang, Y.; Susac, L.; Chan, H.; Basu, R.; Zhou, Z.H.; Feigon, J.  
Deposited on : 2018-04-22  
Resolution : 4.80 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

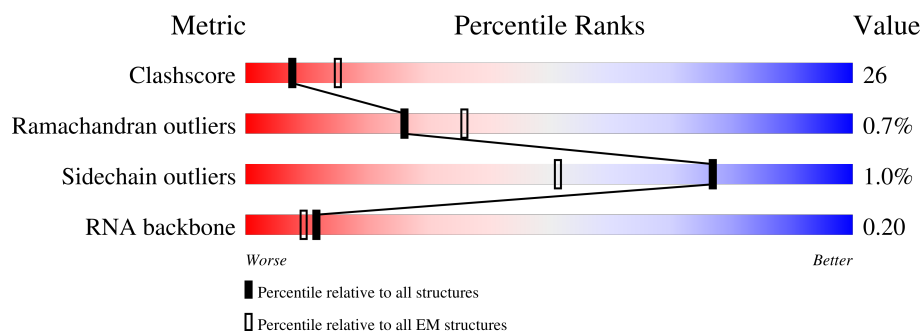
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	1117	
2	D	701	
3	F	121	
4	E	269	
5	B	159	
6	C	19	
7	G	157	

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Mol	Chain	Length	Quality of chain
8	H	542	<div><div><div></div><div></div><div></div></div><div>20%15%5%80%</div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17317 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 Telomerase reverse transcriptase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	980	Total	C	N	O	S	0	0
			8253	5357	1369	1498	29		

- Molecule 2 is a protein called Telomerase-associated protein 82.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	185	Total	C	N	O	S	0	0
			1538	985	255	290	8		

- Molecule 3 is a protein called Telomerase holoenzyme TEB heterotrimer Teb3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	113	Total	C	N	O	S	0	0
			919	580	155	180	4		

- Molecule 4 is a protein called Telomerase holoenzyme Teb2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	149	Total	C	N	O	S	0	0
			1207	765	211	223	8		

- Molecule 5 is a RNA chain called RNA (159-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	159	Total	C	N	O	P	0	0
			3322	1494	568	1102	158		

- Molecule 6 is a DNA chain called DNA (5'-D(P\*GP\*TP\*TP\*GP\*GP\*GP\*GP\*TP\*TP\*GP\*GP\*GP\*TP\*TP\*GP\*GP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	19	Total	C	N	O	P	0	0
			406	190	77	120	19		

- Molecule 7 is a protein called Telomerase-associated protein 50.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	157	Total	C	N	O	0	0
			785	471	157	157		

- Molecule 8 is a protein called Telomerase associated protein p65.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	108	Total	C	N	O	S	0	0
			886	563	156	162	5		

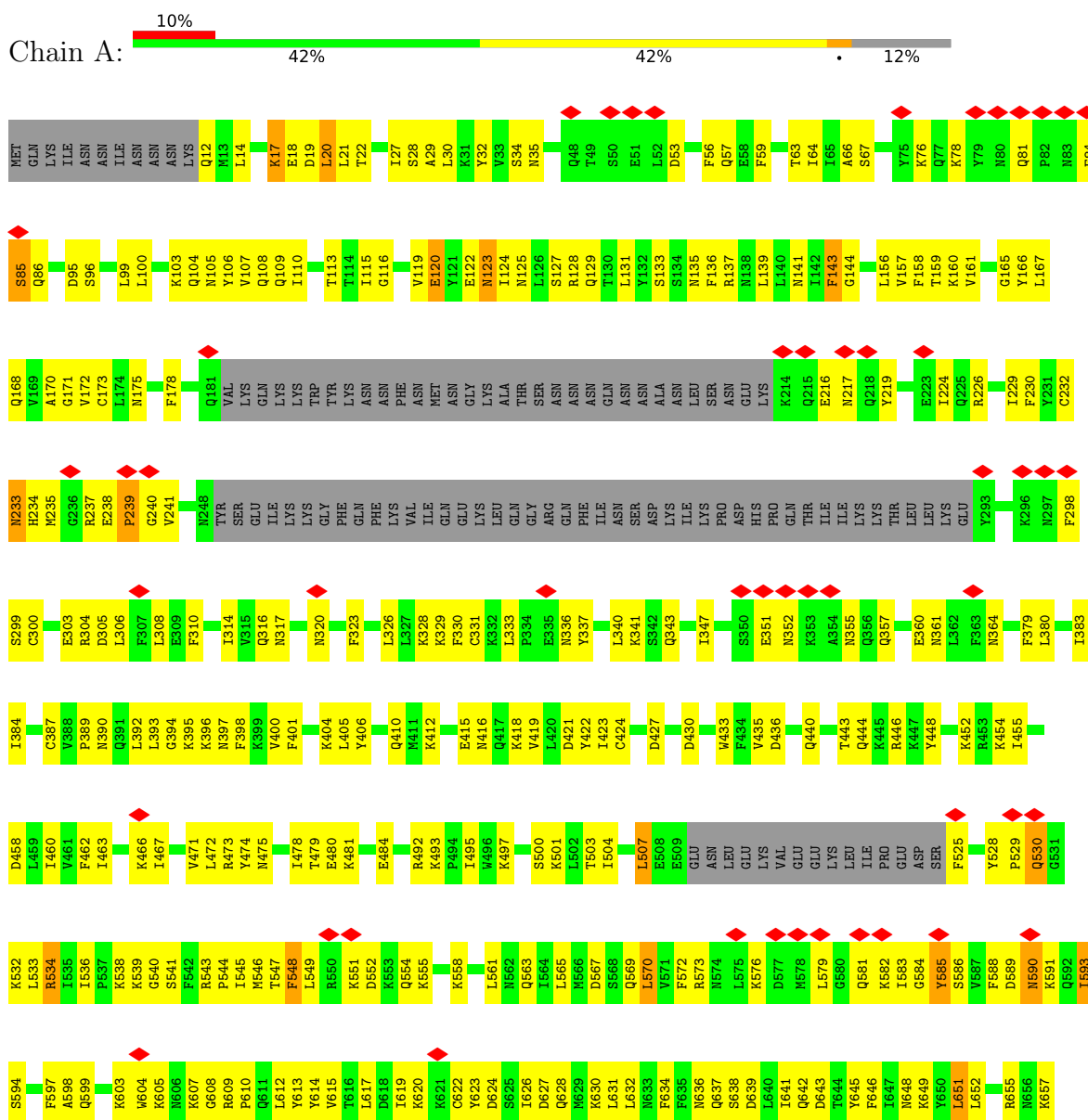
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Zn	0
			1	1	

### 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: Telomerase reverse transcriptase











ASN LYS	M481	M482	M483	M484	M485	K486	L487	Q488	E489	I491	R492	G493	Q494	I495	C496	D497	V498	I499	S500	T501	I502	P503	E504	D505	E506	E507	R508	N509	Y510	W511	N512	Y513	T514	K515	F516	K517	K518	N519	E520	F521	R522	K523	F524	F525	F526	M527	K528	K529	Q530	Q531	K532	LYS	GLN	ASN	ILE	THR	GLN	ASN	TYR	SER	ARG	LYS	ALA	SER	ASP	GLU	PHE	VAL	SER	ILE	ASP	VAL	GLU	ILE	LYS	GLN	N378	C379	L380	I381	K382	I383	I384	N385	I386	P387	Q388	G389	T390	L391	K392	A393	E394	V395	V396	L397	A398	V399	R400	H401	L402	G403	Y404	E405	F406	Y407	C408	D409	Y410	I411	D412	GLU	ASN	SER	ASN	GLN	ILE	ASN	SER

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52506	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.156	Depositor
Minimum map value	-0.054	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	348.16, 348.16, 348.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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: ZN

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	0.73	1/8418 (0.0%)	0.89	16/11318 (0.1%)
2	D	0.69	0/1566	0.77	1/2101 (0.0%)
3	F	0.59	0/934	0.73	0/1262
4	E	0.64	0/1230	0.82	1/1655 (0.1%)
5	B	1.13	9/3711 (0.2%)	2.03	208/5768 (3.6%)
6	C	1.56	2/456 (0.4%)	1.49	10/707 (1.4%)
8	H	0.31	1/899 (0.1%)	0.35	0/1205
All	All	0.84	13/17214 (0.1%)	1.25	236/24016 (1.0%)

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	25
3	F	0	4
4	E	0	5
7	G	0	6
All	All	0	40

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	44	A	N9-C4	-6.88	1.33	1.37
6	C	9	DT	C3'-O3'	6.75	1.52	1.44
5	B	33	A	N9-C4	-6.42	1.33	1.37
5	B	47	C	N1-C6	-6.41	1.33	1.37
5	B	69	A	N9-C4	-6.27	1.34	1.37
6	C	15	DT	C3'-O3'	-5.76	1.36	1.44
8	H	527	MET	CG-SD	5.68	1.96	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	22	A	N9-C4	-5.67	1.34	1.37
5	B	49	C	C4-C5	-5.61	1.38	1.43
5	B	49	C	C5-C6	-5.52	1.29	1.34
5	B	29	A	N9-C4	5.49	1.41	1.37
1	A	120	GLU	CB-CG	5.37	1.62	1.52
5	B	148	A	N7-C5	-5.10	1.36	1.39

