



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:59 PM UTC

PDB ID : 5OA3 / pdb_00005oa3
EMDB ID : EMD-3770
Title : Human 40S-eIF2D-re-initiation complex
Authors : Weisser, M.; Schaefer, T.; Leibundgut, M.; Boehringer, D.; Aylett, C.H.S.;
Ban, N.
Deposited on : 2017-06-20
Resolution : 4.20 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:

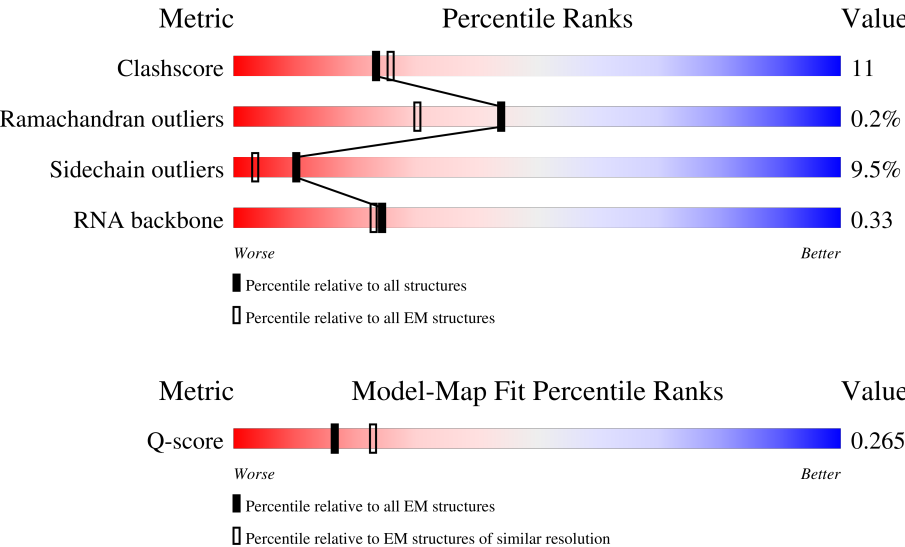
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

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	0	584	60% 60% 19% • 18%
2	1	75	32% 31% 37% 32%
3	2	1868	• 39% 35% 15% 11%

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Mol	Chain	Length	Quality of chain
4	3	275	
5	A	295	
6	B	264	
7	C	293	
8	D	243	
9	E	263	
10	F	204	
11	G	249	
12	H	194	
13	I	208	
14	J	194	
15	K	165	
16	L	158	
17	M	132	
18	N	151	
19	O	151	
20	P	145	
21	Q	146	
22	R	135	
23	S	152	
24	T	145	
25	U	119	
26	V	83	
27	W	130	
28	X	143	

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Mol	Chain	Length	Quality of chain
29	Y	130	
30	Z	125	
31	a	101	
32	b	82	
33	c	61	
34	d	55	
35	e	56	
36	f	72	
37	g	315	
38	h	24	

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 83675 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 Eukaryotic translation initiation factor 2D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	479	Total	C	N	O	S	0	0
			3740	2392	643	684	21		

- Molecule 2 is a RNA chain called initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	75	Total	C	N	O	P	0	0
			1608	716	297	520	75		

- Molecule 3 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	1661	Total	C	N	O	P	0	0
			35466	15831	6370	11604	1661		

- Molecule 4 is a RNA chain called IRES mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	186	Total	C	N	O	P	0	0
			3976	1770	713	1307	186		

- Molecule 5 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 6 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 7 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 8 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 9 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 10 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 12 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 13 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	205	Total	C	N	O	S	0	0
			1675	1053	328	289	5		

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 15 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	95	Total	C	N	O	S	0	0
			800	522	142	131	5		

- Molecule 16 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 17 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 18 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 19 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 20 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 21 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 22 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 23 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 24 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 25 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 26 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 27 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 28 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 30 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 31 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 33 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 34 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 35 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	56	Total	C	N	O	S	0	0
			442	273	96	72	1		

- Molecule 36 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	72	Total	C	N	O	S	0	0
			585	366	114	97	8		

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

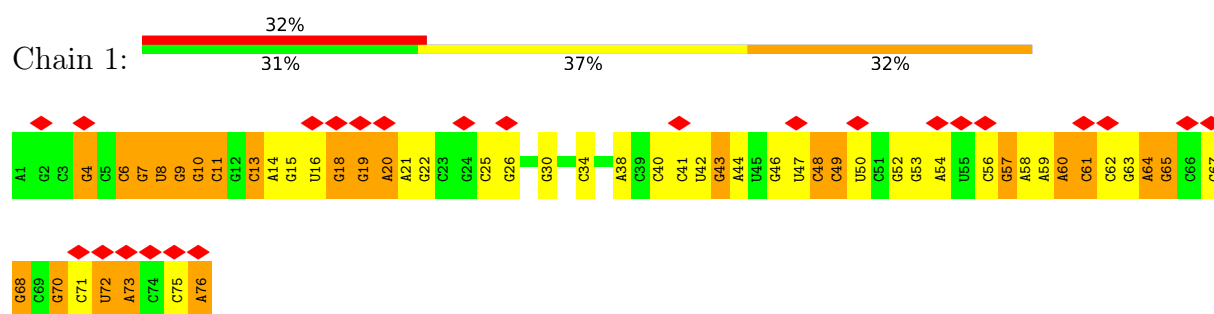
Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 38 is a protein called RIBOSOMAL PROTEIN EL41.

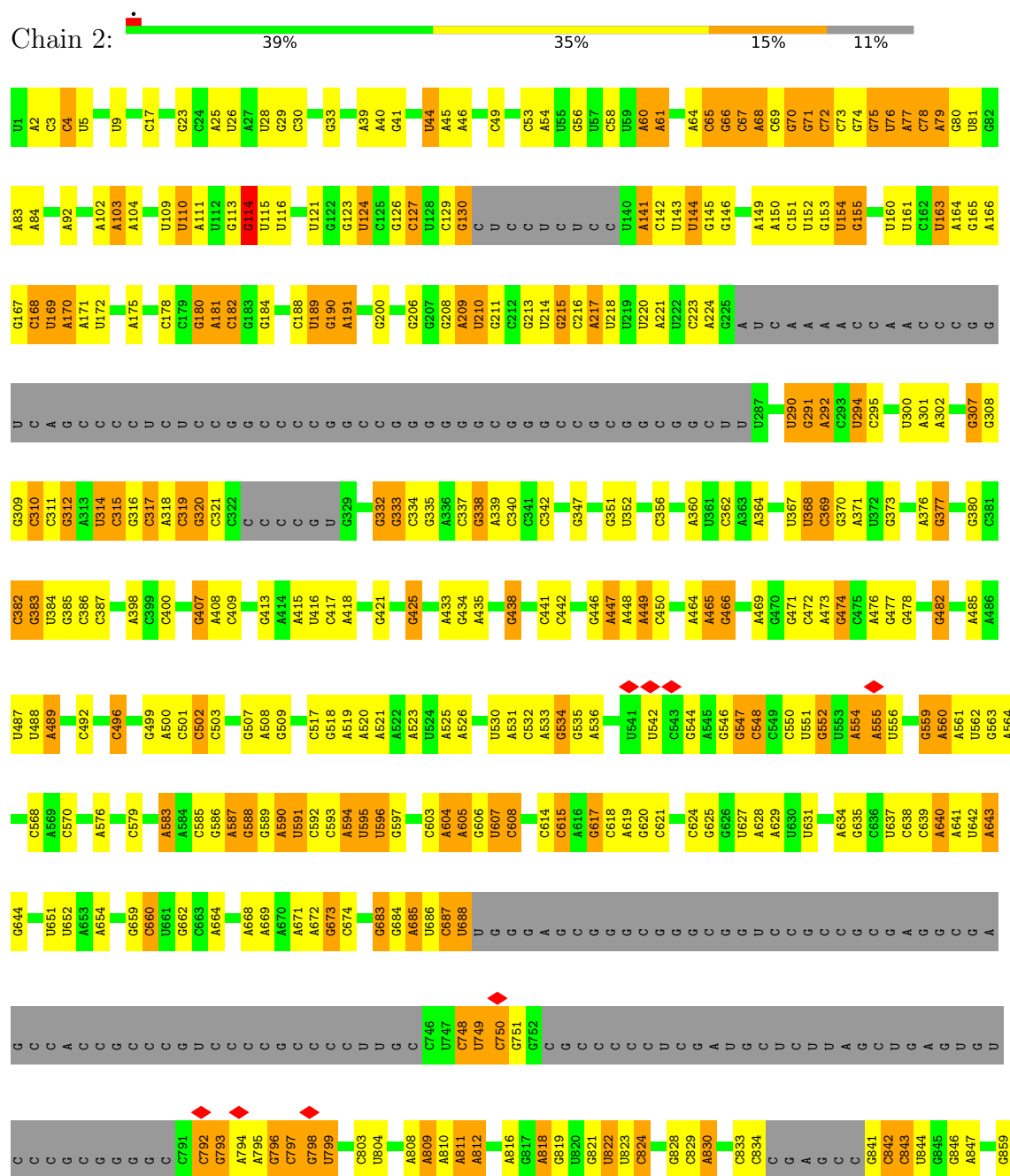
Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	24	Total	C	N	O	S	0	0
			231	140	63	26	2		

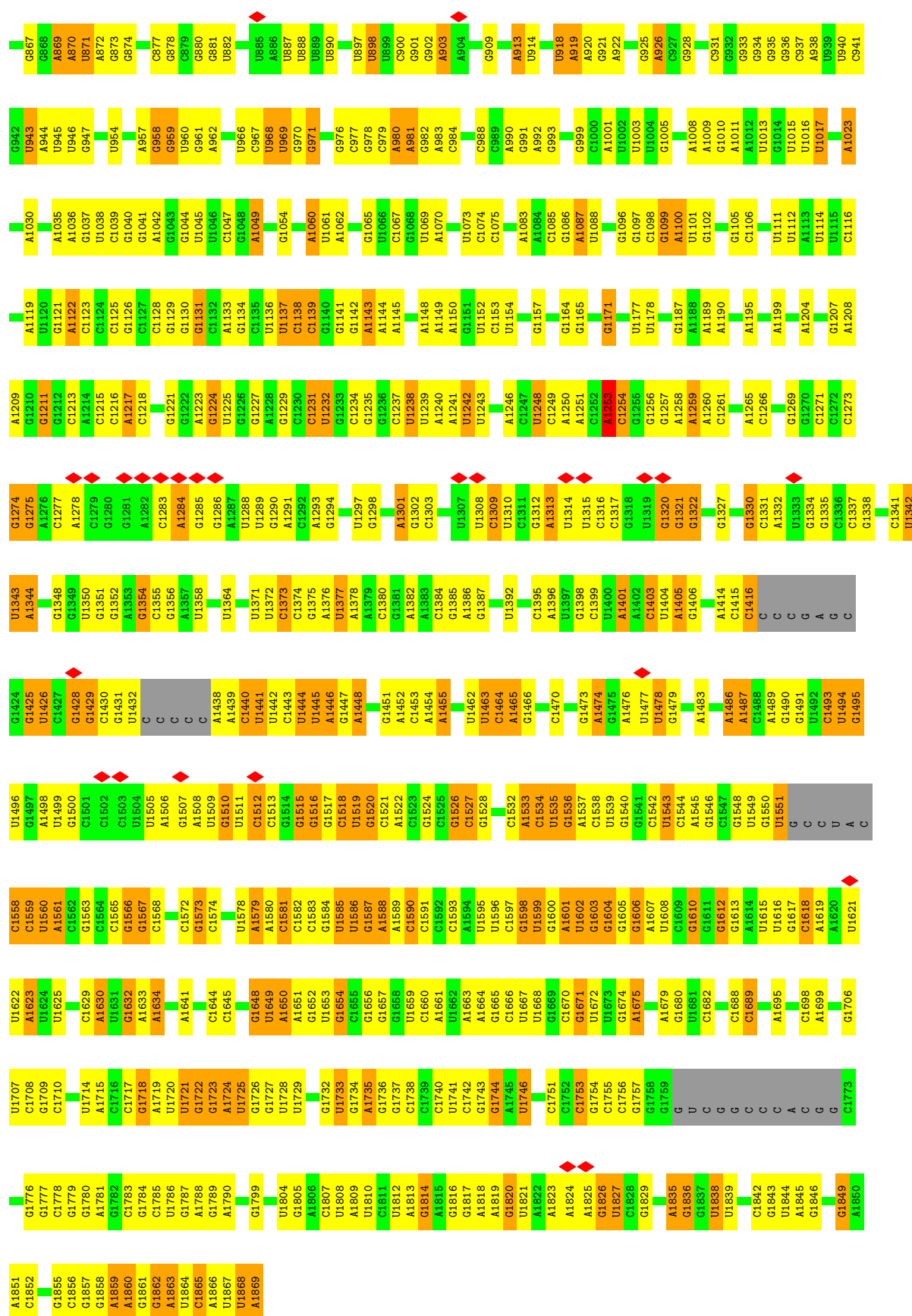
- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

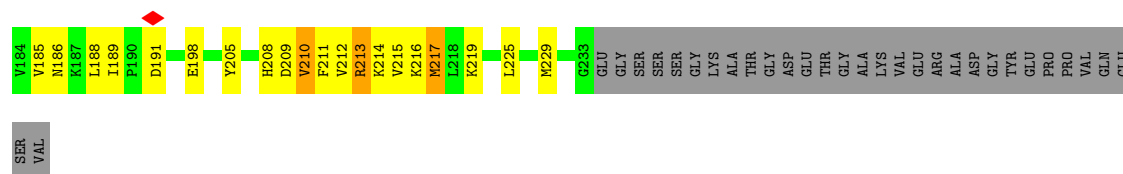
Mol	Chain	Residues	Atoms		AltConf
39	a	1	Total	Zn	0
			1	1	
39	d	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	



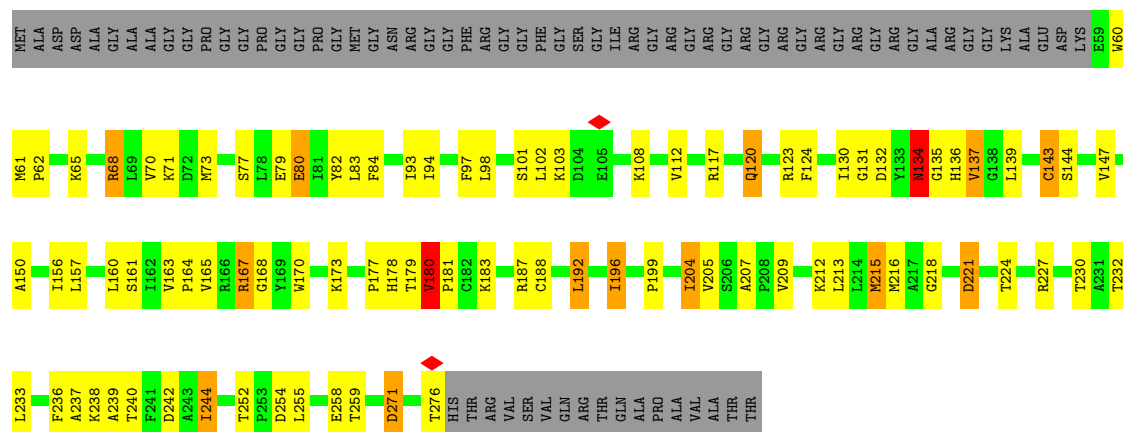
• Molecule 3: 18S ribosomal RNA



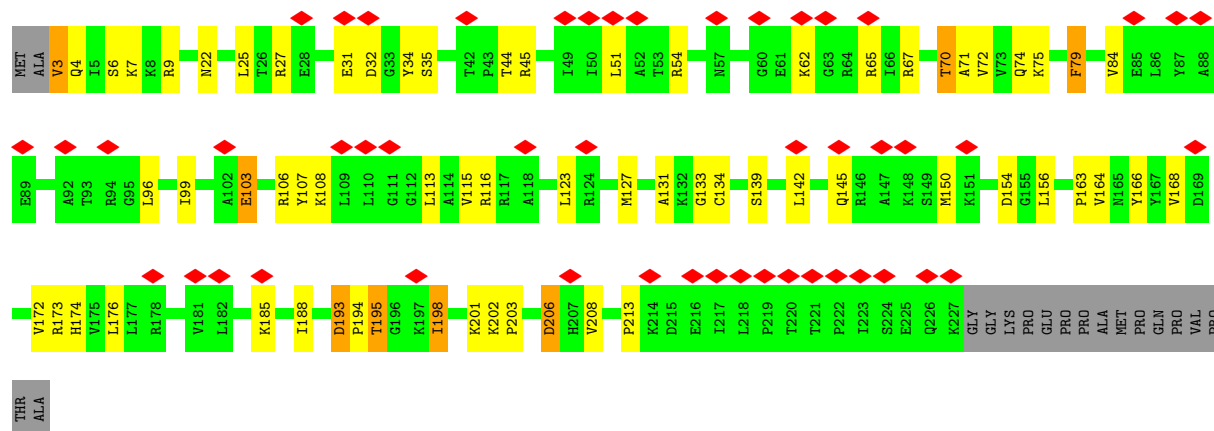




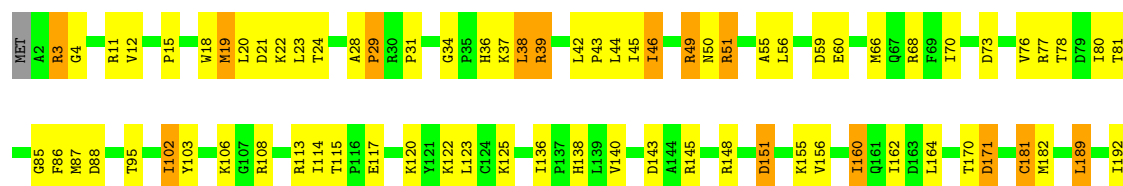
• Molecule 7: 40S ribosomal protein S2

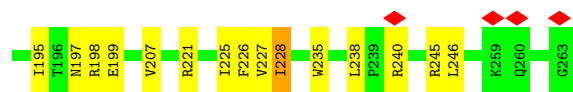


• Molecule 8: 40S ribosomal protein S3

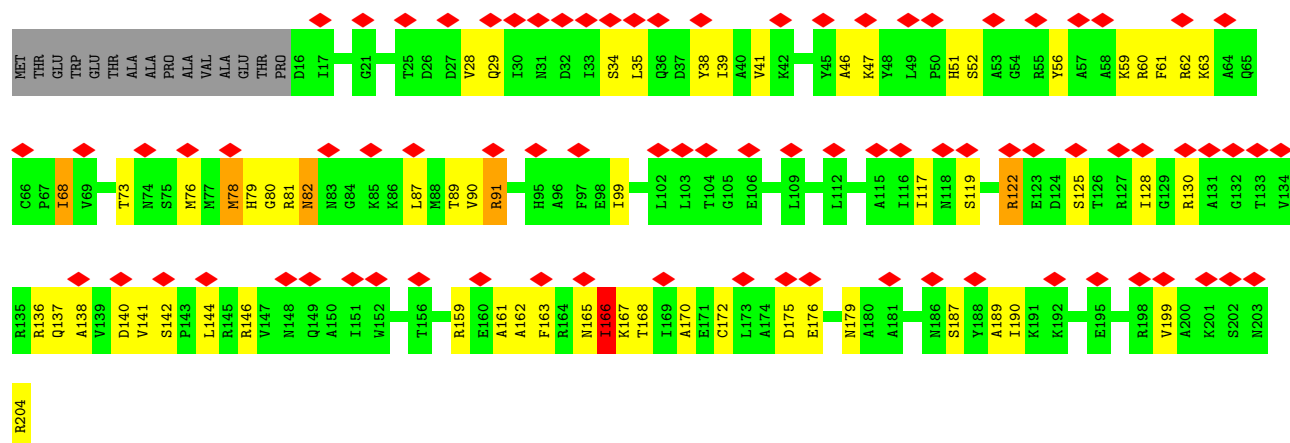
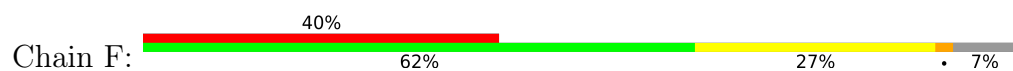


• Molecule 9: 40S ribosomal protein S4, X isoform

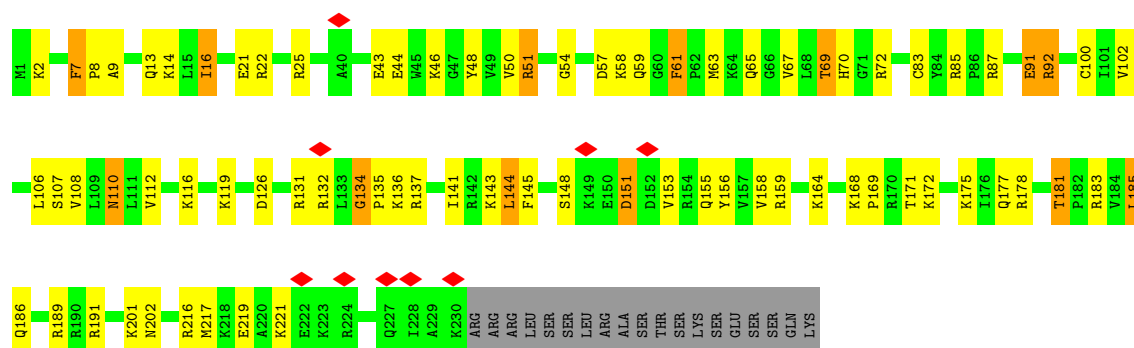




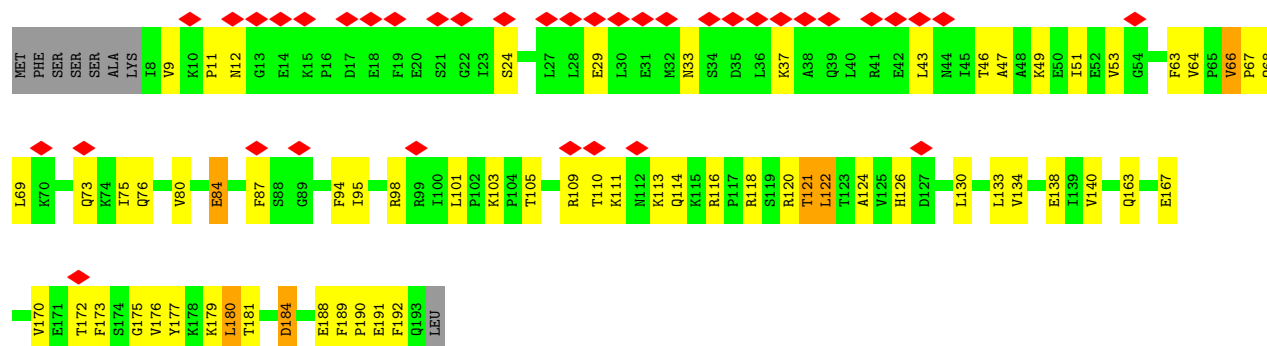
• Molecule 10: 40S ribosomal protein S5



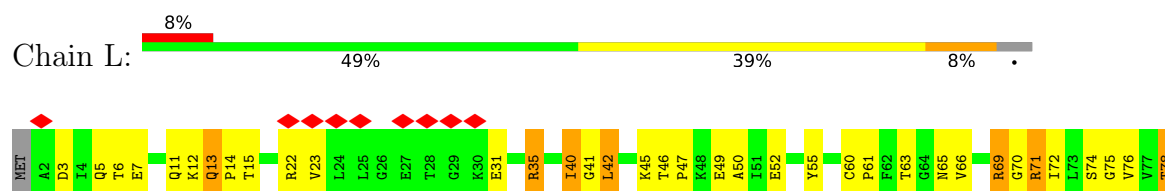
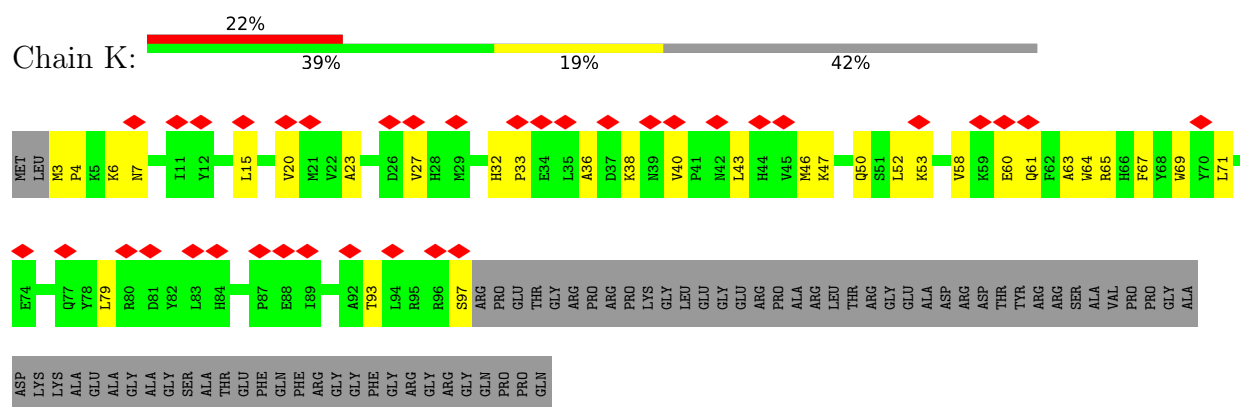
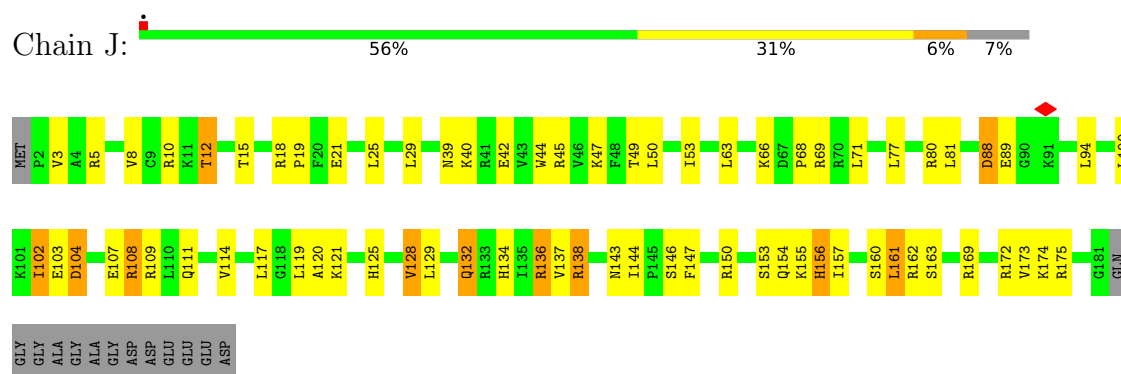
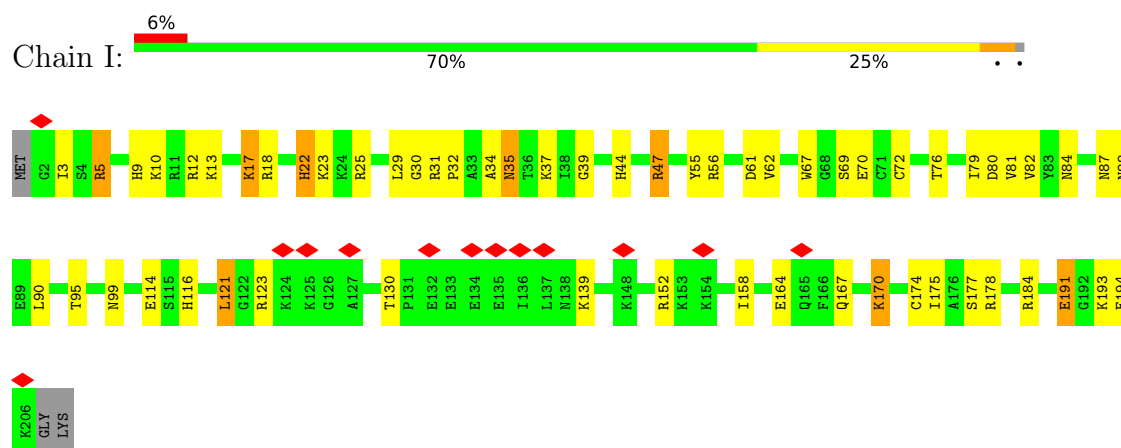
• Molecule 11: 40S ribosomal protein S6

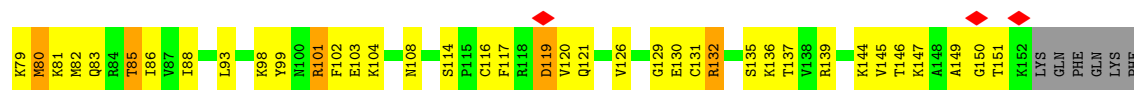


• Molecule 12: 40S ribosomal protein S7

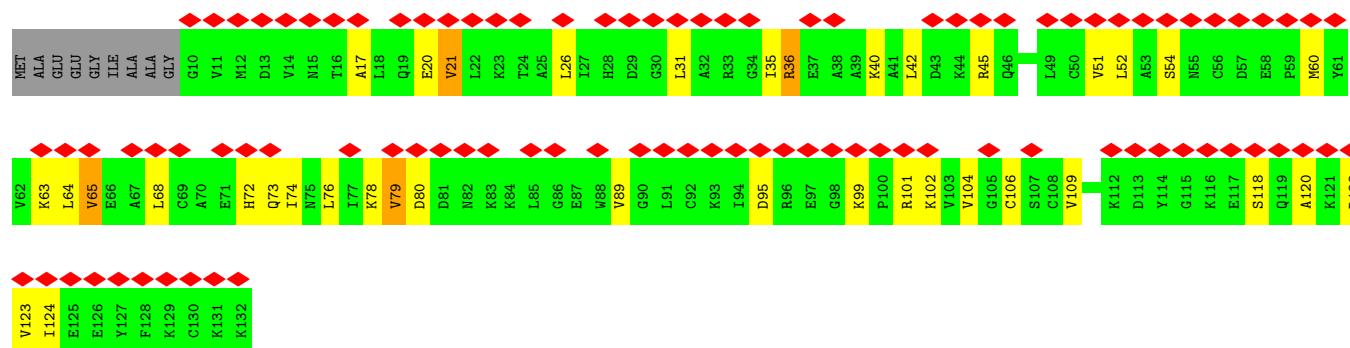


- Molecule 13: 40S ribosomal protein S8

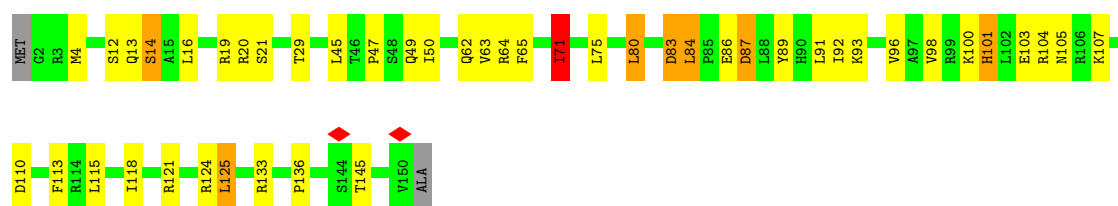




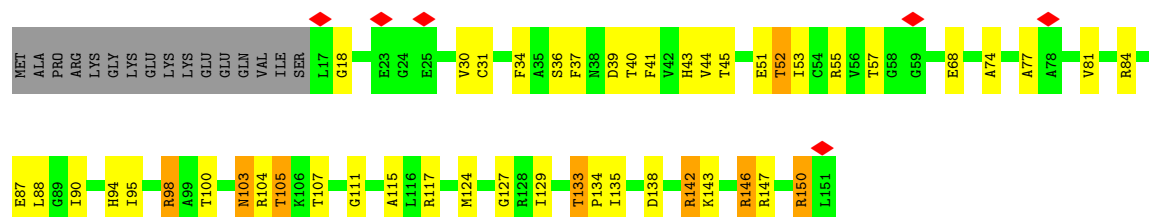
- Molecule 17: 40S ribosomal protein S12



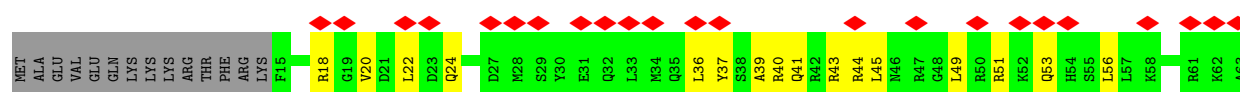
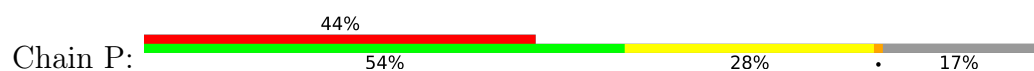
- Molecule 18: 40S ribosomal protein S13

