



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:41 PM UTC

PDB ID : 5XY3 / pdb_00005xy3
EMDB ID : EMD-6784
Title : Large subunit of Trichomonas vaginalis ribosome
Authors : Li, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.
Deposited on : 2017-07-06
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

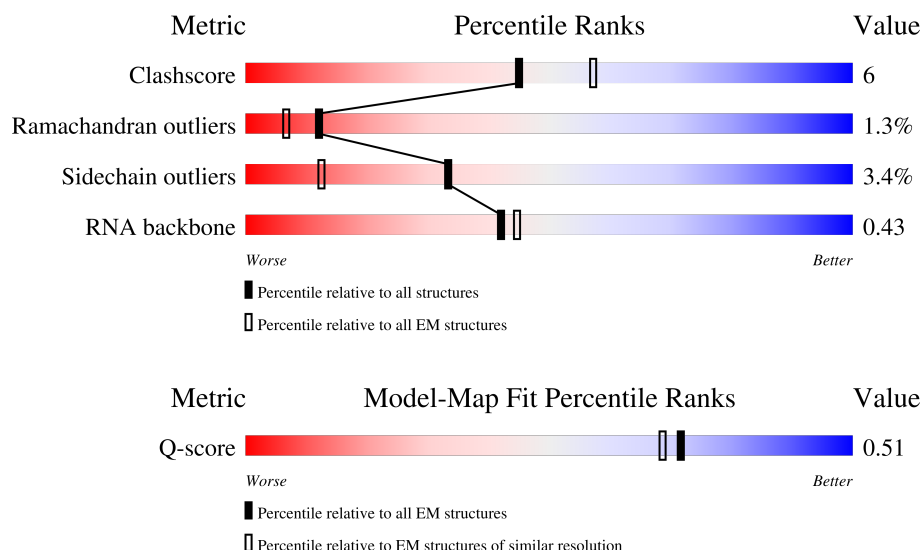
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	2765	
2	3	118	
3	4	162	

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Mol	Chain	Length	Quality of chain
4	A	251	
5	B	415	
6	C	370	
7	D	308	
8	E	151	
9	F	239	
10	G	244	
11	H	197	
12	I	209	
13	J	169	
14	L	189	
15	M	128	
16	N	204	
17	O	200	
18	P	164	
19	Q	186	
20	R	178	
21	S	176	
22	T	159	
23	U	106	
24	V	140	
25	W	113	
26	X	140	
27	Y	138	
28	Z	139	

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Mol	Chain	Length	Quality of chain
29	a	151	
30	b	58	
31	c	112	
32	d	110	
33	e	132	
34	f	102	
35	g	116	
36	h	124	
37	i	91	
38	j	81	
39	k	74	
40	l	51	
41	m	132	
42	o	104	
43	p	92	

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 107145 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 RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2544	Total	C	N	O	P	0	0
			54325	24285	9748	17748	2544		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	117	Total	C	N	O	P	0	0
			2493	1112	449	815	117		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	154	Total	C	N	O	P	0	0
			3289	1472	595	1068	154		

- Molecule 4 is a protein called Ribosomal protein L8, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	237	Total	C	N	O	S	0	0
			1785	1105	365	306	9		

- Molecule 5 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	400	Total	C	N	O	S	0	0
			3175	2002	608	554	11		

- Molecule 6 is a protein called Ribosomal protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	362	Total	C	N	O	S	0	0
			2772	1751	513	501	7		

- Molecule 7 is a protein called Ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	272	Total	C	N	O	S	0	0
			2167	1384	394	384	5		

- Molecule 8 is a protein called 60S ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	135	Total	C	N	O	S	0	0
			1014	651	180	181	2		

- Molecule 9 is a protein called Ribosomal protein L30p/L7e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	231	Total	C	N	O	S	0	0
			1832	1174	330	324	4		

- Molecule 10 is a protein called Ribosomal protein L7Ae, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	174	Total	C	N	O	S	0	0
			1384	892	245	239	8		

- Molecule 11 is a protein called Ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	192	Total	C	N	O	S	0	0
			1556	994	274	281	7		

- Molecule 12 is a protein called Ribosomal protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	195	Total	C	N	O	S	0	0
			1569	989	304	264	12		

- Molecule 13 is a protein called 60S ribosomal protein L11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	164	Total	C	N	O	S	0	0
			1320	827	258	230	5		

- Molecule 14 is a protein called Ribosomal protein L13e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	185	Total	C	N	O	S	0	0
			1498	947	296	252	3		

- Molecule 15 is a protein called Ribosomal protein L14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	124	Total	C	N	O	S	0	0
			1004	650	176	177	1		

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	202	Total	C	N	O	S	0	0
			1696	1076	343	271	6		

- Molecule 17 is a protein called Ribosomal protein L13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	196	Total	C	N	O	S	0	0
			1559	988	295	271	5		

- Molecule 18 is a protein called Ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	155	Total	C	N	O	S	0	0
			1230	781	231	211	7		

- Molecule 19 is a protein called 60S ribosomal protein L18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	185	Total	C	N	O	S	0	0
			1465	907	295	255	8		

- Molecule 20 is a protein called 60S ribosomal protein L19-3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	162	Total	C	N	O	S	0	0
			1299	805	277	213	4		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	175	Total	C	N	O	S	0	0
			1384	882	252	247	3		

- Molecule 22 is a protein called Ribosomal protein L21e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	158	Total	C	N	O	S	0	0
			1255	797	249	207	2		

- Molecule 23 is a protein called 60S ribosomal protein L22-1, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	97	Total	C	N	O	S	0	0
			794	511	140	141	2		

- Molecule 24 is a protein called 60S ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	134	Total	C	N	O	S	0	0
			986	622	185	172	7		

- Molecule 25 is a protein called Ribosomal protein L24e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	59	Total	C	N	O	S	0	0
			513	323	108	79	3		

- Molecule 26 is a protein called Ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	101	Total	C	N	O	S	0	0
			803	518	141	141	3		

- Molecule 27 is a protein called Ribosomal protein L24, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	134	Total	C	N	O	S	0	0
			1068	671	204	188	5		

- Molecule 28 is a protein called Ribosomal protein L27e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	135	Total	C	N	O	S	0	0
			1042	682	184	172	4		

- Molecule 29 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	149	Total	C	N	O	S	0	0
			1179	749	229	196	5		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	50	Total	C	N	O	S	0	0
			415	256	92	65	2		

- Molecule 31 is a protein called 60S ribosomal protein L30, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	96	Total	C	N	O	S	0	0
			727	462	121	140	4		

- Molecule 32 is a protein called Ribosomal protein L31e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	99	Total	C	N	O	S	0	0
			783	497	149	134	3		

- Molecule 33 is a protein called Ribosomal protein L32, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	123	Total	C	N	O	S	0	0
			1003	633	198	169	3		

- Molecule 34 is a protein called Ribosomal protein L35Ae, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	97	Total	C	N	O	S	0	0
			781	511	137	131	2		

- Molecule 35 is a protein called Ribosomal protein L34e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	115	Total	C	N	O	S	0	0
			921	565	191	158	7		

- Molecule 36 is a protein called Ribosomal protein L29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	122	Total	C	N	O	S	0	0
			984	623	190	169	2		

- Molecule 37 is a protein called Ribosomal protein L36e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	73	Total	C	N	O	S	0	0
			616	385	128	101	2		

- Molecule 38 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	77	Total	C	N	O	S	0	0
			616	380	128	101	7		

- Molecule 39 is a protein called Ribosomal protein L38e, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	68	Total	C	N	O	0	0
			547	358	90	99		

- Molecule 40 is a protein called 60S ribosomal protein L39, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	50	Total	C	N	O	S	0	0
			428	267	97	59	5		

- Molecule 41 is a protein called Ubiquitin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	52	Total	C	N	O	S	0	0
			417	254	89	69	5		

- Molecule 42 is a protein called 60S ribosomal protein L44, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	93	Total	C	N	O	S	0	0
			773	486	158	121	8		

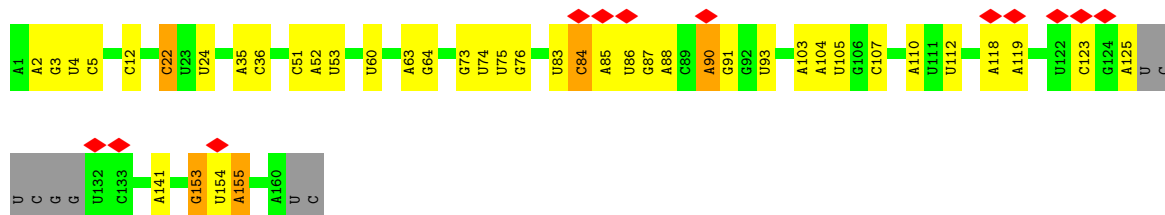
- Molecule 43 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	89	Total	C	N	O	S	0	0
			678	426	133	114	5		

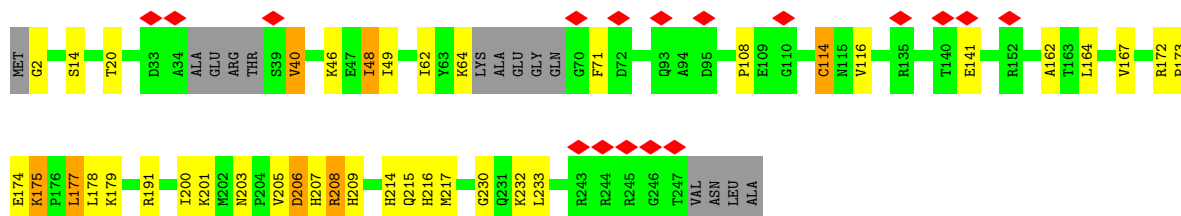
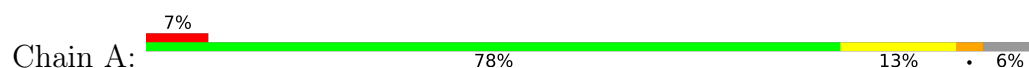




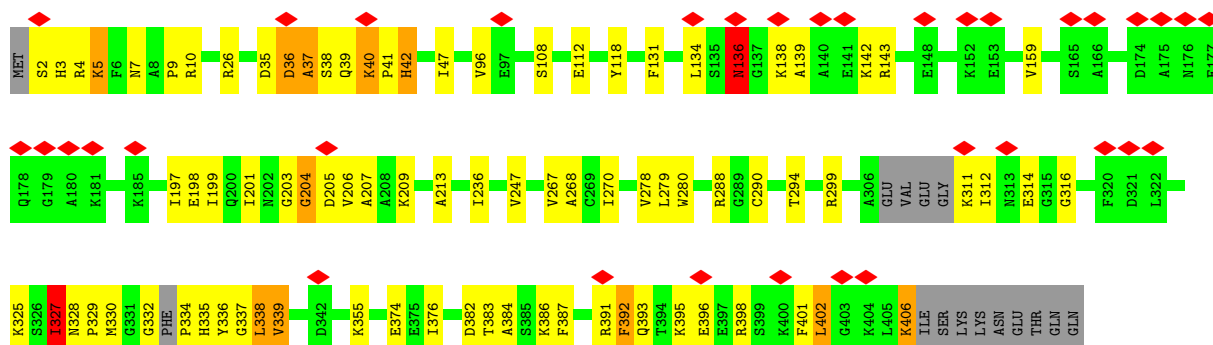
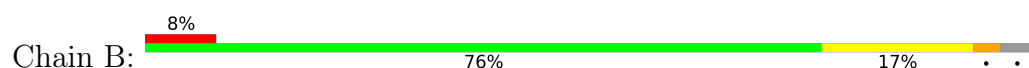
• Molecule 3: 5.8S ribosomal RNA



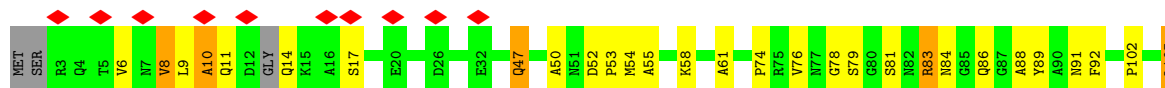
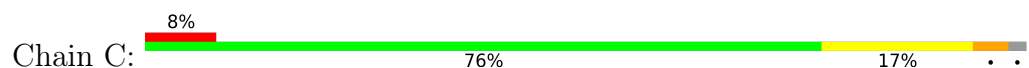
• Molecule 4: Ribosomal protein L8, putative

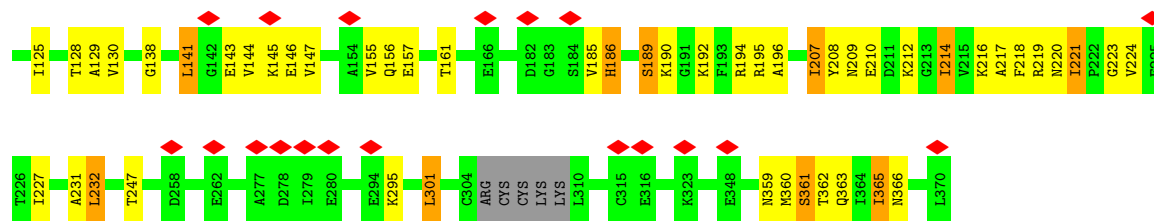


• Molecule 5: Uncharacterized protein

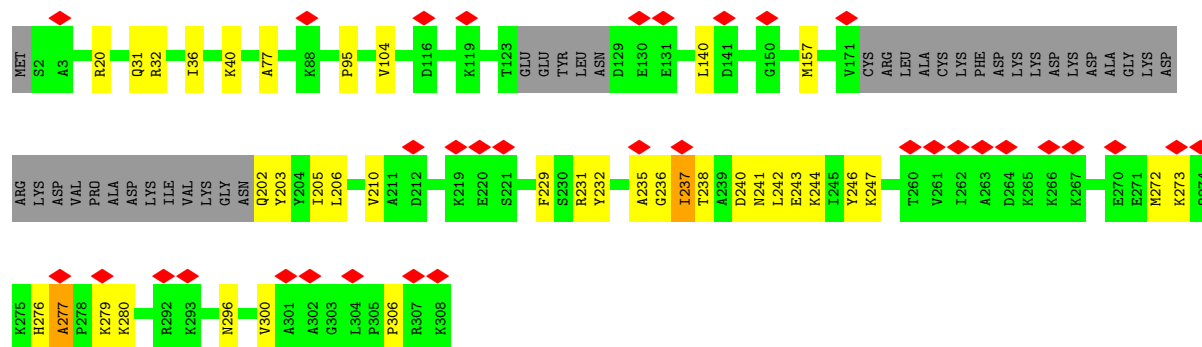
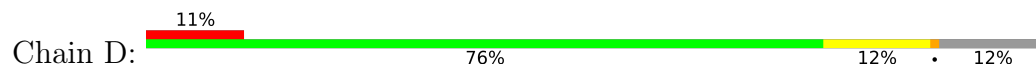


• Molecule 6: Ribosomal protein, putative

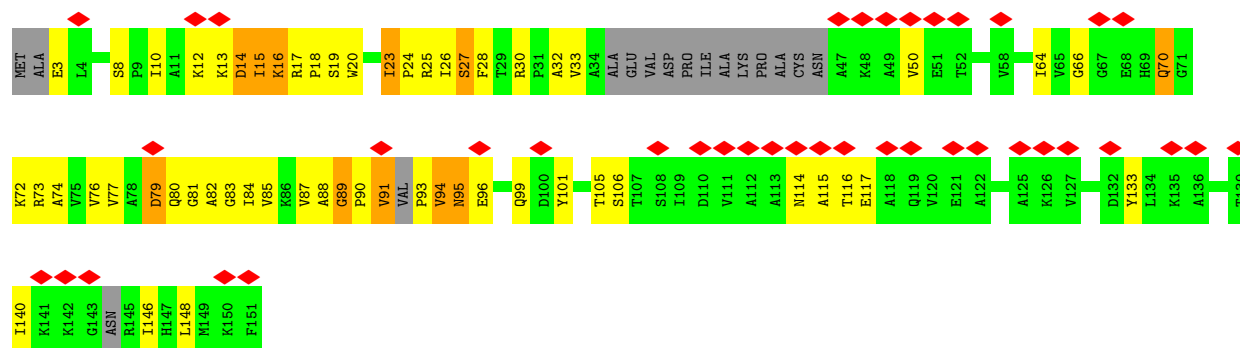




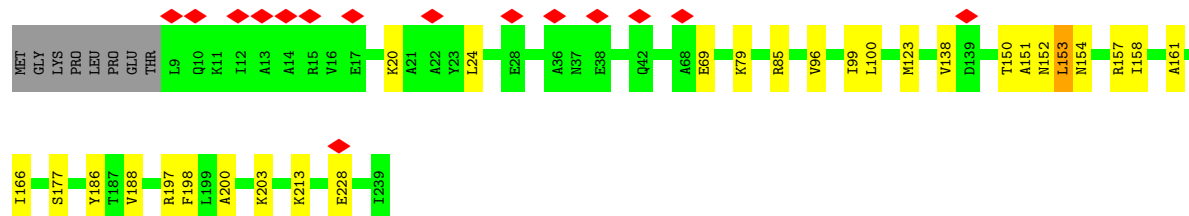
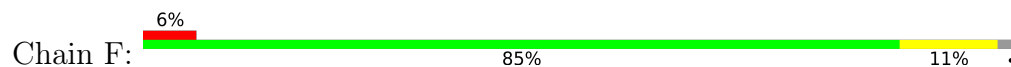
• Molecule 7: Ribosomal protein L5



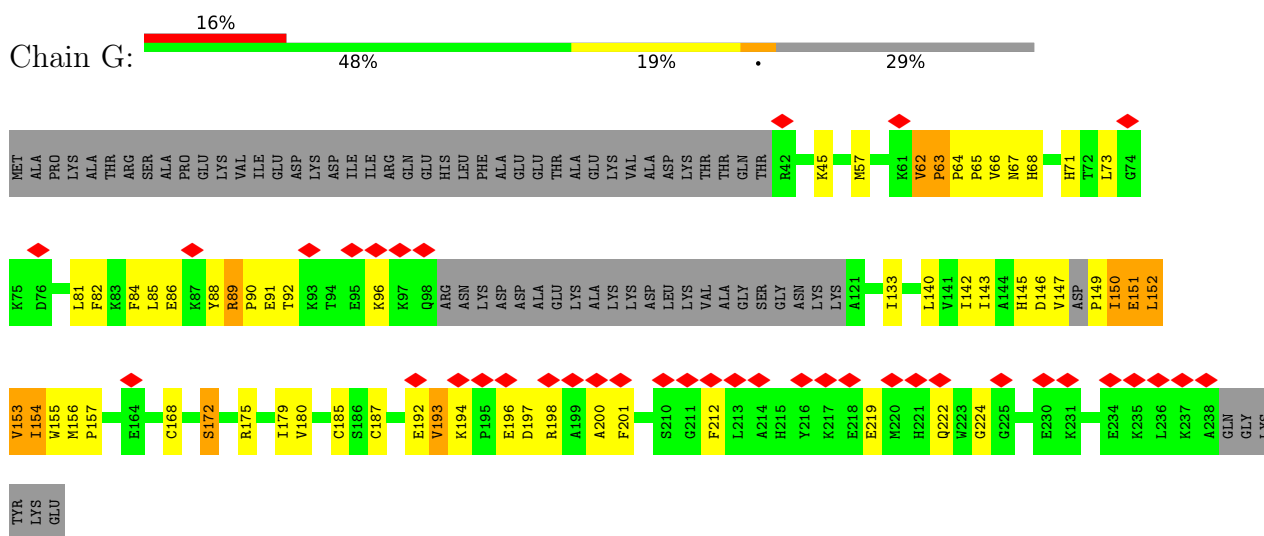
• Molecule 8: 60S ribosomal protein L6, putative



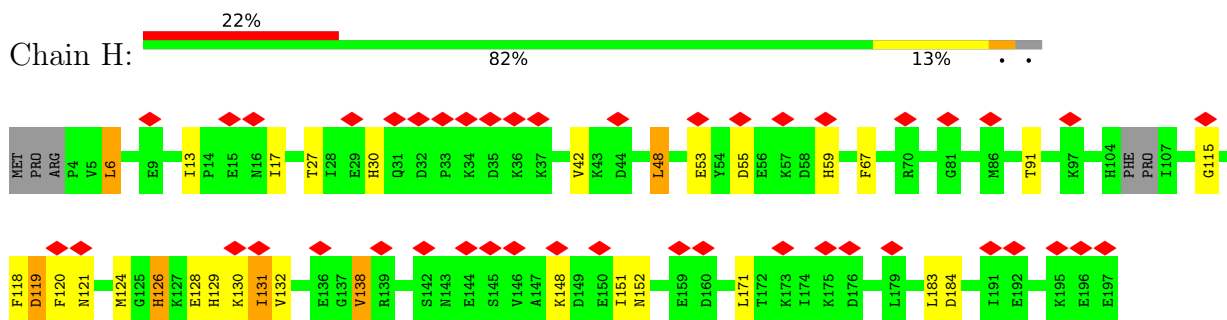
• Molecule 9: Ribosomal protein L30p/L7e, putative



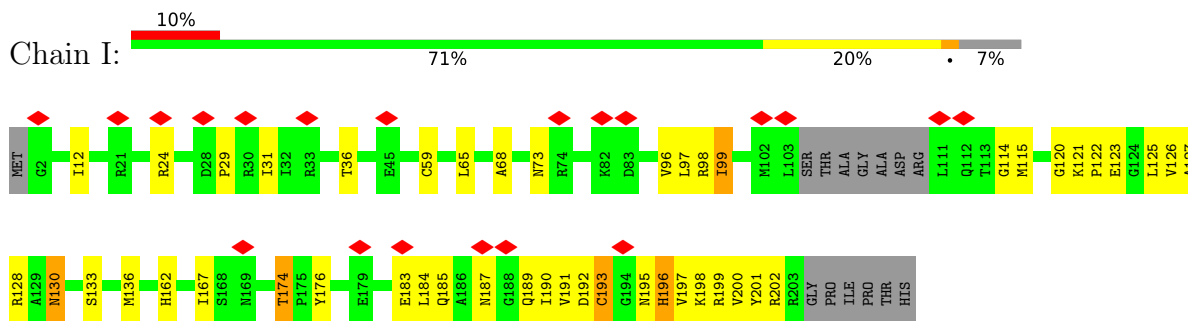
• Molecule 10: Ribosomal protein L7Ae, putative



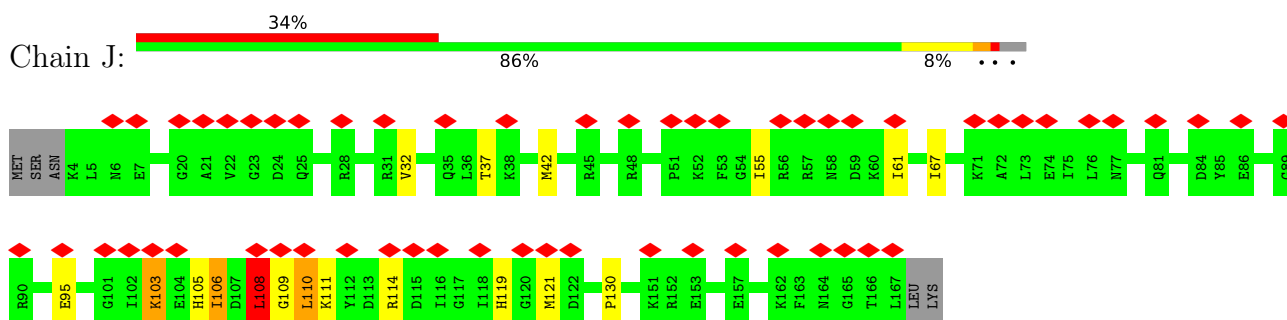
- Molecule 11: Ribosomal protein L6, putative



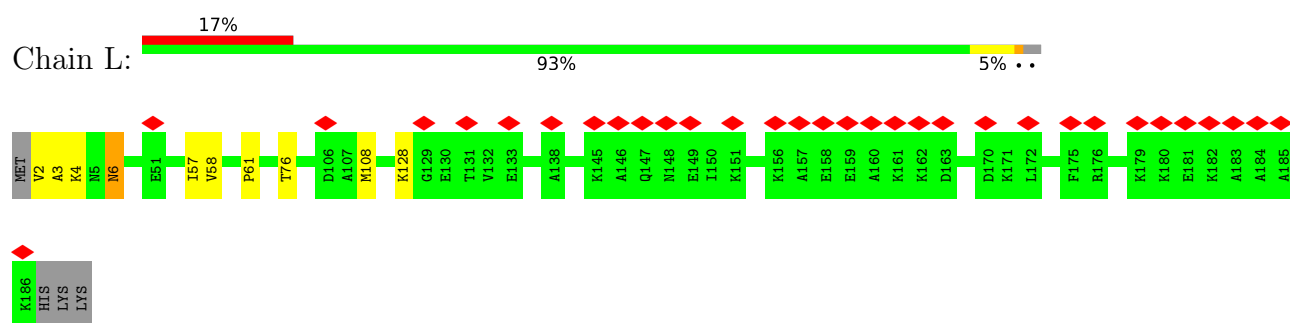
- Molecule 12: Ribosomal protein, putative



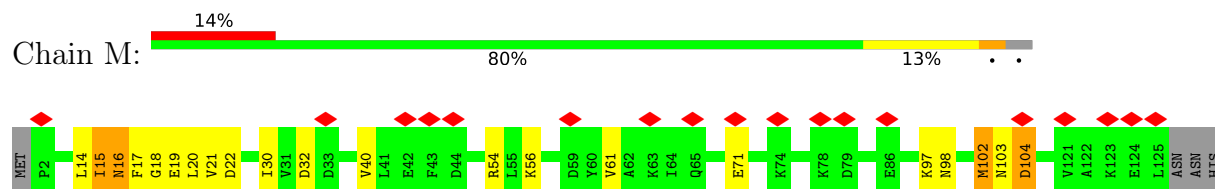
- Molecule 13: 60S ribosomal protein L11, putative



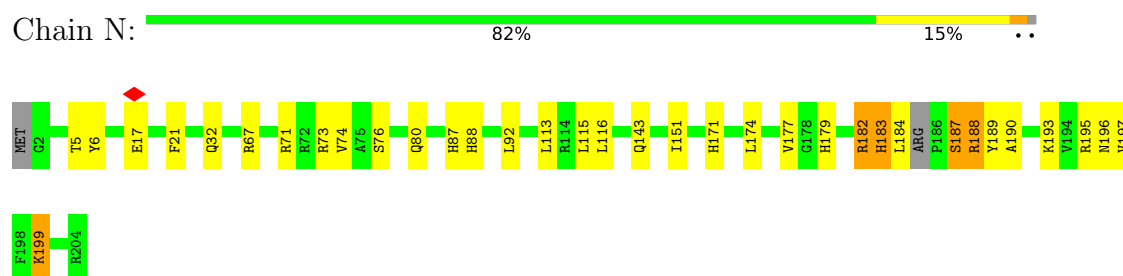
- Molecule 14: Ribosomal protein L13e, putative



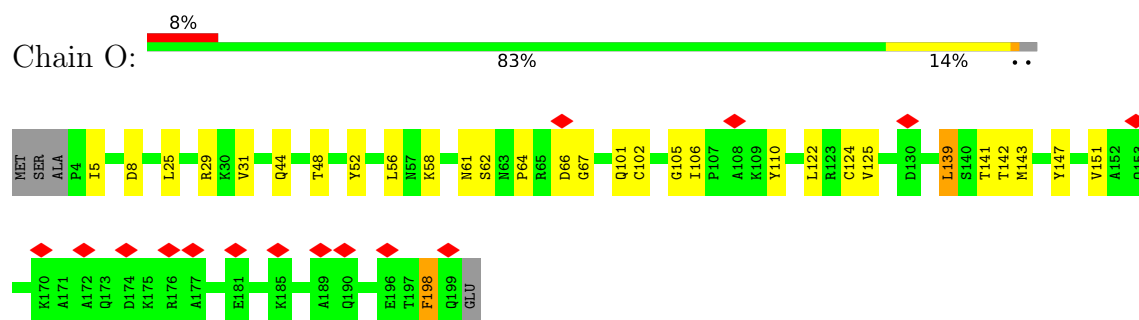
- Molecule 15: Ribosomal protein L14, putative