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	46	C	O4'-C1'-N1	22.24	125.99	108.20
5	B	47	C	C5-C6-N1	16.33	129.16	121.00
5	B	47	C	C6-N1-C2	-14.86	114.36	120.30
5	B	48	C	C5-C6-N1	14.04	128.02	121.00
5	B	145	U	N1-C2-O2	13.35	132.15	122.80
5	B	49	C	C2-N1-C1'	13.19	133.30	118.80
5	B	25	U	C2-N1-C1'	12.88	133.15	117.70
5	B	120	C	N1-C2-O2	12.79	126.57	118.90
5	B	145	U	N3-C2-O2	-12.34	113.56	122.20
5	B	17	U	N3-C2-O2	-12.03	113.78	122.20
5	B	49	C	C5-C4-N4	-11.96	111.82	120.20
5	B	145	U	C2-N1-C1'	11.82	131.88	117.70
5	B	53	A	O5'-P-OP2	-11.63	95.24	105.70
5	B	48	C	C6-N1-C2	-11.54	115.68	120.30
5	B	49	C	C5-C6-N1	11.23	126.62	121.00
5	B	25	U	N1-C2-O2	10.72	130.31	122.80
5	B	123	C	N1-C2-O2	10.68	125.31	118.90
5	B	17	U	N1-C2-O2	10.61	130.22	122.80
5	B	49	C	C6-N1-C1'	-10.52	108.17	120.80
5	B	112	A	N1-C6-N6	10.43	124.86	118.60
5	B	120	C	N3-C2-O2	-9.73	115.09	121.90
5	B	82	U	N3-C2-O2	-9.71	115.40	122.20
5	B	102	U	C5-C6-N1	9.36	127.38	122.70
5	B	145	U	C6-N1-C1'	-9.30	108.18	121.20
5	B	25	U	C6-N1-C1'	-9.21	108.31	121.20
5	B	35	C	N1-C2-O2	9.20	124.42	118.90
6	C	14	DT	O4'-C1'-N1	9.20	114.44	108.00
5	B	148	A	C6-C5-N7	-9.12	125.91	132.30
5	B	70	A	N9-C4-C5	-9.03	102.19	105.80
5	B	152	C	C5-C6-N1	9.01	125.50	121.00
5	B	88	C	N3-C4-C5	8.85	125.44	121.90
5	B	123	C	N3-C2-O2	-8.72	115.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	49	C	N3-C4-N4	8.70	124.09	118.00
5	B	81	U	N3-C2-O2	-8.64	116.15	122.20
5	B	33	A	O4'-C1'-N9	8.58	115.06	108.20
5	B	120	C	C2-N1-C1'	8.56	128.22	118.80
5	B	25	U	N3-C2-O2	-8.51	116.24	122.20
5	B	137	U	N1-C2-O2	8.47	128.73	122.80
5	B	137	U	C2-N1-C1'	8.41	127.80	117.70
5	B	82	U	N1-C2-O2	8.22	128.56	122.80
5	B	84	G	N7-C8-N9	8.08	117.14	113.10
1	A	651	LEU	CA-CB-CG	8.06	133.84	115.30
5	B	3	A	P-O3'-C3'	8.04	129.34	119.70
5	B	69	A	N3-C4-N9	-7.96	121.03	127.40
5	B	85	G	N7-C8-N9	7.90	117.05	113.10
5	B	52	A	C2-N3-C4	7.89	114.54	110.60
5	B	118	A	O5'-P-OP1	-7.83	98.65	105.70
1	A	830	LEU	CA-CB-CG	7.78	133.19	115.30
5	B	103	G	C4-C5-N7	7.75	113.90	110.80
5	B	35	C	N3-C2-O2	-7.73	116.49	121.90
5	B	150	G	N7-C8-N9	7.71	116.95	113.10
5	B	49	C	N1-C2-O2	7.67	123.50	118.90
5	B	33	A	C8-N9-C1'	7.66	141.49	127.70
5	B	6	C	C5-C6-N1	7.65	124.82	121.00
5	B	17	U	C2-N1-C1'	7.55	126.76	117.70
5	B	81	U	N1-C2-O2	7.53	128.07	122.80
5	B	8	C	C5-C6-N1	7.51	124.76	121.00
5	B	137	U	N3-C2-O2	-7.46	116.98	122.20
5	B	69	A	C6-C5-N7	7.43	137.50	132.30
5	B	52	A	N3-C4-N9	7.34	133.28	127.40
5	B	33	A	C4-N9-C1'	-7.30	113.17	126.30
5	B	47	C	O4'-C1'-N1	7.23	113.98	108.20
5	B	114	G	C4-C5-N7	7.20	113.68	110.80
5	B	57	U	C2-N1-C1'	7.15	126.28	117.70
5	B	57	U	N1-C2-O2	7.13	127.79	122.80
5	B	120	C	C6-N1-C1'	-7.12	112.26	120.80
5	B	48	C	C4-C5-C6	-7.09	113.86	117.40
5	B	148	A	C4-C5-N7	7.04	114.22	110.70
5	B	46	C	P-O5'-C5'	7.02	132.14	120.90
5	B	112	A	C5-C6-N6	-7.01	118.09	123.70
5	B	112	A	C4-C5-N7	6.99	114.19	110.70
5	B	69	A	N1-C2-N3	6.97	132.78	129.30
5	B	96	U	N3-C2-O2	-6.96	117.32	122.20
5	B	84	G	C5-N7-C8	-6.96	100.82	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	70	A	C4-C5-N7	6.89	114.14	110.70
5	B	103	G	C5-N7-C8	-6.88	100.86	104.30
1	A	922	SER	C-N-CA	6.79	138.67	121.70
5	B	62	C	N3-C2-O2	-6.78	117.16	121.90
5	B	49	C	C4-C5-C6	-6.74	114.03	117.40
5	B	33	A	N3-C4-N9	-6.73	122.02	127.40
5	B	123	C	C5-C6-N1	6.71	124.35	121.00
5	B	85	G	C5-N7-C8	-6.67	100.97	104.30
5	B	95	G	N3-C4-N9	6.66	130.00	126.00
6	C	1	DG	P-O3'-C3'	6.65	127.67	119.70
5	B	114	G	C5-N7-C8	-6.60	101.00	104.30
5	B	53	A	N9-C4-C5	6.60	108.44	105.80
5	B	69	A	C4-N9-C1'	-6.59	114.43	126.30
5	B	73	U	N3-C2-O2	-6.59	117.58	122.20
5	B	73	U	N1-C2-O2	6.57	127.40	122.80
5	B	47	C	N3-C4-N4	6.57	122.60	118.00
5	B	88	C	C6-N1-C2	6.57	122.93	120.30
5	B	18	U	N1-C2-O2	6.56	127.39	122.80
5	B	69	A	C2-N3-C4	-6.56	107.32	110.60
5	B	8	C	N1-C2-O2	6.54	122.83	118.90
5	B	70	A	N1-C6-N6	6.54	122.52	118.60
5	B	80	A	N1-C2-N3	-6.51	126.05	129.30
5	B	134	C	N1-C2-O2	6.51	122.80	118.90
5	B	150	G	C5-N7-C8	-6.45	101.08	104.30
5	B	148	A	N9-C4-C5	-6.45	103.22	105.80
5	B	25	U	C5-C6-N1	6.40	125.90	122.70
5	B	83	A	N7-C8-N9	6.37	116.98	113.80
5	B	47	C	C2-N3-C4	6.35	123.08	119.90
5	B	54	A	O5'-P-OP1	-6.34	100.00	105.70
5	B	148	A	N1-C6-N6	6.27	122.36	118.60
5	B	148	A	N7-C8-N9	6.27	116.94	113.80
5	B	57	U	C6-N1-C1'	-6.26	112.43	121.20
5	B	41	U	OP1-P-O3'	6.19	118.82	105.20
5	B	8	C	C2-N1-C1'	6.16	125.58	118.80
5	B	42	U	C6-N1-C2	-6.15	117.31	121.00
5	B	77	C	N1-C2-O2	6.13	122.58	118.90
5	B	69	A	C8-N9-C1'	6.11	138.70	127.70
5	B	29	A	C2-N3-C4	6.10	113.65	110.60
5	B	123	C	C6-N1-C2	-6.07	117.87	120.30
5	B	69	A	C4-C5-C6	-6.05	113.98	117.00
5	B	152	C	C4-C5-C6	-6.04	114.38	117.40
6	C	1	DG	OP2-P-O3'	5.99	118.38	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	62	C	N1-C2-O2	5.98	122.49	118.90
5	B	137	U	C6-N1-C1'	-5.97	112.83	121.20
1	A	989	LEU	CA-CB-CG	-5.95	101.62	115.30
5	B	73	U	C5-C6-N1	5.93	125.67	122.70
5	B	103	G	N7-C8-N9	5.88	116.04	113.10
5	B	111	A	C6-N1-C2	5.88	122.13	118.60
5	B	69	A	N3-C4-C5	5.86	130.90	126.80
5	B	94	A	N1-C2-N3	-5.86	126.37	129.30
5	B	114	G	N1-C6-O6	5.86	123.41	119.90
5	B	46	C	C6-N1-C2	5.85	122.64	120.30
5	B	20	A	N9-C4-C5	-5.83	103.47	105.80
5	B	77	C	C5-C6-N1	5.82	123.91	121.00
5	B	124	A	C8-N9-C4	-5.81	103.47	105.80
5	B	42	U	C5-C6-N1	5.79	125.60	122.70
5	B	112	A	C5-N7-C8	-5.77	101.02	103.90
5	B	36	U	N3-C2-O2	-5.75	118.17	122.20
5	B	112	A	N9-C4-C5	-5.75	103.50	105.80
6	C	14	DT	C1'-O4'-C4'	-5.74	104.36	110.10
6	C	9	DT	P-O3'-C3'	5.73	126.58	119.70
5	B	33	A	P-O3'-C3'	5.72	126.57	119.70
1	A	507	LEU	CA-CB-CG	5.71	128.44	115.30
6	C	2	DT	O4'-C4'-C3'	-5.70	102.22	104.50
5	B	8	C	C6-N1-C2	-5.69	118.02	120.30
5	B	46	C	C1'-O4'-C4'	-5.69	105.35	109.90
5	B	29	A	N3-C4-N9	5.68	131.95	127.40
1	A	731	VAL	CG1-CB-CG2	-5.67	101.82	110.90
5	B	114	G	N7-C8-N9	5.66	115.93	113.10
5	B	103	G	N1-C6-O6	5.65	123.29	119.90
2	D	646	LEU	CA-CB-CG	-5.65	102.31	115.30
5	B	148	A	C4-C5-C6	5.64	119.82	117.00
5	B	69	A	N9-C4-C5	5.64	108.06	105.80
1	A	1050	LEU	CA-CB-CG	-5.63	102.34	115.30
5	B	96	U	C6-N1-C2	-5.63	117.62	121.00
5	B	148	A	N3-C4-N9	5.61	131.89	127.40
5	B	136	A	P-O3'-C3'	5.61	126.43	119.70
1	A	703	ILE	CG1-CB-CG2	-5.60	99.08	111.40
5	B	22	A	N3-C4-N9	-5.60	122.92	127.40
1	A	658	ARG	NE-CZ-NH2	-5.59	117.51	120.30
4	E	140	ALA	N-CA-CB	-5.57	102.30	110.10
5	B	83	A	C8-N9-C4	-5.57	103.57	105.80
5	B	20	A	N1-C2-N3	-5.56	126.52	129.30
5	B	77	C	C6-N1-C2	-5.55	118.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	137	U	P-O3'-C3'	5.53	126.33	119.70
5	B	148	A	C5-N7-C8	-5.53	101.14	103.90
5	B	52	A	N9-C4-C5	-5.52	103.59	105.80
5	B	29	A	C4-N9-C1'	5.51	136.22	126.30
1	A	627	ASP	N-CA-C	-5.50	96.14	111.00
6	C	7	DG	O4'-C1'-N9	5.50	111.85	108.00
1	A	707	LEU	CA-CB-CG	5.49	127.93	115.30
5	B	20	A	C4-C5-N7	5.49	113.45	110.70
5	B	136	A	OP2-P-O3'	5.47	117.24	105.20
5	B	113	A	N7-C8-N9	5.47	116.54	113.80
5	B	60	U	P-O3'-C3'	5.47	126.26	119.70
5	B	86	U	N3-C2-O2	-5.47	118.37	122.20
5	B	22	A	C2-N3-C4	-5.46	107.87	110.60
5	B	47	C	N3-C4-C5	-5.45	119.72	121.90
1	A	570	LEU	CA-CB-CG	-5.45	102.76	115.30
5	B	88	C	O4'-C1'-N1	5.45	112.56	108.20
5	B	9	U	N1-C2-O2	5.43	126.60	122.80
5	B	42	U	O4'-C1'-N1	5.43	112.54	108.20
5	B	9	U	C5-C6-N1	5.42	125.41	122.70
5	B	47	C	C4-C5-C6	-5.42	114.69	117.40
5	B	152	C	C5-C4-N4	-5.40	116.42	120.20
5	B	49	C	N3-C4-C5	5.40	124.06	121.90
5	B	57	U	N3-C2-O2	-5.40	118.42	122.20
5	B	33	A	C4-C5-C6	-5.39	114.30	117.00
5	B	59	G	P-O3'-C3'	5.38	126.16	119.70
5	B	95	G	C8-N9-C1'	-5.38	120.00	127.00
5	B	33	A	N3-C4-C5	5.38	130.57	126.80
5	B	75	C	N1-C2-O2	5.37	122.12	118.90
5	B	58	A	O4'-C1'-N9	5.37	112.50	108.20
1	A	585	TYR	CA-CB-CG	5.35	123.56	113.40
5	B	112	A	C6-C5-N7	-5.34	128.56	132.30
5	B	113	A	N1-C6-N6	5.34	121.80	118.60
5	B	29	A	N7-C8-N9	5.30	116.45	113.80
5	B	53	A	N3-C4-N9	-5.30	123.16	127.40
5	B	44	A	C2-N3-C4	-5.30	107.95	110.60
1	A	590	ASN	C-N-CA	5.30	134.94	121.70
5	B	78	C	C5-C6-N1	5.29	123.65	121.00
5	B	103	G	C6-C5-N7	-5.29	127.22	130.40
5	B	152	C	C6-N1-C2	-5.29	118.18	120.30
5	B	114	G	C6-C5-N7	-5.29	127.23	130.40
5	B	70	A	C5-N7-C8	-5.29	101.26	103.90
5	B	59	G	N3-C4-N9	5.28	129.17	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	85	G	C6-C5-N7	-5.28	127.23	130.40
5	B	85	G	C4-C5-N7	5.28	112.91	110.80
5	B	52	A	N3-C4-C5	-5.27	123.11	126.80
5	B	49	C	C6-N1-C2	-5.26	118.20	120.30
5	B	42	U	C6-N1-C1'	5.25	128.54	121.20
5	B	66	U	O5'-P-OP1	-5.23	100.99	105.70
5	B	29	A	N3-C4-C5	-5.18	123.17	126.80
6	C	11	DG	OP2-P-O3'	5.18	116.60	105.20
6	C	15	DT	N3-C4-O4	5.18	123.01	119.90
5	B	18	U	N3-C2-O2	-5.17	118.58	122.20
1	A	593	ILE	CG1-CB-CG2	-5.17	100.02	111.40
5	B	41	U	P-O3'-C3'	5.17	125.90	119.70
5	B	138	U	O4'-C1'-N1	5.16	112.33	108.20
5	B	80	A	C6-N1-C2	5.15	121.69	118.60
5	B	84	G	C4-C5-N7	5.14	112.86	110.80
5	B	52	A	N1-C2-N3	-5.14	126.73	129.30
5	B	44	A	N3-C4-N9	-5.12	123.30	127.40
5	B	132	C	C2-N1-C1'	5.12	124.43	118.80
5	B	69	A	N1-C6-N6	-5.12	115.53	118.60
5	B	124	A	N7-C8-N9	5.11	116.36	113.80
5	B	73	U	C2-N1-C1'	5.11	123.83	117.70
6	C	10	DG	P-O3'-C3'	5.10	125.81	119.70
5	B	6	C	C2-N3-C4	5.08	122.44	119.90
1	A	20	LEU	CA-CB-CG	-5.07	103.64	115.30
5	B	62	C	O4'-C1'-N1	5.07	112.25	108.20
5	B	129	A	N9-C4-C5	-5.07	103.77	105.80
5	B	37	G	N3-C4-C5	5.06	131.13	128.60
5	B	84	G	C6-C5-N7	-5.04	127.38	130.40
5	B	24	C	N1-C2-O2	5.03	121.92	118.90
5	B	53	A	C8-N9-C1'	5.02	136.74	127.70
5	B	83	A	C5-N7-C8	-5.02	101.39	103.90
5	B	29	A	C8-N9-C4	-5.02	103.79	105.80
5	B	62	C	OP2-P-O3'	5.02	116.24	105.20
5	B	44	A	N3-C4-C5	5.01	130.31	126.80
5	B	20	A	C5-C6-N1	5.01	120.20	117.70
5	B	42	U	C2'-C3'-O3'	5.00	121.70	113.70

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1004	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	1007	LEU	Peptide
1	A	122	GLU	Peptide
1	A	144	GLY	Peptide
1	A	17	LYS	Peptide
1	A	217	ASN	Peptide
1	A	233	ASN	Peptide
1	A	238	GLU	Peptide
1	A	240	GLY	Peptide
1	A	299	SER	Peptide
1	A	300	CYS	Peptide
1	A	548	PHE	Peptide
1	A	584	GLY	Peptide
1	A	698	LEU	Peptide
1	A	724	SER	Peptide
1	A	725	ASP	Peptide
1	A	760	PHE	Peptide
1	A	805	GLY	Peptide
1	A	84	PHE	Peptide
1	A	851	THR	Peptide
1	A	853	ASN	Peptide
1	A	865	HIS	Peptide
1	A	924	PHE	Peptide
1	A	933	ASN	Peptide
1	A	936	ILE	Peptide
4	E	122	ASN	Peptide
4	E	123	ASN	Peptide
4	E	125	ASN	Peptide
4	E	61	TYR	Peptide
4	E	81	ASP	Peptide
3	F	21	PHE	Peptide
3	F	58	ASN	Peptide
3	F	65	ASN	Peptide
3	F	97	PHE	Peptide
7	G	108	UNK	Peptide
7	G	109	UNK	Peptide
7	G	110	UNK	Peptide
7	G	136	UNK	Peptide
7	G	62	UNK	Peptide
7	G	66	UNK	Peptide

## 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	8253	0	8327	437	0
2	D	1538	0	1524	76	0
3	F	919	0	898	36	0
4	E	1207	0	1198	75	0
5	B	3322	0	1686	140	0
6	C	406	0	216	16	0
7	G	785	0	177	42	0
8	H	886	0	880	73	0
9	D	1	0	0	0	0
All	All	17317	0	14906	795	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 26.