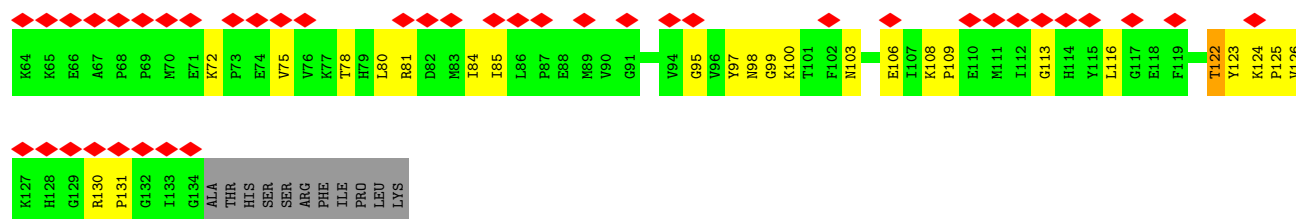


- Molecule 19: 40S ribosomal protein S14

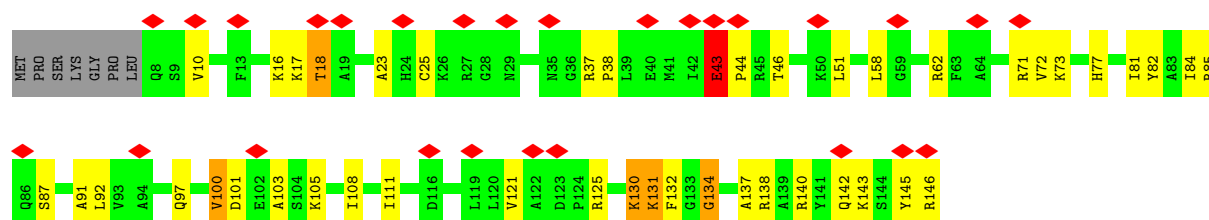


- Molecule 20: 40S ribosomal protein S15

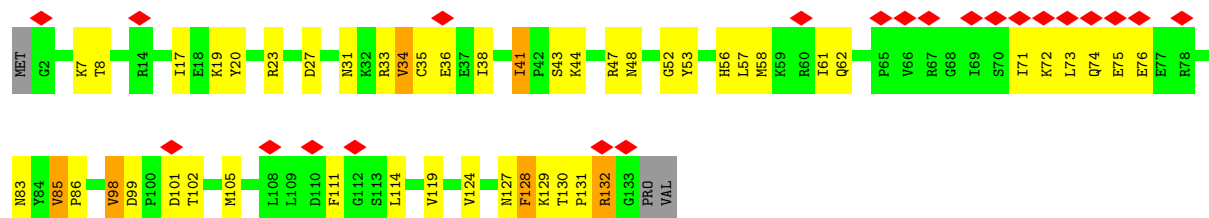




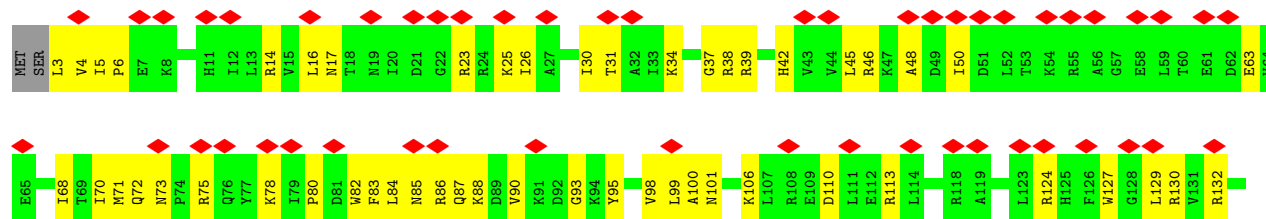
• Molecule 21: 40S ribosomal protein S16



• Molecule 22: 40S ribosomal protein S17

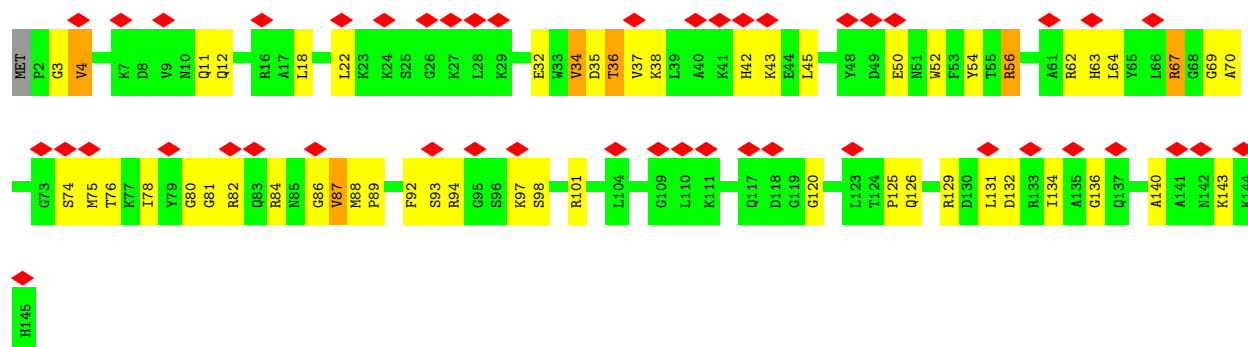


• Molecule 23: 40S ribosomal protein S18

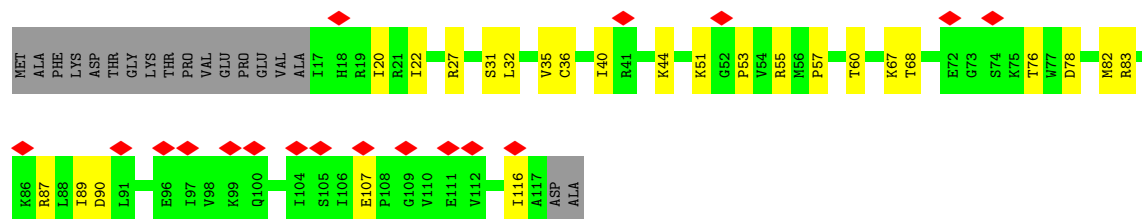


• Molecule 24: 40S ribosomal protein S19

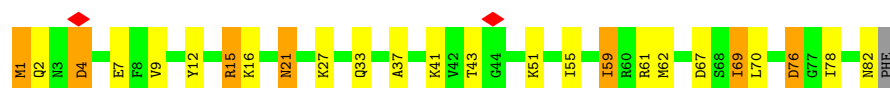




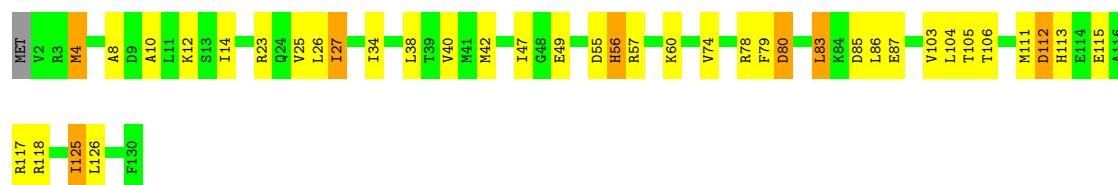
- Molecule 25: 40S ribosomal protein S20



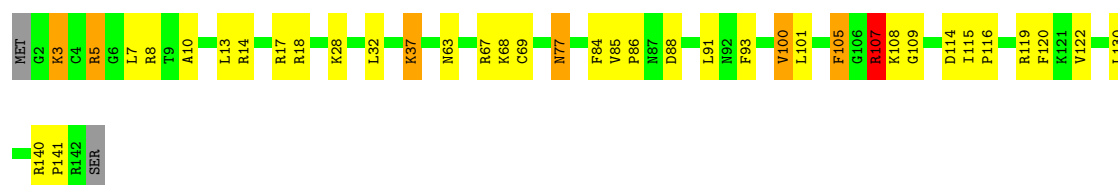
- Molecule 26: 40S ribosomal protein S21



- Molecule 27: 40S ribosomal protein S15a

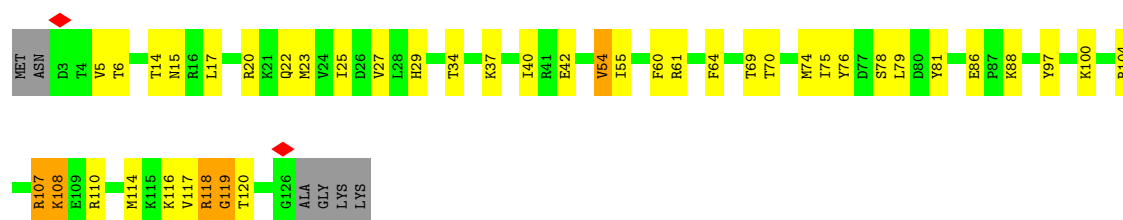


- Molecule 28: 40S ribosomal protein S23

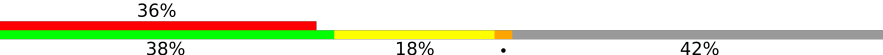


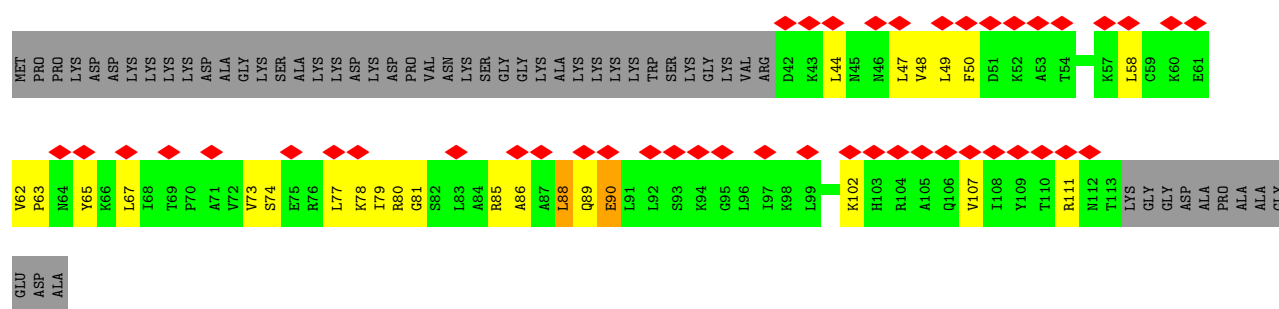
- Molecule 29: 40S ribosomal protein S24

Chain Y: 



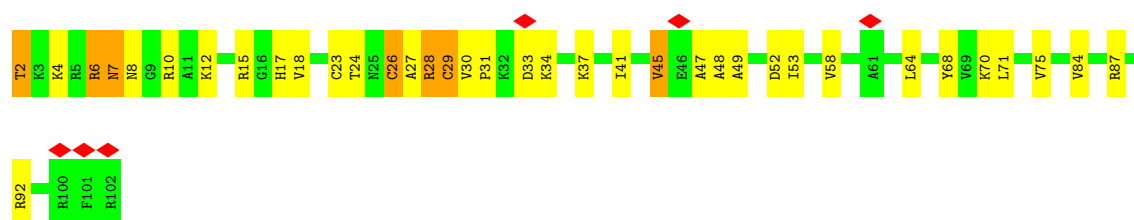
- Molecule 30: 40S ribosomal protein S25

Chain Z: 



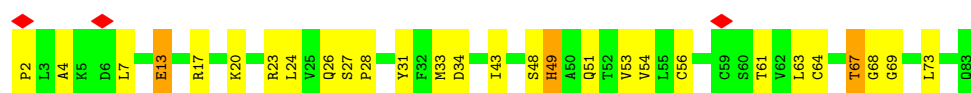
- Molecule 31: 40S ribosomal protein S26

Chain a: 



- Molecule 32: 40S ribosomal protein S27

Chain b: 

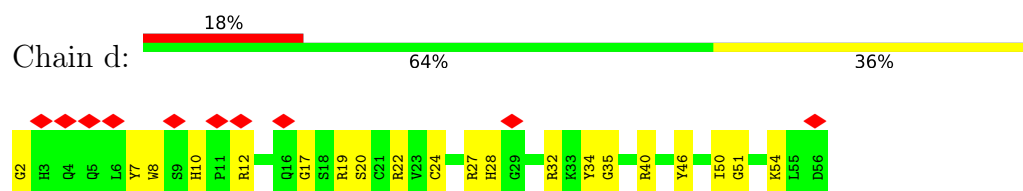


- Molecule 33: 40S ribosomal protein S28

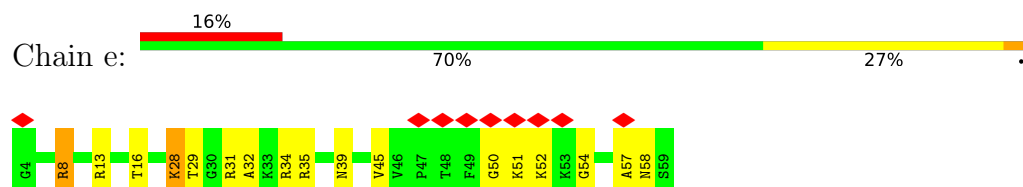
Chain c: 



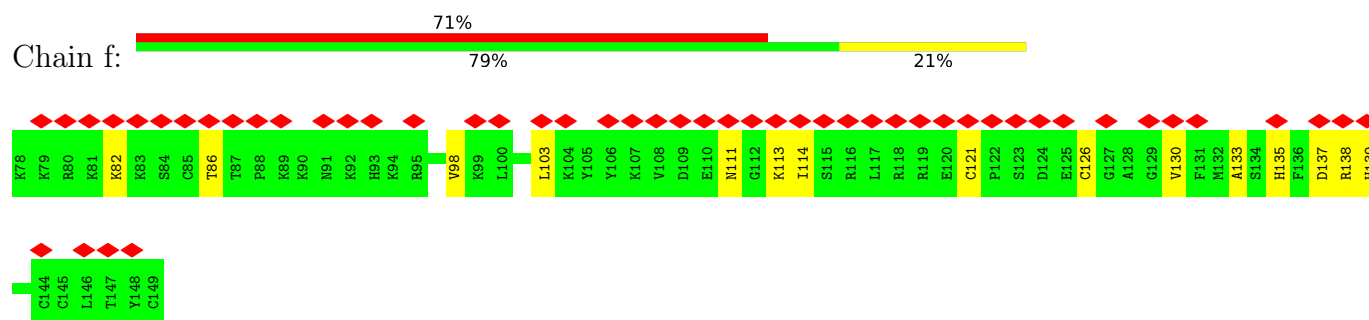
- Molecule 34: 40S ribosomal protein S29



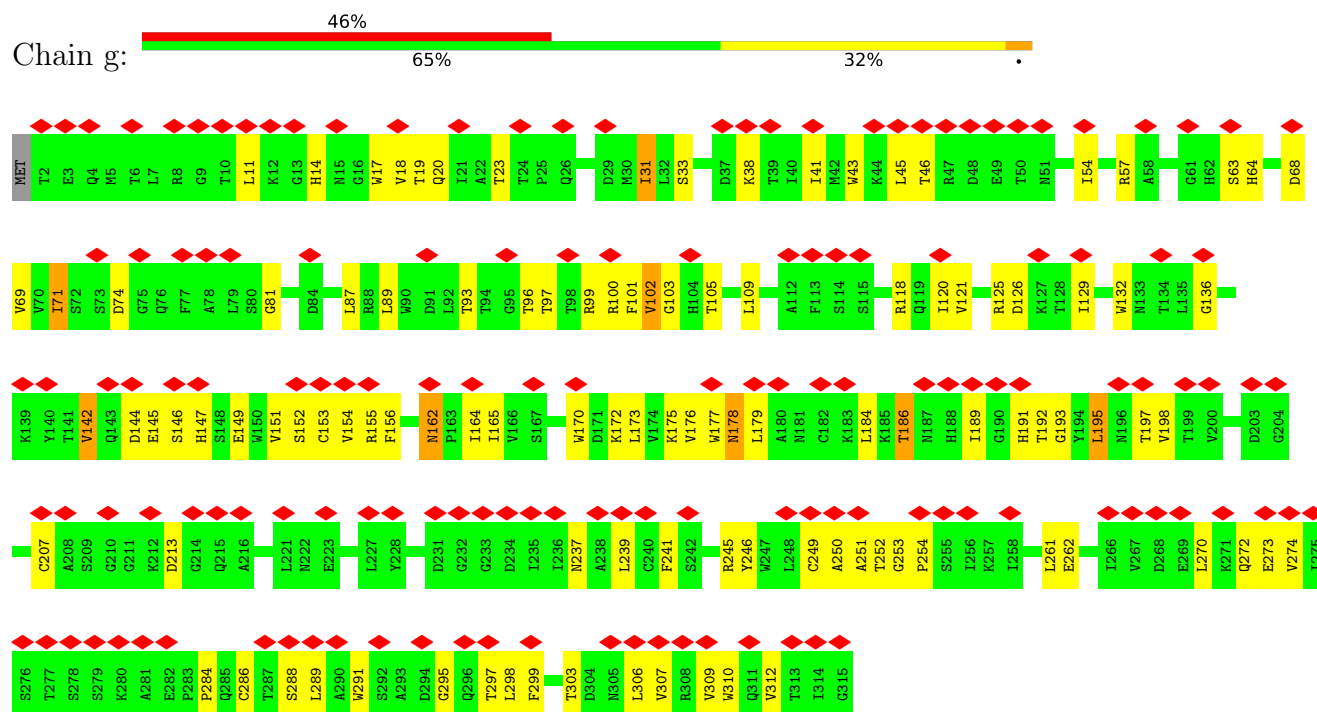
- Molecule 35: 40S ribosomal protein S30



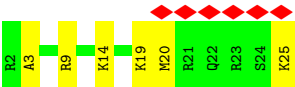
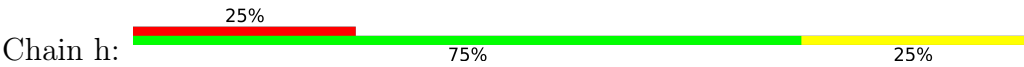
- Molecule 36: Ribosomal protein S27a



- Molecule 37: Receptor of activated protein C kinase 1



- Molecule 38: RIBOSOMAL PROTEIN EL41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62177	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.881	Depositor
Minimum map value	-0.648	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	274.4, 274.4, 274.4	wwPDB
Map dimensions	196, 196, 196	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0	0.85	5/3816 (0.1%)	1.14	24/5171 (0.5%)
2	1	0.18	0/1798	0.41	0/2801
3	2	0.22	0/39659	0.41	4/61804 (0.0%)
4	3	0.16	0/4440	0.36	0/6916
5	A	0.44	0/1742	0.86	2/2367 (0.1%)
6	B	0.39	0/1756	0.83	1/2350 (0.0%)
7	C	0.48	0/1726	0.90	7/2332 (0.3%)
8	D	0.36	0/1780	0.82	2/2397 (0.1%)
9	E	0.41	0/2118	0.91	8/2849 (0.3%)
10	F	0.43	0/1516	0.85	1/2037 (0.0%)
11	G	0.39	0/1885	0.87	8/2510 (0.3%)
12	H	0.42	0/1524	0.91	3/2042 (0.1%)
13	I	0.39	0/1704	0.86	1/2274 (0.0%)
14	J	0.40	0/1524	0.89	4/2035 (0.2%)
15	K	0.33	0/824	0.79	0/1112
16	L	0.45	0/1250	0.95	5/1673 (0.3%)
17	M	0.36	0/963	0.76	0/1291
18	N	0.44	0/1226	0.91	4/1649 (0.2%)
19	O	0.42	0/1023	0.95	0/1372
20	P	0.35	0/1003	0.78	2/1341 (0.1%)
21	Q	0.36	0/1126	0.93	4/1506 (0.3%)
22	R	0.58	2/1081 (0.2%)	0.98	4/1449 (0.3%)
23	S	0.33	0/1202	0.77	2/1610 (0.1%)
24	T	0.36	0/1142	0.82	0/1530
25	U	0.37	0/813	0.81	0/1092
26	V	0.42	0/631	0.82	0/844
27	W	0.51	0/1051	0.90	1/1406 (0.1%)
28	X	0.48	0/1116	0.94	2/1490 (0.1%)
29	Y	0.40	0/1031	0.83	1/1370 (0.1%)
30	Z	0.42	0/580	0.77	0/780
31	a	0.44	0/828	0.90	0/1109
32	b	0.42	0/653	0.87	1/876 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.42	0/481	0.81	1/643 (0.2%)
34	d	0.35	0/469	0.87	1/623 (0.2%)
35	e	0.40	0/447	0.84	0/587
36	f	0.32	0/595	0.81	2/785 (0.3%)
37	g	0.36	0/2497	0.80	2/3399 (0.1%)
38	h	0.35	0/232	0.79	0/295
All	All	0.36	7/89252 (0.0%)	0.67	97/129717 (0.1%)

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
8	D	0	1
28	X	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	277	LYS	CA-C	8.82	1.60	1.52
1	0	120	PRO	CA-C	8.22	1.59	1.52
1	0	301	CYS	C-O	-6.33	1.18	1.24
22	R	71	ILE	C-O	-6.30	1.14	1.23
1	0	278	CYS	C-O	-5.28	1.17	1.24
1	0	345	VAL	CA-CB	5.20	1.61	1.54
22	R	71	ILE	CA-CB	5.08	1.61	1.54

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	377	HIS	CA-C-N	12.32	133.06	120.38
1	0	377	HIS	C-N-CA	12.32	133.06	120.38
1	0	378	PRO	N-CA-C	9.58	122.39	110.70
16	L	41	GLY	N-CA-C	9.17	123.73	112.73
1	0	160	GLY	N-CA-C	-8.87	102.42	115.63
21	Q	43	GLU	CA-C-N	-8.53	110.94	119.90
21	Q	43	GLU	C-N-CA	-8.53	110.94	119.90
12	H	111	LYS	N-CA-C	-8.48	102.95	113.38
10	F	80	GLY	N-CA-C	8.32	122.71	112.64
21	Q	134	GLY	CA-C-N	8.30	127.94	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Q	134	GLY	C-N-CA	8.30	127.94	119.56
9	E	34	GLY	CA-C-N	7.41	127.28	119.05
9	E	34	GLY	C-N-CA	7.41	127.28	119.05
1	0	277	LYS	N-CA-C	7.05	121.80	112.13
22	R	74	GLN	N-CA-C	-6.93	104.86	113.38
1	0	32	THR	N-CA-C	-6.79	105.00	113.28
28	X	85	VAL	CA-C-N	6.58	125.81	118.97
28	X	85	VAL	C-N-CA	6.58	125.81	118.97
22	R	72	LYS	CA-C-O	-6.51	109.73	120.80
1	0	16	GLY	N-CA-C	6.51	120.54	112.73
11	G	7	PHE	CA-C-N	6.50	125.94	118.85
11	G	7	PHE	C-N-CA	6.50	125.94	118.85
16	L	114	SER	CA-C-N	6.49	126.18	119.56
16	L	114	SER	C-N-CA	6.49	126.18	119.56
14	J	144	ILE	CA-C-N	6.49	125.98	119.24
14	J	144	ILE	C-N-CA	6.49	125.98	119.24
22	R	75	GLU	N-CA-C	-6.40	104.17	112.23
34	d	35	GLY	N-CA-C	-6.37	105.90	115.32
16	L	13	GLN	CA-C-N	6.35	126.84	119.47
16	L	13	GLN	C-N-CA	6.35	126.84	119.47
1	0	120	PRO	N-CA-C	6.28	118.37	110.70
6	B	45	GLY	N-CA-C	6.10	118.81	110.58
18	N	71	ILE	N-CA-C	6.08	116.74	110.36
9	E	4	GLY	CA-C-N	6.07	126.03	120.03
9	E	4	GLY	C-N-CA	6.07	126.03	120.03
37	g	162	ASN	CA-C-N	6.06	126.08	119.90
37	g	162	ASN	C-N-CA	6.06	126.08	119.90
5	A	140	VAL	N-CA-C	5.86	117.80	112.29
1	0	30	PHE	CA-C-N	5.83	127.12	119.84
1	0	30	PHE	C-N-CA	5.83	127.12	119.84
32	b	7	LEU	N-CA-C	-5.82	106.14	113.18
14	J	144	ILE	N-CA-C	5.75	114.83	108.05
1	0	303	GLU	N-CA-C	-5.74	106.25	113.20
1	0	99	TRP	CD2-CE2-CZ2	-5.72	116.67	122.40
18	N	136	PRO	CA-C-N	-5.72	112.69	119.84
18	N	136	PRO	C-N-CA	-5.72	112.69	119.84
5	A	144	THR	N-CA-C	5.69	117.68	108.34
12	H	66	VAL	CB-CA-C	-5.68	108.33	114.35
11	G	181	THR	CA-C-N	5.65	125.76	119.32
11	G	181	THR	C-N-CA	5.65	125.76	119.32
20	P	130	ARG	CA-C-N	5.56	125.55	120.21
20	P	130	ARG	C-N-CA	5.56	125.55	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	114	LEU	CA-C-N	-5.53	113.92	119.56
1	0	114	LEU	C-N-CA	-5.53	113.92	119.56
11	G	61	PHE	CA-C-N	5.52	125.51	120.21
11	G	61	PHE	C-N-CA	5.52	125.51	120.21
12	H	37	LYS	N-CA-C	5.37	117.56	111.11
27	W	111	MET	N-CA-C	5.32	115.56	108.38
18	N	13	GLN	N-CA-C	5.32	114.86	107.73
1	0	552	GLN	N-CA-C	5.29	119.83	113.17
9	E	136	ILE	CA-C-N	5.28	125.19	119.85
9	E	136	ILE	C-N-CA	5.28	125.19	119.85
33	c	23	SER	N-CA-C	-5.28	105.17	111.03
7	C	180	VAL	CA-C-N	5.27	124.90	119.05
7	C	180	VAL	C-N-CA	5.27	124.90	119.05
1	0	159	SER	N-CA-C	5.25	118.79	112.38
22	R	71	ILE	CA-C-O	-5.24	115.64	121.98
13	I	139	LYS	CB-CA-C	-5.22	109.03	116.34
29	Y	119	GLY	N-CA-C	5.20	125.51	113.18
9	E	29	PRO	N-CA-C	5.20	120.36	113.86
1	0	100	PRO	CA-C-N	5.19	127.76	120.28
1	0	100	PRO	C-N-CA	5.19	127.76	120.28
8	D	79	PHE	CA-C-N	5.19	125.18	119.89
8	D	79	PHE	C-N-CA	5.19	125.18	119.89
3	2	1253	A	P-O3'-C3'	5.18	127.97	120.20
11	G	134	GLY	CA-C-N	5.18	125.47	119.93
11	G	134	GLY	C-N-CA	5.18	125.47	119.93
3	2	1253	A	C2'-C3'-O3'	5.17	117.25	109.50
7	C	163	VAL	CA-C-N	5.16	125.06	119.85
7	C	163	VAL	C-N-CA	5.16	125.06	119.85
1	0	476	LEU	CA-C-N	5.14	125.14	119.90
1	0	476	LEU	C-N-CA	5.14	125.14	119.90
7	C	209	VAL	CA-C-N	-5.12	114.39	119.56
7	C	209	VAL	C-N-CA	-5.12	114.39	119.56
1	0	499	ALA	CB-CA-C	-5.12	110.65	116.54
14	J	138	ARG	CB-CA-C	-5.12	110.27	117.23
3	2	114	G	C2'-C3'-O3'	5.09	117.14	109.50
23	S	73	ASN	CA-C-N	5.09	124.39	118.85
23	S	73	ASN	C-N-CA	5.09	124.39	118.85
1	0	375	PRO	N-CA-C	5.08	122.92	112.47
1	0	379	PRO	N-CA-C	5.04	119.12	111.11
1	0	279	ARG	N-CA-C	5.03	116.61	108.41
7	C	134	ASN	N-CA-C	5.03	121.51	110.80
36	f	121	CYS	CA-C-N	5.02	124.63	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	f	121	CYS	C-N-CA	5.02	124.63	119.56
9	E	228	ILE	N-CA-C	5.01	115.68	110.82
3	2	1838	U	C2'-C3'-O3'	5.01	117.01	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	193	ASP	Peptide
28	X	107	ARG	Peptide

5.2 Too-close contacts [i](#)

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	0	3740	0	3855	79	0
2	1	1608	0	816	24	0
3	2	35466	0	17905	622	0
4	3	3976	0	2013	47	0
5	A	1705	0	1706	60	0
6	B	1729	0	1803	59	0
7	C	1690	0	1777	47	0
8	D	1752	0	1848	47	0
9	E	2076	0	2177	55	0
10	F	1495	0	1549	44	0
11	G	1862	0	2018	79	0
12	H	1501	0	1593	37	0
13	I	1675	0	1755	36	0
14	J	1499	0	1618	48	0
15	K	800	0	818	22	0
16	L	1229	0	1302	44	0
17	M	953	0	990	25	0
18	N	1202	0	1289	31	0
19	O	1010	0	1034	47	0
20	P	984	0	1028	33	0
21	Q	1109	0	1174	34	0
22	R	1068	0	1120	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	S	1184	0	1244	47	0
24	T	1122	0	1153	53	0
25	U	803	0	873	20	0
26	V	625	0	628	18	0
27	W	1034	0	1080	20	0
28	X	1098	0	1167	33	0
29	Y	1014	0	1082	28	0
30	Z	574	0	627	20	0
31	a	814	0	863	29	0
32	b	640	0	665	15	0
33	c	479	0	507	15	0
34	d	458	0	448	15	0
35	e	442	0	487	10	0
36	f	585	0	615	10	0
37	g	2440	0	2396	61	0
38	h	231	0	277	3	0
39	a	1	0	0	0	0
39	d	1	0	0	0	0
39	f	1	0	0	0	0
All	All	83675	0	65300	1627	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 11.

