



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:03 PM UTC

PDB ID : 6N8K / pdb_00006n8k
EMDB ID : EMD-0370
Title : Cryo-EM structure of early cytoplasmic-immediate (ECI) pre-60S ribosomal subunit
Authors : Zhou, Y.; Musalgaonkar, S.; Johnson, A.W.; Taylor, D.W.
Deposited on : 2018-11-29
Resolution : 3.60 Å(reported)
Based on initial model : 3JCT

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

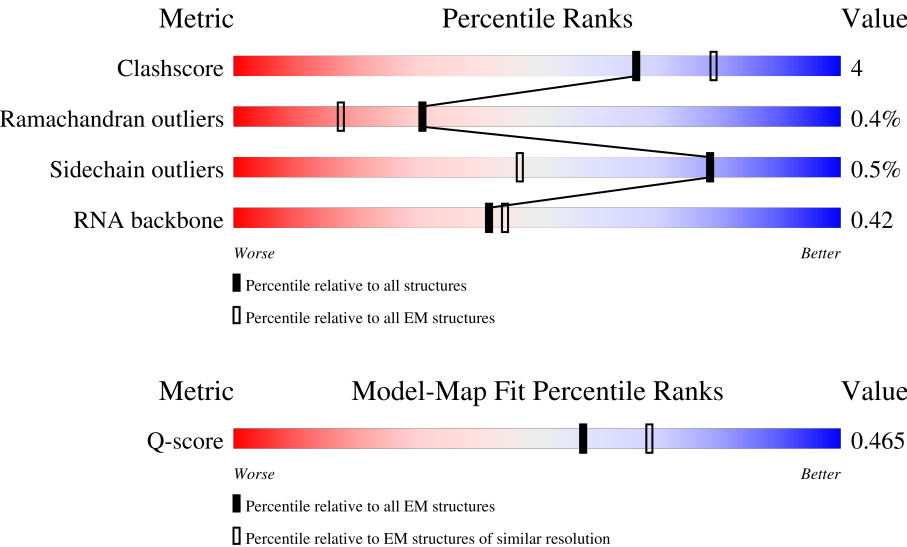
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



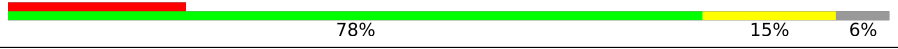
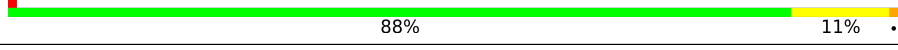
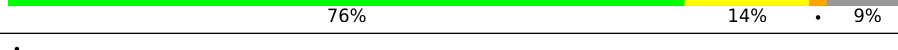
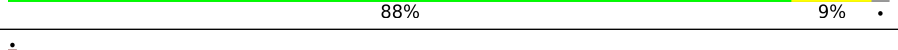
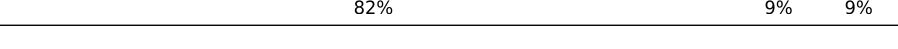
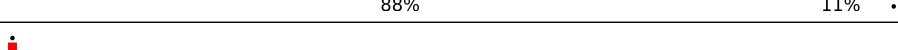
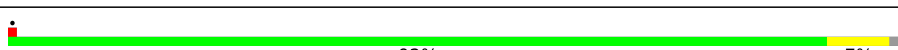
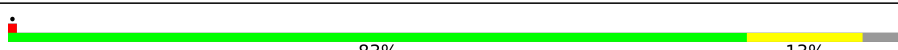
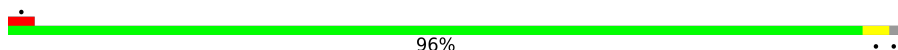
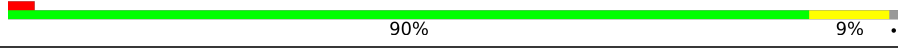
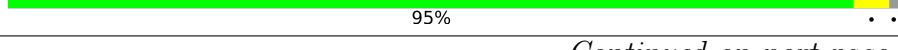
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	s	217	8% 96% ..
2	v	518	41% 8% 51%
3	A	254	84% 12% .

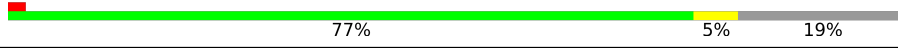
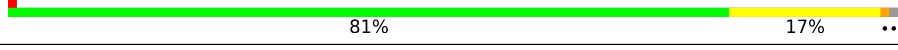
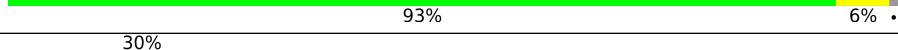
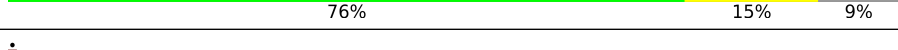
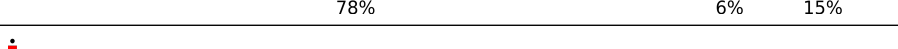
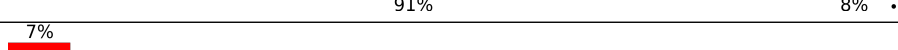
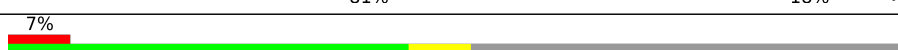
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Mol	Chain	Length	Quality of chain
4	a	149	
5	B	387	
6	b	647	
7	C	362	
8	c	105	
9	d	113	
10	E	176	
11	e	130	
12	F	244	
13	f	107	
14	G	256	
15	g	121	
16	I	166	
17	H	191	
18	h	120	
19	i	100	
20	j	88	
21	k	78	
22	L	199	
23	l	51	
24	M	138	
25	p	92	
26	N	204	
27	u	199	
28	O	199	

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Mol	Chain	Length	Quality of chain
29	P	184	
30	Q	186	
31	R	189	
32	S	172	
33	T	160	
34	U	121	
35	V	137	
36	W	236	
37	X	142	
38	Y	127	
39	y	245	
40	Z	136	
41	z	106	
42	D	297	
43	J	174	
44	q	106	
45	o	59	
46	1	3396	
47	2	121	
48	3	158	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 132821 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal Protein uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	s	210	Total	C	N	O	0	0
			1050	630	210	210		

- Molecule 2 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	252	Total	C	N	O	S	0	0
			1970	1261	329	373	7		

- Molecule 3 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	245	Total	C	N	O	S	0	0
			1863	1162	376	324	1		

- Molecule 4 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	94	Total	C	N	O	S	0	0
			742	484	131	126	1		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 6 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	606	Total	C	N	O	S	0	0
			4895	3073	876	920	26		

- Molecule 7 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 8 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 9 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 10 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	160	Total	C	N	O	S	0	0
			1274	820	230	223	1		

- Molecule 11 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 12 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 13 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 14 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 15 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 16 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	131	Total	C	N	O	S	0	0
			1056	660	195	198	3		

- Molecule 17 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	188	Total	C	N	O	S	0	0
			1493	948	271	270	4		

- Molecule 18 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 19 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	96	Total	C	N	O	S	0	0
			743	465	148	128	2		

- Molecule 20 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	85	Total	C	N	O	S	0	0
			670	408	146	111	5		

- Molecule 21 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 22 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	L	187	Total	C	N	O	0	0
			1491	929	306	256		

- Molecule 23 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 24 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 25 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 26 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 27 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	149	Total	C	N	O	S	0	0
			1256	788	252	207	9		

- Molecule 28 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 29 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	178	Total	C	N	O		0	0
			1409	876	281	252			

- Molecule 30 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	154	Total	C	N	O	S	0	0
			1191	753	231	205	2		

- Molecule 31 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	154	Total	C	N	O		0	0
			1241	772	262	207			

- Molecule 32 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	170	Total	C	N	O	S	0	0
			1425	916	265	241	3		

- Molecule 33 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	61	Total	C	N	O	S	0	0
			476	295	95	85	1		

- Molecule 34 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	U	104	Total	C	N	O		0	0
			826	535	136	155			

- Molecule 35 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 36 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	W	215	Total	C	N	O	S	0	0
			1690	1068	282	335	5		

- Molecule 37 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	X	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 38 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 39 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	y	242	Total	C	N	O	S	0	0
			1826	1131	317	372	6		

- Molecule 40 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Z	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 41 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	z	55	Total	C	N	O		0	0
			444	273	88	83			

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	D	251	Total	C	N	O	S	0	0
			1983	1253	353	375	2		

- Molecule 43 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	J	164	Total	C	N	O	S	0	0
			1304	816	243	242	3		

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	97	Total	C	N	O	S	0	0
			783	493	158	127	5		

- Molecule 45 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	o	54	Total	C	N	O	0	0
			433	271	94	68		

- Molecule 46 is a RNA chain called *Saccharomyces cerevisiae* S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	3201	Total	C	N	O	P	0	0
			68471	30584	12345	22341	3201		

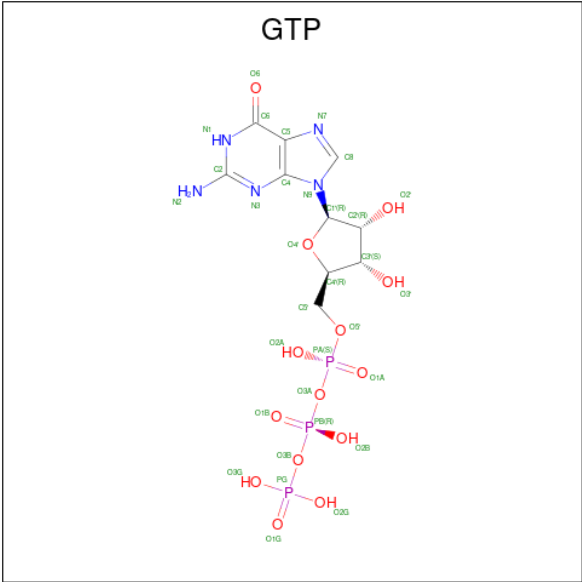
- Molecule 47 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 48 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3	157	Total	C	N	O	P	0	0
			3333	1491	584	1101	157		

- Molecule 49 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
49	b	1	Total	C	N	O	P	0
			32	10	5	14	3	

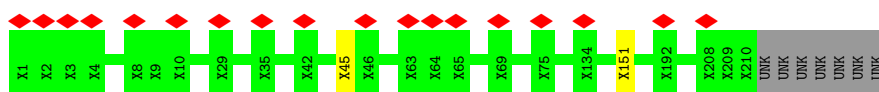
- Molecule 50 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
50	b	1	Total	Mg	0
			1	1	

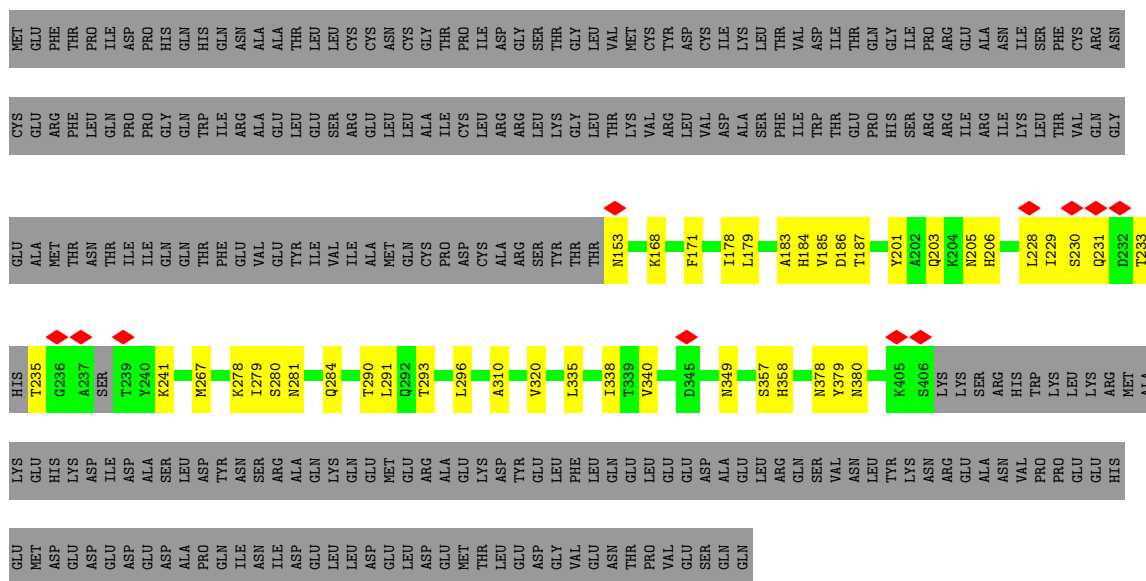
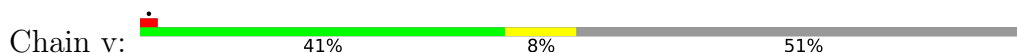
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

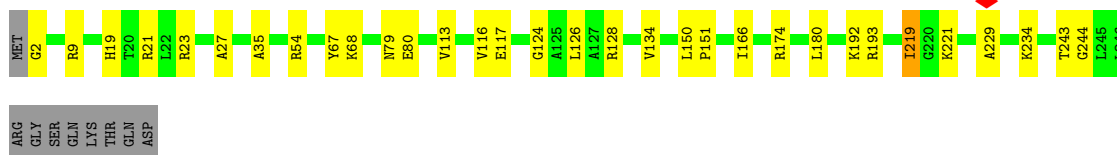
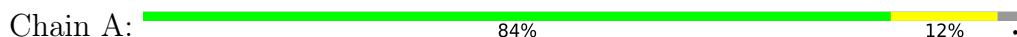
• Molecule 1: Ribosomal Protein uL1



• Molecule 2: 60S ribosomal export protein NMD3

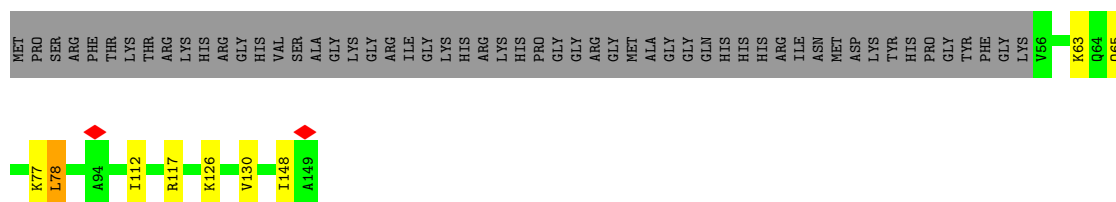


• Molecule 3: 60S ribosomal protein L2-A



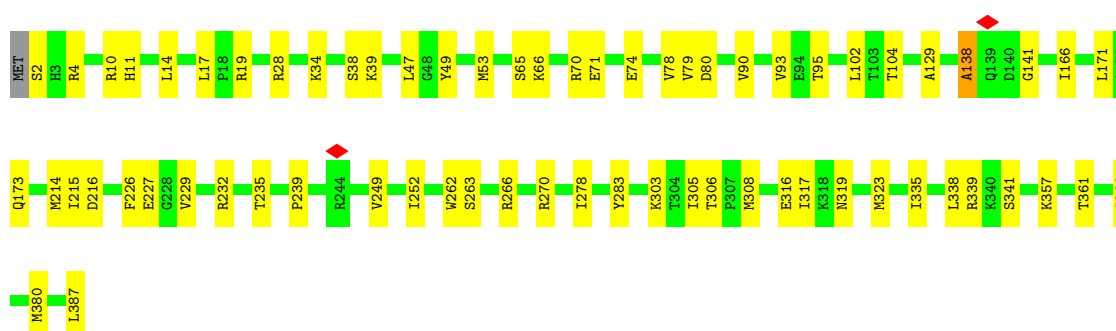
- Molecule 4: 60S ribosomal protein L28

Chain a: 



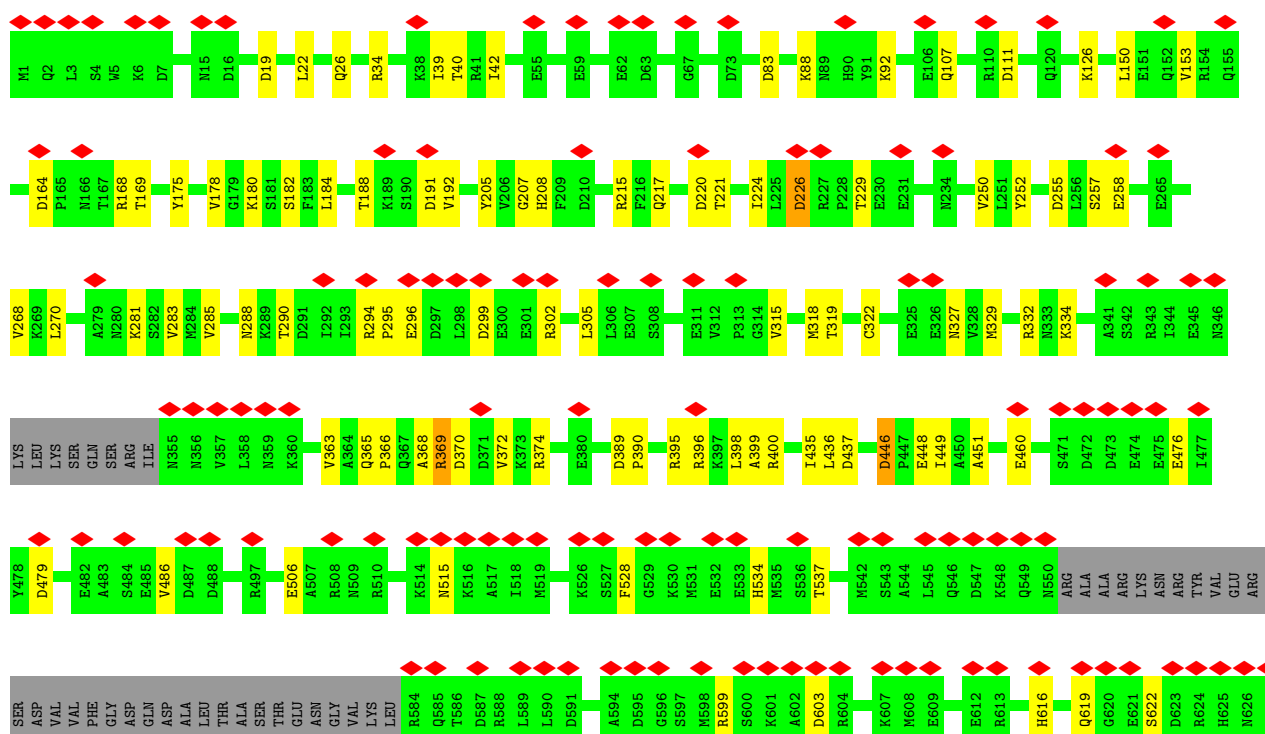
- Molecule 5: 60S ribosomal protein L3

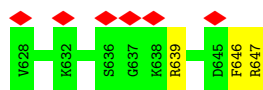
Chain B: 



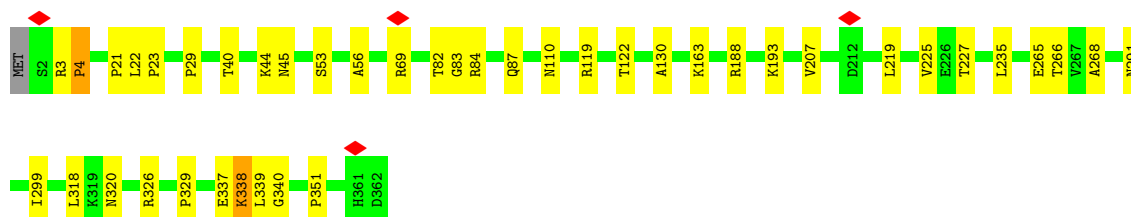
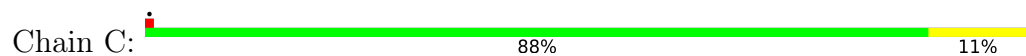
- Molecule 6: Nucleolar GTP-binding protein 1

Chain b: 

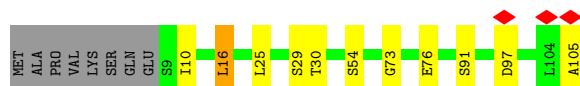
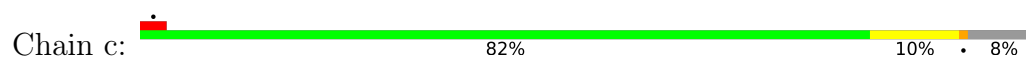




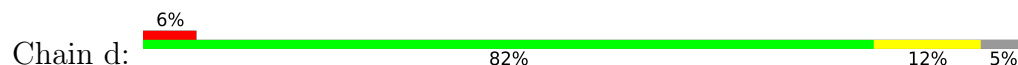
- Molecule 7: 60S ribosomal protein L4-A



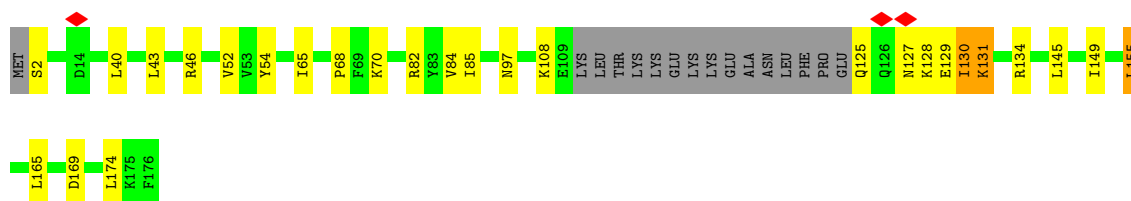
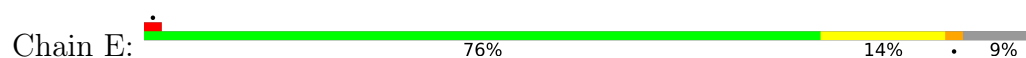
- Molecule 8: 60S ribosomal protein L30



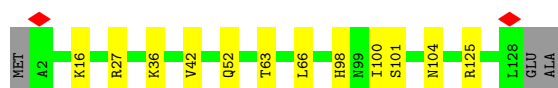
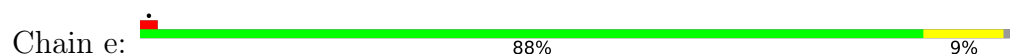
- Molecule 9: 60S ribosomal protein L31-A



- Molecule 10: 60S ribosomal protein L6-A

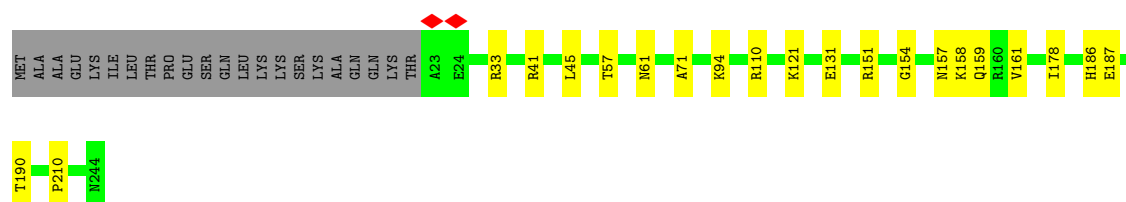


- Molecule 11: 60S ribosomal protein L32



- Molecule 12: 60S ribosomal protein L7-A

Chain F: 



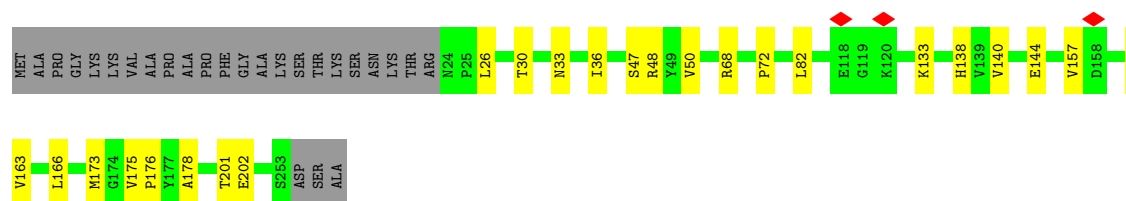
- Molecule 13: 60S ribosomal protein L33-A