All (795) 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)
7:G:98:UNK:HA	7:G:123:UNK:CB	1.28	1.60
1:A:530:GLN:HG2	1:A:757:VAL:CG1	1.13	1.59
7:G:75:UNK:HA	7:G:110:UNK:CB	1.37	1.54
7:G:51:UNK:CB	7:G:73:UNK:O	1.64	1.45
7:G:50:UNK:O	7:G:74:UNK:CB	1.69	1.38
8:H:412:ASP:C	8:H:460:GLY:HA3	1.46	1.35
7:G:51:UNK:HA	7:G:74:UNK:CB	1.57	1.33
1:A:530:GLN:CG	1:A:757:VAL:CG1	2.07	1.32
4:E:140:ALA:O	4:E:141:GLN:HG2	1.28	1.31
5:B:122:A:N7	8:H:518:LYS:HD2	1.45	1.29
5:B:121:G:P	8:H:518:LYS:HA	1.72	1.27
7:G:51:UNK:CA	7:G:74:UNK:CB	2.19	1.21
5:B:140:A:H5'	8:H:396:VAL:CG1	1.74	1.16
7:G:50:UNK:C	7:G:74:UNK:CB	2.24	1.15
7:G:98:UNK:CA	7:G:123:UNK:CB	2.24	1.15
7:G:75:UNK:CA	7:G:110:UNK:CB	2.23	1.15
5:B:121:G:OP1	8:H:518:LYS:HA	1.45	1.14
1:A:626:ILE:CG1	1:A:770:GLY:HA2	1.76	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:122:A:N7	8:H:518:LYS:CD	2.10	1.14
5:B:122:A:C8	8:H:518:LYS:HG2	1.85	1.11
4:E:135:LYS:HE2	4:E:137:ARG:HD3	1.22	1.11
4:E:65:GLU:OE2	4:E:136:MET:O	1.67	1.10
4:E:46:ALA:HB1	4:E:138:LYS:HE3	1.31	1.10
5:B:140:A:C5'	8:H:396:VAL:HG11	1.81	1.10
4:E:140:ALA:O	4:E:141:GLN:CG	1.98	1.09
1:A:530:GLN:HG2	1:A:757:VAL:HG12	1.16	1.08
5:B:140:A:H5'	8:H:396:VAL:HG11	1.34	1.08
4:E:135:LYS:HE2	4:E:137:ARG:CD	1.83	1.07
1:A:529:PRO:CB	1:A:554:GLN:HG2	1.83	1.07
5:B:121:G:C1'	8:H:517:LYS:HA	1.86	1.06
4:E:58:TYR:HE2	4:E:136:MET:HG2	1.16	1.05
4:E:135:LYS:CE	4:E:137:ARG:HD3	1.86	1.05
1:A:530:GLN:CG	1:A:757:VAL:HG12	1.76	1.04
7:G:47:UNK:O	7:G:77:UNK:O	1.76	1.04
1:A:626:ILE:HG12	1:A:770:GLY:HA2	1.33	1.03
5:B:121:G:C1'	8:H:520:GLU:HB3	1.89	1.02
1:A:529:PRO:HA	1:A:554:GLN:HE21	1.23	1.02
1:A:530:GLN:HG2	1:A:757:VAL:HG13	1.03	1.00
1:A:824:GLN:O	1:A:828:LEU:HB2	1.62	1.00
5:B:121:G:OP1	8:H:518:LYS:CA	2.10	1.00
5:B:122:A:N7	8:H:518:LYS:CG	2.26	0.99
5:B:121:G:C1'	8:H:517:LYS:CA	2.40	0.99
1:A:593:ILE:O	1:A:597:PHE:HB3	1.63	0.98
5:B:146:G:O2'	8:H:528:LYS:HE3	1.63	0.98
1:A:912:LEU:O	1:A:916:LEU:HB2	1.63	0.98
7:G:51:UNK:CA	7:G:73:UNK:O	2.12	0.98
4:E:58:TYR:CE2	4:E:136:MET:HG2	2.01	0.95
5:B:121:G:P	8:H:518:LYS:CA	2.53	0.95
1:A:530:GLN:HG2	1:A:757:VAL:HG11	1.48	0.94
7:G:51:UNK:CB	7:G:73:UNK:C	2.44	0.94
7:G:97:UNK:O	7:G:123:UNK:CB	2.17	0.92
2:D:577:GLN:OE1	2:D:579:ILE:HB	1.69	0.91
1:A:626:ILE:HB	1:A:770:GLY:N	1.86	0.90
5:B:140:A:H5'	8:H:396:VAL:HG12	1.52	0.89
1:A:529:PRO:HB2	1:A:554:GLN:HG2	1.53	0.89
1:A:626:ILE:HG13	1:A:771:ILE:HG12	1.54	0.88
1:A:626:ILE:CD1	1:A:771:ILE:HG12	2.04	0.88
5:B:121:G:OP1	8:H:518:LYS:CB	2.23	0.86
7:G:51:UNK:HA	7:G:73:UNK:C	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:122:A:C8	8:H:518:LYS:CG	2.58	0.86
1:A:530:GLN:CG	1:A:757:VAL:HG13	1.87	0.85
4:E:140:ALA:C	4:E:141:GLN:HG2	1.97	0.85
1:A:787:GLY:O	1:A:791:GLU:HB2	1.76	0.85
1:A:658:ARG:HH22	1:A:697:ASN:HB2	1.42	0.84
8:H:412:ASP:C	8:H:460:GLY:CA	2.40	0.83
1:A:462:PHE:O	1:A:466:LYS:HB2	1.79	0.82
1:A:1017:ILE:O	1:A:1021:PHE:HB2	1.81	0.81
1:A:626:ILE:CG1	1:A:771:ILE:HG12	2.10	0.81
1:A:984:THR:O	1:A:988:PHE:HB3	1.81	0.80
7:G:75:UNK:CB	7:G:110:UNK:C	2.58	0.80
1:A:529:PRO:CA	1:A:554:GLN:HG2	2.11	0.80
7:G:51:UNK:N	7:G:74:UNK:CB	2.45	0.80
5:B:122:A:H2	8:H:407:TYR:CG	2.00	0.79
5:B:117:U:C1'	8:H:526:PHE:HB2	2.12	0.79
2:D:572:CYS:SG	2:D:579:ILE:HB	2.23	0.79
4:E:136:MET:HG3	4:E:142:ILE:HD11	1.65	0.79
5:B:120:C:C4	8:H:522:ARG:HA	2.18	0.79
7:G:75:UNK:CB	7:G:110:UNK:O	2.32	0.78
5:B:86:U:O2	5:B:88:C:N4	2.17	0.77
1:A:626:ILE:CG1	1:A:770:GLY:CA	2.60	0.77
1:A:582:LYS:HA	1:A:787:GLY:HA2	1.67	0.76
4:E:39:ILE:HD11	4:E:136:MET:CE	2.15	0.76
5:B:117:U:O4'	8:H:526:PHE:HD2	1.69	0.76
4:E:39:ILE:HD11	4:E:136:MET:HE3	1.67	0.75
7:G:51:UNK:HA	7:G:74:UNK:CA	2.16	0.75
1:A:549:LEU:O	1:A:554:GLN:OE1	2.04	0.75
4:E:59:GLU:HA	4:E:63:ALA:HA	1.70	0.74
5:B:128:G:N2	5:B:142:C:O2	2.18	0.74
5:B:140:A:O2'	8:H:393:ALA:HA	1.88	0.73
1:A:530:GLN:HG3	1:A:757:VAL:HG12	1.68	0.73
3:F:42:VAL:HG13	3:F:58:ASN:HD21	1.53	0.73
5:B:121:G:OP1	8:H:518:LYS:HG2	1.88	0.73
4:E:135:LYS:NZ	4:E:137:ARG:HD3	2.03	0.73
1:A:651:LEU:HD23	1:A:700:GLU:HB3	1.71	0.73
5:B:121:G:OP2	8:H:521:PHE:CB	2.34	0.73
1:A:766:ARG:HH22	1:A:772:PRO:HD3	1.54	0.72
1:A:529:PRO:CA	1:A:554:GLN:HE21	1.99	0.72
1:A:529:PRO:HA	1:A:554:GLN:NE2	2.01	0.72
1:A:617:LEU:HB3	1:A:817:TYR:HB3	1.73	0.71
1:A:889:LYS:HA	1:A:945:GLN:HE22	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:141:U:H4'	8:H:392:LYS:HD3	1.73	0.70
3:F:33:CYS:H	3:F:44:GLU:HA	1.54	0.70
7:G:74:UNK:O	7:G:111:UNK:N	2.25	0.70
1:A:103:LYS:HG3	2:D:640:ARG:HH22	1.56	0.70
5:B:128:G:N1	5:B:142:C:N3	2.36	0.70
5:B:122:A:C8	8:H:518:LYS:CD	2.75	0.69
1:A:558:LYS:HA	1:A:561:LEU:HD12	1.75	0.69
5:B:94:A:H3'	5:B:95:G:H21	1.57	0.69
2:D:572:CYS:SG	2:D:579:ILE:CG2	2.80	0.69
4:E:135:LYS:HE2	4:E:137:ARG:CG	2.23	0.69
4:E:46:ALA:CB	4:E:138:LYS:HE3	2.18	0.68
5:B:70:A:H2	5:B:88:C:H41	1.40	0.68
1:A:630:LYS:O	1:A:788:LYS:NZ	2.25	0.68
5:B:121:G:H2'	8:H:517:LYS:HB3	1.76	0.68
8:H:412:ASP:O	8:H:460:GLY:HA3	1.93	0.68
1:A:626:ILE:CB	1:A:770:GLY:HA2	2.23	0.68
5:B:43:C:H4'	5:B:44:A:H5'	1.74	0.67
5:B:122:A:C2	8:H:407:TYR:CG	2.82	0.67
1:A:790:GLU:OE2	1:A:812:ARG:NH1	2.26	0.67
1:A:944:ARG:O	1:A:948:HIS:HB2	1.93	0.67
4:E:56:ASN:HA	4:E:138:LYS:HB2	1.76	0.67
5:B:140:A:C4'	8:H:396:VAL:HG11	2.25	0.67
2:D:514:TYR:HA	2:D:536:TYR:HB3	1.77	0.67
3:F:14:LEU:HD21	3:F:47:PRO:HD2	1.77	0.67
1:A:528:TYR:HB3	1:A:530:GLN:NE2	2.09	0.66
1:A:643:ASP:H	1:A:740:ILE:HA	1.59	0.66
5:B:121:G:OP1	8:H:518:LYS:CG	2.42	0.66
5:B:149:U:H2'	5:B:150:G:H8	1.60	0.66
2:D:612:ASN:HD22	2:D:620:VAL:HG13	1.59	0.66
1:A:615:VAL:HB	1:A:819:PHE:HB2	1.77	0.66
1:A:923:LEU:HA	1:A:927:GLN:HE21	1.61	0.66
7:G:75:UNK:CB	7:G:110:UNK:CB	2.73	0.66
1:A:1051:LEU:HA	1:A:1054:ILE:HD12	1.77	0.66
7:G:100:UNK:HA	7:G:121:UNK:CB	2.26	0.66
5:B:140:A:C5'	8:H:396:VAL:CG1	2.52	0.65
2:D:564:LYS:HB3	6:C:6:DG:H4'	1.78	0.65
4:E:140:ALA:O	4:E:141:GLN:CB	2.44	0.65
1:A:626:ILE:HB	1:A:770:GLY:CA	2.26	0.65
1:A:481:LYS:HB3	1:A:484:GLU:HB2	1.79	0.65
5:B:121:G:O4'	8:H:521:PHE:N	2.29	0.65
5:B:122:A:N7	8:H:518:LYS:HG2	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:71:UNK:O	7:G:73:UNK:N	2.29	0.65
1:A:168:GLN:NE2	1:A:172:VAL:O	2.28	0.65
1:A:331:CYS:O	1:A:492:ARG:NH1	2.30	0.65
2:D:572:CYS:SG	2:D:577:GLN:O	2.52	0.64
8:H:464:ILE:HD12	8:H:464:ILE:N	2.12	0.64
1:A:127:SER:O	1:A:131:LEU:N	2.29	0.64
1:A:913:LYS:NZ	5:B:58:A:N7	2.41	0.64
4:E:88:LYS:HG2	4:E:97:GLU:HG2	1.79	0.64
7:G:49:UNK:O	7:G:75:UNK:O	2.15	0.64
1:A:139:LEU:O	1:A:143:PHE:HB2	1.97	0.64
2:D:577:GLN:OE1	2:D:579:ILE:CB	2.43	0.64
5:B:121:G:H2'	8:H:517:LYS:HD2	1.79	0.64
3:F:100:ASP:OD1	3:F:104:LYS:NZ	2.32	0.63
2:D:631:ILE:HA	2:D:636:GLU:HB3	1.81	0.63
1:A:229:ILE:HD11	1:A:472:LEU:HB2	1.80	0.63
1:A:528:TYR:CB	1:A:530:GLN:NE2	2.62	0.63
1:A:538:LYS:HE2	1:A:543:ARG:HD3	1.79	0.63
1:A:1103:LEU:O	1:A:1107:ILE:N	2.30	0.63
3:F:104:LYS:O	3:F:108:LEU:HB2	1.98	0.63
4:E:118:ILE:HG23	4:E:126:ARG:HG2	1.79	0.63
1:A:113:THR:HB	1:A:120:GLU:H	1.63	0.63
1:A:1007:LEU:HD13	1:A:1009:PHE:HB2	1.80	0.63
4:E:68:ILE:HG12	4:E:133:MET:HG2	1.79	0.63
1:A:539:LYS:HG3	1:A:541:SER:H	1.62	0.63
1:A:626:ILE:HD11	1:A:771:ILE:HG12	1.81	0.63
2:D:553:TYR:HA	2:D:583:VAL:HA	1.80	0.63
7:G:84:UNK:HA	7:G:99:UNK:HA	1.81	0.62
5:B:126:U:H3	5:B:144:A:H2	1.45	0.62
7:G:51:UNK:CA	7:G:73:UNK:C	2.66	0.62
1:A:397:ASN:ND2	1:A:427:ASP:O	2.33	0.62
1:A:460:ILE:HA	1:A:463:ILE:HD12	1.82	0.62
1:A:594:SER:O	1:A:598:ALA:HB3	2.00	0.62
1:A:579:LEU:O	1:A:581:GLN:NE2	2.31	0.62
1:A:605:LYS:HG2	1:A:610:PRO:HA	1.81	0.62
1:A:412:LYS:NZ	1:A:899:ILE:O	2.32	0.62
1:A:975:TYR:O	1:A:979:TYR:HB2	2.00	0.62
1:A:945:GLN:O	1:A:949:HIS:ND1	2.25	0.62
1:A:1070:GLN:NE2	1:A:1074:SER:OG	2.33	0.62
1:A:224:ILE:O	1:A:416:ASN:ND2	2.33	0.61
1:A:314:ILE:HG23	1:A:387:CYS:HB3	1.82	0.61
1:A:589:ASP:OD1	1:A:590:ASN:ND2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:107:G:H3'	5:B:108:A:H8	1.65	0.61
1:A:702:GLN:NE2	1:A:703:ILE:O	2.30	0.61
1:A:1103:LEU:HA	1:A:1106:LYS:HB2	1.81	0.61
1:A:63:THR:HG23	1:A:159:THR:HG22	1.83	0.61
1:A:626:ILE:HG13	1:A:770:GLY:HA2	1.80	0.60
2:D:560:LYS:N	6:C:2:DT:OP1	2.33	0.60
1:A:1080:LEU:HA	1:A:1084:GLU:HB3	1.81	0.60
7:G:51:UNK:HA	7:G:74:UNK:N	2.15	0.60
7:G:139:UNK:O	7:G:143:UNK:N	2.35	0.60
2:D:652:ILE:HB	2:D:676:GLU:HB2	1.83	0.60
2:D:573:GLU:O	2:D:576:GLN:NE2	2.34	0.60
2:D:642:LEU:HD12	2:D:645:LYS:HD2	1.84	0.60
2:D:689:LYS:O	2:D:693:HIS:ND1	2.31	0.60
1:A:881:ILE:HG12	1:A:888:ILE:HG23	1.82	0.60
1:A:626:ILE:HB	1:A:770:GLY:H	1.64	0.60
3:F:78:LEU:HB2	3:F:82:ILE:HB	1.83	0.60
1:A:949:HIS:O	1:A:953:THR:OG1	2.20	0.59
5:B:120:C:N3	8:H:522:ARG:CB	2.65	0.59
7:G:51:UNK:C	7:G:74:UNK:CB	2.79	0.59
1:A:125:ASN:OD1	1:A:127:SER:OG	2.17	0.59
1:A:241:VAL:HG21	1:A:471:VAL:HG22	1.84	0.59
5:B:110:A:OP2	5:B:155:A:N6	2.35	0.59
1:A:539:LYS:HE3	1:A:541:SER:HB3	1.83	0.59
1:A:750:LYS:HG2	1:A:754:GLN:HE22	1.66	0.59
1:A:615:VAL:HG21	1:A:831:ILE:HD11	1.85	0.59
1:A:888:ILE:O	1:A:945:GLN:NE2	2.34	0.59
3:F:110:GLN:O	3:F:115:SER:OG	2.20	0.59
5:B:95:G:OP2	5:B:95:G:N2	2.35	0.59
5:B:60:U:O2'	5:B:61:G:N2	2.35	0.59
5:B:140:A:H4'	8:H:396:VAL:CG1	2.33	0.59
1:A:463:ILE:O	1:A:467:ILE:HB	2.02	0.59
1:A:648:ASN:ND2	1:A:705:TYR:OH	2.36	0.59
1:A:1008:GLN:HB3	1:A:1012:GLU:HB2	1.85	0.59
1:A:1098:GLN:NE2	1:A:1102:THR:OG1	2.35	0.59
1:A:157:VAL:HB	1:A:170:ALA:HB3	1.84	0.59
1:A:237:ARG:NE	5:B:36:U:O4	2.36	0.59
1:A:471:VAL:O	1:A:475:ASN:ND2	2.36	0.59
1:A:533:LEU:HA	1:A:546:MET:HG3	1.83	0.59
1:A:975:TYR:O	1:A:979:TYR:CB	2.51	0.59
1:A:161:VAL:HG22	1:A:167:LEU:HD11	1.85	0.59
1:A:239:PRO:HB2	1:A:323:PHE:HD2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:ARG:HD2	7:G:3:UNK:HA	1.84	0.59
5:B:32:G:H2'	5:B:33:A:C8	2.37	0.59
5:B:122:A:N3	8:H:407:TYR:CD2	2.71	0.58
3:F:74:ARG:NH2	4:E:129:TYR:OH	2.35	0.58
5:B:146:G:H4'	5:B:147:G:H4'	1.86	0.58
1:A:528:TYR:HB2	1:A:530:GLN:HE22	1.68	0.58
1:A:594:SER:HA	1:A:597:PHE:HD2	1.69	0.58
4:E:36:CYS:O	4:E:40:ASN:ND2	2.36	0.58
1:A:555:LYS:HA	1:A:558:LYS:HE2	1.84	0.58
1:A:812:ARG:HE	1:A:817:TYR:HB2	1.69	0.58
5:B:140:A:H4'	8:H:396:VAL:HG11	1.85	0.58
5:B:47:C:H2'	5:B:48:C:C6	2.39	0.58
5:B:117:U:O4'	8:H:526:PHE:CD2	2.55	0.58
1:A:357:GLN:HE21	1:A:361:ASN:HD21	1.51	0.58
1:A:655:ARG:NH2	5:B:51:A:O3'	2.36	0.58
4:E:67:ALA:HB3	4:E:134:LEU:HB2	1.86	0.58
7:G:78:UNK:N	7:G:105:UNK:O	2.36	0.58
1:A:583:ILE:HG13	1:A:790:GLU:HB3	1.85	0.58
1:A:984:THR:O	1:A:988:PHE:CB	2.51	0.58
3:F:14:LEU:HD11	3:F:47:PRO:HG2	1.86	0.58
7:G:89:UNK:O	7:G:94:UNK:N	2.36	0.58
2:D:572:CYS:SG	2:D:579:ILE:CB	2.90	0.58
4:E:114:GLN:OE1	4:E:147:PHE:N	2.37	0.57
4:E:43:VAL:HG12	4:E:47:LYS:HE3	1.85	0.57
5:B:117:U:C1'	8:H:526:PHE:HD2	2.17	0.57
5:B:149:U:H2'	5:B:150:G:C8	2.39	0.57
1:A:882:ASP:O	1:A:887:GLU:N	2.36	0.57
2:D:564:LYS:HD3	6:C:5:DG:H2''	1.85	0.57
1:A:981:LYS:HE3	1:A:983:ASN:HB2	1.86	0.57
1:A:971:LYS:NZ	5:B:137:U:OP2	2.33	0.57
2:D:563:LEU:N	2:D:571:PHE:O	2.38	0.57
1:A:110:ILE:O	1:A:734:GLN:NE2	2.37	0.57
1:A:796:PHE:HB2	1:A:797:LEU:HD22	1.86	0.57
1:A:849:LYS:H	1:A:869:SER:HB3	1.69	0.57
5:B:102:U:H2'	5:B:103:G:H8	1.69	0.57
7:G:75:UNK:CB	7:G:110:UNK:CA	2.83	0.57
1:A:156:LEU:HD11	1:A:172:VAL:HG12	1.87	0.57
1:A:1030:TRP:HA	1:A:1033:ILE:HD12	1.86	0.57
1:A:390:ASN:O	1:A:394:GLY:N	2.38	0.56
4:E:73:PHE:HA	4:E:89:LEU:HG	1.87	0.56
6:C:9:DT:H2''	6:C:10:DG:H3'	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:SER:OG	1:A:35:ASN:N	2.37	0.56
1:A:333:LEU:HD12	5:B:15:C:H2'	1.86	0.56
3:F:18:MET:SD	3:F:22:ARG:NH2	2.79	0.56
1:A:787:GLY:O	1:A:791:GLU:CB	2.53	0.56
1:A:880:SER:O	1:A:889:LYS:N	2.33	0.56
3:F:78:LEU:N	3:F:82:ILE:O	2.36	0.56
1:A:394:GLY:O	1:A:398:PHE:N	2.35	0.56
5:B:117:U:C1'	8:H:526:PHE:CB	2.83	0.56
1:A:794:THR:HG22	1:A:798:LYS:HE2	1.88	0.56
2:D:687:LEU:HD21	3:F:104:LYS:HD2	1.88	0.56
1:A:110:ILE:HG22	1:A:734:GLN:HG3	1.87	0.56