All (1627) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:9:LYS:NZ	3:2:966:U:OP1	1.92	1.02
7:C:60:TRP:O	7:C:71:LYS:NZ	1.93	1.01
3:2:615:C:O2'	35:e:8:ARG:NH1	1.94	0.99
37:g:245:ARG:HH12	37:g:312:VAL:HG11	1.29	0.93
9:E:11:ARG:NH1	9:E:24:THR:OG1	2.03	0.92
5:A:37:TYR:OH	5:A:57:LYS:NZ	2.05	0.89
3:2:1075:C:OP1	18:N:107:LYS:NZ	2.06	0.89
1:0:378:PRO:HB2	1:0:477:PRO:HG2	1.56	0.88
6:B:87:ILE:HG12	6:B:101:HIS:HB2	1.60	0.82
4:3:42:C:H42	4:3:120:C:H42	1.28	0.81
3:2:146:G:OP1	11:G:143:LYS:NZ	2.13	0.80
3:2:943:U:OP1	6:B:214:LYS:NZ	2.14	0.80
3:2:171:A:H5''	11:G:177:GLN:HG2	1.63	0.80
3:2:1100:A:O5'	22:R:132:ARG:NH1	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1601:A:H4'	3:2:1602:U:H5'	1.64	0.80
11:G:72:ARG:HG3	11:G:72:ARG:HH11	1.45	0.80
3:2:1661:A:OP2	34:d:32:ARG:NH1	2.15	0.80
3:2:384:U:O4	13:I:5:ARG:NH2	2.15	0.79
34:d:17:GLY:HA2	34:d:27:ARG:HD3	1.64	0.79
24:T:69:GLY:HA2	24:T:120:GLY:HA3	1.64	0.79
23:S:23:ARG:HB2	30:Z:48:VAL:HG21	1.64	0.79
5:A:117:ARG:HG3	5:A:119:PRO:HD3	1.66	0.78
3:2:1309:C:H4'	36:f:133:ALA:HB2	1.62	0.78
23:S:16:LEU:HD21	23:S:72:GLN:HE22	1.48	0.77
28:X:93:PHE:O	28:X:140:ARG:NH1	2.17	0.77
3:2:76:U:H3'	3:2:77:A:H5'	1.66	0.77
3:2:64:A:H2	3:2:83:A:H62	1.32	0.77
3:2:68:A:OP2	11:G:164:LYS:NZ	2.17	0.77
20:P:22:LEU:HD11	20:P:109:PRO:HB3	1.66	0.77
16:L:80:MET:HB3	16:L:86:ILE:HG22	1.66	0.77
24:T:140:ALA:HA	24:T:143:LYS:HE2	1.66	0.77
11:G:44:GLU:HA	11:G:119:LYS:HD2	1.67	0.76
3:2:1863:A:OP2	31:a:4:LYS:NZ	2.18	0.76
24:T:52:TRP:HZ3	24:T:56:ARG:HH12	1.34	0.76
14:J:77:LEU:HA	14:J:80:ARG:NH1	2.00	0.75
28:X:68:LYS:HB3	28:X:91:LEU:HD22	1.68	0.75
11:G:159:ARG:HH11	11:G:171:THR:HG21	1.52	0.75
3:2:913:A:H2	12:H:98:ARG:HA	1.51	0.75
3:2:318:A:H61	11:G:186:GLN:HE22	1.33	0.75
3:2:1610:G:N2	23:S:85:ASN:OD1	2.19	0.74
19:O:74:ALA:HB1	19:O:115:ALA:HB2	1.69	0.74
3:2:1649:U:OP2	3:2:1674:G:N1	2.20	0.74
1:0:281:LYS:NZ	1:0:298:PHE:HB2	2.03	0.74
3:2:190:G:O2'	3:2:209:A:N6	2.20	0.74
7:C:131:GLY:HA3	7:C:216:MET:HB3	1.70	0.73
2:1:9:G:H2'	2:1:11:C:H41	1.53	0.73
3:2:121:U:H5''	9:E:77:ARG:HH21	1.53	0.73
3:2:1332:A:O2'	8:D:145:GLN:OE1	2.07	0.73
17:M:20:GLU:HB3	17:M:120:ALA:HB2	1.69	0.73
3:2:387:C:OP2	13:I:10:LYS:NZ	2.21	0.73
6:B:65:ARG:NH2	19:O:51:GLU:OE2	2.22	0.73
3:2:150:A:N6	3:2:169:U:O2	2.21	0.73
8:D:127:MET:HE3	8:D:154:ASP:HB3	1.71	0.72
7:C:187:ARG:HD3	7:C:192:LEU:HD23	1.71	0.72
22:R:41:ILE:HD13	22:R:47:ARG:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1036:A:N3	3:2:1844:U:O2'	2.23	0.72
3:2:919:A:OP2	18:N:64:ARG:NH1	2.19	0.72
25:U:51:LYS:HB2	25:U:90:ASP:HB2	1.69	0.72
3:2:168:C:OP1	11:G:131:ARG:NE	2.23	0.72
30:Z:48:VAL:HG22	30:Z:80:ARG:HH11	1.55	0.72
4:3:150:G:H1	4:3:242:C:H42	1.37	0.71
10:F:78:MET:H	10:F:159:ARG:HH22	1.35	0.71
1:0:14:ILE:HD11	1:0:50:ILE:HG13	1.71	0.71
12:H:76:GLN:HE22	12:H:94:PHE:HB2	1.55	0.71
19:O:117:ARG:HH12	31:a:48:ALA:HB3	1.55	0.71
11:G:59:GLN:HG3	11:G:72:ARG:NH2	2.06	0.71
31:a:26:CYS:HB3	31:a:28:ARG:H	1.56	0.71
12:H:184:ASP:N	12:H:184:ASP:OD1	2.23	0.71
15:K:23:ALA:HB3	15:K:67:PHE:HB2	1.73	0.71
37:g:87:LEU:HB3	37:g:101:PHE:HB2	1.73	0.71
6:B:144:LYS:HB2	6:B:208:HIS:HB2	1.72	0.70
6:B:146:ARG:HA	6:B:146:ARG:HH11	1.56	0.70
3:2:1738:C:OP1	11:G:92:ARG:NH2	2.25	0.70
3:2:76:U:H5'	11:G:159:ARG:HH22	1.57	0.70
3:2:1608:U:H4'	23:S:130:ARG:NH1	2.07	0.70
4:3:243:A:O2'	4:3:244:A:OP1	2.08	0.70
6:B:128:LYS:HG3	6:B:134:LEU:HD13	1.74	0.70
8:D:62:LYS:O	8:D:67:ARG:NH2	2.24	0.70
9:E:55:ALA:HB1	9:E:60:GLU:HB2	1.74	0.70
16:L:35:ARG:NH2	16:L:55:TYR:O	2.24	0.70
32:b:23:ARG:HH11	32:b:27:SER:HB2	1.56	0.70
3:2:1275:G:N2	3:2:1506:A:OP2	2.25	0.69
3:2:1351:G:H2'	3:2:1352:G:H8	1.55	0.69
3:2:525:A:H2'	3:2:526:A:C8	2.27	0.69
20:P:72:LYS:NZ	20:P:106:GLU:OE2	2.23	0.69
32:b:23:ARG:NH1	32:b:27:SER:HB2	2.06	0.69
3:2:1126:G:OP2	22:R:129:LYS:NZ	2.21	0.69
28:X:100:VAL:HG13	28:X:122:VAL:HG13	1.74	0.69
3:2:944:A:H5''	19:O:134:PRO:HB3	1.73	0.69
19:O:40:THR:HG21	19:O:111:GLY:HA3	1.74	0.69
8:D:99:ILE:HG23	8:D:173:ARG:HH21	1.58	0.68
19:O:103:ASN:N	19:O:103:ASN:OD1	2.23	0.68
23:S:34:LYS:HB2	23:S:100:ALA:HA	1.73	0.68
21:Q:82:TYR:HE1	21:Q:85:ARG:NH1	1.90	0.68
24:T:76:THR:HG22	24:T:94:ARG:HB3	1.74	0.68
3:2:1649:U:O2'	3:2:1650:A:OP1	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:7:ASN:ND2	31:a:10:ARG:O	2.26	0.68
3:2:109:U:O2'	16:L:71:ARG:NH2	2.27	0.68
3:2:368:U:O2'	3:2:369:C:OP1	2.09	0.68
3:2:1605:G:OP1	24:T:84:ARG:NH2	2.26	0.68
23:S:90:VAL:HG21	23:S:113:ARG:NH1	2.09	0.68
3:2:1428:G:O6	21:Q:71:ARG:NH2	2.27	0.68
3:2:619:A:N1	28:X:114:ASP:HB2	2.08	0.68
15:K:27:VAL:HG13	15:K:43:LEU:HD13	1.76	0.68
15:K:65:ARG:NH1	34:d:20:SER:OG	2.27	0.68
3:2:1819:A:H2'	3:2:1820:G:C8	2.29	0.67
7:C:168:GLY:N	7:C:179:THR:O	2.27	0.67
3:2:808:A:O2'	3:2:809:A:O5'	2.11	0.67
3:2:152:U:H4'	11:G:132:ARG:NH1	2.09	0.67
6:B:209:ASP:HB3	6:B:211:PHE:HE1	1.58	0.67
23:S:83:PHE:HE2	24:T:36:THR:HG23	1.59	0.67
3:2:685:A:H62	3:2:918:U:H3	1.42	0.67
3:2:1284:A:O2'	17:M:106:CYS:SG	2.50	0.67
3:2:1259:A:H61	3:2:1519:U:H5'	1.60	0.67
37:g:147:HIS:HD2	37:g:151:VAL:HG22	1.60	0.67
3:2:1612:G:H1'	23:S:87:GLN:HG3	1.75	0.67
1:0:13:ALA:HB3	3:2:1069:U:H4'	1.77	0.67
3:2:560:A:H5'	14:J:174:LYS:HG3	1.76	0.67
28:X:67:ARG:HG3	28:X:115:ILE:HG12	1.77	0.67
3:2:1341:C:H4'	3:2:1342:U:H5'	1.77	0.66
11:G:72:ARG:HG3	11:G:72:ARG:NH1	2.08	0.66
11:G:85:ARG:HH21	11:G:87:ARG:HH12	1.43	0.66
37:g:172:LYS:HE2	37:g:193:GLY:H	1.59	0.66
3:2:1387:G:N1	8:D:206:ASP:OD1	2.28	0.66
5:A:198:MET:HG2	5:A:200:ASP:HB2	1.76	0.66
13:I:13:LYS:NZ	16:L:108:ASN:O	2.28	0.66
20:P:18:ARG:HG3	20:P:36:LEU:HB3	1.76	0.66
23:S:86:ARG:HD2	23:S:106:LYS:HD3	1.77	0.66
3:2:617:G:H4'	28:X:88:ASP:HB3	1.78	0.66
23:S:6:PRO:HG2	30:Z:49:LEU:HD13	1.77	0.66
31:a:33:ASP:OD1	31:a:34:LYS:N	2.29	0.66
1:0:549:GLN:NE2	3:2:1829:G:OP1	2.29	0.66
19:O:98:ARG:HH11	19:O:98:ARG:CG	2.09	0.66
3:2:1478:U:H2'	3:2:1479:G:C8	2.31	0.65
14:J:136:ARG:HD2	14:J:160:SER:HA	1.77	0.65
22:R:34:VAL:HG13	22:R:38:ILE:HD12	1.76	0.65
23:S:38:ARG:O	23:S:42:HIS:ND1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:7:G:H5'	2:1:8:U:H5''	1.77	0.65
3:2:145:G:H2'	3:2:146:G:C8	2.31	0.65
3:2:1234:C:H5'	3:2:1246:A:H61	1.62	0.65
3:2:1377:U:C4	5:A:102:ARG:NH1	2.64	0.65
1:0:19:ARG:HG2	1:0:23:ARG:HH12	1.61	0.65
5:A:73:ASP:HB3	5:A:120:ARG:HB2	1.77	0.65
20:P:98:ASN:ND2	20:P:103:ASN:OD1	2.29	0.65
3:2:53:C:O2'	3:2:507:G:N7	2.26	0.65
20:P:41:GLN:NE2	20:P:113:GLY:O	2.28	0.65
3:2:1509:U:O4	36:f:82:LYS:NZ	2.30	0.65
4:3:252:A:H4'	4:3:253:G:H5'	1.79	0.65
27:W:86:LEU:HD21	27:W:113:HIS:HB2	1.77	0.65
3:2:1598:G:H2'	30:Z:81:GLY:H	1.62	0.65
3:2:660:C:OP2	28:X:3:LYS:NZ	2.31	0.64
3:2:1396:A:O2'	3:2:1398:G:N7	2.30	0.64
3:2:1606:G:H5'	24:T:86:GLY:HA2	1.79	0.64
3:2:1630:A:OP1	23:S:37:GLY:N	2.26	0.64
4:3:294:U:H2'	4:3:295:G:H2'	1.78	0.64
1:0:103:LEU:HD13	1:0:137:LEU:HD11	1.80	0.64
18:N:101:HIS:CE1	18:N:105:ASN:HD22	2.15	0.64
25:U:20:ILE:HG23	25:U:116:ILE:HG12	1.79	0.64
27:W:80:ASP:OD1	27:W:80:ASP:N	2.30	0.64
3:2:168:C:O2'	11:G:132:ARG:O	2.15	0.64
13:I:3:ILE:O	13:I:30:GLY:N	2.19	0.64
16:L:116:CYS:SG	16:L:117:PHE:N	2.71	0.64
3:2:1240:A:C4	20:P:100:LYS:HB2	2.33	0.64
3:2:928:G:H1	3:2:1013:U:H3	1.44	0.64
3:2:1269:G:H1	3:2:1513:C:H42	1.43	0.64
11:G:137:ARG:NH1	11:G:178:ARG:NH1	2.45	0.64
3:2:640:A:H2'	3:2:641:A:C8	2.33	0.64
13:I:121:LEU:HD21	13:I:158:ILE:HD12	1.79	0.64
2:1:15:G:H22	2:1:48:C:H42	1.43	0.64
12:H:47:ALA:HB3	12:H:63:PHE:HB2	1.80	0.64
3:2:75:G:H22	11:G:155:GLN:HG3	1.62	0.63
3:2:1310:U:OP2	17:M:36:ARG:NH2	2.30	0.63
4:3:333:C:O2'	4:3:334:C:OP1	2.14	0.63
3:2:1337:C:H2'	3:2:1338:G:H8	1.63	0.63
3:2:1399:C:OP1	37:g:100:ARG:NH1	2.32	0.63
6:B:125:VAL:HG22	6:B:169:MET:HG3	1.80	0.63
3:2:319:C:O2'	3:2:320:G:OP1	2.16	0.63
3:2:1229:G:H21	24:T:87:VAL:HG12	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:109:ARG:HH12	14:J:111:GLN:HB3	1.62	0.63
1:O:135:ILE:HB	1:O:145:ALA:HB3	1.80	0.63
3:2:570:C:O2'	29:Y:34:THR:O	2.15	0.63
1:O:22:LEU:O	1:O:26:VAL:HG23	1.99	0.63
3:2:1528:G:O2'	3:2:1666:C:OP1	2.17	0.63
3:2:1546:G:H5'	21:Q:18:THR:HG21	1.80	0.63
7:C:167:ARG:HB2	7:C:177:PRO:HB2	1.81	0.63
1:O:269:GLN:O	1:O:273:LEU:HB2	1.98	0.63
3:2:1225:U:H1'	21:Q:142:GLN:HE22	1.64	0.63
18:N:118:ILE:HG12	18:N:121:ARG:HH12	1.63	0.63
37:g:120:ILE:HB	37:g:132:TRP:HB2	1.81	0.63
3:2:1256:G:H21	3:2:1659:U:H5'	1.63	0.63
3:2:918:U:H5''	18:N:64:ARG:HH22	1.64	0.63
3:2:1265:A:O2'	3:2:1327:G:OP2	2.17	0.63
3:2:1542:C:H4'	24:T:11:GLN:HB2	1.80	0.63
19:O:98:ARG:HH11	19:O:98:ARG:HG3	1.64	0.62
2:1:18:G:O2'	2:1:57:G:N2	2.31	0.62
3:2:1496:U:H4'	34:d:24:CYS:HB2	1.79	0.62
3:2:1860:A:H5'	31:a:8:ASN:HB3	1.80	0.62
3:2:1265:A:N6	3:2:1518:C:O2	2.33	0.62
5:A:53:ARG:NH2	26:V:82:ASN:O	2.32	0.62
8:D:67:ARG:NH1	15:K:93:THR:O	2.32	0.62
3:2:925:G:H1	3:2:1017:U:H3	1.46	0.62
8:D:22:ASN:OD1	8:D:34:TYR:OH	2.17	0.62
14:J:47:LYS:HA	14:J:102:ILE:HD11	1.80	0.62
24:T:52:TRP:HZ3	24:T:56:ARG:NH1	1.97	0.62
29:Y:15:ASN:ND2	29:Y:22:GLN:OE1	2.33	0.62
4:3:254:C:H4'	4:3:255:C:OP1	2.00	0.62
31:a:10:ARG:NH1	31:a:12:LYS:HD3	2.14	0.62
3:2:809:A:H4'	9:E:221:ARG:NH1	2.15	0.62
3:2:870:A:H4'	3:2:871:U:H5'	1.80	0.62
19:O:43:HIS:CE1	19:O:52:THR:HB	2.34	0.62
22:R:20:TYR:HD2	22:R:23:ARG:HD2	1.63	0.62
22:R:44:LYS:NZ	22:R:47:ARG:HH12	1.96	0.62
27:W:55:ASP:OD1	27:W:56:HIS:N	2.32	0.62
3:2:1610:G:N2	23:S:85:ASN:O	2.33	0.62
13:I:87:ASN:HD22	13:I:88:ASN:H	1.48	0.62
37:g:173:LEU:HD22	37:g:189:ILE:HG12	1.82	0.62
4:3:329:U:O2'	4:3:330:A:O5'	2.12	0.61
5:A:85:ARG:HH21	5:A:201:LEU:HD12	1.65	0.61
22:R:44:LYS:HZ2	22:R:47:ARG:NH1	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:506:VAL:HG22	1:0:547:GLN:HG2	1.82	0.61
3:2:1392:U:H3	3:2:1478:U:H3	1.49	0.61
3:2:1650:A:OP1	21:Q:138:ARG:HB2	2.00	0.61
11:G:58:LYS:HA	11:G:107:SER:HB2	1.82	0.61
17:M:72:HIS:O	17:M:73:GLN:HG2	2.00	0.61
3:2:913:A:N6	12:H:120:ARG:HG3	2.15	0.61
3:2:1622:U:O4	20:P:81:ARG:NH2	2.33	0.61
3:2:925:G:H2'	3:2:926:A:H5''	1.82	0.61
14:J:77:LEU:HA	14:J:80:ARG:HH11	1.63	0.61
3:2:1446:A:OP1	25:U:57:PRO:HA	1.99	0.61
12:H:9:VAL:HG12	12:H:11:PRO:HD3	1.83	0.61
19:O:117:ARG:NH1	31:a:48:ALA:HB3	2.15	0.61
3:2:1189:A:H2'	3:2:1190:A:H8	1.65	0.61
3:2:1199:A:H5'	31:a:2:THR:HB	1.83	0.61
3:2:1606:G:O2'	3:2:1633:A:N6	2.33	0.61
10:F:168:THR:HG22	10:F:170:ALA:H	1.65	0.61
19:O:30:VAL:HG22	19:O:94:HIS:HB2	1.82	0.61
3:2:1342:U:H4'	3:2:1343:U:O5'	2.01	0.61
4:3:146:G:H1	4:3:247:C:H42	1.48	0.61
20:P:56:LEU:HD22	20:P:80:LEU:HD12	1.82	0.61
3:2:76:U:OP1	11:G:159:ARG:NH1	2.31	0.61
3:2:151:C:OP1	29:Y:120:THR:OG1	2.08	0.61
3:2:1428:G:H4'	3:2:1429:G:H5'	1.82	0.61
3:2:73:C:O2'	3:2:74:G:O4'	2.16	0.61
31:a:49:ALA:HA	31:a:52:ASP:HB2	1.82	0.61
1:0:124:LEU:HD21	1:0:156:MET:HE2	1.83	0.60
7:C:137:VAL:HG21	7:C:244:ILE:HD12	1.81	0.60
19:O:105:THR:HG22	19:O:107:THR:H	1.66	0.60
3:2:1337:C:H2'	3:2:1338:G:C8	2.35	0.60
7:C:259:THR:HG21	26:V:16:LYS:H	1.67	0.60
11:G:159:ARG:HB3	11:G:171:THR:HG23	1.83	0.60
14:J:132:GLN:HB3	14:J:134:HIS:CD2	2.35	0.60
3:2:643:A:OP1	14:J:39:ASN:ND2	2.34	0.60
3:2:1395:C:H1'	3:2:1474:A:C4	2.37	0.60
10:F:35:LEU:HD21	10:F:146:ARG:HD2	1.83	0.60
7:C:259:THR:HG21	26:V:15:ARG:HA	1.83	0.60
11:G:59:GLN:HG3	11:G:72:ARG:HH21	1.65	0.60
3:2:943:U:O2'	19:O:135:ILE:O	2.19	0.60
5:A:42:LYS:HE2	5:A:46:ILE:HB	1.83	0.60
29:Y:78:SER:HB3	29:Y:81:TYR:HD2	1.67	0.60
37:g:20:GLN:HE22	37:g:155:ARG:HH22	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:830:A:OP2	3:2:846:G:N2	2.34	0.60
4:3:253:G:O2'	4:3:254:C:H5'	2.02	0.60
14:J:109:ARG:NH2	14:J:146:SER:OG	2.31	0.60
2:1:9:G:O2'	2:1:10:G:N7	2.35	0.60
3:2:1293:A:H2'	3:2:1294:G:C8	2.37	0.60
27:W:112:ASP:OD1	27:W:112:ASP:N	2.34	0.60
37:g:176:VAL:HB	37:g:186:THR:HB	1.83	0.60
29:Y:25:ILE:HG21	29:Y:40:ILE:HD11	1.84	0.60
1:0:281:LYS:HZ3	1:0:298:PHE:HB2	1.66	0.60
3:2:1536:G:H2'	3:2:1537:A:C8	2.36	0.60
8:D:127:MET:HE1	8:D:133:GLY:HA2	1.83	0.60
25:U:55:ARG:HG2	25:U:87:ARG:HH11	1.67	0.60
3:2:1010:G:H2'	3:2:1011:A:C8	2.37	0.59
6:B:123:ALA:HB2	6:B:165:ARG:HG3	1.83	0.59
18:N:83:ASP:N	18:N:83:ASP:OD1	2.35	0.59
3:2:943:U:OP2	6:B:216:LYS:NZ	2.28	0.59
3:2:1351:G:H2'	3:2:1352:G:C8	2.37	0.59
2:1:8:U:OP1	2:1:49:C:H5''	2.01	0.59
3:2:317:C:OP2	11:G:183:ARG:NH2	2.36	0.59
3:2:797:C:O2'	3:2:798:G:OP1	2.15	0.59
3:2:1297:U:O2'	3:2:1301:A:N6	2.35	0.59
3:2:1565:C:H3'	3:2:1566:G:H5''	1.84	0.59
23:S:82:TRP:HA	23:S:87:GLN:HE22	1.66	0.59
3:2:1241:A:O2'	3:2:1266:C:O2'	2.18	0.59
7:C:134:ASN:O	7:C:167:ARG:NH2	2.36	0.59
10:F:138:ALA:O	33:c:63:ARG:NH1	2.35	0.59
16:L:135:SER:OG	16:L:136:LYS:N	2.34	0.59
11:G:159:ARG:HH11	11:G:171:THR:CG2	2.14	0.59
16:L:22:ARG:HH22	16:L:31:GLU:HG3	1.68	0.59
24:T:18:LEU:HD13	24:T:134:ILE:HD13	1.83	0.59
3:2:104:A:OP1	13:I:12:ARG:NE	2.31	0.59
3:2:594:A:H4'	3:2:595:U:OP1	2.03	0.59
3:2:1566:G:N7	24:T:98:SER:HB2	2.18	0.59
21:Q:62:ARG:HH12	21:Q:111:ILE:HD12	1.67	0.59
1:0:59:ASP:HB3	1:0:75:LEU:HD11	1.83	0.59
3:2:446:G:OP2	13:I:47:ARG:NH2	2.36	0.59
4:3:330:A:O2'	4:3:331:G:O5'	2.14	0.59
18:N:4:MET:SD	18:N:124:ARG:NH1	2.76	0.59
1:0:19:ARG:HG3	1:0:48:LEU:HD22	1.85	0.59
3:2:625:G:O6	28:X:63:ASN:HB2	2.03	0.59
3:2:874:G:H21	12:H:114:GLN:HE22	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:126:ASP:OD1	11:G:126:ASP:N	2.35	0.59
35:e:13:ARG:O	35:e:16:THR:OG1	2.21	0.59
26:V:51:LYS:HD2	26:V:78:ILE:HD11	1.85	0.59
14:J:89:GLU:OE2	14:J:89:GLU:N	2.35	0.58
1:0:317:LEU:HB2	3:2:1722:G:H4'	1.83	0.58
4:3:163:G:O2'	4:3:164:U:H4'	2.02	0.58
5:A:134:LEU:HD23	5:A:144:THR:HG21	1.86	0.58
3:2:792:C:H2'	3:2:793:G:C8	2.38	0.58
6:B:82:ARG:NH1	6:B:191:ASP:HB2	2.19	0.58
9:E:68:ARG:NH1	9:E:68:ARG:HB3	2.17	0.58
11:G:141:ILE:HG21	11:G:153:VAL:HG13	1.86	0.58
16:L:12:LYS:HE3	16:L:14:PRO:HA	1.86	0.58
30:Z:48:VAL:HG22	30:Z:80:ARG:NH1	2.18	0.58
37:g:11:LEU:HB2	37:g:307:VAL:HB	1.85	0.58
3:2:816:A:P	14:J:10:ARG:HH22	2.27	0.58
6:B:62:LEU:HA	6:B:65:ARG:HE	1.67	0.58
10:F:28:VAL:HG12	10:F:29:GLN:H	1.69	0.58
1:0:279:ARG:HG2	1:0:280:VAL:HA	1.86	0.58
7:C:134:ASN:HA	7:C:218:GLY:HA3	1.85	0.58
11:G:7:PHE:HE1	11:G:9:ALA:HB3	1.69	0.58
3:2:1470:C:OP2	10:F:59:LYS:NZ	2.36	0.58
1:0:146:ILE:HB	1:0:170:HIS:HB3	1.86	0.58
1:0:275:ALA:HA	1:0:281:LYS:HB3	1.85	0.58
3:2:496:C:OP1	9:E:49:ARG:NH2	2.37	0.58
19:O:117:ARG:HD2	31:a:49:ALA:HB2	1.86	0.58
3:2:520:A:H2'	3:2:521:A:H8	1.69	0.58
3:2:1744:G:O2'	3:2:1790:A:N6	2.36	0.58
3:2:1753:C:H2'	3:2:1754:G:C8	2.39	0.58
12:H:29:GLU:O	12:H:33:ASN:ND2	2.36	0.58
3:2:1141:G:H5'	3:2:1142:G:OP2	2.04	0.58
17:M:21:VAL:HG23	17:M:120:ALA:HB1	1.84	0.58
3:2:1616:U:OP2	20:P:43:ARG:NH2	2.37	0.58
1:0:272:PHE:HE2	1:0:324:MET:HE1	1.69	0.57
5:A:84:GLN:O	5:A:88:LEU:HG	2.03	0.57
8:D:195:THR:HG22	8:D:201:LYS:HE2	1.86	0.57
12:H:53:VAL:HG21	12:H:172:THR:HA	1.85	0.57
11:G:148:SER:OG	11:G:151:ASP:OD1	2.22	0.57
12:H:126:HIS:CD2	12:H:181:THR:HG23	2.39	0.57
37:g:252:THR:HG22	37:g:254:PRO:HD2	1.86	0.57
3:2:312:G:H2'	11:G:191:ARG:NH1	2.19	0.57
3:2:1857:G:H3'	19:O:146:ARG:NH2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:115:GLU:HA	27:W:118:ARG:NH1	2.19	0.57
1:0:83:VAL:HG23	1:0:170:HIS:CD2	2.39	0.57
1:0:124:LEU:HG	1:0:153:THR:HG23	1.86	0.57
3:2:1512:C:O2'	34:d:7:TYR:O	2.22	0.57
3:2:1521:C:OP2	23:S:124:ARG:NH1	2.35	0.57
4:3:162:A:O2'	4:3:163:G:O4'	2.21	0.57
6:B:101:HIS:O	6:B:217:MET:HG3	2.04	0.57
16:L:119:ASP:O	16:L:147:LYS:NZ	2.36	0.57
20:P:20:VAL:HG13	20:P:24:GLN:HB2	1.87	0.57
29:Y:78:SER:HB3	29:Y:81:TYR:CD2	2.40	0.57
1:0:96:PHE:HZ	1:0:127:VAL:HB	1.70	0.57
3:2:958:G:H2'	3:2:959:G:O4'	2.04	0.57
4:3:144:U:H2'	4:3:145:G:H8	1.69	0.57
23:S:78:LYS:NZ	24:T:32:GLU:HB2	2.19	0.57
3:2:1856:C:H2'	3:2:1857:G:H8	1.68	0.57
3:2:65:C:N4	11:G:134:GLY:O	2.33	0.57
10:F:56:TYR:HB3	10:F:63:LYS:HA	1.87	0.57
17:M:64:LEU:HD11	36:f:103:LEU:HA	1.85	0.57
37:g:191:HIS:CE1	37:g:195:LEU:HD21	2.39	0.57
3:2:1579:A:H4'	3:2:1581:C:H5	1.70	0.57
3:2:1598:G:H3'	30:Z:80:ARG:HG2	1.87	0.57
8:D:115:VAL:HG21	8:D:142:LEU:HD22	1.86	0.57
3:2:314:U:H2'	3:2:315:C:H6	1.67	0.56
3:2:1060:A:O2'	3:2:1062:A:N7	2.31	0.56
3:2:1715:A:H61	3:2:1818:A:H62	1.52	0.56
3:2:1866:A:N1	31:a:87:ARG:NH1	2.51	0.56
6:B:137:LEU:HD22	6:B:215:VAL:HG22	1.87	0.56
8:D:27:ARG:HG3	15:K:63:ALA:HB2	1.88	0.56
8:D:194:PRO:HA	8:D:201:LYS:HD3	1.87	0.56
13:I:80:ASP:OD1	13:I:81:VAL:N	2.38	0.56
2:1:8:U:H2'	2:1:13:C:H41	1.70	0.56
16:L:93:LEU:HB3	16:L:102:PHE:HB3	1.86	0.56
22:R:98:VAL:HG13	22:R:102:THR:HB	1.87	0.56
3:2:525:A:H2'	3:2:526:A:H8	1.65	0.56
3:2:824:C:H4'	14:J:147:PHE:HD1	1.69	0.56
3:2:980:A:H2'	3:2:981:A:C8	2.40	0.56
3:2:1223:A:H2'	3:2:1224:G:O4'	2.04	0.56
3:2:1239:U:H5''	20:P:124:LYS:HD3	1.87	0.56
3:2:1584:G:C4	3:2:1586:U:H1'	2.40	0.56
3:2:1589:A:N3	3:2:1653:U:O2'	2.35	0.56
3:2:1670:C:H2'	3:2:1671:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:31:ARG:HB3	35:e:31:ARG:NH1	2.21	0.56
3:2:30:C:O2'	3:2:596:U:OP1	2.23	0.56
6:B:198:GLU:HB2	6:B:210:VAL:HG11	1.87	0.56
3:2:683:G:H4'	27:W:4:MET:HB3	1.86	0.56
3:2:1144:A:H2'	3:2:1145:A:C8	2.41	0.56
3:2:1865:C:H5	31:a:6:ARG:H	1.54	0.56
5:A:42:LYS:NZ	22:R:99:ASP:OD2	2.29	0.56
3:2:1258:A:C2	3:2:1663:A:H2'	2.41	0.56
3:2:1671:G:H2'	3:2:1672:U:C6	2.41	0.56
5:A:14:ASP:OD1	5:A:14:ASP:N	2.37	0.56
3:2:499:G:H2'	3:2:501:C:C5	2.41	0.56
3:2:1047:C:H5''	19:O:143:LYS:HA	1.88	0.56
3:2:1516:G:O5'	20:P:81:ARG:NH1	2.32	0.56
20:P:44:ARG:HD2	20:P:84:ILE:HD11	1.87	0.56
3:2:380:G:C6	3:2:382:C:H5''	2.41	0.56
3:2:579:C:O2	29:Y:61:ARG:NH2	2.39	0.56
1:0:65:VAL:HG21	1:0:182:LYS:HG3	1.87	0.56
3:2:591:U:O2'	3:2:592:C:H3'	2.06	0.56
3:2:918:U:H5''	18:N:64:ARG:NH2	2.21	0.56
5:A:121:LEU:HD12	5:A:143:PRO:HB2	1.88	0.56
6:B:34:LYS:HE2	6:B:42:ARG:HH11	1.71	0.56
10:F:125:SER:HB3	10:F:136:ARG:HB3	1.88	0.56
34:d:19:ARG:HH11	34:d:32:ARG:HD2	1.71	0.56
6:B:30:TRP:CE2	6:B:48:LEU:HD13	2.41	0.55
17:M:79:VAL:HG12	17:M:80:ASP:H	1.70	0.55
19:O:84:ARG:O	19:O:87:GLU:HB3	2.06	0.55
1:0:71:ILE:HG22	1:0:72:LEU:HG	1.87	0.55
12:H:80:VAL:O	12:H:84:GLU:HB2	2.06	0.55
19:O:43:HIS:HE1	19:O:52:THR:HB	1.72	0.55
37:g:245:ARG:NH1	37:g:312:VAL:HG21	2.21	0.55
1:0:380:ASP:HB3	1:0:475:THR:HB	1.88	0.55
3:2:1271:C:N4	3:2:1510:G:O6	2.39	0.55
4:3:304:C:N4	4:3:305:U:O4	2.39	0.55
27:W:78:ARG:HG2	27:W:78:ARG:HH11	1.71	0.55
14:J:121:LYS:H	14:J:125:HIS:HD2	1.54	0.55
16:L:47:PRO:HG2	16:L:50:ALA:HB2	1.89	0.55
23:S:50:ILE:CD1	23:S:63:GLU:HB3	2.36	0.55
3:2:1293:A:H2'	3:2:1294:G:H8	1.70	0.55
4:3:150:G:H1	4:3:242:C:N4	2.05	0.55
14:J:169:ARG:HE	14:J:175:ARG:HH21	1.54	0.55
21:Q:58:LEU:HD13	21:Q:92:LEU:HD23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:38:LYS:NZ	37:g:63:SER:O	2.39	0.55
1:0:9:LYS:HZ3	3:2:966:U:P	2.24	0.55
18:N:100:LYS:O	18:N:103:GLU:HG2	2.07	0.55
23:S:83:PHE:CE2	24:T:36:THR:HG23	2.40	0.55
33:c:22:GLY:HA2	33:c:68:LEU:HD12	1.89	0.55
7:C:70:VAL:HG21	7:C:93:ILE:HG23	1.88	0.55
23:S:84:LEU:HD12	23:S:95:TYR:HB3	1.89	0.55
3:2:1629:C:H5'	23:S:39:ARG:HG2	1.89	0.55
11:G:151:ASP:OD1	11:G:151:ASP:N	2.39	0.55
9:E:68:ARG:HB3	9:E:68:ARG:HH11	1.70	0.55
3:2:981:A:H2'	3:2:982:G:C8	2.41	0.54
3:2:1105:G:O3'	32:b:69:GLY:HA3	2.07	0.54
8:D:208:VAL:HG12	22:R:41:ILE:HG22	1.88	0.54
19:O:36:SER:OG	19:O:37:PHE:N	2.41	0.54
37:g:105:THR:OG1	37:g:126:ASP:OD2	2.19	0.54
3:2:1589:A:OP1	24:T:80:GLY:HA3	2.08	0.54
3:2:1596:U:OP2	30:Z:85:ARG:NH2	2.40	0.54
3:2:1615:U:O4	20:P:40:ARG:NH1	2.40	0.54
5:A:63:ARG:NH1	26:V:78:ILE:HG23	2.22	0.54
7:C:188:CYS:HB3	7:C:239:ALA:HB2	1.89	0.54
16:L:71:ARG:HH11	16:L:71:ARG:HG2	1.71	0.54
17:M:21:VAL:HG21	17:M:124:ILE:HD12	1.89	0.54
21:Q:130:LYS:NZ	21:Q:134:GLY:O	2.24	0.54
21:Q:82:TYR:HE1	21:Q:85:ARG:HH11	1.54	0.54
1:0:38:VAL:O	1:0:42:VAL:N	2.30	0.54
3:2:1550:G:H1	3:2:1582:C:H42	1.54	0.54
10:F:73:THR:O	10:F:89:THR:HG21	2.06	0.54
16:L:78:THR:OG1	16:L:79:LYS:N	2.40	0.54
37:g:153:CYS:SG	37:g:155:ARG:NH1	2.81	0.54
9:E:66:MET:HE1	9:E:78:THR:HB	1.90	0.54
19:O:39:ASP:HB3	19:O:68:GLU:HB3	1.90	0.54
3:2:4:C:H4'	7:C:207:ALA:HB2	1.89	0.54
3:2:373:G:OP1	16:L:137:THR:OG1	2.25	0.54
3:2:624:C:H41	28:X:63:ASN:HD22	1.55	0.54
18:N:47:PRO:HA	18:N:50:ILE:HD12	1.88	0.54
23:S:50:ILE:HD11	23:S:63:GLU:HB3	1.88	0.54
23:S:68:ILE:O	23:S:72:GLN:HG2	2.08	0.54
3:2:181:A:H2'	3:2:182:C:H2'	1.89	0.54
3:2:1038:U:H2'	3:2:1039:C:H6	1.73	0.54
3:2:1855:G:OP2	19:O:147:ARG:NH2	2.41	0.54
3:2:1858:G:OP2	19:O:146:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:183:LYS:HB3	7:C:196:ILE:HG23	1.90	0.54
10:F:161:ALA:O	10:F:165:ASN:ND2	2.40	0.54
12:H:101:LEU:O	12:H:116:ARG:NH1	2.40	0.54
32:b:31:TYR:O	32:b:48:SER:HB2	2.07	0.54
1:0:261:GLN:O	1:0:265:ASP:HB2	2.08	0.54
27:W:79:PHE:H	27:W:125:ILE:HG22	1.72	0.54
34:d:46:TYR:O	34:d:50:ILE:HG13	2.08	0.54
3:2:61:A:H5'	3:2:316:G:H4'	1.89	0.54
3:2:1534:C:H4'	3:2:1535:U:O5'	2.08	0.54
3:2:1565:C:OP2	24:T:101:ARG:NH1	2.41	0.54
10:F:137:GLN:HE21	33:c:63:ARG:HH22	1.55	0.54
13:I:22:HIS:HB2	13:I:25:ARG:NH2	2.23	0.54
23:S:86:ARG:NH2	23:S:110:ASP:OD2	2.41	0.54
25:U:27:ARG:NH1	34:d:51:GLY:HA3	2.23	0.54
37:g:33:SER:HG	37:g:43:TRP:CD1	2.26	0.54
14:J:114:VAL:HG13	14:J:119:LEU:HB2	1.89	0.54
19:O:95:ILE:HB	19:O:129:ILE:HD13	1.88	0.54
3:2:1231:C:H42	3:2:1527:C:H41	1.55	0.53
3:2:1273:C:O2'	3:2:1506:A:N1	2.37	0.53
3:2:1335:G:OP1	8:D:139:SER:OG	2.25	0.53
4:3:230:G:O2'	4:3:231:G:OP1	2.25	0.53
16:L:70:GLY:HA3	16:L:130:GLU:HB3	1.90	0.53
25:U:78:ASP:OD1	34:d:54:LYS:NZ	2.27	0.53
29:Y:29:HIS:NE2	29:Y:69:THR:OG1	2.40	0.53
3:2:1399:C:H5''	37:g:100:ARG:NH1	2.23	0.53
14:J:109:ARG:NH1	14:J:111:GLN:HB3	2.22	0.53
2:1:72:U:O2'	2:1:73:A:H4'	2.08	0.53
32:b:67:THR:HG22	32:b:68:GLY:H	1.73	0.53
1:0:74:GLU:HB3	1:0:79:LEU:HD23	1.89	0.53
1:0:281:LYS:HZ1	1:0:298:PHE:HB2	1.73	0.53
7:C:144:SER:HB3	7:C:150:ALA:HB2	1.89	0.53
9:E:122:LYS:NZ	9:E:143:ASP:OD2	2.32	0.53
9:E:122:LYS:HD2	9:E:164:LEU:HD21	1.90	0.53
12:H:9:VAL:HG23	12:H:24:SER:HB3	1.89	0.53
36:f:126:CYS:HB2	36:f:130:VAL:HB	1.90	0.53
8:D:35:SER:N	8:D:51:LEU:O	2.41	0.53
17:M:76:LEU:HD21	17:M:78:LYS:HE3	1.91	0.53
28:X:28:LYS:O	28:X:32:LEU:HB2	2.08	0.53
30:Z:44:LEU:HD11	30:Z:78:LYS:HZ3	1.73	0.53
37:g:251:ALA:HB2	37:g:289:LEU:HD22	1.90	0.53
3:2:554:A:H4'	3:2:555:A:OP1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:590:A:OP1	3:2:590:A:H3'	2.09	0.53
3:2:1401:A:N6	3:2:1441:U:O2'	2.41	0.53
3:2:1558:C:O2'	3:2:1559:C:O5'	2.26	0.53
5:A:90:PHE:O	5:A:94:THR:OG1	2.22	0.53
1:0:378:PRO:CB	1:0:477:PRO:HG2	2.35	0.53
3:2:1284:A:H61	3:2:1313:A:H2'	1.74	0.53
3:2:1674:G:OP1	10:F:51:HIS:NE2	2.42	0.53
32:b:64:CYS:HB3	32:b:73:LEU:HD23	1.90	0.53
35:e:31:ARG:HB3	35:e:31:ARG:CZ	2.38	0.53
37:g:245:ARG:NH1	37:g:312:VAL:HG11	2.11	0.53
3:2:170:A:H4'	11:G:136:LYS:HD3	1.90	0.53
3:2:1177:U:H2'	3:2:1178:U:H6	1.74	0.53
3:2:1189:A:H2'	3:2:1190:A:C8	2.44	0.53
3:2:1344:A:N6	3:2:1386:A:H5'	2.24	0.53
3:2:1464:C:O2'	3:2:1465:A:OP1	2.24	0.53
29:Y:55:ILE:HG22	29:Y:75:ILE:HG12	1.91	0.53
3:2:300:U:H2'	3:2:301:A:H8	1.74	0.53
3:2:913:A:O2'	12:H:67:PRO:HD3	2.09	0.53
4:3:312:U:H2'	4:3:313:G:C8	2.44	0.53
37:g:245:ARG:HH12	37:g:312:VAL:CG1	2.12	0.53
3:2:64:A:H2	3:2:83:A:N6	2.06	0.53
3:2:92:A:C6	3:2:446:G:C6	2.97	0.53
3:2:583:A:OP1	14:J:162:ARG:NH2	2.42	0.53
3:2:1122:A:H4'	6:B:205:TYR:CE1	2.43	0.53
3:2:1415:C:O2'	24:T:132:ASP:OD2	2.25	0.53
5:A:121:LEU:HD11	5:A:145:ILE:HD11	1.91	0.53
10:F:122:ARG:HE	33:c:57:THR:HG21	1.74	0.53
3:2:124:U:C5'	11:G:201:LYS:HZ3	2.22	0.52
3:2:979:C:H2'	3:2:980:A:H8	1.75	0.52
3:2:1016:U:H5''	18:N:14:SER:HB3	1.90	0.52
3:2:1289:U:H2'	3:2:1290:G:C8	2.44	0.52
9:E:125:LYS:NZ	9:E:225:ILE:O	2.39	0.52
10:F:87:LEU:HA	10:F:90:VAL:HG22	1.91	0.52
12:H:176:VAL:O	12:H:180:LEU:HG	2.09	0.52
3:2:1537:A:O2'	3:2:1604:G:OP1	2.27	0.52
31:a:24:THR:HG21	31:a:71:LEU:HD22	1.92	0.52
37:g:17:TRP:CE2	37:g:303:THR:HG23	2.44	0.52
1:0:290:SER:HB2	3:2:1721:U:H1'	1.92	0.52
3:2:434:G:H2'	3:2:435:A:C8	2.45	0.52
3:2:1355:C:H2'	3:2:1356:G:O4'	2.10	0.52
10:F:79:HIS:O	10:F:82:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:108:ARG:NH2	14:J:154:GLN:OE1	2.42	0.52
3:2:1177:U:H2'	3:2:1178:U:C6	2.44	0.52
3:2:1277:C:H2'	3:2:1278:A:C8	2.44	0.52
3:2:1590:C:H41	21:Q:77:HIS:CE1	2.27	0.52
3:2:1710:C:H42	3:2:1823:A:H61	1.56	0.52
1:0:443:ILE:HG21	1:0:464:CYS:SG	2.49	0.52
3:2:1606:G:N2	3:2:1632:G:H2'	2.24	0.52