Chain f: 



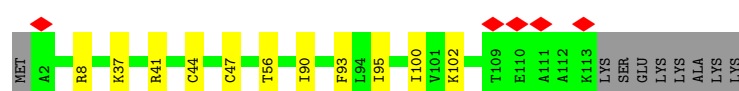
- Molecule 14: 60S ribosomal protein L8-A

Chain G: 



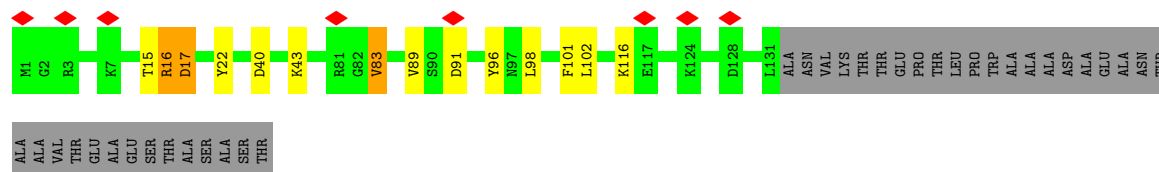
- Molecule 15: 60S ribosomal protein L34-A

Chain g: 



- Molecule 16: Bud site selection protein 20

Chain I: 

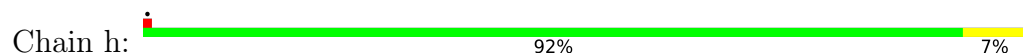


- Molecule 17: 60S ribosomal protein L9-A

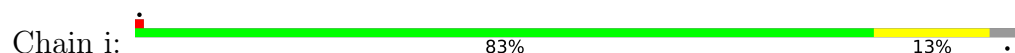
Chain H: 



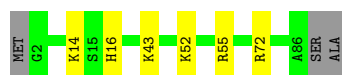
- Molecule 18: 60S ribosomal protein L35-A



- Molecule 19: 60S ribosomal protein L36-A



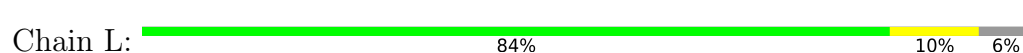
- Molecule 20: 60S ribosomal protein L37-A



- Molecule 21: 60S ribosomal protein L38



- Molecule 22: 60S ribosomal protein L13-A

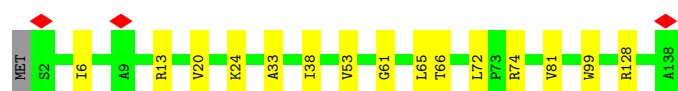


- Molecule 23: 60S ribosomal protein L39



- Molecule 24: 60S ribosomal protein L14-A

Chain M: 



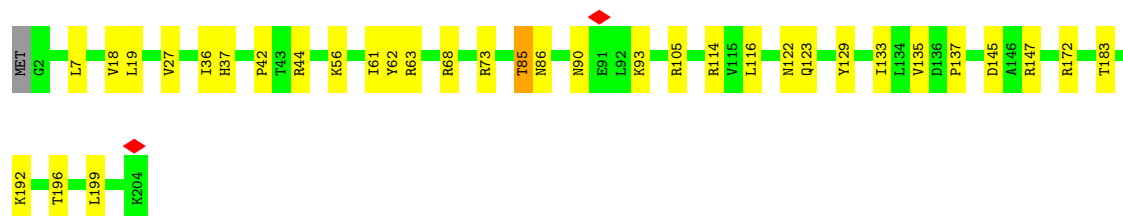
- Molecule 25: 60S ribosomal protein L43-A

Chain p: 



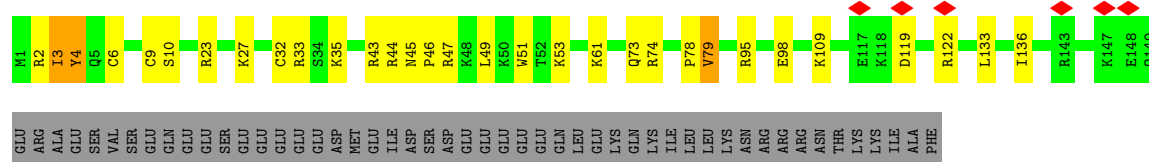
- Molecule 26: 60S ribosomal protein L15-A

Chain N: 

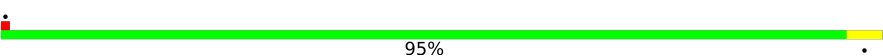


- Molecule 27: Ribosome biogenesis protein RLP24

Chain u: 



- Molecule 28: 60S ribosomal protein L16-A

Chain O: 

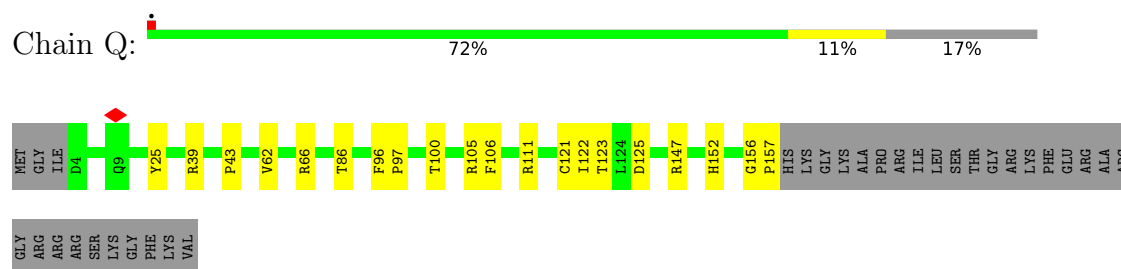


- Molecule 29: 60S ribosomal protein L17-A

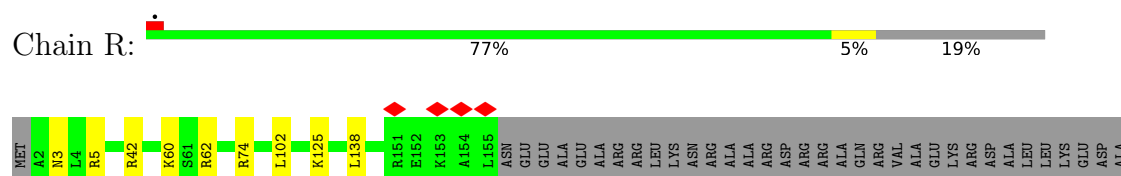
Chain P: 



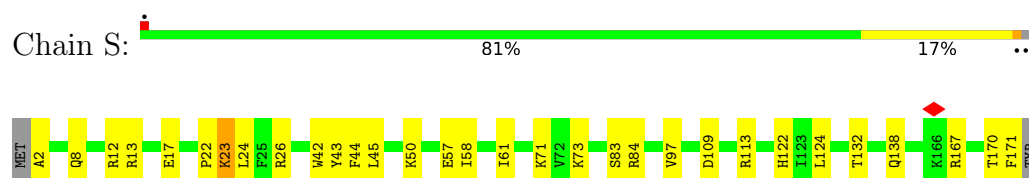
- Molecule 30: 60S ribosomal protein L18-A



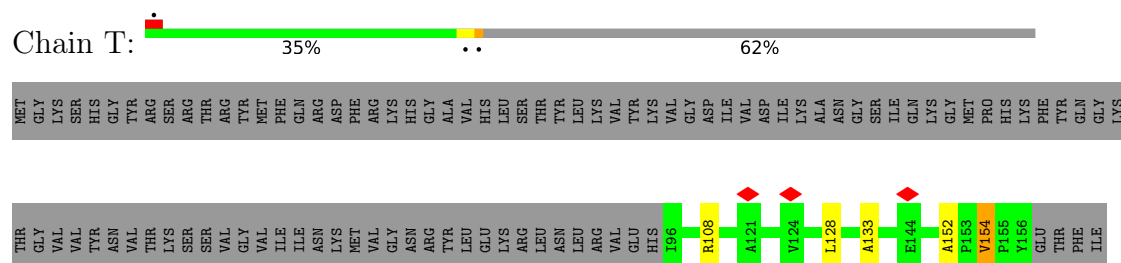
- Molecule 31: 60S ribosomal protein L19-A



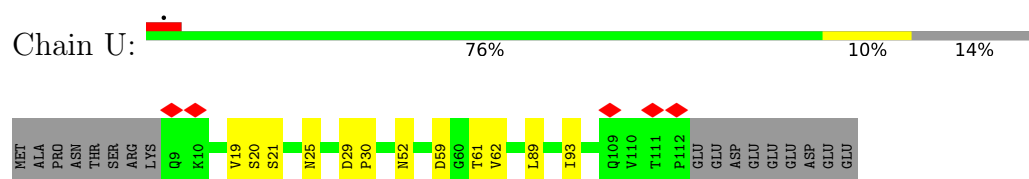
- Molecule 32: 60S ribosomal protein L20-A



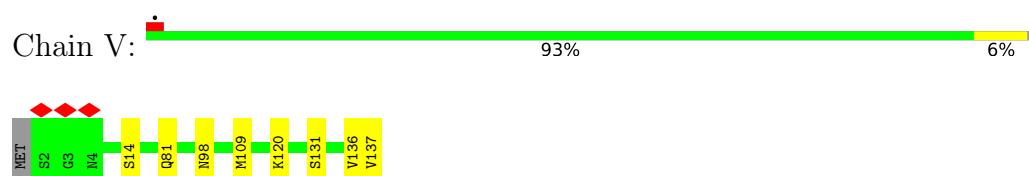
- Molecule 33: 60S ribosomal protein L21-A



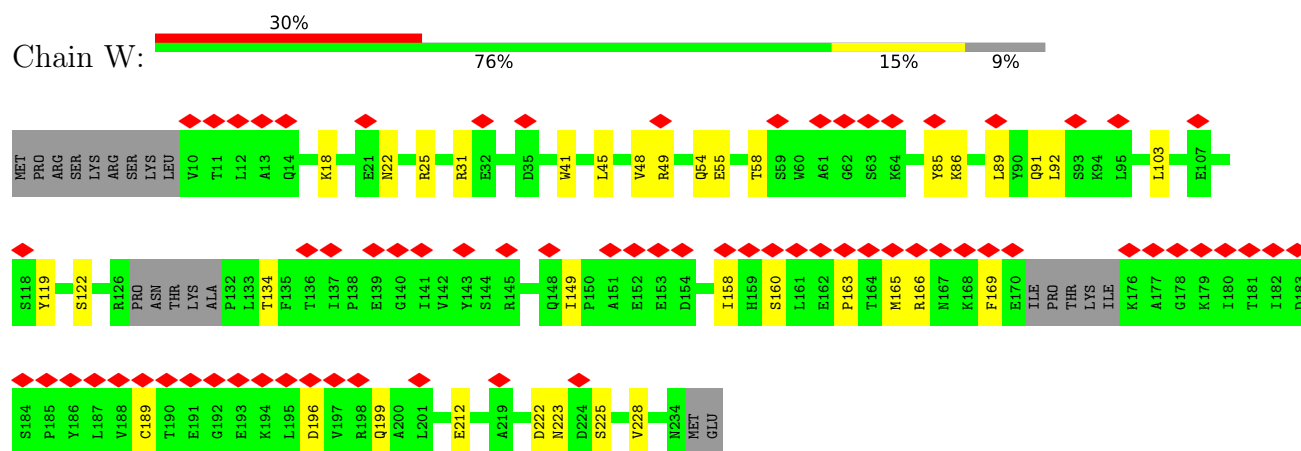
- Molecule 34: 60S ribosomal protein L22-A



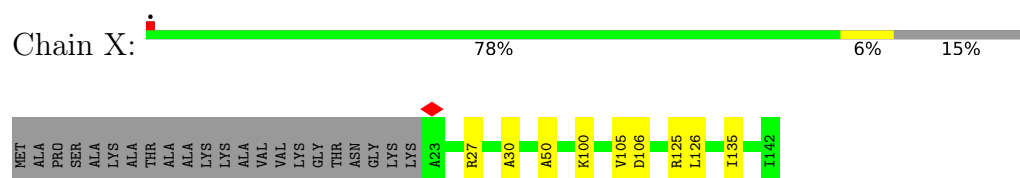
- Molecule 35: 60S ribosomal protein L23-A



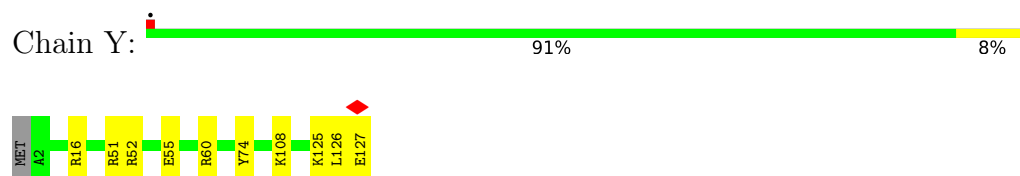
- Molecule 36: Ribosome assembly factor MRT4



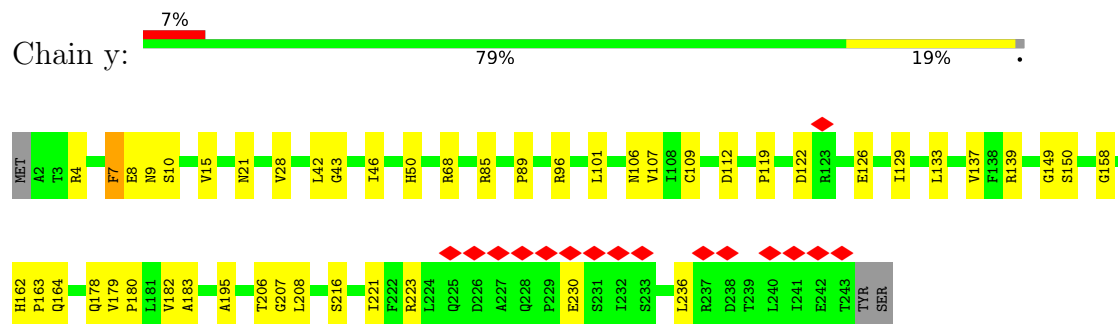
- Molecule 37: 60S ribosomal protein L25



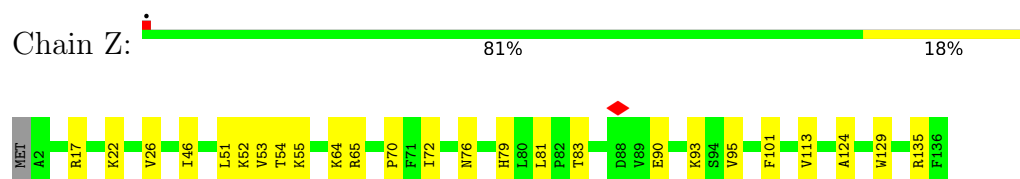
- Molecule 38: 60S ribosomal protein L26-A



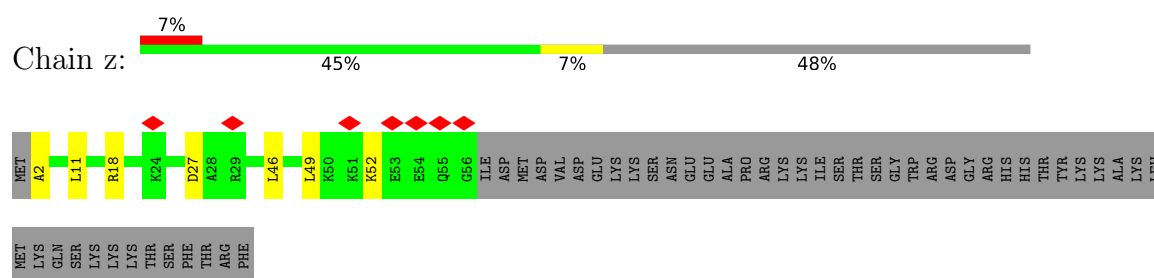
- Molecule 39: Eukaryotic translation initiation factor 6



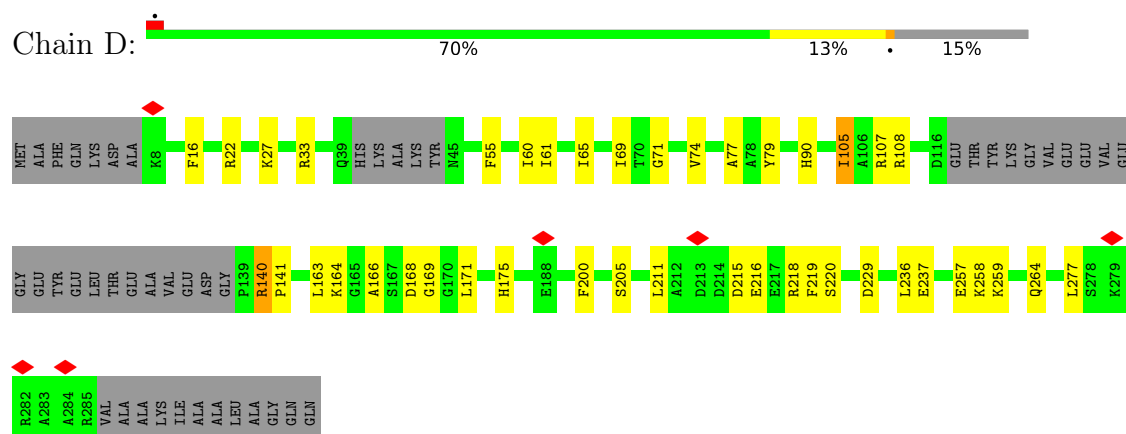
- Molecule 40: 60S ribosomal protein L27-A



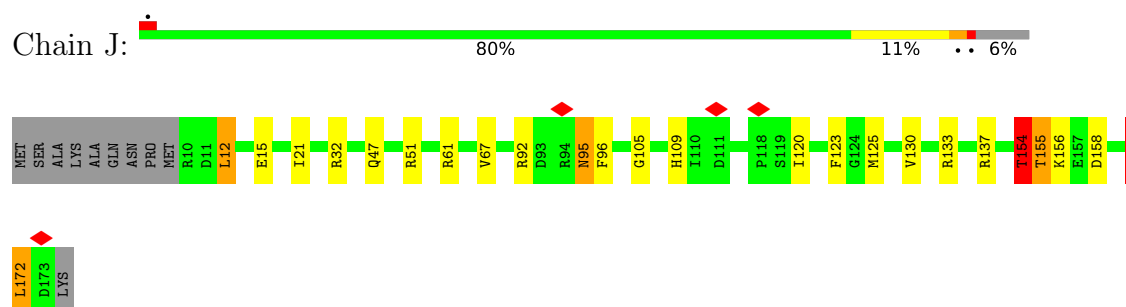
- Molecule 41: UPF0642 protein YBL028C



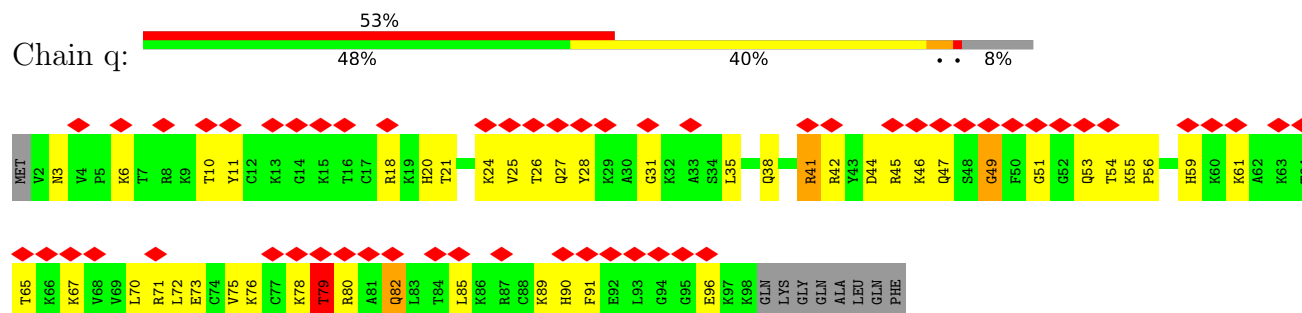
- Molecule 42: 60S ribosomal protein L5



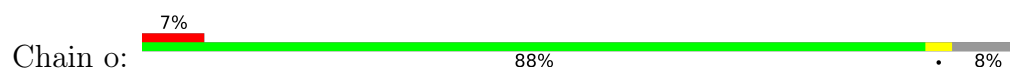
- Molecule 43: 60S ribosomal protein L11-A