1:A:347:ILE:HA	1:A:351:GLU:HB3	1.86	0.56
1:A:881:ILE:HG23	1:A:888:ILE:HG12	1.88	0.55
2:D:661:GLU:HG2	2:D:663:ASN:H	1.71	0.55
5:B:52:A:O2'	5:B:53:A:O4'	2.24	0.55
5:B:111:A:H2'	5:B:112:A:C8	2.41	0.55
7:G:53:UNK:CB	7:G:62:UNK:CB	2.84	0.55
1:A:576:LYS:HZ3	1:A:586:SER:HB3	1.71	0.55
2:D:537:VAL:HG23	2:D:653:PHE:HB2	1.87	0.55
1:A:156:LEU:HG	1:A:171:GLY:HA3	1.89	0.55
3:F:57:ASP:OD1	3:F:60:ARG:NH2	2.39	0.55
4:E:136:MET:HG3	4:E:142:ILE:CD1	2.35	0.55
5:B:52:A:N6	6:C:13:DG:OP1	2.34	0.55
5:B:124:A:O2'	5:B:148:A:O2'	2.16	0.55
1:A:303:GLU:HA	1:A:306:LEU:HD12	1.87	0.55
2:D:562:VAL:HA	2:D:572:CYS:HA	1.88	0.55
4:E:39:ILE:CG1	4:E:136:MET:HE1	2.36	0.55
1:A:129:GLN:NE2	7:G:107:UNK:O	2.40	0.55
5:B:140:A:O2'	8:H:393:ALA:CA	2.54	0.55
1:A:944:ARG:NH2	1:A:1108:SER:O	2.39	0.55
3:F:40:SER:O	3:F:60:ARG:NH2	2.35	0.55
5:B:121:G:C2'	8:H:517:LYS:HB3	2.37	0.55
1:A:233:ASN:H	1:A:234:HIS:CD2	2.25	0.54
1:A:786:PHE:O	1:A:790:GLU:HB2	2.07	0.54
5:B:102:U:H2'	5:B:103:G:C8	2.42	0.54
1:A:234:HIS:CD2	5:B:39:C:H2'	2.42	0.54
1:A:1000:VAL:HA	1:A:1003:ILE:HG22	1.89	0.54
1:A:229:ILE:HG23	1:A:478:ILE:HG21	1.88	0.54
7:G:99:UNK:O	7:G:121:UNK:O	2.24	0.54
1:A:626:ILE:HG13	1:A:770:GLY:C	2.27	0.54
5:B:47:C:H2'	5:B:48:C:H6	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:LYS:HB3	1:A:850:ILE:HG23	1.90	0.54
3:F:40:SER:HB3	3:F:60:ARG:HE	1.72	0.54
2:D:553:TYR:OH	2:D:564:LYS:NZ	2.37	0.54
4:E:39:ILE:HG12	4:E:136:MET:HE1	1.90	0.54
5:B:115:A:N1	5:B:152:C:N4	2.56	0.54
1:A:694:TYR:HB2	1:A:696:PHE:HE1	1.73	0.54
4:E:39:ILE:HD11	4:E:136:MET:HE1	1.89	0.54
1:A:501:LYS:HA	1:A:504:ILE:HD12	1.89	0.54
1:A:961:MET:O	1:A:965:PHE:CB	2.55	0.54
1:A:96:SER:HA	1:A:99:LEU:HD12	1.90	0.54
1:A:533:LEU:HD23	1:A:760:PHE:HB2	1.90	0.54
4:E:135:LYS:HZ1	4:E:137:ARG:HD3	1.72	0.54
2:D:606:GLN:NE2	2:D:673:LEU:O	2.42	0.53
1:A:78:LYS:HZ3	4:E:104:LYS:HE3	1.74	0.53
1:A:106:TYR:HB2	1:A:109:GLN:HG3	1.91	0.53
1:A:530:GLN:CB	1:A:757:VAL:HG13	2.37	0.53
1:A:723:GLN:NE2	1:A:724:SER:O	2.41	0.53
1:A:826:ASN:O	1:A:830:LEU:HB2	2.08	0.53
1:A:360:GLU:O	1:A:364:ASN:ND2	2.42	0.53
1:A:649:LYS:HB3	1:A:731:VAL:HG12	1.91	0.53
2:D:543:SER:O	2:D:545:GLN:NE2	2.42	0.53
1:A:588:PHE:HE2	1:A:591:LYS:H	1.55	0.53
1:A:981:LYS:HG2	1:A:983:ASN:H	1.74	0.53
4:E:130:VAL:HG12	4:E:149:ILE:HA	1.90	0.53
2:D:524:ALA:HB1	2:D:668:ILE:HG21	1.89	0.53
2:D:660:LYS:NZ	6:C:4:DG:O6	2.42	0.53
4:E:100:ILE:HA	4:E:143:GLN:HE22	1.73	0.53
1:A:626:ILE:HG13	1:A:770:GLY:CA	2.36	0.53
5:B:112:A:H2'	5:B:113:A:C8	2.43	0.53
1:A:384:ILE:HG21	1:A:401:PHE:HE2	1.72	0.53
2:D:656:GLN:HB2	2:D:673:LEU:HD11	1.90	0.53
1:A:626:ILE:HB	1:A:770:GLY:HA2	1.90	0.53
1:A:340:LEU:HA	1:A:343:GLN:HE21	1.73	0.52
1:A:626:ILE:CB	1:A:770:GLY:CA	2.86	0.52
1:A:336:ASN:OD1	1:A:336:ASN:N	2.43	0.52
1:A:536:ILE:HB	1:A:544:PRO:HA	1.89	0.52
1:A:827:ALA:HA	1:A:830:LEU:HD13	1.91	0.52
2:D:535:PHE:N	2:D:655:ILE:O	2.42	0.52
1:A:604:TRP:O	1:A:608:GLY:N	2.43	0.52
2:D:514:TYR:HE1	2:D:685:LYS:HB3	1.74	0.52
4:E:58:TYR:CE1	4:E:138:LYS:HD3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ASP:HA	1:A:308:LEU:HD12	1.92	0.52
1:A:626:ILE:HG13	1:A:771:ILE:N	2.24	0.52
5:B:121:G:O5'	8:H:518:LYS:HA	2.09	0.52
2:D:586:MET:O	2:D:588:ARG:NH1	2.41	0.52
1:A:125:ASN:HB2	1:A:734:GLN:NE2	2.25	0.52
1:A:454:LYS:NZ	1:A:458:ASP:OD2	2.41	0.52
1:A:28:SER:HB3	1:A:693:PRO:HD2	1.91	0.52
1:A:30:LEU:HD13	1:A:66:ALA:HB1	1.91	0.52
1:A:623:TYR:O	1:A:626:ILE:HG12	2.10	0.52
1:A:790:GLU:O	1:A:794:THR:OG1	2.20	0.52
1:A:907:ILE:O	1:A:915:GLN:NE2	2.39	0.52
2:D:515:SER:N	2:D:536:TYR:O	2.40	0.52
2:D:572:CYS:N	2:D:577:GLN:O	2.33	0.52
7:G:97:UNK:C	7:G:123:UNK:CB	2.88	0.52
1:A:166:TYR:O	1:A:730:ILE:N	2.38	0.52
1:A:815:ASP:OD1	1:A:815:ASP:N	2.43	0.52
1:A:860:ASP:HA	1:A:863:LEU:HD12	1.90	0.52
3:F:27:THR:HA	3:F:74:ARG:HG2	1.91	0.52
5:B:140:A:H4'	8:H:396:VAL:HB	1.92	0.52
1:A:85:SER:OG	1:A:86:GLN:OE1	2.22	0.51
1:A:528:TYR:CB	1:A:530:GLN:HE22	2.23	0.51
3:F:112:ASP:OD2	3:F:113:LYS:NZ	2.41	0.51
3:F:15:PHE:HA	3:F:21:PHE:HZ	1.75	0.51
7:G:53:UNK:O	7:G:61:UNK:N	2.43	0.51
1:A:479:THR:OG1	1:A:480:GLU:N	2.44	0.51
4:E:141:GLN:O	4:E:142:ILE:HD13	2.10	0.51
1:A:317:ASN:ND2	1:A:387:CYS:O	2.43	0.51
1:A:440:GLN:HA	1:A:443:THR:HB	1.91	0.51
1:A:593:ILE:HD13	1:A:811:MET:HG3	1.93	0.51
1:A:741:THR:OG1	1:A:742:LYS:N	2.43	0.51
1:A:1034:VAL:HG22	1:A:1054:ILE:HD13	1.91	0.51
4:E:46:ALA:HB1	4:E:138:LYS:CE	2.22	0.51
4:E:107:ASP:HA	4:E:110:PRO:HD2	1.92	0.51
1:A:599:GLN:NE2	1:A:934:PRO:O	2.42	0.51
4:E:125:ASN:O	4:E:128:LYS:NZ	2.44	0.51
4:E:58:TYR:CE2	4:E:136:MET:CG	2.84	0.51
4:E:91:ASP:OD1	4:E:94:GLY:N	2.44	0.51
3:F:55:VAL:HB	3:F:82:ILE:HA	1.91	0.51
1:A:81:GLN:HE22	4:E:82:SER:H	1.57	0.51
4:E:58:TYR:HE2	4:E:136:MET:CG	2.05	0.51
1:A:64:ILE:N	1:A:158:PHE:O	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:GLN:HA	1:A:740:ILE:HG23	1.93	0.51
1:A:916:LEU:HG	1:A:992:ILE:HG12	1.93	0.51
1:A:916:LEU:HA	1:A:919:LYS:HB2	1.92	0.50
5:B:122:A:C2	8:H:407:TYR:CD2	2.98	0.50
1:A:534:ARG:HH11	1:A:545:ILE:HD11	1.76	0.50
1:A:882:ASP:OD1	1:A:884:ASN:ND2	2.44	0.50
3:F:112:ASP:O	3:F:116:SER:N	2.43	0.50
6:C:17:DG:H2'	6:C:18:DG:C8	2.46	0.50
1:A:632:LEU:O	1:A:636:ASN:ND2	2.44	0.50
5:B:141:U:C5'	8:H:392:LYS:HD3	2.41	0.50
1:A:507:LEU:HD21	1:A:765:PHE:HB2	1.93	0.50
1:A:1038:LYS:NZ	5:B:71:C:OP2	2.31	0.50
1:A:481:LYS:NZ	1:A:539:LYS:O	2.35	0.50
1:A:337:TYR:OH	5:B:16:A:O3'	2.27	0.50
1:A:746:HIS:HA	1:A:749:LEU:HD12	1.93	0.50
1:A:905:VAL:HA	1:A:960:PHE:HE1	1.76	0.50
2:D:552:TYR:N	2:D:584:HIS:O	2.40	0.50
1:A:626:ILE:CD1	1:A:771:ILE:CG1	2.86	0.50
1:A:934:PRO:HB2	1:A:937:ASN:H	1.75	0.50
1:A:436:ASP:OD1	1:A:448:TYR:OH	2.29	0.50
1:A:594:SER:O	1:A:598:ALA:CB	2.60	0.50
1:A:924:PHE:CE1	5:B:51:A:H2'	2.46	0.50
2:D:517:ILE:HD11	2:D:591:VAL:HG12	1.94	0.50
1:A:624:ASP:HA	1:A:770:GLY:HA3	1.94	0.50
1:A:1017:ILE:O	1:A:1021:PHE:CB	2.55	0.50
8:H:474:LEU:O	8:H:477:GLN:HG2	2.11	0.50
1:A:608:GLY:O	1:A:609:ARG:NH1	2.38	0.49
1:A:947:TYR:HB2	1:A:1032:ILE:HD11	1.94	0.49
2:D:533:LYS:HB3	2:D:657:PHE:CE1	2.47	0.49
1:A:749:LEU:HD23	1:A:752:ILE:HD11	1.93	0.49
1:A:123:ASN:HA	1:A:736:LYS:HE3	1.93	0.49
1:A:953:THR:O	1:A:957:PHE:HB2	2.13	0.49
1:A:53:ASP:O	1:A:57:GLN:N	2.46	0.49
1:A:614:TYR:O	1:A:851:THR:OG1	2.30	0.49
1:A:235:MET:O	5:B:18:U:N3	2.46	0.49
5:B:139:U:O2'	8:H:400:ARG:NH1	2.46	0.49
1:A:412:LYS:N	1:A:415:GLU:OE1	2.45	0.49
5:B:120:C:C4	8:H:522:ARG:CA	2.94	0.49
1:A:658:ARG:NH2	1:A:697:ASN:HB2	2.20	0.49
2:D:518:GLU:HB2	2:D:595:THR:HB	1.94	0.49
2:D:564:LYS:NZ	6:C:6:DG:N3	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ILE:HG21	1:A:695:TYR:HA	1.94	0.48
1:A:891:ILE:O	1:A:948:HIS:NE2	2.45	0.48
1:A:937:ASN:HB2	1:A:942:LEU:HD21	1.93	0.48
1:A:1039:LYS:O	1:A:1041:LYS:NZ	2.44	0.48
5:B:121:G:O4'	8:H:520:GLU:HB3	2.11	0.48
1:A:14:LEU:HA	1:A:1002:LYS:HD2	1.96	0.48
1:A:452:LYS:HA	1:A:455:ILE:HD12	1.94	0.48
2:D:602:ILE:HG13	2:D:672:VAL:HG21	1.95	0.48
5:B:120:C:C5	8:H:522:ARG:HA	2.49	0.48
1:A:882:ASP:N	1:A:887:GLU:O	2.45	0.48
1:A:926:ASN:N	1:A:926:ASN:OD1	2.44	0.48
2:D:529:ILE:HG21	2:D:663:ASN:HD21	1.78	0.48
5:B:2:U:H4'	5:B:3:A:H8	1.78	0.48
1:A:563:GLN:HG3	1:A:645:TYR:OH	2.13	0.48
1:A:585:TYR:CD1	1:A:593:ILE:HG13	2.49	0.48
1:A:619:ILE:HA	1:A:845:PHE:HB3	1.96	0.48
1:A:701:ARG:CZ	1:A:703:ILE:HG12	2.44	0.48
1:A:1053:LYS:NZ	5:B:61:G:N7	2.62	0.48
5:B:153:U:H2'	5:B:154:U:C2	2.49	0.48
1:A:390:ASN:HB2	1:A:395:LYS:HA	1.95	0.48
1:A:400:VAL:O	1:A:404:LYS:HG2	2.13	0.48
1:A:446:ARG:HH21	5:B:134:C:H1'	1.78	0.48
4:E:44:LYS:HA	4:E:47:LYS:HD2	1.96	0.48
5:B:113:A:H2'	5:B:114:G:C8	2.47	0.48
5:B:121:G:H2'	8:H:517:LYS:CB	2.43	0.48
5:B:61:G:O2'	5:B:63:U:OP1	2.23	0.48
7:G:48:UNK:HA	7:G:77:UNK:O	2.13	0.48
4:E:65:GLU:OE2	4:E:137:ARG:HA	2.14	0.48
8:H:487:LEU:CB	8:H:498:VAL:HG22	2.43	0.48
1:A:492:ARG:HB2	1:A:495:ILE:HD12	1.94	0.48
1:A:652:LEU:HD11	1:A:727:ARG:HG3	1.96	0.48
1:A:738:ARG:NH1	7:G:2:UNK:O	2.47	0.48
1:A:742:LYS:HA	1:A:745:ILE:HD12	1.96	0.48
1:A:944:ARG:HA	1:A:947:TYR:CE1	2.49	0.48
5:B:117:U:C1'	8:H:526:PHE:CD2	2.96	0.48
1:A:108:GLN:OE1	1:A:108:GLN:N	2.42	0.48
1:A:124:ILE:HG13	1:A:736:LYS:HG2	1.95	0.48
1:A:897:GLN:HA	1:A:900:ASN:HD22	1.78	0.48
2:D:560:LYS:HB3	2:D:573:GLU:HB2	1.96	0.48
6:C:9:DT:H1'	6:C:10:DG:H8	1.78	0.48
1:A:32:TYR:HB3	1:A:67:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:LYS:HA	1:A:759:SER:H	1.79	0.47
1:A:1019:GLU:O	1:A:1023:ASN:ND2	2.47	0.47
1:A:1044:LYS:HA	1:A:1047:LEU:HB2	1.96	0.47
2:D:608:SER:HA	2:D:611:ILE:HD12	1.95	0.47
5:B:122:A:N6	8:H:514:ILE:CB	2.77	0.47
5:B:146:G:N2	5:B:148:A:N7	2.60	0.47
1:A:694:TYR:HB2	1:A:696:PHE:CE1	2.49	0.47
8:H:515:LYS:NZ	8:H:515:LYS:HB3	2.29	0.47
1:A:298:PHE:HD2	1:A:304:ARG:HB2	1.80	0.47
1:A:529:PRO:C	1:A:554:GLN:NE2	2.68	0.47
1:A:614:TYR:HB2	1:A:818:LEU:HD11	1.96	0.47
1:A:529:PRO:C	1:A:554:GLN:HE21	2.17	0.47
1:A:910:LYS:HD2	5:B:135:U:H1'	1.95	0.47
4:E:39:ILE:CD1	4:E:136:MET:HE1	2.45	0.47
5:B:140:A:H4'	8:H:396:VAL:CB	2.44	0.47
6:C:14:DT:H1'	6:C:15:DT:C6	2.49	0.47
2:D:606:GLN:HE22	2:D:674:LYS:HD2	1.79	0.47
2:D:651:PHE:HB2	2:D:653:PHE:CZ	2.50	0.47
3:F:10:TYR:CG	3:F:74:ARG:HD3	2.48	0.47
4:E:70:THR:HG23	4:E:150:VAL:HG21	1.96	0.47
7:G:51:UNK:HA	7:G:73:UNK:O	1.94	0.47
1:A:761:ASN:OD1	1:A:762:LYS:N	2.48	0.47
1:A:123:ASN:HB2	1:A:734:GLN:HB3	1.96	0.47
1:A:500:SER:O	1:A:503:THR:OG1	2.24	0.47
1:A:565:LEU:HD13	1:A:777:ILE:HB	1.96	0.47
1:A:961:MET:O	1:A:965:PHE:HB3	2.15	0.47
2:D:554:ARG:N	2:D:582:GLN:O	2.33	0.47
5:B:19:C:HO2'	5:B:20:A:H8	1.63	0.47
1:A:124:ILE:H	1:A:734:GLN:HB3	1.79	0.47
1:A:314:ILE:HA	1:A:317:ASN:HD22	1.79	0.47
1:A:603:LYS:O	1:A:607:LYS:N	2.37	0.47
2:D:584:HIS:ND1	2:D:604:ASP:OD2	2.43	0.47
3:F:19:ALA:O	3:F:24:LYS:NZ	2.39	0.47
4:E:69:ILE:HA	4:E:159:HIS:CE1	2.50	0.47
1:A:418:LYS:N	1:A:421:ASP:OD2	2.41	0.47
1:A:612:LEU:HD23	1:A:822:ASP:HB3	1.97	0.47
1:A:1027:TRP:CD1	1:A:1058:ARG:HG2	2.49	0.47
1:A:997:VAL:HA	1:A:1000:VAL:HG12	1.96	0.46
1:A:1098:GLN:O	1:A:1102:THR:CB	2.63	0.46
1:A:565:LEU:HD22	1:A:777:ILE:HA	1.96	0.46
1:A:954:VAL:O	1:A:957:PHE:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:TYR:HE1	1:A:1040:LYS:HG2	1.80	0.46
1:A:1097:ILE:HD12	1:A:1100:ILE:HB	1.98	0.46
1:A:107:VAL:HG21	1:A:168:GLN:HG2	1.96	0.46
1:A:624:ASP:HB3	1:A:767:GLN:HE22	1.80	0.46
1:A:849:LYS:HB3	1:A:850:ILE:H	1.44	0.46
1:A:795:GLN:O	1:A:799:ASN:ND2	2.49	0.46
1:A:28:SER:OG	1:A:693:PRO:O	2.23	0.46
1:A:341:LYS:NZ	5:B:17:U:OP1	2.48	0.46
1:A:614:TYR:CG	1:A:874:CYS:HB2	2.51	0.46
3:F:35:GLU:O	3:F:37:GLN:NE2	2.48	0.46
5:B:71:C:H4'	5:B:89:A:H61	1.80	0.46
1:A:404:LYS:HB3	1:A:422:TYR:CZ	2.51	0.46
5:B:46:C:HO2'	5:B:47:C:C5'	2.28	0.46
1:A:657:LYS:HD2	1:A:1002:LYS:HD2	1.97	0.46
2:D:646:LEU:HD23	2:D:646:LEU:HA	1.78	0.46
1:A:100:LEU:HD22	1:A:103:LYS:HD2	1.98	0.46
1:A:395:LYS:N	1:A:430:ASP:OD2	2.49	0.46
2:D:591:VAL:HG23	2:D:600:VAL:HG21	1.97	0.46
5:B:43:C:O4'	6:C:7:DG:N2	2.37	0.46
1:A:53:ASP:OD2	1:A:56:PHE:N	2.37	0.45
1:A:380:LEU:HD21	1:A:405:LEU:HD22	1.98	0.45
2:D:598:ILE:HG22	2:D:600:VAL:HG13	1.97	0.45
4:E:136:MET:HA	4:E:142:ILE:HD12	1.97	0.45
1:A:241:VAL:HG22	1:A:475:ASN:HD21	1.82	0.45
1:A:594:SER:HA	1:A:597:PHE:CD2	2.50	0.45
1:A:232:CYS:HB3	1:A:493:LYS:HZ1	1.80	0.45
1:A:658:ARG:HH12	1:A:697:ASN:HD22	1.63	0.45
1:A:767:GLN:NE2	1:A:769:ARG:O	2.49	0.45
4:E:121:GLN:HE22	4:E:128:LYS:HG3	1.81	0.45
6:C:7:DG:H1'	6:C:8:DT:C4	2.51	0.45
1:A:435:VAL:O	1:A:452:LYS:NZ	2.39	0.45
2:D:585:LEU:HD22	2:D:587:LEU:HD21	1.99	0.45
8:H:484:ASN:OD1	8:H:486:LYS:HG2	2.15	0.45
1:A:790:GLU:O	1:A:794:THR:CB	2.63	0.45
5:B:141:U:C4'	8:H:392:LYS:HD3	2.45	0.45
1:A:849:LYS:HD3	1:A:849:LYS:HA	1.81	0.45
1:A:1097:ILE:HD11	1:A:1101:LYS:HE3	1.98	0.45
1:A:19:ASP:O	1:A:22:THR:OG1	2.26	0.45
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.84	0.45
1:A:738:ARG:H	1:A:738:ARG:HD3	1.82	0.45