5:A:57:LYS:HD2	5:A:159:ILE:HD11	1.91	0.52
8:D:103:GLU:OE1	8:D:106:ARG:NH1	2.42	0.52
22:R:57:LEU:O	22:R:61:ILE:HG13	2.10	0.52
3:2:144:U:OP2	3:2:144:U:H6	1.93	0.52
3:2:1241:A:H2'	3:2:1242:U:H4'	1.91	0.52
3:2:1613:G:H5''	20:P:39:ALA:HB2	1.92	0.52
3:2:1842:C:OP1	38:h:3:ALA:HB3	2.09	0.52
6:B:225:LEU:O	6:B:229:MET:HG2	2.10	0.52
16:L:150:GLY:HA3	18:N:133:ARG:NH2	2.25	0.52
3:2:688:U:H5	12:H:103:LYS:H	1.57	0.52
3:2:1778:C:H2'	3:2:1779:G:C8	2.45	0.52
14:J:88:ASP:OD1	14:J:88:ASP:N	2.42	0.52
15:K:15:LEU:HG	15:K:71:LEU:HD11	1.91	0.52
21:Q:58:LEU:HD22	21:Q:108:ILE:HG12	1.90	0.52
3:2:66:G:OP1	11:G:172:LYS:NZ	2.35	0.52
3:2:925:G:H5''	18:N:91:LEU:HD21	1.91	0.52
4:3:172:A:H2'	4:3:173:A:C8	2.45	0.52
8:D:163:PRO:HA	8:D:166:TYR:CZ	2.45	0.52
13:I:79:ILE:HG13	13:I:170:LYS:HZ1	1.75	0.52
1:0:19:ARG:HG2	1:0:23:ARG:NH1	2.25	0.52
1:0:19:ARG:CG	1:0:23:ARG:HH12	2.21	0.52
3:2:307:G:C2	13:I:44:HIS:HB3	2.45	0.52
6:B:144:LYS:HE2	6:B:146:ARG:HH12	1.75	0.52
10:F:34:SER:HA	33:c:55:VAL:HG13	1.92	0.52
13:I:87:ASN:HD22	13:I:88:ASN:N	2.08	0.52
14:J:103:GLU:O	14:J:107:GLU:HG2	2.10	0.52
9:E:106:LYS:HD2	9:E:108:ARG:HH22	1.75	0.51
13:I:69:SER:OG	13:I:191:GLU:OE1	2.20	0.51
13:I:84:ASN:HD21	13:I:90:LEU:HD12	1.75	0.51
22:R:33:ARG:O	22:R:36:GLU:HG2	2.10	0.51
22:R:44:LYS:HZ2	22:R:47:ARG:HH12	1.54	0.51
24:T:22:LEU:HB3	24:T:54:TYR:HD2	1.75	0.51
3:2:294:U:C4	16:L:65:ASN:HB2	2.45	0.51
3:2:1216:C:N4	3:2:1342:U:OP1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:51:ARG:HA	9:E:51:ARG:HH11	1.76	0.51
11:G:216:ARG:O	11:G:219:GLU:HG2	2.09	0.51
21:Q:132:PHE:O	21:Q:140:ARG:NH1	2.44	0.51
5:A:198:MET:HG3	5:A:199:PRO:HD2	1.92	0.51
6:B:82:ARG:NH1	6:B:188:LEU:O	2.43	0.51
11:G:91:GLU:HG2	11:G:92:ARG:N	2.25	0.51
12:H:69:LEU:O	12:H:73:GLN:HG2	2.11	0.51
13:I:31:ARG:HH11	13:I:31:ARG:HG3	1.75	0.51
16:L:101:ARG:HB3	28:X:7:LEU:O	2.11	0.51
3:2:1808:U:H2'	3:2:1809:A:C8	2.46	0.51
17:M:52:LEU:HD21	17:M:65:VAL:HG11	1.92	0.51
25:U:40:ILE:O	25:U:44:LYS:HB2	2.10	0.51
36:f:137:ASP:OD1	36:f:138:ARG:NH1	2.43	0.51
37:g:129:ILE:HD11	37:g:151:VAL:HG11	1.91	0.51
3:2:60:A:O2'	3:2:61:A:O5'	2.27	0.51
4:3:134:A:H61	4:3:290:U:H3	1.57	0.51
5:A:128:ARG:NH1	5:A:153:PRO:HD3	2.26	0.51
12:H:43:LEU:HD22	12:H:68:GLN:HB3	1.91	0.51
16:L:120:VAL:HG22	16:L:145:VAL:HG11	1.92	0.51
37:g:246:TYR:CE2	37:g:262:GLU:HG3	2.45	0.51
1:0:272:PHE:CE2	1:0:324:MET:HE1	2.46	0.51
7:C:79:GLU:HB3	26:V:12:TYR:HB3	1.91	0.51
8:D:164:VAL:O	8:D:168:VAL:HG22	2.10	0.51
10:F:146:ARG:HH22	33:c:57:THR:HB	1.76	0.51
15:K:64:TRP:HZ3	34:d:22:ARG:HD2	1.74	0.51
18:N:84:LEU:HD13	18:N:89:TYR:HB2	1.93	0.51
1:0:439:LEU:O	1:0:443:ILE:HG13	2.11	0.51
3:2:65:C:O2'	3:2:67:C:OP2	2.28	0.51
3:2:114:G:OP1	16:L:69:ARG:NH1	2.43	0.51
3:2:870:A:H4'	3:2:871:U:C5'	2.41	0.51
3:2:1515:G:N2	20:P:99:GLY:O	2.44	0.51
3:2:1536:G:H2'	3:2:1537:A:H8	1.74	0.51
5:A:85:ARG:NE	5:A:201:LEU:O	2.44	0.51
20:P:37:TYR:HB3	20:P:41:GLN:HB2	1.93	0.51
24:T:80:GLY:HA2	24:T:92:PHE:HE1	1.76	0.51
37:g:89:LEU:HB3	37:g:99:ARG:HB2	1.93	0.51
7:C:204:ILE:HD11	7:C:215:MET:HE3	1.93	0.51
10:F:128:ILE:HD11	33:c:68:LEU:HD22	1.93	0.51
15:K:60:GLU:HG2	15:K:69:TRP:CD1	2.45	0.51
30:Z:63:PRO:O	30:Z:111:ARG:HB2	2.10	0.51
1:0:124:LEU:HD11	1:0:156:MET:CE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:465:A:H4'	3:2:466:G:O5'	2.11	0.51
3:2:967:C:H3'	3:2:968:U:H5''	1.92	0.51
3:2:1428:G:H4'	3:2:1429:G:C5'	2.41	0.51
4:3:153:G:H4'	4:3:154:A:OP2	2.11	0.51
9:E:151:ASP:OD2	11:G:216:ARG:NH2	2.44	0.51
12:H:109:ARG:HG2	12:H:110:THR:H	1.76	0.51
14:J:134:HIS:ND1	14:J:163:SER:HB2	2.26	0.51
18:N:93:LYS:O	18:N:96:VAL:HB	2.11	0.51
23:S:5:ILE:HG23	30:Z:50:PHE:O	2.10	0.51
1:0:554:HIS:HB3	1:0:579:LYS:O	2.11	0.51
3:2:919:A:OP1	18:N:20:ARG:NE	2.44	0.51
3:2:1566:G:O6	24:T:97:LYS:HB2	2.09	0.50
5:A:134:LEU:CD2	5:A:144:THR:HG21	2.40	0.50
1:0:296:HIS:O	1:0:303:GLU:HG3	2.11	0.50
3:2:434:G:OP1	13:I:23:LYS:HG2	2.11	0.50
3:2:792:C:H2'	3:2:793:G:H8	1.75	0.50
3:2:976:G:H2'	3:2:977:C:C6	2.46	0.50
3:2:1284:A:N6	3:2:1313:A:H2'	2.26	0.50
13:I:31:ARG:HB3	13:I:32:PRO:HD2	1.93	0.50
22:R:44:LYS:NZ	22:R:47:ARG:NH1	2.56	0.50
3:2:180:G:O2'	3:2:181:A:OP1	2.26	0.50
3:2:811:A:H2'	3:2:812:A:H8	1.76	0.50
3:2:1590:C:H41	21:Q:77:HIS:HE1	1.60	0.50
14:J:68:PRO:HA	14:J:71:LEU:HD12	1.93	0.50
23:S:17:ASN:HD22	23:S:101:ASN:HD21	1.59	0.50
1:0:9:LYS:NZ	3:2:966:U:P	2.84	0.50
3:2:687:C:N3	12:H:118:ARG:NH2	2.60	0.50
3:2:828:G:OP1	9:E:22:LYS:NZ	2.31	0.50
4:3:150:G:N2	4:3:242:C:N3	2.53	0.50
4:3:256:G:H5'	4:3:257:A:H5''	1.93	0.50
6:B:29:ASP:OD1	6:B:30:TRP:N	2.44	0.50
6:B:65:ARG:NH1	19:O:51:GLU:OE1	2.36	0.50
6:B:117:TRP:HA	6:B:117:TRP:CE3	2.46	0.50
23:S:34:LYS:HD2	23:S:100:ALA:HA	1.93	0.50
1:0:102:VAL:HG12	1:0:106:LEU:HG	1.93	0.50
3:2:936:G:H2'	3:2:937:C:H6	1.77	0.50
10:F:165:ASN:CG	10:F:167:LYS:HB2	2.36	0.50
23:S:46:ARG:NE	24:T:50:GLU:OE1	2.44	0.50
3:2:1542:C:OP1	24:T:62:ARG:NH1	2.38	0.50
3:2:1543:U:O2'	21:Q:43:GLU:OE2	2.28	0.50
8:D:44:THR:HG22	8:D:45:ARG:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:22:ARG:HA	11:G:25:ARG:HG2	1.93	0.50
12:H:49:LYS:HD3	12:H:179:LYS:HZ2	1.76	0.50
37:g:241:PHE:HE1	37:g:261:LEU:HD11	1.76	0.50
37:g:298:LEU:HB2	37:g:310:TRP:HB2	1.93	0.50
3:2:1284:A:O4'	3:2:1312:G:N2	2.45	0.50
4:3:232:C:H2'	4:3:233:G:H5''	1.93	0.50
18:N:101:HIS:HE1	18:N:105:ASN:HD22	1.58	0.50
24:T:75:MET:HE2	24:T:78:ILE:HG13	1.93	0.50
30:Z:74:SER:OG	30:Z:79:ILE:O	2.23	0.50
1:0:391:MET:HE2	1:0:394:LEU:HD23	1.93	0.50
3:2:957:A:H2'	3:2:958:G:H5'	1.92	0.50
10:F:119:SER:OG	10:F:189:ALA:HB1	2.12	0.50
23:S:90:VAL:HG21	23:S:113:ARG:HH12	1.77	0.50
1:0:105:LYS:HG3	2:1:76:A:C4	2.47	0.50
3:2:559:G:O2'	3:2:560:A:H8	1.95	0.50
3:2:1217:A:H2'	3:2:1218:C:C6	2.47	0.50
7:C:170:TRP:CE2	7:C:199:PRO:HG3	2.47	0.50
21:Q:82:TYR:CE1	21:Q:85:ARG:NH1	2.72	0.50
24:T:74:SER:O	24:T:78:ILE:HG12	2.11	0.50
32:b:49:HIS:N	32:b:49:HIS:CD2	2.80	0.50
3:2:180:G:O2'	3:2:181:A:H5'	2.12	0.49
3:2:590:A:H3'	3:2:590:A:P	2.52	0.49
5:A:77:ILE:HG12	5:A:99:ILE:HB	1.93	0.49
5:A:163:CYS:SG	5:A:174:MET:HG3	2.52	0.49
3:2:44:U:O2'	3:2:45:A:H2'	2.12	0.49
3:2:70:G:H2'	3:2:71:G:O4'	2.12	0.49
3:2:124:U:H5'	11:G:201:LYS:HZ3	1.76	0.49
3:2:407:G:H2'	3:2:407:G:N3	2.27	0.49
3:2:563:G:N7	3:2:586:G:N2	2.60	0.49
3:2:1373:C:OP1	22:R:7:LYS:N	2.45	0.49
3:2:1724:A:H5'	3:2:1725:U:OP2	2.13	0.49
37:g:109:LEU:HD13	37:g:152:SER:HA	1.95	0.49
3:2:104:A:H62	3:2:356:C:H5	1.60	0.49
3:2:945:U:H2'	3:2:946:U:C6	2.47	0.49
3:2:1856:C:H2'	3:2:1857:G:C8	2.45	0.49
10:F:35:LEU:HD12	10:F:117:ILE:HG12	1.94	0.49
11:G:44:GLU:H	11:G:44:GLU:CD	2.21	0.49
16:L:104:LYS:NZ	28:X:8:ARG:HH11	2.10	0.49
20:P:44:ARG:HH21	20:P:53:GLN:NE2	2.10	0.49
22:R:33:ARG:HG3	37:g:125:ARG:NH1	2.27	0.49
3:2:1259:A:H3'	3:2:1259:A:N3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1374:C:O2'	3:2:1464:C:O2	2.27	0.49
5:A:26:GLY:HA3	5:A:150:THR:HG23	1.93	0.49
9:E:80:ILE:HG13	9:E:81:THR:HG23	1.94	0.49
11:G:135:PRO:HG2	11:G:141:ILE:HD13	1.94	0.49
1:0:124:LEU:HD11	1:0:156:MET:HE1	1.95	0.49
1:0:305:ARG:O	1:0:307:LEU:HG	2.13	0.49
3:2:1549:U:OP1	34:d:34:TYR:OH	2.30	0.49
3:2:1630:A:OP2	23:S:39:ARG:HB3	2.12	0.49
6:B:129:THR:OG1	6:B:131:ASP:OD1	2.18	0.49
18:N:98:VAL:HG11	18:N:115:LEU:HB2	1.95	0.49
37:g:270:LEU:HB3	37:g:310:TRP:CZ2	2.47	0.49
37:g:273:GLU:OE2	37:g:284:PRO:HD2	2.11	0.49
2:1:8:U:H2'	2:1:13:C:N4	2.26	0.49
3:2:4:C:H5'	7:C:230:THR:HG21	1.93	0.49
3:2:65:C:OP1	11:G:136:LYS:NZ	2.45	0.49
3:2:309:G:OP2	13:I:55:TYR:OH	2.24	0.49
5:A:135:THR:O	5:A:138:SER:HB3	2.11	0.49
5:A:155:ARG:HD2	26:V:61:ARG:O	2.13	0.49
8:D:72:VAL:O	8:D:75:LYS:HB2	2.13	0.49
20:P:45:LEU:HD23	20:P:49:LEU:HD21	1.93	0.49
24:T:37:VAL:HG13	24:T:38:LYS:O	2.13	0.49
3:2:1723:G:H2'	3:2:1724:A:O4'	2.13	0.49
4:3:332:A:H3'	4:3:333:C:H5'	1.94	0.49
6:B:146:ARG:HA	6:B:146:ARG:NH1	2.27	0.49
14:J:25:LEU:HA	14:J:40:LYS:NZ	2.28	0.49
19:O:44:VAL:HG12	19:O:53:ILE:HD12	1.94	0.49
23:S:46:ARG:NH1	24:T:35:ASP:HA	2.27	0.49
3:2:332:G:H4'	3:2:333:G:OP1	2.13	0.49
3:2:1447:G:OP1	25:U:87:ARG:NH2	2.46	0.49
3:2:1868:U:H3'	3:2:1869:A:H5'	1.95	0.49
7:C:108:LYS:HD2	7:C:233:LEU:HD22	1.95	0.49
8:D:67:ARG:HH21	15:K:97:SER:HB3	1.78	0.49
8:D:96:LEU:HD12	8:D:198:ILE:HD13	1.93	0.49
9:E:31:PRO:HG3	9:E:43:PRO:HG3	1.95	0.49
11:G:145:PHE:CD2	11:G:156:TYR:HB3	2.47	0.49
14:J:128:VAL:O	14:J:132:GLN:HB2	2.13	0.49
3:2:1384:C:H2'	3:2:1385:G:H8	1.77	0.49
3:2:1498:A:OP2	8:D:27:ARG:NH1	2.37	0.49
3:2:1644:C:H2'	3:2:1645:C:H6	1.78	0.49
3:2:1010:G:H2'	3:2:1011:A:H8	1.77	0.49
4:3:165:A:N6	4:3:237:C:O2'	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:263:G:H1'	4:3:271:G:N2	2.28	0.49
21:Q:130:LYS:HA	21:Q:137:ALA:HA	1.95	0.49
29:Y:88:LYS:HB3	29:Y:97:TYR:CE2	2.48	0.49
36:f:133:ALA:O	36:f:139:HIS:HA	2.13	0.49
37:g:162:ASN:HD21	37:g:178:ASN:HD22	1.61	0.49
3:2:312:G:N2	3:2:338:G:H1'	2.28	0.48
3:2:617:G:N7	28:X:67:ARG:NH1	2.51	0.48
3:2:634:A:H2'	3:2:635:G:C8	2.47	0.48
3:2:1354:G:H5'	3:2:1355:C:OP2	2.13	0.48
3:2:1425:G:O2'	3:2:1426:U:OP1	2.26	0.48
3:2:1786:U:H2'	3:2:1787:G:H8	1.78	0.48
32:b:13:GLU:H	32:b:13:GLU:HG3	1.36	0.48
3:2:1269:G:H1	3:2:1513:C:N4	2.11	0.48
3:2:1826:G:H2'	3:2:1827:U:O4'	2.13	0.48
9:E:160:ILE:HD12	9:E:162:ILE:HD11	1.94	0.48
11:G:135:PRO:HG3	11:G:144:LEU:HD12	1.95	0.48
12:H:133:LEU:HD11	12:H:176:VAL:HG11	1.94	0.48
16:L:101:ARG:NH1	28:X:5:ARG:O	2.46	0.48
1:0:100:PRO:O	1:0:103:LEU:HB3	2.12	0.48
1:0:559:LEU:O	1:0:563:GLU:HB2	2.14	0.48
3:2:69:C:N4	3:2:70:G:O6	2.47	0.48
3:2:165:G:H2'	3:2:166:A:H8	1.77	0.48
3:2:551:U:H2'	3:2:552:G:C8	2.49	0.48
3:2:867:G:H5'	16:L:149:ALA:HB1	1.94	0.48
3:2:869:A:C5	12:H:114:GLN:HB2	2.48	0.48
9:E:106:LYS:HD2	9:E:108:ARG:NH2	2.28	0.48
14:J:136:ARG:HB3	14:J:160:SER:HB3	1.96	0.48
14:J:137:VAL:HG22	14:J:157:ILE:HG12	1.95	0.48
14:J:169:ARG:HH21	14:J:175:ARG:NH2	2.11	0.48
17:M:95:ASP:HB2	17:M:99:LYS:HB2	1.93	0.48
3:2:28:U:H2'	3:2:29:G:C8	2.49	0.48
3:2:588:G:OP2	3:2:588:G:N2	2.42	0.48
6:B:104:ASP:OD1	6:B:104:ASP:N	2.45	0.48
37:g:18:VAL:HG21	37:g:307:VAL:HG22	1.96	0.48
37:g:164:ILE:HG23	37:g:176:VAL:HG13	1.95	0.48
3:2:502:C:H5''	3:2:503:C:H5	1.77	0.48
3:2:1779:G:H2'	3:2:1780:G:C8	2.48	0.48
4:3:42:C:H42	4:3:120:C:N4	2.05	0.48
10:F:136:ARG:HH11	10:F:199:VAL:HG11	1.77	0.48
21:Q:145:TYR:O	21:Q:146:ARG:HG2	2.14	0.48
24:T:42:HIS:CD2	24:T:43:LYS:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:37:LYS:HA	29:Y:40:ILE:HG22	1.95	0.48
2:1:43:G:H5'	2:1:43:G:H8	1.78	0.48
3:2:1101:U:H2'	3:2:1102:G:C8	2.48	0.48
3:2:1567:G:H2'	24:T:37:VAL:HG21	1.96	0.48
3:2:1654:G:OP1	24:T:82:ARG:NE	2.33	0.48
5:A:130:ASP:OD1	5:A:130:ASP:N	2.46	0.48
8:D:3:VAL:HG12	8:D:4:GLN:H	1.79	0.48
10:F:99:ILE:HG23	30:Z:67:LEU:HD13	1.95	0.48
11:G:48:TYR:CZ	11:G:116:LYS:HG3	2.49	0.48
12:H:163:GLN:O	12:H:167:GLU:HB2	2.12	0.48
1:0:412:ARG:HG2	1:0:461:LEU:HD13	1.96	0.48
3:2:127:C:HO2'	3:2:215:G:HO2'	1.59	0.48
3:2:314:U:O2'	3:2:315:C:O5'	2.29	0.48
3:2:1375:G:H2'	3:2:1376:A:H8	1.78	0.48
6:B:134:LEU:HB3	6:B:219:LYS:H	1.78	0.48
16:L:22:ARG:NH2	16:L:31:GLU:HG3	2.28	0.48
18:N:125:LEU:HD23	18:N:125:LEU:HA	1.68	0.48
37:g:81:GLY:HA2	37:g:87:LEU:HD12	1.96	0.48
3:2:520:A:H2'	3:2:521:A:C8	2.48	0.48
3:2:941:C:H5''	6:B:136:ARG:HH21	1.79	0.48
3:2:976:G:H2'	3:2:977:C:H6	1.78	0.48
3:2:1650:A:H1'	3:2:1675:A:N6	2.29	0.48
4:3:257:A:H4'	4:3:258:G:OP1	2.14	0.48
23:S:48:ALA:HB2	23:S:70:ILE:HD12	1.95	0.48
3:2:1238:U:H3	3:2:1242:U:H3	1.61	0.48
5:A:12:GLU:CD	22:R:114:LEU:HD22	2.38	0.48
9:E:115:THR:HG22	9:E:117:GLU:HG2	1.94	0.48
37:g:14:HIS:HD1	37:g:18:VAL:HG22	1.79	0.48
3:2:749:U:O4	3:2:750:C:N4	2.46	0.48
3:2:969:U:H5'	3:2:971:G:H1'	1.94	0.48
3:2:1038:U:H2'	3:2:1039:C:C6	2.49	0.48
3:2:1560:U:H4'	3:2:1583:C:O2'	2.13	0.48
3:2:1857:G:N7	19:O:146:ARG:NH1	2.60	0.48
5:A:178:LEU:O	5:A:182:VAL:HG22	2.13	0.48
8:D:116:ARG:HG2	8:D:150:MET:HE1	1.96	0.48
1:0:86:LEU:HD22	1:0:146:ILE:HD11	1.96	0.47
15:K:32:HIS:ND1	15:K:33:PRO:HD2	2.29	0.47
28:X:84:PHE:CE2	28:X:86:PRO:HA	2.48	0.47
3:2:1035:A:H2'	3:2:1036:A:O4'	2.15	0.47
3:2:1585:U:O3'	3:2:1586:U:H4'	2.14	0.47
3:2:1732:G:H2'	3:2:1733:U:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:38:LEU:HG	9:E:39:ARG:N	2.29	0.47
13:I:34:ALA:HB2	13:I:56:ARG:HD3	1.95	0.47
19:O:34:PHE:HB3	19:O:41:PHE:HB2	1.96	0.47
3:2:1532:C:H5''	3:2:1533:A:O4'	2.13	0.47
3:2:1585:U:H2'	24:T:67:ARG:HH22	1.80	0.47
3:2:1649:U:HO2'	3:2:1650:A:P	2.37	0.47
6:B:33:VAL:HB	6:B:44:ILE:CG1	2.44	0.47
30:Z:44:LEU:HD11	30:Z:78:LYS:NZ	2.28	0.47
37:g:11:LEU:HB3	37:g:43:TRP:CH2	2.49	0.47
37:g:23:THR:HG22	37:g:31:ILE:HG23	1.95	0.47
37:g:291:TRP:HE1	37:g:295:GLY:HA2	1.80	0.47
1:0:23:ARG:HD2	1:0:38:VAL:HG11	1.96	0.47
3:2:1005:G:OP2	6:B:162:ARG:NH2	2.47	0.47
3:2:1445:U:O2'	3:2:1446:A:OP1	2.27	0.47
3:2:1590:C:H3'	3:2:1591:C:C6	2.49	0.47
5:A:120:ARG:O	5:A:143:PRO:HD2	2.15	0.47
17:M:118:SER:O	17:M:122:ASP:HB2	2.14	0.47
28:X:119:ARG:HB2	28:X:120:PHE:CE1	2.49	0.47
30:Z:86:ALA:HA	30:Z:89:GLN:HB2	1.96	0.47
3:2:1623:A:C6	23:S:132:ARG:NH1	2.83	0.47
3:2:1820:G:H2'	3:2:1821:U:O4'	2.14	0.47
3:2:1845:A:H2'	3:2:1846:G:C8	2.50	0.47
6:B:69:VAL:HG11	6:B:74:LEU:HD21	1.96	0.47
9:E:87:MET:HE2	9:E:123:LEU:HB2	1.97	0.47
16:L:103:GLU:HB3	28:X:10:ALA:HB3	1.97	0.47
29:Y:76:TYR:OH	29:Y:86:GLU:OE1	2.32	0.47
30:Z:58:LEU:HD12	30:Z:62:VAL:HG21	1.96	0.47
3:2:958:G:N2	19:O:68:GLU:OE2	2.47	0.47
3:2:1320:G:H2'	3:2:1321:G:H5'	1.96	0.47
3:2:1447:G:H2'	3:2:1448:A:H8	1.80	0.47
4:3:144:U:H2'	4:3:145:G:C8	2.49	0.47
5:A:68:ILE:HD11	5:A:121:LEU:HB2	1.97	0.47
6:B:82:ARG:HH12	6:B:191:ASP:HB2	1.78	0.47
9:E:85:GLY:O	9:E:88:ASP:HB2	2.15	0.47
26:V:2:GLN:HA	26:V:7:GLU:O	2.14	0.47
1:0:329:ILE:HG22	1:0:330:ILE:HG23	1.95	0.47
3:2:413:G:C5	3:2:425:G:C2	3.03	0.47
3:2:533:A:H2'	3:2:534:G:O4'	2.15	0.47
3:2:586:G:N7	14:J:172:ARG:HD3	2.30	0.47
3:2:634:A:H2'	3:2:635:G:H8	1.78	0.47
3:2:659:G:O4'	3:2:662:G:N2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:811:A:O2'	3:2:812:A:OP1	2.30	0.47
3:2:1073:U:H2'	3:2:1074:C:H6	1.78	0.47
3:2:1440:C:O2'	3:2:1441:U:O5'	2.24	0.47
3:2:1623:A:C8	23:S:132:ARG:HD2	2.49	0.47
7:C:103:LYS:O	7:C:130:ILE:HG13	2.15	0.47
7:C:178:HIS:H	7:C:178:HIS:CD2	2.33	0.47
10:F:187:SER:HB3	10:F:190:ILE:HG12	1.95	0.47
16:L:104:LYS:HZ1	28:X:8:ARG:HH11	1.62	0.47
22:R:111:PHE:O	22:R:114:LEU:HG	2.13	0.47
31:a:12:LYS:HB2	31:a:33:ASP:OD2	2.14	0.47
37:g:68:ASP:OD1	37:g:69:VAL:N	2.48	0.47
37:g:101:PHE:CE2	37:g:136:GLY:HA2	2.49	0.47
3:2:651:U:H2'	3:2:652:U:C6	2.50	0.47
3:2:1164:G:O2'	3:2:1165:G:H5'	2.14	0.47
3:2:1334:G:O2'	8:D:174:HIS:HD2	1.97	0.47
4:3:146:G:H1	4:3:247:C:N4	2.12	0.47
6:B:21:VAL:HG12	6:B:22:VAL:HG23	1.97	0.47
6:B:25:PHE:CE2	19:O:88:LEU:HD13	2.50	0.47
6:B:38:MET:HE2	6:B:38:MET:HB3	1.75	0.47
11:G:63:MET:HE3	11:G:100:CYS:HA	1.96	0.47
16:L:61:PRO:HA	16:L:66:VAL:HG22	1.97	0.47
16:L:75:GLY:HA3	16:L:88:ILE:HD12	1.95	0.47
29:Y:100:LYS:NZ	29:Y:107:ARG:HD3	2.30	0.47
3:2:70:G:N2	3:2:80:G:N3	2.63	0.47
3:2:339:A:H2'	3:2:340:C:C5	2.50	0.47
3:2:803:C:H2'	3:2:804:U:H6	1.79	0.47
3:2:1518:C:OP1	3:2:1520:G:H8	1.98	0.47
3:2:1585:U:H3	21:Q:73:LYS:HZ3	1.61	0.47
3:2:1590:C:H3'	3:2:1591:C:H6	1.79	0.47
4:3:135:G:N2	4:3:290:U:O2	2.48	0.47
8:D:213:PRO:HD3	22:R:19:LYS:HD3	1.96	0.47
10:F:38:TYR:CE2	10:F:144:LEU:HB2	2.50	0.47
12:H:121:THR:HG22	12:H:124:ALA:HB3	1.97	0.47
29:Y:20:ARG:NH1	29:Y:74:MET:SD	2.88	0.47
35:e:50:GLY:HA3	35:e:52:LYS:HE3	1.96	0.47
37:g:156:PHE:HE1	37:g:179:LEU:HD11	1.80	0.47
3:2:561:A:OP2	14:J:173:VAL:HB	2.15	0.47
19:O:31:CYS:N	19:O:94:HIS:O	2.30	0.47
24:T:42:HIS:CG	24:T:81:GLY:HA3	2.50	0.47
3:2:607:U:O2'	3:2:608:C:OP1	2.28	0.46
3:2:1494:U:H1'	3:2:1495:G:OP2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1866:A:C6	31:a:87:ARG:NH1	2.83	0.46
5:A:121:LEU:HG	5:A:122:LEU:N	2.30	0.46
6:B:186:ASN:HA	6:B:189:ILE:HD12	1.95	0.46
11:G:2:LYS:HB2	11:G:108:VAL:HG22	1.96	0.46
11:G:61:PHE:HD2	11:G:72:ARG:HD2	1.80	0.46
16:L:7:GLU:HB2	16:L:11:GLN:HE21	1.79	0.46
17:M:52:LEU:HD11	17:M:65:VAL:HB	1.98	0.46
23:S:3:LEU:N	30:Z:90:GLU:OE2	2.48	0.46
3:2:291:G:C2	3:2:292:A:C4	3.03	0.46
3:2:1238:U:H1'	20:P:126:VAL:HG13	1.96	0.46
3:2:1710:C:N4	3:2:1823:A:H61	2.13	0.46
7:C:271:ASP:OD1	7:C:271:ASP:N	2.47	0.46
9:E:199:GLU:HG3	9:E:207:VAL:HB	1.95	0.46
11:G:21:GLU:O	11:G:25:ARG:HG2	2.15	0.46
11:G:54:GLY:H	11:G:110:ASN:HB2	1.79	0.46
11:G:110:ASN:N	11:G:110:ASN:OD1	2.45	0.46
15:K:15:LEU:HD23	15:K:79:LEU:HD11	1.97	0.46
18:N:63:VAL:HG21	18:N:71:ILE:HD11	1.98	0.46
23:S:26:ILE:O	23:S:30:ILE:HG12	2.14	0.46
23:S:98:VAL:HG11	23:S:106:LYS:HD2	1.97	0.46
29:Y:110:ARG:O	29:Y:114:MET:HG2	2.15	0.46
2:1:43:G:H2'	2:1:44:A:O4'	2.16	0.46
3:2:1566:G:C5	24:T:98:SER:HB2	2.51	0.46
5:A:39:TYR:CD2	5:A:40:LYS:HG2	2.51	0.46
16:L:79:LYS:HG2	16:L:81:LYS:NZ	2.30	0.46
18:N:80:LEU:HD22	18:N:80:LEU:H	1.79	0.46
23:S:26:ILE:HD11	23:S:45:LEU:HD22	1.97	0.46
3:2:465:A:H5'	3:2:466:G:C4	2.50	0.46
3:2:913:A:C2	12:H:98:ARG:HA	2.41	0.46
3:2:1453:C:OP1	22:R:48:ASN:ND2	2.40	0.46
7:C:124:PHE:O	7:C:143:CYS:HA	2.15	0.46
8:D:31:GLU:HG2	8:D:107:TYR:HE2	1.80	0.46
14:J:132:GLN:HB3	14:J:134:HIS:HD2	1.80	0.46
15:K:58:VAL:HG12	15:K:71:LEU:HD23	1.96	0.46
1:0:271:CYS:SG	1:0:305:ARG:NE	2.89	0.46
1:0:321:LEU:HB3	1:0:332:VAL:HG11	1.96	0.46
3:2:39:A:H2'	3:2:40:A:O4'	2.14	0.46
3:2:165:G:OP2	3:2:165:G:N2	2.38	0.46
3:2:936:G:H2'	3:2:937:C:C6	2.50	0.46
3:2:1073:U:H2'	3:2:1074:C:C6	2.51	0.46
8:D:74:GLN:HE21	8:D:84:VAL:HG12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:15:PRO:HG2	9:E:18:TRP:CE2	2.51	0.46
16:L:131:CYS:SG	16:L:132:ARG:N	2.89	0.46
17:M:51:VAL:HB	17:M:109:VAL:HB	1.96	0.46
19:O:43:HIS:HD2	19:O:55:ARG:HD3	1.81	0.46
22:R:73:LEU:HA	22:R:76:GLU:HB3	1.97	0.46
1:O:81:PRO:HD2	1:O:132:LEU:HD21	1.98	0.46
3:2:67:C:O2'	3:2:68:A:H3'	2.15	0.46
3:2:352:U:H5''	16:L:139:ARG:HG2	1.98	0.46
3:2:816:A:OP2	14:J:10:ARG:NH2	2.48	0.46
3:2:1097:G:H4'	5:A:32:PHE:CD1	2.51	0.46
3:2:1204:A:OP1	7:C:117:ARG:HB3	2.15	0.46
3:2:1538:C:O2'	24:T:45:LEU:HD12	2.15	0.46
3:2:1735:A:H2'	3:2:1736:G:O4'	2.15	0.46
4:3:153:G:H3'	4:3:154:A:H5'	1.97	0.46
13:I:79:ILE:HG13	13:I:170:LYS:NZ	2.31	0.46
19:O:90:ILE:O	19:O:124:MET:HE1	2.16	0.46
21:Q:25:CYS:SG	21:Q:91:ALA:HB1	2.56	0.46
25:U:82:MET:HE2	34:d:51:GLY:C	2.41	0.46
3:2:314:U:H2'	3:2:315:C:C6	2.48	0.46
3:2:822:U:H2'	3:2:824:C:OP2	2.16	0.46
3:2:1493:C:H5'	3:2:1494:U:H2'	1.97	0.46
3:2:1558:C:H4'	3:2:1559:C:OP1	2.16	0.46
3:2:1561:A:N6	3:2:1573:G:O6	2.48	0.46
3:2:1585:U:H2'	24:T:67:ARG:NH2	2.31	0.46
3:2:1648:G:H1'	3:2:1649:U:OP2	2.16	0.46
7:C:161:SER:HA	26:V:27:LYS:NZ	2.30	0.46
9:E:19:MET:HB2	9:E:51:ARG:NH2	2.31	0.46
11:G:185:LEU:HD12	11:G:185:LEU:HA	1.67	0.46
14:J:63:LEU:HD11	14:J:69:ARG:NH1	2.31	0.46
17:M:101:ARG:HG3	17:M:102:LYS:N	2.30	0.46
21:Q:100:VAL:HG12	21:Q:101:ASP:H	1.81	0.46
24:T:37:VAL:HG22	24:T:38:LYS:H	1.80	0.46
32:b:31:TYR:HE1	32:b:33:MET:HE2	1.81	0.46
33:c:10:LYS:HD2	33:c:34:PHE:HE1	1.81	0.46
35:e:51:LYS:HD2	35:e:51:LYS:HA	1.60	0.46
37:g:121:VAL:HG12	37:g:154:VAL:HG11	1.97	0.46
3:2:1515:G:H21	20:P:99:GLY:CA	2.29	0.46
3:2:1651:A:H2'	3:2:1652:G:H8	1.81	0.46
9:E:182:MET:HB2	9:E:228:ILE:HD11	1.98	0.46
26:V:59:ILE:H	26:V:59:ILE:HG13	1.55	0.46
29:Y:88:LYS:HD2	29:Y:97:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:26:GLN:H	33:c:26:GLN:HG2	1.44	0.46
3:2:309:G:O2'	3:2:310:C:OP2	2.30	0.46
3:2:501:C:O2	3:2:501:C:H2'	2.16	0.46
3:2:587:A:H5'	3:2:592:C:H41	1.81	0.46
8:D:96:LEU:HD12	8:D:198:ILE:HG21	1.98	0.46
9:E:245:ARG:O	9:E:246:LEU:HD23	2.16	0.46
23:S:78:LYS:HZ2	24:T:32:GLU:HB2	1.79	0.46
37:g:19:THR:O	37:g:288:SER:HB2	2.16	0.46
3:2:103:A:OP2	3:2:356:C:N4	2.48	0.46
3:2:300:U:H2'	3:2:301:A:C8	2.51	0.46
3:2:926:A:H61	3:2:1015:U:H3	1.62	0.46
3:2:1598:G:H21	10:F:166:ILE:HG22	1.81	0.46
3:2:1726:G:H2'	3:2:1727:G:C8	2.51	0.46
3:2:1735:A:H62	3:2:1799:G:H21	1.63	0.46
3:2:1804:U:H2'	3:2:1805:G:C8	2.51	0.46
12:H:53:VAL:HG12	12:H:175:GLY:HA3	1.98	0.46
16:L:98:LYS:HD3	16:L:99:TYR:CE1	2.51	0.46
19:O:37:PHE:HE2	19:O:105:THR:HG21	1.81	0.46
23:S:80:PRO:HB2	23:S:83:PHE:HD2	1.81	0.46
32:b:2:PRO:C	32:b:4:ALA:H	2.24	0.46
1:0:70:PRO:HB2	1:0:82:THR:HG21	1.98	0.45
3:2:900:C:H2'	3:2:901:G:H8	1.81	0.45
3:2:1415:C:H5''	24:T:129:ARG:HG3	1.96	0.45
3:2:1522:A:N1	20:P:131:PRO:HD3	2.31	0.45
7:C:82:TYR:CE2	7:C:164:PRO:HD3	2.51	0.45
8:D:133:GLY:HA3	8:D:156:LEU:O	2.17	0.45
10:F:59:LYS:HG3	10:F:62:ARG:HB2	1.97	0.45
15:K:7:ASN:HB3	15:K:40:VAL:HG13	1.99	0.45
37:g:57:ARG:NH1	37:g:93:THR:O	2.49	0.45
3:2:1374:C:H2'	3:2:1375:G:O4'	2.16	0.45
3:2:1753:C:H2'	3:2:1754:G:H8	1.81	0.45
4:3:265:U:O2'	4:3:266:G:H5'	2.16	0.45
6:B:38:MET:HE1	6:B:182:LYS:O	2.15	0.45
6:B:52:THR:HG22	6:B:54:GLY:H	1.81	0.45
7:C:233:LEU:HD12	7:C:233:LEU:HA	1.72	0.45
9:E:11:ARG:NH2	9:E:20:LEU:HD22	2.31	0.45
11:G:102:VAL:HG13	11:G:106:LEU:HD12	1.98	0.45
16:L:101:ARG:HH12	28:X:5:ARG:HA	1.82	0.45
21:Q:16:LYS:HG3	21:Q:17:LYS:HG3	1.99	0.45
25:U:67:LYS:HE2	25:U:78:ASP:OD1	2.16	0.45
3:2:415:A:H2'	3:2:416:U:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:521:A:OP1	14:J:45:ARG:NH1	2.49	0.45
3:2:811:A:H2'	3:2:812:A:C8	2.52	0.45
3:2:897:U:H2'	3:2:898:U:O4'	2.15	0.45
3:2:1453:C:O2'	22:R:52:GLY:HA3	2.17	0.45
3:2:1859:A:H5'	3:2:1860:A:OP2	2.16	0.45
4:3:334:C:H41	31:a:47:ALA:HB3	1.81	0.45
9:E:73:ASP:HA	9:E:164:LEU:HD13	1.97	0.45
30:Z:77:LEU:HB2	30:Z:79:ILE:HG13	1.98	0.45
34:d:19:ARG:NH1	34:d:32:ARG:HD2	2.30	0.45
3:2:465:A:H5'	3:2:466:G:C5	2.51	0.45
3:2:1595:U:OP1	30:Z:102:LYS:NZ	2.36	0.45
7:C:221:ASP:OD1	7:C:221:ASP:N	2.49	0.45
10:F:41:VAL:HG13	10:F:46:ALA:HA	1.99	0.45
21:Q:132:PHE:HE2	25:U:76:THR:HA	1.82	0.45
25:U:22:ILE:HB	25:U:89:ILE:HG23	1.99	0.45
27:W:87:GLU:HG2	27:W:117:ARG:NH2	2.31	0.45
31:a:10:ARG:HH11	31:a:12:LYS:HD3	1.78	0.45
1:0:265:ASP:O	1:0:269:GLN:HB2	2.17	0.45
3:2:127:C:O2'	3:2:215:G:O2'	2.30	0.45
3:2:152:U:H4'	11:G:132:ARG:HH12	1.78	0.45
3:2:488:U:H3'	3:2:489:A:H5'	1.99	0.45
6:B:144:LYS:HB2	6:B:208:HIS:CB	2.45	0.45
9:E:36:HIS:NE2	9:E:88:ASP:OD2	2.49	0.45
11:G:7:PHE:HA	11:G:8:PRO:HD3	1.75	0.45
24:T:34:VAL:HG13	24:T:52:TRP:NE1	2.32	0.45
24:T:52:TRP:O	24:T:56:ARG:HB2	2.17	0.45
36:f:111:ASN:HD22	36:f:113:LYS:HE3	1.81	0.45
3:2:92:A:H1'	9:E:3:ARG:HB2	1.99	0.45
3:2:190:G:C6	3:2:208:G:C6	3.04	0.45
3:2:1445:U:O4	3:2:1446:A:N6	2.50	0.45
3:2:1566:G:H4'	3:2:1566:G:OP1	2.16	0.45
3:2:1656:G:H1	3:2:1668:U:H3	1.63	0.45
6:B:68:GLU:HG3	6:B:83:LYS:HE2	1.99	0.45
8:D:108:LYS:O	8:D:113:LEU:HB2	2.17	0.45
16:L:60:CYS:SG	16:L:63:THR:OG1	2.74	0.45
1:0:34:GLY:O	1:0:38:VAL:N	2.50	0.45
1:0:291:THR:O	1:0:295:SER:HB2	2.17	0.45
3:2:161:U:H5'	29:Y:116:LYS:HB3	1.97	0.45
3:2:209:A:H2'	3:2:210:U:H5'	1.99	0.45
3:2:993:G:N7	31:a:15:ARG:NH1	2.65	0.45
3:2:1440:C:HO2'	3:2:1441:U:C5'	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:147:LYS:HB3	16:L:151:THR:OG1	2.16	0.45
20:P:108:LYS:HB3	20:P:109:PRO:HD2	1.97	0.45
28:X:77:ASN:OD1	28:X:77:ASN:N	2.39	0.45
28:X:115:ILE:HA	28:X:116:PRO:HD3	1.82	0.45
1:O:97:THR:HA	1:O:136:SER:O	2.16	0.45
3:2:70:G:N2	3:2:79:A:H62	2.15	0.45
3:2:624:C:N4	28:X:63:ASN:HD22	2.14	0.45
3:2:1277:C:H2'	3:2:1278:A:H8	1.81	0.45
3:2:1605:G:O2'	3:2:1634:A:N6	2.49	0.45
3:2:1744:G:H2'	3:2:1789:G:H22	1.82	0.45
9:E:68:ARG:NH1	9:E:76:VAL:HG11	2.31	0.45
11:G:61:PHE:CD2	11:G:72:ARG:HD2	2.51	0.45
20:P:78:THR:HG22	20:P:95:GLY:O	2.17	0.45
23:S:25:LYS:HA	23:S:25:LYS:HD3	1.75	0.45
25:U:40:ILE:HD12	25:U:53:PRO:HD3	1.98	0.45
26:V:15:ARG:HH12	26:V:33:GLN:HB2	1.81	0.45
3:2:1373:C:H2'	3:2:1374:C:C6	2.52	0.45
10:F:162:ALA:HB2	10:F:172:CYS:SG	2.57	0.45
12:H:140:VAL:HG22	18:N:19:ARG:HH21	1.81	0.45
13:I:84:ASN:ND2	13:I:90:LEU:HD12	2.32	0.45
15:K:53:LYS:HD2	15:K:60:GLU:HG3	1.99	0.45
1:O:529:GLN:NE2	3:2:1849:G:O2'	2.49	0.45
3:2:1842:C:N4	3:2:1843:G:O6	2.49	0.45
3:2:1866:A:C2	31:a:87:ARG:NH1	2.66	0.45
13:I:193:LYS:O	13:I:196:GLU:HG2	2.17	0.45
37:g:192:THR:O	37:g:213:ASP:HB3	2.16	0.45
2:1:4:G:C2	2:1:70:G:C2	3.06	0.44
3:2:979:C:H2'	3:2:980:A:C8	2.51	0.44
3:2:1258:A:N1	3:2:1663:A:H2'	2.32	0.44
3:2:1535:U:H4'	10:F:91:ARG:HH12	1.83	0.44
3:2:1740:C:H2'	3:2:1741:U:C6	2.52	0.44
4:3:260:A:C2	4:3:261:G:H1'	2.52	0.44
4:3:263:G:C2	4:3:264:U:H5	2.35	0.44