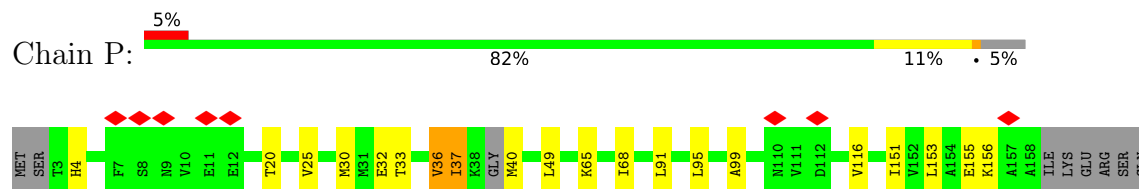
- Molecule 16: Ribosomal protein L15



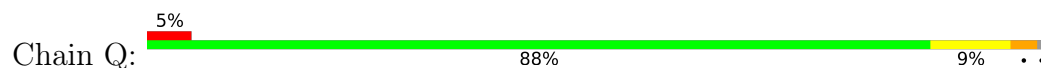
- Molecule 17: Ribosomal protein L13, putative



- Molecule 18: Ribosomal protein L22, putative

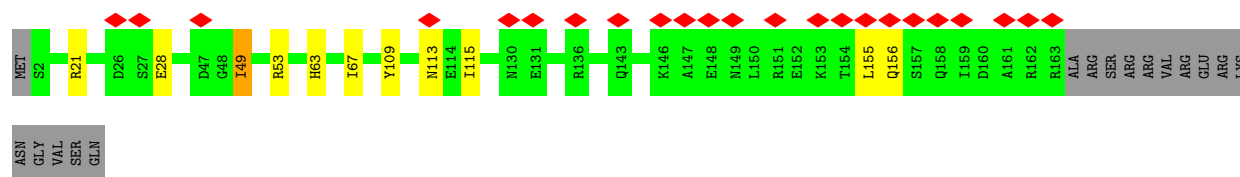
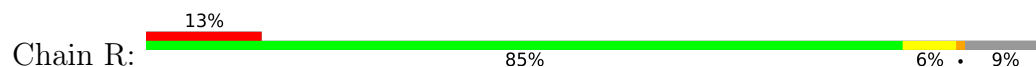


- Molecule 19: 60S ribosomal protein L18, putative

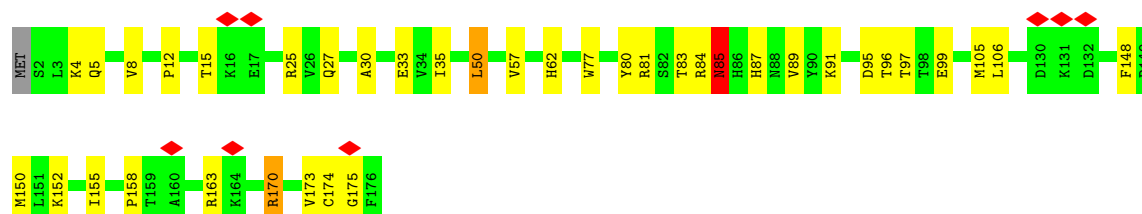
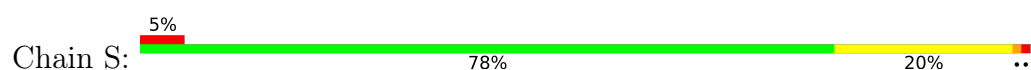




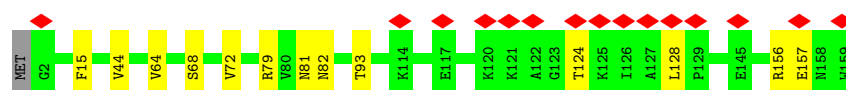
- Molecule 20: 60S ribosomal protein L19-3, putative



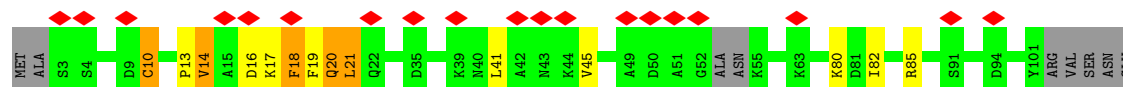
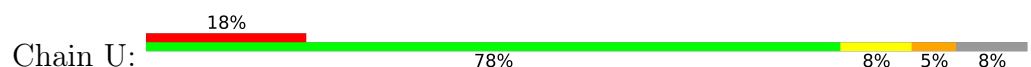
- Molecule 21: 60S ribosomal protein L18a



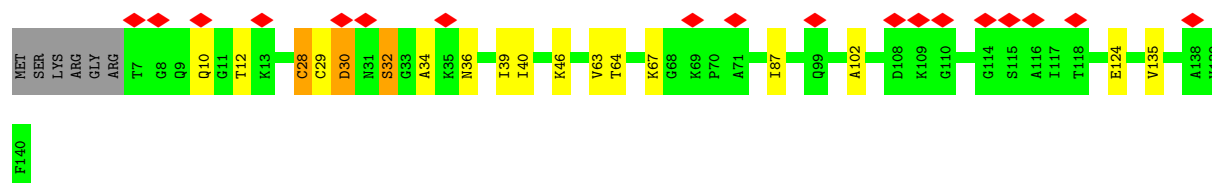
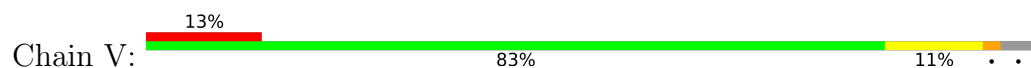
- Molecule 22: Ribosomal protein L21e, putative



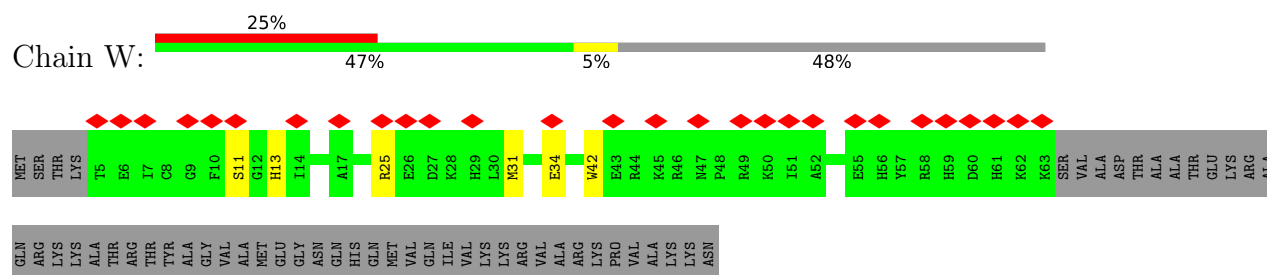
- Molecule 23: 60S ribosomal protein L22-1, putative



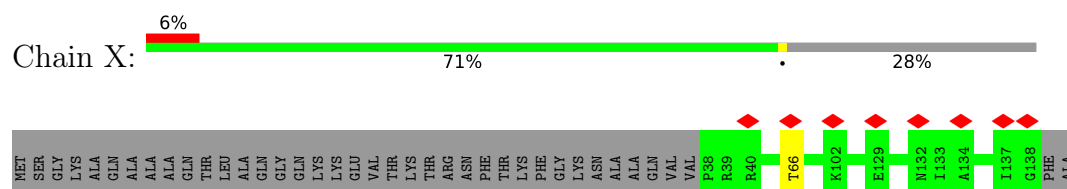
- Molecule 24: 60S ribosomal protein L23, putative



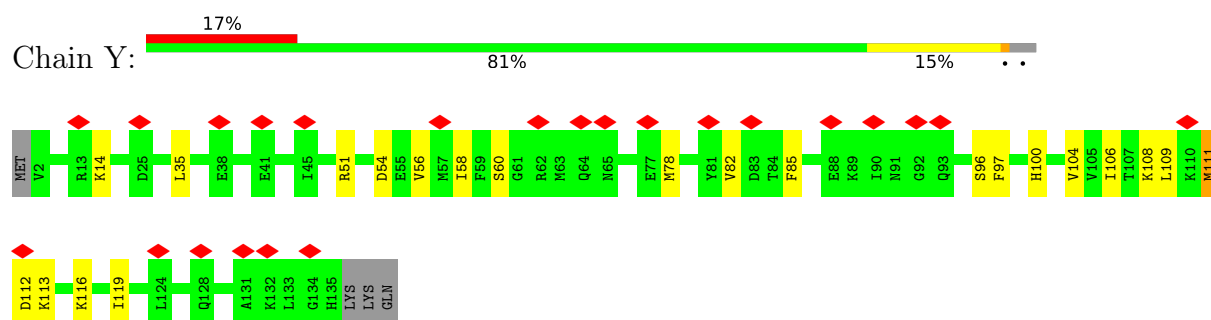
- Molecule 25: Ribosomal protein L24e, putative



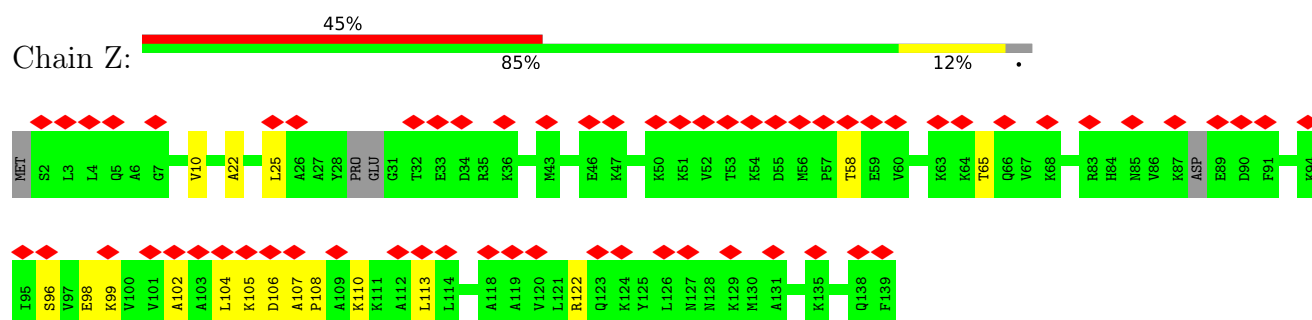
- Molecule 26: Ribosomal protein L23, putative



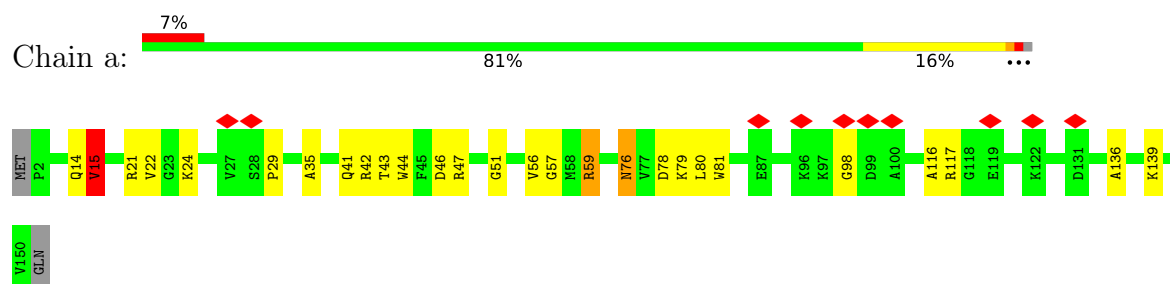
- Molecule 27: Ribosomal protein L24, putative



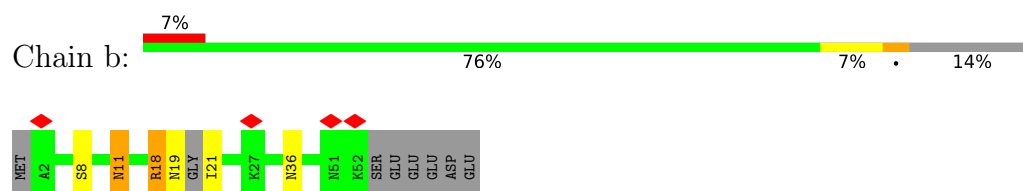
- Molecule 28: Ribosomal protein L27e, putative



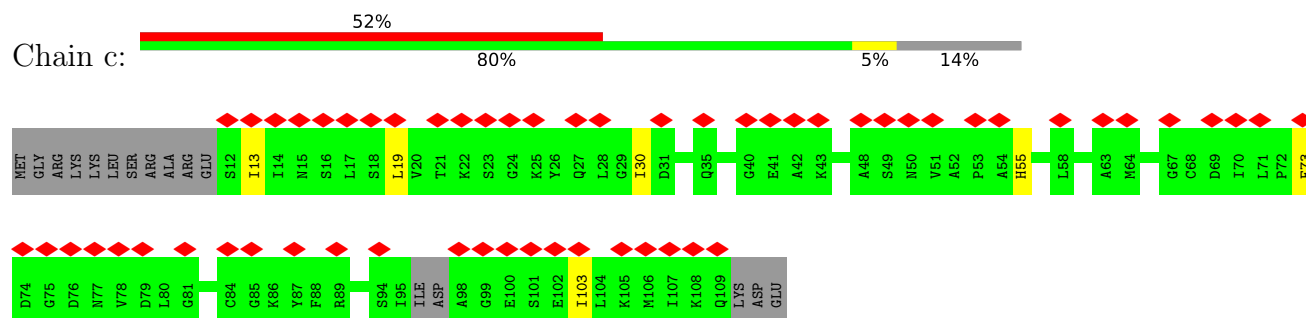
- Molecule 29: Uncharacterized protein



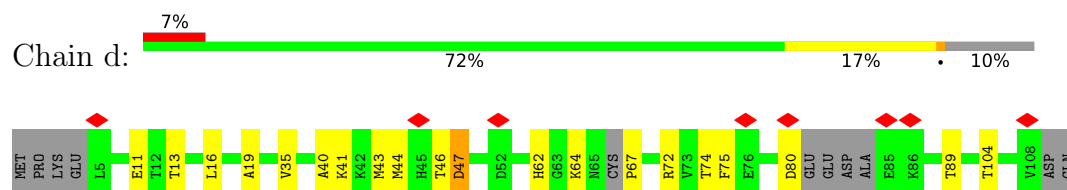
- Molecule 30: 60S ribosomal protein L29



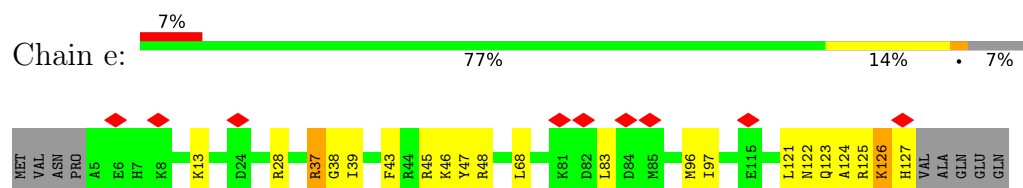
- Molecule 31: 60S ribosomal protein L30, putative



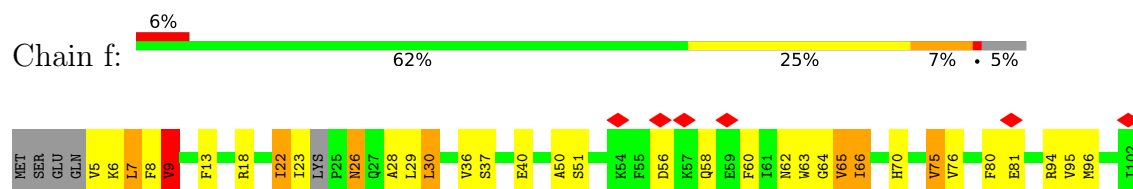
- Molecule 32: Ribosomal protein L31e, putative



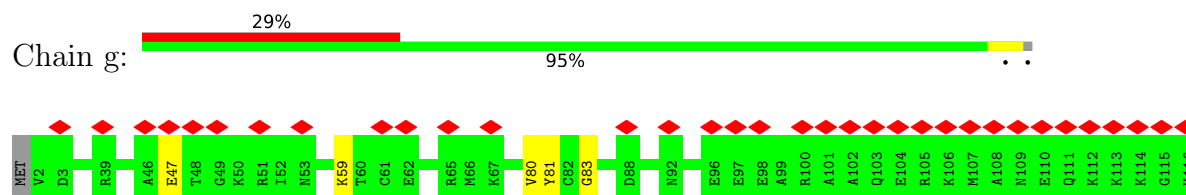
- Molecule 33: Ribosomal protein L32, putative



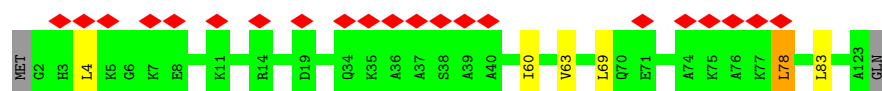
- Molecule 34: Ribosomal protein L35Ae, putative



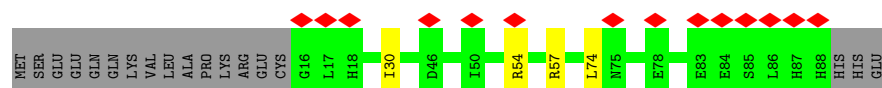
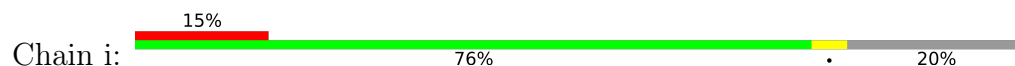
- Molecule 35: Ribosomal protein L34e, putative



- Molecule 36: Ribosomal protein L29, putative



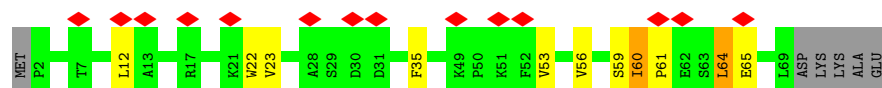
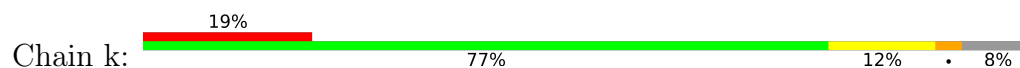
- Molecule 37: Ribosomal protein L36e, putative



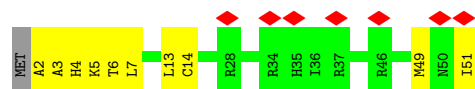
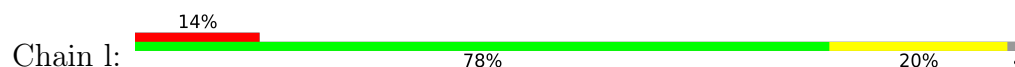
- Molecule 38: Ribosomal protein L37



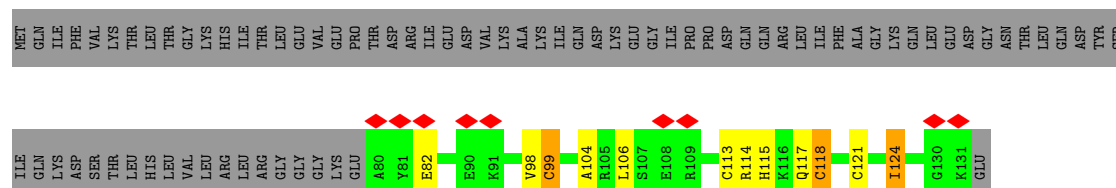
- Molecule 39: Ribosomal protein L38e, putative



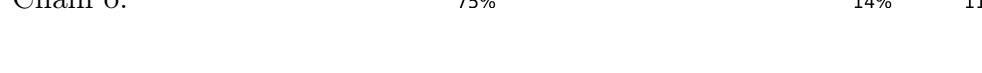
- Molecule 40: 60S ribosomal protein L39, putative

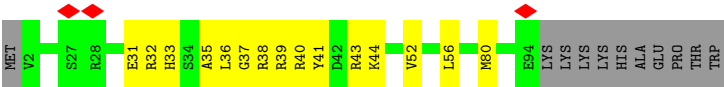


- Molecule 41: Ubiquitin, putative

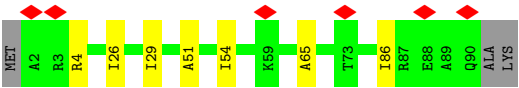
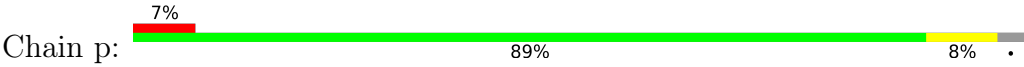


- Molecule 42: 60S ribosomal protein L44, putative





• Molecule 43: Uncharacterized protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57162	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.399	Depositor
Minimum map value	-0.231	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.044	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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	1	0.36	0/60789	0.67	35/94723 (0.0%)
2	3	0.38	0/2785	0.68	2/4339 (0.0%)
3	4	0.36	0/3681	0.66	1/5732 (0.0%)
4	A	0.55	0/1822	0.81	4/2450 (0.2%)
5	B	0.52	0/3237	0.81	9/4340 (0.2%)
6	C	0.58	0/2819	0.93	13/3816 (0.3%)
7	D	0.53	0/2201	0.84	7/2950 (0.2%)
8	E	0.59	0/1028	1.02	8/1388 (0.6%)
9	F	0.54	0/1864	0.82	2/2507 (0.1%)
10	G	0.64	0/1409	1.00	9/1892 (0.5%)
11	H	0.50	0/1589	0.74	1/2136 (0.0%)
12	I	0.53	0/1603	0.83	3/2151 (0.1%)
13	J	0.51	0/1341	0.78	2/1797 (0.1%)
14	L	0.51	0/1525	0.76	0/2042
15	M	0.50	0/1020	0.85	2/1371 (0.1%)
16	N	0.53	0/1739	0.83	4/2332 (0.2%)
17	O	0.57	0/1591	0.85	3/2141 (0.1%)
18	P	0.49	0/1260	0.76	2/1701 (0.1%)
19	Q	0.54	0/1488	0.82	4/1996 (0.2%)
20	R	0.53	0/1314	0.84	2/1754 (0.1%)
21	S	0.55	0/1416	0.80	3/1922 (0.2%)
22	T	0.51	0/1288	0.69	0/1743
23	U	0.54	0/809	0.86	3/1085 (0.3%)
24	V	0.52	0/1000	0.71	1/1346 (0.1%)
25	W	0.51	0/530	0.68	0/705
26	X	0.51	0/819	0.71	0/1106
27	Y	0.53	0/1082	0.78	1/1447 (0.1%)
28	Z	0.52	0/1061	0.76	0/1428
29	a	0.53	0/1209	0.77	1/1619 (0.1%)
30	b	0.51	0/423	0.79	1/559 (0.2%)
31	c	0.55	0/735	0.76	0/987
32	d	0.57	0/794	0.81	2/1065 (0.2%)
33	e	0.51	0/1027	0.79	2/1381 (0.1%)
34	f	0.56	0/799	0.86	3/1075 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	g	0.51	0/933	0.75	0/1243
36	h	0.55	0/993	0.80	0/1316
37	i	0.51	0/627	0.82	0/835
38	j	0.61	0/631	0.98	5/839 (0.6%)
39	k	0.52	0/557	0.84	2/752 (0.3%)
40	l	0.51	0/436	0.83	0/580
41	m	0.53	0/422	0.89	1/558 (0.2%)
42	o	0.48	0/788	0.67	1/1038 (0.1%)
43	p	0.52	0/688	0.74	0/919
All	All	0.44	0/115172	0.73	139/169106 (0.1%)

There are no bond length outliers.