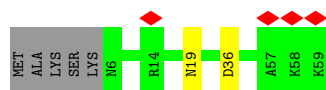


- Molecule 44: 60S ribosomal protein L42-A

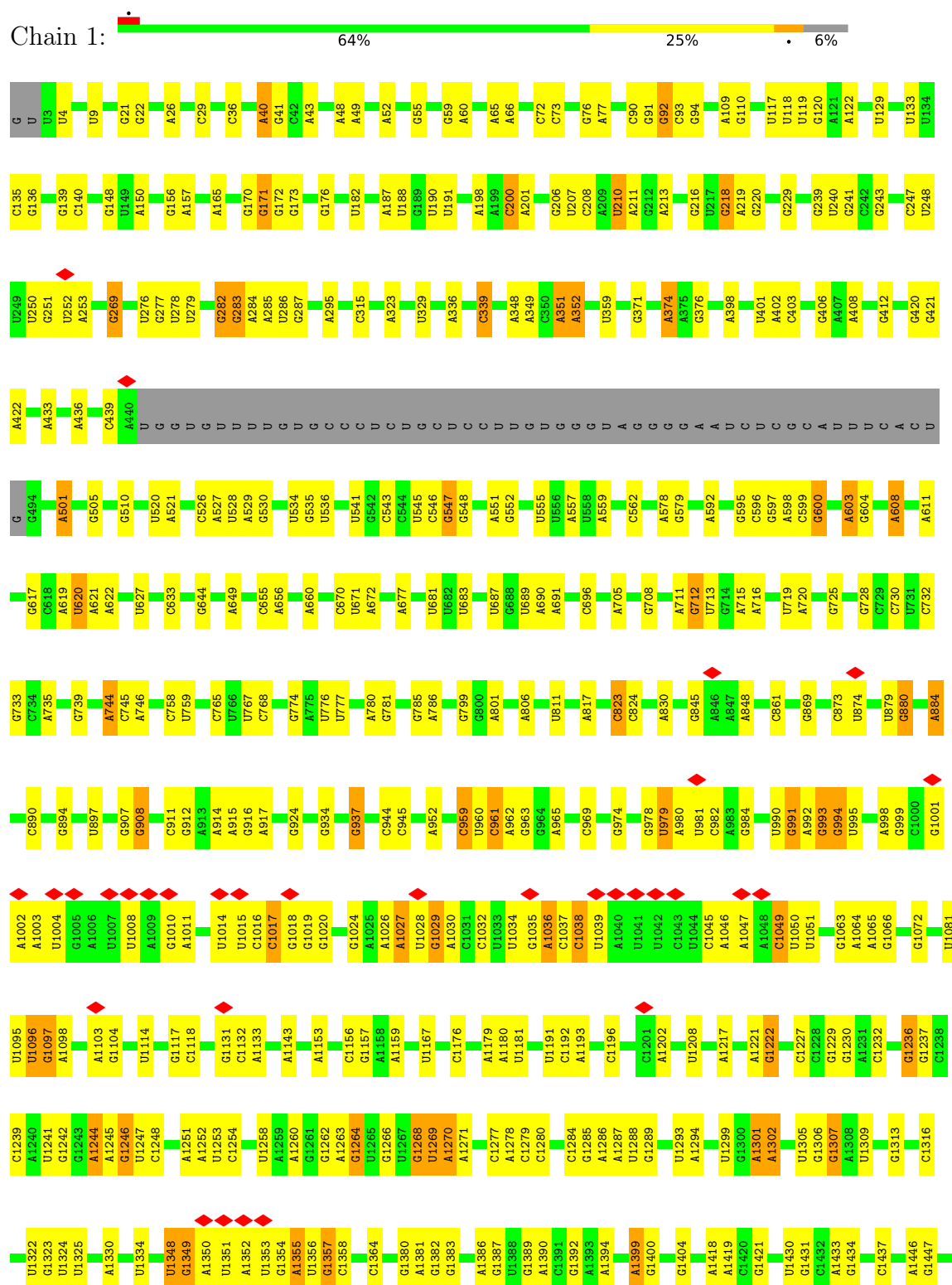


- Molecule 45: 60S ribosomal protein L29

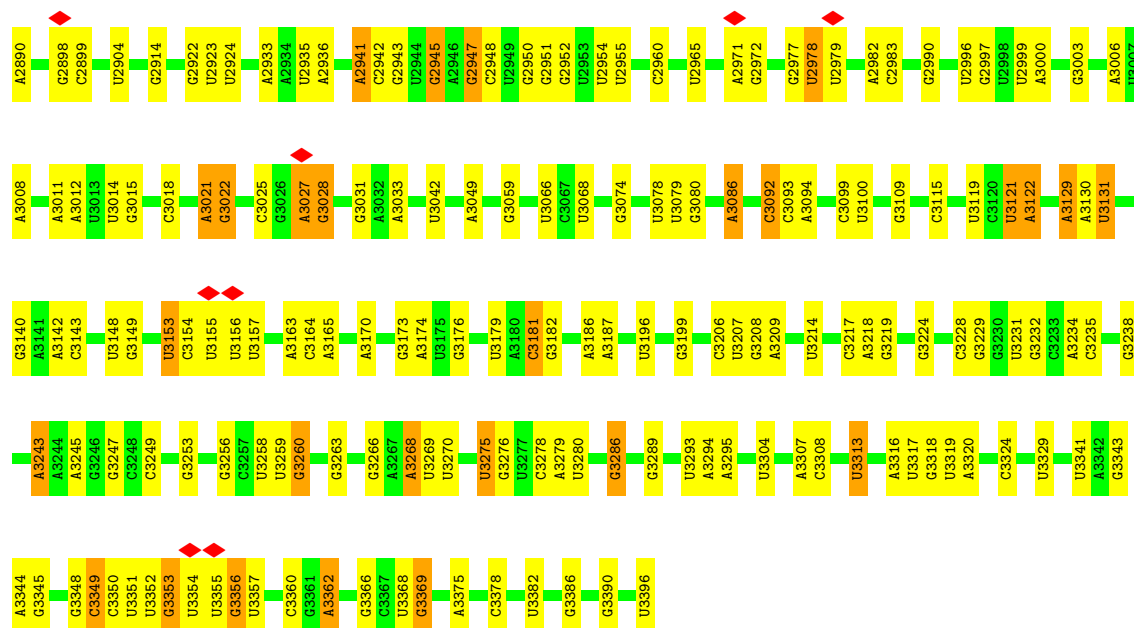




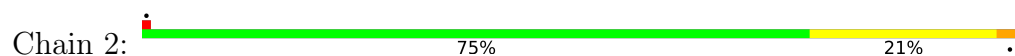
- Molecule 46: *Saccharomyces cerevisiae* S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA



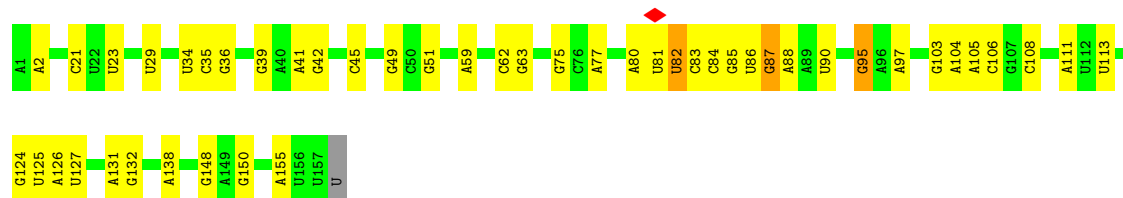




• Molecule 47: 5S rRNA



• Molecule 48: 5.8S rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	43797	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG

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	$\# Z > 5$
2	v	0.32	0/2008	0.66	1/2727 (0.0%)
3	A	0.38	0/1897	0.74	0/2550
4	a	0.34	0/758	0.61	0/1023
5	B	0.39	0/3152	0.80	3/4239 (0.1%)
6	b	0.27	0/4977	0.70	2/6689 (0.0%)
7	C	0.33	0/2801	0.67	4/3792 (0.1%)
8	c	0.28	0/751	0.57	0/1008
9	d	0.36	0/887	0.65	2/1191 (0.2%)
10	E	0.29	0/1295	0.61	0/1740
11	e	0.32	0/1041	0.63	0/1394
12	F	0.33	0/1821	0.70	3/2451 (0.1%)
13	f	0.35	0/868	0.57	0/1168
14	G	0.33	0/1830	0.71	0/2469
15	g	0.36	0/891	0.65	0/1191
16	I	0.26	0/1072	0.65	0/1440
17	H	0.30	0/1514	0.60	0/2039
18	h	0.30	0/978	0.58	0/1301
19	i	0.29	0/749	0.68	1/995 (0.1%)
20	j	0.37	0/685	0.71	0/908
21	k	0.31	0/618	0.61	0/826
22	L	0.34	0/1516	0.74	2/2037 (0.1%)
23	l	0.35	0/443	0.68	0/588
24	M	0.30	0/1074	0.60	0/1446
25	p	0.32	0/701	0.68	0/934
26	N	0.40	0/1757	0.68	0/2354
27	u	0.35	0/1278	0.76	1/1699 (0.1%)
28	O	0.34	0/1585	0.62	2/2128 (0.1%)
29	P	0.34	0/1431	0.60	0/1921
30	Q	0.33	0/1211	0.62	0/1633
31	R	0.34	0/1258	0.63	0/1679
32	S	0.32	0/1460	0.66	4/1962 (0.2%)
33	T	0.26	0/483	0.66	0/650

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	U	0.27	0/843	0.65	0/1143
35	V	0.34	0/1018	0.60	0/1369
36	W	0.22	0/1716	0.54	0/2317
37	X	0.31	0/974	0.60	0/1314
38	Y	0.30	0/1004	0.58	0/1341
39	y	0.30	0/1848	0.63	0/2516
40	Z	0.32	0/1118	0.65	0/1497
41	z	0.19	0/445	0.50	0/585
42	D	0.30	0/2023	0.64	2/2729 (0.1%)
43	J	0.27	0/1324	0.77	4/1778 (0.2%)
44	q	0.51	0/795	1.11	2/1050 (0.2%)
45	o	0.35	0/444	0.64	0/592
46	1	0.32	1/76644 (0.0%)	0.38	10/119495 (0.0%)
47	2	0.26	0/2883	0.28	0/4491
48	3	0.33	0/3724	0.34	0/5798
All	All	0.32	1/141593 (0.0%)	0.51	43/208187 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	v	0	1
3	A	0	2
5	B	0	1
6	b	0	5
7	C	0	3
10	E	0	1
12	F	0	1
14	G	0	1
16	I	0	1
17	H	0	1
18	h	0	1
22	L	0	1
26	N	0	1
30	Q	0	1
32	S	0	2
33	T	0	1
38	Y	0	1
39	y	0	1
40	Z	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	D	0	3
43	J	0	2
44	q	0	5
All	All	0	37

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	1	2260	U	C1'-N1	5.58	1.55	1.47

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	q	82	GLN	N-CA-C	7.06	118.94	110.19
6	b	515	ASN	CA-C-N	-6.99	113.09	121.90
6	b	515	ASN	C-N-CA	-6.99	113.09	121.90
12	F	157	ASN	CA-C-N	6.60	134.15	121.54
12	F	157	ASN	C-N-CA	6.60	134.15	121.54
43	J	154	THR	CA-C-N	6.50	133.94	121.54
43	J	154	THR	C-N-CA	6.50	133.94	121.54
32	S	23	LYS	CA-C-N	6.09	133.16	121.54
32	S	23	LYS	C-N-CA	6.09	133.16	121.54
5	B	38	SER	N-CA-C	-5.87	107.35	114.75
9	d	86	LYS	CA-C-N	5.87	136.12	121.80
9	d	86	LYS	C-N-CA	5.87	136.12	121.80
46	1	2112	U	P-O3'-C3'	5.74	128.81	120.20
46	1	2541	U	P-O3'-C3'	5.74	128.81	120.20
43	J	171	VAL	CA-C-N	5.61	132.25	121.54
43	J	171	VAL	C-N-CA	5.61	132.25	121.54
19	i	28	TYR	N-CA-C	-5.52	107.20	114.04
46	1	1576	G	P-O3'-C3'	5.50	128.44	120.20
2	v	185	VAL	N-CA-C	-5.49	107.51	112.12
46	1	1029	G	P-O3'-C3'	5.42	128.33	120.20
7	C	337	GLU	CA-C-N	5.40	131.86	121.54
7	C	337	GLU	C-N-CA	5.40	131.86	121.54
46	1	979	U	P-O3'-C3'	5.37	128.26	120.20
46	1	1815	U	P-O3'-C3'	5.32	128.17	120.20
12	F	159	GLN	N-CA-C	5.28	121.56	113.28
44	q	49	GLY	N-CA-C	5.24	120.57	111.14
27	u	32	CYS	CA-CB-SG	-5.16	102.53	114.40
46	1	1038	C	P-O3'-C3'	5.15	127.93	120.20
7	C	130	ALA	CA-C-N	5.11	127.74	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	130	ALA	C-N-CA	5.11	127.74	120.53
22	L	75	PHE	CA-C-N	5.11	131.31	121.54
22	L	75	PHE	C-N-CA	5.11	131.31	121.54
46	1	2819	A	P-O3'-C3'	5.11	127.87	120.20
46	1	1027	A	P-O3'-C3'	5.09	127.83	120.20
32	S	17	GLU	CA-C-N	5.08	131.24	121.54
32	S	17	GLU	C-N-CA	5.08	131.24	121.54
28	O	186	ALA	CA-C-N	5.05	131.18	121.54
28	O	186	ALA	C-N-CA	5.05	131.18	121.54
46	1	2769	A	P-O3'-C3'	5.03	127.74	120.20
5	B	4	ARG	CA-C-N	5.02	131.12	121.54
5	B	4	ARG	C-N-CA	5.02	131.12	121.54
42	D	215	ASP	CA-C-N	5.01	127.70	120.38
42	D	215	ASP	C-N-CA	5.01	127.70	120.38

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	219	ILE	Peptide
3	A	229	ALA	Peptide
5	B	138	ALA	Peptide
7	C	318	LEU	Peptide
7	C	338	LYS	Peptide
7	C	4	PRO	Peptide
42	D	140	ARG	Peptide
42	D	257	GLU	Peptide
42	D	259	LYS	Peptide
10	E	97	ASN	Peptide
12	F	158	LYS	Peptide
14	G	30	THR	Peptide
17	H	21	LYS	Peptide
16	I	16	ARG	Peptide
43	J	154	THR	Peptide
43	J	171	VAL	Peptide
22	L	131	LYS	Peptide
26	N	85	THR	Peptide
30	Q	152	HIS	Peptide
32	S	22	PRO	Peptide
32	S	23	LYS	Peptide
33	T	154	VAL	Peptide
38	Y	125	LYS	Peptide

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Mol	Chain	Res	Type	Group
40	Z	124	ALA	Peptide
6	b	226	ASP	Peptide
6	b	368	ALA	Peptide
6	b	369	ARG	Peptide
6	b	446	ASP	Peptide
6	b	528	PHE	Peptide
18	h	83	LYS	Peptide
44	q	31	GLY	Peptide
44	q	35	LEU	Peptide
44	q	41	ARG	Peptide
44	q	46	LYS	Peptide
44	q	79	THR	Peptide
2	v	278	LYS	Peptide
39	y	7	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	s	1050	0	237	1	0
2	v	1970	0	1954	28	0
3	A	1863	0	1930	25	0
4	a	742	0	785	4	0
5	B	3081	0	3165	47	0
6	b	4895	0	4930	63	0
7	C	2749	0	2863	25	0
8	c	743	0	797	6	0
9	d	873	0	914	9	0
10	E	1274	0	1361	41	0
11	e	1020	0	1090	9	0
12	F	1784	0	1862	17	0
13	f	850	0	880	8	0
14	G	1798	0	1894	18	0
15	g	881	0	945	7	0
16	I	1056	0	1084	8	0
17	H	1493	0	1566	11	0
18	h	969	0	1078	7	0
19	i	743	0	822	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	j	670	0	675	5	0
21	k	612	0	682	1	0
22	L	1491	0	1543	12	0
23	l	436	0	475	12	0
24	M	1059	0	1154	9	0
25	p	694	0	734	7	0
26	N	1720	0	1779	23	0
27	u	1256	0	1308	21	0
28	O	1555	0	1659	6	0
29	P	1409	0	1450	11	0
30	Q	1191	0	1265	14	0
31	R	1241	0	1330	8	0
32	S	1425	0	1466	16	0
33	T	476	0	499	5	0
34	U	826	0	843	6	0
35	V	1003	0	1048	6	0
36	W	1690	0	1661	21	0
37	X	959	0	1023	8	0
38	Y	993	0	1081	6	0
39	y	1826	0	1813	31	0
40	Z	1092	0	1155	16	0
41	z	444	0	478	6	0
42	D	1983	0	1937	23	0
43	J	1304	0	1318	16	0
44	q	783	0	853	48	0
45	o	433	0	455	2	0
46	1	68471	0	34407	353	0
47	2	2579	0	1304	14	0
48	3	3333	0	1685	14	0
49	b	32	0	12	2	0
50	b	1	0	0	0	0
All	All	132821	0	97249	798	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 4.