12:H:133:LEU:O	12:H:173:PHE:HE1	2.01	0.44
13:I:25:ARG:HA	13:I:25:ARG:HD3	1.63	0.44
17:M:42:LEU:HG	17:M:74:ILE:HD13	1.99	0.44
23:S:68:ILE:HG23	23:S:72:GLN:HE21	1.81	0.44
24:T:4:VAL:HG23	24:T:136:GLY:HA2	1.99	0.44
31:a:45:VAL:HG13	31:a:49:ALA:HB3	1.99	0.44
33:c:34:PHE:CE2	33:c:40:ARG:HD3	2.52	0.44
1:O:30:PHE:HB3	1:O:31:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:154:U:H3'	3:2:155:G:H5''	1.99	0.44
3:2:318:A:H61	11:G:186:GLN:NE2	2.06	0.44
3:2:1721:U:H2'	3:2:1722:G:O4'	2.17	0.44
13:I:99:ASN:HA	13:I:174:CYS:SG	2.57	0.44
3:2:316:G:P	11:G:183:ARG:NH1	2.90	0.44
3:2:902:G:H2'	3:2:903:A:O4'	2.18	0.44
3:2:1551:U:OP1	8:D:9:ARG:NH2	2.50	0.44
3:2:1599:U:C5	10:F:166:ILE:HD12	2.52	0.44
3:2:1718:G:C6	3:2:1814:G:C6	3.05	0.44
4:3:123:C:O2'	4:3:124:C:OP1	2.35	0.44
4:3:166:C:H5	4:3:231:G:OP1	1.99	0.44
5:A:68:ILE:HD13	5:A:120:ARG:HB3	1.99	0.44
6:B:33:VAL:HA	6:B:96:CYS:HB2	1.99	0.44
17:M:68:LEU:HD23	36:f:114:ILE:HD13	2.00	0.44
19:O:142:ARG:NH1	19:O:142:ARG:HG2	2.33	0.44
21:Q:23:ALA:HB2	21:Q:87:SER:HB2	1.99	0.44
21:Q:131:LYS:HE3	21:Q:131:LYS:HB2	1.57	0.44
25:U:32:LEU:HD21	25:U:87:ARG:HG3	1.99	0.44
27:W:115:GLU:HA	27:W:118:ARG:HH11	1.80	0.44
28:X:17:ARG:NH1	28:X:17:ARG:HA	2.32	0.44
37:g:149:GLU:HB3	37:g:170:TRP:HB2	2.00	0.44
37:g:253:GLY:HA2	37:g:286:CYS:H	1.81	0.44
3:2:518:G:H2'	3:2:519:A:H8	1.81	0.44
3:2:1338:G:OP1	25:U:67:LYS:HD2	2.18	0.44
4:3:159:G:H8	4:3:159:G:OP2	2.01	0.44
7:C:135:GLY:C	7:C:136:HIS:CG	2.95	0.44
13:I:17:LYS:H	13:I:17:LYS:HG3	1.45	0.44
15:K:32:HIS:CG	15:K:33:PRO:HD2	2.52	0.44
16:L:104:LYS:HB2	16:L:104:LYS:HE3	1.74	0.44
29:Y:118:ARG:HA	29:Y:118:ARG:HD2	1.68	0.44
31:a:23:CYS:HB3	31:a:27:ALA:H	1.82	0.44
1:0:86:LEU:HD21	1:0:134:ALA:HB2	1.98	0.44
3:2:130:G:H1	3:2:182:C:H42	1.65	0.44
3:2:552:G:OP1	35:e:39:ASN:ND2	2.51	0.44
3:2:1425:G:H2'	3:2:1426:U:C6	2.52	0.44
3:2:1618:C:H5'	3:2:1619:A:OP2	2.17	0.44
4:3:252:A:H4'	4:3:253:G:C5'	2.45	0.44
5:A:89:LYS:HE3	5:A:201:LEU:HD11	1.99	0.44
7:C:179:THR:OG1	7:C:180:VAL:N	2.50	0.44
8:D:32:ASP:OD2	8:D:65:ARG:NH1	2.50	0.44
10:F:47:LYS:NZ	10:F:52:SER:CB	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:60:MET:SD	17:M:63:LYS:HD2	2.57	0.44
24:T:125:PRO:O	24:T:129:ARG:HG3	2.18	0.44
37:g:177:TRP:CZ3	37:g:184:LEU:HB2	2.53	0.44
37:g:239:LEU:HD23	37:g:250:ALA:HA	1.99	0.44
38:h:20:MET:O	38:h:25:LYS:NZ	2.27	0.44
3:2:380:G:P	13:I:56:ARG:HH22	2.41	0.44
3:2:991:G:C6	3:2:1134:G:H4'	2.53	0.44
3:2:1644:C:OP1	21:Q:143:LYS:HD3	2.18	0.44
11:G:217:MET:O	11:G:221:LYS:HG3	2.17	0.44
12:H:130:LEU:HB2	12:H:177:TYR:CE1	2.52	0.44
12:H:138:GLU:OE2	18:N:21:SER:OG	2.25	0.44
16:L:72:ILE:HA	16:L:129:GLY:HA2	1.99	0.44
17:M:36:ARG:HE	17:M:40:LYS:NZ	2.16	0.44
18:N:45:LEU:HB3	18:N:49:GLN:HB2	1.98	0.44
24:T:88:MET:HB3	24:T:89:PRO:HD2	2.00	0.44
26:V:21:ASN:O	26:V:21:ASN:ND2	2.50	0.44
27:W:10:ALA:HB1	27:W:27:ILE:HD12	1.99	0.44
31:a:41:ILE:HG12	31:a:68:TYR:HD1	1.83	0.44
1:0:75:LEU:O	1:0:77:LYS:HB2	2.17	0.44
3:2:1314:U:O2'	15:K:3:MET:HG2	2.18	0.44
3:2:1486:A:N6	3:2:1487:A:C6	2.86	0.44
3:2:1819:A:H2'	3:2:1820:G:H8	1.79	0.44
8:D:202:LYS:HA	8:D:203:PRO:HD3	1.75	0.44
9:E:117:GLU:O	9:E:120:LYS:HG3	2.17	0.44
9:E:181:CYS:SG	9:E:195:ILE:HG13	2.58	0.44
25:U:31:SER:O	25:U:35:VAL:HG23	2.18	0.44
28:X:101:LEU:HD12	28:X:101:LEU:HA	1.68	0.44
28:X:140:ARG:HD2	28:X:141:PRO:HD2	2.00	0.44
29:Y:88:LYS:HB3	29:Y:97:TYR:CD2	2.53	0.44
1:0:309:ILE:O	1:0:309:ILE:HG13	2.17	0.44
2:1:71:C:H2'	2:1:72:U:O4'	2.18	0.44
3:2:71:G:H5''	3:2:72:C:OP2	2.18	0.44
3:2:797:C:HO2'	3:2:798:G:P	2.37	0.44
3:2:824:C:H4'	14:J:147:PHE:CD1	2.49	0.44
3:2:841:G:H2'	3:2:842:C:C6	2.53	0.44
3:2:1136:U:C2'	3:2:1137:U:H5'	2.48	0.44
3:2:1137:U:O2'	3:2:1138:C:OP1	2.34	0.44
3:2:1416:C:O2'	24:T:3:GLY:HA3	2.17	0.44
3:2:1425:G:HO2'	3:2:1426:U:P	2.38	0.44
3:2:1534:C:P	10:F:81:ARG:HH22	2.40	0.44
8:D:72:VAL:HG22	15:K:20:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:73:ASP:HB3	9:E:164:LEU:HD22	1.99	0.44
25:U:60:THR:HG23	25:U:83:ARG:HG2	1.99	0.44
3:2:124:U:C5'	11:G:201:LYS:NZ	2.81	0.44
3:2:319:C:HO2'	3:2:320:G:P	2.38	0.44
3:2:795:A:C2	3:2:796:G:H1'	2.52	0.44
3:2:1274:G:H4'	15:K:47:LYS:HE2	1.99	0.44
5:A:26:GLY:O	5:A:46:ILE:HG23	2.18	0.44
6:B:28:LYS:HB3	6:B:48:LEU:HD11	2.00	0.44
6:B:49:VAL:HG21	6:B:62:LEU:HD13	1.99	0.44
18:N:110:ASP:O	18:N:113:PHE:HB3	2.17	0.44
19:O:146:ARG:HG3	19:O:146:ARG:HH11	1.83	0.44
1:0:118:VAL:CG2	1:0:161:LEU:HG	2.48	0.43
3:2:65:C:O2'	3:2:66:G:OP1	2.30	0.43
3:2:191:A:N6	3:2:208:G:O2'	2.49	0.43
3:2:223:C:H2'	3:2:224:A:C8	2.52	0.43
3:2:596:U:H2'	3:2:597:G:O4'	2.18	0.43
3:2:843:C:H2'	3:2:844:U:O4'	2.18	0.43
3:2:1231:C:H2'	3:2:1232:U:O4'	2.18	0.43
10:F:60:ARG:HG2	10:F:61:PHE:CD2	2.53	0.43
17:M:52:LEU:HD12	17:M:76:LEU:HD13	1.99	0.43
22:R:20:TYR:CD2	22:R:23:ARG:HD2	2.50	0.43
30:Z:73:VAL:HG12	30:Z:79:ILE:HD12	1.99	0.43
33:c:46:VAL:HG21	33:c:50:VAL:HG21	1.99	0.43
2:1:34:C:H4'	3:2:1248:U:H1'	2.00	0.43
3:2:70:G:C2	3:2:80:G:C2	3.07	0.43
3:2:160:U:O2	3:2:469:A:H5'	2.17	0.43
3:2:587:A:H5'	3:2:592:C:N4	2.33	0.43
3:2:604:A:H4'	3:2:605:A:OP1	2.19	0.43
3:2:1237:C:H2'	3:2:1238:U:O4'	2.18	0.43
3:2:1845:A:H2'	3:2:1846:G:H8	1.82	0.43
6:B:181:LEU:O	6:B:185:VAL:HG23	2.18	0.43
8:D:172:VAL:HG22	8:D:185:LYS:HG2	2.00	0.43
9:E:29:PRO:HG2	9:E:46:ILE:HD11	1.99	0.43
9:E:235:TRP:CD1	9:E:235:TRP:N	2.85	0.43
12:H:191:GLU:O	12:H:192:PHE:HB2	2.19	0.43
13:I:31:ARG:HG3	13:I:31:ARG:NH1	2.33	0.43
27:W:86:LEU:HD12	27:W:86:LEU:HA	1.87	0.43
31:a:37:LYS:HE2	31:a:37:LYS:HB2	1.79	0.43
2:1:20:A:N6	2:1:57:G:O2'	2.51	0.43
3:2:39:A:OP2	14:J:5:ARG:NH1	2.52	0.43
3:2:811:A:HO2'	3:2:812:A:P	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1152:U:H2'	27:W:12:LYS:NZ	2.34	0.43
3:2:1722:G:H3'	3:2:1723:G:H8	1.84	0.43
8:D:25:LEU:HD23	8:D:25:LEU:HA	1.82	0.43
9:E:73:ASP:OD2	9:E:122:LYS:NZ	2.52	0.43
13:I:9:HIS:CG	13:I:9:HIS:O	2.70	0.43
16:L:80:MET:H	16:L:80:MET:HG3	1.55	0.43
21:Q:51:LEU:HD13	21:Q:81:ILE:HG23	1.99	0.43
33:c:12:ALA:O	33:c:55:VAL:HA	2.18	0.43
36:f:135:HIS:HB2	36:f:138:ARG:HG2	2.00	0.43
37:g:197:THR:OG1	37:g:237:ASN:O	2.33	0.43
3:2:1102:G:N2	3:2:1131:G:C4	2.87	0.43
7:C:236:PHE:O	7:C:240:THR:HG22	2.18	0.43
37:g:173:LEU:HD12	37:g:175:LYS:NZ	2.34	0.43
3:2:70:G:N2	3:2:80:G:C2	2.86	0.43
3:2:918:U:H5'	18:N:20:ARG:CZ	2.48	0.43
3:2:1259:A:H61	3:2:1519:U:C5'	2.29	0.43
3:2:1746:U:H4'	11:G:65:GLN:NE2	2.34	0.43
5:A:38:ILE:HD11	5:A:47:TYR:HB3	2.00	0.43
6:B:77:ASP:OD1	6:B:77:ASP:N	2.51	0.43
7:C:102:LEU:HD23	7:C:102:LEU:HA	1.84	0.43
9:E:103:TYR:CD1	9:E:189:LEU:HD11	2.53	0.43
10:F:61:PHE:HB3	33:c:51:ARG:NH1	2.34	0.43
16:L:61:PRO:HA	16:L:66:VAL:CG2	2.49	0.43
21:Q:37:ARG:HA	21:Q:38:PRO:HD3	1.90	0.43
27:W:117:ARG:HG3	27:W:117:ARG:HH11	1.83	0.43
28:X:14:ARG:HD3	28:X:18:ARG:HH12	1.82	0.43
28:X:105:PHE:HB2	28:X:119:ARG:O	2.17	0.43
32:b:27:SER:HA	32:b:28:PRO:HD2	1.91	0.43
37:g:146:SER:O	37:g:147:HIS:CG	2.72	0.43
3:2:53:C:O3'	29:Y:108:LYS:HG2	2.19	0.43
3:2:163:U:O3'	11:G:83:CYS:HA	2.18	0.43
3:2:166:A:H1'	11:G:13:GLN:NE2	2.33	0.43
3:2:919:A:H5'	18:N:16:LEU:HD12	2.00	0.43
3:2:1644:C:H2'	3:2:1645:C:C6	2.53	0.43
5:A:5:LEU:HD21	26:V:41:LYS:HA	2.01	0.43
5:A:126:ASP:HA	5:A:127:PRO:HD2	1.90	0.43
5:A:169:HIS:HA	5:A:203:PHE:CE1	2.54	0.43
8:D:27:ARG:HB3	15:K:61:GLN:HE21	1.82	0.43
8:D:71:ALA:O	8:D:75:LYS:HG2	2.19	0.43
13:I:164:GLU:O	13:I:167:GLN:HB2	2.17	0.43
37:g:142:VAL:HG12	37:g:144:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:71:G:O2'	3:2:79:A:N6	2.52	0.43
3:2:76:U:H5'	11:G:159:ARG:NH2	2.29	0.43
3:2:748:C:O2'	3:2:749:U:OP1	2.31	0.43
3:2:957:A:OP1	19:O:57:THR:OG1	2.34	0.43
5:A:65:ILE:HD12	5:A:182:VAL:HG11	2.01	0.43
7:C:77:SER:HA	7:C:97:PHE:HE1	1.84	0.43
8:D:96:LEU:HD22	8:D:131:ALA:HB2	2.00	0.43
14:J:143:ASN:HB2	29:Y:64:PHE:CZ	2.53	0.43
19:O:77:ALA:O	19:O:81:VAL:HG12	2.19	0.43
24:T:42:HIS:HB3	24:T:93:SER:HB2	2.00	0.43
24:T:126:GLN:HA	24:T:129:ARG:HD2	2.01	0.43
25:U:55:ARG:HE	25:U:87:ARG:HH12	1.67	0.43
28:X:130:LEU:HD23	28:X:130:LEU:HA	1.73	0.43
37:g:45:LEU:HD11	37:g:299:PHE:HZ	1.84	0.43
1:0:65:VAL:HG22	1:0:70:PRO:HA	2.01	0.43
3:2:842:C:C2'	3:2:843:C:H5'	2.49	0.43
3:2:1377:U:C5	5:A:102:ARG:NH1	2.87	0.43
3:2:1601:A:H4'	3:2:1602:U:C5'	2.44	0.43
5:A:180:ARG:HD2	5:A:184:ARG:CZ	2.49	0.43
9:E:44:LEU:HD21	9:E:70:ILE:HG21	2.00	0.43
15:K:4:PRO:HB2	15:K:6:LYS:HG2	2.01	0.43
23:S:75:ARG:CZ	23:S:95:TYR:HB2	2.49	0.43
29:Y:55:ILE:HG22	29:Y:75:ILE:HG23	1.99	0.43
1:0:400:HIS:CD2	1:0:406:LEU:HD21	2.54	0.43
3:2:70:G:C6	3:2:71:G:C4	3.07	0.43
3:2:946:U:H2'	3:2:947:G:C8	2.53	0.43
7:C:168:GLY:HA3	7:C:181:PRO:HA	2.01	0.43
9:E:56:LEU:HB2	9:E:60:GLU:OE2	2.18	0.43
9:E:181:CYS:HB3	9:E:227:VAL:HA	2.01	0.43
11:G:51:ARG:HH11	11:G:112:VAL:HG21	1.84	0.43
12:H:189:PHE:HA	12:H:190:PRO:HD3	1.86	0.43
13:I:116:HIS:CD2	13:I:152:ARG:HD3	2.54	0.43
17:M:101:ARG:HG3	17:M:102:LYS:H	1.83	0.43
21:Q:97:GLN:OE1	21:Q:105:LYS:NZ	2.30	0.43
22:R:31:ASN:HA	22:R:34:VAL:HB	2.00	0.43
28:X:7:LEU:HD23	28:X:7:LEU:HA	1.86	0.43
29:Y:54:VAL:HG22	29:Y:76:TYR:HB2	2.01	0.43
32:b:24:LEU:HD12	32:b:24:LEU:HA	1.91	0.43
3:2:69:C:OP2	11:G:164:LYS:NZ	2.49	0.43
3:2:829:C:OP1	9:E:21:ASP:HB2	2.18	0.43
3:2:940:U:H1'	3:2:1003:U:O2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1535:U:N3	10:F:76:MET:O	2.50	0.43
3:2:1599:U:C6	10:F:166:ILE:HD12	2.54	0.43
4:3:263:G:N3	4:3:264:U:H5	2.17	0.43
6:B:23:ASP:HA	6:B:24:PRO:HD3	1.86	0.43
9:E:138:HIS:CD2	9:E:148:ARG:HB3	2.53	0.43
9:E:155:LYS:HA	9:E:155:LYS:HD3	1.86	0.43
14:J:15:THR:HG22	14:J:44:TRP:CZ3	2.54	0.43
14:J:53:ILE:HG21	14:J:81:LEU:HD11	2.01	0.43
14:J:104:ASP:OD1	14:J:104:ASP:N	2.52	0.43
16:L:42:LEU:HD13	16:L:42:LEU:HA	1.81	0.43
16:L:104:LYS:HZ1	28:X:8:ARG:HD3	1.84	0.43
21:Q:132:PHE:CE2	25:U:76:THR:HA	2.54	0.43
24:T:64:LEU:HD23	24:T:64:LEU:HA	1.76	0.43
24:T:80:GLY:HA2	24:T:92:PHE:CE1	2.54	0.43
3:2:433:A:N6	3:2:434:G:O6	2.52	0.42
3:2:941:C:H5'	6:B:136:ARG:NH2	2.34	0.42
9:E:164:LEU:HA	9:E:164:LEU:HD23	1.76	0.42
11:G:137:ARG:HH11	11:G:178:ARG:NH1	2.17	0.42
13:I:67:TRP:HE1	13:I:70:GLU:CG	2.32	0.42
2:1:48:C:H6	2:1:48:C:O5'	2.02	0.42
3:2:552:G:H8	3:2:552:G:OP2	2.02	0.42
3:2:984:C:O2'	19:O:138:ASP:HB3	2.19	0.42
3:2:1232:U:H3	3:2:1526:G:H1	1.66	0.42
3:2:1356:G:H5'	7:C:238:LYS:NZ	2.34	0.42
6:B:87:ILE:HG12	6:B:101:HIS:CB	2.41	0.42
6:B:136:ARG:C	6:B:137:LEU:HD23	2.44	0.42
13:I:35:ASN:HB2	13:I:37:LYS:HE2	2.00	0.42
24:T:37:VAL:HG22	24:T:38:LYS:N	2.34	0.42
37:g:102:VAL:HG12	37:g:103:GLY:H	1.84	0.42
2:1:64:A:H2'	2:1:65:G:O4'	2.19	0.42
3:2:149:A:H2'	3:2:150:A:C8	2.53	0.42
3:2:376:A:H2'	3:2:377:G:O4'	2.18	0.42
3:2:1291:A:OP1	34:d:2:GLY:N	2.52	0.42
3:2:1447:G:H2'	3:2:1448:A:C8	2.55	0.42
3:2:1544:C:H5	3:2:1588:A:OP2	2.01	0.42
7:C:173:LYS:O	26:V:4:ASP:HB2	2.19	0.42
8:D:7:LYS:HA	8:D:7:LYS:HD3	1.78	0.42
20:P:122:THR:HG22	20:P:123:TYR:HD2	1.84	0.42
22:R:58:MET:HG2	22:R:61:ILE:HD12	2.00	0.42
2:1:60:A:H5'	2:1:61:C:C5	2.53	0.42
3:2:871:U:H4'	3:2:871:U:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1105:G:H2'	3:2:1106:C:C6	2.55	0.42
3:2:1593:C:O2'	24:T:12:GLN:NE2	2.43	0.42
3:2:1607:A:H1'	3:2:1633:A:C2	2.55	0.42
5:A:108:PHE:HB3	5:A:140:VAL:HG21	2.00	0.42
5:A:111:GLN:HE21	5:A:111:GLN:HB2	1.47	0.42
7:C:258:GLU:OE1	7:C:258:GLU:N	2.46	0.42
2:1:19:G:H5'	2:1:20:A:H5'	2.02	0.42
3:2:1143:A:H5''	3:2:1144:A:OP2	2.19	0.42
3:2:1648:G:C6	21:Q:125:ARG:NH1	2.87	0.42
5:A:167:GLY:O	5:A:171:VAL:HG23	2.20	0.42
10:F:175:ASP:OD1	10:F:179:ASN:ND2	2.53	0.42
11:G:14:LYS:HE2	11:G:16:ILE:HG13	2.01	0.42
14:J:129:LEU:HD23	14:J:129:LEU:HA	1.82	0.42
14:J:155:LYS:HE3	14:J:156:HIS:CE1	2.55	0.42
19:O:146:ARG:HD3	31:a:29:CYS:HB2	2.02	0.42
22:R:27:ASP:O	22:R:31:ASN:ND2	2.51	0.42
28:X:107:ARG:O	28:X:109:GLY:N	2.53	0.42
30:Z:88:LEU:HD12	30:Z:88:LEU:HA	1.71	0.42
3:2:124:U:H5'	11:G:201:LYS:NZ	2.34	0.42
3:2:1451:G:H1'	3:2:1474:A:N6	2.33	0.42
4:3:160:U:O2'	4:3:161:G:OP1	2.32	0.42
5:A:42:LYS:HG3	5:A:43:SER:O	2.20	0.42
5:A:85:ARG:HD3	5:A:203:PHE:O	2.19	0.42
8:D:195:THR:H	8:D:201:LYS:HE2	1.85	0.42
10:F:59:LYS:HE3	10:F:59:LYS:HB2	1.82	0.42
20:P:125:PRO:HG3	23:S:127:TRP:CH2	2.55	0.42
33:c:12:ALA:HB1	33:c:32:VAL:HG13	2.02	0.42
35:e:28:LYS:HB3	35:e:28:LYS:HE2	1.76	0.42
37:g:121:VAL:HG11	37:g:165:ILE:HD12	2.02	0.42
3:2:68:A:H2'	3:2:69:C:O4'	2.19	0.42
3:2:121:U:H5''	9:E:77:ARG:NH2	2.25	0.42
3:2:960:U:H2'	3:2:962:A:OP2	2.19	0.42
3:2:1740:C:O5'	3:2:1740:C:H6	2.03	0.42
3:2:1856:C:OP2	19:O:146:ARG:HB2	2.19	0.42
4:3:330:A:HO2'	4:3:331:G:P	2.39	0.42
8:D:79:PHE:CE2	8:D:84:VAL:HB	2.55	0.42
10:F:78:MET:N	10:F:159:ARG:HH22	2.09	0.42
18:N:62:GLN:HB2	18:N:65:PHE:CD2	2.54	0.42
27:W:26:LEU:HD11	27:W:60:LYS:HB3	2.00	0.42
3:2:75:G:N2	11:G:155:GLN:HG3	2.29	0.42
3:2:220:U:H2'	3:2:221:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:642:U:P	14:J:39:ASN:HB2	2.59	0.42
3:2:1171:G:N2	3:2:1187:G:H2'	2.35	0.42
3:2:1464:C:HO2'	3:2:1465:A:P	2.42	0.42
3:2:1737:G:H2'	3:2:1738:C:C6	2.54	0.42
3:2:1737:G:C5	3:2:1738:C:C4	3.08	0.42
18:N:20:ARG:HE	27:W:56:HIS:CD2	2.37	0.42
22:R:53:TYR:O	22:R:57:LEU:HB2	2.20	0.42
3:2:818:A:H5''	3:2:819:G:OP2	2.20	0.42
3:2:1049:A:C5	3:2:1070:A:C2	3.08	0.42
3:2:1231:C:O2'	3:2:1232:U:P	2.78	0.42
3:2:1403:C:OP2	3:2:1405:A:N6	2.53	0.42
4:3:244:A:H1'	4:3:245:G:P	2.60	0.42
5:A:136:GLU:O	5:A:140:VAL:HG23	2.19	0.42
7:C:102:LEU:HD13	7:C:130:ILE:HD11	2.01	0.42
9:E:11:ARG:HA	9:E:28:ALA:HB2	2.02	0.42
9:E:46:ILE:O	9:E:50:ASN:HB2	2.20	0.42
12:H:63:PHE:HA	12:H:95:ILE:O	2.20	0.42
20:P:85:ILE:HG12	20:P:116:LEU:HG	2.01	0.42
22:R:130:THR:HA	22:R:131:PRO:HD3	1.79	0.42
3:2:383:G:C6	3:2:384:U:C4	3.08	0.42
3:2:499:G:H2'	3:2:501:C:H5	1.84	0.42
4:3:263:G:C2	4:3:264:U:C5	3.08	0.42
6:B:42:ARG:HD3	6:B:42:ARG:HA	1.83	0.42
6:B:63:LYS:HG3	6:B:89:GLU:O	2.19	0.42
16:L:40:ILE:HD13	16:L:40:ILE:HA	1.63	0.42
19:O:146:ARG:NH1	19:O:146:ARG:HG3	2.35	0.42
23:S:16:LEU:HD13	23:S:99:LEU:HD13	2.02	0.42
24:T:64:LEU:HD21	24:T:70:ALA:HB3	2.02	0.42
27:W:8:ALA:HA	27:W:74:VAL:HG11	2.02	0.42
27:W:83:LEU:HD12	27:W:83:LEU:HA	1.78	0.42
3:2:291:G:H2'	3:2:292:A:C8	2.55	0.41
3:2:1139:C:H5	3:2:1149:A:H62	1.66	0.41
3:2:1578:U:O2'	8:D:6:SER:HA	2.19	0.41
12:H:122:LEU:HD22	12:H:122:LEU:HA	1.87	0.41
13:I:114:GLU:OE1	13:I:123:ARG:NH2	2.48	0.41
14:J:45:ARG:O	14:J:49:THR:HG23	2.19	0.41
19:O:98:ARG:CG	19:O:98:ARG:NH1	2.75	0.41
20:P:124:LYS:HA	20:P:125:PRO:HD3	1.93	0.41
23:S:31:THR:HG23	23:S:37:GLY:HA2	2.02	0.41
25:U:32:LEU:HD21	25:U:87:ARG:CG	2.49	0.41
1:0:305:ARG:HD3	1:0:305:ARG:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:385:TYR:CZ	1:0:465:LEU:HD22	2.55	0.41
3:2:109:U:H2'	3:2:110:U:O4'	2.20	0.41
3:2:944:A:C6	3:2:945:U:C4	3.08	0.41
3:2:1086:G:O2'	3:2:1087:A:H5'	2.20	0.41
3:2:1231:C:H42	3:2:1527:C:N4	2.15	0.41
3:2:1443:C:H2'	3:2:1444:U:H5'	2.02	0.41
3:2:1455:A:OP2	22:R:56:HIS:ND1	2.53	0.41
5:A:147:LEU:O	5:A:165:ASN:ND2	2.53	0.41
7:C:80:GLU:O	7:C:84:PHE:HD2	2.04	0.41
8:D:67:ARG:O	8:D:70:THR:HG22	2.20	0.41
8:D:134:CYS:HB2	8:D:188:ILE:HD13	2.01	0.41
15:K:36:ALA:C	15:K:38:LYS:H	2.28	0.41
15:K:47:LYS:HE3	15:K:50:GLN:OE1	2.20	0.41
17:M:17:ALA:HB3	17:M:123:VAL:HG11	2.01	0.41
17:M:102:LYS:HD2	17:M:102:LYS:HA	1.86	0.41
20:P:44:ARG:HH21	20:P:53:GLN:HE22	1.68	0.41
26:V:51:LYS:HD3	26:V:76:ASP:CG	2.45	0.41
1:0:491:ILE:HD13	1:0:510:LEU:HD23	2.01	0.41
3:2:367:U:H4'	3:2:371:A:C8	2.55	0.41
3:2:803:C:H2'	3:2:804:U:C6	2.54	0.41
3:2:1023:A:O5'	3:2:1023:A:H8	2.03	0.41
20:P:18:ARG:NE	23:S:88:LYS:HD3	2.35	0.41
22:R:58:MET:O	22:R:62:GLN:HG2	2.19	0.41
24:T:82:ARG:NH1	24:T:84:ARG:HD3	2.35	0.41
3:2:54:A:P	29:Y:108:LYS:HZ2	2.43	0.41
3:2:141:A:N7	3:2:178:C:H1'	2.35	0.41
3:2:290:U:H5'	3:2:291:G:OP2	2.20	0.41
3:2:957:A:C6	3:2:958:G:C5	3.08	0.41
3:2:1445:U:HO2'	3:2:1446:A:P	2.44	0.41
3:2:1516:G:P	20:P:81:ARG:HD3	2.60	0.41
7:C:65:LYS:HA	7:C:68:ARG:HH12	1.84	0.41
9:E:86:PHE:HE1	9:E:102:ILE:HG23	1.85	0.41
19:O:94:HIS:ND1	19:O:127:GLY:HA3	2.36	0.41
38:h:19:LYS:HA	38:h:19:LYS:HD3	1.85	0.41
1:0:450:HIS:ND1	1:0:450:HIS:N	2.68	0.41
3:2:78:C:O2'	11:G:175:LYS:HB2	2.20	0.41
3:2:477:G:H2'	3:2:478:G:H8	1.85	0.41
3:2:673:G:H2'	3:2:674:C:C6	2.55	0.41
3:2:1218:C:O2'	33:c:24:GLN:HG2	2.21	0.41
3:2:1275:G:H4'	3:2:1322:G:H22	1.86	0.41
3:2:1463:U:H4'	3:2:1464:C:H5'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1587:G:H1	24:T:67:ARG:CG	2.33	0.41
5:A:123:VAL:HG13	5:A:145:ILE:HB	2.02	0.41
6:B:129:THR:HG22	6:B:176:VAL:HG13	2.02	0.41
11:G:201:LYS:HG2	11:G:202:ASN:N	2.34	0.41
20:P:18:ARG:HA	23:S:93:GLY:HA3	2.01	0.41
37:g:213:ASP:OD1	37:g:213:ASP:N	2.52	0.41
3:2:164:A:H3'	3:2:165:G:N2	2.35	0.41
3:2:189:U:H5'	3:2:190:G:OP2	2.21	0.41
3:2:210:U:H2'	3:2:211:G:C8	2.55	0.41
3:2:959:G:O2'	3:2:1065:G:H4'	2.20	0.41
3:2:1098:C:H2'	3:2:1099:G:C8	2.55	0.41
5:A:50:ASN:HA	22:R:105:MET:SD	2.60	0.41
5:A:63:ARG:HB3	26:V:37:ALA:HB3	2.03	0.41
6:B:30:TRP:HE1	19:O:18:GLY:HA2	1.85	0.41
11:G:69:THR:HG22	11:G:70:HIS:H	1.84	0.41
19:O:43:HIS:CE1	19:O:45:THR:HG22	2.55	0.41
19:O:147:ARG:NH1	19:O:150:ARG:HH12	2.17	0.41
37:g:71:ILE:H	37:g:71:ILE:HG13	1.75	0.41
3:2:84:A:O3'	29:Y:119:GLY:HA2	2.21	0.41
3:2:332:G:O2'	3:2:333:G:O5'	2.34	0.41
3:2:520:A:H5''	14:J:12:THR:OG1	2.20	0.41
3:2:946:U:H2'	3:2:947:G:H8	1.86	0.41
3:2:1037:G:H4'	3:2:1845:A:H4'	2.02	0.41
3:2:1862:G:H4'	3:2:1863:A:OP1	2.20	0.41
6:B:110:MET:HE1	6:B:213:ARG:HB2	2.03	0.41
13:I:84:ASN:HB3	13:I:87:ASN:O	2.20	0.41
18:N:87:ASP:OD1	18:N:87:ASP:N	2.31	0.41
22:R:85:VAL:HG13	22:R:86:PRO:O	2.21	0.41
32:b:56:CYS:HB3	32:b:61:THR:HB	2.02	0.41
37:g:165:ILE:HG13	37:g:177:TRP:HB2	2.03	0.41
1:0:289:THR:HG21	1:0:317:LEU:HD11	2.03	0.41
3:2:1539:U:H2'	3:2:1540:G:C8	2.55	0.41
3:2:1584:G:O4'	3:2:1586:U:O2'	2.33	0.41
3:2:1679:A:H5''	3:2:1680:G:O5'	2.21	0.41
7:C:120:GLN:H	7:C:120:GLN:HG2	1.50	0.41
11:G:186:GLN:O	11:G:189:ARG:HG3	2.21	0.41
14:J:120:ALA:HB2	14:J:129:LEU:HD12	2.02	0.41
21:Q:72:VAL:HG21	21:Q:84:ILE:HG12	2.02	0.41
21:Q:92:LEU:HD12	21:Q:92:LEU:HA	1.92	0.41
27:W:34:ILE:O	27:W:38:LEU:HG	2.20	0.41
34:d:8:TRP:CH2	34:d:12:ARG:NH1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:6:C:O2	2:1:68:G:N2	2.54	0.41
2:1:44:A:H8	2:1:44:A:OP2	2.03	0.41
3:2:77:A:H5''	3:2:77:A:H8	1.86	0.41
3:2:913:A:N3	12:H:66:VAL:HG21	2.36	0.41
3:2:1128:C:O2'	3:2:1129:G:H5'	2.20	0.41
3:2:1350:U:O2'	5:A:110:ASN:OD1	2.31	0.41
3:2:1550:G:H1	3:2:1582:C:N4	2.19	0.41
3:2:1599:U:C4	10:F:166:ILE:HG23	2.55	0.41
3:2:1657:G:H1	3:2:1667:U:H3	1.69	0.41
5:A:39:TYR:CE2	5:A:40:LYS:HG2	2.56	0.41
5:A:41:ARG:HB2	5:A:47:TYR:CE1	2.56	0.41
7:C:61:MET:HA	7:C:62:PRO:HD2	1.98	0.41
7:C:139:LEU:HD21	7:C:237:ALA:HB1	2.03	0.41
9:E:19:MET:SD	9:E:108:ARG:HD2	2.61	0.41
9:E:170:THR:OG1	9:E:171:ASP:N	2.54	0.41
9:E:182:MET:HE2	9:E:192:ILE:HD11	2.02	0.41
10:F:141:VAL:HG12	10:F:142:SER:O	2.21	0.41
12:H:113:LYS:HD3	12:H:113:LYS:HA	1.90	0.41
14:J:18:ARG:HA	14:J:19:PRO:HD3	1.83	0.41
17:M:31:LEU:HD23	17:M:31:LEU:HA	1.96	0.41
18:N:100:LYS:HE2	18:N:104:ARG:HH22	1.86	0.41
27:W:103:VAL:HG12	27:W:126:LEU:HB2	2.02	0.41
28:X:13:LEU:HD23	28:X:13:LEU:HA	1.91	0.41
28:X:37:LYS:HB3	28:X:37:LYS:HE2	1.62	0.41
36:f:135:HIS:HB2	36:f:138:ARG:CG	2.50	0.41
1:0:82:THR:HG22	1:0:176:LEU:HD21	2.02	0.41
3:2:316:G:P	11:G:183:ARG:HH11	2.44	0.41
6:B:107:ARG:NH2	19:O:133:THR:O	2.53	0.41
7:C:77:SER:O	7:C:80:GLU:HG2	2.21	0.41
9:E:125:LYS:HB2	9:E:226:PHE:CE2	2.56	0.41
29:Y:6:THR:O	29:Y:27:VAL:HA	2.22	0.41
35:e:54:GLY:H	35:e:57:ALA:HB2	1.85	0.41
1:0:566:LEU:HA	1:0:567:PRO:HD3	1.95	0.40
3:2:65:C:H4'	11:G:172:LYS:HD3	2.03	0.40
3:2:447:A:C6	3:2:449:A:C6	3.10	0.40
3:2:547:G:H1'	3:2:548:C:OP2	2.22	0.40
3:2:1224:G:H2'	3:2:1225:U:C6	2.56	0.40
3:2:1414:A:N6	3:2:1425:G:O6	2.54	0.40
3:2:1788:A:H2'	3:2:1789:G:O4'	2.21	0.40
4:3:142:A:H2'	4:3:143:G:C8	2.56	0.40
6:B:179:ASN:HB3	6:B:183:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:85:ARG:HE	11:G:87:ARG:NH1	2.18	0.40
13:I:39:GLY:O	13:I:61:ASP:HB2	2.21	0.40
20:P:97:TYR:CE2	20:P:99:GLY:HA2	2.56	0.40
22:R:43:SER:HB3	22:R:44:LYS:H	1.59	0.40
31:a:31:PRO:HG2	31:a:34:LYS:HB3	2.03	0.40
31:a:87:ARG:HE	31:a:92:ARG:HA	1.86	0.40
35:e:32:ALA:O	35:e:35:ARG:HB3	2.20	0.40
1:0:277:LYS:O	1:0:283:ALA:HA	2.21	0.40
2:1:6:C:N4	2:1:7:G:O6	2.55	0.40
2:1:42:U:H2'	2:1:43:G:H5''	2.02	0.40
3:2:438:G:H5''	3:2:438:G:N3	2.36	0.40
3:2:474:G:H2'	3:2:474:G:N3	2.37	0.40
3:2:798:G:H3'	3:2:799:U:C5'	2.50	0.40
3:2:900:C:H2'	3:2:901:G:C8	2.56	0.40
3:2:921:G:OP1	32:b:26:GLN:NE2	2.54	0.40
3:2:1211:G:N2	3:2:1689:C:C2	2.90	0.40
3:2:1253:A:H1'	3:2:1254:C:OP2	2.21	0.40
3:2:1710:C:H42	3:2:1823:A:N6	2.19	0.40
11:G:48:TYR:OH	11:G:116:LYS:HG3	2.21	0.40
14:J:109:ARG:HH21	14:J:146:SER:HG	1.65	0.40
21:Q:43:GLU:HB2	21:Q:44:PRO:HD3	2.04	0.40
29:Y:104:ARG:NH2	29:Y:108:LYS:HE2	2.36	0.40
3:2:217:A:H5'	3:2:218:U:OP2	2.21	0.40
3:2:482:G:N1	3:2:485:A:OP2	2.53	0.40
5:A:68:ILE:HD12	5:A:74:VAL:HG22	2.03	0.40
5:A:120:ARG:HH11	5:A:120:ARG:HG2	1.85	0.40
6:B:131:ASP:OD2	6:B:180:ASP:HB2	2.22	0.40
6:B:188:LEU:HD23	6:B:188:LEU:HA	1.94	0.40
7:C:205:VAL:O	7:C:224:THR:HB	2.20	0.40
11:G:168:LYS:HA	11:G:169:PRO:HD3	1.89	0.40
16:L:82:MET:HB3	16:L:85:THR:HG23	2.03	0.40
26:V:55:ILE:HD11	26:V:69:ILE:HG12	2.01	0.40
29:Y:60:PHE:HA	29:Y:70:THR:O	2.21	0.40
32:b:51:GLN:H	32:b:51:GLN:HG3	1.73	0.40
1:0:290:SER:OG	1:0:291:THR:N	2.53	0.40
3:2:808:A:HO2'	3:2:809:A:P	2.43	0.40
3:2:841:G:H2'	3:2:842:C:H6	1.86	0.40
3:2:1125:C:H4'	22:R:128:PHE:HZ	1.86	0.40
3:2:1714:U:H2'	3:2:1715:A:C8	2.56	0.40
3:2:1835:A:H1'	3:2:1836:G:OP1	2.21	0.40
7:C:254:ASP:HB3	26:V:1:MET:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:43:GLU:O	11:G:46:LYS:HG3	2.21	0.40
17:M:54:SER:OG	17:M:78:LYS:HB3	2.22	0.40
21:Q:103:ALA:HB2	37:g:54:ILE:HG21	2.03	0.40
3:2:413:G:C6	3:2:425:G:C2	3.10	0.40
3:2:988:C:OP2	31:a:70:LYS:HE3	2.22	0.40
3:2:1330:G:N7	3:2:1493:C:OP2	2.55	0.40
3:2:1587:G:N2	24:T:67:ARG:NH1	2.70	0.40
3:2:1597:C:H4'	3:2:1603:G:C6	2.56	0.40
3:2:1606:G:N2	3:2:1633:A:OP2	2.41	0.40
5:A:71:PRO:HB2	5:A:95:GLY:O	2.21	0.40
10:F:39:ILE:HG23	10:F:68:ILE:HD12	2.04	0.40
10:F:76:MET:HE2	10:F:76:MET:HB2	1.96	0.40
14:J:66:LYS:HD3	14:J:66:LYS:HA	1.85	0.40
31:a:28:ARG:CG	31:a:28:ARG:HH11	2.35	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	0	473/584 (81%)	451 (95%)	20 (4%)	2 (0%)	30	66
5	A	214/295 (72%)	202 (94%)	11 (5%)	1 (0%)	24	62
6	B	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
7	C	216/293 (74%)	215 (100%)	1 (0%)	0	100	100
8	D	223/243 (92%)	214 (96%)	8 (4%)	1 (0%)	30	66
9	E	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
10	F	187/204 (92%)	172 (92%)	13 (7%)	2 (1%)	11	45
11	G	228/249 (92%)	218 (96%)	10 (4%)	0	100	100
12	H	184/194 (95%)	174 (95%)	9 (5%)	1 (0%)	24	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	203/208 (98%)	196 (97%)	7 (3%)	0	100	100
14	J	178/194 (92%)	173 (97%)	4 (2%)	1 (1%)	21	58
15	K	93/165 (56%)	89 (96%)	4 (4%)	0	100	100
16	L	149/158 (94%)	145 (97%)	4 (3%)	0	100	100
17	M	121/132 (92%)	111 (92%)	10 (8%)	0	100	100
18	N	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
19	O	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
20	P	118/145 (81%)	117 (99%)	1 (1%)	0	100	100
21	Q	137/146 (94%)	131 (96%)	6 (4%)	0	100	100
22	R	128/135 (95%)	121 (94%)	7 (6%)	0	100	100
23	S	141/152 (93%)	136 (96%)	5 (4%)	0	100	100
24	T	142/145 (98%)	137 (96%)	4 (3%)	1 (1%)	18	54
25	U	99/119 (83%)	94 (95%)	5 (5%)	0	100	100
26	V	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
27	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
28	X	139/143 (97%)	131 (94%)	7 (5%)	1 (1%)	18	54
29	Y	122/130 (94%)	118 (97%)	4 (3%)	0	100	100
30	Z	70/125 (56%)	65 (93%)	5 (7%)	0	100	100
31	a	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
32	b	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
33	c	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
34	d	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
35	e	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
36	f	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
37	g	312/315 (99%)	295 (95%)	16 (5%)	1 (0%)	36	71
38	h	22/24 (92%)	22 (100%)	0	0	100	100
All	All	5272/5967 (88%)	5046 (96%)	215 (4%)	11 (0%)	44	77