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	108	LEU	N-CA-C	10.29	122.08	111.07
5	B	338	LEU	N-CA-C	9.14	121.24	111.28
8	E	20	TRP	N-CA-C	9.09	121.27	111.36
1	1	1348	U	C4'-C3'-O3'	9.03	122.95	109.40
9	F	158	ILE	N-CA-C	8.56	116.98	109.02
23	U	16	ASP	N-CA-C	8.50	120.62	111.36
1	1	1766	U	C4'-C3'-O3'	8.43	122.05	109.40
1	1	806	C	C4'-C3'-O3'	8.37	121.96	109.40
2	3	112	U	C4'-C3'-O3'	8.23	121.74	109.40
1	1	1258	U	C4'-C3'-O3'	8.20	121.70	109.40
3	4	90	A	C4'-C3'-O3'	8.18	121.67	109.40
15	M	16	ASN	N-CA-C	8.08	120.17	111.36
1	1	1903	U	C2'-C3'-O3'	7.97	121.46	109.50
13	J	103	LYS	N-CA-C	-7.86	98.17	110.36
1	1	1072	U	C4'-C3'-O3'	7.82	121.13	109.40
20	R	155	LEU	N-CA-C	7.72	119.48	111.14
1	1	308	G	C2'-C3'-O3'	-7.69	102.16	113.70
1	1	2042	A	C2'-C3'-O3'	7.64	120.95	109.50
1	1	2039	C	C4'-C3'-O3'	7.63	120.84	109.40
1	1	1030	A	C2'-C3'-O3'	7.50	120.75	109.50
5	B	136	ASN	N-CA-C	7.43	119.38	111.28
10	G	62	VAL	CA-C-N	-7.29	114.41	119.66
10	G	62	VAL	C-N-CA	-7.29	114.41	119.66
1	1	2743	G	C2'-C3'-O3'	7.28	120.42	109.50
16	N	183	HIS	N-CA-C	7.24	120.22	111.82
5	B	139	ALA	N-CA-C	7.22	118.94	111.14
1	1	152	A	C2'-C3'-O3'	-7.16	98.76	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	j	39	TYR	C-N-CD	7.16	136.35	120.60
29	a	47	ARG	N-CA-C	7.14	119.14	111.36
6	C	194	ARG	N-CA-C	7.07	121.61	112.92
1	1	2225	U	C2'-C3'-O3'	7.02	120.03	109.50
1	1	1787	C	C4'-C3'-O3'	6.95	119.82	109.40
1	1	807	U	C4'-C3'-O3'	6.94	119.81	109.40
10	G	63	PRO	O-C-N	6.89	124.39	121.15
10	G	153	VAL	N-CA-C	6.83	118.66	112.17
5	B	204	GLY	N-CA-C	6.83	120.95	112.14
1	1	271	G	C2'-C3'-O3'	6.64	119.45	109.50
1	1	1373	U	C2'-C3'-O3'	6.52	119.28	109.50
1	1	225	A	C4'-C3'-O3'	6.49	119.14	109.40
1	1	1628	U	C2'-C3'-O3'	6.49	119.24	109.50
6	C	189	SER	N-CA-C	6.46	118.35	110.41
19	Q	161	THR	N-CA-C	6.40	121.09	113.16
38	j	27	PHE	N-CA-C	-6.39	98.79	109.07
2	3	51	A	C2'-C3'-O3'	6.38	119.07	109.50
27	Y	111	MET	N-CA-C	6.37	119.48	110.50
23	U	14	VAL	N-CA-C	6.36	116.53	110.42
4	A	179	LYS	N-CA-C	6.26	119.68	109.59
6	C	78	GLY	N-CA-C	-6.24	102.07	110.56
7	D	237	ILE	N-CA-C	6.22	116.97	110.62
1	1	1014	U	C2'-C3'-O3'	6.17	118.76	109.50
12	I	193	CYS	N-CA-C	-6.12	101.90	110.35
16	N	196	ASN	N-CA-C	6.09	120.71	113.28
10	G	63	PRO	CA-C-N	-6.03	114.17	120.38
10	G	63	PRO	C-N-CA	-6.03	114.17	120.38
5	B	327	ILE	N-CA-C	6.01	116.79	110.72
18	P	37	ILE	N-CA-C	6.01	118.56	111.05
41	m	124	ILE	N-CA-C	5.99	116.74	108.12
7	D	277	ALA	CA-C-N	-5.93	113.66	119.76
7	D	277	ALA	C-N-CA	-5.93	113.66	119.76
17	O	61	ASN	N-CA-C	5.91	117.72	111.28
4	A	206	ASP	N-CA-C	5.90	117.80	111.36
8	E	27	SER	N-CA-C	5.90	117.72	111.28
10	G	154	ILE	CB-CA-C	-5.86	104.23	112.14
8	E	16	LYS	N-CA-C	-5.84	104.99	111.36
5	B	142	LYS	N-CA-C	5.82	117.63	111.28
8	E	30	ARG	CA-C-N	-5.79	114.30	120.03
8	E	30	ARG	C-N-CA	-5.79	114.30	120.03
19	Q	153	ALA	CA-C-N	-5.77	113.84	119.78
19	Q	153	ALA	C-N-CA	-5.77	113.84	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2722	G	C4'-C3'-O3'	5.76	121.65	113.00
1	1	1614	A	C2'-C3'-O3'	5.76	118.14	109.50
7	D	244	LYS	N-CA-C	5.75	117.55	111.28
1	1	1618	U	C3'-C2'-O2'	5.75	119.32	110.70
6	C	83	ARG	N-CA-C	-5.72	105.12	111.36
30	b	18	ARG	N-CA-C	-5.72	105.04	111.28
23	U	10	CYS	N-CA-C	5.70	119.82	112.41
19	Q	152	ALA	N-CA-C	-5.63	102.56	110.50
9	F	158	ILE	CB-CA-C	-5.63	105.48	111.00
4	A	175	LYS	CA-C-N	-5.63	114.79	120.31
4	A	175	LYS	C-N-CA	-5.63	114.79	120.31
1	1	2451	A	C2'-C3'-O3'	5.63	117.94	109.50
1	1	457	U	C4'-C3'-O3'	5.59	117.78	109.40
18	P	155	GLU	N-CA-C	-5.58	103.17	110.53
32	d	67	PRO	CA-C-N	-5.52	114.07	119.76
32	d	67	PRO	C-N-CA	-5.52	114.07	119.76
7	D	280	LYS	CA-C-N	-5.50	114.29	119.85
7	D	280	LYS	C-N-CA	-5.50	114.29	119.85
16	N	188	ARG	N-CA-C	-5.49	105.20	111.07
1	1	2678	U	C2'-C3'-O3'	5.49	117.73	109.50
1	1	1619	C	C2'-C3'-O3'	-5.47	105.49	113.70
8	E	89	GLY	CA-C-N	-5.45	113.71	120.79
8	E	89	GLY	C-N-CA	-5.45	113.71	120.79
1	1	113	A	C2'-C3'-O3'	5.45	117.67	109.50
38	j	32	SER	N-CA-C	5.43	119.07	111.74
21	S	170	ARG	CA-C-N	-5.42	114.37	119.85
21	S	170	ARG	C-N-CA	-5.42	114.37	119.85
5	B	138	LYS	N-CA-C	5.40	116.97	111.14
42	o	31	GLU	N-CA-C	5.39	118.05	110.23
1	1	1327	C	C4'-C3'-O3'	5.39	117.48	109.40
6	C	221	ILE	CA-C-N	-5.37	114.23	119.76
6	C	221	ILE	C-N-CA	-5.37	114.23	119.76
1	1	1070	A	C2'-C3'-O3'	5.37	117.56	109.50
6	C	10	ALA	N-CA-C	-5.37	103.44	110.53
6	C	47	GLN	CA-C-N	-5.35	114.41	119.76
6	C	47	GLN	C-N-CA	-5.35	114.41	119.76
15	M	15	ILE	N-CA-C	5.33	114.94	107.37
6	C	207	ILE	N-CA-C	5.33	115.57	108.11
6	C	221	ILE	N-CA-C	-5.32	101.77	108.05
1	1	2047	A	C4'-C3'-O3'	5.32	117.38	109.40
17	O	67	GLY	CA-C-N	-5.31	114.09	119.83
17	O	67	GLY	C-N-CA	-5.31	114.09	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	89	ARG	CA-C-N	-5.31	114.49	119.85
10	G	89	ARG	C-N-CA	-5.31	114.49	119.85
24	V	30	ASP	N-CA-C	5.31	117.53	110.53
7	D	240	ASP	N-CA-C	5.29	117.05	111.28
38	j	29	ILE	N-CA-C	5.29	115.50	110.42
6	C	223	GLY	N-CA-C	5.22	122.30	115.36
39	k	60	ILE	CA-C-N	-5.22	114.39	119.76
39	k	60	ILE	C-N-CA	-5.22	114.39	119.76
11	H	131	ILE	N-CA-C	5.20	115.39	108.11
1	1	1070	A	C4'-C3'-O3'	5.19	117.19	109.40
6	C	186	HIS	N-CA-C	5.18	118.56	110.32
21	S	85	ASN	N-CA-C	5.17	116.70	108.79
20	R	156	GLN	N-CA-C	5.16	116.71	111.14
16	N	199	LYS	N-CA-C	5.16	116.93	108.52
1	1	643	G	C2'-C3'-O3'	-5.16	105.97	113.70
34	f	9	VAL	CA-C-N	-5.13	114.49	119.78
34	f	9	VAL	C-N-CA	-5.13	114.49	119.78
33	e	124	ALA	N-CA-C	5.12	118.46	111.39
1	1	147	C	C2'-C3'-O3'	5.10	121.35	113.70
33	e	123	GLN	N-CA-C	5.10	117.13	109.23
12	I	121	LYS	CA-C-N	-5.09	114.67	119.76
12	I	121	LYS	C-N-CA	-5.09	114.67	119.76
34	f	22	ILE	N-CA-C	5.08	116.59	108.87
1	1	457	U	C2'-C3'-O3'	5.05	117.08	109.50
5	B	40	LYS	CA-C-N	-5.05	113.72	118.97
5	B	40	LYS	C-N-CA	-5.05	113.72	118.97
8	E	14	ASP	N-CA-C	5.03	116.76	111.28
38	j	20	ARG	N-CA-C	5.00	116.42	111.07

There are no chirality outliers.

There are no planarity outliers.

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	1	54325	0	27334	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3	2493	0	1268	6	0
3	4	3289	0	1657	12	0
4	A	1785	0	1814	46	0
5	B	3175	0	3279	128	0
6	C	2772	0	2885	101	0
7	D	2167	0	2281	54	0
8	E	1014	0	1076	99	0
9	F	1832	0	1902	26	0
10	G	1384	0	1464	110	0
11	H	1556	0	1555	33	0
12	I	1569	0	1606	78	0
13	J	1320	0	1360	23	0
14	L	1498	0	1574	12	0
15	M	1004	0	1049	27	0
16	N	1696	0	1738	33	0
17	O	1559	0	1598	29	0
18	P	1230	0	1245	14	0
19	Q	1465	0	1513	19	0
20	R	1299	0	1353	3	0
21	S	1384	0	1419	35	0
22	T	1255	0	1294	16	0
23	U	794	0	806	27	0
24	V	986	0	1047	8	0
25	W	513	0	496	13	0
26	X	803	0	853	0	0
27	Y	1068	0	1137	35	0
28	Z	1042	0	1071	15	0
29	a	1179	0	1197	33	0
30	b	415	0	420	14	0
31	c	727	0	748	2	0
32	d	783	0	834	13	0
33	e	1003	0	1032	26	0
34	f	781	0	815	47	0
35	g	921	0	963	1	0
36	h	984	0	1085	2	0
37	i	616	0	640	2	0
38	j	616	0	606	22	0
39	k	547	0	590	15	0
40	l	428	0	471	16	0
41	m	417	0	444	15	0
42	o	773	0	820	18	0
43	p	678	0	727	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	107145	0	79066	1170	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 6.