All (798) 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)
10:E:130:ILE:O	10:E:131:LYS:O	1.87	0.91
10:E:2:SER:N	46:1:1387:G:HO2'	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:130:ILE:HG22	10:E:134:ARG:HB3	1.52	0.89
10:E:130:ILE:HD11	46:1:3268:A:O2'	1.72	0.88
10:E:128:LYS:HD3	10:E:128:LYS:H	1.45	0.80
26:N:85:THR:HG21	44:q:51:GLY:H	1.47	0.80
10:E:130:ILE:CG2	10:E:134:ARG:HG2	2.11	0.79
5:B:10:ARG:HD2	46:1:2883:U:OP1	1.82	0.79
10:E:130:ILE:CD1	46:1:3268:A:O2'	2.31	0.78
46:1:2813:A:N6	46:1:2814:G:C6	2.52	0.78
10:E:130:ILE:HD11	46:1:3268:A:C2'	2.15	0.77
44:q:80:ARG:HA	46:1:2769:A:H3'	1.66	0.77
5:B:10:ARG:CD	46:1:2883:U:OP1	2.33	0.76
25:p:49:ARG:HH21	25:p:52:ALA:HB2	1.52	0.75
10:E:130:ILE:HG21	10:E:134:ARG:HG2	1.67	0.74
10:E:128:LYS:HD3	10:E:128:LYS:N	2.04	0.73
10:E:129:GLU:OE1	10:E:129:GLU:N	2.24	0.71
5:B:10:ARG:NE	46:1:2883:U:OP1	2.23	0.71
44:q:41:ARG:HG2	44:q:44:ASP:HB2	1.71	0.71
20:j:52:LYS:HG2	20:j:55:ARG:HH21	1.56	0.70
10:E:130:ILE:O	10:E:131:LYS:C	2.33	0.70
2:v:378:ASN:HA	44:q:90:HIS:HB2	1.74	0.70
46:1:3350:C:H42	46:1:3353:G:H1	1.39	0.69
22:L:46:ILE:HG22	22:L:49:ARG:HB2	1.74	0.69
46:1:993:G:N2	46:1:2637:A:C5	2.61	0.68
46:1:2831:G:H1	46:1:2857:C:H42	1.40	0.68
44:q:10:THR:HG21	44:q:72:LEU:HD13	1.76	0.67
44:q:42:ARG:NH2	46:1:90:C:O2	2.28	0.67
10:E:128:LYS:H	10:E:128:LYS:CD	2.07	0.67
46:1:2813:A:C6	46:1:2814:G:C5	2.83	0.67
6:b:175:TYR:HE1	6:b:270:LEU:HD13	1.58	0.66
46:1:2881:C:H2'	46:1:2882:U:H6	1.60	0.66
10:E:130:ILE:HG22	10:E:134:ARG:CB	2.25	0.66
10:E:127:ASN:HD22	10:E:127:ASN:C	2.04	0.65
15:g:8:ARG:NH2	46:1:1597:C:OP1	2.29	0.65
36:W:31:ARG:HH21	36:W:85:TYR:HB2	1.62	0.65
46:1:2425:G:H1	46:1:2604:U:H3	1.45	0.65
46:1:993:G:C2	46:1:2637:A:C4	2.85	0.64
27:u:44:ARG:NH2	46:1:2111:G:N3	2.45	0.64
5:B:215:ILE:HD13	5:B:338:LEU:HD12	1.80	0.64
46:1:2260:U:O4	46:1:2262:A:N6	2.31	0.64
42:D:77:ALA:O	42:D:108:ARG:NH1	2.32	0.63
30:Q:86:THR:HG22	30:Q:105:ARG:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:q:79:THR:HB	46:1:2770:G:H3'	1.81	0.63
6:b:182:SER:HG	6:b:322:CYS:HG	1.44	0.63
44:q:41:ARG:NH1	46:1:283:G:OP2	2.30	0.63
15:g:90:ILE:HD12	40:Z:81:LEU:HD13	1.81	0.63
39:y:119:PRO:O	39:y:139:ARG:NH2	2.32	0.62
6:b:619:GLN:HG3	23:l:46:ARG:HH21	1.64	0.62
11:e:42:VAL:HG12	11:e:52:GLN:HE21	1.64	0.62
3:A:192:LYS:HB3	3:A:193:ARG:HE	1.64	0.62
46:1:2401:A:N3	46:1:2404:A:N6	2.48	0.62
10:E:70:LYS:NZ	46:1:3266:G:OP2	2.33	0.62
31:R:3:ASN:HD21	31:R:5:ARG:HH11	1.47	0.61
46:1:1236:G:N2	46:1:1244:A:OP1	2.32	0.61
44:q:82:GLN:NE2	46:1:2768:U:O2	2.33	0.61
41:z:2:ALA:N	46:1:3015:G:OP2	2.33	0.61
5:B:11:HIS:CD2	46:1:2882:U:OP1	2.54	0.61
35:V:81:GLN:O	35:V:98:ASN:ND2	2.33	0.61
2:v:378:ASN:HB2	44:q:89:LYS:HB2	1.83	0.61
44:q:24:LYS:HB2	44:q:73:GLU:HB3	1.81	0.61
46:1:3022:G:H22	46:1:3031:G:H2'	1.66	0.61
7:C:265:GLU:HG2	7:C:266:THR:HG23	1.82	0.60
10:E:130:ILE:CG2	10:E:134:ARG:CG	2.79	0.60
3:A:19:HIS:O	3:A:23:ARG:NH1	2.35	0.60
7:C:193:LYS:NZ	48:3:21:C:OP1	2.31	0.60
5:B:227:GLU:HG2	5:B:270:ARG:HE	1.66	0.60
14:G:33:ASN:ND2	46:1:2549:G:N7	2.50	0.60
31:R:60:LYS:NZ	46:1:1671:C:OP1	2.34	0.60
36:W:54:GLN:NE2	46:1:1232:C:O2	2.34	0.60
5:B:28:ARG:NH2	46:1:3140:G:N7	2.48	0.60
44:q:47:GLN:OE1	44:q:54:THR:N	2.35	0.60
23:l:27:ILE:O	23:l:33:ASN:ND2	2.35	0.60
43:J:47:GLN:HG2	43:J:67:VAL:HG12	1.83	0.60
19:i:50:LEU:HB2	19:i:55:ARG:HE	1.66	0.59
43:J:96:PHE:HB2	43:J:156:LYS:HE3	1.84	0.59
46:1:2483:G:H21	46:1:2485:A:H8	1.51	0.59
6:b:622:SER:OG	23:l:46:ARG:NH1	2.35	0.59
9:d:80:ASN:ND2	9:d:84:ASP:OD2	2.36	0.59
22:L:174:ARG:HH12	46:1:712:G:H5'	1.67	0.59
46:1:526:C:N3	46:1:527:A:N6	2.51	0.59
7:C:329:PRO:HB3	12:F:41:ARG:HH21	1.68	0.59
32:S:42:TRP:HE1	32:S:58:ILE:HD11	1.68	0.59
44:q:3:ASN:ND2	44:q:96:GLU:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1:3164:C:N4	46:1:3286:G:O6	2.35	0.59
26:N:37:HIS:HE1	26:N:63:ARG:HH11	1.50	0.59
43:J:109:HIS:HD2	43:J:123:PHE:H	1.49	0.59
46:1:993:G:N2	46:1:2637:A:C4	2.71	0.59
44:q:49:GLY:HA2	46:1:278:U:H3'	1.85	0.58
39:y:85:ARG:NH1	39:y:89:PRO:O	2.36	0.58
46:1:3349:C:O2	46:1:3356:G:N2	2.36	0.58
5:B:214:MET:O	5:B:341:SER:OG	2.22	0.58
5:B:266:ARG:NH2	46:1:2392:C:O2'	2.37	0.58
5:B:47:LEU:HD12	5:B:335:ILE:HD11	1.85	0.58
23:l:2:ALA:N	46:1:1493:G:O6	2.37	0.58
23:l:43:ASN:OD1	23:l:46:ARG:NH1	2.37	0.58
46:1:2727:A:OP2	46:1:2728:G:N2	2.36	0.58
19:i:9:ILE:HG21	22:L:174:ARG:HH21	1.69	0.58
39:y:106:ASN:ND2	39:y:150:SER:OG	2.33	0.58
7:C:188:ARG:NH1	46:1:1382:G:OP2	2.37	0.58
18:h:85:THR:OG1	48:3:36:G:OP2	2.22	0.58
27:u:44:ARG:NH2	46:1:2111:G:O2'	2.36	0.58
42:D:71:GLY:O	47:2:7:G:O2'	2.20	0.58
44:q:18:ARG:NH2	46:1:759:U:OP2	2.37	0.58
46:1:2841:G:N2	46:1:2846:U:OP1	2.36	0.57
5:B:90:VAL:HG22	5:B:104:THR:HG22	1.86	0.57
6:b:302:ARG:HA	6:b:305:LEU:HD13	1.86	0.57
12:F:178:ILE:HD11	12:F:187:GLU:HG3	1.85	0.57
5:B:11:HIS:HD2	46:1:2882:U:OP1	1.88	0.57
46:1:2876:C:OP1	46:1:2942:C:N4	2.37	0.57
18:h:118:ILE:HG12	22:L:123:ILE:HG22	1.87	0.57
20:j:16:HIS:HD1	46:1:359:U:HO2'	1.52	0.57
22:L:18:TRP:NE1	46:1:799:G:O2'	2.32	0.57
34:U:89:LEU:HB3	34:U:93:ILE:HD12	1.86	0.57
24:M:72:LEU:HD11	24:M:81:VAL:HG22	1.87	0.57
38:Y:126:LEU:HD12	38:Y:127:GLU:HG2	1.86	0.57
46:1:1222:G:HO2'	46:1:1285:G:H1	1.45	0.57
46:1:1485:G:H1	46:1:1857:C:H42	1.52	0.57
19:i:5:THR:HG23	19:i:12:ASN:HB2	1.85	0.57
36:W:163:PRO:HA	36:W:166:ARG:HG2	1.87	0.57
39:y:21:ASN:ND2	39:y:112:ASP:OD2	2.38	0.57
7:C:291:ASN:ND2	46:1:1350:A:OP1	2.37	0.57
46:1:198:A:N3	46:1:218:G:O2'	2.37	0.57
37:X:125:ARG:NH2	46:1:1609:C:OP1	2.38	0.56
6:b:435:ILE:HG12	27:u:3:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:55:LEU:HB2	9:d:95:PRO:HD3	1.87	0.56
36:W:18:LYS:HE3	46:1:1260:A:H5''	1.86	0.56
46:1:1268:G:N2	46:1:1269:U:O4	2.37	0.56
5:B:66:LYS:O	5:B:70:ARG:NH2	2.38	0.56
37:X:27:ARG:NH2	48:3:150:G:OP1	2.38	0.56
46:1:2770:G:H22	46:1:2789:U:H1'	1.70	0.56
5:B:173:GLN:NE2	46:1:3313:U:O5'	2.39	0.56
15:g:102:LYS:NZ	46:1:2552:C:OP1	2.36	0.56
39:y:9:ASN:ND2	46:1:3018:C:OP1	2.34	0.56
31:R:42:ARG:NH2	46:1:1600:U:OP1	2.39	0.56
39:y:158:GLY:HA2	39:y:179:VAL:HB	1.88	0.56
46:1:2253:G:H1	46:1:2263:C:H41	1.51	0.56
46:1:2466:G:H1	46:1:2489:C:H42	1.54	0.56
12:F:33:ARG:NH2	46:1:595:G:OP1	2.38	0.56
30:Q:39:ARG:NH1	46:1:1348:U:OP2	2.38	0.56
40:Z:52:LYS:O	40:Z:65:ARG:NH1	2.39	0.56
6:b:318:MET:SD	6:b:334:LYS:NZ	2.75	0.56
6:b:370:ASP:HB3	6:b:372:VAL:H	1.71	0.56
36:W:158:ILE:HG22	36:W:160:SER:H	1.70	0.56
2:v:229:ILE:HB	46:1:2873:U:H3'	1.88	0.56
44:q:78:LYS:O	46:1:2772:C:N4	2.36	0.56
9:d:62:ARG:NH1	9:d:68:GLU:OE2	2.38	0.56
18:h:77:PRO:HD2	18:h:80:LEU:HD12	1.88	0.56
31:R:102:LEU:HD22	31:R:138:LEU:HD13	1.87	0.56
32:S:132:THR:OG1	46:1:534:U:OP1	2.24	0.56
43:J:32:ARG:NH1	43:J:120:ILE:O	2.39	0.56
10:E:40:LEU:HD13	10:E:84:VAL:HG11	1.89	0.55
10:E:43:LEU:HD11	10:E:85:ILE:HG13	1.88	0.55
15:g:41:ARG:HD2	15:g:56:THR:HG21	1.87	0.55
44:q:42:ARG:HA	44:q:45:ARG:HB3	1.86	0.55
2:v:205:ASN:ND2	46:1:2284:C:O2	2.38	0.55
7:C:122:THR:HG22	7:C:235:LEU:HB2	1.89	0.55
10:E:46:ARG:NH2	46:1:3268:A:OP1	2.40	0.55
14:G:48:ARG:NH1	46:1:2526:C:N3	2.54	0.55
23:l:11:GLN:NE2	48:3:45:C:O2'	2.40	0.55
46:1:1004:U:O4	46:1:1045:C:N4	2.38	0.55
4:a:112:ILE:HB	4:a:130:VAL:HG12	1.88	0.55
9:d:62:ARG:HE	46:1:3074:G:H4'	1.72	0.55
46:1:991:G:C6	46:1:992:A:C6	2.93	0.55
10:E:54:TYR:HA	10:E:65:ILE:HG22	1.87	0.55
14:G:68:ARG:NH1	46:1:2514:U:OP1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:24:LYS:NZ	24:M:61:GLY:O	2.40	0.55
28:O:49:ARG:NH1	46:1:1191:U:OP2	2.38	0.55
46:1:1597:C:H42	46:1:1610:G:H1	1.53	0.55
3:A:2:GLY:N	46:1:2415:C:OP1	2.40	0.55
7:C:69:ARG:NH2	46:1:2400:G:OP2	2.40	0.55
7:C:326:ARG:NH1	46:1:608:A:O3'	2.40	0.55
17:H:44:THR:OG1	46:1:3186:A:N3	2.38	0.55
35:V:136:VAL:HG12	35:V:137:VAL:HG23	1.88	0.55
36:W:91:GLN:HB2	36:W:228:VAL:HG21	1.89	0.55
6:b:178:VAL:HG13	6:b:255:ASP:HB2	1.89	0.54
14:G:48:ARG:NH2	46:1:2526:C:O2	2.40	0.54
22:L:53:LEU:HB2	22:L:55:ARG:HH12	1.72	0.54
34:U:21:SER:O	34:U:25:ASN:ND2	2.40	0.54
39:y:68:ARG:NH1	39:y:112:ASP:O	2.39	0.54
46:1:1863:G:N1	46:1:1866:C:OP2	2.40	0.54
10:E:127:ASN:OD1	29:P:181:ARG:NH1	2.33	0.54
37:X:100:LYS:NZ	37:X:106:ASP:OD1	2.40	0.54
6:b:164:ASP:H	6:b:217:GLN:HE22	1.54	0.54
12:F:57:THR:O	12:F:61:ASN:ND2	2.39	0.54
46:1:2883:U:H2'	46:1:2883:U:O2	2.06	0.54
29:P:56:ARG:NH1	29:P:75:GLU:OE2	2.40	0.54
11:e:101:SER:HB3	46:1:1389:G:H5''	1.88	0.54
43:J:15:GLU:HB3	43:J:130:VAL:HG13	1.89	0.54
46:1:1348:U:O2	46:1:1349:G:N2	2.40	0.54
46:1:2483:G:N2	46:1:2486:A:OP2	2.39	0.54
2:v:290:THR:HA	2:v:335:LEU:HD11	1.90	0.54
3:A:221:LYS:NZ	46:1:2965:U:O2	2.41	0.54
10:E:68:PRO:HG3	10:E:145:LEU:HD23	1.89	0.54
26:N:18:VAL:HG13	26:N:19:LEU:HD12	1.90	0.54
44:q:71:ARG:NH2	46:1:2769:A:OP1	2.41	0.54
46:1:2882:U:H2'	46:1:2882:U:O2	2.06	0.54
47:2:96:U:H2'	47:2:97:A:H8	1.73	0.54
2:v:168:LYS:HB3	2:v:171:PHE:HB3	1.90	0.54
3:A:244:GLY:HA2	46:1:2153:U:H4'	1.90	0.54
33:T:128:LEU:HD11	46:1:1096:U:H5'	1.89	0.54
43:J:51:ARG:O	43:J:61:ARG:NH2	2.41	0.54
46:1:1645:U:H3	46:1:1810:A:H61	1.54	0.54
5:B:53:MET:HB2	46:1:3049:A:H5''	1.88	0.54
10:E:127:ASN:O	10:E:127:ASN:ND2	2.40	0.54
32:S:109:ASP:OD1	32:S:113:ARG:NH1	2.41	0.54
44:q:38:GLN:NE2	46:1:90:C:OP1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:h:67:ARG:NH2	48:3:97:A:OP1	2.42	0.53
36:W:22:ASN:HD21	36:W:25:ARG:HH21	1.57	0.53
3:A:54:ARG:NH2	46:1:2176:U:OP1	2.39	0.53
6:b:22:LEU:HD12	46:1:2828:G:H21	1.74	0.53
7:C:329:PRO:HB2	12:F:45:LEU:HD12	1.91	0.53
26:N:42:PRO:HG3	26:N:61:ILE:HG13	1.89	0.53
29:P:167:ARG:HE	46:1:620:U:H4'	1.73	0.53
36:W:49:ARG:HH21	46:1:1230:G:H5'	1.73	0.53
2:v:380:ASN:HD21	44:q:65:THR:HA	1.73	0.53
42:D:205:SER:HB3	42:D:236:LEU:HD23	1.90	0.53
46:1:1468:A:N6	46:1:1508:C:O2	2.41	0.53
39:y:4:ARG:HB3	39:y:208:LEU:HD23	1.91	0.53
46:1:600:G:N2	46:1:603:A:OP2	2.40	0.53
6:b:268:VAL:HG21	6:b:305:LEU:HB3	1.89	0.53
34:U:59:ASP:HB3	34:U:62:VAL:H	1.73	0.53
43:J:133:ARG:NH2	43:J:158:ASP:OD2	2.41	0.53
6:b:436:LEU:HD23	6:b:437:ASP:H	1.73	0.53
11:e:16:LYS:NZ	46:1:1404:G:O6	2.42	0.53
46:1:52:A:N3	46:1:811:U:O2'	2.42	0.53
46:1:1390:A:N6	46:1:1418:A:O2'	2.42	0.53
48:3:41:A:N6	48:3:103:G:O2'	2.42	0.53
6:b:290:THR:HG21	6:b:319:THR:HB	1.90	0.53
24:M:128:ARG:NH1	46:1:3214:U:OP2	2.42	0.53
39:y:42:LEU:HD13	39:y:46:ILE:HD11	1.91	0.53
46:1:348:A:N3	46:1:352:A:O2'	2.42	0.53
46:1:2844:C:N3	46:1:2847:A:N6	2.57	0.53
7:C:338:LYS:O	7:C:340:GLY:N	2.42	0.53
42:D:16:PHE:O	47:2:11:A:N6	2.42	0.53
46:1:371:G:N1	46:1:374:A:OP2	2.39	0.53
46:1:2451:G:N2	46:1:2495:C:N3	2.57	0.53
26:N:56:LYS:NZ	26:N:145:ASP:OD2	2.42	0.53
44:q:45:ARG:NH1	46:1:283:G:OP1	2.38	0.53
1:s:45:UNK:O	1:s:151:UNK:N	2.42	0.52
5:B:216:ASP:HB3	5:B:278:ILE:HA	1.90	0.52
25:p:73:THR:HG23	25:p:76:ALA:H	1.73	0.52
46:1:41:G:N2	46:1:2803:A:N7	2.57	0.52
46:1:36:C:O2'	46:1:934:G:N3	2.42	0.52
4:a:126:LYS:HB3	4:a:148:ILE:HG12	1.90	0.52
32:S:44:PHE:HE1	32:S:122:HIS:HD2	1.57	0.52
32:S:124:LEU:HD22	33:T:154:VAL:HA	1.91	0.52
39:y:180:PRO:HB2	39:y:221:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:178:ILE:HG13	2:v:183:ALA:HB3	1.91	0.52
14:G:157:VAL:HG21	14:G:163:VAL:HG21	1.90	0.52
20:j:72:ARG:NH1	48:3:95:G:OP2	2.40	0.52
46:1:998:A:O2'	47:2:103:A:N3	2.40	0.52
46:1:1524:A:O2'	46:1:1526:U:OP2	2.27	0.52
46:1:937:G:N2	46:1:961:C:OP1	2.41	0.52
3:A:67:TYR:OH	46:1:2525:G:N7	2.42	0.52
36:W:196:ASP:HB3	36:W:199:GLN:H	1.74	0.52
16:I:17:ASP:OD2	27:u:23:ARG:NH1	2.42	0.52
16:I:89:VAL:HG22	16:I:101:PHE:HE1	1.75	0.52
28:O:117:ARG:NH2	46:1:3182:G:OP1	2.40	0.52
7:C:207:VAL:HB	7:C:227:THR:HG22	1.91	0.52
36:W:45:LEU:HD12	36:W:48:VAL:HG11	1.92	0.52
36:W:55:GLU:HA	36:W:58:THR:HG22	1.92	0.52
46:1:2112:U:H4'	46:1:2113:A:H5'	1.92	0.52
46:1:3343:G:H21	46:1:3362:A:H2	1.58	0.52
5:B:39:LYS:NZ	41:z:27:ASP:OD1	2.41	0.52
6:b:83:ASP:HA	6:b:88:LYS:HG3	1.92	0.52
6:b:126:LYS:NZ	46:1:2826:U:OP2	2.43	0.52
42:D:218:ARG:NH2	47:2:31:U:O2'	2.43	0.52
43:J:137:ARG:NH2	47:2:44:C:OP2	2.42	0.52
6:b:226:ASP:O	6:b:229:THR:N	2.42	0.51
46:1:1288:U:H2'	46:1:1289:G:H8	1.75	0.51
12:F:33:ARG:NH1	46:1:596:C:OP1	2.44	0.51
3:A:9:ARG:NH1	46:1:912:G:OP2	2.43	0.51
18:h:77:PRO:HG2	37:X:50:ALA:HB2	1.93	0.51
24:M:13:ARG:NH1	24:M:65:LEU:O	2.43	0.51
46:1:2452:G:N1	46:1:2494:A:N1	2.51	0.51
5:B:10:ARG:NH1	5:B:11:HIS:O	2.43	0.51
24:M:6:ILE:HG21	46:1:3199:G:H5''	1.93	0.51
45:o:19:ASN:ND2	46:1:969:C:OP1	2.41	0.51
46:1:2813:A:N6	46:1:2814:G:O6	2.42	0.51
6:b:257:SER:OG	6:b:258:GLU:N	2.44	0.51
6:b:639:ARG:HH21	46:1:2401:A:H5'	1.75	0.51
14:G:47:SER:OG	46:1:2585:G:O6	2.28	0.51
40:Z:26:VAL:O	40:Z:93:LYS:NZ	2.41	0.51
40:Z:90:GLU:HA	40:Z:93:LYS:HG2	1.93	0.51
46:1:908:G:N2	46:1:2609:A:OP1	2.44	0.51
2:v:153:ASN:OD1	2:v:241:LYS:NZ	2.44	0.51
10:E:130:ILE:HG21	10:E:134:ARG:CG	2.36	0.51
10:E:130:ILE:C	10:E:131:LYS:O	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:b:299:ASP:HB2	6:b:302:ARG:HG2	1.92	0.51
13:f:6:ARG:NH1	13:f:8:TYR:O	2.42	0.51
44:q:27:GLN:HG2	44:q:28:TYR:H	1.76	0.51
46:1:1246:G:N2	46:1:1264:G:O2'	2.44	0.51
46:1:3042:U:OP2	46:1:3092:C:N4	2.44	0.51
2:v:379:TYR:H	44:q:90:HIS:CD2	2.29	0.51
5:B:138:ALA:O	5:B:141:GLY:N	2.39	0.51
10:E:82:ARG:NH2	46:1:501:A:OP1	2.43	0.51
12:F:151:ARG:HH22	46:1:1334:U:H4'	1.76	0.51
46:1:2770:G:N2	46:1:2789:U:O2	2.43	0.51
6:b:184:LEU:HD22	6:b:220:ASP:HB2	1.93	0.51
7:C:299:ILE:HG23	30:Q:39:ARG:HB3	1.93	0.51
29:P:107:LEU:HD23	29:P:152:GLU:HG3	1.93	0.51
39:y:163:PRO:HA	39:y:183:ALA:HB1	1.93	0.51
46:1:3129:A:N6	46:1:3131:U:O2	2.44	0.51
3:A:117:GLU:HG2	3:A:124:GLY:H	1.76	0.50
32:S:73:LYS:NZ	32:S:97:VAL:O	2.41	0.50
35:V:131:SER:O	39:y:106:ASN:ND2	2.44	0.50
39:y:15:VAL:HG23	39:y:195:ALA:HB1	1.94	0.50
5:B:366:GLY:HA2	46:1:3086:A:H4'	1.94	0.50
14:G:201:THR:HG22	14:G:202:GLU:HG2	1.93	0.50
38:Y:55:GLU:HB2	38:Y:108:LYS:HB2	1.93	0.50
46:1:21:G:OP2	48:3:36:G:N2	2.41	0.50
5:B:129:ALA:O	46:1:3149:G:O2'	2.25	0.50
13:f:99:ARG:NH1	46:1:3275:U:O2'	2.45	0.50
19:i:59:ASP:O	19:i:63:ASN:ND2	2.44	0.50
23:l:48:LYS:NZ	46:1:1492:G:O2'	2.44	0.50
46:1:2140:U:H1'	46:1:2978:U:H5'	1.94	0.50
5:B:2:SER:OG	46:1:2943:G:OP2	2.28	0.50
10:E:52:VAL:HG11	10:E:65:ILE:HD13	1.93	0.50
22:L:24:VAL:HG12	26:N:199:LEU:HB2	1.92	0.50
46:1:2260:U:C5	46:1:2262:A:C5	2.99	0.50
39:y:8:GLU:HB3	46:1:3018:C:H5''	1.94	0.50
41:z:49:LEU:HD23	41:z:52:LYS:HD2	1.93	0.50
44:q:45:ARG:NE	46:1:282:G:OP2	2.44	0.50
12:F:186:HIS:O	12:F:190:THR:OG1	2.28	0.50
30:Q:106:PHE:HB2	30:Q:111:ARG:HH21	1.77	0.50
46:1:2950:G:N2	46:1:2950:G:OP2	2.45	0.50
6:b:646:PHE:O	46:1:884:A:N6	2.45	0.50
6:b:647:ARG:HD2	46:1:880:G:H22	1.77	0.50
43:J:137:ARG:NH1	47:2:28:C:OP1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1:1293:U:O4	46:1:1294:A:N6	2.45	0.50
46:1:2945:G:O2'	46:1:2948:C:OP2	2.28	0.50
9:d:57:GLN:NE2	46:1:1474:A:O2'	2.45	0.50
26:N:90:ASN:ND2	46:1:2424:A:OP1	2.44	0.50
17:H:20:ILE:HG21	17:H:45:PHE:HD2	1.76	0.50
30:Q:43:PRO:HB2	46:1:728:G:H5''	1.94	0.50
46:1:1242:G:N2	46:1:1270:A:O2'	2.45	0.50
6:b:180:LYS:NZ	6:b:221:THR:O	2.44	0.49
7:C:163:LYS:NZ	46:1:208:C:OP2	2.34	0.49
12:F:154:GLY:O	12:F:161:VAL:N	2.45	0.49
6:b:26:GLN:HE21	46:1:1302:A:H61	1.60	0.49
5:B:380:MET:O	46:1:3369:G:N1	2.44	0.49
46:1:2406:C:O2	46:1:2816:G:N2	2.46	0.49
3:A:113:VAL:HG12	3:A:166:ILE:HD13	1.94	0.49
5:B:71:GLU:OE2	5:B:357:LYS:NZ	2.40	0.49
18:h:66:VAL:HG11	37:X:50:ALA:HB1	1.94	0.49
30:Q:123:THR:OG1	30:Q:125:ASP:OD1	2.30	0.49
39:y:4:ARG:HD3	39:y:208:LEU:HA	1.94	0.49
44:q:26:THR:H	44:q:71:ARG:HG2	1.76	0.49
5:B:305:ILE:HD11	5:B:317:ILE:HG21	1.95	0.49
6:b:188:THR:HG21	6:b:207:GLY:HA3	1.95	0.49
24:M:33:ALA:HB2	24:M:53:VAL:HG11	1.95	0.49
46:1:993:G:C2	46:1:2637:A:C5	3.01	0.49
2:v:228:LEU:HG	46:1:2874:G:H5'	1.94	0.49
6:b:19:ASP:HA	46:1:2828:G:H22	1.78	0.49
17:H:89:LYS:HG2	17:H:145:VAL:HG22	1.94	0.49
27:u:33:ARG:HH11	27:u:35:LYS:HD3	1.77	0.49
6:b:168:ARG:HH21	6:b:215:ARG:H	1.59	0.49
24:M:74:ARG:NH2	46:1:534:U:O4	2.45	0.49
31:R:125:LYS:NZ	46:1:1724:U:O4	2.44	0.49
36:W:134:THR:HA	36:W:189:CYS:HB2	1.94	0.49
43:J:105:GLY:HA3	46:1:2674:A:H5''	1.94	0.49
5:B:317:ILE:O	5:B:319:ASN:N	2.46	0.49
8:c:54:SER:OG	46:1:2552:C:N4	2.46	0.49
5:B:216:ASP:OD1	5:B:216:ASP:N	2.45	0.49
6:b:390:PRO:O	6:b:395:ARG:NH1	2.39	0.49
48:3:131:A:H2'	48:3:132:G:H8	1.78	0.49
26:N:114:ARG:HD3	26:N:137:PRO:HG3	1.94	0.49
30:Q:66:ARG:NH1	46:1:744:A:OP1	2.46	0.49
32:S:50:LYS:NZ	47:2:76:A:N3	2.59	0.49
44:q:67:LYS:HE3	46:1:2793:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1:3006:A:H62	46:1:3140:G:H21	1.60	0.48
16:I:91:ASP:HB3	16:I:96:TYR:HD2	1.78	0.48
46:1:2137:U:OP2	46:1:2142:A:N6	2.47	0.48
46:1:2947:G:OP1	46:1:2982:A:N6	2.40	0.48
7:C:40:THR:O	7:C:44:LYS:NZ	2.43	0.48
16:I:83:VAL:HG13	27:u:47:ARG:HH22	1.78	0.48
46:1:339:C:OP1	46:1:1380:G:O2'	2.31	0.48
46:1:1493:G:OP2	46:1:1493:G:N2	2.45	0.48
6:b:446:ASP:H	6:b:449:ILE:HD11	1.79	0.48
2:v:187:THR:HG22	2:v:201:TYR:HE1	1.78	0.48
18:h:59:ASN:ND2	48:3:97:A:O2'	2.46	0.48
46:1:2890:A:O2'	46:1:2933:A:N3	2.45	0.48
2:v:280:SER:OG	2:v:281:ASN:N	2.46	0.48
7:C:82:THR:HG23	7:C:84:ARG:H	1.78	0.48
23:l:24:PRO:HD2	23:l:27:ILE:HD12	1.95	0.48
42:D:61:ILE:HG23	42:D:79:TYR:HE1	1.79	0.48
14:G:162:LEU:HD23	26:N:7:LEU:HD21	1.95	0.48
46:1:1889:G:O6	46:1:2345:A:N6	2.47	0.48
3:A:21:ARG:HD3	46:1:824:C:H5''	1.94	0.48
7:C:29:PRO:HB3	30:Q:25:TYR:HE2	1.78	0.48
12:F:151:ARG:NH2	46:1:1334:U:O3'	2.47	0.48
10:E:149:ILE:HG23	10:E:155:LEU:HD12	1.95	0.48
10:E:165:LEU:HD11	13:f:102:LEU:HD11	1.95	0.48
26:N:73:ARG:NH1	26:N:86:ASN:O	2.47	0.48
46:1:3021:A:N6	46:1:3033:A:OP2	2.45	0.48
40:Z:64:LYS:NZ	46:1:1812:G:N7	2.59	0.47
42:D:33:ARG:NH1	47:2:7:G:OP1	2.47	0.47
6:b:616:HIS:HA	29:P:126:ARG:HB2	1.95	0.47
26:N:172:ARG:NH2	46:1:29:C:O3'	2.47	0.47
27:u:74:ARG:HH21	39:y:96:ARG:HH11	1.62	0.47
33:T:108:ARG:NH1	46:1:1097:G:O2'	2.43	0.47
36:W:122:SER:HA	36:W:212:GLU:HA	1.96	0.47
42:D:216:GLU:O	42:D:220:SER:N	2.46	0.47
42:D:264:GLN:HB3	47:2:121:U:H3	1.77	0.47
2:v:186:ASP:OD2	2:v:206:HIS:ND1	2.48	0.47
46:1:3231:U:H2'	46:1:3232:G:H8	1.80	0.47
3:A:68:LYS:NZ	46:1:1580:A:OP1	2.48	0.47
3:A:174:ARG:NH1	46:1:1793:C:O2	2.48	0.47
5:B:93:VAL:HG23	5:B:102:LEU:HD22	1.96	0.47
46:1:2816:G:O6	46:1:2817:A:N6	2.47	0.47
46:1:2881:C:H2'	46:1:2882:U:C6	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:203:GLN:HB3	2:v:206:HIS:HD2	1.78	0.47
3:A:180:LEU:HD11	25:p:26:VAL:HG21	1.97	0.47
26:N:27:VAL:HG23	26:N:129:TYR:HE2	1.79	0.47
27:u:45:ASN:HD22	27:u:46:PRO:HD2	1.79	0.47
46:1:2116:G:OP1	46:1:2118:C:N4	2.48	0.47
46:1:2570:U:H3	46:1:2573:G:H1	1.63	0.47
3:A:243:THR:O	46:1:2153:U:O2'	2.26	0.47
9:d:31:ARG:NH2	46:1:1884:A:OP1	2.39	0.47
17:H:8:GLN:HB3	17:H:72:LYS:HD2	1.96	0.47
25:p:49:ARG:NH2	46:1:1793:C:OP2	2.38	0.47
35:V:120:LYS:HB2	35:V:137:VAL:HG22	1.96	0.47
38:Y:74:TYR:OH	48:3:75:G:OP2	2.31	0.47
46:1:2813:A:C5	46:1:2814:G:N7	2.83	0.47
6:b:319:THR:O	6:b:327:ASN:ND2	2.46	0.47