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	189	ILE
12	H	170	VAL

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Mol	Chain	Res	Type
14	J	161	LEU
28	X	108	LYS
37	g	145	GLU
1	0	278	CYS
10	F	163	PHE
1	0	76	GLU
24	T	4	VAL
10	F	166	ILE
8	D	193	ASP

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	0	417/511 (82%)	402 (96%)	15 (4%)	31	52
5	A	180/243 (74%)	155 (86%)	25 (14%)	3	16
6	B	194/231 (84%)	173 (89%)	21 (11%)	6	22
7	C	184/225 (82%)	148 (80%)	36 (20%)	1	9
8	D	189/202 (94%)	180 (95%)	9 (5%)	23	45
9	E	224/225 (100%)	195 (87%)	29 (13%)	4	18
10	F	159/170 (94%)	149 (94%)	10 (6%)	16	39
11	G	200/218 (92%)	186 (93%)	14 (7%)	14	37
12	H	167/174 (96%)	153 (92%)	14 (8%)	10	31
13	I	176/180 (98%)	155 (88%)	21 (12%)	5	20
14	J	160/168 (95%)	138 (86%)	22 (14%)	3	16
15	K	86/136 (63%)	84 (98%)	2 (2%)	44	64
16	L	135/142 (95%)	107 (79%)	28 (21%)	1	7
17	M	104/108 (96%)	95 (91%)	9 (9%)	9	30
18	N	130/131 (99%)	116 (89%)	14 (11%)	6	22
19	O	105/119 (88%)	95 (90%)	10 (10%)	8	26
20	P	107/130 (82%)	104 (97%)	3 (3%)	38	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	Q	115/121 (95%)	107 (93%)	8 (7%)	14	37
22	R	119/122 (98%)	105 (88%)	14 (12%)	5	20
23	S	124/132 (94%)	119 (96%)	5 (4%)	28	49
24	T	114/115 (99%)	107 (94%)	7 (6%)	17	40
25	U	93/107 (87%)	90 (97%)	3 (3%)	34	56
26	V	66/67 (98%)	54 (82%)	12 (18%)	2	11
27	W	112/113 (99%)	93 (83%)	19 (17%)	2	12
28	X	113/115 (98%)	105 (93%)	8 (7%)	13	36
29	Y	108/112 (96%)	97 (90%)	11 (10%)	7	24
30	Z	64/103 (62%)	59 (92%)	5 (8%)	11	33
31	a	88/88 (100%)	73 (83%)	15 (17%)	2	12
32	b	74/74 (100%)	64 (86%)	10 (14%)	4	17
33	c	54/54 (100%)	51 (94%)	3 (6%)	19	42
34	d	48/48 (100%)	45 (94%)	3 (6%)	16	39
35	e	45/45 (100%)	39 (87%)	6 (13%)	4	17
36	f	65/65 (100%)	63 (97%)	2 (3%)	35	56
37	g	272/273 (100%)	250 (92%)	22 (8%)	11	32
38	h	23/23 (100%)	21 (91%)	2 (9%)	9	30
All	All	4614/5090 (91%)	4177 (90%)	437 (10%)	10	26

All (437) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	38	VAL
1	0	50	ILE
1	0	99	TRP
1	0	100	PRO
1	0	102	VAL
1	0	117	LEU
1	0	121	PRO
1	0	127	VAL
1	0	137	LEU
1	0	309	ILE
1	0	317	LEU
1	0	339	VAL
1	0	343	VAL

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Mol	Chain	Res	Type
1	0	423	ASP
1	0	450	HIS
5	A	5	LEU
5	A	14	ASP
5	A	38	ILE
5	A	53	ARG
5	A	60	LEU
5	A	78	SER
5	A	80	ARG
5	A	94	THR
5	A	111	GLN
5	A	120	ARG
5	A	130	ASP
5	A	131	HIS
5	A	136	GLU
5	A	140	VAL
5	A	145	ILE
5	A	154	LEU
5	A	157	VAL
5	A	159	ILE
5	A	178	LEU
5	A	180	ARG
5	A	185	MET
5	A	188	THR
5	A	189	ILE
5	A	192	GLU
5	A	200	ASP
6	B	25	PHE
6	B	33	VAL
6	B	38	MET
6	B	57	ILE
6	B	76	ASN
6	B	77	ASP
6	B	79	VAL
6	B	88	THR
6	B	95	ASN
6	B	98	THR
6	B	106	THR
6	B	107	ARG
6	B	125	VAL
6	B	131	ASP
6	B	146	ARG

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Mol	Chain	Res	Type
6	B	147	ASN
6	B	169	MET
6	B	210	VAL
6	B	212	VAL
6	B	213	ARG
6	B	217	MET
7	C	68	ARG
7	C	73	MET
7	C	80	GLU
7	C	83	LEU
7	C	94	ILE
7	C	98	LEU
7	C	101	SER
7	C	112	VAL
7	C	120	GLN
7	C	123	ARG
7	C	132	ASP
7	C	134	ASN
7	C	137	VAL
7	C	143	CYS
7	C	147	VAL
7	C	156	ILE
7	C	157	LEU
7	C	160	LEU
7	C	165	VAL
7	C	167	ARG
7	C	180	VAL
7	C	192	LEU
7	C	196	ILE
7	C	204	ILE
7	C	212	LYS
7	C	213	LEU
7	C	215	MET
7	C	221	ASP
7	C	227	ARG
7	C	232	THR
7	C	242	ASP
7	C	244	ILE
7	C	252	THR
7	C	255	LEU
7	C	271	ASP
7	C	276	THR

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Mol	Chain	Res	Type
8	D	3	VAL
8	D	54	ARG
8	D	70	THR
8	D	103	GLU
8	D	123	LEU
8	D	176	LEU
8	D	195	THR
8	D	198	ILE
8	D	206	ASP
9	E	3	ARG
9	E	12	VAL
9	E	19	MET
9	E	23	LEU
9	E	37	LYS
9	E	38	LEU
9	E	39	ARG
9	E	42	LEU
9	E	45	ILE
9	E	46	ILE
9	E	49	ARG
9	E	51	ARG
9	E	59	ASP
9	E	95	THR
9	E	102	ILE
9	E	113	ARG
9	E	114	ILE
9	E	140	VAL
9	E	145	ARG
9	E	151	ASP
9	E	156	VAL
9	E	160	ILE
9	E	171	ASP
9	E	181	CYS
9	E	189	LEU
9	E	197	ASN
9	E	198	ARG
9	E	238	LEU
9	E	240	ARG
10	F	68	ILE
10	F	78	MET
10	F	82	ASN
10	F	91	ARG