All (1170) 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)
4:A:64:LYS:HB2	4:A:71:PHE:CD1	1.22	1.67
23:U:17:LYS:HE3	23:U:85:ARG:CD	1.42	1.45
21:S:5:GLN:NE2	21:S:27:GLN:HE21	1.14	1.37
23:U:17:LYS:CE	23:U:85:ARG:HD3	1.53	1.37
28:Z:102:ALA:HB1	28:Z:110:LYS:CG	1.57	1.35
28:Z:25:LEU:HD22	28:Z:96:SER:CB	1.57	1.33
4:A:64:LYS:HB2	4:A:71:PHE:CE1	1.62	1.31
21:S:5:GLN:NE2	21:S:27:GLN:NE2	1.79	1.29
8:E:93:PRO:HB2	8:E:117:GLU:OE2	1.24	1.29
28:Z:102:ALA:CB	28:Z:110:LYS:HG3	1.60	1.28
4:A:64:LYS:CB	4:A:71:PHE:CD1	2.18	1.26
8:E:93:PRO:CB	8:E:117:GLU:OE2	1.83	1.26
38:j:22:CYS:SG	38:j:37:CYS:SG	2.36	1.23
1:1:889:G:OP2	34:f:26:ASN:OD1	1.53	1.21
4:A:64:LYS:CB	4:A:71:PHE:CE1	2.25	1.19
1:1:189:U:OP1	6:C:219:ARG:HD2	1.43	1.18
21:S:5:GLN:HE21	21:S:27:GLN:NE2	1.37	1.18
1:1:2691:A:H4'	5:B:387:PHE:O	1.38	1.17
1:1:2691:A:C4'	5:B:387:PHE:O	1.93	1.17
8:E:77:VAL:HG11	8:E:115:ALA:N	1.58	1.16
12:I:12:ILE:HG23	12:I:128:ARG:NH2	1.58	1.16
1:1:1126:A:OP1	33:e:125:ARG:O	1.62	1.16
8:E:66:GLY:HA3	8:E:101:TYR:HD1	1.09	1.15
4:A:64:LYS:HG3	4:A:71:PHE:HE1	1.07	1.14
12:I:130:ASN:OD1	12:I:133:SER:OG	1.66	1.13
4:A:64:LYS:CG	4:A:71:PHE:HE1	1.62	1.12
5:B:41:PRO:HA	5:B:203:GLY:CA	1.79	1.12
12:I:189:GLN:O	12:I:200:VAL:HB	1.49	1.12
8:E:25:ARG:HG3	9:F:154:ASN:HB3	1.29	1.12
27:Y:106:ILE:CG2	27:Y:109:LEU:HD21	1.80	1.11
7:D:229:PHE:HD1	7:D:232:TYR:CE2	1.67	1.11
8:E:16:LYS:NZ	19:Q:13:GLN:OE1	1.83	1.11
1:1:188:U:O2	6:C:216:LYS:NZ	1.84	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:64:LYS:HG3	4:A:71:PHE:CE1	1.86	1.10
10:G:84:PHE:CZ	10:G:201:PHE:N	2.20	1.10
7:D:202:GLN:HA	7:D:205:ILE:HD12	1.29	1.10
7:D:206:LEU:HD13	7:D:247:LYS:HE2	1.27	1.09
23:U:17:LYS:HZ2	23:U:85:ARG:NE	1.51	1.09
23:U:17:LYS:NZ	23:U:85:ARG:CZ	2.15	1.09
13:J:108:LEU:HD12	13:J:108:LEU:H	1.16	1.08
4:A:64:LYS:CG	4:A:71:PHE:CE1	2.37	1.07
5:B:41:PRO:HA	5:B:203:GLY:HA3	1.28	1.07
13:J:110:LEU:HD23	13:J:110:LEU:H	1.18	1.07
10:G:91:GLU:OE2	10:G:96:LYS:HA	1.55	1.07
32:d:46:THR:HG21	32:d:89:THR:OG1	1.54	1.07
10:G:84:PHE:HZ	10:G:201:PHE:N	1.53	1.07
10:G:89:ARG:HG3	10:G:179:ILE:O	1.55	1.06
10:G:151:GLU:OE1	10:G:151:GLU:N	1.88	1.06
1:1:2690:U:H5"	5:B:330:MET:HE2	1.38	1.06
10:G:67:ASN:ND2	10:G:224:GLY:H	1.51	1.06
5:B:4:ARG:NH1	5:B:7:ASN:OD1	1.88	1.05
6:C:363:GLN:HE21	6:C:365:ILE:HG12	1.20	1.05
23:U:17:LYS:HZ1	23:U:85:ARG:CZ	1.68	1.05
12:I:115:MET:HE3	12:I:115:MET:HA	1.39	1.04
6:C:214:ILE:HD11	6:C:218:PHE:CE2	1.93	1.04
10:G:63:PRO:HD2	10:G:66:VAL:HG21	1.32	1.04
14:L:2:VAL:HG11	29:a:44:TRP:CE3	1.93	1.03
7:D:95:PRO:HB2	7:D:246:TYR:CE1	1.94	1.03
10:G:91:GLU:OE2	10:G:96:LYS:HG2	1.58	1.03
8:E:25:ARG:HG3	9:F:154:ASN:CB	1.88	1.03
1:1:1743:C:OP1	42:o:33:HIS:CE1	2.13	1.02
5:B:401:PHE:HD2	5:B:402:LEU:HD22	1.19	1.02
14:L:2:VAL:CG1	29:a:44:TRP:CD2	2.43	1.02
15:M:102:MET:HE1	17:O:198:PHE:CD1	1.95	1.02
23:U:17:LYS:NZ	23:U:85:ARG:NE	2.08	1.02
17:O:52:TYR:HD2	17:O:143:MET:HE2	1.20	1.01
1:1:256:G:P	42:o:43:ARG:NH1	2.32	1.01
27:Y:51:ARG:NH1	27:Y:112:ASP:OD2	1.92	1.01
1:1:1901:G:O2'	17:O:66:ASP:OD1	1.76	1.01
8:E:26:ILE:HD12	9:F:153:LEU:HD21	1.41	1.01
8:E:66:GLY:HA3	8:E:101:TYR:CD1	1.95	1.01
27:Y:106:ILE:HG21	27:Y:109:LEU:CD2	1.91	1.01
4:A:64:LYS:CB	4:A:71:PHE:HD1	1.66	1.00
10:G:63:PRO:HD2	10:G:66:VAL:CG2	1.92	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:106:ILE:HG21	27:Y:109:LEU:HD21	1.36	1.00
8:E:74:ALA:HB1	8:E:87:VAL:HG13	1.42	1.00
5:B:401:PHE:CD2	5:B:402:LEU:HD22	1.97	0.99
1:1:2721:C:H2'	1:1:2722:G:H5''	1.44	0.99
18:P:37:ILE:HA	18:P:40:MET:CE	1.92	0.99
6:C:6:VAL:HG23	6:C:146:GLU:OE2	1.61	0.99
1:1:1618:U:HO2'	1:1:1619:C:H6	1.00	0.98
7:D:229:PHE:CD1	7:D:232:TYR:CE2	2.52	0.98
27:Y:106:ILE:CG2	27:Y:109:LEU:CD2	2.41	0.97
7:D:206:LEU:CD1	7:D:247:LYS:HE2	1.94	0.97
8:E:77:VAL:HG23	8:E:88:ALA:HB3	1.47	0.96
16:N:73:ARG:HD2	16:N:80:GLN:NE2	1.79	0.96
17:O:52:TYR:CD2	17:O:143:MET:HE2	2.00	0.96
1:1:1619:C:O2'	1:1:1620:A:O5'	1.83	0.95
11:H:124:MET:CE	11:H:184:ASP:CB	2.44	0.95
1:1:256:G:P	42:o:43:ARG:HH12	1.90	0.95
29:a:79:LYS:HG3	29:a:80:LEU:H	1.31	0.95
2:3:49:A:H5''	7:D:231:ARG:HD2	1.49	0.95
1:1:1617:A:O2'	1:1:1618:U:O5'	1.85	0.95
23:U:17:LYS:CE	23:U:85:ARG:CD	2.26	0.94
10:G:68:HIS:CE1	10:G:219:GLU:OE1	2.19	0.94
1:1:66:C:H4'	16:N:177:VAL:HG12	1.47	0.94
1:1:151:U:O2'	1:1:152:A:OP2	1.85	0.94
7:D:229:PHE:HD1	7:D:232:TYR:CD2	1.86	0.93
16:N:73:ARG:HH11	16:N:88:HIS:CE1	1.85	0.93
8:E:70:GLN:NE2	34:f:6:LYS:O	2.01	0.93
4:A:208:ARG:NH1	4:A:208:ARG:HB2	1.82	0.93
10:G:85:LEU:HD11	10:G:142:ILE:CD1	1.97	0.93
10:G:67:ASN:HD22	10:G:224:GLY:H	1.07	0.93
1:1:2721:C:C2'	1:1:2722:G:H5''	1.98	0.92
5:B:41:PRO:CA	5:B:203:GLY:HA3	1.98	0.92
38:j:18:ILE:HD11	40:l:51:ILE:HG23	1.50	0.92
15:M:17:PHE:HB3	15:M:54:ARG:HB2	1.50	0.92
1:1:1205:G:O6	40:l:2:ALA:HB3	1.70	0.92
1:1:47:U:O4	16:N:188:ARG:HD3	1.70	0.92
4:A:2:GLY:HA2	4:A:205:VAL:HG23	1.53	0.91
8:E:106:SER:OG	15:M:103:ASN:OD1	1.86	0.91
12:I:12:ILE:CG2	12:I:128:ARG:NH2	2.32	0.91
12:I:29:PRO:HB3	12:I:125:LEU:CD1	2.01	0.91
3:4:84:C:H4'	27:Y:113:LYS:HE2	1.53	0.90
10:G:81:LEU:HD11	10:G:168:CYS:SG	2.12	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:121:ASN:ND2	11:H:129:HIS:HE1	1.67	0.90
6:C:360:MET:CE	21:S:77:TRP:HD1	1.83	0.90
8:E:77:VAL:CG2	8:E:88:ALA:CB	2.50	0.90
7:D:206:LEU:HD13	7:D:247:LYS:CE	2.00	0.90
11:H:121:ASN:ND2	11:H:129:HIS:CE1	2.40	0.90
11:H:124:MET:HE3	11:H:184:ASP:HB3	1.50	0.90
14:L:2:VAL:CG1	29:a:44:TRP:CE3	2.55	0.89
22:T:82:ASN:O	30:b:21:ILE:HA	1.72	0.89
8:E:77:VAL:HG23	8:E:88:ALA:CB	2.01	0.89
10:G:85:LEU:HD11	10:G:142:ILE:HD13	1.52	0.89
11:H:124:MET:HE3	11:H:184:ASP:CB	2.03	0.89
6:C:214:ILE:CD1	6:C:218:PHE:CE2	2.56	0.89
10:G:91:GLU:OE2	10:G:96:LYS:CA	2.20	0.88
12:I:191:VAL:HG23	12:I:200:VAL:HG23	1.55	0.88
7:D:206:LEU:HD11	7:D:247:LYS:HZ3	1.39	0.88
10:G:67:ASN:ND2	10:G:224:GLY:N	2.21	0.88
1:1:2722:G:HO2'	1:1:2723:A:H2	1.21	0.88
8:E:74:ALA:HB1	8:E:87:VAL:CG1	2.03	0.88
11:H:124:MET:HE2	11:H:184:ASP:CG	1.99	0.88
27:Y:108:LYS:O	27:Y:109:LEU:HD23	1.74	0.87
15:M:22:ASP:OD2	15:M:97:LYS:HE3	1.75	0.87
6:C:8:VAL:HG12	6:C:17:SER:O	1.75	0.86
1:1:543:A:H8	38:j:15:THR:OG1	1.59	0.86
5:B:41:PRO:HB3	5:B:201:ILE:CG2	2.06	0.86
5:B:325:LYS:HD2	5:B:383:THR:OG1	1.75	0.86
8:E:77:VAL:HG11	8:E:115:ALA:H	1.35	0.86
1:1:1348:U:O2'	1:1:1349:A:C5'	2.23	0.86
1:1:2488:C:C2	11:H:126:HIS:HB2	2.10	0.86
5:B:39:GLN:O	5:B:40:LYS:HD2	1.76	0.85
23:U:21:LEU:HD12	23:U:21:LEU:H	1.40	0.85
11:H:13:ILE:HG22	11:H:59:HIS:O	1.75	0.85
12:I:183:GLU:O	12:I:187:ASN:ND2	2.10	0.85
13:J:110:LEU:O	13:J:111:LYS:HG3	1.77	0.85
1:1:543:A:H8	38:j:15:THR:HG1	0.94	0.85
5:B:41:PRO:HB3	5:B:201:ILE:HG22	1.57	0.84
7:D:229:PHE:CD1	7:D:232:TYR:CD2	2.64	0.84
17:O:139:LEU:HD12	17:O:139:LEU:O	1.77	0.84
34:f:13:PHE:HE1	34:f:28:ALA:HB1	1.41	0.84
5:B:39:GLN:C	5:B:40:LYS:HD2	2.01	0.84
12:I:29:PRO:HB3	12:I:125:LEU:HD13	1.60	0.84
10:G:71:HIS:NE2	10:G:219:GLU:HG2	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:12:ILE:HG23	12:I:128:ARG:HH21	1.40	0.84
10:G:68:HIS:ND1	10:G:219:GLU:OE1	2.10	0.84
1:1:1743:C:OP1	42:o:33:HIS:HE1	1.56	0.84
10:G:91:GLU:OE2	10:G:96:LYS:CG	2.26	0.84
40:l:6:THR:HG22	40:l:7:LEU:N	1.91	0.84
17:O:124:CYS:SG	21:S:173:VAL:HB	2.17	0.84
32:d:46:THR:CG2	32:d:89:THR:OG1	2.25	0.84
38:j:39:TYR:CD1	38:j:40:PRO:HA	2.13	0.83
5:B:42:HIS:O	5:B:42:HIS:ND1	2.11	0.83
27:Y:106:ILE:HG22	27:Y:109:LEU:HD21	1.58	0.83
7:D:206:LEU:CD1	7:D:247:LYS:CE	2.55	0.83
1:1:1903:U:O2'	1:1:1904:A:O5'	1.97	0.83
11:H:121:ASN:HD22	11:H:129:HIS:HE1	1.25	0.83
12:I:199:ARG:HD2	12:I:201:TYR:CZ	2.13	0.83
10:G:73:LEU:HD13	10:G:212:PHE:HE2	1.44	0.82
18:P:37:ILE:HA	18:P:40:MET:HE3	1.61	0.82
39:k:12:LEU:HD11	39:k:59:SER:OG	1.80	0.82
5:B:391:ARG:HH11	25:W:13:HIS:CG	1.98	0.82
6:C:141:LEU:HD11	6:C:145:LYS:HA	1.61	0.82
5:B:203:GLY:O	5:B:209:LYS:HE3	1.80	0.81
1:1:1348:U:O2'	1:1:1349:A:O5'	1.98	0.81
7:D:229:PHE:HD1	7:D:232:TYR:HE2	1.27	0.81
13:J:110:LEU:O	13:J:111:LYS:CG	2.28	0.81
39:k:12:LEU:CD1	39:k:59:SER:OG	2.28	0.81
8:E:77:VAL:CG1	8:E:115:ALA:N	2.41	0.81
41:m:99:CYS:SG	41:m:113:CYS:SG	2.78	0.81
8:E:77:VAL:HG11	8:E:115:ALA:CA	2.11	0.81
8:E:77:VAL:CG2	8:E:88:ALA:HB3	2.10	0.81
5:B:201:ILE:O	5:B:209:LYS:HE2	1.80	0.81
10:G:73:LEU:HD13	10:G:212:PHE:CE2	2.16	0.81
28:Z:102:ALA:HB1	28:Z:110:LYS:HG3	0.82	0.81
33:e:68:LEU:CD1	33:e:121:LEU:HD13	2.11	0.81
1:1:889:G:P	34:f:26:ASN:OD1	2.38	0.80
24:V:28:CYS:HB3	24:V:34:ALA:O	1.81	0.80
5:B:159:VAL:HG23	5:B:201:ILE:HD11	1.63	0.80
10:G:133:ILE:CD1	10:G:156:MET:HE1	2.11	0.80
6:C:360:MET:O	6:C:361:SER:OG	1.99	0.80
7:D:237:ILE:HD13	7:D:242:LEU:CD2	2.12	0.80
1:1:1618:U:O2'	1:1:1619:C:O5'	1.99	0.80
14:L:2:VAL:HG12	29:a:44:TRP:CD2	2.17	0.80
15:M:98:ASN:ND2	17:O:198:PHE:O	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:206:LEU:HD11	7:D:247:LYS:NZ	1.96	0.80
5:B:327:ILE:HD12	5:B:328:ASN:N	1.97	0.79
5:B:391:ARG:NH1	25:W:13:HIS:CG	2.50	0.79
10:G:194:LYS:NZ	10:G:196:GLU:OE1	2.13	0.79
5:B:38:SER:O	5:B:39:GLN:HG2	1.81	0.79
10:G:84:PHE:CZ	10:G:201:PHE:CA	2.65	0.79
8:E:93:PRO:HB3	8:E:117:GLU:OE2	1.81	0.79
22:T:79:ARG:CZ	30:b:21:ILE:HD13	2.12	0.79
2:3:49:A:C5'	7:D:231:ARG:HD2	2.12	0.79
6:C:363:GLN:HE21	6:C:365:ILE:CG1	1.95	0.79
1:1:189:U:OP1	6:C:219:ARG:CD	2.30	0.78
12:I:115:MET:HE3	12:I:115:MET:CA	2.13	0.78
7:D:237:ILE:HD13	7:D:242:LEU:HD23	1.64	0.78
38:j:18:ILE:HD11	40:l:51:ILE:CG2	2.14	0.78
1:1:66:C:H4'	16:N:177:VAL:CG1	2.13	0.78
6:C:81:SER:HB3	6:C:84:ASN:ND2	1.97	0.78
33:e:97:ILE:N	33:e:122:ASN:HD21	1.81	0.78
27:Y:51:ARG:CZ	27:Y:112:ASP:OD2	2.31	0.78
10:G:84:PHE:CE2	10:G:200:ALA:C	2.62	0.77
1:1:2414:C:OP1	4:A:215:GLN:NE2	2.16	0.77
1:1:97:A:OP1	16:N:195:ARG:HD2	1.85	0.77
10:G:81:LEU:HD23	10:G:81:LEU:O	1.84	0.77
10:G:143:ILE:HD11	10:G:156:MET:HB3	1.66	0.77
21:S:5:GLN:HE22	21:S:27:GLN:NE2	1.81	0.77
12:I:184:LEU:HB3	12:I:190:ILE:HG23	1.66	0.77
5:B:311:LYS:NZ	5:B:312:ILE:HD11	2.00	0.77
6:C:214:ILE:HD11	6:C:218:PHE:CD2	2.18	0.77
11:H:124:MET:CE	11:H:184:ASP:HB2	2.15	0.76
1:1:256:G:OP2	42:o:43:ARG:NH1	2.17	0.76
34:f:9:VAL:HG13	34:f:95:VAL:HB	1.68	0.76
5:B:311:LYS:HG2	5:B:312:ILE:HD12	1.68	0.76
18:P:36:VAL:O	18:P:40:MET:HE2	1.84	0.76
4:A:208:ARG:HB2	4:A:208:ARG:HH11	1.51	0.76
1:1:2691:A:O4'	5:B:387:PHE:O	2.02	0.76
4:A:208:ARG:NH1	4:A:233:LEU:HD12	2.00	0.76
11:H:132:VAL:CG2	11:H:171:LEU:HD11	2.16	0.76
34:f:13:PHE:CE1	34:f:28:ALA:HB1	2.19	0.76
6:C:214:ILE:CD1	6:C:218:PHE:HE2	1.98	0.75
12:I:191:VAL:HG23	12:I:200:VAL:CG2	2.17	0.75
10:G:81:LEU:CD1	10:G:168:CYS:SG	2.74	0.75
22:T:79:ARG:NH2	30:b:21:ILE:HD13	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:108:LEU:H	13:J:108:LEU:CD1	1.95	0.75
1:1:2221:U:OP2	42:o:32:ARG:NH1	2.19	0.75
6:C:141:LEU:C	6:C:141:LEU:HD12	2.12	0.75
7:D:202:GLN:CA	7:D:205:ILE:HD12	2.15	0.75
1:1:308:G:OP2	27:Y:14:LYS:NZ	2.18	0.74
15:M:98:ASN:HB3	17:O:198:PHE:HB2	1.69	0.74
6:C:360:MET:CE	21:S:77:TRP:CD1	2.69	0.74
11:H:121:ASN:HD22	11:H:129:HIS:CE1	2.03	0.74
8:E:76:VAL:HG13	8:E:85:VAL:CG1	2.17	0.74
40:l:6:THR:HG22	40:l:7:LEU:H	1.52	0.74
5:B:136:ASN:HD22	5:B:136:ASN:H	1.36	0.74
1:1:1346:G:H2'	1:1:1347:G:H5'	1.70	0.74
4:A:49:ILE:O	4:A:49:ILE:HD12	1.87	0.74
4:A:207:HIS:HD2	4:A:209:HIS:H	1.35	0.74
6:C:214:ILE:CD1	6:C:218:PHE:CD2	2.70	0.74
7:D:202:GLN:HA	7:D:205:ILE:CD1	2.16	0.74
6:C:363:GLN:NE2	6:C:365:ILE:HG12	2.02	0.73
11:H:124:MET:HE2	11:H:184:ASP:CB	2.16	0.73
16:N:73:ARG:CD	16:N:80:GLN:HE21	2.01	0.73
21:S:96:THR:HG23	21:S:97:THR:HG22	1.71	0.73
3:4:84:C:O3'	27:Y:113:LYS:HE2	1.88	0.73
21:S:163:ARG:HG3	34:f:36:VAL:HG11	1.69	0.73
10:G:84:PHE:CZ	10:G:200:ALA:C	2.66	0.73
33:e:96:MET:HE3	33:e:121:LEU:HB2	1.71	0.73
7:D:206:LEU:CD1	7:D:247:LYS:NZ	2.51	0.73
29:a:79:LYS:HG3	29:a:80:LEU:N	2.03	0.73
16:N:73:ARG:NH1	16:N:88:HIS:CE1	2.55	0.73
6:C:221:ILE:HD11	6:C:224:VAL:HG21	1.70	0.73
6:C:363:GLN:HG2	6:C:365:ILE:HG13	1.69	0.73
10:G:88:TYR:OH	10:G:194:LYS:HB2	1.89	0.73
13:J:106:ILE:HA	13:J:109:GLY:O	1.89	0.73
5:B:327:ILE:HD12	5:B:327:ILE:C	2.14	0.73
6:C:360:MET:HE1	21:S:77:TRP:HD1	1.52	0.73
10:G:67:ASN:HD21	10:G:224:GLY:HA3	1.52	0.73
13:J:110:LEU:H	13:J:110:LEU:CD2	1.95	0.73
38:j:18:ILE:CD1	40:l:51:ILE:HG23	2.17	0.73
29:a:59:ARG:HH11	29:a:59:ARG:HB2	1.53	0.72
5:B:401:PHE:HD2	5:B:402:LEU:CD2	1.99	0.72
4:A:64:LYS:C	4:A:64:LYS:HD3	2.14	0.72
5:B:398:ARG:O	5:B:402:LEU:HD23	1.90	0.72
1:1:2488:C:C2	11:H:126:HIS:CB	2.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2691:A:H4'	5:B:387:PHE:C	2.15	0.72
7:D:229:PHE:CD1	7:D:232:TYR:HE2	2.02	0.72
8:E:89:GLY:O	8:E:93:PRO:HB3	1.90	0.72
12:I:198:LYS:HG3	12:I:198:LYS:O	1.90	0.72
33:e:97:ILE:O	33:e:122:ASN:ND2	2.22	0.72
10:G:133:ILE:HD11	10:G:156:MET:HE1	1.72	0.72
12:I:115:MET:HA	12:I:115:MET:CE	2.19	0.72
1:I:2571:C:C5	41:m:114:ARG:NH1	2.58	0.71
34:f:66:ILE:CG2	34:f:76:VAL:HG21	2.20	0.71
34:f:70:HIS:O	34:f:75:VAL:HG23	1.91	0.71
8:E:84:ILE:HG21	8:E:96:GLU:OE2	1.91	0.71
16:N:73:ARG:HD2	16:N:80:GLN:HE21	1.52	0.71
11:H:124:MET:HE2	11:H:184:ASP:OD2	1.91	0.71
12:I:29:PRO:CB	12:I:125:LEU:CD1	2.68	0.71
10:G:193:VAL:HG12	10:G:194:LYS:N	2.06	0.71
5:B:159:VAL:CG2	5:B:201:ILE:HD11	2.20	0.70
12:I:185:GLN:NE2	12:I:185:GLN:HA	2.06	0.70
28:Z:102:ALA:CA	28:Z:110:LYS:HG3	2.19	0.70
34:f:7:LEU:C	34:f:7:LEU:HD23	2.16	0.70
5:B:39:GLN:HG3	5:B:40:LYS:H	1.55	0.70
8:E:93:PRO:C	8:E:94:VAL:HG23	2.15	0.70
14:L:3:ALA:O	14:L:6:ASN:ND2	2.24	0.70
8:E:23:ILE:HD12	8:E:23:ILE:C	2.16	0.70
38:j:19:CYS:HB2	38:j:27:PHE:HB2	1.72	0.70
12:I:176:TYR:CE1	12:I:199:ARG:NH2	2.59	0.70
13:J:105:HIS:ND1	13:J:106:ILE:HG13	2.07	0.70
5:B:402:LEU:HD23	5:B:402:LEU:N	2.06	0.70
10:G:67:ASN:HD21	10:G:224:GLY:CA	2.04	0.70
12:I:174:THR:HG21	12:I:197:VAL:HB	1.73	0.70
2:3:63:C:N3	12:I:202:ARG:HG3	2.06	0.70
27:Y:111:MET:HB3	27:Y:116:LYS:HE2	1.73	0.70
5:B:4:ARG:HH11	5:B:7:ASN:CG	2.00	0.70
16:N:73:ARG:CD	16:N:80:GLN:NE2	2.55	0.70
5:B:402:LEU:HD23	5:B:402:LEU:H	1.56	0.70
23:U:21:LEU:HD12	23:U:21:LEU:N	2.05	0.70
5:B:316:GLY:HA3	5:B:325:LYS:O	1.91	0.69
11:H:13:ILE:CG2	11:H:59:HIS:O	2.39	0.69
12:I:29:PRO:CB	12:I:125:LEU:HD12	2.23	0.69
33:e:37:ARG:HG2	33:e:37:ARG:HH21	1.57	0.69
8:E:77:VAL:CG2	8:E:88:ALA:HB2	2.22	0.69
12:I:29:PRO:CA	12:I:125:LEU:HD12	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:143:GLU:OE2	6:C:144:VAL:HG22	1.93	0.69
10:G:143:ILE:CG2	10:G:153:VAL:HG11	2.22	0.69
12:I:29:PRO:HB3	12:I:125:LEU:HD12	1.71	0.69
19:Q:159:SER:HB2	19:Q:161:THR:HG23	1.75	0.69
23:U:10:CYS:C	23:U:13:PRO:HD2	2.18	0.69
23:U:18:PHE:HE2	23:U:80:LYS:O	1.74	0.69
6:C:360:MET:HE1	21:S:77:TRP:CD1	2.28	0.69
1:1:2527:G:H5'	32:d:62:HIS:O	1.93	0.68
39:k:35:PHE:CE2	39:k:56:VAL:HG11	2.27	0.68
7:D:237:ILE:CD1	7:D:242:LEU:HD23	2.23	0.68
1:1:2393:G:N7	5:B:2:SER:HB2	2.07	0.68
21:S:105:MET:HE2	21:S:106:LEU:HD12	1.75	0.68
1:1:2722:G:O2'	1:1:2723:A:C2	2.46	0.68
1:1:1348:U:O2'	1:1:1349:A:H5''	1.93	0.68
13:J:105:HIS:HB2	13:J:119:HIS:O	1.93	0.68
1:1:2690:U:H5''	5:B:330:MET:CE	2.18	0.68
10:G:143:ILE:HG23	10:G:153:VAL:HG11	1.75	0.68
8:E:76:VAL:CG1	8:E:85:VAL:HG11	2.23	0.68
10:G:68:HIS:ND1	10:G:219:GLU:CD	2.51	0.68
12:I:191:VAL:HG12	12:I:192:ASP:N	2.09	0.68
21:S:5:GLN:HE21	21:S:27:GLN:HE21	0.68	0.68
33:e:37:ARG:HH21	33:e:37:ARG:CG	2.07	0.68
10:G:145:HIS:CD2	10:G:172:SER:H	2.12	0.68
3:4:84:C:C4'	27:Y:113:LYS:HE2	2.22	0.67
17:O:48:THR:HG22	17:O:139:LEU:HD22	1.75	0.67
10:G:193:VAL:HG12	10:G:194:LYS:H	1.58	0.67
12:I:68:ALA:HB1	12:I:136:MET:HE1	1.75	0.67
6:C:8:VAL:CG1	6:C:17:SER:O	2.41	0.67
33:e:97:ILE:N	33:e:122:ASN:ND2	2.43	0.67
1:1:506:C:H4'	19:Q:162:ARG:HG3	1.76	0.67
15:M:16:ASN:O	15:M:21:VAL:HG12	1.95	0.67
16:N:197:VAL:HG11	16:N:199:LYS:HZ1	1.60	0.67
6:C:209:ASN:OD1	6:C:210:GLU:N	2.27	0.67
8:E:90:PRO:O	8:E:91:VAL:HG22	1.95	0.67
1:1:1133:G:N7	6:C:186:HIS:HD2	1.92	0.67
5:B:4:ARG:O	5:B:5:LYS:HB3	1.95	0.67
14:L:6:ASN:ND2	14:L:6:ASN:H	1.91	0.66
34:f:66:ILE:HG21	34:f:76:VAL:HG21	1.77	0.66
6:C:143:GLU:OE2	6:C:144:VAL:HA	1.95	0.66
41:m:104:ALA:CB	41:m:115:HIS:HE1	2.08	0.66
8:E:105:THR:HG23	15:M:104:ASP:CB	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:88:ALA:O	6:C:89:TYR:HB2	1.95	0.66
6:C:207:ILE:HD12	6:C:247:THR:CG2	2.26	0.66
8:E:93:PRO:HB2	8:E:117:GLU:CD	2.16	0.66
10:G:90:PRO:HG3	10:G:180:VAL:HG13	1.76	0.66
10:G:192:GLU:O	10:G:193:VAL:HB	1.95	0.66
38:j:28:HIS:CD2	38:j:31:LYS:HB3	2.30	0.66
23:U:41:LEU:HD22	23:U:45:VAL:HG22	1.77	0.66
5:B:108:SER:HA	5:B:143:ARG:NH2	2.11	0.66
6:C:360:MET:HE3	21:S:77:TRP:HD1	1.61	0.66
12:I:189:GLN:O	12:I:200:VAL:CB	2.36	0.66
16:N:182:ARG:HH21	16:N:182:ARG:HG3	1.61	0.65
5:B:37:ALA:O	5:B:38:SER:OG	2.10	0.65
6:C:10:ALA:N	6:C:14:GLN:O	2.27	0.65
8:E:74:ALA:CB	8:E:87:VAL:CG1	2.73	0.65
6:C:52:ASP:HB3	6:C:55:ALA:HB2	1.79	0.65
6:C:157:GLU:OE2	6:C:212:LYS:HG3	1.95	0.65
10:G:82:PHE:CE2	10:G:175:ARG:CZ	2.79	0.65
12:I:183:GLU:O	12:I:187:ASN:CG	2.39	0.65
3:4:84:C:H4'	27:Y:113:LYS:CE	2.27	0.65
20:R:63:HIS:CE1	20:R:67:ILE:HD11	2.32	0.65
6:C:295:LYS:O	8:E:32:ALA:HB2	1.97	0.65
27:Y:58:ILE:HD12	27:Y:85:PHE:CE1	2.32	0.65
33:e:125:ARG:O	33:e:126:LYS:HB2	1.95	0.65
40:l:6:THR:CG2	40:l:7:LEU:N	2.60	0.65
1:1:2488:C:O2	11:H:126:HIS:HB2	1.96	0.65
5:B:4:ARG:HH11	5:B:7:ASN:HA	1.61	0.65
8:E:77:VAL:CG1	8:E:115:ALA:H	2.04	0.65
10:G:84:PHE:HZ	10:G:201:PHE:H	1.42	0.65
4:A:208:ARG:NH1	4:A:233:LEU:CD1	2.58	0.65
5:B:41:PRO:CB	5:B:201:ILE:CG2	2.75	0.65
6:C:10:ALA:HB3	6:C:14:GLN:CB	2.27	0.64
8:E:23:ILE:HD12	8:E:23:ILE:O	1.96	0.64
17:O:139:LEU:HD12	17:O:139:LEU:C	2.22	0.64
34:f:66:ILE:CG2	34:f:76:VAL:CG2	2.75	0.64
8:E:90:PRO:O	8:E:91:VAL:HG13	1.96	0.64
5:B:316:GLY:HA2	5:B:327:ILE:HG22	1.79	0.64
6:C:220:ASN:O	6:C:220:ASN:ND2	2.31	0.64
41:m:106:LEU:CD1	41:m:124:ILE:HD13	2.27	0.64
33:e:97:ILE:H	33:e:122:ASN:ND2	1.94	0.64
8:E:74:ALA:CB	8:E:87:VAL:HG13	2.24	0.64
42:o:35:ALA:O	42:o:39:ARG:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:229:PHE:HB3	7:D:232:TYR:HD2	1.63	0.64
13:J:108:LEU:HD12	13:J:108:LEU:N	2.01	0.64
13:J:108:LEU:N	13:J:109:GLY:HA3	2.13	0.64
27:Y:111:MET:HE1	27:Y:119:ILE:HD12	1.78	0.64
1:1:1348:U:HO2'	1:1:1349:A:H8	1.46	0.63
8:E:76:VAL:HG13	8:E:85:VAL:HG11	1.78	0.63
11:H:53:GLU:HA	11:H:53:GLU:OE1	1.97	0.63
17:O:56:LEU:HD11	17:O:143:MET:CE	2.28	0.63
1:1:1618:U:C2	1:1:1619:C:C5	2.86	0.63
10:G:67:ASN:ND2	10:G:224:GLY:CA	2.62	0.63
8:E:83:GLY:HA2	8:E:99:GLN:HE22	1.63	0.63
12:I:162:HIS:NE2	21:S:84:ARG:NE	2.46	0.63
10:G:84:PHE:HE2	10:G:200:ALA:C	2.07	0.63
1:1:97:A:O2'	16:N:183:HIS:CE1	2.52	0.63
1:1:529:C:H4'	6:C:91:ASN:ND2	2.13	0.63
8:E:90:PRO:C	8:E:91:VAL:HG13	2.24	0.63
14:L:2:VAL:HG11	29:a:44:TRP:CD2	2.22	0.63
32:d:41:LYS:HG3	32:d:46:THR:O	1.99	0.63
23:U:17:LYS:CE	23:U:85:ARG:NE	2.60	0.62
24:V:40:ILE:HD11	24:V:64:THR:HG23	1.80	0.62
5:B:5:LYS:HD2	5:B:5:LYS:O	2.00	0.62
39:k:12:LEU:CD2	39:k:59:SER:OG	2.47	0.62
6:C:359:ASN:O	22:T:156:ARG:NH2	2.32	0.62
10:G:149:PRO:HG2	10:G:152:LEU:HD11	1.80	0.62
10:G:156:MET:HB2	10:G:157:PRO:HD3	1.81	0.62
34:f:8:PHE:CD2	34:f:94:ARG:HG2	2.33	0.62
4:A:208:ARG:HH11	4:A:233:LEU:HD12	1.63	0.62
10:G:86:GLU:HA	10:G:179:ILE:HD11	1.81	0.62
12:I:176:TYR:HE1	12:I:199:ARG:NH2	1.97	0.62
10:G:150:ILE:O	10:G:154:ILE:HG13	2.00	0.62
39:k:22:TRP:HA	39:k:64:LEU:CD2	2.30	0.62
7:D:206:LEU:O	7:D:243:GLU:HA	2.00	0.62
34:f:5:VAL:O	34:f:96:MET:HE1	1.99	0.62
15:M:98:ASN:CB	17:O:198:PHE:HB2	2.29	0.62
29:a:42:ARG:NH1	29:a:46:ASP:OD2	2.33	0.62
29:a:79:LYS:O	29:a:80:LEU:HB2	1.99	0.62
34:f:36:VAL:HG12	34:f:36:VAL:O	2.00	0.62
38:j:36:LYS:O	38:j:57:ARG:NH1	2.32	0.62
1:1:1618:U:O2'	1:1:1619:C:H6	1.78	0.61
1:1:1619:C:O2'	1:1:1620:A:C5'	2.48	0.61
8:E:25:ARG:NH1	9:F:154:ASN:HB2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:62:VAL:HG12	10:G:66:VAL:CG2	2.29	0.61
1:1:1126:A:H5''	33:e:126:LYS:HD3	1.82	0.61
5:B:406:LYS:C	5:B:406:LYS:HE2	2.26	0.61
8:E:105:THR:CG2	15:M:104:ASP:CB	2.77	0.61
10:G:81:LEU:HD21	10:G:142:ILE:HD11	1.80	0.61
1:1:2722:G:O2'	1:1:2723:A:H2	1.81	0.61
23:U:17:LYS:HZ2	23:U:85:ARG:CZ	1.96	0.61
34:f:64:GLY:H	34:f:80:PHE:HA	1.66	0.61
1:1:2705:A:C2	1:1:2722:G:N2	2.68	0.61
10:G:84:PHE:CZ	10:G:200:ALA:HB3	2.35	0.61
3:4:22:C:OP1	6:C:192:LYS:NZ	2.33	0.61
3:4:84:C:C3'	27:Y:113:LYS:HE2	2.30	0.61
8:E:10:ILE:HG21	8:E:12:LYS:HD2	1.81	0.61
10:G:67:ASN:ND2	10:G:224:GLY:HA3	2.16	0.61
10:G:197:ASP:O	10:G:198:ARG:HB3	2.00	0.61
33:e:126:LYS:O	33:e:127:HIS:HB2	2.00	0.61
5:B:41:PRO:HA	5:B:203:GLY:N	2.15	0.61
5:B:338:LEU:O	5:B:339:VAL:HB	2.00	0.61
6:C:6:VAL:HG23	6:C:146:GLU:CD	2.26	0.61
1:1:330:U:H1'	6:C:79:SER:O	2.00	0.61
14:L:2:VAL:HG12	29:a:44:TRP:CG	2.35	0.61
23:U:17:LYS:HZ1	23:U:85:ARG:NH1	1.98	0.61
32:d:47:ASP:OD2	32:d:47:ASP:N	2.33	0.61
4:A:208:ARG:HB2	4:A:208:ARG:CZ	2.31	0.60
27:Y:106:ILE:HG22	27:Y:109:LEU:CD2	2.21	0.60
7:D:95:PRO:HB2	7:D:246:TYR:CD1	2.34	0.60
12:I:185:GLN:HA	12:I:185:GLN:HE21	1.66	0.60
22:T:79:ARG:NH2	30:b:21:ILE:CD1	2.64	0.60
5:B:334:PRO:O	5:B:335:HIS:HB2	2.01	0.60
15:M:18:GLY:O	15:M:21:VAL:HG13	2.01	0.60
19:Q:8:ARG:NH1	30:b:18:ARG:HH21	1.99	0.60
28:Z:25:LEU:CD2	28:Z:96:SER:CB	2.54	0.60
8:E:25:ARG:HG3	9:F:154:ASN:HB2	1.76	0.60
29:a:116:ALA:HB2	29:a:136:ALA:HA	1.83	0.60
32:d:41:LYS:HE3	32:d:47:ASP:HA	1.82	0.60
1:1:1617:A:HO2'	1:1:1618:U:C5'	2.09	0.60
12:I:114:GLY:O	12:I:115:MET:HB2	2.02	0.60
17:O:8:ASP:OD1	21:S:170:ARG:NH2	2.34	0.60
5:B:4:ARG:NH1	5:B:7:ASN:HA	2.17	0.60
3:4:84:C:C4'	27:Y:113:LYS:HG3	2.31	0.60
8:E:77:VAL:HG21	8:E:88:ALA:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:21:ILE:HG22	30:b:21:ILE:O	2.02	0.60
12:I:191:VAL:CG2	12:I:200:VAL:CG2	2.80	0.59
8:E:105:THR:HG23	15:M:104:ASP:HB2	1.83	0.59
34:f:7:LEU:HD23	34:f:7:LEU:O	2.01	0.59
6:C:221:ILE:HD11	6:C:224:VAL:HG11	1.83	0.59
19:Q:159:SER:O	19:Q:160:LYS:HB2	2.02	0.59
8:E:19:SER:HB2	8:E:23:ILE:O	2.02	0.59
1:l:529:C:H4'	6:C:91:ASN:HD21	1.67	0.59
12:I:176:TYR:OH	12:I:199:ARG:NH2	2.35	0.59
22:T:79:ARG:CZ	30:b:21:ILE:CD1	2.80	0.59
11:H:132:VAL:HG22	11:H:171:LEU:HD11	1.84	0.59
3:4:84:C:H4'	27:Y:113:LYS:HG3	1.84	0.59
4:A:64:LYS:HB2	4:A:71:PHE:HD1	0.85	0.59
5:B:118:TYR:CE2	5:B:131:PHE:HE2	2.20	0.59
1:l:1617:A:H2'	1:l:1618:U:C6	2.38	0.59
6:C:221:ILE:CG1	6:C:224:VAL:HG22	2.33	0.59
10:G:62:VAL:HG12	10:G:66:VAL:HG23	1.84	0.59
21:S:152:LYS:HD2	21:S:173:VAL:CG1	2.33	0.59
6:C:11:GLN:CD	6:C:155:VAL:HG12	2.28	0.59
10:G:90:PRO:HD2	10:G:180:VAL:HA	1.85	0.59
39:k:12:LEU:HD21	39:k:59:SER:OG	2.03	0.59
39:k:22:TRP:HA	39:k:64:LEU:HD21	1.84	0.59
40:l:2:ALA:HB1	40:l:5:LYS:NZ	2.17	0.59
4:A:49:ILE:HD12	4:A:49:ILE:C	2.28	0.58
6:C:214:ILE:HD12	6:C:218:PHE:CD2	2.38	0.58
8:E:25:ARG:CG	9:F:154:ASN:CB	2.75	0.58
27:Y:108:LYS:C	27:Y:109:LEU:HD23	2.28	0.58
40:l:6:THR:CG2	40:l:7:LEU:H	2.15	0.58
8:E:17:ARG:HB3	8:E:25:ARG:CZ	2.33	0.58
5:B:236:ILE:HD12	5:B:294:THR:HG22	1.86	0.58
5:B:236:ILE:HG23	5:B:294:THR:HG22	1.83	0.58
11:H:124:MET:CE	11:H:184:ASP:HB3	2.17	0.58
19:Q:154:PRO:HA	19:Q:159:SER:OG	2.04	0.58
34:f:29:LEU:C	34:f:30:LEU:HD12	2.28	0.58
41:m:106:LEU:HD12	41:m:124:ILE:HD13	1.85	0.58
15:M:103:ASN:HD22	15:M:104:ASP:N	2.01	0.58
16:N:182:ARG:HH21	16:N:182:ARG:CG	2.15	0.58
29:a:78:ASP:OD1	29:a:79:LYS:N	2.36	0.58
16:N:73:ARG:NH1	16:N:88:HIS:HE1	1.98	0.58
7:D:235:ALA:N	7:D:236:GLY:HA2	2.18	0.58
23:U:21:LEU:H	23:U:21:LEU:CD1	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2416:G:N7	4:A:214:HIS:NE2	2.50	0.58
21:S:163:ARG:CG	34:f:36:VAL:HG11	2.34	0.58
41:m:104:ALA:CB	41:m:115:HIS:CE1	2.86	0.58
1:1:1346:G:C2'	1:1:1347:G:H5'	2.34	0.58
5:B:312:ILE:HD12	5:B:312:ILE:N	2.18	0.58
4:A:64:LYS:CB	4:A:71:PHE:HE1	1.82	0.57
33:e:97:ILE:C	33:e:122:ASN:HD21	2.12	0.57
4:A:208:ARG:HH12	4:A:233:LEU:HD11	1.69	0.57
5:B:325:LYS:HZ2	5:B:383:THR:HG21	1.69	0.57
6:C:143:GLU:HA	6:C:144:VAL:C	2.29	0.57
6:C:363:GLN:HG2	6:C:365:ILE:CG1	2.34	0.57
7:D:279:LYS:HE3	7:D:279:LYS:HA	1.85	0.57
10:G:153:VAL:HG13	10:G:156:MET:CG	2.34	0.57
5:B:336:TYR:CD2	5:B:337:GLY:N	2.72	0.57
10:G:86:GLU:CA	10:G:179:ILE:HD11	2.33	0.57
23:U:18:PHE:N	23:U:18:PHE:CD1	2.72	0.57
10:G:153:VAL:HG12	10:G:153:VAL:O	2.03	0.57
9:F:157:ARG:HH21	9:F:203:LYS:HD2	1.70	0.57
16:N:73:ARG:HD2	16:N:80:GLN:HE22	1.69	0.57
1:1:2489:U:H4'	11:H:128:GLU:HG3	1.86	0.57
4:A:207:HIS:CD2	4:A:209:HIS:H	2.21	0.57
18:P:37:ILE:HG22	18:P:116:VAL:HG11	1.86	0.57
4:A:208:ARG:HH12	4:A:233:LEU:CD1	2.17	0.57
5:B:392:PHE:N	5:B:392:PHE:CD2	2.73	0.57
10:G:64:PRO:HG2	10:G:65:PRO:HD3	1.86	0.57
29:a:79:LYS:O	29:a:81:TRP:N	2.37	0.57
33:e:97:ILE:CA	33:e:122:ASN:HD21	2.16	0.57
6:C:144:VAL:HG12	6:C:146:GLU:H	1.69	0.57
39:k:23:VAL:HG23	39:k:64:LEU:HD13	1.85	0.57
40:l:3:ALA:O	40:l:4:HIS:HB2	2.05	0.57
1:1:1348:U:O2'	1:1:1349:A:H8	1.87	0.57
4:A:46:LYS:HD2	4:A:46:LYS:O	2.05	0.56
8:E:77:VAL:HG21	8:E:88:ALA:HB2	1.85	0.56
12:I:29:PRO:CB	12:I:125:LEU:HD13	2.33	0.56
12:I:191:VAL:CG2	12:I:200:VAL:HG23	2.33	0.56
8:E:81:GLY:O	8:E:82:ALA:HB3	2.05	0.56
12:I:99:ILE:CG1	12:I:123:GLU:HB2	2.35	0.56
27:Y:111:MET:CB	27:Y:116:LYS:HE2	2.34	0.56
1:1:27:C:OP1	16:N:190:ALA:HB2	2.06	0.56
1:1:1619:C:O2'	1:1:1620:A:P	2.63	0.56
9:F:79:LYS:HB3	9:F:188:VAL:HG11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:125:VAL:HG11	21:S:155:ILE:HD12	1.87	0.56
23:U:10:CYS:O	23:U:13:PRO:HD2	2.04	0.56
32:d:44:MET:SD	32:d:44:MET:N	2.78	0.56
12:I:196:HIS:CD2	12:I:197:VAL:N	2.73	0.56
1:1:309:A:H2	6:C:47:GLN:HE22	1.51	0.56
1:1:1067:U:OP1	8:E:25:ARG:HD3	2.05	0.56
8:E:105:THR:CG2	15:M:104:ASP:HB3	2.35	0.56
10:G:62:VAL:CG1	10:G:66:VAL:HG23	2.35	0.56
10:G:63:PRO:HD2	10:G:66:VAL:HG22	1.84	0.56
41:m:104:ALA:HB2	41:m:115:HIS:HE1	1.71	0.56
5:B:311:LYS:HZ2	5:B:312:ILE:HD11	1.69	0.56
7:D:242:LEU:O	7:D:246:TYR:HD2	1.89	0.56
14:L:2:VAL:CG1	29:a:44:TRP:CE2	2.89	0.56
23:U:19:PHE:O	23:U:20:GLN:HG3	2.06	0.56
24:V:30:ASP:CG	24:V:32:SER:HG	2.12	0.56
42:o:38:ARG:NH1	42:o:41:TYR:CD2	2.74	0.56
1:1:2219:C:O3'	42:o:37:GLY:HA3	2.05	0.56
6:C:207:ILE:HD12	6:C:247:THR:HG23	1.86	0.56
10:G:153:VAL:HG13	10:G:156:MET:HG3	1.87	0.56
17:O:56:LEU:HD11	17:O:143:MET:HE1	1.87	0.56
1:1:97:A:HO2'	16:N:183:HIS:CE1	2.24	0.56
23:U:10:CYS:O	23:U:14:VAL:HG23	2.06	0.56
23:U:18:PHE:CE2	23:U:80:LYS:O	2.58	0.56
34:f:6:LYS:O	34:f:7:LEU:HB3	2.05	0.56
34:f:66:ILE:HG23	34:f:76:VAL:HG22	1.88	0.56
38:j:34:CYS:SG	38:j:37:CYS:SG	3.02	0.56
5:B:311:LYS:NZ	5:B:312:ILE:CD1	2.69	0.56
10:G:150:ILE:N	10:G:151:GLU:OE1	2.39	0.56
5:B:391:ARG:CZ	25:W:34:GLU:CD	2.79	0.56
40:l:2:ALA:HB2	40:l:5:LYS:HE3	1.88	0.56
42:o:36:LEU:HD21	42:o:40:ARG:NH2	2.21	0.56
10:G:84:PHE:CE2	10:G:201:PHE:HA	2.42	0.55
10:G:145:HIS:CD2	10:G:172:SER:N	2.73	0.55
5:B:39:GLN:HG3	5:B:40:LYS:N	2.20	0.55
13:J:105:HIS:O	13:J:106:ILE:HB	2.07	0.55
18:P:95:LEU:HB3	18:P:151:ILE:HD12	1.88	0.55
34:f:58:GLN:HG2	34:f:60:PHE:CE1	2.40	0.55
5:B:316:GLY:CA	5:B:325:LYS:O	2.54	0.55
7:D:229:PHE:CB	7:D:232:TYR:HD2	2.20	0.55
10:G:67:ASN:HD21	10:G:224:GLY:N	1.97	0.55
23:U:17:LYS:HD2	23:U:82:ILE:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:256:G:O5'	42:o:43:ARG:NH1	2.36	0.55