5:B:145:U:H5'	5:B:146:G:H2'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ILE:HD13	1:A:536:ILE:HA	1.77	0.45
1:A:551:LYS:HB2	1:A:554:GLN:HB2	1.97	0.45
1:A:658:ARG:HH12	1:A:697:ASN:ND2	2.15	0.45
2:D:566:HIS:HB3	5:B:42:U:C4	2.51	0.45
3:F:58:ASN:O	3:F:60:ARG:NH2	2.49	0.45
1:A:160:LYS:HD2	1:A:166:TYR:HE1	1.82	0.45
1:A:230:PHE:O	1:A:473:ARG:NH1	2.48	0.45
1:A:620:LYS:HG2	1:A:845:PHE:HA	1.98	0.45
1:A:769:ARG:NH2	1:A:842:GLY:O	2.50	0.45
1:A:911:ASN:N	1:A:911:ASN:OD1	2.50	0.45
1:A:961:MET:O	1:A:965:PHE:HB2	2.17	0.45
2:D:564:LYS:HZ1	6:C:6:DG:H21	1.65	0.45
1:A:239:PRO:HA	1:A:474:TYR:HE2	1.82	0.45
1:A:131:LEU:HA	1:A:136:PHE:CE2	2.52	0.44
1:A:529:PRO:HA	1:A:554:GLN:CG	2.47	0.44
1:A:583:ILE:HA	1:A:794:THR:HG21	1.98	0.44
1:A:927:GLN:OE1	1:A:953:THR:OG1	2.32	0.44
1:A:1004:LEU:HD21	1:A:1022:LYS:HB3	1.99	0.44
1:A:389:PRO:HB2	1:A:392:LEU:H	1.83	0.44
1:A:825:GLN:O	1:A:829:ASN:ND2	2.50	0.44
1:A:849:LYS:HB2	1:A:869:SER:H	1.82	0.44
4:E:146:TYR:HE2	4:E:148:SER:HB2	1.82	0.44
1:A:641:ILE:HG22	1:A:642:GLN:H	1.82	0.44
1:A:912:LEU:HB3	1:A:975:TYR:CE2	2.52	0.44
1:A:979:TYR:CE1	1:A:987:ASN:HB2	2.52	0.44
1:A:76:LYS:H	1:A:76:LYS:HG2	1.65	0.44
1:A:760:PHE:H	1:A:763:VAL:HG12	1.82	0.44
1:A:958:TYR:O	1:A:962:THR:OG1	2.22	0.44
2:D:588:ARG:NH2	6:C:3:DT:O2	2.51	0.44
3:F:12:ARG:HG2	3:F:27:THR:HB	2.00	0.44
4:E:170:ARG:HE	4:E:174:ILE:HD11	1.83	0.44
4:E:114:GLN:HB3	4:E:147:PHE:HB3	1.98	0.44
5:B:96:U:H2'	5:B:97:G:C8	2.53	0.44
7:G:137:UNK:O	7:G:139:UNK:N	2.50	0.44
1:A:12:GLN:O	1:A:1002:LYS:NZ	2.36	0.44
1:A:337:TYR:CZ	1:A:341:LYS:HD2	2.53	0.44
1:A:628:GLN:NE2	1:A:768:LYS:O	2.49	0.44
4:E:63:ALA:H	4:E:170:ARG:NH2	2.16	0.44
1:A:797:LEU:HD11	1:A:833:GLN:NE2	2.32	0.44
5:B:46:C:O2'	5:B:47:C:H6	2.01	0.44
1:A:552:ASP:N	1:A:552:ASP:OD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:GLN:HE21	1:A:573:ARG:NH2	2.16	0.44
1:A:1046:TYR:HD1	1:A:1049:LYS:HG3	1.82	0.44
1:A:809:LEU:HA	1:A:810:LEU:HD12	2.00	0.44
2:D:568:ASP:HB3	2:D:571:PHE:HB2	1.99	0.44
2:D:682:GLU:HA	2:D:685:LYS:HG2	2.00	0.44
4:E:77:GLN:HB3	4:E:86:MET:HB3	2.00	0.44
4:E:79:ILE:HD11	4:E:86:MET:HB2	1.99	0.44
1:A:115:ILE:HG12	2:D:590:PHE:CE2	2.53	0.43
1:A:137:ARG:O	1:A:141:ASN:ND2	2.51	0.43
1:A:340:LEU:HD23	1:A:343:GLN:HE21	1.81	0.43
1:A:932:PHE:HZ	1:A:946:LEU:HB2	1.83	0.43
4:E:102:LYS:HB2	4:E:107:ASP:H	1.83	0.43
4:E:117:GLU:HB2	4:E:147:PHE:HE2	1.83	0.43
5:B:31:A:H5''	5:B:32:G:H8	1.83	0.43
1:A:20:LEU:HD22	1:A:166:TYR:HD2	1.84	0.43
1:A:525:PHE:CZ	1:A:751:HIS:HD2	2.37	0.43
1:A:985:ASN:HD22	1:A:989:LEU:HD12	1.82	0.43
3:F:40:SER:O	3:F:58:ASN:N	2.45	0.43
4:E:130:VAL:HG12	4:E:149:ILE:HG13	2.00	0.43
1:A:355:ASN:OD1	1:A:355:ASN:N	2.49	0.43
1:A:889:LYS:HD2	1:A:945:GLN:NE2	2.34	0.43
5:B:71:C:O2'	5:B:90:A:N6	2.47	0.43
5:B:140:A:O2'	8:H:393:ALA:CB	2.66	0.43
1:A:229:ILE:HA	1:A:229:ILE:HD12	1.75	0.43
1:A:642:GLN:O	1:A:708:TYR:HB3	2.18	0.43
5:B:125:U:H2'	5:B:126:U:C6	2.53	0.43
1:A:567:ASP:OD1	1:A:567:ASP:N	2.49	0.43
1:A:613:TYR:CD2	1:A:824:GLN:HB2	2.53	0.43
1:A:622:CYS:HB2	1:A:786:PHE:HE2	1.83	0.43
2:D:654:GLU:HG2	2:D:673:LEU:HD12	2.00	0.43
5:B:44:A:HO2'	5:B:45:A:H8	1.64	0.43
5:B:124:A:H2'	5:B:125:U:C6	2.54	0.43
1:A:113:THR:O	1:A:119:VAL:HA	2.19	0.43
1:A:809:LEU:HA	1:A:809:LEU:HD23	1.73	0.43
4:E:60:TRP:HD1	4:E:167:TYR:CE1	2.36	0.43
1:A:696:PHE:HD2	1:A:699:LYS:HE2	1.84	0.43
1:A:894:GLN:HE22	1:A:896:GLN:HB3	1.84	0.43
2:D:593:ASP:OD1	2:D:596:GLY:N	2.34	0.43
1:A:393:LEU:HD12	1:A:398:PHE:HD1	1.84	0.43
1:A:440:GLN:OE1	1:A:444:GLN:N	2.51	0.43
1:A:797:LEU:HA	1:A:797:LEU:HD13	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:ILE:HG23	5:B:135:U:C5	2.54	0.43
1:A:979:TYR:OH	1:A:983:ASN:O	2.28	0.43
1:A:1001:CYS:O	1:A:1022:LYS:HD2	2.19	0.43
2:D:572:CYS:SG	2:D:579:ILE:HG21	2.56	0.43
5:B:90:A:H2'	5:B:91:A:C8	2.54	0.43
5:B:94:A:H3'	5:B:95:G:N2	2.30	0.43
5:B:119:U:H2'	5:B:120:C:O4'	2.19	0.43
1:A:481:LYS:HA	1:A:481:LYS:HD3	1.78	0.43
1:A:637:GLN:NE2	1:A:639:ASP:OD2	2.52	0.43
1:A:797:LEU:HD12	1:A:830:LEU:HG	2.00	0.43
1:A:873:GLU:HG3	1:A:882:ASP:HA	2.01	0.43
1:A:1079:GLN:NE2	1:A:1081:ASN:OD1	2.40	0.43
2:D:554:ARG:HD3	2:D:559:GLY:HA2	2.00	0.43
1:A:316:GLN:O	1:A:320:ASN:ND2	2.52	0.42
1:A:392:LEU:HA	1:A:433:TRP:HE1	1.83	0.42
1:A:396:LYS:N	1:A:430:ASP:OD2	2.38	0.42
1:A:912:LEU:HB3	1:A:975:TYR:HE2	1.83	0.42
5:B:22:A:H2'	5:B:23:U:C6	2.53	0.42
5:B:37:G:H2'	5:B:38:U:C6	2.54	0.42
1:A:993:LEU:HD11	1:A:1033:ILE:HD13	2.00	0.42
3:F:33:CYS:HB3	3:F:43:ILE:HG22	2.01	0.42
1:A:105:ASN:HB3	1:A:173:CYS:SG	2.59	0.42
1:A:565:LEU:O	1:A:565:LEU:HG	2.18	0.42
1:A:565:LEU:HD21	1:A:780:VAL:HB	2.01	0.42
1:A:882:ASP:HB3	1:A:887:GLU:HB3	2.01	0.42
1:A:622:CYS:SG	1:A:623:TYR:N	2.92	0.42
2:D:534:GLU:OE2	2:D:656:GLN:NE2	2.52	0.42
4:E:74:GLU:HA	4:E:127:HIS:CD2	2.55	0.42
1:A:623:TYR:HD2	1:A:773:GLN:HG2	1.84	0.42
1:A:1017:ILE:HD12	1:A:1020:ILE:HB	2.02	0.42
2:D:682:GLU:H	2:D:682:GLU:HG2	1.53	0.42
3:F:79:ASN:OD1	3:F:79:ASN:N	2.51	0.42
3:F:114:LEU:O	3:F:118:PHE:N	2.43	0.42
4:E:134:LEU:HD22	4:E:142:ILE:HG22	2.00	0.42
6:C:16:DG:H2'	6:C:17:DG:C8	2.55	0.42
1:A:21:LEU:HD21	1:A:64:ILE:HD12	2.02	0.42
1:A:103:LYS:O	1:A:104:GLN:NE2	2.53	0.42
1:A:175:ASN:O	1:A:178:PHE:N	2.47	0.42
1:A:406:TYR:O	1:A:410:GLN:HB2	2.19	0.42
1:A:593:ILE:HD13	1:A:593:ILE:HG21	1.85	0.42
1:A:920:LEU:HD13	1:A:920:LEU:HA	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:127:HIS:H	4:E:128:LYS:HZ3	1.65	0.42
5:B:101:A:H2'	5:B:102:U:H6	1.85	0.42
1:A:29:ALA:N	1:A:695:TYR:HE2	2.18	0.42
1:A:396:LYS:NZ	1:A:430:ASP:OD1	2.36	0.42
1:A:939:PHE:HA	1:A:942:LEU:HD12	2.02	0.42
8:H:487:LEU:HB3	8:H:498:VAL:HG22	2.02	0.42
4:E:29:GLN:HE22	4:E:65:GLU:HB3	1.85	0.42
5:B:138:U:O2'	5:B:139:U:O4'	2.37	0.42
1:A:131:LEU:HA	1:A:136:PHE:HE2	1.85	0.42
1:A:216:GLU:HB3	1:A:219:TYR:HD1	1.84	0.42
1:A:232:CYS:SG	1:A:233:ASN:N	2.93	0.42
1:A:328:LYS:HG2	5:B:15:C:N1	2.35	0.42
1:A:548:PHE:HE2	1:A:775:LEU:HA	1.85	0.42
1:A:912:LEU:N	1:A:975:TYR:OH	2.47	0.42
1:A:1068:SER:HA	1:A:1071:LEU:HD12	2.00	0.42
3:F:21:PHE:HB2	3:F:22:ARG:HG3	2.01	0.42
4:E:108:GLU:O	4:E:111:GLU:HB3	2.20	0.42
5:B:66:U:O2'	5:B:68:U:OP2	2.37	0.42
1:A:380:LEU:HA	1:A:383:ILE:HD12	2.01	0.42
1:A:645:TYR:CD2	1:A:737:PRO:HB2	2.55	0.42
1:A:822:ASP:OD1	1:A:823:SER:N	2.53	0.42
1:A:979:TYR:CE2	1:A:981:LYS:HB3	2.55	0.42
2:D:625:GLN:O	2:D:629:ASN:ND2	2.52	0.42
1:A:128:ARG:HA	1:A:131:LEU:HB2	2.01	0.41
1:A:424:CYS:HB3	5:B:136:A:C8	2.55	0.41
1:A:534:ARG:NH1	1:A:545:ILE:HD11	2.35	0.41
1:A:622:CYS:HB3	1:A:815:ASP:HB3	2.02	0.41
1:A:1003:ILE:HD12	1:A:1003:ILE:HA	1.92	0.41
1:A:570:LEU:HD23	1:A:570:LEU:HA	1.81	0.41
1:A:638:SER:HA	1:A:742:LYS:HE3	2.01	0.41
1:A:727:ARG:HA	1:A:728:PRO:HD2	1.83	0.41
1:A:909:ILE:N	1:A:911:ASN:OD1	2.53	0.41
1:A:969:LEU:HD22	1:A:971:LYS:HE2	2.02	0.41
1:A:989:LEU:HA	1:A:992:ILE:HG22	2.02	0.41
1:A:995:TYR:O	1:A:998:GLU:HB3	2.20	0.41
2:D:514:TYR:CE1	2:D:685:LYS:HB3	2.54	0.41
4:E:138:LYS:HA	4:E:138:LYS:HD2	1.81	0.41
4:E:168:LEU:HA	4:E:168:LEU:HD13	1.86	0.41
5:B:86:U:H1'	5:B:90:A:N1	2.34	0.41
1:A:95:ASP:O	1:A:99:LEU:N	2.46	0.41
1:A:1063:LYS:NZ	5:B:65:A:H5'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLY:N	1:A:728:PRO:HB3	2.34	0.41
1:A:310:PHE:HD2	1:A:392:LEU:HD13	1.85	0.41
1:A:528:TYR:O	1:A:530:GLN:OE1	2.39	0.41
1:A:588:PHE:CE2	1:A:593:ILE:HG22	2.56	0.41
1:A:916:LEU:HA	1:A:916:LEU:HD12	1.92	0.41
5:B:151:U:H2'	5:B:152:C:C6	2.54	0.41
8:H:486:LYS:HE2	8:H:497:ASP:OD2	2.19	0.41
1:A:59:PHE:CE2	1:A:135:ASN:HB3	2.56	0.41
1:A:389:PRO:HD2	1:A:392:LEU:HD23	2.02	0.41
1:A:224:ILE:HB	1:A:416:ASN:HD21	1.86	0.41
1:A:326:LEU:HD13	1:A:329:LYS:HD2	2.02	0.41
1:A:497:LYS:HE2	1:A:497:LYS:HB3	1.88	0.41
1:A:530:GLN:N	1:A:554:GLN:NE2	2.68	0.41
1:A:547:THR:HG22	5:B:46:C:H5'	2.02	0.41
1:A:582:LYS:HG2	1:A:790:GLU:OE1	2.21	0.41
1:A:1037:LEU:HB3	1:A:1047:LEU:HD22	2.02	0.41
5:B:111:A:N1	5:B:154:U:H2'	2.36	0.41
1:A:226:ARG:HD3	1:A:415:GLU:O	2.21	0.41
2:D:544:ILE:H	2:D:544:ILE:HG13	1.69	0.41
2:D:556:THR:OG1	2:D:584:HIS:NE2	2.52	0.41
4:E:84:LYS:HA	4:E:84:LYS:HD3	1.80	0.41
5:B:67:A:O2'	5:B:68:U:O4'	2.36	0.41
1:A:59:PHE:HE2	1:A:139:LEU:HD11	1.86	0.41
1:A:125:ASN:HB2	1:A:734:GLN:HE21	1.86	0.41
1:A:492:ARG:HA	1:A:492:ARG:HD2	1.92	0.41
3:F:105:LEU:O	3:F:109:SER:OG	2.28	0.41
4:E:166:ARG:O	4:E:170:ARG:HB2	2.21	0.41
6:C:15:DT:H2'	6:C:16:DG:C8	2.56	0.41
8:H:464:ILE:N	8:H:464:ILE:CD1	2.81	0.41
1:A:20:LEU:HD22	1:A:166:TYR:CD2	2.56	0.41
1:A:330:PHE:HD2	1:A:379:PHE:HD1	1.67	0.41
1:A:364:ASN:OD1	1:A:540:GLY:HA3	2.21	0.41
1:A:1002:LYS:HA	1:A:1002:LYS:HD3	1.88	0.41
1:A:1010:GLU:HB3	1:A:1086:GLU:HG3	2.01	0.41
2:D:563:LEU:HB2	2:D:573:GLU:HG2	2.02	0.41
3:F:20:GLN:HA	3:F:24:LYS:HD2	2.03	0.41
4:E:61:TYR:CD2	4:E:171:LYS:HB2	2.56	0.41
5:B:6:C:H2'	5:B:7:G:H8	1.86	0.41
5:B:93:A:H2'	5:B:94:A:H8	1.86	0.41
1:A:106:TYR:H	1:A:109:GLN:CD	2.24	0.41
1:A:106:TYR:CD1	1:A:172:VAL:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:SER:OG	1:A:136:PHE:N	2.45	0.41
1:A:1098:GLN:O	1:A:1102:THR:OG1	2.32	0.41
2:D:566:HIS:HB2	5:B:41:U:C5	2.56	0.41
4:E:84:LYS:HG3	4:E:102:LYS:HG2	2.02	0.41
1:A:446:ARG:HG3	5:B:137:U:C4	2.56	0.40
1:A:572:PHE:O	1:A:576:LYS:HB3	2.22	0.40
1:A:921:ARG:C	1:A:923:LEU:H	2.24	0.40
3:F:69:LYS:HB2	3:F:69:LYS:HE2	1.90	0.40
4:E:100:ILE:HG22	4:E:144:LEU:HB3	2.03	0.40
5:B:140:A:C4'	8:H:396:VAL:CG1	2.93	0.40
7:G:71:UNK:C	7:G:73:UNK:N	2.84	0.40
8:H:487:LEU:HB2	8:H:498:VAL:HG22	2.02	0.40
1:A:361:ASN:HA	1:A:364:ASN:HD22	1.86	0.40
1:A:419:VAL:HG12	1:A:423:ILE:HD11	2.04	0.40
1:A:987:ASN:HA	1:A:990:LYS:HB3	2.03	0.40
1:A:1093:LEU:C	1:A:1098:GLN:HE21	2.24	0.40
2:D:627:VAL:HG13	2:D:639:ILE:HG21	2.04	0.40
3:F:51:ASN:HA	3:F:53:HIS:CD2	2.56	0.40
3:F:71:VAL:HG22	3:F:90:GLU:HG2	2.03	0.40
8:H:382:LYS:O	8:H:498:VAL:HA	2.20	0.40
1:A:440:GLN:HB3	1:A:448:TYR:HD1	1.87	0.40
1:A:646:PHE:HE2	1:A:707:LEU:HB3	1.86	0.40
1:A:646:PHE:CZ	1:A:707:LEU:HD23	2.56	0.40
1:A:1068:SER:O	1:A:1072:ILE:HG12	2.21	0.40
2:D:554:ARG:HB3	2:D:584:HIS:CD2	2.56	0.40
2:D:563:LEU:HG	2:D:565:TYR:HB2	2.04	0.40
2:D:572:CYS:SG	2:D:579:ILE:HG22	2.59	0.40
5:B:121:G:OP1	8:H:518:LYS:HB3	2.14	0.40
1:A:536:ILE:H	1:A:544:PRO:HA	1.87	0.40
1:A:886:LEU:HA	1:A:886:LEU:HD12	1.89	0.40
1:A:934:PRO:HB3	1:A:937:ASN:ND2	2.36	0.40
1:A:996:THR:HA	1:A:999:ASP:OD2	2.22	0.40
2:D:516:SER:HB2	2:D:595:THR:HG21	2.04	0.40
3:F:10:TYR:CE1	3:F:25:LYS:HB3	2.57	0.40
4:E:65:GLU:CD	4:E:136:MET:O	2.51	0.40
5:B:140:A:H2'	5:B:141:U:C6	2.57	0.40
2:D:591:VAL:O	2:D:598:ILE:N	2.42	0.40
2:D:661:GLU:HG2	2:D:663:ASN:N	2.34	0.40
5:B:21:G:O2'	5:B:22:A:O4'	2.40	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	970/1117 (87%)	784 (81%)	178 (18%)	8 (1%)	19	59
2	D	183/701 (26%)	162 (88%)	19 (10%)	2 (1%)	14	51
3	F	111/121 (92%)	93 (84%)	18 (16%)	0	100	100
4	E	147/269 (55%)	122 (83%)	24 (16%)	1 (1%)	22	62
8	H	104/542 (19%)	104 (100%)	0	0	100	100
All	All	1515/2750 (55%)	1265 (84%)	239 (16%)	11 (1%)	26	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	GLN
1	A	123	ASN
4	E	141	GLN
2	D	661	GLU
2	D	662	PHE
1	A	17	LYS
1	A	18	GLU
1	A	1006	TYR
1	A	85	SER
1	A	116	GLY
1	A	239	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	931/1069 (87%)	920 (99%)	11 (1%)	71	84
2	D	172/657 (26%)	171 (99%)	1 (1%)	86	92
3	F	107/114 (94%)	105 (98%)	2 (2%)	57	75
4	E	132/242 (54%)	132 (100%)	0	100	100
8	H	95/517 (18%)	94 (99%)	1 (1%)	73	85
All	All	1437/2599 (55%)	1422 (99%)	15 (1%)	77	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	PHE
1	A	352	ASN
1	A	534	ARG
1	A	631	LEU
1	A	634	PHE
1	A	738	ARG
1	A	851	THR
1	A	933	ASN
1	A	960	PHE
1	A	985	ASN
1	A	1004	LEU
2	D	640	ARG
3	F	61	ARG
3	F	100	ASP
8	H	498	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	141	ASN
1	A	234	HIS
1	A	248	ASN
1	A	317	ASN
1	A	319	HIS
1	A	320	ASN
1	A	343	GLN
1	A	352	ASN
1	A	357	GLN
1	A	361	ASN