10:E:127:ASN:C	10:E:127:ASN:ND2	2.73	0.47
36:W:41:TRP:HB2	36:W:103:LEU:HB3	1.97	0.47
38:Y:60:ARG:NH1	46:1:200:C:OP2	2.43	0.47
2:v:379:TYR:H	44:q:90:HIS:HD2	1.62	0.47
5:B:308:MET:HE2	46:1:3329:U:H5''	1.95	0.47
14:G:72:PRO:HG3	26:N:18:VAL:HA	1.97	0.47
45:o:36:ASP:OD1	46:1:2737:C:O2'	2.33	0.47
46:1:1489:A:OP2	46:1:1838:G:N1	2.45	0.47
46:1:90:C:O2'	46:1:282:G:OP1	2.23	0.47
46:1:3121:U:H1'	46:1:3122:A:H5''	1.97	0.47
10:E:129:GLU:N	10:E:129:GLU:CD	2.73	0.46
27:u:10:SER:HB2	27:u:53:LYS:HB2	1.97	0.46
46:1:655:C:H2'	46:1:656:A:C8	2.50	0.46
5:B:10:ARG:HH21	5:B:263:SER:HB2	1.80	0.46
5:B:387:LEU:HD13	27:u:109:LYS:HZ3	1.80	0.46
7:C:320:ASN:ND2	46:1:505:G:OP1	2.48	0.46
8:c:25:LEU:O	8:c:29:SER:OG	2.33	0.46
36:W:89:LEU:HD12	36:W:92:LEU:HD21	1.96	0.46
40:Z:72:ILE:HD12	40:Z:101:PHE:HE1	1.80	0.46
41:z:11:LEU:HD22	46:1:3100:U:H2'	1.98	0.46
5:B:166:ILE:HD11	5:B:171:LEU:HD22	1.98	0.46
16:I:40:ASP:HB3	16:I:43:LYS:HD3	1.98	0.46
24:M:20:VAL:O	24:M:66:THR:OG1	2.32	0.46
40:Z:46:ILE:HA	40:Z:70:PRO:HA	1.96	0.46
46:1:9:U:O2	48:3:150:G:N2	2.49	0.46
46:1:528:U:H2'	46:1:529:A:H8	1.80	0.46
46:1:2451:G:H21	46:1:2496:C:H5	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:2:SER:N	46:1:1387:G:O2'	2.43	0.46
22:L:171:ARG:HH12	46:1:713:U:H5'	1.80	0.46
42:D:200:PHE:HB3	42:D:237:GLU:HG3	1.97	0.46
3:A:27:ALA:O	3:A:128:ARG:NH2	2.49	0.46
5:B:78:VAL:HG22	5:B:323:MET:HG2	1.97	0.46
16:I:98:LEU:O	16:I:102:LEU:N	2.41	0.46
26:N:44:ARG:NH1	46:1:269:G:OP2	2.41	0.46
46:1:408:A:N3	46:1:655:C:O2'	2.45	0.46
10:E:2:SER:O	46:1:1421:G:N2	2.48	0.46
15:g:37:LYS:NZ	46:1:1591:G:OP1	2.49	0.46
17:H:16:VAL:HG12	17:H:29:GLY:HA3	1.97	0.46
28:O:74:ARG:NH1	46:1:3008:A:OP2	2.49	0.46
39:y:28:VAL:HG12	39:y:50:HIS:HB3	1.97	0.46
42:D:211:LEU:HB3	42:D:219:PHE:HB2	1.96	0.46
46:1:1899:G:N2	46:1:2335:G:OP2	2.39	0.46
11:e:104:ASN:ND2	46:1:1389:G:OP1	2.40	0.46
46:1:545:U:H5''	46:1:547:G:H21	1.80	0.46
46:1:2537:U:H1'	46:1:2538:U:H4'	1.97	0.46
8:c:73:GLY:N	8:c:76:GLU:OE2	2.47	0.46
29:P:62:ARG:NH1	46:1:412:G:OP1	2.48	0.46
6:b:396:ARG:HH22	39:y:43:GLY:HA2	1.81	0.46
9:d:75:ILE:HG12	9:d:93:VAL:HG22	1.98	0.46
26:N:192:LYS:O	26:N:196:THR:OG1	2.31	0.46
46:1:2185:G:O2'	46:1:2314:U:OP2	2.26	0.46
46:1:2262:A:N1	46:1:2263:C:N4	2.63	0.46
11:e:100:ILE:O	11:e:125:ARG:NH1	2.49	0.46
27:u:78:PRO:HG2	39:y:85:ARG:HB2	1.98	0.46
37:X:105:VAL:HG21	37:X:135:ILE:HD12	1.96	0.46
6:b:184:LEU:HD23	6:b:192:VAL:HG21	1.97	0.45
36:W:222:ASP:HB3	36:W:225:SER:HB3	1.97	0.45
46:1:1627:U:H3	46:1:1816:A:H61	1.64	0.45
10:E:130:ILE:HD11	46:1:3268:A:H2'	1.94	0.45
14:G:144:GLU:HA	14:G:173:MET:HG3	1.98	0.45
29:P:25:SER:OG	46:1:1447:G:N7	2.46	0.45
29:P:29:THR:HA	29:P:32:THR:HG22	1.98	0.45
46:1:1284:C:N3	46:1:1285:G:N2	2.64	0.45
2:v:229:ILE:N	46:1:2874:G:OP1	2.31	0.45
2:v:310:ALA:HB2	2:v:379:TYR:HE1	1.81	0.45
2:v:338:ILE:HD12	2:v:357:SER:HB2	1.99	0.45
11:e:63:THR:HA	11:e:66:LEU:HD12	1.97	0.45
30:Q:62:VAL:HG13	30:Q:66:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1:999:G:N2	46:1:1050:U:O2	2.49	0.45
46:1:1306:G:N2	46:1:1307:G:N7	2.61	0.45
46:1:1322:U:H2'	46:1:1323:G:H8	1.81	0.45
46:1:2094:C:H2'	46:1:2095:G:H8	1.81	0.45
4:a:63:LYS:NZ	4:a:65:GLN:OE1	2.48	0.45
26:N:68:ARG:NH2	26:N:123:GLN:OE1	2.50	0.45
32:S:170:THR:OG1	32:S:171:PHE:N	2.47	0.45
46:1:1017:C:H4'	46:1:1036:A:H2'	1.98	0.45
27:u:2:ARG:O	27:u:4:TYR:N	2.36	0.45
41:z:18:ARG:NH2	46:1:3100:U:OP1	2.41	0.45
41:z:46:LEU:HD23	41:z:49:LEU:HD12	1.99	0.45
46:1:745:C:H2'	46:1:746:A:H8	1.81	0.45
15:g:44:CYS:HB3	15:g:47:CYS:HB2	1.75	0.45
19:i:34:SER:HG	19:i:37:THR:H	1.57	0.45
39:y:126:GLU:HG3	39:y:137:VAL:HG11	1.98	0.45
46:1:40:A:H61	46:1:963:G:H21	1.65	0.45
22:L:174:ARG:NH1	46:1:712:G:OP1	2.50	0.45
46:1:994:G:H5'	46:1:2637:A:O2'	2.16	0.45
46:1:2955:U:OP2	46:1:2977:G:N1	2.47	0.45
2:v:230:SER:H	46:1:2873:U:H3'	1.81	0.45
6:b:363:VAL:HG12	39:y:182:VAL:HG22	1.97	0.45
6:b:448:GLU:HB3	6:b:451:ALA:HB3	1.99	0.45
26:N:36:ILE:HD11	26:N:105:ARG:HB3	1.99	0.45
42:D:65:ILE:HG12	42:D:74:VAL:HG22	1.98	0.45
44:q:41:ARG:CZ	46:1:283:G:H5'	2.47	0.45
44:q:82:GLN:HB2	46:1:2790:A:H2	1.81	0.45
46:1:845:G:O2'	46:1:848:A:N6	2.50	0.45
46:1:1354:G:H1	46:1:1358:C:H5'	1.82	0.45
6:b:506:GLU:HA	9:d:97:LEU:HD13	1.98	0.45
13:f:52:VAL:HG22	13:f:66:VAL:HG22	1.98	0.45
31:R:62:ARG:NH1	46:1:3068:U:OP2	2.40	0.45
42:D:22:ARG:HE	42:D:27:LYS:HB2	1.82	0.45
46:1:1004:U:H3	46:1:1046:A:H61	1.65	0.45
46:1:3348:G:H1	46:1:3357:U:H3	1.65	0.45
6:b:34:ARG:HD2	46:1:2825:C:H41	1.81	0.44
17:H:18:VAL:HG12	17:H:27:VAL:HG22	1.99	0.44
21:k:28:ASN:O	21:k:40:GLN:N	2.44	0.44
36:W:55:GLU:OE2	36:W:119:TYR:OH	2.31	0.44
5:B:95:THR:HG22	46:1:3243:A:H4'	1.99	0.44
10:E:169:ASP:HB3	10:E:174:LEU:HD11	1.99	0.44
14:G:82:LEU:HD21	14:G:178:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:j:14:LYS:HD3	23:l:51:ILE:HD11	2.00	0.44
46:1:1861:G:O2'	46:1:3066:U:OP1	2.35	0.44
46:1:2568:C:OP1	46:1:2569:A:N6	2.50	0.44
3:A:80:GLU:HG3	25:p:66:GLY:HA2	2.00	0.44
44:q:55:LYS:HA	44:q:56:PRO:HD3	1.87	0.44
3:A:35:ALA:HA	14:G:36:ILE:HD11	1.98	0.44
14:G:133:LYS:HG2	14:G:138:HIS:HE1	1.82	0.44
20:j:43:LYS:NZ	46:1:55:G:OP1	2.48	0.44
32:S:2:ALA:HA	46:1:1324:U:H5'	1.98	0.44
34:U:29:ASP:N	34:U:29:ASP:OD1	2.50	0.44
42:D:22:ARG:NE	42:D:27:LYS:HE3	2.32	0.44
46:1:959:C:O2	46:1:2614:G:O2'	2.34	0.44
6:b:479:ASP:OD1	6:b:479:ASP:N	2.51	0.44
14:G:140:VAL:HG22	14:G:166:LEU:HD21	1.99	0.44
19:i:4:LYS:HA	19:i:12:ASN:HB3	1.98	0.44
22:L:27:ASP:HB3	48:3:29:U:H5''	1.98	0.44
6:b:294:ARG:O	6:b:296:GLU:N	2.50	0.44
42:D:90:HIS:NE2	42:D:229:ASP:OD2	2.43	0.44
42:D:105:ILE:H	42:D:105:ILE:HG13	1.67	0.44
44:q:70:LEU:HB2	44:q:85:LEU:HD11	2.00	0.44
46:1:1355:A:H5''	46:1:1357:G:H1'	1.98	0.44
2:v:291:LEU:HD11	2:v:358:HIS:HB3	2.00	0.44
31:R:74:ARG:NH1	46:1:1942:U:OP2	2.51	0.44
46:1:171:G:O6	46:1:248:U:N3	2.50	0.44
46:1:188:U:O2'	46:1:207:U:O2	2.33	0.44
46:1:1718:G:H2'	46:1:1719:G:H8	1.82	0.44
2:v:179:LEU:HA	2:v:184:HIS:HE1	1.83	0.44
7:C:53:SER:HB3	7:C:56:ALA:HB2	1.99	0.44
23:l:21:ARG:HH22	23:l:24:PRO:HG3	1.83	0.44
26:N:122:ASN:HB3	26:N:129:TYR:HD2	1.82	0.44
46:1:1529:A:OP2	46:1:1592:G:N2	2.47	0.44
46:1:2349:U:O2'	46:1:3307:A:N3	2.51	0.44
10:E:130:ILE:CG2	10:E:134:ARG:CB	2.96	0.44
39:y:216:SER:HB2	39:y:236:LEU:HD13	1.99	0.44
43:J:172:LEU:HD23	43:J:172:LEU:HA	1.83	0.44
46:1:1381:A:H2'	46:1:1382:G:H8	1.83	0.44
44:q:56:PRO:HG2	46:1:92:G:H1'	2.00	0.43
46:1:991:G:C6	46:1:992:A:C5	3.05	0.43
6:b:250:VAL:HG13	6:b:283:VAL:HG13	2.01	0.43
13:f:57:LYS:NZ	46:1:433:A:OP2	2.42	0.43
33:T:152:ALA:O	33:T:154:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:y:101:LEU:HD13	39:y:107:VAL:HG21	1.98	0.43
46:1:1899:G:O2'	46:1:2334:U:O4	2.34	0.43
12:F:110:ARG:NH1	46:1:1364:C:OP1	2.50	0.43
44:q:6:LYS:HA	44:q:25:VAL:HB	2.00	0.43
46:1:1288:U:H2'	46:1:1289:G:C8	2.54	0.43
46:1:2344:U:H2'	46:1:2345:A:C8	2.53	0.43
14:G:144:GLU:HA	14:G:173:MET:HE2	2.01	0.43
44:q:21:THR:HB	44:q:76:LYS:HD2	1.99	0.43
25:p:44:LYS:NZ	46:1:1727:G:OP1	2.49	0.43
40:Z:135:ARG:HH22	46:1:1807:G:H5''	1.83	0.43
44:q:11:TYR:HA	44:q:20:HIS:HA	2.00	0.43
3:A:234:LYS:NZ	46:1:2162:U:OP1	2.39	0.43
10:E:108:LYS:NZ	46:1:617:G:OP1	2.42	0.43
13:f:14:LEU:HD11	13:f:31:LYS:HB2	2.00	0.43
27:u:95:ARG:NH1	27:u:98:GLU:OE1	2.51	0.43
44:q:67:LYS:HG2	46:1:2792:A:H2'	2.00	0.43
46:1:991:G:O6	46:1:992:A:C6	2.72	0.43
46:1:2108:C:H1'	46:1:3344:A:H8	1.82	0.43
46:1:2941:A:OP1	46:1:2943:G:O2'	2.33	0.43
3:A:193:ARG:NH1	46:1:2174:G:OP2	2.52	0.43
6:b:150:LEU:HA	6:b:153:VAL:HG22	2.01	0.43
16:I:15:THR:OG1	27:u:43:ARG:NH1	2.49	0.43
30:Q:106:PHE:CE2	30:Q:121:CYS:HB2	2.54	0.43
42:D:164:LYS:NZ	42:D:168:ASP:OD2	2.47	0.43
46:1:1543:G:N2	46:1:1551:C:O2	2.52	0.43
5:B:252:ILE:HG22	46:1:2394:G:H5'	2.00	0.43
6:b:476:GLU:HG3	6:b:486:VAL:HG11	2.00	0.43
27:u:133:LEU:HD23	27:u:136:ILE:HD12	2.00	0.43
29:P:118:GLN:HE22	46:1:412:G:H21	1.66	0.43
39:y:162:HIS:NE2	39:y:164:GLN:HB2	2.34	0.43
43:J:154:THR:OG1	43:J:155:THR:N	2.51	0.43
6:b:252:TYR:HB3	6:b:285:VAL:HG22	2.01	0.43
17:H:124:ARG:NH1	17:H:164:ILE:O	2.52	0.43
36:W:86:LYS:HE2	36:W:223:ASN:HB3	2.00	0.43
43:J:21:ILE:HD11	43:J:125:MET:HG2	2.01	0.43
46:1:1132:C:H2'	46:1:1133:A:H8	1.84	0.43
48:3:82:U:H4'	48:3:87:G:H4'	2.01	0.43
29:P:118:GLN:NE2	46:1:412:G:H21	2.17	0.42
30:Q:100:THR:HG23	30:Q:122:ILE:HD13	2.01	0.42
42:D:166:ALA:HB1	42:D:171:LEU:HD12	1.99	0.42
46:1:2537:U:N3	46:1:2543:U:O4	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:233:THR:OG1	46:1:2875:U:O2	2.32	0.42
6:b:322:CYS:N	49:b:701:GTP:O6	2.52	0.42
12:F:210:PRO:O	46:1:1167:U:O2'	2.35	0.42
40:Z:22:LYS:NZ	40:Z:129:TRP:O	2.52	0.42
46:1:708:G:N2	46:1:711:A:OP2	2.53	0.42
46:1:2344:U:H2'	46:1:2345:A:H8	1.83	0.42
10:E:130:ILE:HD13	46:1:3268:A:O2'	2.15	0.42
27:u:6:CYS:HB3	27:u:9:CYS:HB2	1.85	0.42
40:Z:95:VAL:HG21	40:Z:113:VAL:HG11	2.01	0.42
44:q:67:LYS:HE2	46:1:2792:A:C5	2.54	0.42
4:a:117:ARG:NH1	46:1:716:A:N1	2.67	0.42
6:b:192:VAL:HG13	6:b:205:TYR:HD2	1.84	0.42
14:G:50:VAL:HG12	37:X:30:ALA:HA	2.01	0.42
17:H:90:MET:HE2	17:H:179:ILE:HG22	2.02	0.42
34:U:20:SER:HB3	34:U:61:THR:HB	2.01	0.42
39:y:109:CYS:HB3	39:y:149:GLY:HA2	2.01	0.42
39:y:206:THR:OG1	39:y:207:GLY:N	2.52	0.42
46:1:201:A:OP1	46:1:220:G:O2'	2.29	0.42
46:1:730:C:H42	46:1:739:G:H1	1.67	0.42
46:1:2813:A:N6	46:1:2814:G:C5	2.87	0.42
46:1:1480:G:O2'	46:1:1871:U:O4	2.33	0.42
8:c:16:LEU:HD11	8:c:97:ASP:HB3	2.01	0.42
11:e:27:ARG:N	46:1:655:C:OP1	2.52	0.42
12:F:121:LYS:HB2	33:T:133:ALA:HB3	2.02	0.42
36:W:49:ARG:NH2	46:1:1230:G:OP1	2.53	0.42
42:D:277:LEU:HD23	47:2:62:U:H5'	2.02	0.42
43:J:92:ARG:H	43:J:95:ASN:ND2	2.18	0.42
6:b:107:GLN:NE2	6:b:111:ASP:OD2	2.46	0.42
10:E:125:GLN:C	10:E:125:GLN:CD	2.87	0.42
22:L:189:GLU:HA	22:L:192:GLU:HG2	2.02	0.42
27:u:119:ASP:OD1	27:u:122:ARG:NH1	2.48	0.42
29:P:4:TYR:HE1	29:P:18:ARG:HD2	1.83	0.42
46:1:1277:C:O2'	46:1:1278:A:O5'	2.34	0.42
46:1:1718:G:H2'	46:1:1719:G:C8	2.55	0.42
46:1:3153:U:H3	46:1:3293:U:H3	1.67	0.42
6:b:168:ARG:H	6:b:168:ARG:HD3	1.85	0.42
6:b:389:ASP:HA	6:b:390:PRO:HD3	1.92	0.42
17:H:73:SER:O	17:H:77:ASN:ND2	2.53	0.42
23:l:20:ASN:ND2	23:l:41:ARG:HE	2.18	0.42
30:Q:156:GLY:HA2	30:Q:157:PRO:HD3	1.91	0.42
40:Z:51:LEU:HB2	40:Z:65:ARG:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:D:163:LEU:HD21	42:D:175:HIS:CG	2.55	0.42
43:J:12:LEU:HD22	43:J:12:LEU:HA	1.91	0.42
46:1:129:U:H3	46:1:139:G:H1	1.68	0.42
2:v:203:GLN:HB3	2:v:206:HIS:CD2	2.54	0.42
5:B:65:SER:OG	5:B:66:LYS:N	2.53	0.42
6:b:329:MET:HE3	6:b:332:ARG:HH11	1.85	0.42
46:1:627:U:H4'	46:1:1399:A:H1'	2.01	0.42
46:1:671:U:H2'	46:1:672:A:H8	1.84	0.42
46:1:1490:A:H3'	46:1:1491:A:H8	1.85	0.42
6:b:374:ARG:NH2	39:y:178:GLN:HG3	2.34	0.42
7:C:22:LEU:HA	7:C:23:PRO:HD3	1.89	0.42
24:M:66:THR:HG22	24:M:99:TRP:HZ3	1.85	0.42
27:u:61:LYS:NZ	46:1:3366:G:OP1	2.53	0.42
46:1:1390:A:O4'	46:1:1418:A:N6	2.52	0.42
6:b:92:LYS:HG2	46:1:2863:G:H22	1.85	0.41
6:b:398:LEU:O	6:b:400:ARG:N	2.54	0.41
7:C:3:ARG:HB2	7:C:21:PRO:HB3	2.02	0.41
7:C:45:ASN:HA	7:C:110:ASN:HD22	1.84	0.41
15:g:93:PHE:HZ	40:Z:83:THR:HG23	1.85	0.41
36:W:149:ILE:H	36:W:149:ILE:HG13	1.75	0.41
38:Y:16:ARG:NH1	46:1:216:G:OP1	2.52	0.41
44:q:47:GLN:HE22	44:q:53:GLN:CD	2.28	0.41
44:q:75:VAL:HG23	44:q:76:LYS:HG3	2.02	0.41
44:q:80:ARG:HB3	46:1:2769:A:C5	2.55	0.41
46:1:2960:C:N4	46:1:2972:G:O6	2.51	0.41
2:v:235:THR:HA	46:1:2922:G:H1	1.83	0.41
3:A:134:VAL:HG12	3:A:151:PRO:HD3	2.01	0.41
5:B:74:GLU:OE2	5:B:283:TYR:OH	2.26	0.41
19:i:68:ARG:NH2	46:1:2218:G:OP1	2.53	0.41
26:N:116:LEU:HB2	26:N:135:VAL:HG23	2.02	0.41
28:O:59:ARG:NH1	46:1:1307:G:OP1	2.53	0.41
32:S:43:TYR:OH	47:2:96:U:OP1	2.30	0.41
44:q:67:LYS:HG3	46:1:2793:G:O4'	2.20	0.41
46:1:2815:G:C2	46:1:2816:G:C4	3.09	0.41
10:E:130:ILE:HD12	46:1:3268:A:C4	2.55	0.41
12:F:131:GLU:OE1	47:2:98:C:O2'	2.32	0.41
14:G:175:VAL:HA	14:G:176:PRO:HD3	1.93	0.41
17:H:90:MET:HB2	17:H:144:ILE:HG23	2.02	0.41
26:N:93:LYS:NZ	46:1:276:U:O2	2.54	0.41
44:q:67:LYS:HE2	46:1:2792:A:C4	2.54	0.41
3:A:79:ASN:ND2	3:A:166:ILE:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:49:TYR:O	5:B:80:ASP:N	2.52	0.41
14:G:26:LEU:HB3	40:Z:53:VAL:HG11	2.02	0.41
17:H:1:MET:HE1	32:S:138:GLN:HB3	2.02	0.41
46:1:210:U:O2'	46:1:229:G:O2'	2.34	0.41
46:1:2807:U:O2'	46:1:2809:C:OP1	2.39	0.41
47:2:21:G:H1	47:2:58:C:H42	1.68	0.41
2:v:267:MET:HE1	2:v:296:LEU:HD13	2.02	0.41
6:b:40:THR:HG1	46:1:2874:G:H1	1.66	0.41
6:b:365:GLN:HA	6:b:366:PRO:HD3	1.90	0.41
11:e:36:LYS:NZ	46:1:945:C:OP1	2.53	0.41
32:S:71:LYS:NZ	46:1:562:C:O3'	2.53	0.41
42:D:55:PHE:HE1	42:D:60:ILE:HG23	1.85	0.41
46:1:117:U:O2'	46:1:119:U:OP2	2.28	0.41
46:1:952:A:N3	46:1:1114:U:O2'	2.52	0.41
5:B:216:ASP:OD2	5:B:339:ARG:NH1	2.53	0.41
8:c:30:THR:HG22	8:c:91:SER:HB2	2.03	0.41
12:F:33:ARG:HH22	46:1:595:G:H5''	1.85	0.41
26:N:145:ASP:O	26:N:147:ARG:N	2.54	0.41
32:S:83:SER:OG	32:S:84:ARG:N	2.53	0.41
37:X:105:VAL:HG11	37:X:126:LEU:HD13	2.03	0.41
44:q:59:HIS:O	44:q:61:LYS:N	2.54	0.41
44:q:65:THR:OG1	46:1:2793:G:H5'	2.20	0.41
5:B:19:ARG:HB2	5:B:232:ARG:HH21	1.85	0.41
27:u:3:ILE:H	27:u:3:ILE:HG13	1.61	0.41
27:u:49:LEU:HD23	27:u:51:TRP:HE1	1.86	0.41
32:S:8:GLN:NE2	32:S:26:ARG:HE	2.19	0.41
34:U:19:VAL:HG21	34:U:30:PRO:HB3	2.03	0.41
46:1:1229:G:H2'	46:1:1230:G:C8	2.56	0.41
46:1:2335:G:N2	46:1:2339:C:O2'	2.53	0.41
46:1:3258:U:O2'	46:1:3260:G:OP1	2.33	0.41
3:A:19:HIS:HD2	46:1:823:C:H4'	1.84	0.41
5:B:262:TRP:CD1	5:B:262:TRP:H	2.39	0.41
6:b:180:LYS:NZ	49:b:701:GTP:O3G	2.42	0.41
7:C:83:GLY:O	7:C:87:GLN:NE2	2.53	0.41
23:l:37:TYR:O	46:1:351:A:N6	2.46	0.41
40:Z:54:THR:OG1	40:Z:55:LYS:N	2.54	0.41
40:Z:76:ASN:HB3	40:Z:79:HIS:ND1	2.35	0.41
2:v:284:GLN:HE21	2:v:293:THR:HB	1.86	0.41
3:A:150:LEU:HA	3:A:150:LEU:HD23	1.89	0.41
5:B:306:THR:HG21	5:B:316:GLU:HG2	2.02	0.41
6:b:39:ILE:HA	6:b:42:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:b:169:THR:HG22	6:b:217:GLN:HE21	1.86	0.41
6:b:191:ASP:H	46:1:3027:A:H5'	1.86	0.41
7:C:119:ARG:NH2	46:1:696:C:OP2	2.52	0.41
7:C:219:LEU:HD13	7:C:225:VAL:HG11	2.02	0.41
8:c:10:ILE:HD13	8:c:105:ALA:HB1	2.03	0.41
11:e:98:HIS:NE2	46:1:1394:A:OP1	2.51	0.41
22:L:70:ARG:NH1	46:1:76:G:OP1	2.51	0.41
25:p:49:ARG:HB2	25:p:55:TRP:CZ3	2.56	0.41
31:R:74:ARG:NH2	46:1:1942:U:O5'	2.52	0.41
39:y:129:ILE:HG23	39:y:133:LEU:HD12	2.02	0.41
44:q:47:GLN:HA	44:q:54:THR:HG23	2.03	0.41
46:1:993:G:N3	46:1:2637:A:H2'	2.36	0.41
46:1:2999:U:H2'	46:1:3000:A:H8	1.86	0.41
6:b:208:HIS:CD2	46:1:3028:G:H4'	2.56	0.41
6:b:460:GLU:OE2	27:u:95:ARG:NH2	2.54	0.41
7:C:351:PRO:HA	12:F:71:ALA:HA	2.03	0.41
9:d:35:GLU:O	9:d:39:PHE:N	2.53	0.41
26:N:61:ILE:HD13	26:N:133:ILE:HA	2.02	0.41
26:N:62:TYR:HD1	26:N:62:TYR:HA	1.75	0.41
35:V:109:MET:HE3	35:V:109:MET:HB3	1.96	0.41
46:1:1595:U:O2'	46:1:1606:U:O2	2.38	0.41
5:B:303:LYS:HD2	5:B:361:THR:HG21	2.03	0.40
28:O:119:VAL:HG11	32:S:167:ARG:HH11	1.85	0.40
30:Q:147:ARG:NH2	46:1:670:C:OP2	2.54	0.40
39:y:122:ASP:OD1	39:y:122:ASP:N	2.54	0.40
39:y:223:ARG:HD3	39:y:230:GLU:HB2	2.02	0.40
43:J:32:ARG:HD2	43:J:120:ILE:HA	2.03	0.40
5:B:14:LEU:HA	5:B:17:LEU:HD13	2.03	0.40
6:b:599:ARG:O	6:b:603:ASP:N	2.48	0.40
13:f:16:TYR:OH	13:f:89:LEU:O	2.38	0.40
28:O:164:SER:OG	46:1:3181:C:O2'	2.31	0.40
38:Y:51:ARG:HG2	38:Y:52:ARG:H	1.86	0.40
39:y:7:PHE:O	39:y:10:SER:N	2.47	0.40
44:q:47:GLN:O	44:q:49:GLY:N	2.54	0.40
44:q:67:LYS:NZ	46:1:2766:U:H3	2.19	0.40
3:A:116:VAL:HG13	3:A:126:LEU:HB2	2.02	0.40
5:B:235:THR:HG21	5:B:249:VAL:HG22	2.03	0.40
6:b:534:HIS:O	6:b:537:THR:OG1	2.37	0.40
30:Q:96:PHE:HA	30:Q:97:PRO:HD3	1.93	0.40
35:V:14:SER:OG	46:1:3094:A:OP1	2.31	0.40
40:Z:17:ARG:HG3	46:1:1639:C:H41	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:D:107:ARG:NH1	42:D:169:GLY:O	2.54	0.40
44:q:27:GLN:HG3	44:q:91:PHE:HD2	1.86	0.40
46:1:1868:G:N2	46:1:2118:C:O2	2.53	0.40
5:B:226:PHE:O	46:1:1886:A:O2'	2.38	0.40
12:F:94:LYS:NZ	46:1:1156:C:OP2	2.53	0.40
16:I:22:TYR:CE1	16:I:116:LYS:HE2	2.56	0.40
32:S:12:ARG:NH2	32:S:57:GLU:OE2	2.47	0.40
46:1:999:G:H1	46:1:1049:C:H42	1.70	0.40
46:1:1202:A:N6	46:1:1301:A:O4'	2.54	0.40
46:1:2501:U:H2'	46:1:2502:A:C8	2.55	0.40
2:v:320:VAL:HA	2:v:340:VAL:HG23	2.02	0.40
5:B:19:ARG:N	46:1:2990:G:OP1	2.54	0.40
13:f:21:ARG:O	46:1:633:C:O2'	2.38	0.40
36:W:165:MET:HA	36:W:169:PHE:HD2	1.87	0.40
42:D:69:ILE:H	42:D:69:ILE:HG13	1.77	0.40
46:1:732:C:N4	46:1:733:G:O6	2.55	0.40
46:1:2700:G:O2'	46:1:2705:A:N1	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	v	246/518 (48%)	223 (91%)	21 (8%)	2 (1%)	16	49
3	A	243/254 (96%)	220 (90%)	22 (9%)	1 (0%)	30	61
4	a	92/149 (62%)	85 (92%)	5 (5%)	2 (2%)	5	30
5	B	384/387 (99%)	342 (89%)	40 (10%)	2 (0%)	24	57
6	b	600/647 (93%)	557 (93%)	40 (7%)	3 (0%)	24	57
7	C	359/362 (99%)	329 (92%)	27 (8%)	3 (1%)	16	49
8	c	95/105 (90%)	92 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	d	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
10	E	156/176 (89%)	146 (94%)	8 (5%)	2 (1%)	9	39
11	e	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
12	F	220/244 (90%)	202 (92%)	18 (8%)	0	100	100
13	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
14	G	228/256 (89%)	210 (92%)	18 (8%)	0	100	100
15	g	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
16	I	129/166 (78%)	116 (90%)	11 (8%)	2 (2%)	7	36
17	H	186/191 (97%)	170 (91%)	16 (9%)	0	100	100
18	h	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
19	i	94/100 (94%)	88 (94%)	6 (6%)	0	100	100
20	j	83/88 (94%)	77 (93%)	6 (7%)	0	100	100
21	k	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
22	L	185/199 (93%)	166 (90%)	18 (10%)	1 (0%)	24	57
23	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
24	M	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
25	p	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
26	N	201/204 (98%)	181 (90%)	20 (10%)	0	100	100
27	u	147/199 (74%)	137 (93%)	6 (4%)	4 (3%)	4	27
28	O	195/199 (98%)	190 (97%)	5 (3%)	0	100	100
29	P	174/184 (95%)	167 (96%)	7 (4%)	0	100	100
30	Q	152/186 (82%)	144 (95%)	8 (5%)	0	100	100
31	R	152/189 (80%)	146 (96%)	6 (4%)	0	100	100
32	S	168/172 (98%)	155 (92%)	11 (6%)	2 (1%)	10	41
33	T	59/160 (37%)	52 (88%)	7 (12%)	0	100	100
34	U	102/121 (84%)	95 (93%)	6 (6%)	1 (1%)	12	45
35	V	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
36	W	209/236 (89%)	204 (98%)	5 (2%)	0	100	100
37	X	118/142 (83%)	113 (96%)	5 (4%)	0	100	100
38	Y	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
39	y	240/245 (98%)	229 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	Z	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
41	z	53/106 (50%)	53 (100%)	0	0	100	100
42	D	245/297 (82%)	229 (94%)	13 (5%)	3 (1%)	10	41
43	J	162/174 (93%)	146 (90%)	12 (7%)	4 (2%)	4	28
44	q	95/106 (90%)	69 (73%)	26 (27%)	0	100	100
45	o	52/59 (88%)	47 (90%)	5 (10%)	0	100	100
All	All	7123/8171 (87%)	6624 (93%)	467 (7%)	32 (0%)	31	61