12:I:174:THR:CG2	12:I:197:VAL:HB	2.37	0.55
6:C:10:ALA:HB3	6:C:14:GLN:HB2	1.87	0.55
6:C:83:ARG:O	6:C:86:GLN:HB2	2.06	0.55
7:D:237:ILE:O	7:D:238:THR:OG1	2.19	0.55
16:N:189:TYR:C	16:N:189:TYR:CD2	2.85	0.55
1:1:937:U:O2'	6:C:361:SER:HB3	2.07	0.55
10:G:84:PHE:CZ	10:G:201:PHE:HA	2.39	0.55
12:I:99:ILE:HG12	12:I:123:GLU:HB2	1.87	0.55
29:a:76:ASN:N	29:a:76:ASN:HD22	2.04	0.55
39:k:60:ILE:HG23	39:k:61:PRO:HD2	1.88	0.55
21:S:152:LYS:HD2	21:S:173:VAL:HG11	1.87	0.54
1:1:1619:C:HO2'	1:1:1620:A:P	2.29	0.54
8:E:26:ILE:HD12	9:F:153:LEU:CD2	2.27	0.54
12:I:191:VAL:CG1	12:I:192:ASP:N	2.70	0.54
4:A:200:ILE:HD11	4:A:217:MET:HG3	1.89	0.54
6:C:221:ILE:CG1	6:C:224:VAL:CG2	2.85	0.54
11:H:30:HIS:CD2	11:H:91:THR:HG22	2.43	0.54
15:M:16:ASN:C	15:M:21:VAL:HG12	2.32	0.54
6:C:76:VAL:HG13	6:C:84:ASN:HA	1.89	0.54
28:Z:10:VAL:HG23	28:Z:22:ALA:HB3	1.90	0.54
8:E:77:VAL:HG23	8:E:88:ALA:HB2	1.84	0.54
15:M:21:VAL:HG11	21:S:158:PRO:O	2.08	0.54
19:Q:152:ALA:O	19:Q:161:THR:HG21	2.07	0.54
38:j:28:HIS:O	38:j:32:SER:N	2.41	0.54
6:C:11:GLN:NE2	6:C:155:VAL:HG12	2.23	0.54
6:C:54:MET:O	6:C:54:MET:HG2	2.08	0.54
38:j:16:HIS:HB3	38:j:26:CYS:HA	1.90	0.54
1:1:332:U:O2'	38:j:16:HIS:HD2	1.91	0.54
5:B:391:ARG:HB2	5:B:392:PHE:CD2	2.43	0.54
1:1:1619:C:HO2'	1:1:1620:A:C5'	2.16	0.53
11:H:118:PHE:CE1	11:H:151:ILE:HD12	2.43	0.53
5:B:338:LEU:O	5:B:339:VAL:CB	2.55	0.53
16:N:197:VAL:CG1	16:N:199:LYS:HZ1	2.20	0.53
5:B:335:HIS:O	5:B:355:LYS:HE2	2.09	0.53
7:D:237:ILE:HG12	7:D:241:ASN:HB2	1.90	0.53
8:E:79:ASP:OD1	8:E:79:ASP:N	2.41	0.53
33:e:68:LEU:HD12	33:e:121:LEU:HD13	1.88	0.53
7:D:237:ILE:C	7:D:238:THR:HG23	2.33	0.53
8:E:95:ASN:N	8:E:95:ASN:OD1	2.40	0.53
13:J:108:LEU:CD2	13:J:121:MET:HE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:81:SER:CB	6:C:84:ASN:ND2	2.71	0.53
6:C:221:ILE:CD1	6:C:224:VAL:HG21	2.38	0.53
9:F:157:ARG:O	9:F:157:ARG:HG3	2.09	0.53
10:G:81:LEU:HD23	10:G:81:LEU:C	2.32	0.53
10:G:143:ILE:HD11	10:G:156:MET:CB	2.37	0.53
12:I:199:ARG:HG2	12:I:200:VAL:N	2.23	0.53
17:O:124:CYS:SG	21:S:173:VAL:CB	2.94	0.53
34:f:8:PHE:CD1	34:f:8:PHE:C	2.86	0.53
41:m:117:GLN:O	41:m:117:GLN:HG3	2.09	0.53
1:l:543:A:C8	38:j:15:THR:OG1	2.37	0.53
28:Z:102:ALA:O	28:Z:110:LYS:HD3	2.08	0.53
33:e:68:LEU:HD13	33:e:121:LEU:HD13	1.87	0.53
5:B:136:ASN:HD22	5:B:136:ASN:N	2.03	0.53
10:G:62:VAL:CG1	10:G:66:VAL:CG2	2.87	0.53
34:f:58:GLN:HG2	34:f:60:PHE:CZ	2.43	0.53
5:B:280:TRP:HD1	17:O:62:SER:O	1.91	0.53
6:C:365:ILE:C	6:C:366:ASN:HD22	2.17	0.53
1:l:414:G:OP1	33:e:38:GLY:HA3	2.09	0.53
9:F:152:ASN:HD22	9:F:197:ARG:HH12	1.56	0.53
29:a:59:ARG:HH11	29:a:59:ARG:CB	2.22	0.53
38:j:18:ILE:CD1	40:l:51:ILE:CG2	2.82	0.52
8:E:13:LYS:HG3	8:E:13:LYS:O	2.09	0.52
10:G:193:VAL:CG1	10:G:194:LYS:H	2.21	0.52
18:P:25:VAL:HG21	18:P:91:LEU:HD11	1.92	0.52
6:C:214:ILE:HD12	6:C:218:PHE:HD2	1.74	0.52
7:D:32:ARG:CZ	7:D:36:ILE:HD11	2.39	0.52
10:G:64:PRO:HG2	10:G:65:PRO:CD	2.39	0.52
10:G:145:HIS:NE2	10:G:146:ASP:OD1	2.42	0.52
16:N:187:SER:HB2	16:N:190:ALA:H	1.74	0.52
19:Q:156:ASP:OD2	19:Q:159:SER:HB3	2.09	0.52
4:A:64:LYS:CA	4:A:71:PHE:HD1	2.20	0.52
5:B:312:ILE:HD12	5:B:312:ILE:H	1.75	0.52
9:F:150:THR:OG1	9:F:200:ALA:HB3	2.09	0.52
11:H:27:THR:HG22	11:H:42:VAL:HG22	1.92	0.52
19:Q:156:ASP:OD2	19:Q:159:SER:N	2.43	0.52
34:f:5:VAL:HG12	34:f:96:MET:SD	2.49	0.52
1:l:26:C:OP1	16:N:193:LYS:HE2	2.09	0.52
1:l:1347:G:O2'	1:l:1348:U:H5'	2.10	0.52
27:Y:51:ARG:NE	27:Y:112:ASP:OD2	2.41	0.52
10:G:84:PHE:CE2	10:G:201:PHE:N	2.72	0.52
15:M:102:MET:HE1	17:O:198:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:102:ALA:C	28:Z:110:LYS:HG3	2.35	0.52
34:f:37:SER:HB3	34:f:40:GLU:HB2	1.91	0.52
5:B:402:LEU:CD2	5:B:402:LEU:N	2.73	0.52
5:B:335:HIS:O	5:B:355:LYS:CE	2.58	0.52
6:C:363:GLN:NE2	12:I:167:ILE:O	2.42	0.52
23:U:17:LYS:HE3	23:U:85:ARG:HD3	0.59	0.52
27:Y:35:LEU:CD2	27:Y:109:LEU:HD11	2.40	0.52
10:G:71:HIS:NE2	10:G:219:GLU:CG	2.66	0.52
11:H:6:LEU:HD11	11:H:67:PHE:CE1	2.45	0.52
14:L:4:LYS:O	29:a:44:TRP:NE1	2.37	0.52
15:M:103:ASN:HD22	15:M:104:ASP:H	1.56	0.52
18:P:32:GLU:O	18:P:36:VAL:HG23	2.10	0.52
7:D:210:VAL:CG1	7:D:242:LEU:CD1	2.88	0.51
10:G:73:LEU:CD1	10:G:212:PHE:CE2	2.92	0.51
12:I:126:VAL:HG12	12:I:127:ALA:N	2.25	0.51
13:J:32:VAL:HG13	13:J:105:HIS:NE2	2.25	0.51
24:V:30:ASP:OD1	24:V:32:SER:OG	2.27	0.51
29:a:59:ARG:CB	29:a:59:ARG:NH1	2.73	0.51
40:l:2:ALA:CB	40:l:5:LYS:NZ	2.73	0.51
1:I:2321:U:OP1	12:I:115:MET:HB2	2.09	0.51
21:S:150:MET:O	21:S:175:GLY:HA2	2.09	0.51
27:Y:111:MET:HE1	27:Y:119:ILE:CD1	2.40	0.51
31:c:30:ILE:HD13	31:c:55:HIS:CD2	2.46	0.51
6:C:161:THR:HG22	6:C:217:ALA:O	2.11	0.51
9:F:99:ILE:HD11	9:F:123:MET:HG2	1.91	0.51
5:B:197:ILE:HD11	5:B:199:ILE:HD11	1.92	0.51
5:B:279:LEU:CD2	17:O:62:SER:HA	2.40	0.51
16:N:197:VAL:CG1	16:N:199:LYS:NZ	2.73	0.51
6:C:221:ILE:HD11	6:C:224:VAL:CG2	2.41	0.51
34:f:23:ILE:HG13	34:f:23:ILE:O	2.11	0.51
34:f:50:ALA:HA	34:f:62:ASN:O	2.11	0.51
6:C:301:LEU:CD1	8:E:28:PHE:HE1	2.23	0.51
7:D:272:MET:HE1	7:D:276:HIS:CE1	2.46	0.51
10:G:82:PHE:O	10:G:86:GLU:N	2.36	0.51
40:l:2:ALA:HB1	40:l:5:LYS:HZ2	1.75	0.51
7:D:229:PHE:CD1	7:D:232:TYR:HD2	2.25	0.51
2:3:51:A:O2'	2:3:52:U:O5'	2.23	0.51
7:D:232:TYR:O	7:D:236:GLY:HA2	2.10	0.51
8:E:76:VAL:HG11	8:E:85:VAL:HG11	1.93	0.51
12:I:115:MET:CA	12:I:115:MET:CE	2.86	0.51
10:G:84:PHE:HE2	10:G:200:ALA:O	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:108:LEU:HD22	13:J:121:MET:HE2	1.92	0.51
18:P:65:LYS:HA	18:P:68:ILE:HD12	1.92	0.51
18:P:156:LYS:C	18:P:156:LYS:HD2	2.36	0.51
1:1:1613:G:N2	1:1:1615:A:O2'	2.44	0.50
34:f:30:LEU:N	34:f:30:LEU:CD1	2.73	0.50
39:k:35:PHE:HE2	39:k:56:VAL:HG11	1.71	0.50
1:1:2372:C:OP1	5:B:7:ASN:HB2	2.12	0.50
4:A:175:LYS:HB2	43:p:29:ILE:HD13	1.94	0.50
5:B:36:ASP:OD1	5:B:36:ASP:N	2.44	0.50
43:p:51:ALA:HB3	43:p:54:ILE:HD12	1.91	0.50
8:E:76:VAL:CG1	8:E:85:VAL:CG1	2.86	0.50
10:G:82:PHE:CE2	10:G:175:ARG:NE	2.78	0.50
12:I:99:ILE:O	12:I:120:GLY:HA3	2.12	0.50
19:Q:34:LEU:O	19:Q:38:THR:HG22	2.11	0.50
19:Q:158:ASN:N	19:Q:158:ASN:ND2	2.60	0.50
1:1:696:C:OP1	30:b:19:ASN:ND2	2.33	0.50
5:B:205:ASP:O	5:B:207:ALA:N	2.39	0.50
1:1:2395:A:N7	5:B:3:HIS:ND1	2.59	0.50
29:a:14:GLN:O	29:a:15:VAL:HG22	2.12	0.50
4:A:116:VAL:HG23	4:A:162:ALA:HB2	1.93	0.50
8:E:33:VAL:HG11	9:F:20:LYS:HD2	1.94	0.50
11:H:132:VAL:CG2	11:H:171:LEU:CD1	2.87	0.50
34:f:66:ILE:HG23	34:f:76:VAL:CG2	2.39	0.50
1:1:2488:C:C2	11:H:126:HIS:HB3	2.47	0.50
5:B:36:ASP:HB2	5:B:39:GLN:OE1	2.11	0.50
6:C:362:THR:HB	22:T:157:GLU:HG3	1.92	0.50
1:1:2180:U:O2'	1:1:2182:G:O4'	2.30	0.50
3:4:153:G:O2'	3:4:155:A:OP1	2.29	0.50
5:B:325:LYS:HZ2	5:B:383:THR:CG2	2.25	0.50
8:E:84:ILE:CG2	8:E:96:GLU:OE2	2.59	0.50
17:O:139:LEU:HD12	17:O:143:MET:HG2	1.94	0.50
21:S:83:THR:O	21:S:84:ARG:HB2	2.12	0.50
1:1:1619:C:O2'	1:1:1620:A:O4'	2.29	0.49
4:A:214:HIS:O	4:A:216:HIS:HD2	1.95	0.49
34:f:29:LEU:C	34:f:30:LEU:CD1	2.85	0.49
41:m:118:CYS:SG	41:m:121:CYS:SG	3.02	0.49
1:1:1665:A:H4'	4:A:177:LEU:O	2.13	0.49
5:B:395:LYS:HG3	5:B:396:GLU:N	2.28	0.49
7:D:40:LYS:HE3	22:T:93:THR:HG21	1.93	0.49
11:H:120:PHE:HB2	11:H:130:LYS:H	1.77	0.49
15:M:16:ASN:OD1	15:M:56:LYS:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:59:ARG:HB2	29:a:59:ARG:NH1	2.24	0.49
7:D:235:ALA:HB3	7:D:236:GLY:HA2	1.94	0.49
10:G:193:VAL:CG1	10:G:194:LYS:N	2.72	0.49
12:I:187:ASN:N	12:I:187:ASN:HD22	2.08	0.49
38:j:28:HIS:O	38:j:32:SER:HA	2.11	0.49
5:B:136:ASN:H	5:B:136:ASN:ND2	2.08	0.49
5:B:136:ASN:N	5:B:136:ASN:ND2	2.60	0.49
8:E:93:PRO:O	8:E:94:VAL:HG23	2.11	0.49
10:G:63:PRO:HD3	16:N:21:PHE:CD2	2.47	0.49
29:a:35:ALA:O	29:a:41:GLN:OE1	2.29	0.49
5:B:311:LYS:HZ3	5:B:312:ILE:HD11	1.76	0.49
8:E:33:VAL:HG11	9:F:20:LYS:CD	2.42	0.49
32:d:40:ALA:HB2	32:d:75:PHE:CE1	2.48	0.49
1:l:2221:U:P	42:o:32:ARG:NH1	2.85	0.49
1:l:2489:U:C4'	11:H:128:GLU:HG3	2.43	0.49
5:B:201:ILE:CD1	5:B:213:ALA:HB2	2.41	0.49
6:C:9:LEU:HA	6:C:14:GLN:O	2.11	0.49
34:f:18:ARG:HB3	34:f:23:ILE:HG22	1.94	0.49
8:E:74:ALA:CB	8:E:87:VAL:HG11	2.42	0.49
10:G:143:ILE:HG21	10:G:153:VAL:HG11	1.93	0.49
36:h:69:LEU:HD23	36:h:83:LEU:HD11	1.95	0.49
9:F:151:ALA:CB	9:F:198:PHE:CZ	2.96	0.49
1:l:1617:A:H2'	1:l:1618:U:H6	1.78	0.49
10:G:90:PRO:CD	10:G:180:VAL:HA	2.42	0.49
12:I:31:ILE:HD11	12:I:65:LEU:HB2	1.94	0.49
16:N:182:ARG:CG	16:N:182:ARG:NH2	2.74	0.49
40:l:13:LEU:CD2	40:l:49:MET:HE1	2.42	0.49
8:E:84:ILE:HG21	8:E:96:GLU:CD	2.38	0.49
21:S:85:ASN:N	21:S:85:ASN:ND2	2.60	0.49
38:j:27:PHE:HA	38:j:34:CYS:HA	1.95	0.49
5:B:205:ASP:O	5:B:206:VAL:HB	2.13	0.48
4:A:49:ILE:C	4:A:49:ILE:CD1	2.86	0.48
6:C:10:ALA:HB3	6:C:14:GLN:HB3	1.94	0.48
10:G:91:GLU:OE2	10:G:96:LYS:CB	2.61	0.48
21:S:173:VAL:HG12	21:S:173:VAL:O	2.13	0.48
10:G:67:ASN:HD22	10:G:224:GLY:N	1.89	0.48
5:B:384:ALA:HB2	5:B:393:GLN:HE22	1.79	0.48
7:D:203:TYR:O	7:D:205:ILE:HG13	2.13	0.48
8:E:105:THR:CG2	15:M:104:ASP:OD2	2.61	0.48
1:l:417:U:OP2	29:a:22:VAL:HG12	2.13	0.48
15:M:103:ASN:ND2	15:M:104:ASP:N	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:j:36:LYS:HB2	38:j:36:LYS:NZ	2.28	0.48
1:1:2321:U:OP1	12:I:114:GLY:O	2.31	0.48
10:G:86:GLU:N	10:G:179:ILE:HD11	2.27	0.48
1:1:151:U:HO2'	1:1:152:A:P	2.27	0.48
5:B:36:ASP:O	5:B:37:ALA:HB3	2.13	0.48
7:D:40:LYS:CE	22:T:93:THR:HG21	2.44	0.48
11:H:132:VAL:HG23	11:H:171:LEU:HD11	1.96	0.48
24:V:28:CYS:SG	24:V:30:ASP:CG	2.97	0.48
5:B:311:LYS:HZ2	5:B:312:ILE:CD1	2.27	0.48
10:G:81:LEU:HD11	10:G:168:CYS:HG	1.79	0.48
23:U:19:PHE:C	23:U:20:GLN:HG3	2.39	0.48
32:d:19:ALA:HB1	32:d:35:VAL:HG21	1.94	0.48
5:B:391:ARG:NH2	25:W:34:GLU:OE2	2.46	0.47
12:I:176:TYR:CZ	12:I:199:ARG:NH2	2.82	0.47
12:I:196:HIS:HD2	12:I:197:VAL:N	2.11	0.47
32:d:11:GLU:HG2	32:d:74:THR:HG22	1.95	0.47
5:B:329:PRO:HG2	5:B:332:GLY:O	2.14	0.47
5:B:391:ARG:NH1	25:W:13:HIS:ND1	2.62	0.47
6:C:91:ASN:OD1	6:C:92:PHE:N	2.47	0.47
8:E:77:VAL:HG12	8:E:114:ASN:HA	1.95	0.47
28:Z:102:ALA:HB1	28:Z:110:LYS:HG2	1.79	0.47
1:1:2225:U:O2	1:1:2225:U:O4'	2.31	0.47
4:A:205:VAL:HG13	4:A:206:ASP:N	2.29	0.47
6:C:54:MET:O	6:C:58:LYS:NZ	2.47	0.47
16:N:6:TYR:CE1	37:i:30:ILE:HD11	2.49	0.47
34:f:5:VAL:HG12	34:f:96:MET:HE1	1.97	0.47
39:k:22:TRP:CA	39:k:64:LEU:HD21	2.44	0.47
40:l:2:ALA:CB	40:l:5:LYS:HZ2	2.27	0.47
6:C:52:ASP:OD1	6:C:53:PRO:HD2	2.14	0.47
6:C:81:SER:HB3	6:C:84:ASN:HD21	1.77	0.47
7:D:206:LEU:HD22	7:D:247:LYS:HG3	1.96	0.47
39:k:64:LEU:HD23	39:k:65:GLU:N	2.29	0.47
41:m:106:LEU:CD1	41:m:124:ILE:CD1	2.92	0.47
13:J:37:THR:HG22	13:J:67:ILE:HD11	1.97	0.47
1:1:2571:C:C6	41:m:114:ARG:NH1	2.83	0.47
4:A:208:ARG:CZ	4:A:208:ARG:CB	2.92	0.47
7:D:279:LYS:HA	7:D:279:LYS:CE	2.43	0.47
10:G:84:PHE:CZ	10:G:200:ALA:CB	2.98	0.47
18:P:20:THR:HG23	18:P:95:LEU:HD21	1.96	0.47
29:a:56:VAL:CG1	29:a:57:GLY:N	2.77	0.47
42:o:38:ARG:NH1	42:o:41:TYR:CE2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:26:ARG:CZ	5:B:197:ILE:HG22	2.45	0.47
8:E:72:LYS:HD2	8:E:91:VAL:HG21	1.97	0.47
8:E:140:ILE:HD12	8:E:146:ILE:HD11	1.97	0.47
9:F:166:ILE:HD11	9:F:177:SER:C	2.40	0.47
10:G:90:PRO:HG2	10:G:180:VAL:O	2.15	0.47
6:C:219:ARG:O	6:C:220:ASN:HB3	2.15	0.47
13:J:110:LEU:HD23	13:J:110:LEU:N	2.04	0.47
13:J:110:LEU:O	13:J:111:LYS:HG2	2.12	0.47
6:C:362:THR:O	22:T:156:ARG:HA	2.14	0.47
1:1:1617:A:C5	1:1:1618:U:C4	3.04	0.46
6:C:221:ILE:HG13	6:C:224:VAL:HG22	1.96	0.46
27:Y:111:MET:HE3	27:Y:116:LYS:HG3	1.97	0.46
5:B:39:GLN:CG	5:B:40:LYS:N	2.75	0.46
8:E:8:SER:O	8:E:27:SER:OG	2.31	0.46
10:G:156:MET:CB	10:G:157:PRO:HD3	2.45	0.46
29:a:56:VAL:HG12	29:a:57:GLY:N	2.29	0.46
33:e:97:ILE:HB	33:e:122:ASN:ND2	2.30	0.46
41:m:99:CYS:SG	41:m:121:CYS:SG	3.10	0.46
1:1:2242:G:OP2	42:o:32:ARG:NH2	2.48	0.46
10:G:63:PRO:HD3	16:N:21:PHE:CG	2.50	0.46
6:C:192:LYS:HZ3	6:C:192:LYS:HB2	1.81	0.46
10:G:143:ILE:CD1	10:G:156:MET:CB	2.93	0.46
12:I:191:VAL:HB	12:I:198:LYS:HG3	1.97	0.46
5:B:311:LYS:CG	5:B:312:ILE:HD12	2.44	0.46
6:C:74:PRO:HB2	6:C:88:ALA:O	2.15	0.46
13:J:32:VAL:HG13	13:J:105:HIS:HE2	1.80	0.46
8:E:77:VAL:HG11	8:E:115:ALA:HA	1.97	0.46
10:G:89:ARG:CG	10:G:179:ILE:O	2.46	0.46
12:I:12:ILE:CG2	12:I:128:ARG:CZ	2.93	0.46
15:M:20:LEU:CD2	15:M:40:VAL:HG21	2.45	0.46
21:S:89:VAL:HG12	21:S:91:LYS:HG3	1.96	0.46
33:e:48:ARG:CZ	34:f:22:ILE:HD13	2.45	0.46
17:O:147:TYR:O	17:O:151:VAL:HG23	2.15	0.46
2:3:49:A:O5'	7:D:231:ARG:HD2	2.16	0.46
6:C:189:SER:O	6:C:192:LYS:HG3	2.16	0.46
8:E:15:ILE:O	8:E:15:ILE:HG22	2.15	0.46
8:E:94:VAL:HG12	8:E:94:VAL:O	2.15	0.46
10:G:63:PRO:O	10:G:66:VAL:HG22	2.16	0.46
16:N:116:LEU:HD13	16:N:151:ILE:HD11	1.98	0.46
37:i:57:ARG:HB3	37:i:74:LEU:HD11	1.98	0.46
11:H:119:ASP:CG	11:H:131:ILE:HG12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:126:VAL:CG1	12:I:127:ALA:N	2.78	0.46
1:1:1903:U:O2'	1:1:1904:A:H8	1.99	0.46
6:C:81:SER:CB	6:C:84:ASN:HD21	2.29	0.46
10:G:91:GLU:CD	10:G:96:LYS:HG2	2.34	0.46
3:4:84:C:H4'	27:Y:113:LYS:CD	2.45	0.45
5:B:279:LEU:HD23	17:O:62:SER:HA	1.98	0.45
9:F:151:ALA:HB1	9:F:198:PHE:CZ	2.51	0.45
5:B:270:ILE:HG21	5:B:278:VAL:HG22	1.99	0.45
17:O:139:LEU:CD1	17:O:143:MET:HG2	2.46	0.45
42:o:44:LYS:HD3	42:o:52:VAL:HG11	1.98	0.45
1:1:2446:G:O2'	1:1:2671:G:N7	2.49	0.45
5:B:236:ILE:HD12	5:B:294:THR:CG2	2.47	0.45
6:C:10:ALA:H	6:C:14:GLN:C	2.21	0.45
6:C:362:THR:CB	22:T:157:GLU:HG3	2.46	0.45
12:I:199:ARG:CD	12:I:201:TYR:CE1	3.00	0.45
1:1:2402:G:N3	5:B:268:ALA:HB1	2.31	0.45
8:E:64:ILE:HD11	8:E:74:ALA:HB3	1.98	0.45
8:E:83:GLY:CA	8:E:99:GLN:HE22	2.28	0.45
12:I:195:ASN:O	12:I:196:HIS:CG	2.69	0.45
22:T:68:SER:HA	30:b:36:ASN:HD21	1.81	0.45
34:f:66:ILE:CG2	34:f:76:VAL:HG22	2.46	0.45
1:1:2541:U:OP1	5:B:288:ARG:NH2	2.39	0.45
5:B:391:ARG:HH12	25:W:13:HIS:CE1	2.34	0.45
5:B:401:PHE:CD2	5:B:401:PHE:C	2.94	0.45
6:C:208:TYR:CD1	6:C:208:TYR:O	2.70	0.45
12:I:59:CYS:HB3	12:I:126:VAL:HG11	1.99	0.45
16:N:73:ARG:HG2	16:N:74:VAL:N	2.30	0.45
33:e:96:MET:HG3	33:e:122:ASN:OD1	2.16	0.45
34:f:8:PHE:CG	34:f:94:ARG:HG2	2.51	0.45
35:g:80:VAL:HG13	35:g:81:TYR:CD2	2.52	0.45
8:E:17:ARG:HB3	8:E:25:ARG:NH2	2.32	0.45
10:G:84:PHE:CE1	10:G:201:PHE:HB2	2.52	0.45
12:I:96:VAL:HG11	12:I:122:PRO:HB3	1.99	0.45
39:k:12:LEU:HD13	39:k:59:SER:OG	2.16	0.45
1:1:1347:G:C6	1:1:1348:U:O4	2.70	0.45
1:1:2571:C:OP1	41:m:114:ARG:NH2	2.47	0.45
1:1:2721:C:O2'	1:1:2722:G:H5''	2.15	0.45
5:B:406:LYS:C	5:B:406:LYS:CE	2.89	0.45
8:E:14:ASP:OD2	8:E:17:ARG:NH2	2.50	0.45
8:E:105:THR:HG21	15:M:104:ASP:HB3	1.99	0.45
12:I:98:ARG:HD2	12:I:120:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:334:A:OP1	38:j:36:LYS:NZ	2.50	0.45
3:4:84:C:O4'	27:Y:113:LYS:HG3	2.17	0.45
4:A:208:ARG:HB2	4:A:233:LEU:HD12	1.99	0.45
5:B:4:ARG:HH11	5:B:7:ASN:CA	2.29	0.45
5:B:384:ALA:HB2	5:B:393:GLN:NE2	2.32	0.45
8:E:14:ASP:O	8:E:15:ILE:HB	2.17	0.45
10:G:66:VAL:HG23	10:G:67:ASN:N	2.32	0.45
32:d:13:THR:HG23	32:d:72:ARG:HD3	1.98	0.45
33:e:37:ARG:CG	33:e:37:ARG:NH2	2.72	0.45
34:f:7:LEU:C	34:f:7:LEU:CD2	2.88	0.45
34:f:63:TRP:HA	34:f:64:GLY:HA3	1.83	0.45
5:B:391:ARG:HB2	5:B:392:PHE:CE2	2.51	0.45
12:I:99:ILE:HD11	12:I:123:GLU:HG3	1.99	0.45
5:B:391:ARG:HH11	25:W:13:HIS:CB	2.30	0.44
7:D:229:PHE:HB3	7:D:232:TYR:CD2	2.49	0.44
9:F:138:VAL:HG23	9:F:186:TYR:CD2	2.52	0.44
10:G:152:LEU:HD23	10:G:152:LEU:N	2.32	0.44
27:Y:35:LEU:HD22	27:Y:109:LEU:HD11	1.98	0.44
1:1:308:G:H2'	1:1:309:A:C8	2.53	0.44
1:1:1618:U:O2	1:1:1619:C:C6	2.70	0.44
4:A:46:LYS:HB2	4:A:62:ILE:HD12	2.00	0.44
5:B:42:HIS:O	5:B:42:HIS:CG	2.70	0.44
8:E:83:GLY:C	8:E:99:GLN:NE2	2.76	0.44
42:o:33:HIS:HA	42:o:38:ARG:HG2	1.98	0.44
1:1:2488:C:O2	11:H:128:GLU:HB2	2.17	0.44
8:E:25:ARG:CG	9:F:154:ASN:HB2	2.45	0.44
12:I:193:CYS:SG	12:I:198:LYS:HB3	2.58	0.44
19:Q:46:ILE:CD1	19:Q:136:LEU:HD21	2.47	0.44
19:Q:170:ARG:HD2	29:a:57:GLY:HA3	1.99	0.44
33:e:45:ARG:O	33:e:46:LYS:HB2	2.18	0.44
4:A:114:CYS:SG	4:A:167:VAL:HG22	2.57	0.44
10:G:192:GLU:O	10:G:193:VAL:CB	2.65	0.44
18:P:99:ALA:HB1	18:P:153:LEU:HD12	1.99	0.44
39:k:53:VAL:O	39:k:56:VAL:HG12	2.18	0.44
5:B:312:ILE:CD1	5:B:312:ILE:H	2.31	0.44
5:B:391:ARG:CZ	25:W:34:GLU:OE1	2.66	0.44
8:E:10:ILE:HG22	8:E:12:LYS:HG3	2.00	0.44
4:A:178:LEU:HD11	43:p:26:ILE:HD12	2.00	0.44
6:C:221:ILE:HG12	6:C:224:VAL:HG22	2.00	0.44
12:I:99:ILE:HD11	12:I:123:GLU:CG	2.48	0.44
12:I:125:LEU:O	12:I:126:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:57:ILE:HG22	14:L:108:MET:HE1	1.99	0.44
6:C:301:LEU:HD11	8:E:28:PHE:HE1	1.83	0.44
8:E:25:ARG:CG	9:F:154:ASN:HB3	2.21	0.44
28:Z:102:ALA:CB	28:Z:110:LYS:HA	2.47	0.44
5:B:338:LEU:C	5:B:339:VAL:HG23	2.43	0.44
5:B:391:ARG:CZ	25:W:34:GLU:OE2	2.66	0.44
10:G:81:LEU:C	10:G:81:LEU:CD2	2.91	0.44
13:J:106:ILE:HG22	13:J:106:ILE:O	2.16	0.44
39:k:64:LEU:HD23	39:k:65:GLU:H	1.83	0.44
21:S:80:TYR:CE2	21:S:87:HIS:HB2	2.53	0.44
27:Y:54:ASP:HB2	27:Y:108:LYS:O	2.18	0.44
33:e:126:LYS:HB3	33:e:126:LYS:HE2	1.82	0.44
7:D:206:LEU:HD13	7:D:247:LYS:HG3	1.99	0.43
7:D:210:VAL:HG12	7:D:242:LEU:CD1	2.47	0.43
15:M:21:VAL:O	15:M:22:ASP:HB3	2.18	0.43
1:1:261:G:H4'	16:N:171:HIS:O	2.18	0.43
1:1:2179:U:O2	1:1:2179:U:O4'	2.34	0.43
1:1:2221:U:OP1	42:o:32:ARG:HG2	2.18	0.43
6:C:54:MET:HE2	6:C:54:MET:HB3	1.82	0.43
10:G:140:LEU:HD23	10:G:201:PHE:CZ	2.53	0.43
15:M:15:ILE:O	15:M:21:VAL:HA	2.17	0.43
17:O:5:ILE:HD11	17:O:29:ARG:HD3	2.00	0.43
3:4:84:C:H4'	27:Y:113:LYS:CG	2.49	0.43
24:V:36:ASN:HD22	24:V:67:LYS:HB2	1.83	0.43
25:W:25:ARG:HB2	25:W:31:MET:HE2	2.00	0.43
5:B:336:TYR:CG	5:B:337:GLY:N	2.84	0.43
8:E:64:ILE:HG12	8:E:72:LYS:O	2.19	0.43
8:E:87:VAL:CG1	8:E:88:ALA:N	2.82	0.43
22:T:64:VAL:HG13	22:T:72:VAL:HG13	2.00	0.43
6:C:156:GLN:O	6:C:212:LYS:HB2	2.19	0.43
6:C:221:ILE:HG12	6:C:224:VAL:CG2	2.48	0.43
8:E:10:ILE:CG2	8:E:12:LYS:HG3	2.49	0.43
13:J:55:ILE:HG23	13:J:61:ILE:HD11	1.99	0.43
29:a:76:ASN:N	29:a:76:ASN:ND2	2.67	0.43
31:c:13:ILE:HD11	31:c:73:PHE:CD1	2.53	0.43
1:1:480:A:OP2	29:a:117:ARG:NH1	2.51	0.43
1:1:1347:G:O2'	1:1:1348:U:C6	2.70	0.43
12:I:196:HIS:HD2	12:I:197:VAL:O	2.02	0.43
1:1:1766:U:O2	1:1:1766:U:C2'	2.67	0.43
1:1:2463:G:H5'	17:O:64:PRO:HG2	2.00	0.43
4:A:108:PRO:HG2	43:p:86:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:391:ARG:NH1	25:W:13:HIS:CD2	2.86	0.43
10:G:143:ILE:CD1	10:G:156:MET:HB3	2.44	0.43
29:a:21:ARG:NH2	33:e:39:ILE:HG23	2.33	0.43
34:f:13:PHE:HE1	34:f:28:ALA:CB	2.19	0.43
8:E:76:VAL:HG13	8:E:85:VAL:HG12	2.00	0.43
1:1:1452:C:H42	1:1:1615:A:HO2'	1.64	0.43
6:C:6:VAL:CG2	6:C:146:GLU:OE2	2.48	0.43
6:C:214:ILE:CD1	6:C:218:PHE:HD2	2.26	0.43
6:C:301:LEU:CD1	8:E:28:PHE:CE1	3.01	0.43
6:C:301:LEU:HD12	8:E:28:PHE:CE1	2.54	0.43
7:D:242:LEU:O	7:D:246:TYR:CD2	2.70	0.43
6:C:125:ILE:HD11	6:C:232:LEU:HD13	2.00	0.43
19:Q:8:ARG:NH1	30:b:18:ARG:NH2	2.66	0.43
21:S:8:VAL:O	21:S:25:ARG:HA	2.18	0.43
22:T:15:PHE:CD1	22:T:44:VAL:HG21	2.54	0.43
5:B:201:ILE:HD13	5:B:213:ALA:HB2	2.01	0.42
5:B:395:LYS:O	5:B:398:ARG:HB2	2.19	0.42
10:G:64:PRO:HB3	10:G:222:GLN:O	2.19	0.42
11:H:132:VAL:HG23	11:H:171:LEU:CD1	2.48	0.42
5:B:4:ARG:HH11	5:B:7:ASN:CB	2.31	0.42
6:C:221:ILE:HG13	6:C:221:ILE:O	2.19	0.42
12:I:130:ASN:OD1	12:I:130:ASN:N	2.53	0.42
12:I:202:ARG:O	12:I:202:ARG:HG2	2.19	0.42
19:Q:178:ARG:HG2	29:a:51:GLY:HA3	2.00	0.42
21:S:4:LYS:HB3	21:S:62:HIS:CE1	2.54	0.42
32:d:43:MET:C	32:d:44:MET:SD	3.02	0.42
33:e:97:ILE:CA	33:e:122:ASN:ND2	2.81	0.42
34:f:64:GLY:O	34:f:65:VAL:HG12	2.20	0.42
1:1:42:U:H1'	42:o:52:VAL:HG13	2.01	0.42
1:1:254:G:N7	16:N:183:HIS:HE1	2.17	0.42
1:1:1662:C:OP1	4:A:201:LYS:HD3	2.19	0.42
5:B:118:TYR:CE2	5:B:131:PHE:CE2	3.03	0.42
9:F:99:ILE:HD11	9:F:123:MET:HB3	2.01	0.42
12:I:97:LEU:O	12:I:122:PRO:HA	2.19	0.42
1:1:1071:U:O2	1:1:1071:U:C2'	2.67	0.42
8:E:80:GLN:HB2	8:E:84:ILE:O	2.19	0.42
12:I:125:LEU:C	12:I:126:VAL:HG23	2.44	0.42
12:I:199:ARG:HD3	12:I:201:TYR:CE1	2.54	0.42
4:A:48:ILE:HD12	43:p:65:ALA:HB2	2.02	0.42
9:F:166:ILE:HG22	9:F:198:PHE:CZ	2.55	0.42
12:I:199:ARG:CD	12:I:201:TYR:CZ	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:296:ASN:O	7:D:300:VAL:HG23	2.20	0.42
18:P:30:MET:HE1	18:P:91:LEU:HB2	2.01	0.42
1:1:361:A:O2'	18:P:20:THR:HG22	2.20	0.42
1:1:1618:U:O2'	1:1:1619:C:P	2.78	0.42
1:1:2731:A:P	5:B:406:LYS:HG2	2.60	0.42
5:B:299:ARG:HD2	5:B:376:ILE:HD11	2.02	0.42
6:C:363:GLN:HE21	6:C:365:ILE:CD1	2.31	0.42
34:f:9:VAL:HG12	34:f:95:VAL:O	2.19	0.42
36:h:60:ILE:HA	36:h:63:VAL:HG22	2.02	0.42
5:B:247:VAL:HG11	5:B:267:VAL:HG23	2.02	0.42
7:D:210:VAL:HG11	7:D:242:LEU:CD1	2.50	0.42
8:E:84:ILE:HD13	8:E:96:GLU:OE2	2.19	0.42
12:I:199:ARG:HG3	12:I:199:ARG:HH11	1.84	0.42
19:Q:160:LYS:HB3	19:Q:160:LYS:HE2	1.95	0.42
23:U:18:PHE:HB2	23:U:19:PHE:H	1.63	0.42
27:Y:106:ILE:HG21	27:Y:109:LEU:HD22	1.92	0.42
28:Z:65:THR:HG23	28:Z:122:ARG:NE	2.34	0.42
34:f:51:SER:HB3	34:f:62:ASN:HB3	2.02	0.42
1:1:1618:U:O2'	1:1:1619:C:C5'	2.67	0.42
15:M:14:LEU:HD11	15:M:22:ASP:HA	2.01	0.42
1:1:1373:U:O2'	1:1:1374:A:O5'	2.33	0.42
1:1:2393:G:N7	5:B:2:SER:CB	2.80	0.42
5:B:39:GLN:CG	5:B:40:LYS:H	2.21	0.42
7:D:232:TYR:O	7:D:236:GLY:CA	2.68	0.42
8:E:10:ILE:HG21	8:E:12:LYS:CD	2.50	0.42
9:F:96:VAL:HG12	9:F:96:VAL:O	2.19	0.42
10:G:156:MET:N	10:G:157:PRO:CD	2.83	0.42
17:O:106:ILE:HD11	17:O:110:TYR:O	2.20	0.42
19:Q:63:SER:HA	19:Q:90:LEU:HD22	2.01	0.42
22:T:79:ARG:HH21	30:b:21:ILE:HG23	1.84	0.42
7:D:273:LYS:O	7:D:277:ALA:HB2	2.20	0.41
10:G:82:PHE:HE2	10:G:175:ARG:CZ	2.32	0.41
20:R:28:GLU:CB	20:R:49:ILE:HD11	2.49	0.41
25:W:31:MET:HE1	25:W:42:TRP:CZ2	2.55	0.41
28:Z:98:GLU:O	28:Z:113:LEU:HD23	2.20	0.41
32:d:64:LYS:HB3	32:d:64:LYS:HE2	1.84	0.41
5:B:312:ILE:N	5:B:312:ILE:CD1	2.83	0.41
5:B:325:LYS:NZ	5:B:383:THR:CG2	2.83	0.41
13:J:103:LYS:HE3	13:J:103:LYS:HB2	1.86	0.41
21:S:12:PRO:HD3	21:S:50:LEU:HD11	2.02	0.41
21:S:30:ALA:HB1	21:S:35:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:80:TYR:HE2	21:S:89:VAL:CG2	2.33	0.41
34:f:64:GLY:C	34:f:65:VAL:CG1	2.93	0.41
1:1:1449:U:O2'	1:1:1450:G:O5'	2.32	0.41
6:C:50:ALA:HA	6:C:102:PRO:O	2.20	0.41
14:L:2:VAL:HG13	29:a:44:TRP:CE2	2.55	0.41
33:e:43:PHE:CD2	33:e:43:PHE:N	2.89	0.41
34:f:13:PHE:CE1	34:f:28:ALA:CB	2.98	0.41
1:1:1070:A:N3	1:1:1070:A:H2'	2.35	0.41
7:D:77:ALA:HB3	7:D:104:VAL:HG23	2.03	0.41
12:I:36:THR:HG21	12:I:73:ASN:HD21	1.85	0.41
18:P:37:ILE:HD11	18:P:49:LEU:HD11	2.02	0.41
28:Z:102:ALA:HB1	28:Z:110:LYS:CB	2.39	0.41
5:B:314:GLU:O	5:B:314:GLU:HG2	2.21	0.41
12:I:29:PRO:CD	12:I:125:LEU:CD1	2.99	0.41
12:I:196:HIS:CD2	12:I:196:HIS:C	2.99	0.41
16:N:197:VAL:HG11	16:N:199:LYS:NZ	2.33	0.41
30:b:18:ARG:HD2	30:b:18:ARG:HA	1.74	0.41
1:1:1204:G:H5'	38:j:12:HIS:O	2.21	0.41
5:B:325:LYS:NZ	5:B:383:THR:HG23	2.35	0.41
10:G:91:GLU:HG2	10:G:92:THR:O	2.20	0.41
24:V:29:CYS:SG	24:V:102:ALA:HB1	2.60	0.41
6:C:360:MET:O	6:C:361:SER:CB	2.69	0.41
9:F:85:ARG:CZ	9:F:100:LEU:HD13	2.50	0.41
12:I:199:ARG:HD2	12:I:201:TYR:CE1	2.55	0.41
29:a:116:ALA:HB1	29:a:139:LYS:HD2	2.03	0.41
1:1:1348:U:C2'	1:1:1349:A:H8	2.34	0.41
1:1:2463:G:C5'	17:O:64:PRO:HG2	2.51	0.41
2:3:113:U:O2	2:3:113:U:O4'	2.37	0.41
4:A:208:ARG:NH1	4:A:230:GLY:O	2.54	0.41
6:C:301:LEU:HD12	8:E:28:PHE:HE1	1.86	0.41
10:G:84:PHE:CZ	10:G:201:PHE:HB2	2.56	0.41
17:O:25:LEU:HD21	17:O:31:VAL:HG12	2.03	0.41
22:T:79:ARG:HH22	30:b:21:ILE:HG12	1.86	0.41
27:Y:78:MET:HE3	27:Y:100:HIS:CD2	2.56	0.41
27:Y:106:ILE:CG2	27:Y:109:LEU:HD23	2.44	0.41
30:b:11:ASN:O	30:b:11:ASN:CG	2.62	0.41
41:m:98:VAL:HG12	41:m:99:CYS:O	2.20	0.41
41:m:117:GLN:O	41:m:118:CYS:SG	2.78	0.41
1:1:628:G:OP1	38:j:12:HIS:CE1	2.73	0.41
5:B:96:VAL:HG12	17:O:151:VAL:HG22	2.03	0.41
8:E:73:ARG:NH1	8:E:133:TYR:CE1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:109:TYR:CB	20:R:115:ILE:HD12	2.50	0.41
21:S:89:VAL:CG1	21:S:91:LYS:HG3	2.50	0.41
7:D:140:LEU:HD12	7:D:157:MET:HE3	2.02	0.40
9:F:151:ALA:HB2	9:F:198:PHE:CZ	2.55	0.40
12:I:191:VAL:CG1	12:I:192:ASP:H	2.34	0.40
12:I:196:HIS:HD2	12:I:197:VAL:C	2.29	0.40
15:M:30:ILE:HD11	21:S:148:PHE:CZ	2.56	0.40
19:Q:46:ILE:HD11	19:Q:136:LEU:HD21	2.03	0.40
23:U:17:LYS:HD2	23:U:82:ILE:HD11	2.02	0.40
28:Z:107:ALA:N	28:Z:108:PRO:HD2	2.36	0.40
16:N:67:ARG:O	16:N:71:ARG:NH1	2.42	0.40
24:V:39:ILE:HG22	24:V:63:VAL:HG12	2.02	0.40
25:W:31:MET:HE1	25:W:42:TRP:CH2	2.55	0.40
27:Y:58:ILE:HG12	27:Y:104:VAL:HG22	2.03	0.40
29:a:79:LYS:C	29:a:81:TRP:N	2.76	0.40
34:f:64:GLY:C	34:f:65:VAL:HG13	2.46	0.40
8:E:90:PRO:O	8:E:90:PRO:HG2	2.20	0.40
13:J:105:HIS:CG	13:J:106:ILE:N	2.89	0.40
5:B:134:LEU:HD12	5:B:134:LEU:HA	1.83	0.40
5:B:204:GLY:O	5:B:205:ASP:CB	2.70	0.40
8:E:83:GLY:C	8:E:99:GLN:HE22	2.30	0.40
10:G:147:VAL:HG23	10:G:149:PRO:O	2.22	0.40
1:1:330:U:C1'	6:C:79:SER:O	2.69	0.40
4:A:172:ARG:N	4:A:173:PRO:CD	2.85	0.40
6:C:221:ILE:HD11	6:C:224:VAL:CG1	2.51	0.40
10:G:155:TRP:CD1	10:G:155:TRP:H	2.37	0.40
19:Q:60:TYR:CD2	19:Q:80:LEU:HD11	2.57	0.40
23:U:17:LYS:CE	23:U:85:ARG:CZ	2.98	0.40
34:f:64:GLY:O	34:f:65:VAL:CG1	2.70	0.40
34:f:64:GLY:N	34:f:80:PHE:HA	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	
4	A	231/251 (92%)	210 (91%)	18 (8%)	3 (1%)	9	40
5	B	394/415 (95%)	357 (91%)	32 (8%)	5 (1%)	9	40
6	C	356/370 (96%)	329 (92%)	16 (4%)	11 (3%)	3	22
7	D	266/308 (86%)	238 (90%)	26 (10%)	2 (1%)	16	50
8	E	127/151 (84%)	113 (89%)	8 (6%)	6 (5%)	2	14
9	F	229/239 (96%)	215 (94%)	11 (5%)	3 (1%)	9	40
10	G	168/244 (69%)	151 (90%)	14 (8%)	3 (2%)	6	34
11	H	188/197 (95%)	175 (93%)	8 (4%)	5 (3%)	4	25
12	I	191/209 (91%)	175 (92%)	15 (8%)	1 (0%)	24	59
13	J	162/169 (96%)	155 (96%)	5 (3%)	2 (1%)	10	42
14	L	183/189 (97%)	167 (91%)	14 (8%)	2 (1%)	11	43
15	M	122/128 (95%)	118 (97%)	3 (2%)	1 (1%)	16	50
16	N	198/204 (97%)	189 (96%)	9 (4%)	0	100	100
17	O	194/200 (97%)	188 (97%)	3 (2%)	3 (2%)	8	37
18	P	151/164 (92%)	138 (91%)	12 (8%)	1 (1%)	18	52
19	Q	183/186 (98%)	168 (92%)	14 (8%)	1 (0%)	24	59
20	R	160/178 (90%)	150 (94%)	9 (6%)	1 (1%)	21	56
21	S	173/176 (98%)	166 (96%)	7 (4%)	0	100	100
22	T	156/159 (98%)	145 (93%)	10 (6%)	1 (1%)	21	56
23	U	93/106 (88%)	83 (89%)	9 (10%)	1 (1%)	11	43
24	V	132/140 (94%)	124 (94%)	7 (5%)	1 (1%)	16	50
25	W	57/113 (50%)	54 (95%)	2 (4%)	1 (2%)	6	34
26	X	99/140 (71%)	92 (93%)	7 (7%)	0	100	100
27	Y	132/138 (96%)	124 (94%)	7 (5%)	1 (1%)	16	50
28	Z	129/139 (93%)	117 (91%)	8 (6%)	4 (3%)	3	22
29	a	147/151 (97%)	135 (92%)	8 (5%)	4 (3%)	4	25
30	b	46/58 (79%)	44 (96%)	2 (4%)	0	100	100
31	c	92/112 (82%)	86 (94%)	5 (5%)	1 (1%)	11	43
32	d	93/110 (84%)	91 (98%)	2 (2%)	0	100	100
33	e	121/132 (92%)	113 (93%)	5 (4%)	3 (2%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	f	93/102 (91%)	83 (89%)	8 (9%)	2 (2%)	5	29
35	g	113/116 (97%)	105 (93%)	6 (5%)	2 (2%)	6	34
36	h	120/124 (97%)	112 (93%)	7 (6%)	1 (1%)	16	50
37	i	71/91 (78%)	64 (90%)	7 (10%)	0	100	100
38	j	73/81 (90%)	69 (94%)	4 (6%)	0	100	100
39	k	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
40	l	48/51 (94%)	43 (90%)	5 (10%)	0	100	100
41	m	50/132 (38%)	46 (92%)	3 (6%)	1 (2%)	6	31
42	o	91/104 (88%)	87 (96%)	4 (4%)	0	100	100
43	p	87/92 (95%)	82 (94%)	5 (6%)	0	100	100
All	All	5785/6443 (90%)	5365 (93%)	347 (6%)	73 (1%)	12	40