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Mol	Chain	Res	Type
1	A	364	ASN
1	A	475	ASN
1	A	526	GLN
1	A	554	GLN
1	A	636	ASN
1	A	648	ASN
1	A	697	ASN
1	A	748	HIS
1	A	751	HIS
1	A	754	GLN
1	A	767	GLN
1	A	804	ASN
1	A	839	ASN
1	A	841	ASN
1	A	884	ASN
1	A	896	GLN
1	A	900	ASN
1	A	927	GLN
1	A	945	GLN
1	A	985	ASN
1	A	1016	ASN
1	A	1023	ASN
1	A	1070	GLN
1	A	1098	GLN
2	D	576	GLN
2	D	606	GLN
2	D	612	ASN
2	D	629	ASN
2	D	656	GLN
3	F	52	GLN
4	E	40	ASN
4	E	127	HIS
4	E	143	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	B	158/159 (99%)	103 (65%)	14 (8%)

All (103) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	B	2	U
5	B	3	A
5	B	4	C
5	B	8	C
5	B	9	U
5	B	11	A
5	B	12	A
5	B	13	U
5	B	14	U
5	B	16	A
5	B	19	C
5	B	20	A
5	B	21	G
5	B	22	A
5	B	24	C
5	B	25	U
5	B	26	G
5	B	27	U
5	B	29	A
5	B	30	U
5	B	31	A
5	B	32	G
5	B	33	A
5	B	34	A
5	B	35	C
5	B	36	U
5	B	37	G
5	B	38	U
5	B	39	C
5	B	40	A
5	B	41	U
5	B	42	U
5	B	43	C
5	B	44	A
5	B	45	A
5	B	46	C
5	B	47	C
5	B	49	C
5	B	50	A
5	B	51	A
5	B	53	A
5	B	54	A
5	B	55	U