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	339	LEU
10	E	131	LYS
27	u	3	ILE
42	D	140	ARG
5	B	34	LYS
22	L	63	VAL
27	u	73	GLN
27	u	79	VAL
43	J	95	ASN
43	J	155	THR
2	v	279	ILE
6	b	369	ARG
6	b	399	ALA
7	C	4	PRO
16	I	17	ASP
27	u	4	TYR
43	J	154	THR
2	v	231	GLN
3	A	219	ILE
32	S	24	LEU
4	a	77	LYS
4	a	78	LEU
7	C	268	ALA
16	I	16	ARG
32	S	13	ARG
34	U	52	ASN
42	D	258	LYS
43	J	172	LEU
6	b	295	PRO

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Mol	Chain	Res	Type
42	D	141	PRO
5	B	239	PRO
10	E	130	ILE

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	
2	v	220/467 (47%)	219 (100%)	1 (0%)	81	80
3	A	188/196 (96%)	188 (100%)	0	100	100
4	a	77/119 (65%)	76 (99%)	1 (1%)	61	72
5	B	322/323 (100%)	320 (99%)	2 (1%)	78	79
6	b	537/573 (94%)	533 (99%)	4 (1%)	76	78
7	C	288/289 (100%)	288 (100%)	0	100	100
8	c	81/88 (92%)	80 (99%)	1 (1%)	63	73
9	d	94/97 (97%)	94 (100%)	0	100	100
10	E	138/153 (90%)	137 (99%)	1 (1%)	76	78
11	e	109/111 (98%)	109 (100%)	0	100	100
12	F	186/205 (91%)	186 (100%)	0	100	100
13	f	90/91 (99%)	90 (100%)	0	100	100
14	G	189/208 (91%)	189 (100%)	0	100	100
15	g	95/103 (92%)	93 (98%)	2 (2%)	47	65
16	I	116/141 (82%)	115 (99%)	1 (1%)	70	76
17	H	168/171 (98%)	168 (100%)	0	100	100
18	h	104/105 (99%)	104 (100%)	0	100	100
19	i	78/82 (95%)	77 (99%)	1 (1%)	61	72
20	j	69/71 (97%)	69 (100%)	0	100	100
21	k	68/69 (99%)	68 (100%)	0	100	100
22	L	147/159 (92%)	144 (98%)	3 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	l	45/46 (98%)	45 (100%)	0	100	100
24	M	108/109 (99%)	107 (99%)	1 (1%)	70	76
25	p	71/72 (99%)	71 (100%)	0	100	100
26	N	175/176 (99%)	174 (99%)	1 (1%)	78	79
27	u	132/180 (73%)	130 (98%)	2 (2%)	57	70
28	O	160/162 (99%)	159 (99%)	1 (1%)	78	79
29	P	143/146 (98%)	140 (98%)	3 (2%)	47	65
30	Q	126/151 (83%)	126 (100%)	0	100	100
31	R	127/154 (82%)	127 (100%)	0	100	100
32	S	154/156 (99%)	152 (99%)	2 (1%)	61	72
33	T	50/137 (36%)	50 (100%)	0	100	100
34	U	91/107 (85%)	91 (100%)	0	100	100
35	V	104/105 (99%)	104 (100%)	0	100	100
36	W	184/213 (86%)	184 (100%)	0	100	100
37	X	104/118 (88%)	104 (100%)	0	100	100
38	Y	109/110 (99%)	109 (100%)	0	100	100
39	y	207/211 (98%)	207 (100%)	0	100	100
40	Z	115/116 (99%)	115 (100%)	0	100	100
41	z	48/95 (50%)	48 (100%)	0	100	100
42	D	203/245 (83%)	202 (100%)	1 (0%)	81	80
43	J	140/150 (93%)	138 (99%)	2 (1%)	59	71
44	q	84/91 (92%)	83 (99%)	1 (1%)	63	73
45	o	43/47 (92%)	43 (100%)	0	100	100
All	All	6087/6918 (88%)	6056 (100%)	31 (0%)	78	80

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	v	349	ASN
4	a	78	LEU
5	B	79	VAL
5	B	229	VAL
6	b	224	ILE
6	b	281	LYS

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Mol	Chain	Res	Type
6	b	288	ASN
6	b	315	VAL
8	c	16	LEU
10	E	155	LEU
15	g	95	ILE
15	g	100	ILE
16	I	83	VAL
19	i	60	LEU
22	L	9	ILE
22	L	54	LEU
22	L	124	ILE
24	M	38	ILE
26	N	183	THR
27	u	27	LYS
27	u	79	VAL
28	O	148	LYS
29	P	24	VAL
29	P	114	VAL
29	P	176	ILE
32	S	45	LEU
32	S	61	ILE
42	D	105	ILE
43	J	12	LEU
43	J	171	VAL
44	q	79	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
2	v	284	GLN
2	v	349	ASN
2	v	364	HIS
3	A	132	ASN
4	a	74	ASN
4	a	120	ASN
5	B	11	HIS
5	B	231	HIS
5	B	256	HIS
5	B	293	ASN
5	B	371	GLN
6	b	26	GLN
6	b	70	ASN

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Mol	Chain	Res	Type
6	b	155	GLN
6	b	208	HIS
6	b	217	GLN
6	b	288	ASN
6	b	346	ASN
6	b	384	ASN
6	b	413	ASN
6	b	415	ASN
6	b	515	ASN
6	b	549	GLN
6	b	614	ASN
6	b	616	HIS
6	b	625	HIS
6	b	626	ASN
7	C	110	ASN
7	C	114	ASN
7	C	221	ASN
7	C	320	ASN
9	d	57	GLN
9	d	87	ASN
11	e	13	HIS
11	e	71	HIS
12	F	61	ASN
12	F	81	HIS
12	F	166	ASN
12	F	172	ASN
12	F	244	ASN
14	G	85	ASN
14	G	95	ASN
14	G	138	HIS
14	G	221	ASN
15	g	69	HIS
16	I	110	GLN
17	H	77	ASN
17	H	157	ASN
17	H	183	HIS
18	h	59	ASN
22	L	120	GLN
23	l	11	GLN
23	l	20	ASN
24	M	27	GLN
24	M	41	GLN

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Mol	Chain	Res	Type
26	N	11	GLN
26	N	37	HIS
26	N	70	ASN
26	N	156	HIS
26	N	182	ASN
27	u	24	ASN
27	u	45	ASN
28	O	72	HIS
29	P	96	GLN
29	P	97	ASN
30	Q	5	HIS
30	Q	9	GLN
31	R	3	ASN
31	R	150	GLN
32	S	8	GLN
32	S	46	GLN
32	S	65	ASN
32	S	122	HIS
32	S	157	GLN
33	T	103	GLN
34	U	49	ASN
34	U	87	ASN
35	V	7	GLN
35	V	98	ASN
36	W	22	ASN
36	W	88	ASN
36	W	232	ASN
38	Y	66	GLN
38	Y	110	HIS
39	y	33	ASN
39	y	79	GLN
39	y	140	GLN
39	y	168	GLN
39	y	178	GLN
40	Z	122	HIS
41	z	44	GLN
42	D	45	ASN
42	D	151	GLN
42	D	178	ASN
43	J	95	ASN
44	q	59	HIS
44	q	82	GLN

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Mol	Chain	Res	Type
44	q	90	HIS
45	o	42	ASN
45	o	45	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	1	3197/3396 (94%)	745 (23%)	39 (1%)
47	2	120/121 (99%)	20 (16%)	0
48	3	156/158 (98%)	35 (22%)	2 (1%)
All	All	3473/3675 (94%)	800 (23%)	41 (1%)

All (800) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	1	4	U
46	1	22	G
46	1	26	A
46	1	40	A
46	1	43	A
46	1	48	A
46	1	49	A
46	1	59	G
46	1	60	A
46	1	65	A
46	1	66	A
46	1	72	C
46	1	73	C
46	1	77	A
46	1	91	G
46	1	92	G
46	1	93	C
46	1	94	G
46	1	109	A
46	1	110	G
46	1	118	U
46	1	120	G
46	1	122	A
46	1	133	U
46	1	135	C
46	1	136	G

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Mol	Chain	Res	Type
46	1	140	C
46	1	148	G
46	1	150	A
46	1	156	G
46	1	157	A
46	1	165	A
46	1	170	G
46	1	171	G
46	1	172	G
46	1	173	G
46	1	176	G
46	1	182	U
46	1	187	A
46	1	190	U
46	1	191	U
46	1	200	C
46	1	206	G
46	1	210	U
46	1	211	A
46	1	213	A
46	1	218	G
46	1	219	A
46	1	240	U
46	1	241	G
46	1	243	G
46	1	247	C
46	1	250	U
46	1	251	G
46	1	252	U
46	1	253	A
46	1	269	G
46	1	277	G
46	1	279	U
46	1	282	G
46	1	283	G
46	1	284	A
46	1	285	A
46	1	286	U
46	1	287	G
46	1	295	A
46	1	315	C
46	1	323	A

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Mol	Chain	Res	Type
46	1	329	U
46	1	336	A
46	1	339	C
46	1	349	A
46	1	351	A
46	1	352	A
46	1	374	A
46	1	376	G
46	1	398	A
46	1	401	U
46	1	402	A
46	1	403	C
46	1	406	G
46	1	420	G
46	1	421	G
46	1	422	A
46	1	436	A
46	1	439	C
46	1	501	A
46	1	510	G
46	1	520	U
46	1	521	A
46	1	530	G
46	1	535	G
46	1	536	U
46	1	541	U
46	1	543	C
46	1	546	C
46	1	547	G
46	1	548	G
46	1	551	A
46	1	552	G
46	1	555	U
46	1	557	A
46	1	559	A
46	1	578	A
46	1	579	G
46	1	592	A
46	1	597	G
46	1	598	A
46	1	600	G
46	1	603	A

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Mol	Chain	Res	Type
46	1	604	G
46	1	608	A
46	1	611	A
46	1	619	A
46	1	620	U
46	1	621	A
46	1	622	A
46	1	644	G
46	1	649	A
46	1	660	A
46	1	677	A
46	1	681	U
46	1	683	U
46	1	687	U
46	1	689	U
46	1	690	A
46	1	691	A
46	1	705	A
46	1	712	G
46	1	715	A
46	1	719	U
46	1	720	A
46	1	725	G
46	1	735	A
46	1	744	A
46	1	758	C
46	1	765	C
46	1	767	U
46	1	768	C
46	1	774	G
46	1	776	U
46	1	777	U
46	1	780	A
46	1	781	G
46	1	785	G
46	1	786	A
46	1	801	A
46	1	806	A
46	1	817	A
46	1	823	C
46	1	830	A
46	1	861	C

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Mol	Chain	Res	Type
46	1	869	G
46	1	873	C
46	1	874	U
46	1	879	U
46	1	880	G
46	1	884	A
46	1	890	C
46	1	894	G
46	1	897	U
46	1	907	G
46	1	908	G
46	1	911	C
46	1	914	A
46	1	915	A
46	1	916	G
46	1	917	A
46	1	924	G
46	1	937	G
46	1	944	C
46	1	959	C
46	1	960	U
46	1	961	C
46	1	962	A
46	1	965	A
46	1	974	G
46	1	978	G
46	1	979	U
46	1	980	A
46	1	981	U
46	1	982	C
46	1	984	G
46	1	990	U
46	1	991	G
46	1	993	G
46	1	994	G
46	1	995	U
46	1	1001	G
46	1	1002	A
46	1	1003	A
46	1	1008	U
46	1	1010	G
46	1	1011	A

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Mol	Chain	Res	Type
46	1	1014	U
46	1	1015	U
46	1	1016	C
46	1	1017	C
46	1	1018	G
46	1	1019	G
46	1	1020	G
46	1	1024	G
46	1	1026	A
46	1	1027	A
46	1	1028	U
46	1	1029	G
46	1	1030	A
46	1	1032	C
46	1	1034	U
46	1	1035	G
46	1	1036	A
46	1	1037	C
46	1	1038	C
46	1	1039	U
46	1	1047	A
46	1	1049	C
46	1	1051	U
46	1	1063	G
46	1	1064	A
46	1	1065	A
46	1	1066	G
46	1	1072	G
46	1	1081	U
46	1	1082	U
46	1	1093	A
46	1	1094	U
46	1	1095	U
46	1	1096	U
46	1	1097	G
46	1	1098	A
46	1	1103	A
46	1	1104	G
46	1	1117	G
46	1	1118	C
46	1	1131	G
46	1	1143	A