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	42	HIS
7	D	306	PRO
8	E	15	ILE
8	E	94	VAL
10	G	193	VAL
13	J	106	ILE
15	M	104	ASP
22	T	81	ASN
28	Z	58	THR
4	A	40	VAL
4	A	232	LYS
5	B	339	VAL
7	D	20	ARG
8	E	116	THR
9	F	161	ALA
10	G	172	SER
11	H	48	LEU
11	H	148	LYS
23	U	20	GLN
34	f	56	ASP
4	A	141	GLU
6	C	105	LEU
6	C	129	ALA

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Mol	Chain	Res	Type
6	C	195	ARG
6	C	232	LEU
8	E	18	PRO
9	F	213	LYS
11	H	115	GLY
14	L	61	PRO
17	O	198	PHE
18	P	4	HIS
24	V	10	GLN
28	Z	106	ASP
31	c	103	ILE
33	e	126	LYS
34	f	7	LEU
6	C	138	GLY
6	C	196	ALA
6	C	361	SER
9	F	228	GLU
12	I	24	ARG
14	L	128	LYS
17	O	58	LYS
17	O	105	GLY
19	Q	162	ARG
28	Z	99	LYS
28	Z	105	LYS
33	e	47	TYR
35	g	47	GLU
41	m	82	GLU
6	C	61	ALA
6	C	130	VAL
6	C	231	ALA
6	C	365	ILE
8	E	24	PRO
10	G	45	LYS
13	J	130	PRO
25	W	11	SER
27	Y	60	SER
29	a	24	LYS
33	e	13	LYS
35	g	83	GLY
36	h	78	LEU
5	B	5	LYS
5	B	37	ALA

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Mol	Chain	Res	Type
29	a	15	VAL
29	a	29	PRO
29	a	98	GLY
8	E	50	VAL
5	B	9	PRO
11	H	17	ILE
11	H	138	VAL
20	R	53	ARG

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	
4	A	181/191 (95%)	170 (94%)	11 (6%)	17	49
5	B	333/347 (96%)	318 (96%)	15 (4%)	24	58
6	C	294/301 (98%)	284 (97%)	10 (3%)	32	64
7	D	225/256 (88%)	224 (100%)	1 (0%)	84	86
8	E	106/118 (90%)	99 (93%)	7 (7%)	15	47
9	F	185/192 (96%)	182 (98%)	3 (2%)	55	75
10	G	151/209 (72%)	145 (96%)	6 (4%)	28	61
11	H	171/179 (96%)	163 (95%)	8 (5%)	23	57
12	I	167/177 (94%)	163 (98%)	4 (2%)	43	70
13	J	139/144 (96%)	134 (96%)	5 (4%)	31	63
14	L	150/155 (97%)	147 (98%)	3 (2%)	48	72
15	M	103/107 (96%)	98 (95%)	5 (5%)	22	55
16	N	175/177 (99%)	161 (92%)	14 (8%)	11	40
17	O	160/163 (98%)	153 (96%)	7 (4%)	25	59
18	P	127/135 (94%)	125 (98%)	2 (2%)	55	75
19	Q	151/153 (99%)	148 (98%)	3 (2%)	48	72
20	R	130/156 (83%)	127 (98%)	3 (2%)	44	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	S	149/151 (99%)	140 (94%)	9 (6%)	17	50
22	T	131/132 (99%)	129 (98%)	2 (2%)	57	76
23	U	85/92 (92%)	83 (98%)	2 (2%)	43	70
24	V	103/108 (95%)	96 (93%)	7 (7%)	14	46
25	W	51/94 (54%)	51 (100%)	0	100	100
26	X	89/117 (76%)	88 (99%)	1 (1%)	65	79
27	Y	118/122 (97%)	114 (97%)	4 (3%)	32	64
28	Z	102/119 (86%)	101 (99%)	1 (1%)	68	80
29	a	120/122 (98%)	116 (97%)	4 (3%)	33	65
30	b	42/49 (86%)	40 (95%)	2 (5%)	23	56
31	c	81/95 (85%)	80 (99%)	1 (1%)	63	79
32	d	84/94 (89%)	80 (95%)	4 (5%)	23	56
33	e	108/116 (93%)	105 (97%)	3 (3%)	38	68
34	f	85/90 (94%)	78 (92%)	7 (8%)	10	39
35	g	97/98 (99%)	96 (99%)	1 (1%)	68	80
36	h	103/105 (98%)	101 (98%)	2 (2%)	50	73
37	i	65/82 (79%)	64 (98%)	1 (2%)	57	76
38	j	62/66 (94%)	57 (92%)	5 (8%)	11	39
39	k	63/68 (93%)	62 (98%)	1 (2%)	55	75
40	l	46/47 (98%)	45 (98%)	1 (2%)	45	71
41	m	45/116 (39%)	43 (96%)	2 (4%)	25	59
42	o	84/94 (89%)	82 (98%)	2 (2%)	43	70
43	p	67/69 (97%)	66 (98%)	1 (2%)	57	76
All	All	4928/5406 (91%)	4758 (97%)	170 (3%)	33	64