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Mol	Chain	Res	Type
10	F	122	ARG
10	F	130	ARG
10	F	140	ASP
10	F	166	ILE
10	F	176	GLU
10	F	204	ARG
11	G	16	ILE
11	G	50	VAL
11	G	51	ARG
11	G	57	ASP
11	G	67	VAL
11	G	69	THR
11	G	91	GLU
11	G	92	ARG
11	G	110	ASN
11	G	144	LEU
11	G	151	ASP
11	G	158	VAL
11	G	181	THR
11	G	185	LEU
12	H	12	ASN
12	H	46	THR
12	H	51	ILE
12	H	64	VAL
12	H	75	ILE
12	H	84	GLU
12	H	87	PHE
12	H	105	THR
12	H	121	THR
12	H	122	LEU
12	H	134	VAL
12	H	180	LEU
12	H	184	ASP
12	H	188	GLU
13	I	5	ARG
13	I	17	LYS
13	I	18	ARG
13	I	22	HIS
13	I	29	LEU
13	I	35	ASN
13	I	47	ARG
13	I	62	VAL

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Mol	Chain	Res	Type
13	I	72	CYS
13	I	76	THR
13	I	82	VAL
13	I	95	THR
13	I	121	LEU
13	I	130	THR
13	I	170	LYS
13	I	175	ILE
13	I	177	SER
13	I	178	ARG
13	I	184	ARG
13	I	191	GLU
13	I	194	GLU
14	J	3	VAL
14	J	8	VAL
14	J	12	THR
14	J	21	GLU
14	J	29	LEU
14	J	42	GLU
14	J	50	LEU
14	J	88	ASP
14	J	94	LEU
14	J	100	LEU
14	J	102	ILE
14	J	104	ASP
14	J	108	ARG
14	J	117	LEU
14	J	128	VAL
14	J	132	GLN
14	J	136	ARG
14	J	138	ARG
14	J	150	ARG
14	J	153	SER
14	J	156	HIS
14	J	161	LEU
15	K	46	MET
15	K	52	LEU
16	L	3	ASP
16	L	5	GLN
16	L	6	THR
16	L	13	GLN
16	L	15	THR

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Mol	Chain	Res	Type
16	L	23	VAL
16	L	35	ARG
16	L	40	ILE
16	L	42	LEU
16	L	45	LYS
16	L	46	THR
16	L	49	GLU
16	L	52	GLU
16	L	69	ARG
16	L	71	ARG
16	L	74	SER
16	L	76	VAL
16	L	78	THR
16	L	80	MET
16	L	83	GLN
16	L	85	THR
16	L	101	ARG
16	L	119	ASP
16	L	121	GLN
16	L	126	VAL
16	L	132	ARG
16	L	144	LYS
16	L	146	THR
17	M	21	VAL
17	M	26	LEU
17	M	35	ILE
17	M	36	ARG
17	M	45	ARG
17	M	65	VAL
17	M	79	VAL
17	M	89	VAL
17	M	104	VAL
18	N	12	SER
18	N	14	SER
18	N	29	THR
18	N	71	ILE
18	N	75	LEU
18	N	80	LEU
18	N	83	ASP
18	N	84	LEU
18	N	86	GLU
18	N	87	ASP

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Mol	Chain	Res	Type
18	N	92	ILE
18	N	101	HIS
18	N	125	LEU
18	N	145	THR
19	O	52	THR
19	O	98	ARG
19	O	100	THR
19	O	103	ASN
19	O	104	ARG
19	O	105	THR
19	O	133	THR
19	O	142	ARG
19	O	146	ARG
19	O	150	ARG
20	P	51	ARG
20	P	75	VAL
20	P	122	THR
21	Q	10	VAL
21	Q	18	THR
21	Q	43	GLU
21	Q	46	THR
21	Q	100	VAL
21	Q	121	VAL
21	Q	130	LYS
21	Q	131	LYS
22	R	8	THR
22	R	17	ILE
22	R	34	VAL
22	R	35	CYS
22	R	41	ILE
22	R	83	ASN
22	R	85	VAL
22	R	98	VAL
22	R	101	ASP
22	R	119	VAL
22	R	124	VAL
22	R	127	ASN
22	R	128	PHE
22	R	132	ARG
23	S	4	VAL
23	S	14	ARG
23	S	71	MET

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Mol	Chain	Res	Type
23	S	129	LEU
23	S	138	THR
24	T	34	VAL
24	T	36	THR
24	T	56	ARG
24	T	63	HIS
24	T	67	ARG
24	T	87	VAL
24	T	131	LEU
25	U	36	CYS
25	U	68	THR
25	U	107	GLU
26	V	1	MET
26	V	4	ASP
26	V	9	VAL
26	V	15	ARG
26	V	21	ASN
26	V	43	THR
26	V	59	ILE
26	V	62	MET
26	V	67	ASP
26	V	69	ILE
26	V	70	LEU
26	V	76	ASP
27	W	4	MET
27	W	14	ILE
27	W	23	ARG
27	W	25	VAL
27	W	27	ILE
27	W	40	VAL
27	W	42	MET
27	W	47	ILE
27	W	49	GLU
27	W	56	HIS
27	W	57	ARG
27	W	80	ASP
27	W	83	LEU
27	W	85	ASP
27	W	104	LEU
27	W	105	THR
27	W	106	THR
27	W	112	ASP

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Mol	Chain	Res	Type
27	W	125	ILE
28	X	3	LYS
28	X	5	ARG
28	X	37	LYS
28	X	69	CYS
28	X	77	ASN
28	X	100	VAL
28	X	105	PHE
28	X	107	ARG
29	Y	5	VAL
29	Y	14	THR
29	Y	17	LEU
29	Y	23	MET
29	Y	42	GLU
29	Y	54	VAL
29	Y	79	LEU
29	Y	107	ARG
29	Y	108	LYS
29	Y	117	VAL
29	Y	118	ARG
30	Z	47	LEU
30	Z	65	TYR
30	Z	88	LEU
30	Z	90	GLU
30	Z	107	VAL
31	a	2	THR
31	a	6	ARG
31	a	7	ASN
31	a	17	HIS
31	a	18	VAL
31	a	26	CYS
31	a	28	ARG
31	a	29	CYS
31	a	30	VAL
31	a	45	VAL
31	a	53	ILE
31	a	58	VAL
31	a	64	LEU
31	a	75	VAL
31	a	84	VAL
32	b	13	GLU
32	b	17	ARG

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Mol	Chain	Res	Type
32	b	20	LYS
32	b	34	ASP
32	b	43	ILE
32	b	49	HIS
32	b	53	VAL
32	b	54	VAL
32	b	63	LEU
32	b	67	THR
33	c	26	GLN
33	c	37	ASP
33	c	55	VAL
34	d	10	HIS
34	d	28	HIS
34	d	40	ARG
35	e	8	ARG
35	e	28	LYS
35	e	29	THR
35	e	34	ARG
35	e	45	VAL
35	e	58	ASN
36	f	86	THR
36	f	98	VAL
37	g	31	ILE
37	g	41	ILE
37	g	46	THR
37	g	64	HIS
37	g	71	ILE
37	g	74	ASP
37	g	96	THR
37	g	97	THR
37	g	102	VAL
37	g	118	ARG
37	g	142	VAL
37	g	178	ASN
37	g	186	THR
37	g	195	LEU
37	g	198	VAL
37	g	207	CYS
37	g	249	CYS
37	g	272	GLN
37	g	274	VAL
37	g	297	THR

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Mol	Chain	Res	Type
37	g	306	LEU
37	g	309	VAL
38	h	9	ARG
38	h	14	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	11	ASN
1	0	37	GLN
1	0	69	ASN
1	0	175	HIS
1	0	535	ASN
1	0	549	GLN
1	0	570	HIS
5	A	36	GLN
5	A	111	GLN
6	B	147	ASN
7	C	178	HIS
8	D	56	GLN
8	D	101	GLN
8	D	174	HIS
8	D	226	GLN
9	E	50	ASN
9	E	138	HIS
9	E	142	HIS
9	E	161	GLN
9	E	179	ASN
10	F	110	GLN
10	F	137	GLN
10	F	203	ASN
11	G	56	ASN
11	G	59	GLN
11	G	65	GLN
11	G	186	GLN
12	H	76	GLN
12	H	97	GLN
12	H	112	ASN
12	H	114	GLN
12	H	126	HIS
13	I	35	ASN
13	I	84	ASN

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Mol	Chain	Res	Type
13	I	87	ASN
13	I	116	HIS
13	I	138	ASN
13	I	168	GLN
14	J	125	HIS
15	K	39	ASN
15	K	61	GLN
16	L	11	GLN
16	L	83	GLN
16	L	94	HIS
16	L	100	ASN
18	N	62	GLN
18	N	101	HIS
18	N	105	ASN
19	O	43	HIS
20	P	53	GLN
20	P	114	HIS
21	Q	24	HIS
21	Q	77	HIS
21	Q	142	GLN
22	R	74	GLN
22	R	83	ASN
23	S	72	GLN
23	S	87	GLN
23	S	97	GLN
23	S	101	ASN
27	W	15	ASN
27	W	56	HIS
27	W	64	ASN
27	W	91	ASN
28	X	31	HIS
29	Y	15	ASN
29	Y	63	HIS
29	Y	94	HIS
29	Y	124	ASN
33	c	29	GLN
34	d	5	GLN
35	e	37	GLN
36	f	93	HIS
36	f	111	ASN
37	g	20	GLN
37	g	51	ASN

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Mol	Chain	Res	Type
37	g	64	HIS
37	g	143	GLN
37	g	147	HIS
37	g	159	ASN
37	g	178	ASN
37	g	215	GLN
37	g	226	HIS
37	g	305	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1	74/75 (98%)	47 (63%)	4 (5%)
3	2	1652/1868 (88%)	558 (33%)	62 (3%)
4	3	183/275 (66%)	98 (53%)	18 (9%)
All	All	1909/2218 (86%)	703 (36%)	84 (4%)

All (703) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	1	4	G
2	1	6	C
2	1	7	G
2	1	8	U
2	1	9	G
2	1	10	G
2	1	11	C
2	1	13	C
2	1	14	A
2	1	16	U
2	1	18	G
2	1	19	G
2	1	20	A
2	1	21	A
2	1	22	G
2	1	25	C
2	1	26	G
2	1	30	G
2	1	38	A
2	1	40	C
2	1	41	C

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Mol	Chain	Res	Type
2	1	43	G
2	1	46	G
2	1	47	U
2	1	48	C
2	1	49	C
2	1	50	U
2	1	52	G
2	1	53	G
2	1	54	A
2	1	56	C
2	1	57	G
2	1	58	A
2	1	59	A
2	1	60	A
2	1	61	C
2	1	62	C
2	1	63	G
2	1	64	A
2	1	65	G
2	1	67	G
2	1	68	G
2	1	70	G
2	1	72	U
2	1	73	A
2	1	75	C
2	1	76	A
3	2	3	C
3	2	4	C
3	2	5	U
3	2	9	U
3	2	17	C
3	2	23	G
3	2	25	A
3	2	26	U
3	2	33	G
3	2	41	G
3	2	44	U
3	2	46	A
3	2	49	C
3	2	56	G
3	2	58	C
3	2	60	A

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Mol	Chain	Res	Type
3	2	61	A
3	2	65	C
3	2	66	G
3	2	67	C
3	2	68	A
3	2	70	G
3	2	71	G
3	2	72	C
3	2	75	G
3	2	76	U
3	2	77	A
3	2	78	C
3	2	79	A
3	2	81	U
3	2	103	A
3	2	110	U
3	2	111	A
3	2	113	G
3	2	114	G
3	2	115	U
3	2	116	U
3	2	123	G
3	2	124	U
3	2	126	G
3	2	127	C
3	2	129	C
3	2	130	G
3	2	141	A
3	2	142	C
3	2	143	U
3	2	144	U
3	2	153	G
3	2	154	U
3	2	155	G
3	2	163	U
3	2	167	G
3	2	168	C
3	2	169	U
3	2	170	A
3	2	172	U
3	2	175	A
3	2	181	A

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Mol	Chain	Res	Type
3	2	182	C
3	2	184	G
3	2	188	C
3	2	189	U
3	2	190	G
3	2	191	A
3	2	200	G
3	2	206	G
3	2	209	A
3	2	210	U
3	2	213	G
3	2	214	U
3	2	215	G
3	2	216	C
3	2	217	A
3	2	290	U
3	2	291	G
3	2	292	A
3	2	294	U
3	2	295	C
3	2	302	A
3	2	307	G
3	2	308	G
3	2	310	C
3	2	311	C
3	2	312	G
3	2	315	C
3	2	317	C
3	2	319	C
3	2	320	G
3	2	321	C
3	2	332	G
3	2	333	G
3	2	334	C
3	2	335	G
3	2	337	C
3	2	338	G
3	2	342	C
3	2	347	G
3	2	351	G
3	2	360	A
3	2	362	C

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Mol	Chain	Res	Type
3	2	364	A
3	2	368	U
3	2	369	C
3	2	370	G
3	2	377	G
3	2	382	C
3	2	383	G
3	2	385	G
3	2	386	C
3	2	398	A
3	2	400	C
3	2	407	G
3	2	408	A
3	2	409	C
3	2	417	C
3	2	418	A
3	2	421	G
3	2	425	G
3	2	438	G
3	2	441	C
3	2	442	C
3	2	447	A
3	2	448	A
3	2	449	A
3	2	450	C
3	2	464	A
3	2	465	A
3	2	466	G
3	2	471	G
3	2	472	C
3	2	473	A
3	2	474	G
3	2	476	A
3	2	482	G
3	2	487	U
3	2	489	A
3	2	492	C
3	2	496	C
3	2	500	A
3	2	502	C
3	2	508	A
3	2	509	G

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Mol	Chain	Res	Type
3	2	517	C
3	2	523	A
3	2	530	U
3	2	531	A
3	2	532	C
3	2	534	G
3	2	535	G
3	2	536	A
3	2	542	U
3	2	544	G
3	2	546	G
3	2	548	C
3	2	550	C
3	2	552	G
3	2	554	A
3	2	555	A
3	2	556	U
3	2	559	G
3	2	560	A
3	2	562	U
3	2	564	A
3	2	568	C
3	2	576	A
3	2	583	A
3	2	585	C
3	2	587	A
3	2	588	G
3	2	589	G
3	2	590	A
3	2	591	U
3	2	593	C
3	2	595	U
3	2	596	U
3	2	603	C
3	2	604	A
3	2	605	A
3	2	606	G
3	2	607	U
3	2	608	C
3	2	614	C
3	2	615	C
3	2	617	G

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Mol	Chain	Res	Type
3	2	618	C
3	2	621	C
3	2	627	U
3	2	628	A
3	2	629	A
3	2	631	U
3	2	637	U
3	2	638	C
3	2	639	C
3	2	640	A
3	2	643	A
3	2	644	G
3	2	654	A
3	2	660	C
3	2	664	A
3	2	668	A
3	2	669	A
3	2	671	A
3	2	672	A
3	2	673	G
3	2	683	G
3	2	684	G
3	2	685	A
3	2	686	U
3	2	687	C
3	2	688	U
3	2	748	C
3	2	749	U
3	2	750	C
3	2	751	G
3	2	792	C
3	2	793	G
3	2	794	A
3	2	796	G
3	2	797	C
3	2	798	G
3	2	799	U
3	2	809	A
3	2	810	A
3	2	811	A
3	2	812	A
3	2	818	A

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Mol	Chain	Res	Type
3	2	821	G
3	2	822	U
3	2	823	U
3	2	824	C
3	2	830	A
3	2	833	C
3	2	834	C
3	2	842	C
3	2	843	C
3	2	847	A
3	2	859	G
3	2	869	A
3	2	870	A
3	2	871	U
3	2	872	A
3	2	873	G
3	2	877	C
3	2	878	G
3	2	880	G
3	2	881	G
3	2	882	U
3	2	887	U
3	2	888	U
3	2	890	U
3	2	898	U
3	2	903	A
3	2	909	G
3	2	913	A
3	2	914	U
3	2	918	U
3	2	919	A
3	2	920	A
3	2	922	A
3	2	926	A
3	2	931	C
3	2	933	G
3	2	934	G
3	2	935	G
3	2	938	A
3	2	943	U
3	2	954	U
3	2	959	G

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Mol	Chain	Res	Type
3	2	961	G
3	2	968	U
3	2	969	U
3	2	970	G
3	2	971	G
3	2	978	G
3	2	980	A
3	2	981	A
3	2	983	A
3	2	990	A
3	2	992	A
3	2	999	G
3	2	1001	A
3	2	1008	A
3	2	1009	A
3	2	1017	U
3	2	1023	A
3	2	1030	A
3	2	1040	G
3	2	1041	G
3	2	1042	A
3	2	1044	G
3	2	1045	U
3	2	1049	A
3	2	1054	G
3	2	1060	A
3	2	1061	U
3	2	1067	C
3	2	1083	A
3	2	1085	C
3	2	1087	A
3	2	1088	U
3	2	1096	G
3	2	1099	G
3	2	1100	A
3	2	1111	U
3	2	1112	U
3	2	1114	U
3	2	1116	C
3	2	1119	A
3	2	1121	G
3	2	1122	A

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Mol	Chain	Res	Type
3	2	1123	C
3	2	1130	G
3	2	1131	G
3	2	1133	A
3	2	1137	U
3	2	1138	C
3	2	1139	C
3	2	1143	A
3	2	1148	A
3	2	1150	A
3	2	1153	C
3	2	1154	U
3	2	1157	G
3	2	1171	G
3	2	1195	A
3	2	1207	G
3	2	1208	A
3	2	1209	A
3	2	1211	G
3	2	1213	C
3	2	1215	C
3	2	1217	A
3	2	1221	G
3	2	1224	G
3	2	1227	G
3	2	1232	U
3	2	1235	G
3	2	1238	U
3	2	1242	U
3	2	1243	U
3	2	1248	U
3	2	1249	C
3	2	1250	A
3	2	1251	A
3	2	1253	A
3	2	1254	C
3	2	1257	G
3	2	1259	A
3	2	1260	A
3	2	1261	C
3	2	1274	G
3	2	1275	G

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Mol	Chain	Res	Type
3	2	1283	C
3	2	1284	A
3	2	1285	G
3	2	1286	G
3	2	1288	U
3	2	1298	G
3	2	1301	A
3	2	1302	G
3	2	1303	C
3	2	1308	U
3	2	1309	C
3	2	1313	A
3	2	1315	U
3	2	1317	C
3	2	1320	G
3	2	1321	G
3	2	1322	G
3	2	1330	G
3	2	1331	C
3	2	1343	U
3	2	1344	A
3	2	1348	G
3	2	1354	G
3	2	1358	U
3	2	1364	U
3	2	1371	U
3	2	1372	U
3	2	1373	C
3	2	1377	U
3	2	1378	A
3	2	1380	C
3	2	1382	A
3	2	1401	A
3	2	1404	U
3	2	1405	A
3	2	1406	G
3	2	1416	C
3	2	1426	U
3	2	1428	G
3	2	1429	G
3	2	1430	C
3	2	1431	G

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Mol	Chain	Res	Type
3	2	1432	U
3	2	1439	A
3	2	1441	U
3	2	1442	U
3	2	1444	U
3	2	1446	A
3	2	1448	A
3	2	1452	A
3	2	1454	A
3	2	1455	A
3	2	1462	U
3	2	1463	U
3	2	1464	C
3	2	1465	A
3	2	1466	G
3	2	1473	G
3	2	1474	A
3	2	1477	U
3	2	1478	U
3	2	1483	A
3	2	1486	A
3	2	1487	A
3	2	1489	A
3	2	1490	G
3	2	1491	G
3	2	1493	C
3	2	1494	U
3	2	1495	G
3	2	1499	U
3	2	1500	G
3	2	1505	U
3	2	1507	G
3	2	1508	A
3	2	1510	G
3	2	1512	C
3	2	1515	G
3	2	1516	G
3	2	1517	G
3	2	1518	C
3	2	1519	U
3	2	1520	G
3	2	1524	G

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Mol	Chain	Res	Type
3	2	1526	G
3	2	1527	C
3	2	1533	A
3	2	1535	U
3	2	1536	G
3	2	1543	U
3	2	1545	A
3	2	1548	G
3	2	1551	U
3	2	1559	C
3	2	1560	U
3	2	1561	A
3	2	1563	G
3	2	1566	G
3	2	1567	G
3	2	1568	C
3	2	1572	C
3	2	1573	G
3	2	1574	C
3	2	1579	A
3	2	1580	A
3	2	1581	C
3	2	1585	U
3	2	1586	U
3	2	1587	G
3	2	1588	A
3	2	1590	C
3	2	1598	G
3	2	1599	U
3	2	1600	G
3	2	1601	A
3	2	1602	U
3	2	1603	G
3	2	1604	G
3	2	1606	G
3	2	1610	G
3	2	1612	G
3	2	1617	G
3	2	1618	C
3	2	1621	U
3	2	1623	A
3	2	1625	U

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Mol	Chain	Res	Type
3	2	1630	A
3	2	1632	G
3	2	1634	A
3	2	1641	A
3	2	1648	G
3	2	1649	U
3	2	1650	A
3	2	1654	G
3	2	1660	C
3	2	1664	A
3	2	1665	G
3	2	1671	G
3	2	1675	A
3	2	1682	C
3	2	1688	C
3	2	1689	C
3	2	1695	A
3	2	1698	C
3	2	1699	A
3	2	1706	G
3	2	1707	U
3	2	1708	C
3	2	1709	G
3	2	1717	C
3	2	1718	G
3	2	1719	A
3	2	1720	U
3	2	1721	U
3	2	1722	G
3	2	1723	G
3	2	1724	A
3	2	1725	U
3	2	1728	U
3	2	1729	U
3	2	1733	U
3	2	1734	G
3	2	1735	A
3	2	1742	C
3	2	1744	G
3	2	1746	U
3	2	1751	C
3	2	1753	C

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Mol	Chain	Res	Type
3	2	1755	C
3	2	1756	C
3	2	1757	G
3	2	1776	G
3	2	1777	G
3	2	1781	A
3	2	1783	C
3	2	1784	G
3	2	1785	C
3	2	1807	C
3	2	1810	U
3	2	1812	U
3	2	1813	A
3	2	1814	G
3	2	1816	G
3	2	1817	G
3	2	1820	G
3	2	1824	A
3	2	1825	A
3	2	1826	G
3	2	1827	U
3	2	1835	A
3	2	1836	G
3	2	1838	U
3	2	1839	U
3	2	1849	G
3	2	1851	A
3	2	1852	C
3	2	1859	A
3	2	1860	A
3	2	1861	G
3	2	1862	G
3	2	1863	A
3	2	1864	U
3	2	1865	C
3	2	1867	U
3	2	1868	U
3	2	1869	A
4	3	41	U
4	3	42	C
4	3	43	C
4	3	44	C

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Mol	Chain	Res	Type
4	3	45	C
4	3	47	G
4	3	117	G
4	3	118	G
4	3	120	C
4	3	121	C
4	3	122	C
4	3	123	C
4	3	124	C
4	3	128	C
4	3	129	C
4	3	133	G
4	3	135	G
4	3	137	G
4	3	139	C
4	3	140	A
4	3	141	U
4	3	142	A
4	3	147	U
4	3	150	G
4	3	152	G
4	3	153	G
4	3	154	A
4	3	155	A
4	3	159	G
4	3	160	U
4	3	161	G
4	3	162	A
4	3	163	G
4	3	164	U
4	3	165	A
4	3	166	C
4	3	169	C
4	3	172	A
4	3	175	U
4	3	176	G
4	3	228	U
4	3	229	G
4	3	231	G
4	3	232	C
4	3	233	G
4	3	234	U

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Mol	Chain	Res	Type
4	3	235	G
4	3	236	C
4	3	237	C
4	3	242	C
4	3	243	A
4	3	244	A
4	3	245	G
4	3	246	A
4	3	247	C
4	3	249	G
4	3	251	U
4	3	252	A
4	3	253	G
4	3	254	C
4	3	255	C
4	3	256	G
4	3	257	A
4	3	258	G
4	3	259	U
4	3	264	U
4	3	265	U
4	3	266	G
4	3	269	U
4	3	270	C
4	3	274	A
4	3	278	G
4	3	280	C
4	3	281	U
4	3	282	U
4	3	283	G
4	3	284	U
4	3	285	G
4	3	288	A
4	3	290	U
4	3	297	U
4	3	303	G
4	3	304	C
4	3	306	U
4	3	307	G
4	3	308	C
4	3	310	A
4	3	311	G

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Mol	Chain	Res	Type
4	3	321	A
4	3	322	G
4	3	324	U
4	3	325	C
4	3	328	G
4	3	330	A
4	3	331	G
4	3	332	A
4	3	333	C
4	3	334	C

All (84) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	16	U
2	1	19	G
2	1	48	C
2	1	75	C
3	2	2	A
3	2	60	A
3	2	65	C
3	2	102	A
3	2	114	G
3	2	143	U
3	2	180	G
3	2	291	G
3	2	314	U
3	2	319	C
3	2	332	G
3	2	368	U
3	2	382	C
3	2	465	A
3	2	547	G
3	2	554	A
3	2	590	A
3	2	594	A
3	2	604	A
3	2	620	G
3	2	748	C
3	2	750	C
3	2	793	G
3	2	797	C

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Mol	Chain	Res	Type
3	2	811	A
3	2	870	A
3	2	958	G
3	2	980	A
3	2	1137	U
3	2	1231	C
3	2	1250	A
3	2	1253	A
3	2	1302	G
3	2	1308	U
3	2	1316	C
3	2	1321	G
3	2	1330	G
3	2	1342	U
3	2	1403	C
3	2	1404	U
3	2	1425	G
3	2	1428	G
3	2	1430	C
3	2	1438	A
3	2	1440	C
3	2	1445	U
3	2	1464	C
3	2	1476	A
3	2	1493	C
3	2	1494	U
3	2	1511	U
3	2	1534	C
3	2	1558	C
3	2	1585	U
3	2	1587	G
3	2	1601	A
3	2	1648	G
3	2	1649	U
3	2	1743	G
3	2	1826	G
3	2	1835	A
3	2	1838	U
4	3	116	A
4	3	123	C
4	3	136	A
4	3	160	U

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Mol	Chain	Res	Type
4	3	163	G
4	3	230	G
4	3	243	A
4	3	244	A
4	3	245	G
4	3	252	A
4	3	254	C
4	3	257	A
4	3	280	C
4	3	281	U
4	3	289	C
4	3	306	U
4	3	329	U
4	3	330	A

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 3 ligands modelled in this entry, 3 are 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	72:LYS	C	73:LEU	N	4.52

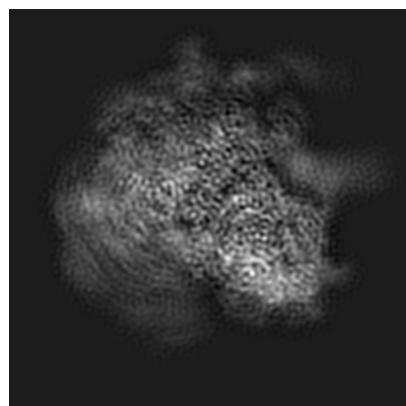
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3770. These allow visual inspection of the internal detail of the map and identification of artifacts.

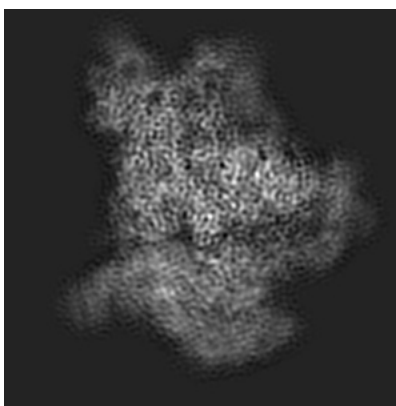
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

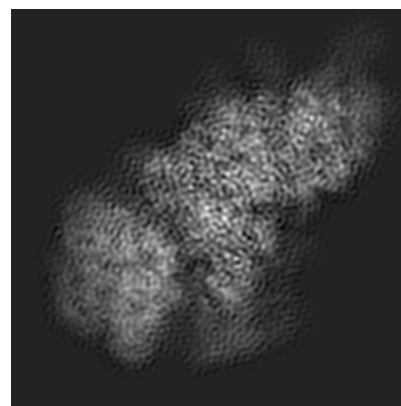
6.1.1 Primary map



X

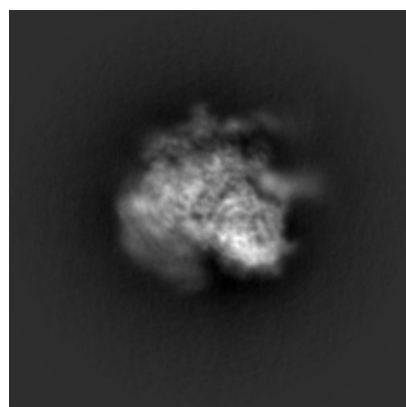


Y

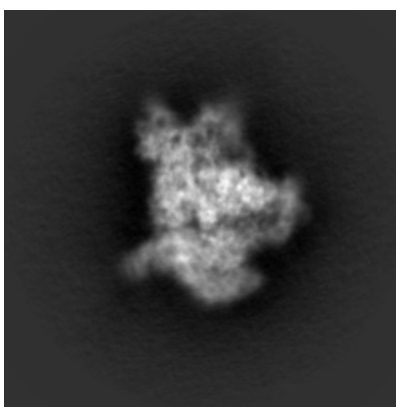


Z

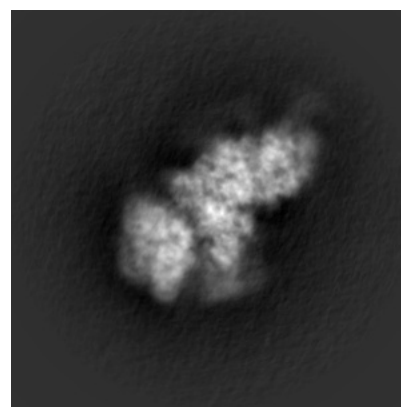
6.1.2 Raw map



X



Y

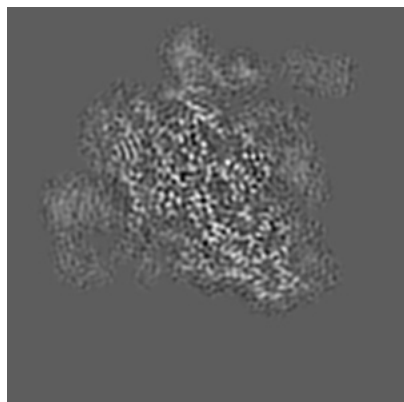


Z

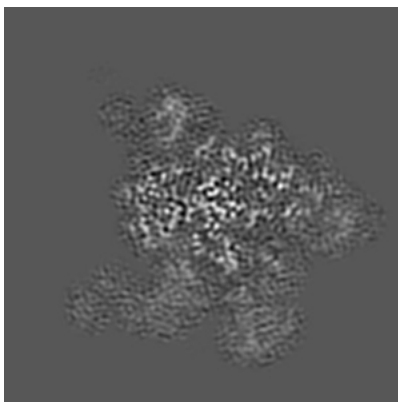
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

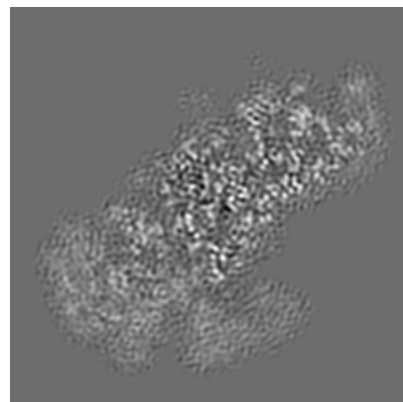
6.2.1 Primary map



X Index: 98

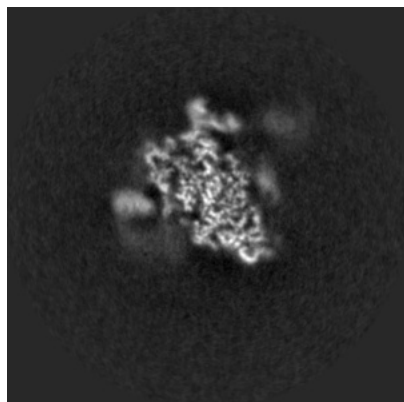


Y Index: 98

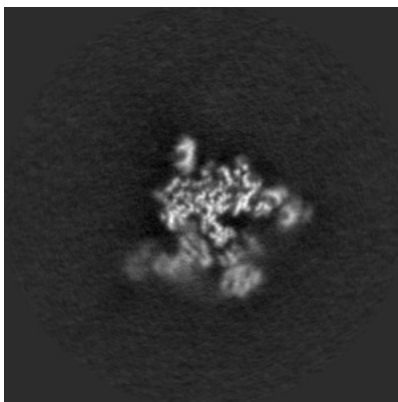


Z Index: 98

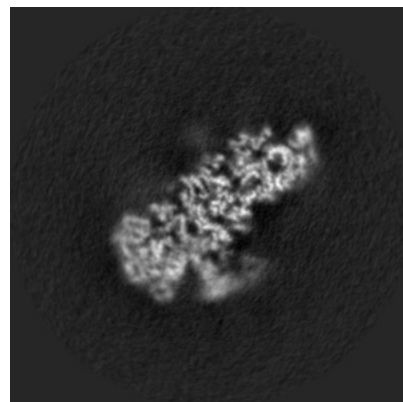
6.2.2 Raw map



X Index: 160



Y Index: 160

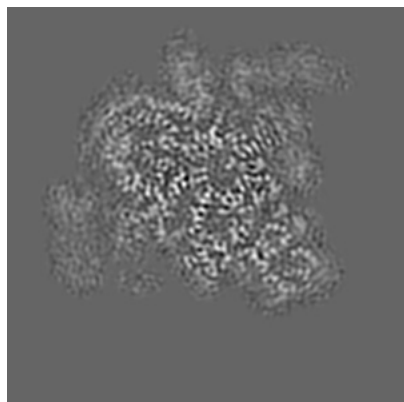


Z Index: 160

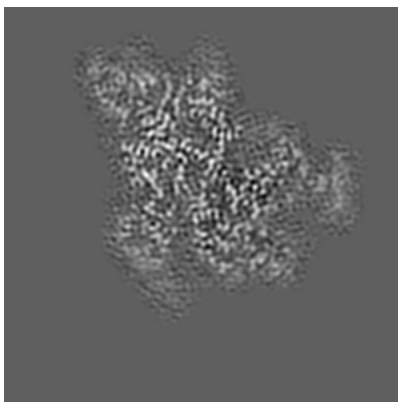
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

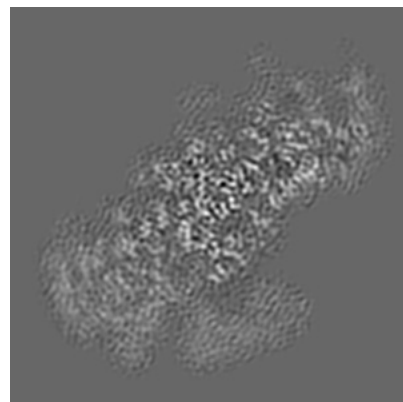
6.3.1 Primary map



X Index: 105

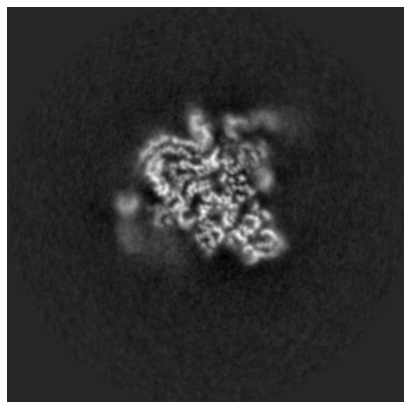


Y Index: 117

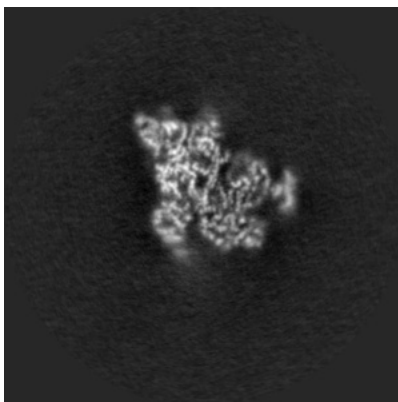


Z Index: 101

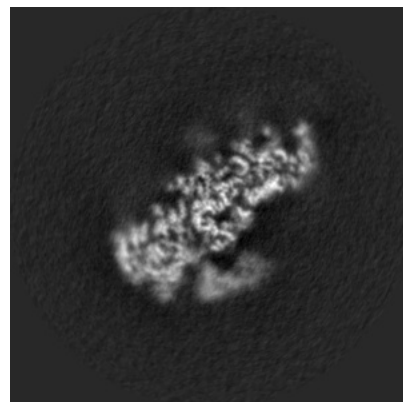
6.3.2 Raw map



X Index: 169



Y Index: 181

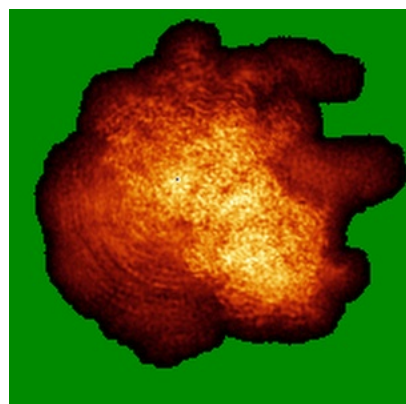


Z Index: 165

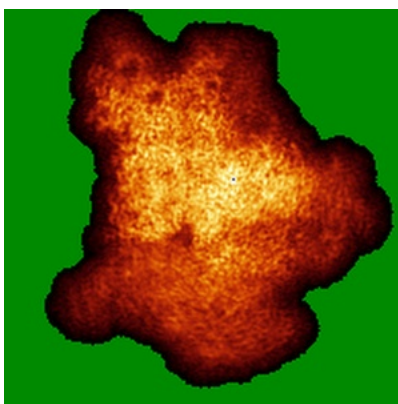
The images above show the largest variance slices of the map in three orthogonal directions.