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Mol	Chain	Res	Type
46	1	1153	A
46	1	1157	G
46	1	1159	A
46	1	1176	C
46	1	1179	A
46	1	1180	A
46	1	1181	U
46	1	1192	C
46	1	1193	A
46	1	1196	C
46	1	1208	U
46	1	1217	A
46	1	1221	A
46	1	1222	G
46	1	1227	C
46	1	1236	G
46	1	1237	G
46	1	1239	C
46	1	1241	U
46	1	1244	A
46	1	1245	A
46	1	1246	G
46	1	1247	U
46	1	1248	C
46	1	1251	A
46	1	1252	A
46	1	1253	U
46	1	1254	C
46	1	1258	U
46	1	1262	G
46	1	1263	A
46	1	1264	G
46	1	1266	G
46	1	1268	G
46	1	1269	U
46	1	1270	A
46	1	1271	A
46	1	1279	C
46	1	1280	C
46	1	1286	A
46	1	1287	A
46	1	1299	U

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Mol	Chain	Res	Type
46	1	1301	A
46	1	1302	A
46	1	1305	U
46	1	1307	G
46	1	1309	U
46	1	1313	G
46	1	1316	C
46	1	1325	U
46	1	1330	A
46	1	1348	U
46	1	1349	G
46	1	1351	U
46	1	1352	A
46	1	1353	U
46	1	1355	A
46	1	1356	U
46	1	1357	G
46	1	1383	G
46	1	1386	A
46	1	1392	G
46	1	1399	A
46	1	1400	G
46	1	1419	A
46	1	1430	U
46	1	1431	G
46	1	1433	A
46	1	1434	G
46	1	1437	C
46	1	1446	A
46	1	1450	G
46	1	1455	U
46	1	1475	A
46	1	1480	G
46	1	1481	A
46	1	1483	G
46	1	1484	U
46	1	1496	C
46	1	1503	A
46	1	1508	C
46	1	1522	U
46	1	1523	U
46	1	1533	U

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Mol	Chain	Res	Type
46	1	1536	G
46	1	1537	A
46	1	1546	A
46	1	1547	G
46	1	1548	C
46	1	1556	C
46	1	1557	A
46	1	1561	G
46	1	1562	C
46	1	1563	C
46	1	1564	U
46	1	1565	G
46	1	1566	A
46	1	1567	U
46	1	1568	U
46	1	1569	U
46	1	1570	U
46	1	1572	U
46	1	1576	G
46	1	1577	G
46	1	1580	A
46	1	1581	C
46	1	1583	A
46	1	1587	A
46	1	1589	A
46	1	1593	A
46	1	1618	G
46	1	1619	A
46	1	1629	U
46	1	1630	U
46	1	1639	C
46	1	1642	A
46	1	1643	A
46	1	1645	U
46	1	1656	A
46	1	1657	C
46	1	1683	A
46	1	1690	C
46	1	1696	A
46	1	1714	A
46	1	1716	U
46	1	1717	U

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Mol	Chain	Res	Type
46	1	1724	U
46	1	1725	C
46	1	1741	A
46	1	1742	U
46	1	1748	G
46	1	1749	A
46	1	1750	A
46	1	1751	G
46	1	1752	A
46	1	1760	A
46	1	1765	U
46	1	1766	G
46	1	1769	G
46	1	1770	G
46	1	1780	G
46	1	1796	G
46	1	1797	A
46	1	1800	A
46	1	1808	G
46	1	1810	A
46	1	1813	A
46	1	1814	A
46	1	1816	A
46	1	1817	G
46	1	1820	U
46	1	1821	U
46	1	1839	A
46	1	1841	A
46	1	1842	A
46	1	1846	C
46	1	1849	C
46	1	1850	A
46	1	1851	G
46	1	1880	U
46	1	1886	A
46	1	1906	G
46	1	1936	A
46	1	1942	U
46	1	1943	C
46	1	1949	G
46	1	1951	C
46	1	1953	G

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Mol	Chain	Res	Type
46	1	1954	G
46	1	2101	C
46	1	2102	U
46	1	2111	G
46	1	2112	U
46	1	2113	A
46	1	2121	G
46	1	2122	G
46	1	2131	A
46	1	2139	A
46	1	2142	A
46	1	2158	A
46	1	2160	G
46	1	2166	A
46	1	2169	G
46	1	2171	G
46	1	2176	U
46	1	2184	U
46	1	2186	U
46	1	2188	A
46	1	2192	C
46	1	2205	U
46	1	2208	A
46	1	2209	U
46	1	2210	G
46	1	2244	A
46	1	2249	G
46	1	2250	G
46	1	2254	U
46	1	2260	U
46	1	2261	G
46	1	2262	A
46	1	2263	C
46	1	2265	C
46	1	2267	C
46	1	2268	U
46	1	2269	U
46	1	2270	A
46	1	2273	G
46	1	2282	U
46	1	2288	G
46	1	2298	U

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Mol	Chain	Res	Type
46	1	2307	G
46	1	2308	C
46	1	2310	U
46	1	2313	A
46	1	2314	U
46	1	2315	G
46	1	2334	U
46	1	2336	U
46	1	2356	A
46	1	2373	A
46	1	2374	C
46	1	2375	G
46	1	2388	U
46	1	2393	G
46	1	2397	A
46	1	2398	A
46	1	2401	A
46	1	2402	A
46	1	2403	G
46	1	2404	A
46	1	2405	C
46	1	2406	C
46	1	2411	U
46	1	2415	C
46	1	2435	G
46	1	2437	G
46	1	2440	G
46	1	2448	G
46	1	2449	A
46	1	2450	G
46	1	2452	G
46	1	2453	U
46	1	2454	G
46	1	2455	U
46	1	2456	A
46	1	2458	A
46	1	2459	A
46	1	2461	A
46	1	2463	G
46	1	2468	A
46	1	2470	C
46	1	2472	U

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Mol	Chain	Res	Type
46	1	2473	C
46	1	2474	G
46	1	2475	G
46	1	2477	G
46	1	2486	A
46	1	2488	A
46	1	2494	A
46	1	2495	C
46	1	2496	C
46	1	2497	U
46	1	2498	U
46	1	2502	A
46	1	2503	G
46	1	2505	U
46	1	2506	U
46	1	2508	U
46	1	2511	A
46	1	2514	U
46	1	2515	A
46	1	2522	G
46	1	2531	C
46	1	2533	G
46	1	2535	A
46	1	2537	U
46	1	2538	U
46	1	2539	C
46	1	2540	A
46	1	2541	U
46	1	2542	U
46	1	2544	U
46	1	2545	C
46	1	2547	A
46	1	2548	C
46	1	2549	G
46	1	2550	U
46	1	2552	C
46	1	2561	A
46	1	2565	U
46	1	2567	C
46	1	2569	A
46	1	2570	U
46	1	2571	U

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Mol	Chain	Res	Type
46	1	2572	C
46	1	2573	G
46	1	2577	C
46	1	2582	C
46	1	2585	G
46	1	2593	A
46	1	2594	C
46	1	2606	G
46	1	2607	G
46	1	2614	G
46	1	2620	G
46	1	2621	G
46	1	2626	A
46	1	2629	U
46	1	2648	G
46	1	2652	U
46	1	2655	U
46	1	2656	A
46	1	2657	A
46	1	2674	A
46	1	2677	G
46	1	2688	U
46	1	2689	A
46	1	2691	A
46	1	2696	A
46	1	2703	A
46	1	2704	A
46	1	2705	A
46	1	2714	G
46	1	2716	U
46	1	2719	U
46	1	2728	G
46	1	2729	U
46	1	2742	C
46	1	2753	G
46	1	2768	U
46	1	2770	G
46	1	2772	C
46	1	2777	G
46	1	2778	G
46	1	2792	A
46	1	2796	G

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Mol	Chain	Res	Type
46	1	2798	C
46	1	2800	G
46	1	2801	A
46	1	2803	A
46	1	2804	A
46	1	2809	C
46	1	2810	C
46	1	2814	G
46	1	2817	A
46	1	2818	U
46	1	2819	A
46	1	2820	A
46	1	2821	C
46	1	2822	U
46	1	2823	G
46	1	2824	G
46	1	2826	U
46	1	2828	G
46	1	2829	U
46	1	2836	C
46	1	2842	U
46	1	2843	U
46	1	2844	C
46	1	2845	A
46	1	2846	U
46	1	2847	A
46	1	2848	G
46	1	2857	C
46	1	2858	U
46	1	2859	U
46	1	2861	U
46	1	2863	G
46	1	2864	A
46	1	2865	U
46	1	2866	U
46	1	2867	C
46	1	2868	U
46	1	2869	U
46	1	2870	C
46	1	2871	G
46	1	2872	A
46	1	2873	U

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Mol	Chain	Res	Type
46	1	2874	G
46	1	2875	U
46	1	2876	C
46	1	2877	G
46	1	2878	G
46	1	2879	C
46	1	2882	U
46	1	2883	U
46	1	2887	A
46	1	2898	G
46	1	2899	C
46	1	2904	U
46	1	2914	G
46	1	2923	U
46	1	2924	U
46	1	2935	U
46	1	2936	A
46	1	2941	A
46	1	2945	G
46	1	2947	G
46	1	2951	G
46	1	2952	G
46	1	2954	U
46	1	2971	A
46	1	2978	U
46	1	2979	U
46	1	2983	C
46	1	2996	U
46	1	2997	G
46	1	3003	G
46	1	3011	A
46	1	3012	A
46	1	3014	U
46	1	3021	A
46	1	3022	G
46	1	3025	C
46	1	3027	A
46	1	3028	G
46	1	3059	G
46	1	3078	U
46	1	3079	U
46	1	3080	G

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Mol	Chain	Res	Type
46	1	3086	A
46	1	3092	C
46	1	3093	C
46	1	3099	C
46	1	3109	G
46	1	3115	C
46	1	3119	U
46	1	3122	A
46	1	3129	A
46	1	3130	A
46	1	3131	U
46	1	3142	A
46	1	3143	C
46	1	3148	U
46	1	3153	U
46	1	3154	C
46	1	3155	U
46	1	3156	U
46	1	3157	U
46	1	3163	A
46	1	3165	A
46	1	3170	A
46	1	3173	G
46	1	3174	A
46	1	3176	G
46	1	3179	U
46	1	3181	C
46	1	3187	A
46	1	3196	U
46	1	3206	C
46	1	3207	U
46	1	3208	G
46	1	3209	A
46	1	3217	C
46	1	3218	A
46	1	3219	G
46	1	3224	G
46	1	3229	G
46	1	3234	A
46	1	3235	C
46	1	3238	G
46	1	3243	A

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Mol	Chain	Res	Type
46	1	3245	A
46	1	3247	G
46	1	3249	C
46	1	3253	G
46	1	3256	G
46	1	3259	U
46	1	3260	G
46	1	3263	G
46	1	3268	A
46	1	3269	U
46	1	3270	U
46	1	3275	U
46	1	3276	G
46	1	3278	C
46	1	3279	A
46	1	3280	U
46	1	3286	G
46	1	3289	G
46	1	3294	A
46	1	3295	A
46	1	3304	U
46	1	3308	C
46	1	3313	U
46	1	3316	A
46	1	3317	U
46	1	3318	G
46	1	3319	U
46	1	3320	A
46	1	3324	C
46	1	3341	U
46	1	3345	G
46	1	3349	C
46	1	3351	U
46	1	3352	U
46	1	3354	U
46	1	3355	U
46	1	3356	G
46	1	3360	C
46	1	3362	A
46	1	3368	U
46	1	3369	G
46	1	3375	A

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Mol	Chain	Res	Type
46	1	3378	C
46	1	3382	U
46	1	3386	G
46	1	3390	G
46	1	3396	U
47	2	10	C
47	2	11	A
47	2	18	C
47	2	22	A
47	2	26	C
47	2	42	A
47	2	49	G
47	2	52	G
47	2	53	U
47	2	54	U
47	2	62	U
47	2	64	A
47	2	65	G
47	2	67	G
47	2	73	C
47	2	76	A
47	2	99	G
47	2	102	A
47	2	112	G
47	2	121	U
48	3	2	A
48	3	23	U
48	3	34	U
48	3	35	C
48	3	39	G
48	3	42	G
48	3	49	G
48	3	51	G
48	3	59	A
48	3	62	C
48	3	63	G
48	3	77	A
48	3	80	A
48	3	81	U
48	3	82	U
48	3	83	C
48	3	84	C

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Mol	Chain	Res	Type
48	3	86	U
48	3	87	G
48	3	88	A
48	3	90	U
48	3	95	G
48	3	104	A
48	3	105	A
48	3	106	C
48	3	108	C
48	3	111	A
48	3	113	U
48	3	124	G
48	3	125	U
48	3	126	A
48	3	127	U
48	3	138	A
48	3	148	G
48	3	155	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	1	239	G
46	1	285	A
46	1	547	G
46	1	599	C
46	1	916	G
46	1	979	U
46	1	1027	A
46	1	1029	G
46	1	1038	C
46	1	1064	A
46	1	1097	G
46	1	1103	A
46	1	1352	A
46	1	1355	A
46	1	1576	G
46	1	1716	U
46	1	1815	U
46	1	2101	C
46	1	2112	U
46	1	2209	U

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Mol	Chain	Res	Type
46	1	2249	G
46	1	2264	U
46	1	2266	U
46	1	2453	U
46	1	2501	U
46	1	2537	U
46	1	2541	U
46	1	2593	A
46	1	2769	A
46	1	2817	A
46	1	2819	A
46	1	2857	C
46	1	2866	U
46	1	3078	U
46	1	3121	U
46	1	3218	A
46	1	3228	C
46	1	3269	U
46	1	3353	G
48	3	82	U
48	3	85	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	GTP	b	701	50	33,34,34	0.93	1 (3%)	50,54,54	1.61	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	GTP	b	701	50	-	3/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	b	701	GTP	C2-N3	2.02	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	b	701	GTP	C5-C4-N3	-4.92	120.56	128.39
49	b	701	GTP	C2-N3-C4	4.66	120.33	112.30
49	b	701	GTP	N9-C4-N3	3.01	131.98	125.95
49	b	701	GTP	C2-N1-C6	-3.00	119.67	125.11
49	b	701	GTP	N9-C8-N7	-2.86	108.11	113.40
49	b	701	GTP	C8-N7-C5	2.70	109.06	104.26
49	b	701	GTP	C5-C6-N1	2.50	119.63	113.25
49	b	701	GTP	O6-C6-C5	-2.37	120.26	126.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

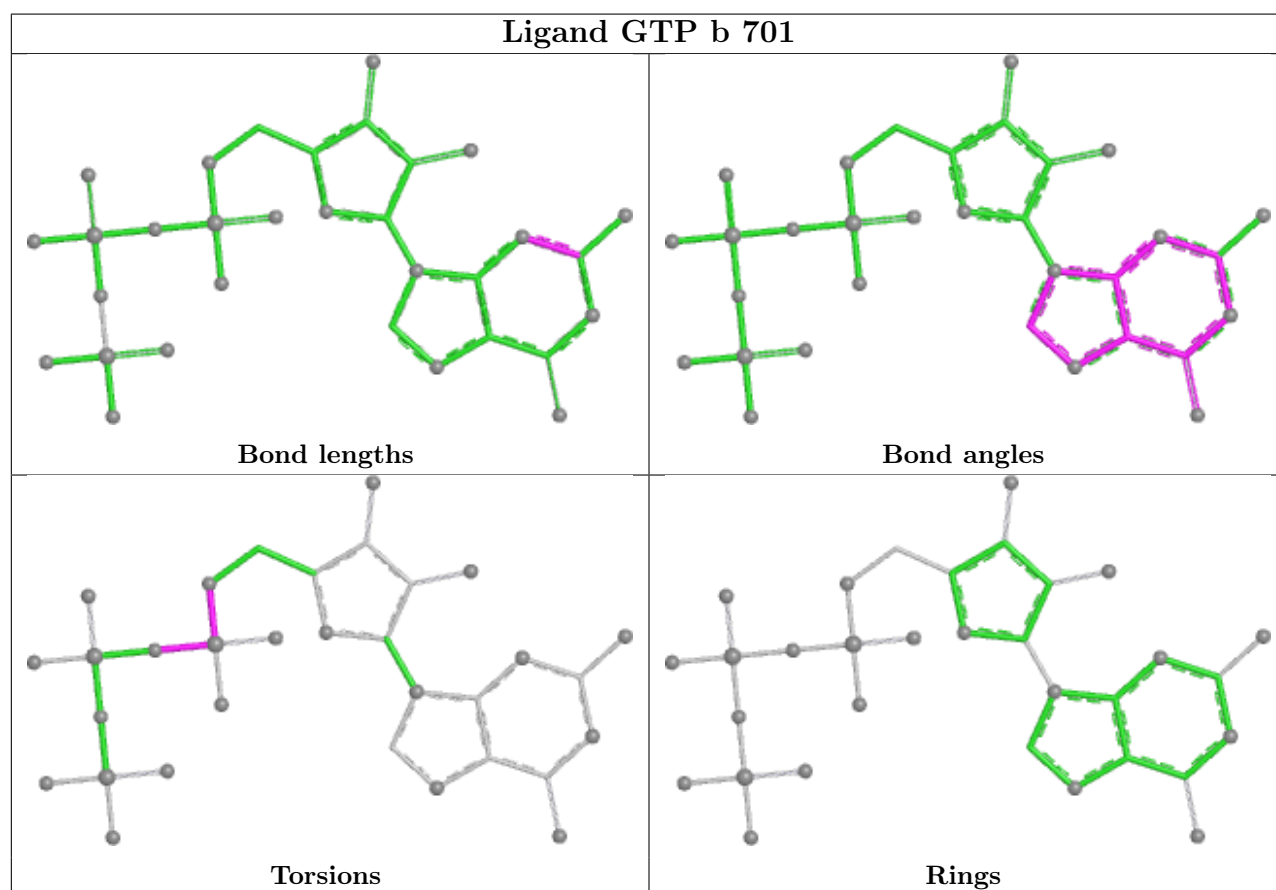
Mol	Chain	Res	Type	Atoms
49	b	701	GTP	C5'-O5'-PA-O1A
49	b	701	GTP	PB-O3A-PA-O1A
49	b	701	GTP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	b	701	GTP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

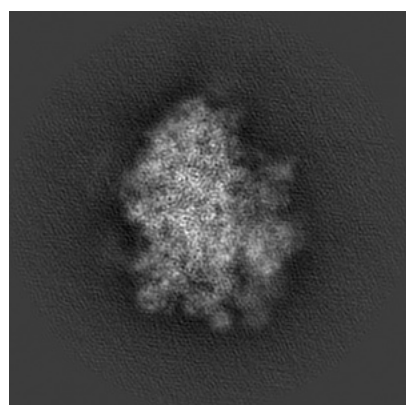
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0370. These allow visual inspection of the internal detail of the map and identification of artifacts.

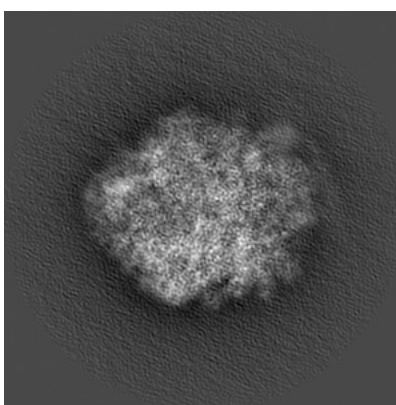
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

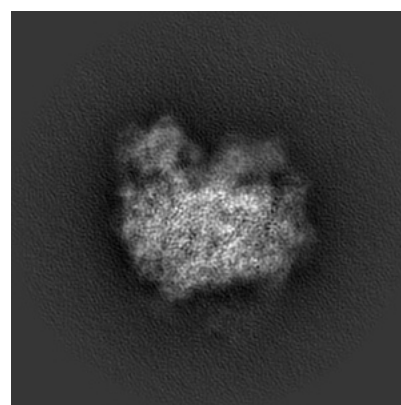
6.1.1 Primary map



X



Y

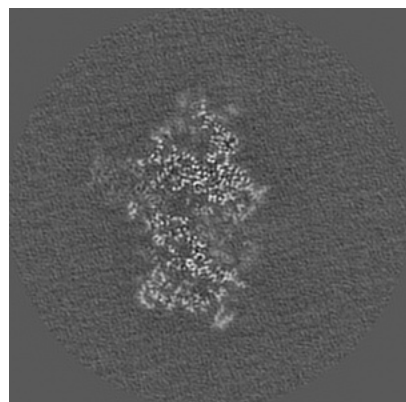


Z

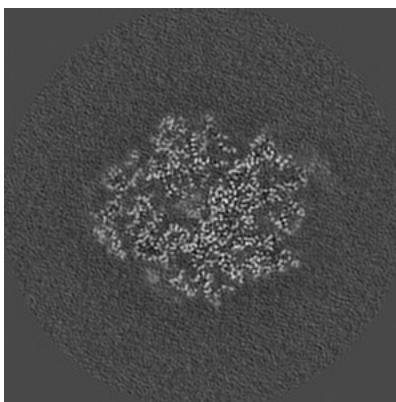
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

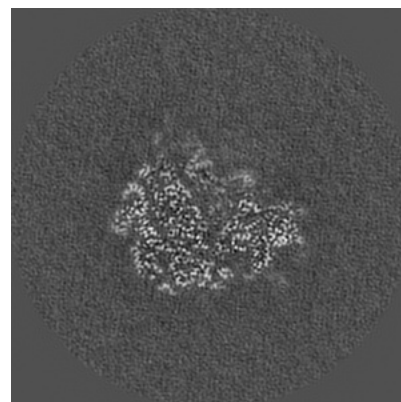
6.2.1 Primary map



X Index: 192



Y Index: 192

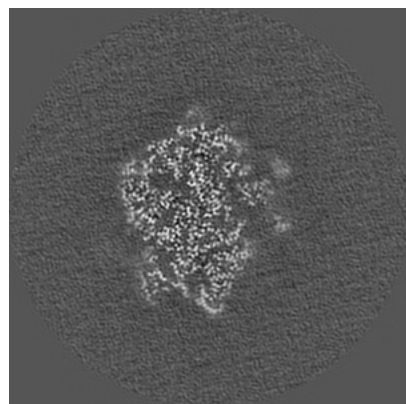


Z Index: 192

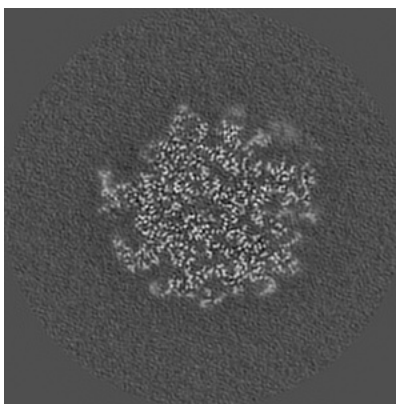
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

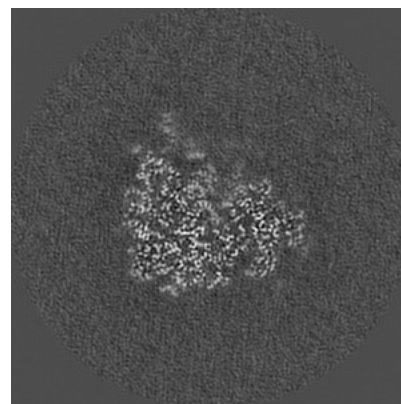
6.3.1 Primary map



X Index: 165



Y Index: 173

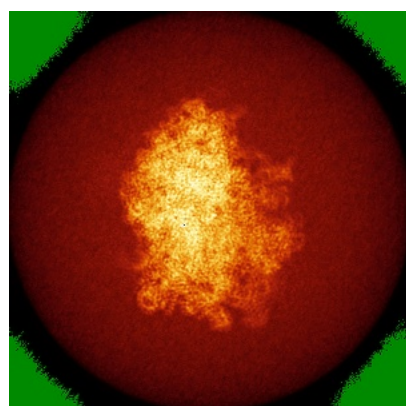


Z Index: 186

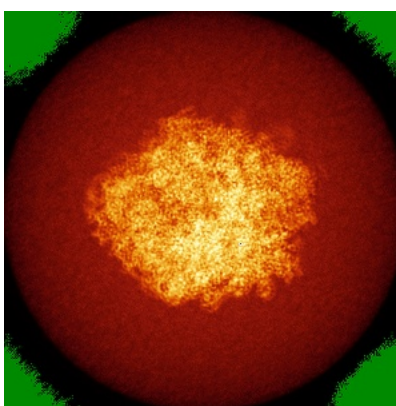
The images above show the largest variance slices of the map in three orthogonal directions.