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	14	SER
4	A	20	THR
4	A	40	VAL
4	A	48	ILE
4	A	114	CYS
4	A	164	LEU

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Mol	Chain	Res	Type
4	A	174	GLU
4	A	177	LEU
4	A	191	ARG
4	A	203	ASN
4	A	208	ARG
5	B	10	ARG
5	B	35	ASP
5	B	36	ASP
5	B	47	ILE
5	B	112	GLU
5	B	136	ASN
5	B	198	GLU
5	B	290	CYS
5	B	327	ILE
5	B	374	GLU
5	B	382	ASP
5	B	386	LYS
5	B	392	PHE
5	B	402	LEU
5	B	406	LYS
6	C	8	VAL
6	C	105	LEU
6	C	128	THR
6	C	141	LEU
6	C	147	VAL
6	C	185	VAL
6	C	190	LYS
6	C	214	ILE
6	C	227	ILE
6	C	301	LEU
7	D	31	GLN
8	E	3	GLU
8	E	23	ILE
8	E	70	GLN
8	E	79	ASP
8	E	91	VAL
8	E	95	ASN
8	E	148	LEU
9	F	24	LEU
9	F	69	GLU
9	F	153	LEU
10	G	57	MET

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Mol	Chain	Res	Type
10	G	150	ILE
10	G	151	GLU
10	G	152	LEU
10	G	185	CYS
10	G	187	CYS
11	H	6	LEU
11	H	48	LEU
11	H	55	ASP
11	H	119	ASP
11	H	126	HIS
11	H	138	VAL
11	H	152	ASN
11	H	183	LEU
12	I	99	ILE
12	I	130	ASN
12	I	174	THR
12	I	196	HIS
13	J	42	MET
13	J	95	GLU
13	J	108	LEU
13	J	110	LEU
13	J	114	ARG
14	L	6	ASN
14	L	58	VAL
14	L	76	THR
15	M	19	GLU
15	M	32	ASP
15	M	61	VAL
15	M	71	GLU
15	M	102	MET
16	N	5	THR
16	N	17	GLU
16	N	32	GLN
16	N	76	SER
16	N	87	HIS
16	N	92	LEU
16	N	113	LEU
16	N	115	LEU
16	N	143	GLN
16	N	174	LEU
16	N	179	HIS
16	N	182	ARG

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Mol	Chain	Res	Type
16	N	184	LEU
16	N	187	SER
17	O	44	GLN
17	O	101	GLN
17	O	102	CYS
17	O	122	LEU
17	O	139	LEU
17	O	141	THR
17	O	142	THR
18	P	33	THR
18	P	36	VAL
19	Q	61	SER
19	Q	80	LEU
19	Q	158	ASN
20	R	21	ARG
20	R	49	ILE
20	R	113	ASN
21	S	15	THR
21	S	33	GLU
21	S	50	LEU
21	S	57	VAL
21	S	81	ARG
21	S	85	ASN
21	S	95	ASP
21	S	99	GLU
21	S	174	CYS
22	T	124	THR
22	T	128	LEU
23	U	18	PHE
23	U	21	LEU
24	V	12	THR
24	V	28	CYS
24	V	32	SER
24	V	46	LYS
24	V	87	ILE
24	V	124	GLU
24	V	135	VAL
26	X	66	THR
27	Y	56	VAL
27	Y	82	VAL
27	Y	96	SER
27	Y	97	PHE

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Mol	Chain	Res	Type
28	Z	104	LEU
29	a	15	VAL
29	a	43	THR
29	a	59	ARG
29	a	76	ASN
30	b	8	SER
30	b	11	ASN
31	c	19	LEU
32	d	16	LEU
32	d	47	ASP
32	d	80	ASP
32	d	104	THR
33	e	28	ARG
33	e	37	ARG
33	e	83	LEU
34	f	9	VAL
34	f	26	ASN
34	f	30	LEU
34	f	65	VAL
34	f	66	ILE
34	f	75	VAL
34	f	81	GLU
35	g	59	LYS
36	h	4	LEU
36	h	78	LEU
37	i	54	ARG
38	j	14	LYS
38	j	18	ILE
38	j	22	CYS
38	j	36	LYS
38	j	40	PRO
39	k	64	LEU
40	l	14	CYS
41	m	99	CYS
41	m	118	CYS
42	o	56	LEU
42	o	80	MET
43	p	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	50	HIS
4	A	83	HIS
4	A	86	GLN
4	A	207	HIS
4	A	216	HIS
5	B	124	GLN
5	B	136	ASN
5	B	191	GLN
5	B	287	GLN
5	B	297	ASN
5	B	328	ASN
5	B	367	ASN
5	B	389	HIS
5	B	393	GLN
6	C	11	GLN
6	C	49	HIS
6	C	84	ASN
6	C	186	HIS
6	C	220	ASN
6	C	242	GLN
6	C	363	GLN
6	C	366	ASN
7	D	8	ASN
7	D	38	GLN
7	D	111	GLN
7	D	226	ASN
7	D	282	GLN
7	D	296	ASN
8	E	99	GLN
9	F	37	ASN
9	F	107	GLN
9	F	109	HIS
9	F	152	ASN
10	G	67	ASN
10	G	71	HIS
10	G	139	GLN
10	G	222	GLN
11	H	8	GLN
11	H	30	HIS
11	H	121	ASN
11	H	129	HIS
12	I	73	ASN
12	I	90	ASN

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Mol	Chain	Res	Type
12	I	112	GLN
12	I	169	ASN
12	I	180	GLN
12	I	185	GLN
12	I	187	ASN
12	I	196	HIS
13	J	6	ASN
13	J	58	ASN
13	J	148	GLN
14	L	10	ASN
14	L	66	ASN
14	L	111	GLN
14	L	147	GLN
14	L	148	ASN
15	M	67	ASN
15	M	92	GLN
16	N	80	GLN
16	N	88	HIS
17	O	42	ASN
17	O	71	GLN
17	O	186	GLN
18	P	110	ASN
18	P	133	HIS
19	Q	23	GLN
19	Q	28	HIS
19	Q	86	ASN
19	Q	158	ASN
20	R	94	GLN
21	S	5	GLN
21	S	62	HIS
21	S	85	ASN
22	T	58	HIS
22	T	70	HIS
22	T	112	ASN
23	U	36	ASN
24	V	36	ASN
26	X	98	ASN
27	Y	65	ASN
27	Y	91	ASN
27	Y	135	HIS
28	Z	85	ASN
29	a	66	ASN

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Mol	Chain	Res	Type
29	a	76	ASN
31	c	39	ASN
31	c	55	HIS
32	d	15	HIS
32	d	56	ASN
32	d	100	ASN
33	e	90	ASN
34	f	26	ASN
34	f	42	GLN
34	f	62	ASN
34	f	72	ASN
35	g	29	ASN
35	g	40	GLN
35	g	44	HIS
35	g	103	GLN
36	h	65	GLN
36	h	87	GLN
36	h	111	HIS
37	i	38	GLN
37	i	75	ASN
38	j	13	ASN
38	j	16	HIS
38	j	24	ASN
38	j	28	HIS
39	k	32	ASN
42	o	33	HIS
42	o	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2532/2765 (91%)	534 (21%)	97 (3%)
2	3	116/118 (98%)	26 (22%)	3 (2%)
3	4	152/162 (93%)	40 (26%)	6 (3%)
All	All	2800/3045 (91%)	600 (21%)	106 (3%)

All (600) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	A
1	1	6	U

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Mol	Chain	Res	Type
1	1	16	G
1	1	20	G
1	1	24	A
1	1	29	C
1	1	38	A
1	1	41	A
1	1	47	U
1	1	57	G
1	1	58	A
1	1	64	A
1	1	67	U
1	1	70	C
1	1	72	A
1	1	83	A
1	1	90	G
1	1	107	A
1	1	108	G
1	1	114	C
1	1	115	G
1	1	116	U
1	1	117	C
1	1	119	U
1	1	120	A
1	1	121	A
1	1	122	U
1	1	130	G
1	1	137	G
1	1	138	U
1	1	141	U
1	1	142	C
1	1	148	A
1	1	150	C
1	1	151	U
1	1	152	A
1	1	153	U
1	1	158	C
1	1	159	U
1	1	164	U
1	1	165	A
1	1	168	U
1	1	178	U
1	1	179	G

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Mol	Chain	Res	Type
1	1	188	U
1	1	189	U
1	1	191	A
1	1	196	A
1	1	197	A
1	1	198	A
1	1	209	G
1	1	212	C
1	1	215	C
1	1	217	G
1	1	218	C
1	1	219	A
1	1	222	C
1	1	223	U
1	1	224	U
1	1	225	A
1	1	226	C
1	1	227	G
1	1	242	G
1	1	243	U
1	1	268	A
1	1	271	G
1	1	272	G
1	1	278	U
1	1	296	A
1	1	302	C
1	1	309	A
1	1	322	A
1	1	323	C
1	1	325	A
1	1	348	A
1	1	349	G
1	1	359	A
1	1	360	C
1	1	366	G
1	1	372	A
1	1	373	G
1	1	375	U
1	1	390	G
1	1	394	U
1	1	395	A
1	1	402	U

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Mol	Chain	Res	Type
1	1	403	U
1	1	405	A
1	1	406	U
1	1	424	A
1	1	433	G
1	1	435	A
1	1	450	C
1	1	452	A
1	1	456	U
1	1	457	U
1	1	458	U
1	1	459	G
1	1	466	A
1	1	480	A
1	1	490	A
1	1	491	C
1	1	496	G
1	1	500	G
1	1	501	C
1	1	502	A
1	1	503	U
1	1	506	C
1	1	511	G
1	1	512	A
1	1	519	C
1	1	526	G
1	1	527	A
1	1	532	A
1	1	539	G
1	1	543	A
1	1	556	A
1	1	557	G
1	1	558	G
1	1	562	A
1	1	573	A
1	1	575	C
1	1	577	C
1	1	580	A
1	1	587	A
1	1	593	C
1	1	594	G
1	1	601	U

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Mol	Chain	Res	Type
1	1	606	U
1	1	607	G
1	1	621	U
1	1	622	G
1	1	623	A
1	1	624	U
1	1	634	G
1	1	635	G
1	1	636	U
1	1	641	A
1	1	643	G
1	1	644	A
1	1	652	A
1	1	664	G
1	1	668	G
1	1	671	U
1	1	686	C
1	1	687	U
1	1	689	A
1	1	694	A
1	1	701	A
1	1	712	U
1	1	720	G
1	1	728	A
1	1	730	G
1	1	766	A
1	1	773	A
1	1	775	C
1	1	777	U
1	1	790	U
1	1	792	A
1	1	793	G
1	1	796	A
1	1	807	U
1	1	808	G
1	1	813	U
1	1	814	G
1	1	816	U
1	1	817	U
1	1	820	A
1	1	823	A
1	1	826	U

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Mol	Chain	Res	Type
1	1	828	G
1	1	841	G
1	1	855	G
1	1	868	A
1	1	869	A
1	1	875	U
1	1	876	G
1	1	877	A
1	1	883	A
1	1	902	A
1	1	904	A
1	1	905	U
1	1	906	G
1	1	915	C
1	1	923	A
1	1	924	U
1	1	925	A
1	1	931	A
1	1	939	U
1	1	941	U
1	1	1014	U
1	1	1015	A
1	1	1016	G
1	1	1018	G
1	1	1026	A
1	1	1030	A
1	1	1031	A
1	1	1032	U
1	1	1036	G
1	1	1040	A
1	1	1054	C
1	1	1068	C
1	1	1070	A
1	1	1071	U
1	1	1072	U
1	1	1073	G
1	1	1089	G
1	1	1090	A
1	1	1098	A
1	1	1118	U
1	1	1127	C
1	1	1132	A

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Mol	Chain	Res	Type
1	1	1147	G
1	1	1150	C
1	1	1154	A
1	1	1159	A
1	1	1163	G
1	1	1165	G
1	1	1168	U
1	1	1177	U
1	1	1183	C
1	1	1184	C
1	1	1194	A
1	1	1195	U
1	1	1197	A
1	1	1198	G
1	1	1200	A
1	1	1220	U
1	1	1227	A
1	1	1236	U
1	1	1244	C
1	1	1246	U
1	1	1256	A
1	1	1257	A
1	1	1259	G
1	1	1266	A
1	1	1270	A
1	1	1284	U
1	1	1297	A
1	1	1303	C
1	1	1304	G
1	1	1306	G
1	1	1311	C
1	1	1314	A
1	1	1316	A
1	1	1328	C
1	1	1329	G
1	1	1337	U
1	1	1344	U
1	1	1345	U
1	1	1346	G
1	1	1347	G
1	1	1348	U
1	1	1349	A

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Mol	Chain	Res	Type
1	1	1373	U
1	1	1374	A
1	1	1376	U
1	1	1379	U
1	1	1390	A
1	1	1391	C
1	1	1396	C
1	1	1399	C
1	1	1409	G
1	1	1410	C
1	1	1411	G
1	1	1421	U
1	1	1424	C
1	1	1425	A
1	1	1426	A
1	1	1443	U
1	1	1450	G
1	1	1451	G
1	1	1452	C
1	1	1453	U
1	1	1461	U
1	1	1470	A
1	1	1481	A
1	1	1484	U
1	1	1485	U
1	1	1504	A
1	1	1505	U
1	1	1506	A
1	1	1507	A
1	1	1508	C
1	1	1511	C
1	1	1513	U
1	1	1514	C
1	1	1530	G
1	1	1531	U
1	1	1543	A
1	1	1544	U
1	1	1550	C
1	1	1551	A
1	1	1560	C
1	1	1571	G
1	1	1572	C

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Mol	Chain	Res	Type
1	1	1585	U
1	1	1591	C
1	1	1595	A
1	1	1614	A
1	1	1615	A
1	1	1616	A
1	1	1617	A
1	1	1618	U
1	1	1619	C
1	1	1620	A
1	1	1628	U
1	1	1629	U
1	1	1632	U
1	1	1637	G
1	1	1638	G
1	1	1647	A
1	1	1650	G
1	1	1661	A
1	1	1674	C
1	1	1685	U
1	1	1686	A
1	1	1687	G
1	1	1688	C
1	1	1703	U
1	1	1711	G
1	1	1722	U
1	1	1723	G
1	1	1724	U
1	1	1726	U
1	1	1740	A
1	1	1742	G
1	1	1745	A
1	1	1759	A
1	1	1761	A
1	1	1763	A
1	1	1766	U
1	1	1767	G
1	1	1772	A
1	1	1773	A
1	1	1774	C
1	1	1776	A
1	1	1780	C

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Mol	Chain	Res	Type
1	1	1784	U
1	1	1786	U
1	1	1787	C
1	1	1788	A
1	1	1791	G
1	1	1792	U
1	1	1798	A
1	1	1799	A
1	1	1800	U
1	1	1801	A
1	1	1824	U
1	1	1825	G
1	1	1826	C
1	1	1828	U
1	1	1831	A
1	1	1832	C
1	1	1833	G
1	1	1852	U
1	1	1853	G
1	1	1854	U
1	1	1875	A
1	1	1890	A
1	1	1891	A
1	1	1892	C
1	1	1893	G
1	1	1901	G
1	1	1902	A
1	1	1903	U
1	1	1904	A
1	1	1911	G
1	1	1915	A
1	1	1920	A
1	1	1921	G
1	1	1922	A
1	1	1929	A
1	1	1937	A
1	1	1940	U
1	1	1942	G
1	1	1953	G
1	1	1956	U
1	1	1957	A
1	1	1959	U

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Mol	Chain	Res	Type
1	1	2025	U
1	1	2026	U
1	1	2032	U
1	1	2033	A
1	1	2039	C
1	1	2040	A
1	1	2041	C
1	1	2043	A
1	1	2047	A
1	1	2048	U
1	1	2058	U
1	1	2060	G
1	1	2061	A
1	1	2068	G
1	1	2080	A
1	1	2092	G
1	1	2102	G
1	1	2106	U
1	1	2109	U
1	1	2110	A
1	1	2125	A
1	1	2126	G
1	1	2128	A
1	1	2131	G
1	1	2132	A
1	1	2135	U
1	1	2144	G
1	1	2148	A
1	1	2150	A
1	1	2168	U
1	1	2180	U
1	1	2182	G
1	1	2183	U
1	1	2194	G
1	1	2206	A
1	1	2207	G
1	1	2209	C
1	1	2225	U
1	1	2226	A
1	1	2227	G
1	1	2228	C
1	1	2229	C

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Mol	Chain	Res	Type
1	1	2232	A
1	1	2233	G
1	1	2234	G
1	1	2235	U
1	1	2236	G
1	1	2237	C
1	1	2252	G
1	1	2255	A
1	1	2256	G
1	1	2257	A
1	1	2258	C
1	1	2259	A
1	1	2260	A
1	1	2266	C
1	1	2270	G
1	1	2273	A
1	1	2293	A
1	1	2294	A
1	1	2298	A
1	1	2301	A
1	1	2317	U
1	1	2323	C
1	1	2327	G
1	1	2328	A
1	1	2329	U
1	1	2331	U
1	1	2332	C
1	1	2337	C
1	1	2342	U
1	1	2343	A
1	1	2344	U
1	1	2345	C
1	1	2355	U
1	1	2356	A
1	1	2366	A
1	1	2367	A
1	1	2374	G
1	1	2376	U
1	1	2379	U
1	1	2390	U
1	1	2391	A
1	1	2396	U

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Mol	Chain	Res	Type
1	1	2400	G
1	1	2402	G
1	1	2426	A
1	1	2438	U
1	1	2445	G
1	1	2450	U
1	1	2451	A
1	1	2452	G
1	1	2466	G
1	1	2482	G
1	1	2501	C
1	1	2503	U
1	1	2509	U
1	1	2510	A
1	1	2530	U
1	1	2531	G
1	1	2532	U
1	1	2537	C
1	1	2542	A
1	1	2549	C
1	1	2557	A
1	1	2559	G
1	1	2560	G
1	1	2567	G
1	1	2568	C
1	1	2573	U
1	1	2574	A
1	1	2581	A
1	1	2582	A
1	1	2593	A
1	1	2594	A
1	1	2595	A
1	1	2596	G
1	1	2597	U
1	1	2599	A
1	1	2602	C
1	1	2621	A
1	1	2622	C
1	1	2624	A
1	1	2625	A
1	1	2627	A
1	1	2628	A

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Mol	Chain	Res	Type
1	1	2655	G
1	1	2666	U
1	1	2667	A
1	1	2668	G
1	1	2678	U
1	1	2679	G
1	1	2680	U
1	1	2681	G
1	1	2688	G
1	1	2689	G
1	1	2696	A
1	1	2702	U
1	1	2705	A
1	1	2706	G
1	1	2709	G
1	1	2721	C
1	1	2722	G
1	1	2723	A
1	1	2730	G
1	1	2736	C
1	1	2739	C
1	1	2741	U
1	1	2742	C
1	1	2743	G
1	1	2744	C
1	1	2745	U
1	1	2753	U
1	1	2754	U
2	3	8	C
2	3	21	G
2	3	26	A
2	3	32	C
2	3	33	U
2	3	36	A
2	3	38	U
2	3	42	A
2	3	48	G
2	3	49	A
2	3	52	U
2	3	53	U
2	3	54	A
2	3	64	G

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Mol	Chain	Res	Type
2	3	88	C
2	3	89	G
2	3	93	U
2	3	100	A
2	3	103	G
2	3	106	C
2	3	107	G
2	3	109	U
2	3	110	G
2	3	113	U
2	3	114	G
2	3	115	C
3	4	2	A
3	4	3	G
3	4	4	U
3	4	5	C
3	4	12	C
3	4	22	C
3	4	24	U
3	4	35	A
3	4	36	C
3	4	51	C
3	4	52	A
3	4	53	U
3	4	60	U
3	4	63	A
3	4	64	G
3	4	73	G
3	4	74	U
3	4	75	U
3	4	76	G
3	4	83	U
3	4	84	C
3	4	85	A
3	4	86	U
3	4	87	G
3	4	88	A
3	4	91	G
3	4	93	U
3	4	103	A
3	4	104	A
3	4	105	U

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Mol	Chain	Res	Type
3	4	107	C
3	4	112	U
3	4	118	A
3	4	119	A
3	4	123	C
3	4	125	A
3	4	141	A
3	4	153	G
3	4	154	U
3	4	155	A

All (106) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	38	A
1	1	113	A
1	1	137	G
1	1	147	C
1	1	149	C
1	1	151	U
1	1	152	A
1	1	164	U
1	1	222	C
1	1	225	A
1	1	271	G
1	1	308	G
1	1	374	U
1	1	394	U
1	1	456	U
1	1	457	U
1	1	525	G
1	1	526	G
1	1	621	U
1	1	623	A
1	1	643	G
1	1	686	C
1	1	806	C
1	1	807	U
1	1	812	A
1	1	822	G
1	1	868	A
1	1	876	G

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Mol	Chain	Res	Type
1	1	1014	U
1	1	1030	A
1	1	1070	A
1	1	1071	U
1	1	1072	U
1	1	1193	G
1	1	1196	G
1	1	1258	U
1	1	1327	C
1	1	1328	C
1	1	1347	G
1	1	1348	U
1	1	1367	U
1	1	1373	U
1	1	1378	A
1	1	1466	C
1	1	1505	U
1	1	1507	A
1	1	1523	U
1	1	1530	G
1	1	1543	A
1	1	1550	C
1	1	1614	A
1	1	1615	A
1	1	1617	A
1	1	1618	U
1	1	1619	C
1	1	1628	U
1	1	1685	U
1	1	1687	G
1	1	1766	U
1	1	1787	C
1	1	1823	C
1	1	1824	U
1	1	1895	U
1	1	1902	A
1	1	1903	U
1	1	1958	G
1	1	2039	C
1	1	2040	A
1	1	2042	A
1	1	2047	A

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Mol	Chain	Res	Type
1	1	2071	U
1	1	2131	G
1	1	2134	A
1	1	2181	U
1	1	2224	A
1	1	2225	U
1	1	2226	A
1	1	2232	A
1	1	2331	U
1	1	2342	U
1	1	2367	A
1	1	2405	G
1	1	2434	U
1	1	2450	U
1	1	2451	A
1	1	2509	U
1	1	2567	G
1	1	2572	U
1	1	2596	G
1	1	2621	A
1	1	2627	A
1	1	2678	U
1	1	2701	G
1	1	2705	A
1	1	2721	C
1	1	2722	G
1	1	2743	G
2	3	53	U
2	3	109	U
2	3	112	U
3	4	4	U
3	4	74	U
3	4	87	G
3	4	90	A
3	4	110	A
3	4	153	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

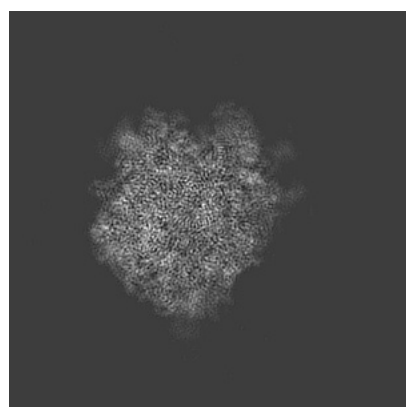
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6784. These allow visual inspection of the internal detail of the map and identification of artifacts.

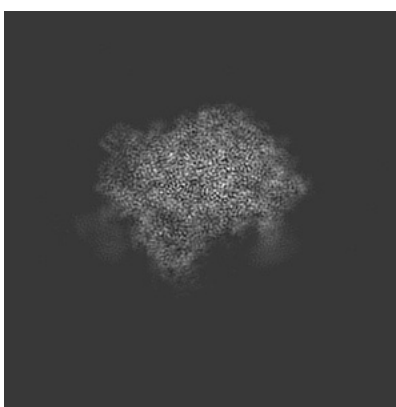
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

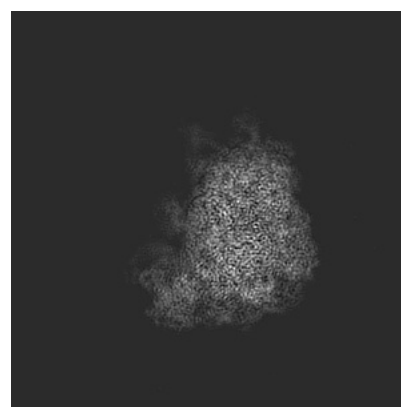
6.1.1 Primary map



X



Y

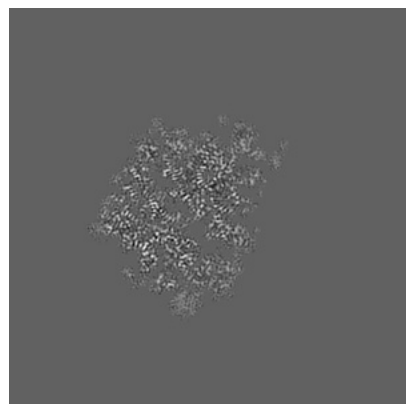


Z

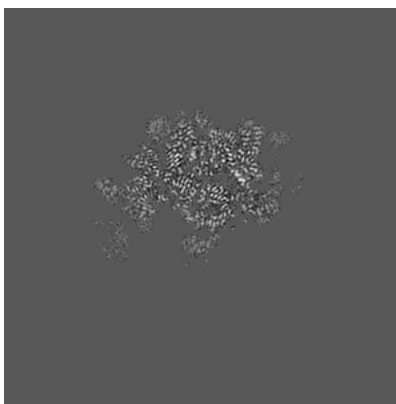
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

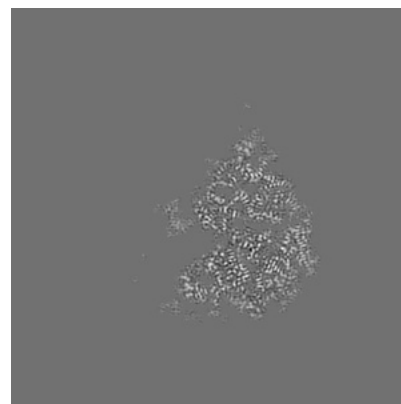
6.2.1 Primary map



X Index: 160



Y Index: 160

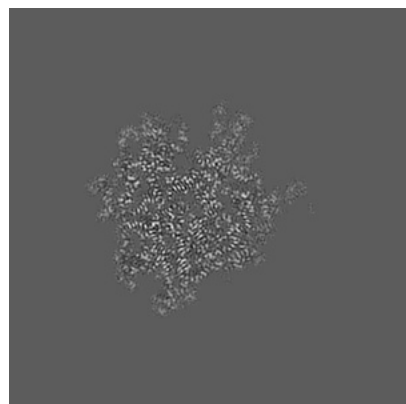


Z Index: 160

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

6.3 Largest variance slices [i](#)

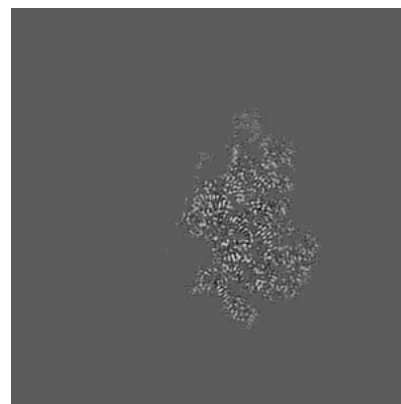
6.3.1 Primary map



X Index: 189



Y Index: 120

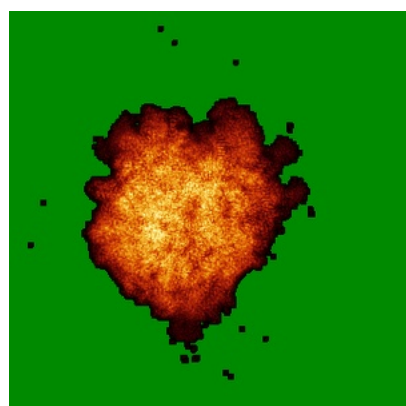


Z Index: 174

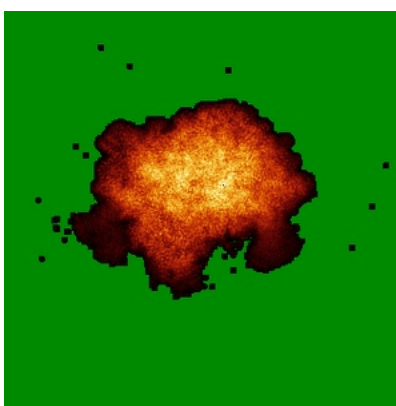
The images above show the largest variance slices of the map in three orthogonal directions.