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Mol	Chain	Res	Type
5	B	56	C
5	B	57	U
5	B	58	A
5	B	59	G
5	B	60	U
5	B	61	G
5	B	62	C
5	B	63	U
5	B	64	G
5	B	66	U
5	B	67	A
5	B	68	U
5	B	69	A
5	B	71	C
5	B	75	C
5	B	76	A
5	B	86	U
5	B	88	C
5	B	89	A
5	B	90	A
5	B	91	A
5	B	92	U
5	B	96	U
5	B	101	A
5	B	106	G
5	B	108	A
5	B	110	A
5	B	111	A
5	B	115	A
5	B	116	C
5	B	117	U
5	B	118	A
5	B	119	U
5	B	122	A
5	B	123	C
5	B	124	A
5	B	125	U
5	B	126	U
5	B	128	G
5	B	129	A
5	B	130	U
5	B	131	A

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Mol	Chain	Res	Type
5	B	132	C
5	B	133	A
5	B	134	C
5	B	135	U
5	B	136	A
5	B	137	U
5	B	138	U
5	B	140	A
5	B	143	A
5	B	144	A
5	B	145	U
5	B	146	G
5	B	147	G
5	B	154	U
5	B	155	A
5	B	156	U
5	B	157	U
5	B	159	U

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	B	3	A
5	B	33	A
5	B	34	A
5	B	39	C
5	B	41	U
5	B	42	U
5	B	43	C
5	B	46	C
5	B	53	A
5	B	60	U
5	B	65	A
5	B	122	A
5	B	136	A
5	B	137	U

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

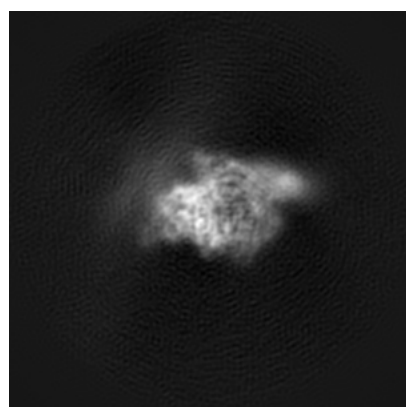
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7821. These allow visual inspection of the internal detail of the map and identification of artifacts.

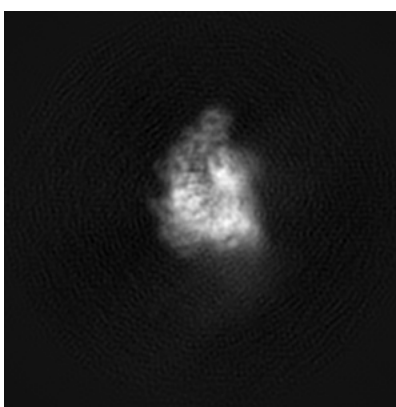
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

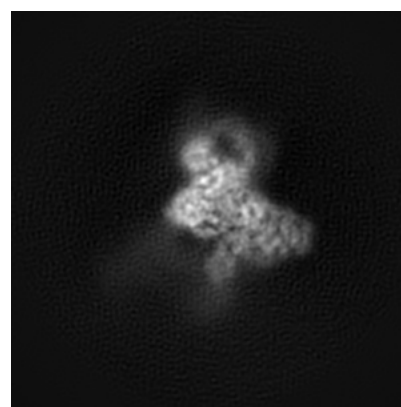
#### 6.1.1 Primary map



X



Y

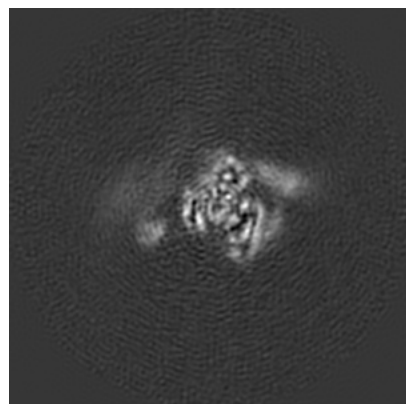


Z

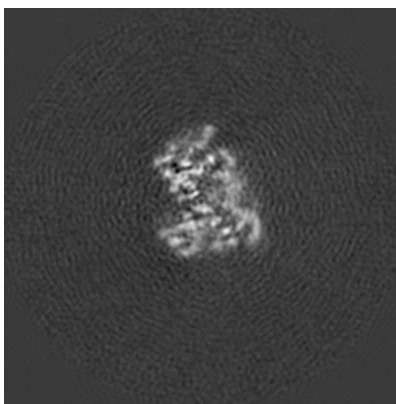
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

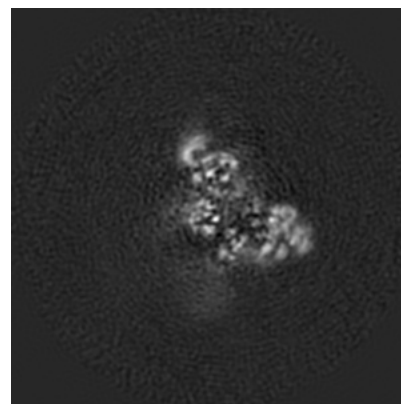
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

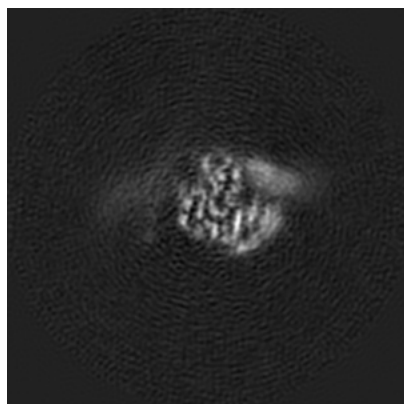


Z Index: 128

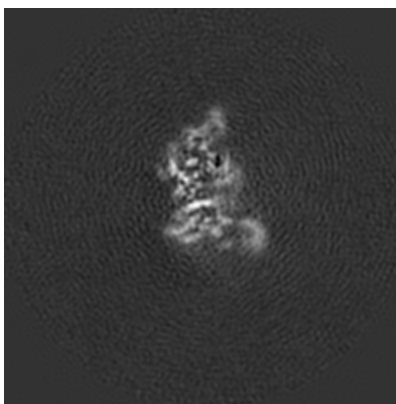
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

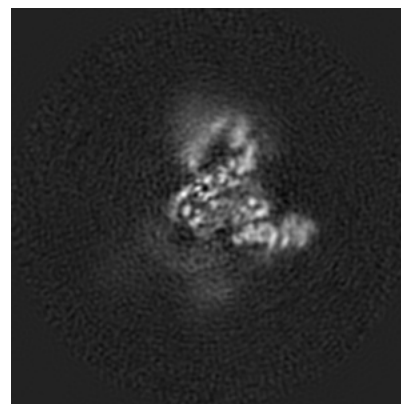
### 6.3.1 Primary map



X Index: 123



Y Index: 121

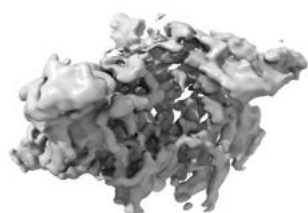


Z Index: 140

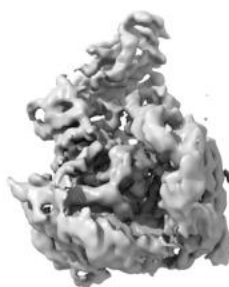
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

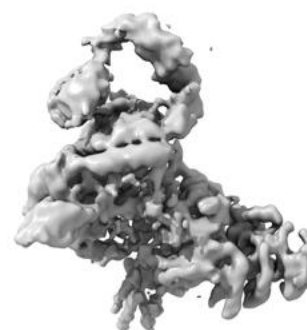
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



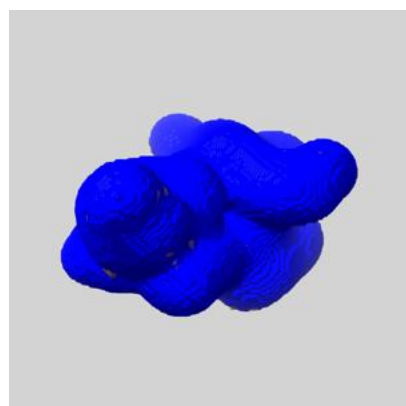
## 6.5 Mask visualisation [i](#)

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

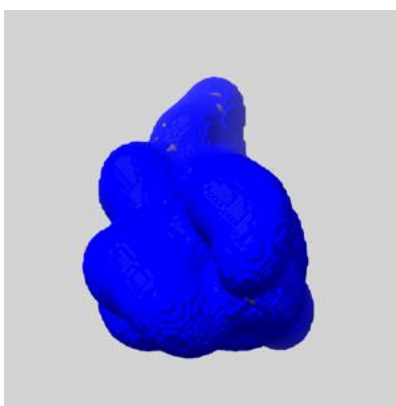
A mask typically either:

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

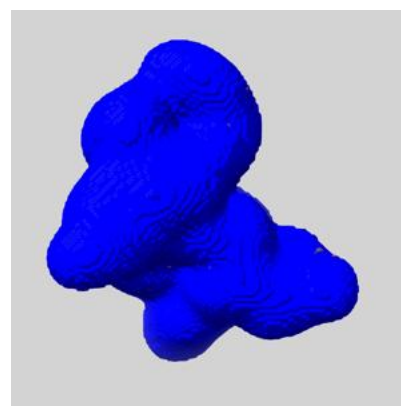
### 6.5.1 emd\_7821\_msk\_1.map [i](#)