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

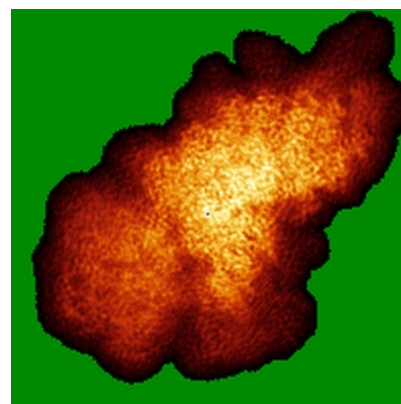
6.4.1 Primary map



X

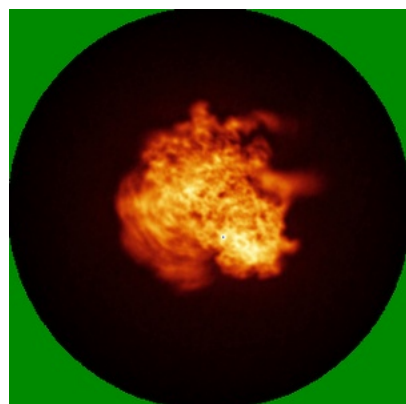


Y

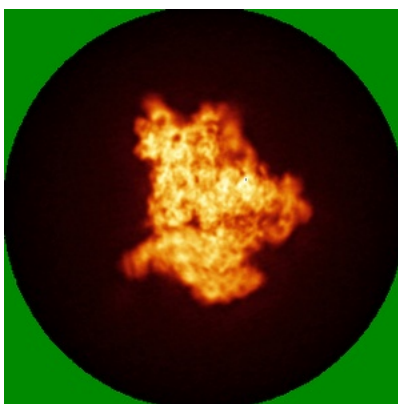


Z

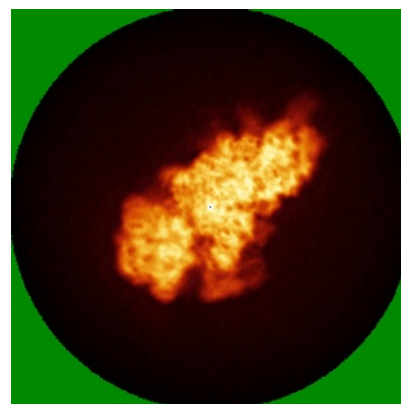
6.4.2 Raw map



X



Y

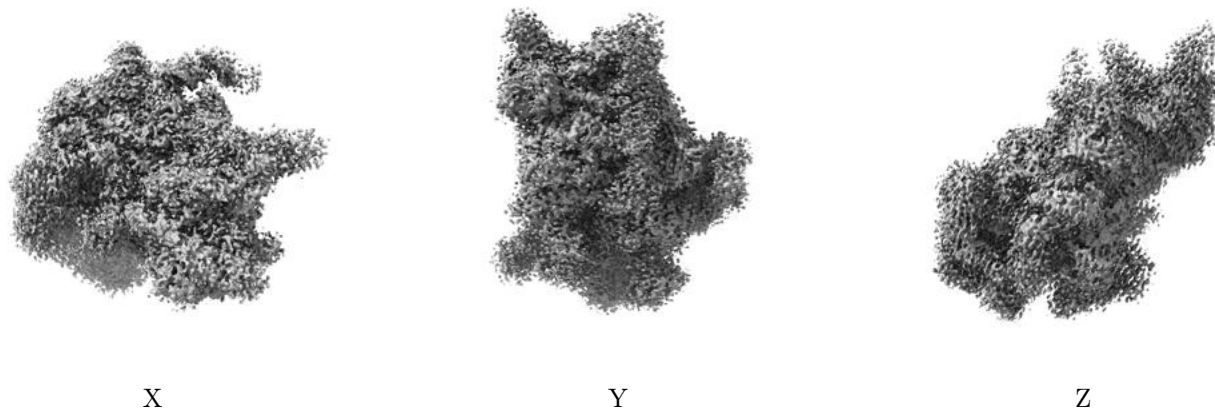


Z

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.

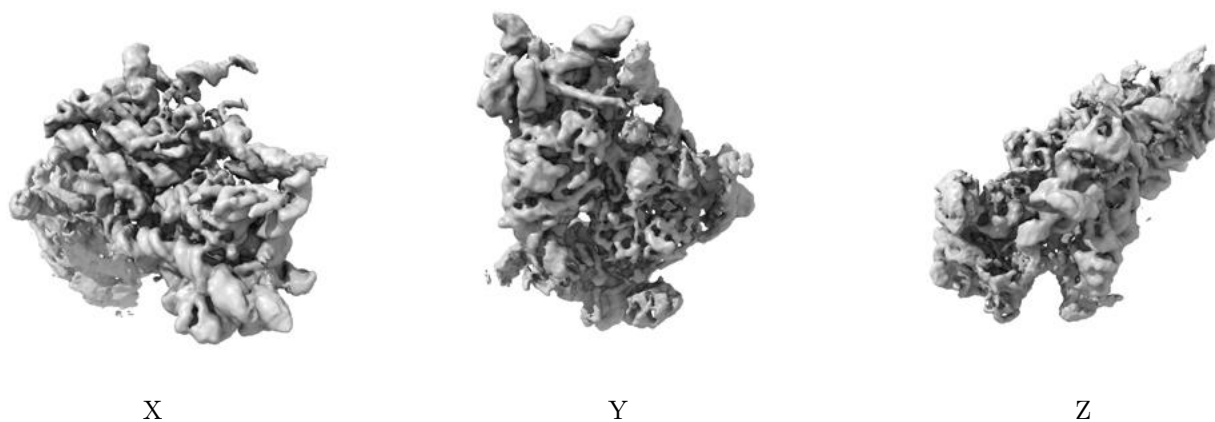
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

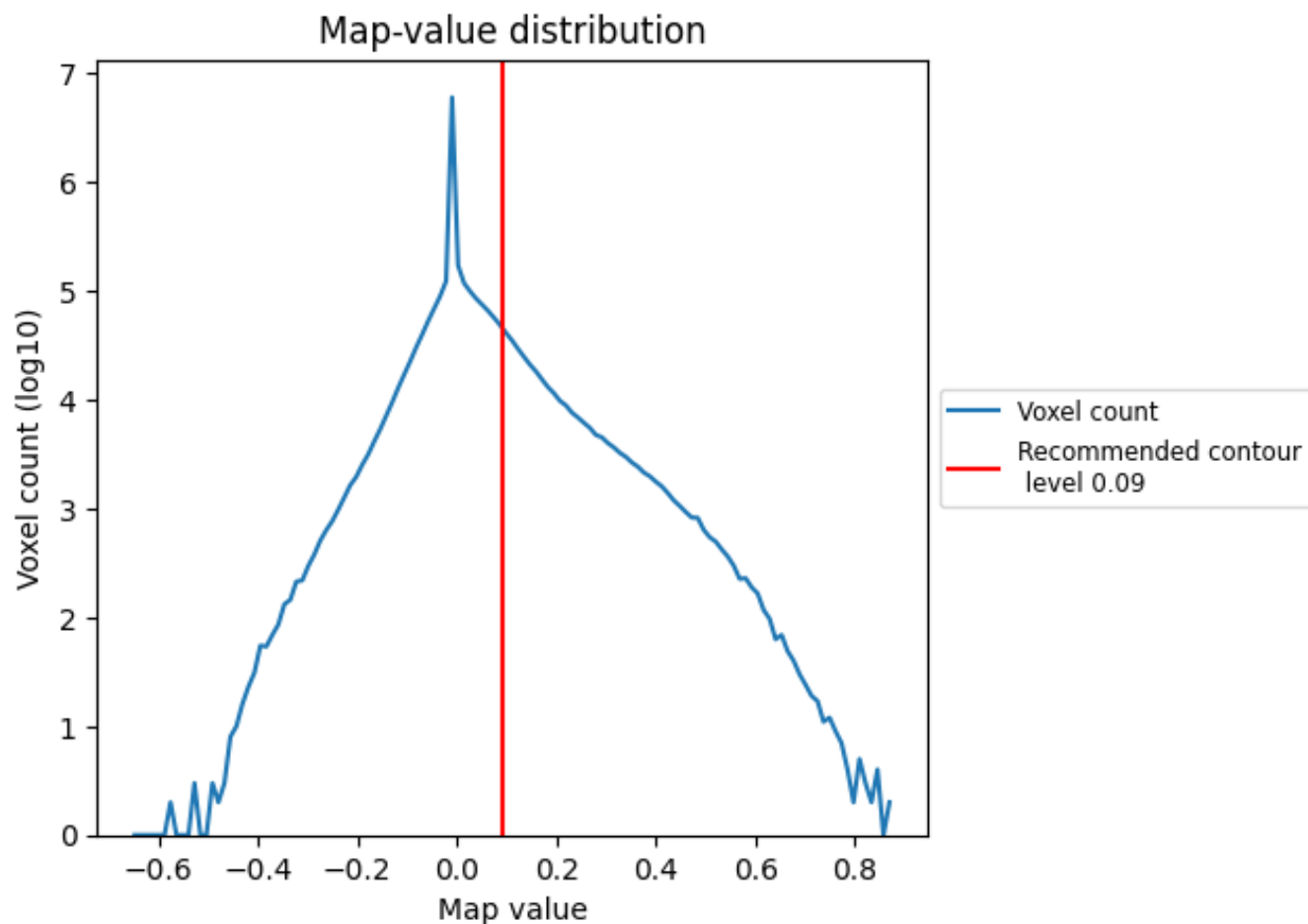
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

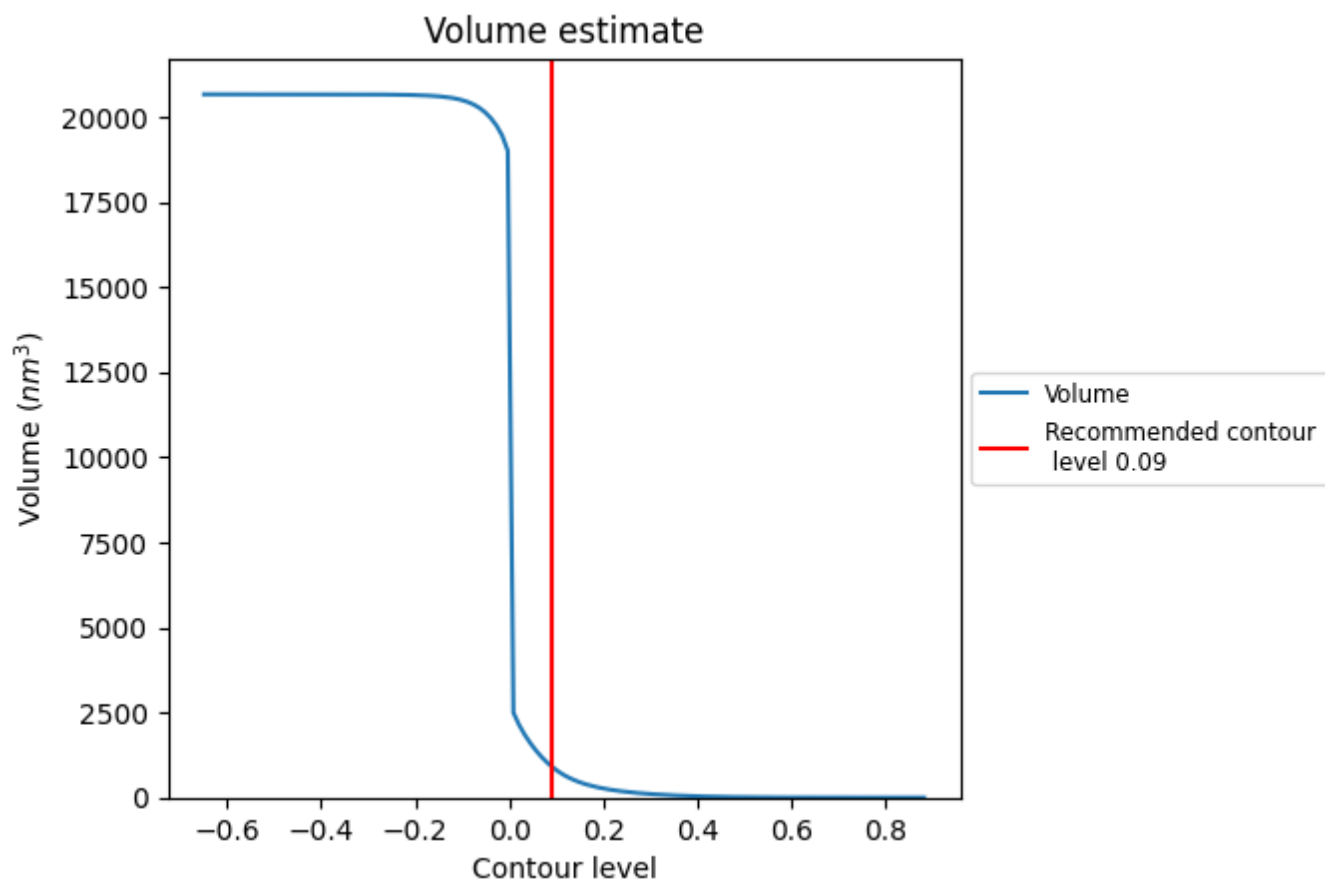
This section contains the results of statistical analysis of the map.

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.

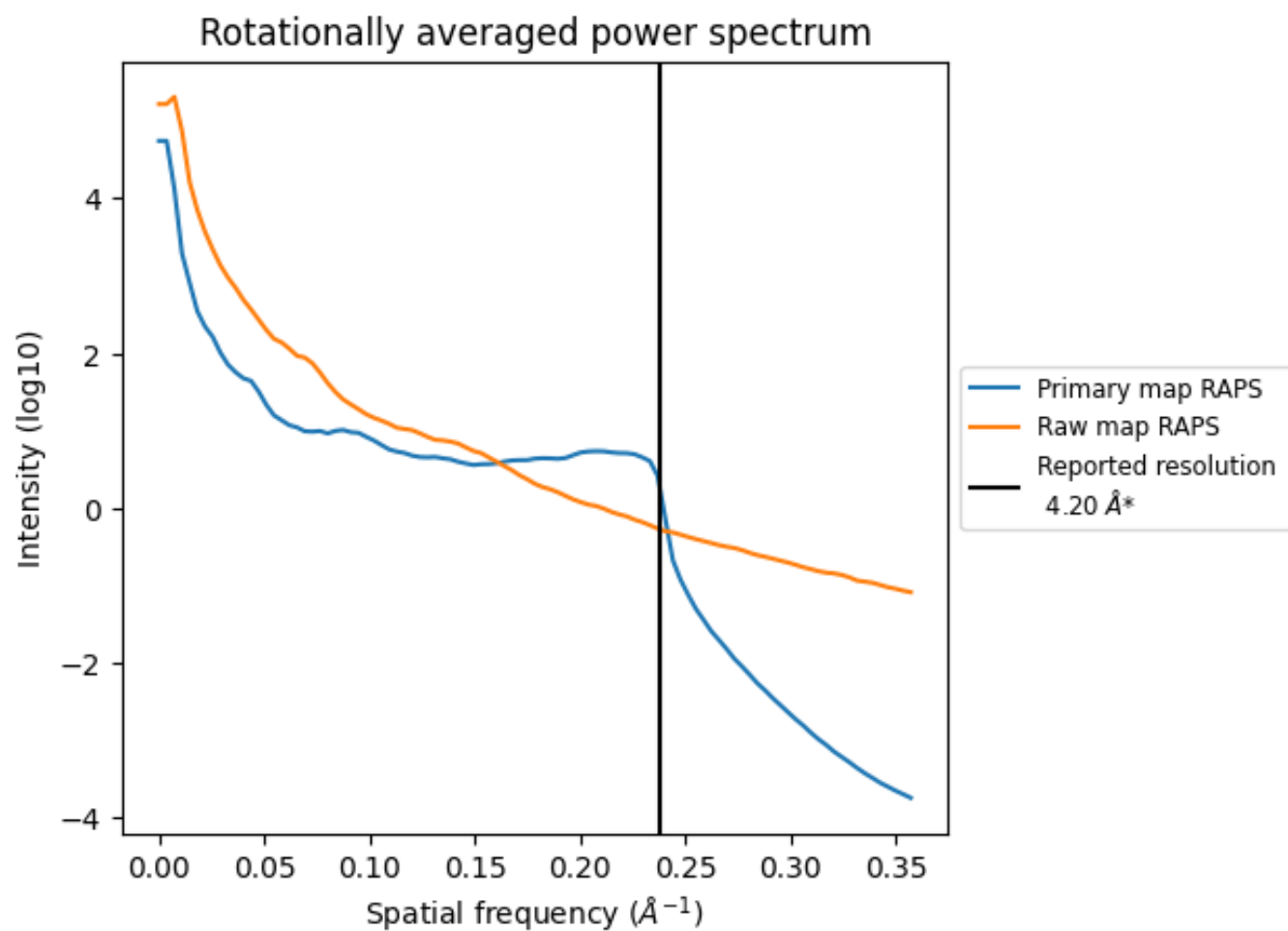
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 916 nm^3 ; this corresponds to an approximate mass of 827 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 ⓘ

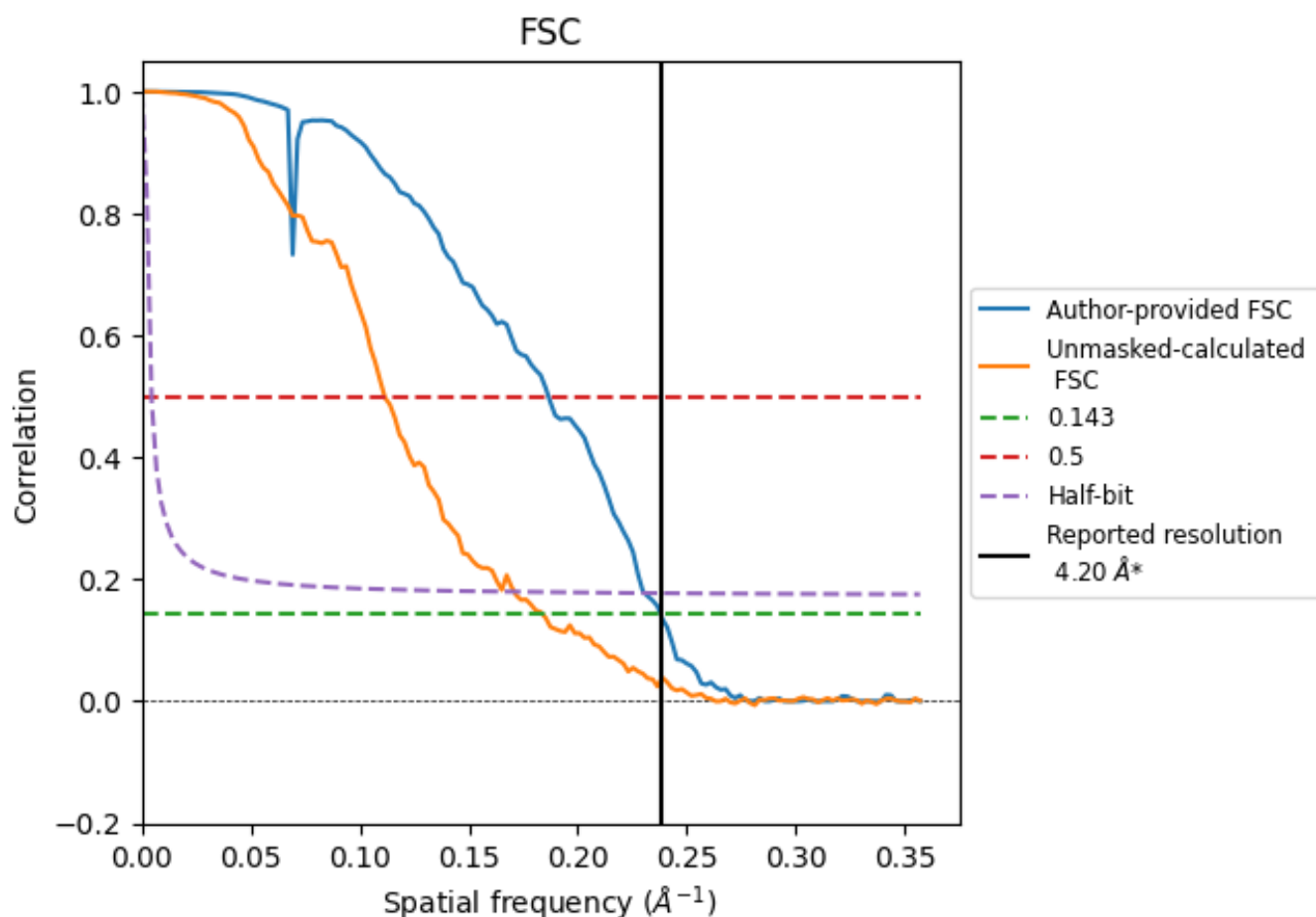


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	5.36	4.33
Unmasked-calculated*	5.44	8.98	5.85

*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 5.44 differs from the reported value 4.2 by more than 10 %

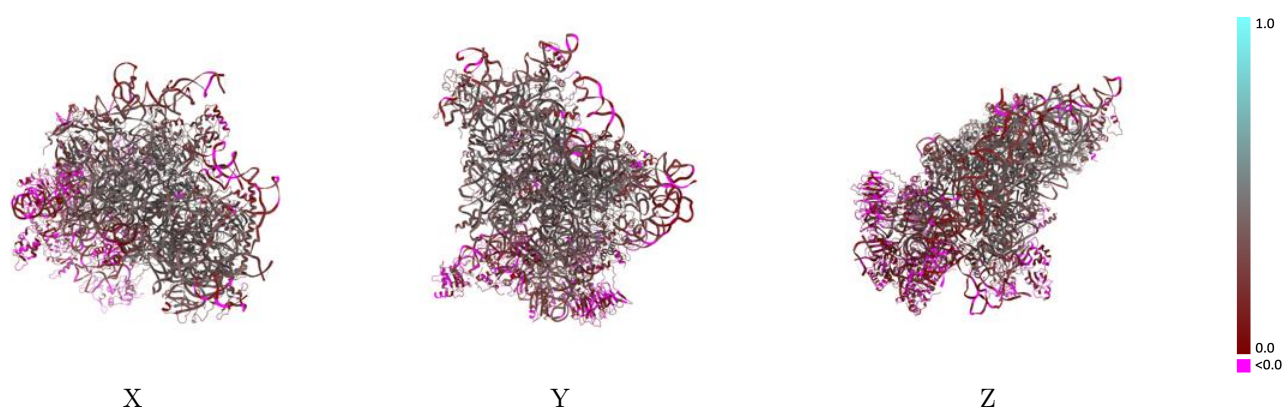
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3770 and PDB model 5OA3. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

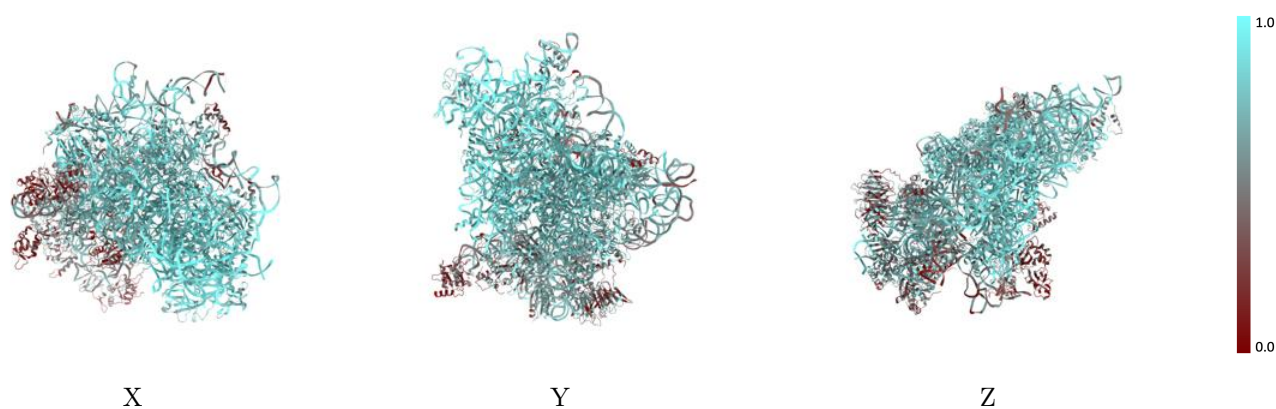
This section was not generated.

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



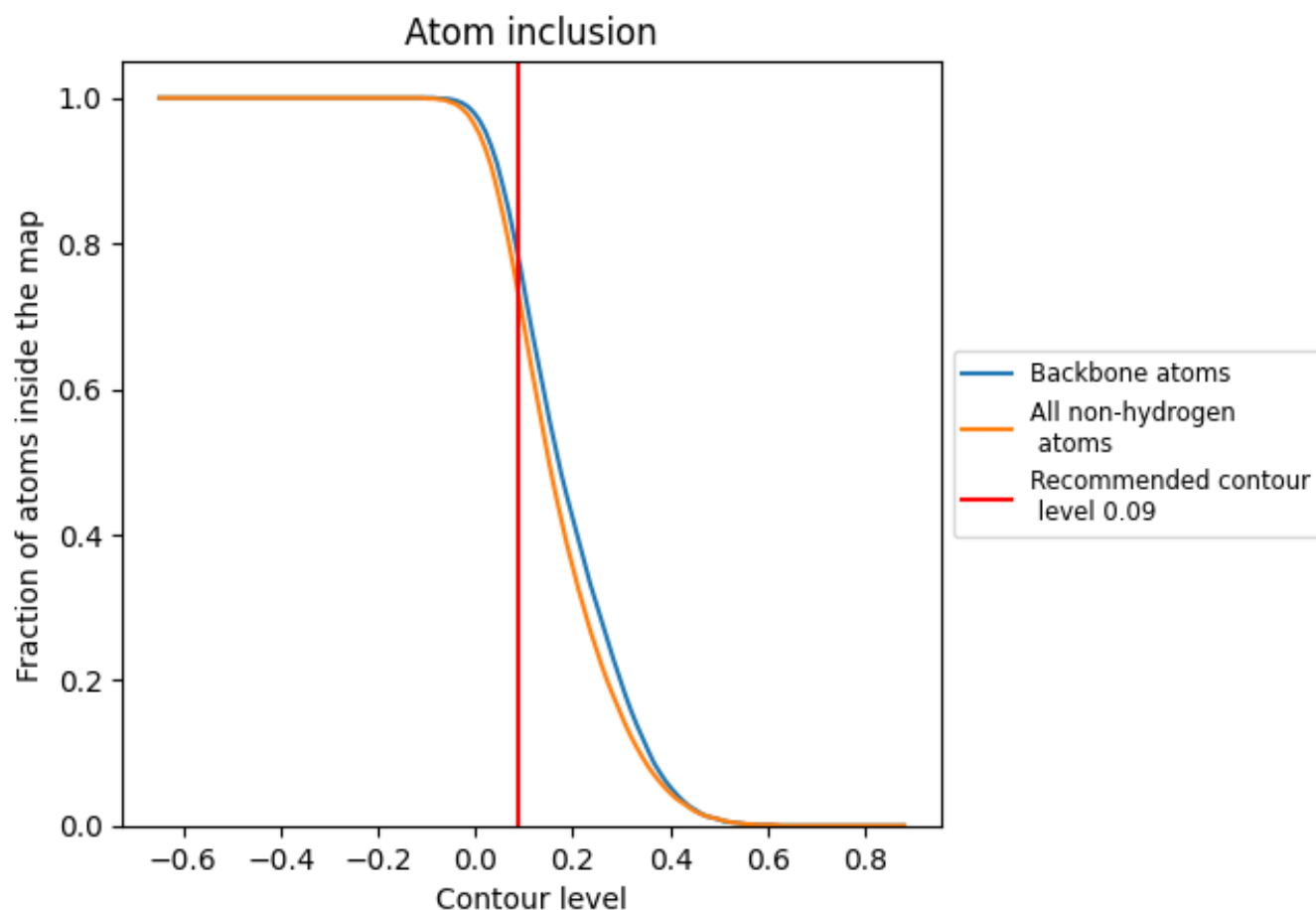
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.2650
0	 0.2800	 0.0960
1	 0.4910	 0.0950
2	 0.8640	 0.3120
3	 0.6250	 0.1520
A	 0.7840	 0.3440
B	 0.7810	 0.3450
C	 0.7940	 0.3880
D	 0.5830	 0.1790
E	 0.8270	 0.3970
F	 0.4720	 0.1010
G	 0.7870	 0.3110
H	 0.6180	 0.2840
I	 0.7680	 0.3290
J	 0.8270	 0.3810
K	 0.4880	 0.1030
L	 0.7680	 0.3780
M	 0.2180	 0.0450
N	 0.8140	 0.3700
O	 0.7490	 0.3300
P	 0.3980	 0.0540
Q	 0.5910	 0.1510
R	 0.6040	 0.2430
S	 0.4960	 0.0970
T	 0.5170	 0.1010
U	 0.6220	 0.2370
V	 0.8000	 0.3710
W	 0.8200	 0.4260
X	 0.8250	 0.4100
Y	 0.8350	 0.3600
Z	 0.3740	 0.0470
a	 0.7760	 0.3810
b	 0.7710	 0.3450
c	 0.4140	 0.1040
d	 0.6120	 0.1920



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Chain	Atom inclusion	Q-score
e	 0.6860	 0.3280
f	 0.2580	 0.0210
g	 0.4360	 0.0400
h	 0.6860	 0.3190