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

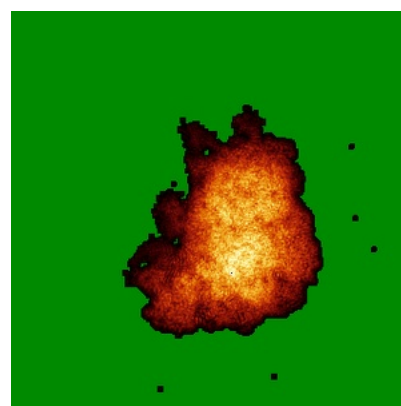
6.4.1 Primary map



X



Y



Z

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 0.044. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

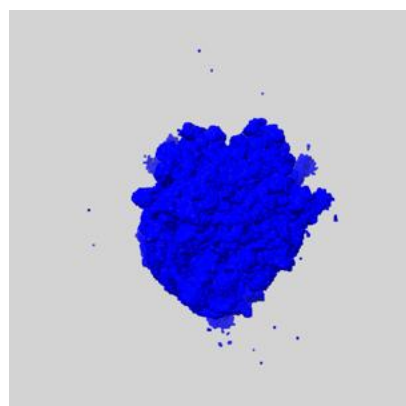
6.6 Mask visualisation [i](#)

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

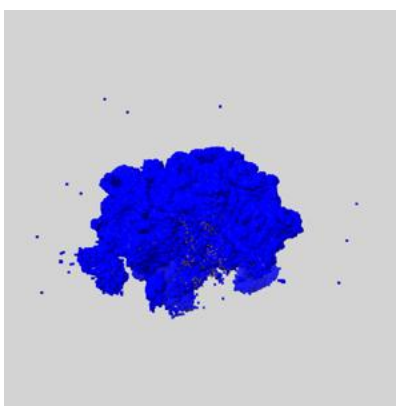
A mask typically either:

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

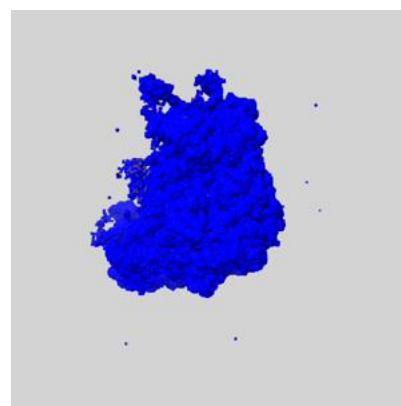
6.6.1 emd_6784_msk_1.map [i](#)



X



Y

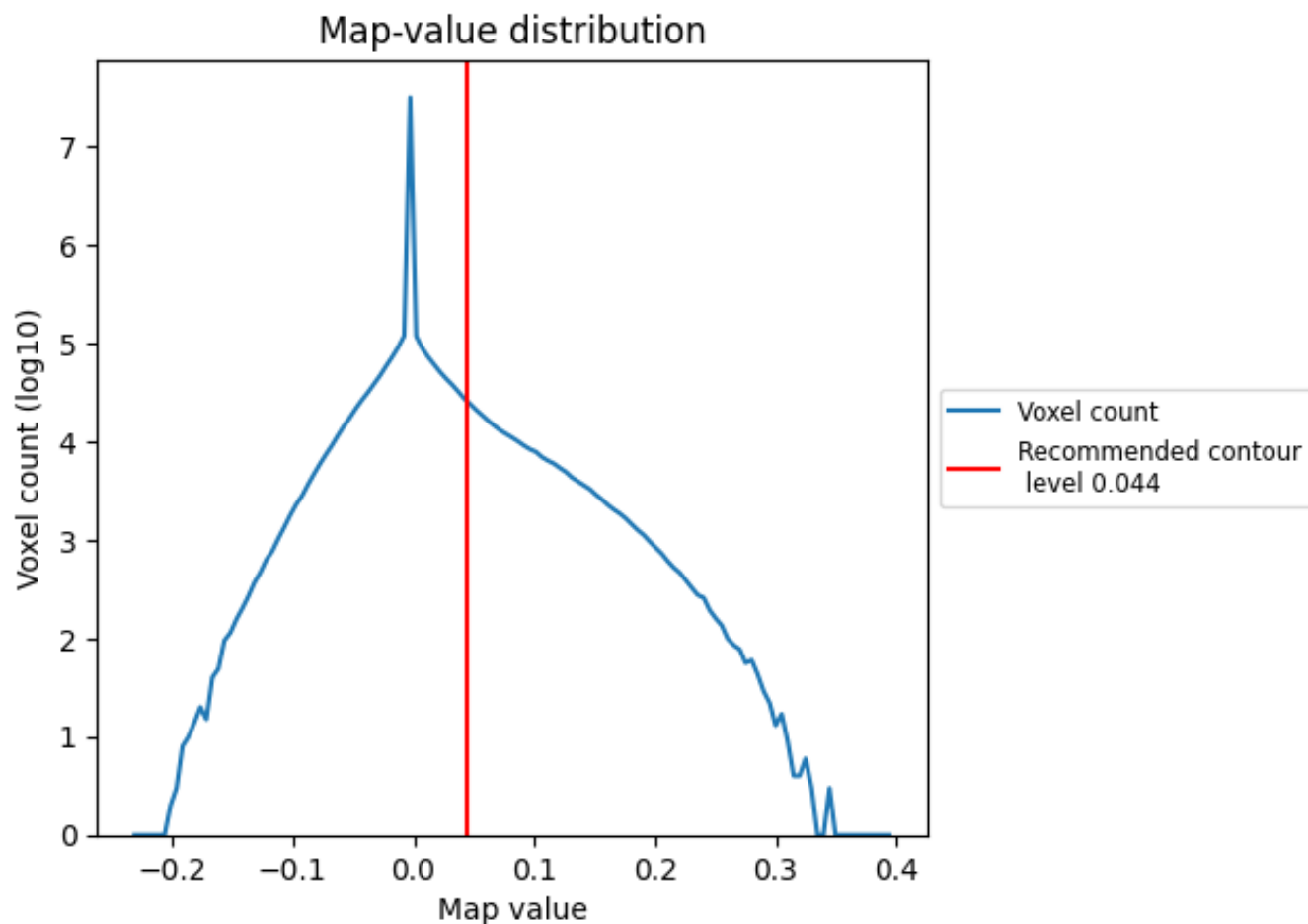


Z

7 Map analysis [i](#)

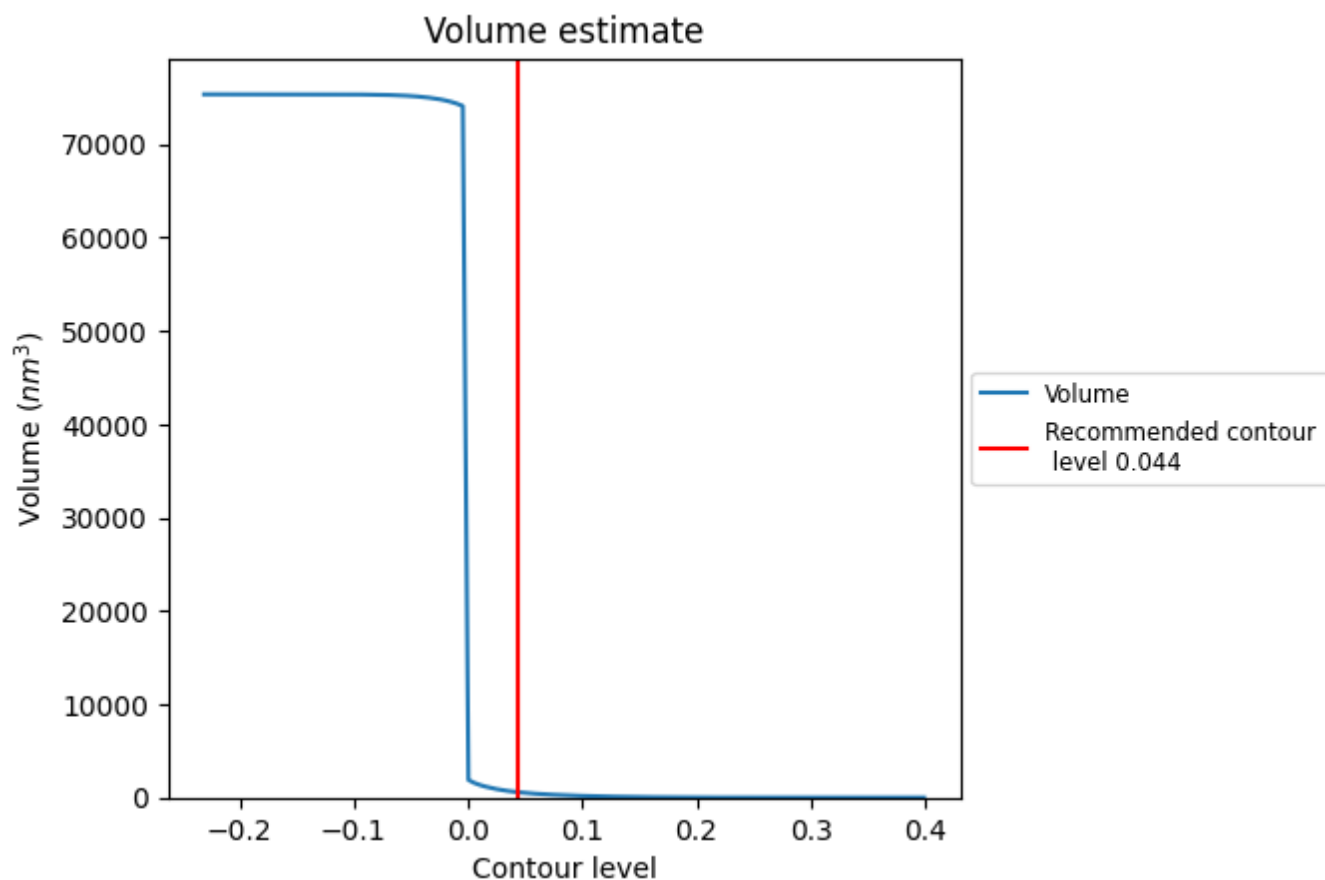
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

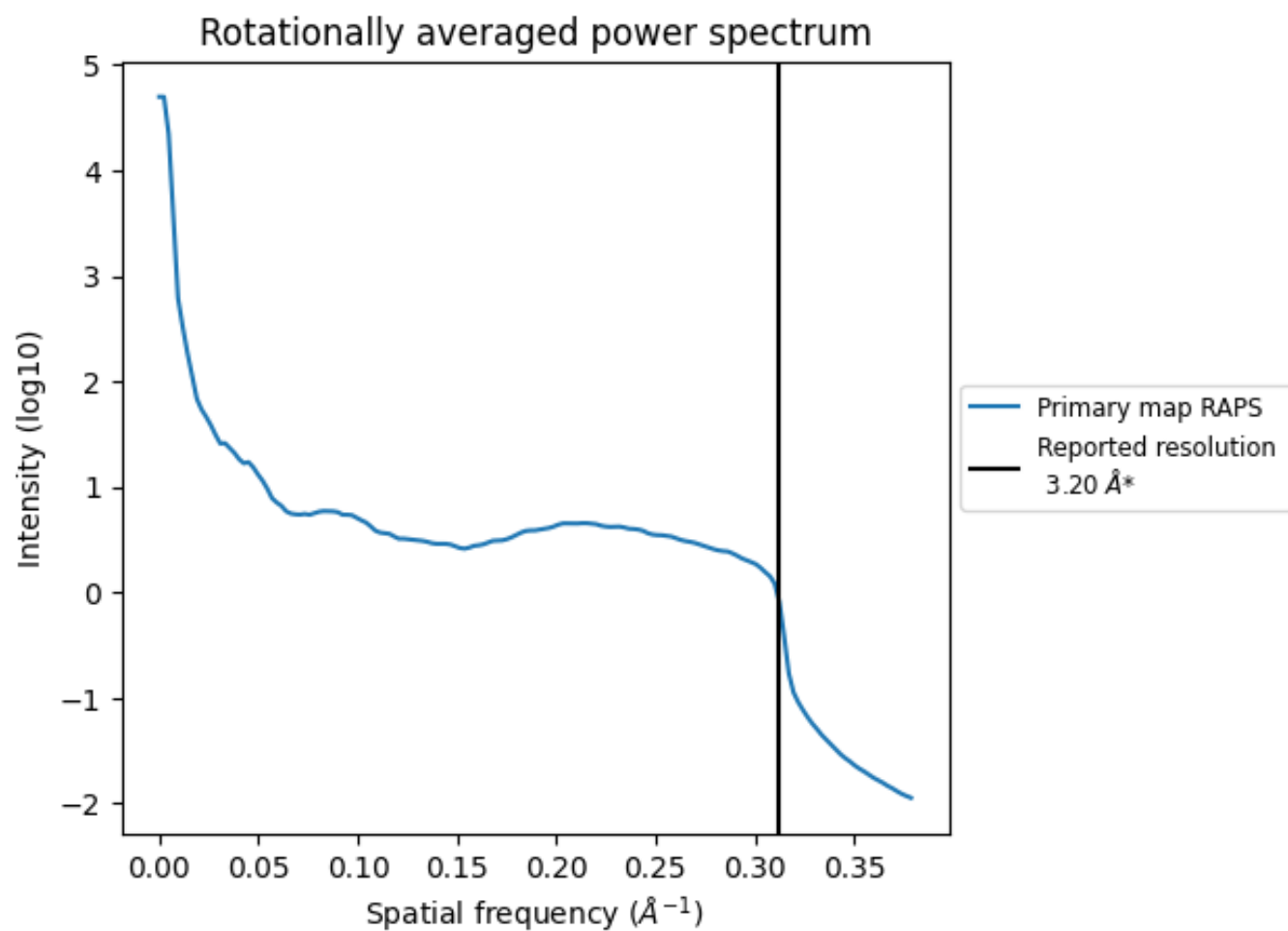
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 572 nm^3 ; this corresponds to an approximate mass of 517 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

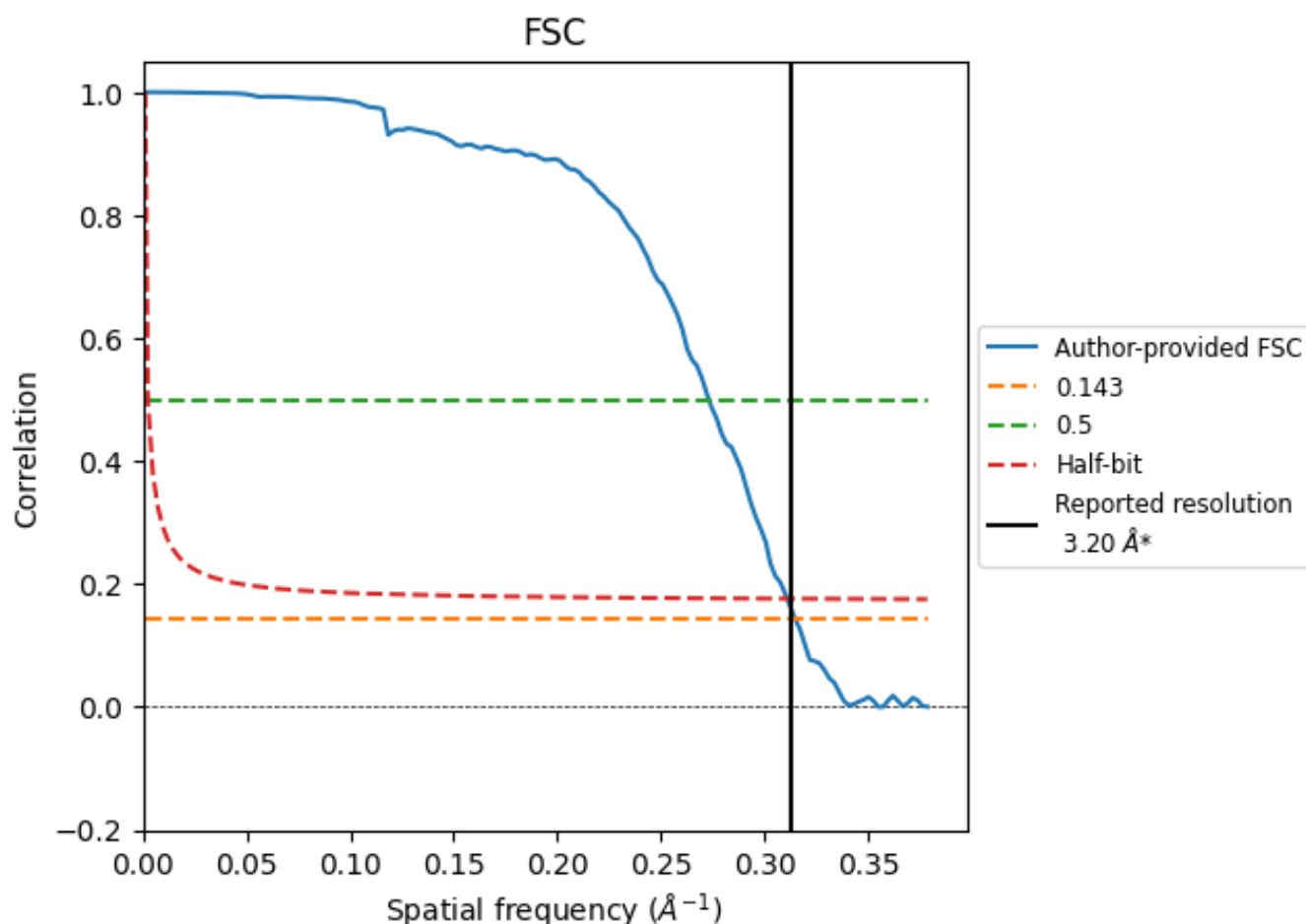


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

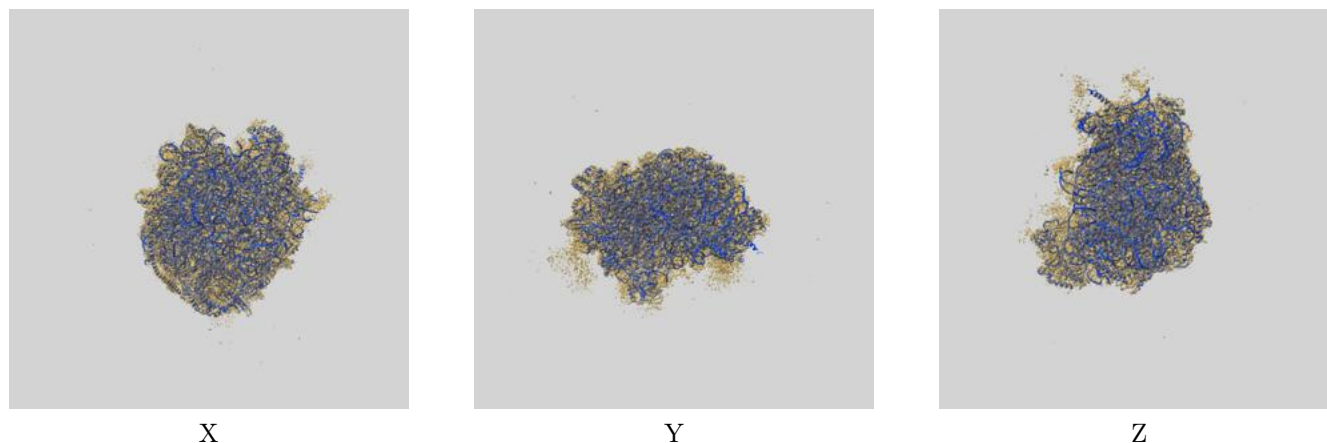
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.66	3.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

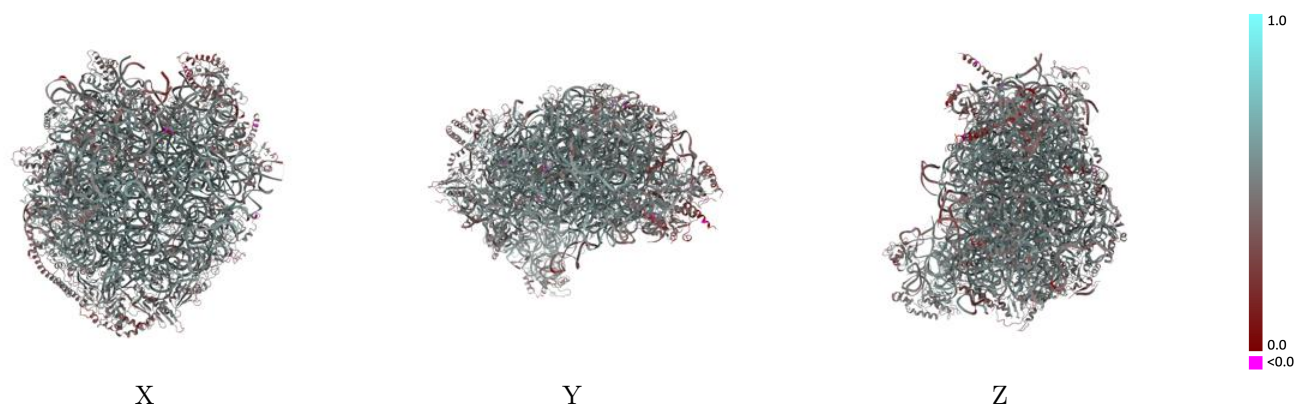
This section contains information regarding the fit between EMDB map EMD-6784 and PDB model 5XY3. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



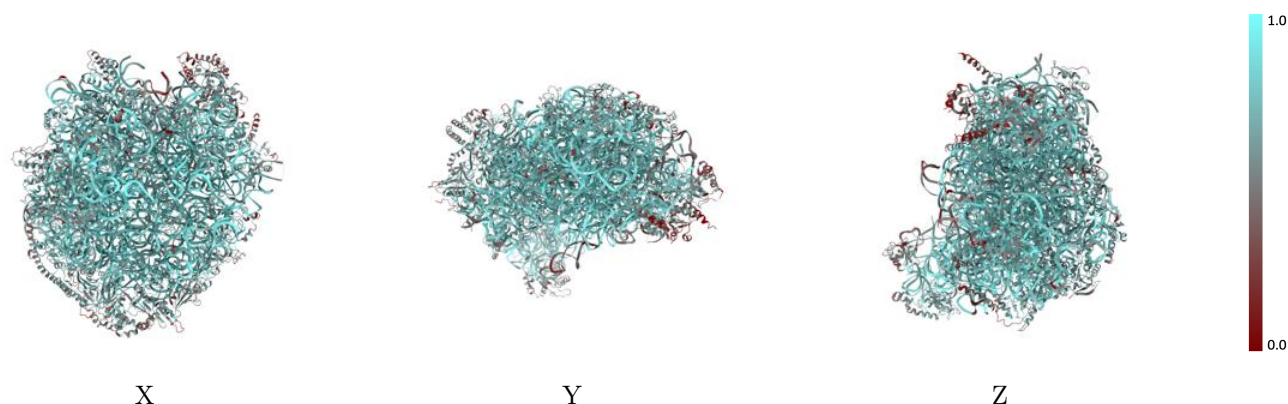
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



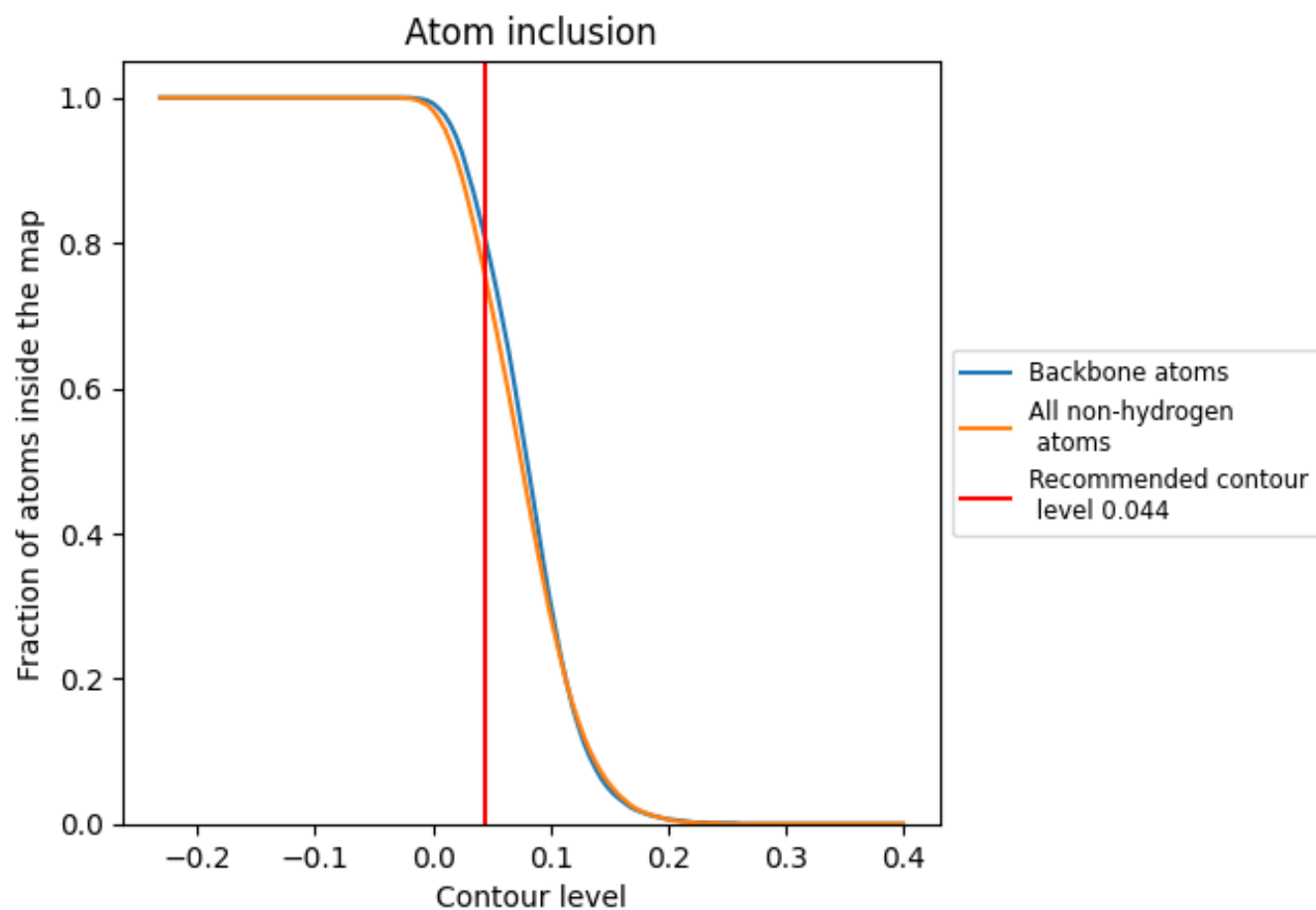
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.044).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.5100
1	 0.8440	 0.5360
3	 0.8460	 0.5180
4	 0.7780	 0.5050
A	 0.7020	 0.5180
B	 0.6950	 0.5050
C	 0.6870	 0.4940
D	 0.6430	 0.4700
E	 0.5510	 0.4410
F	 0.7010	 0.4880
G	 0.5750	 0.4470
H	 0.5680	 0.4500
I	 0.6860	 0.5060
J	 0.4960	 0.4080
L	 0.6440	 0.4690
M	 0.6040	 0.4480
N	 0.7840	 0.5430
O	 0.6870	 0.4990
P	 0.7310	 0.5160
Q	 0.7240	 0.5130
R	 0.6510	 0.4680
S	 0.7070	 0.5060
T	 0.7110	 0.5000
U	 0.5720	 0.4450
V	 0.6490	 0.4880
W	 0.4270	 0.3950
X	 0.6530	 0.4860
Y	 0.6190	 0.4540
Z	 0.4440	 0.3740
a	 0.7400	 0.5220
b	 0.7270	 0.5050
c	 0.3700	 0.3400
d	 0.6800	 0.5040
e	 0.7010	 0.5090
f	 0.7130	 0.5210



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Chain	Atom inclusion	Q-score
g	 0.5440	 0.4090
h	 0.5860	 0.4390
i	 0.6110	 0.4600
j	 0.7870	 0.5490
k	 0.5590	 0.4370
l	 0.7100	 0.5130
m	 0.6140	 0.4650
o	 0.6820	 0.5070
p	 0.6450	 0.4780