X



Y

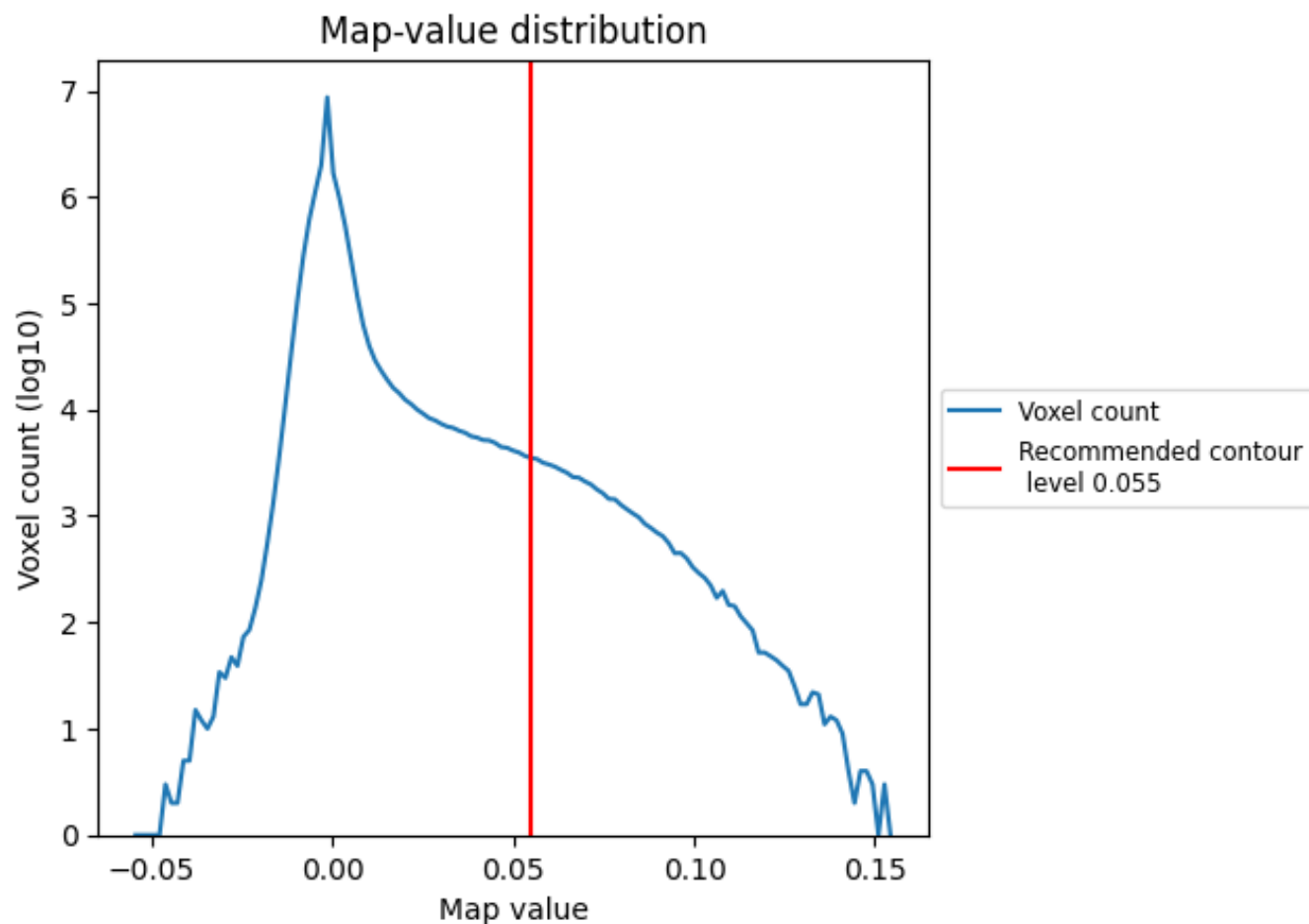


Z

## 7 Map analysis [i](#)

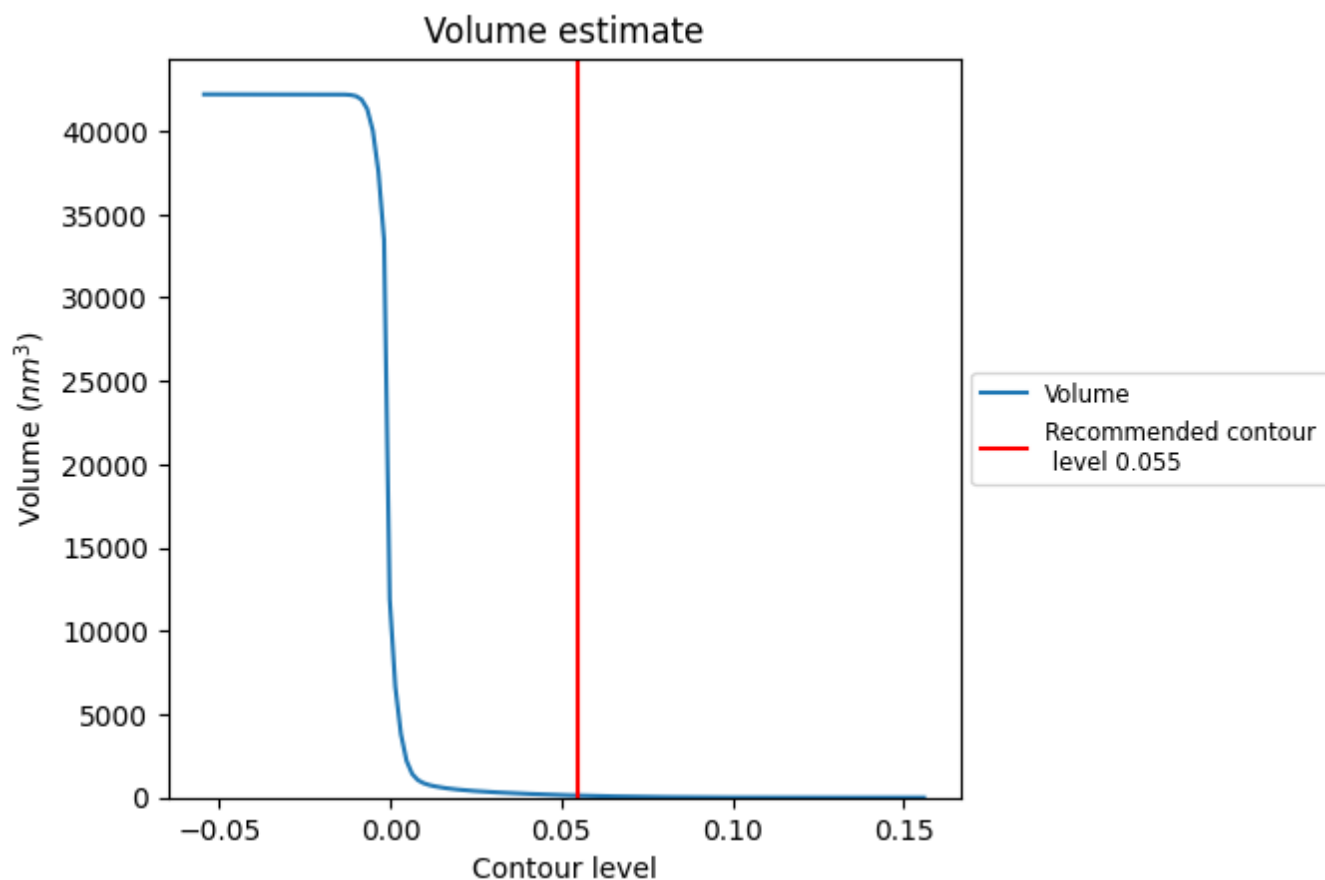
This section contains the results of statistical analysis of the map.

### 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.

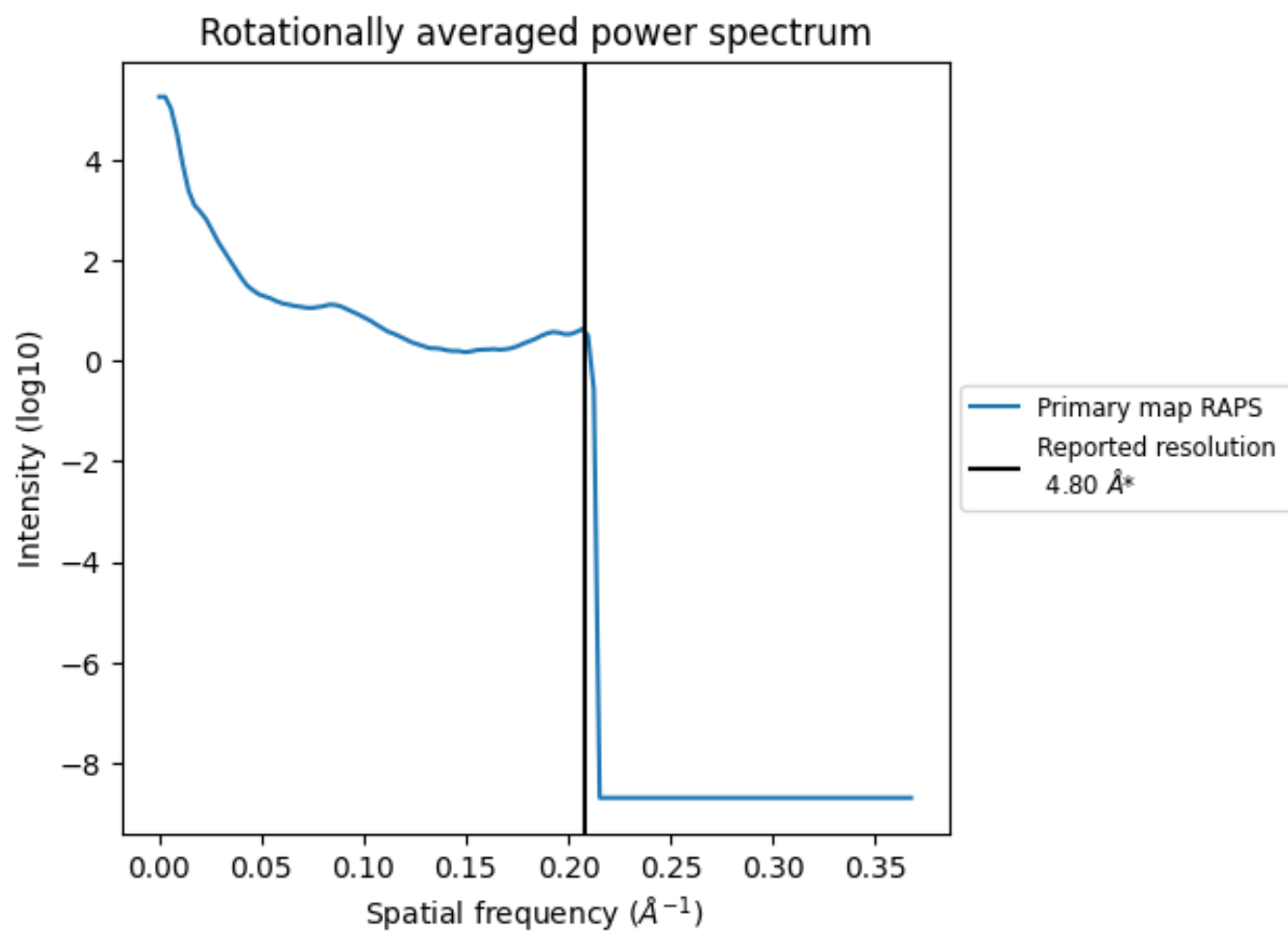
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm<sup>3</sup>; this corresponds to an approximate mass of 109 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 0.208 Å<sup>-1</sup>

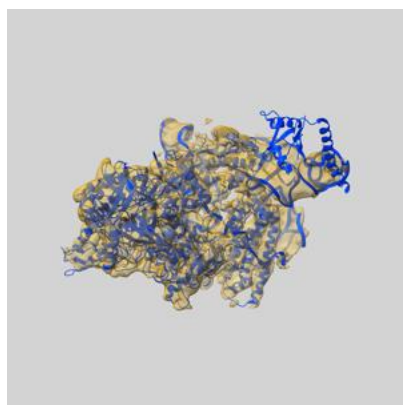
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

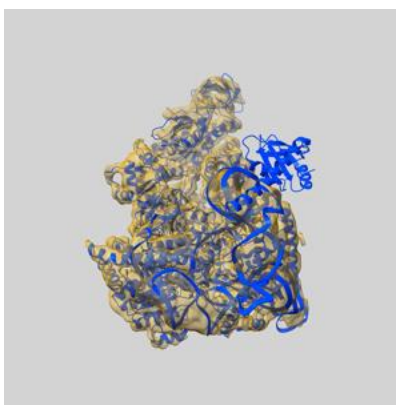
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7821 and PDB model 6D6V. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

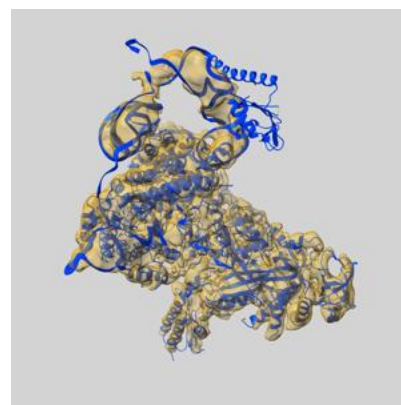
### 9.1 Map-model overlay [i](#)



X



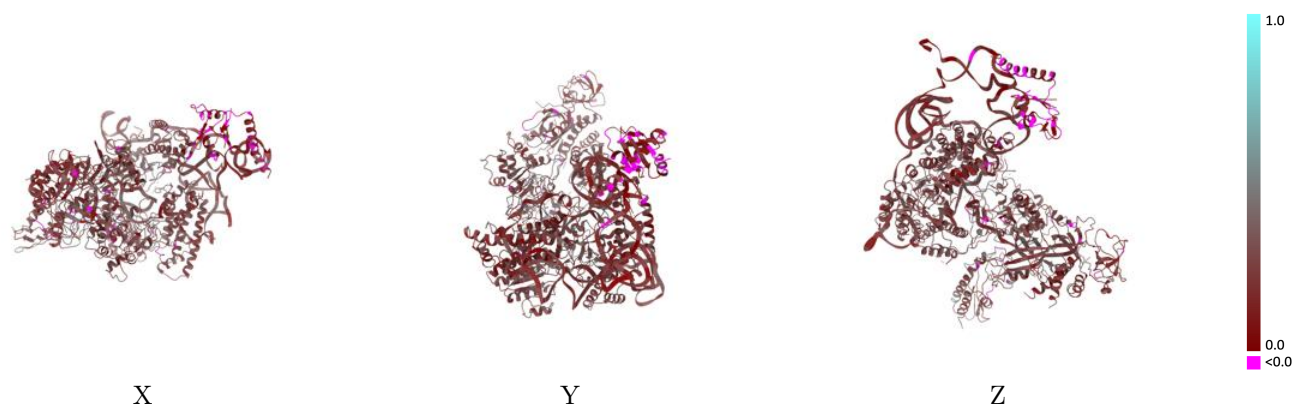
Y



Z

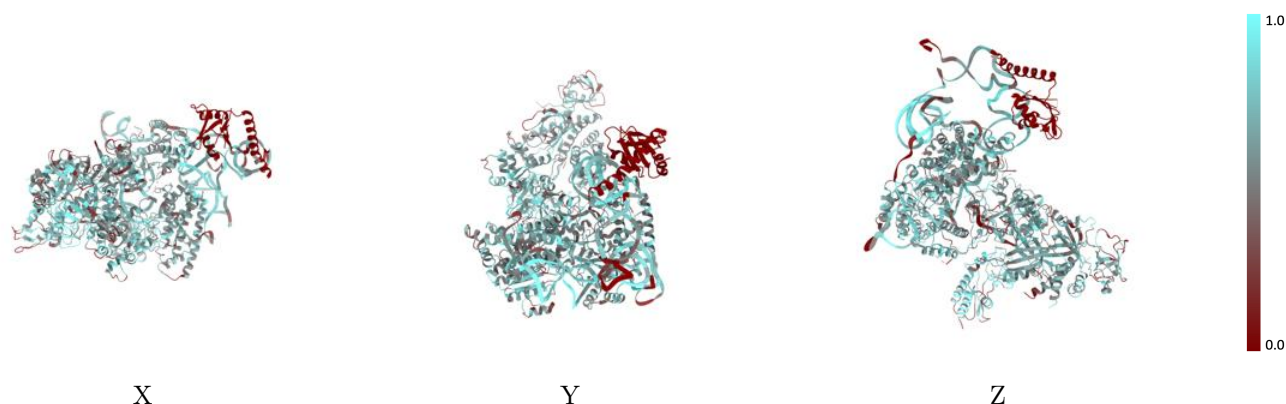
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



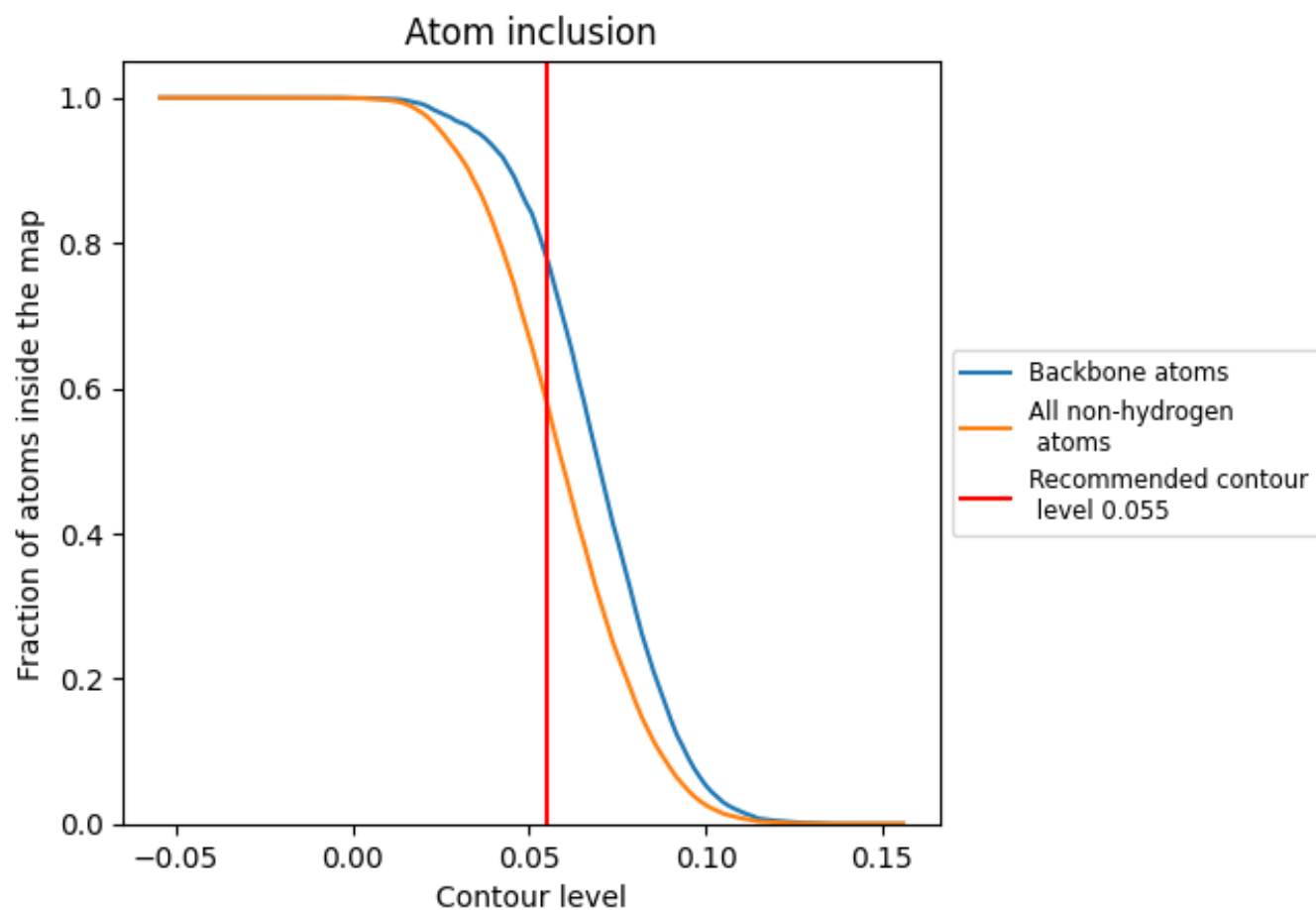
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 58% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5808	<div></div> 0.2430
A	<div></div> 0.6162	<div></div> 0.2620
B	<div></div> 0.6451	<div></div> 0.2200
C	<div></div> 0.5640	<div></div> 0.2710
D	<div></div> 0.5780	<div></div> 0.2640
E	<div></div> 0.5631	<div></div> 0.2470
F	<div></div> 0.5199	<div></div> 0.2240
G	<div></div> 0.6955	<div></div> 0.2920
H	<div></div> 0.0023	<div></div> 0.0720