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

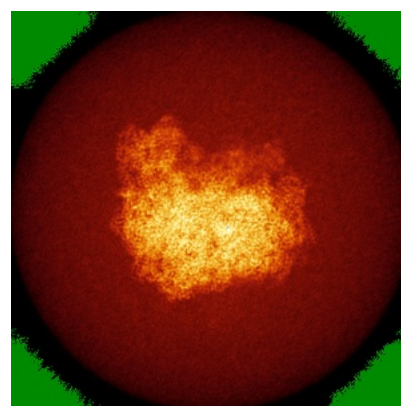
6.4.1 Primary map



X



Y

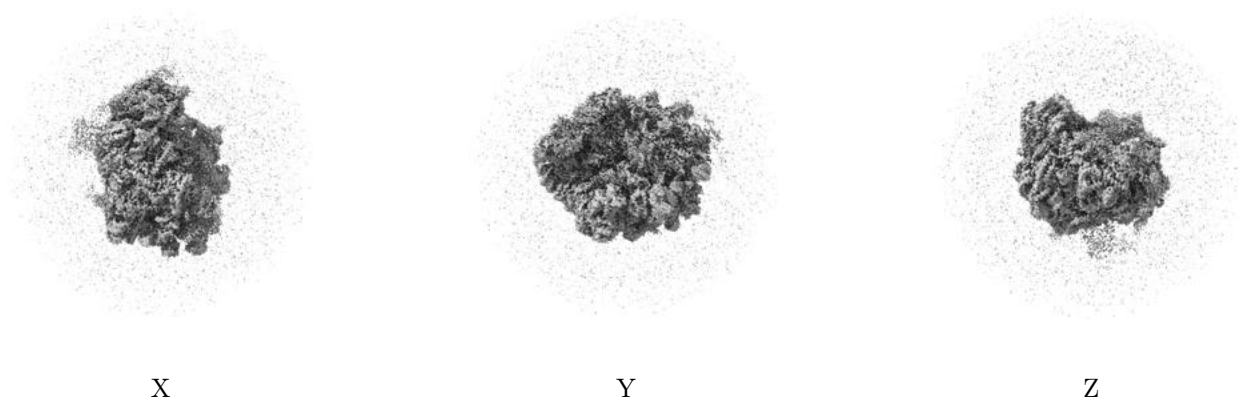


Z

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

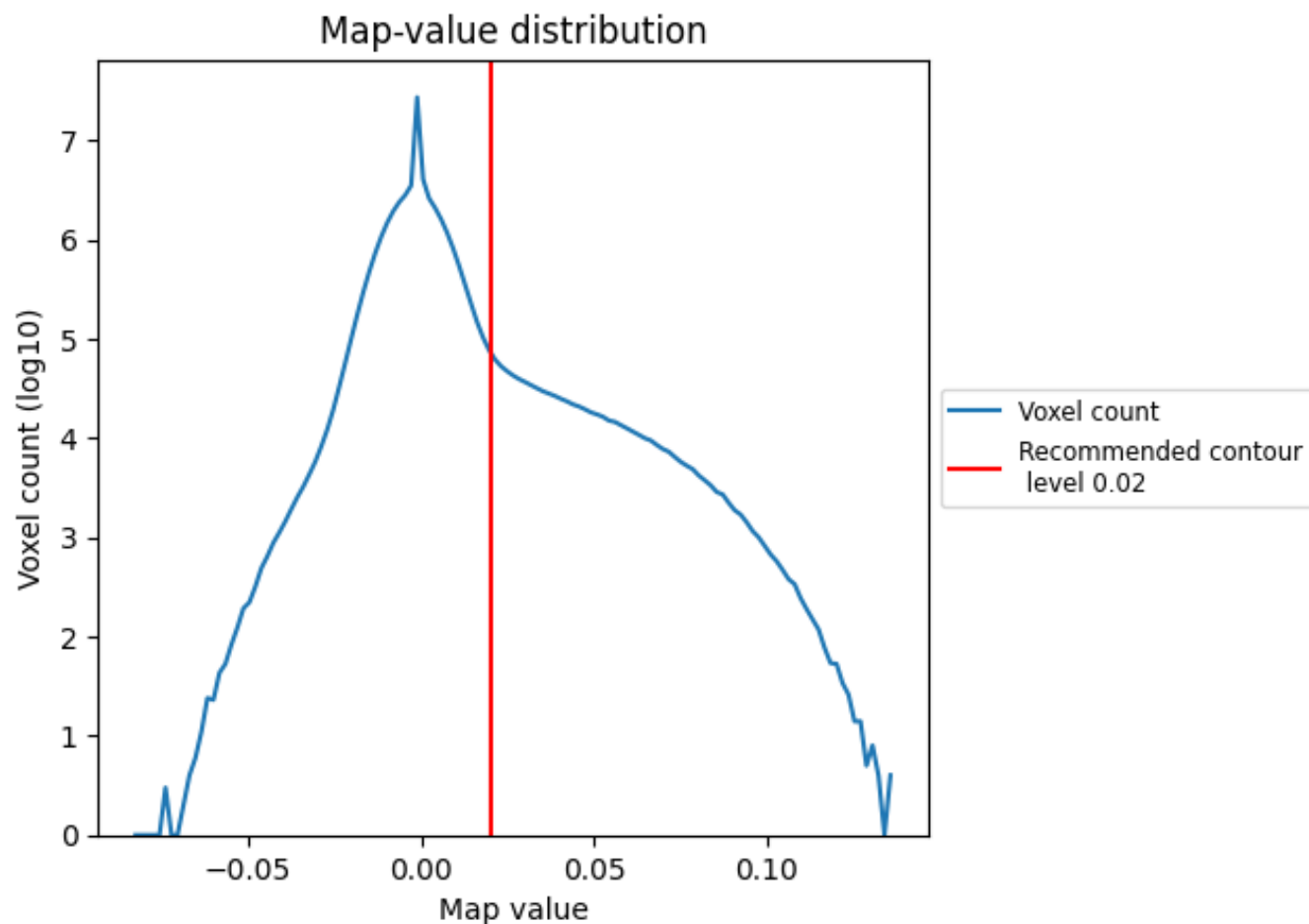
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

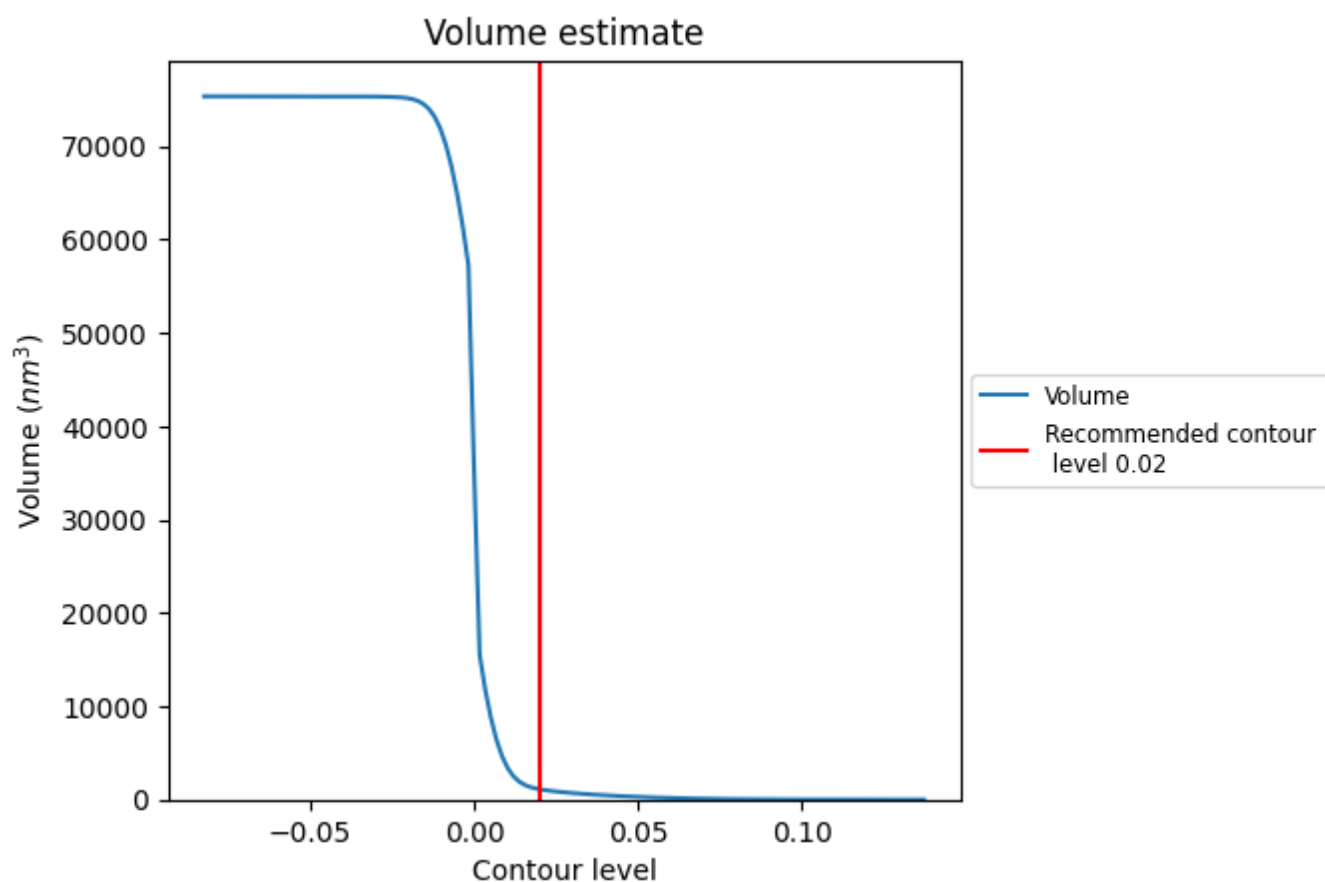
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

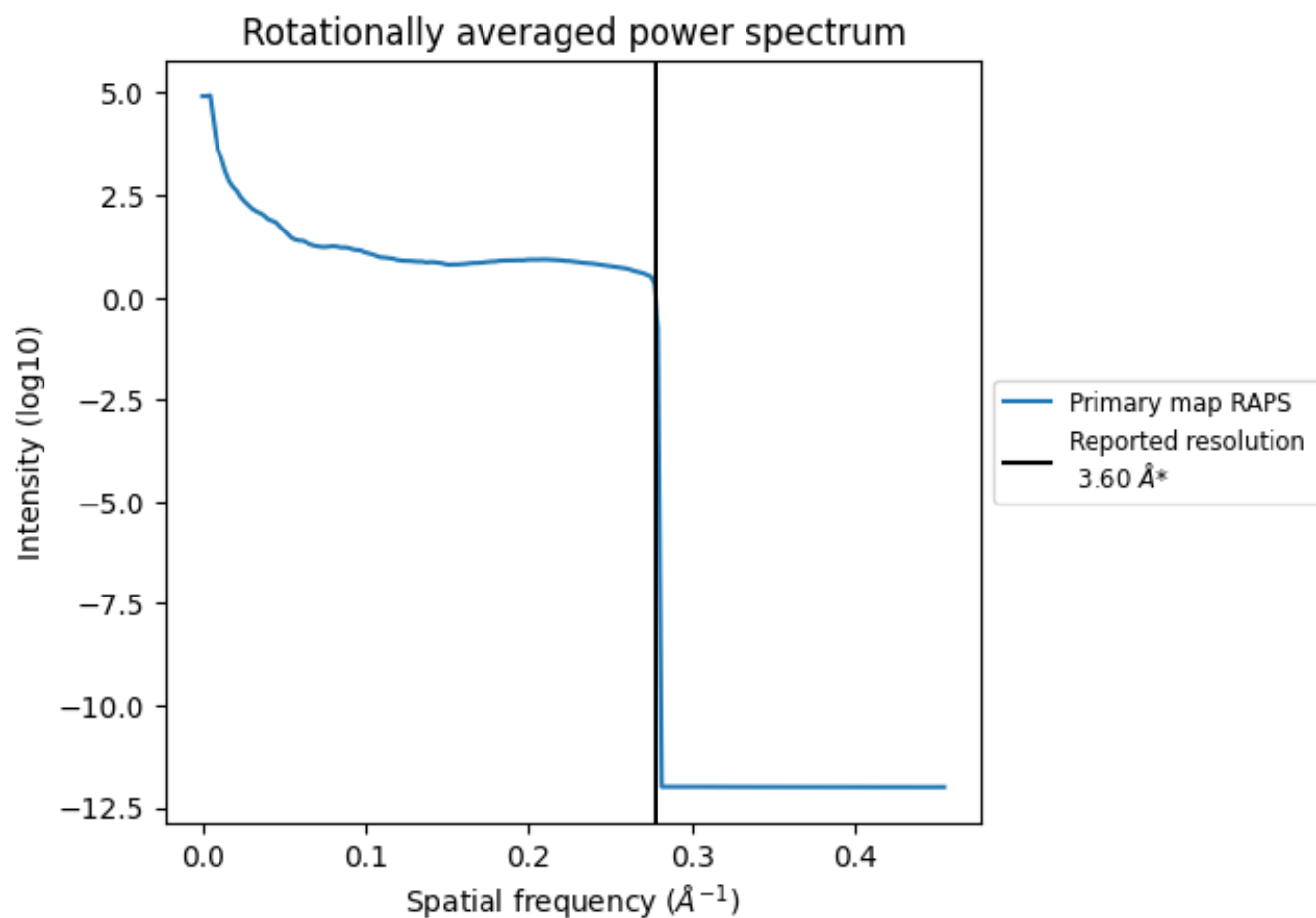
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1106 nm³; this corresponds to an approximate mass of 999 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 ⓘ

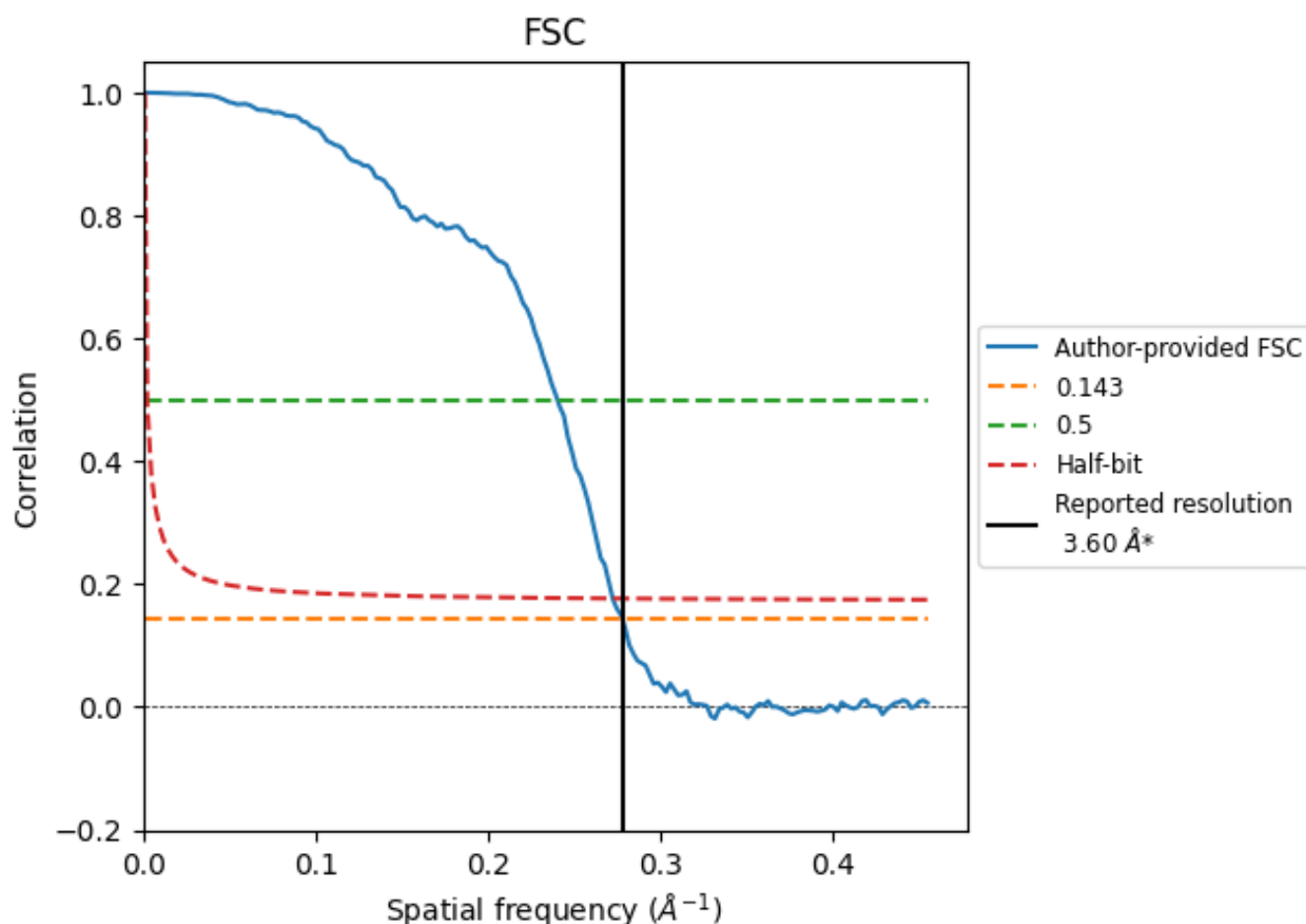


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

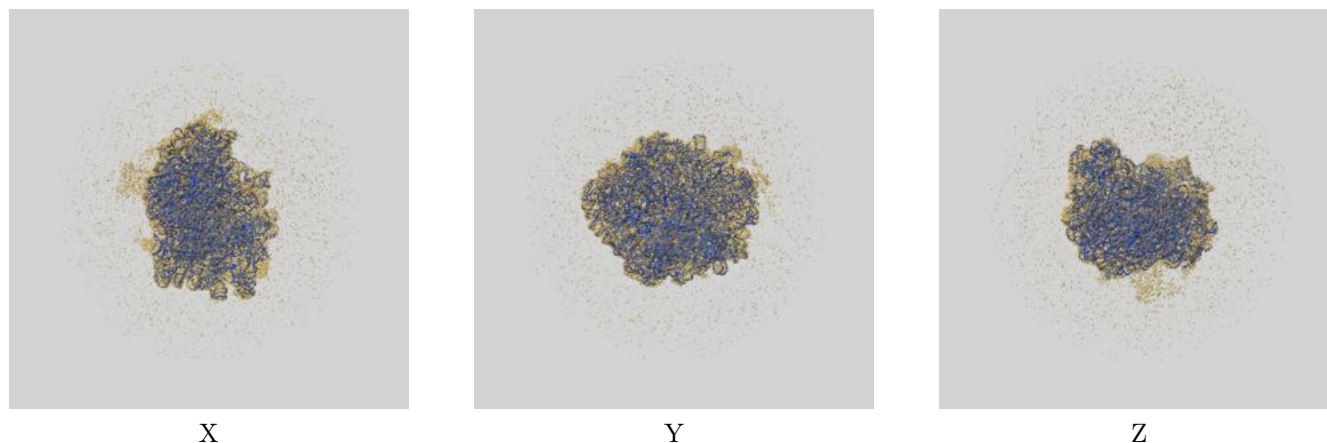
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.16	3.68
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

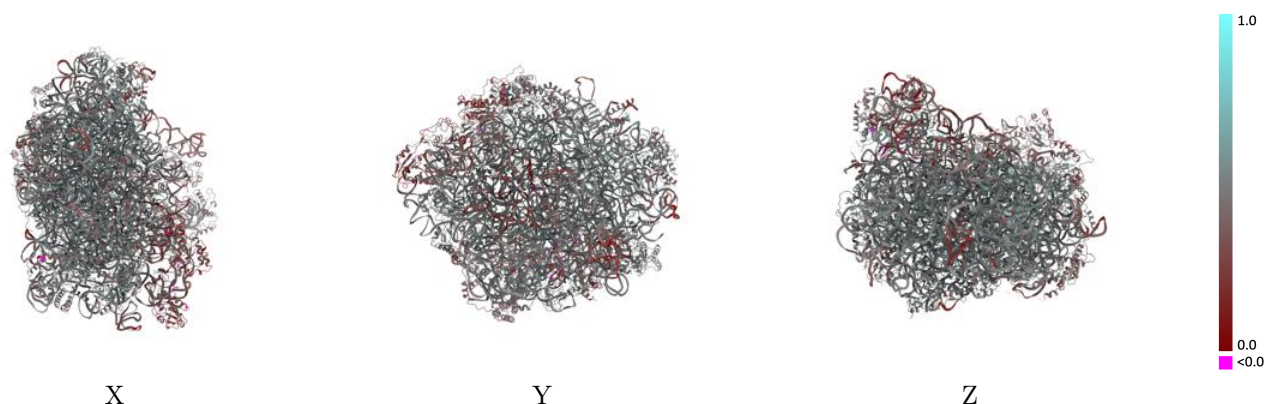
This section contains information regarding the fit between EMDB map EMD-0370 and PDB model 6N8K. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



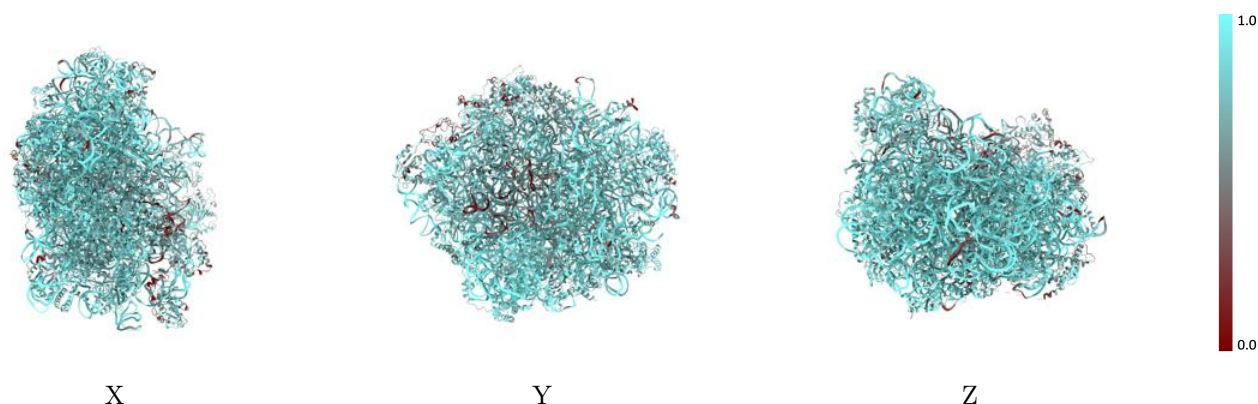
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



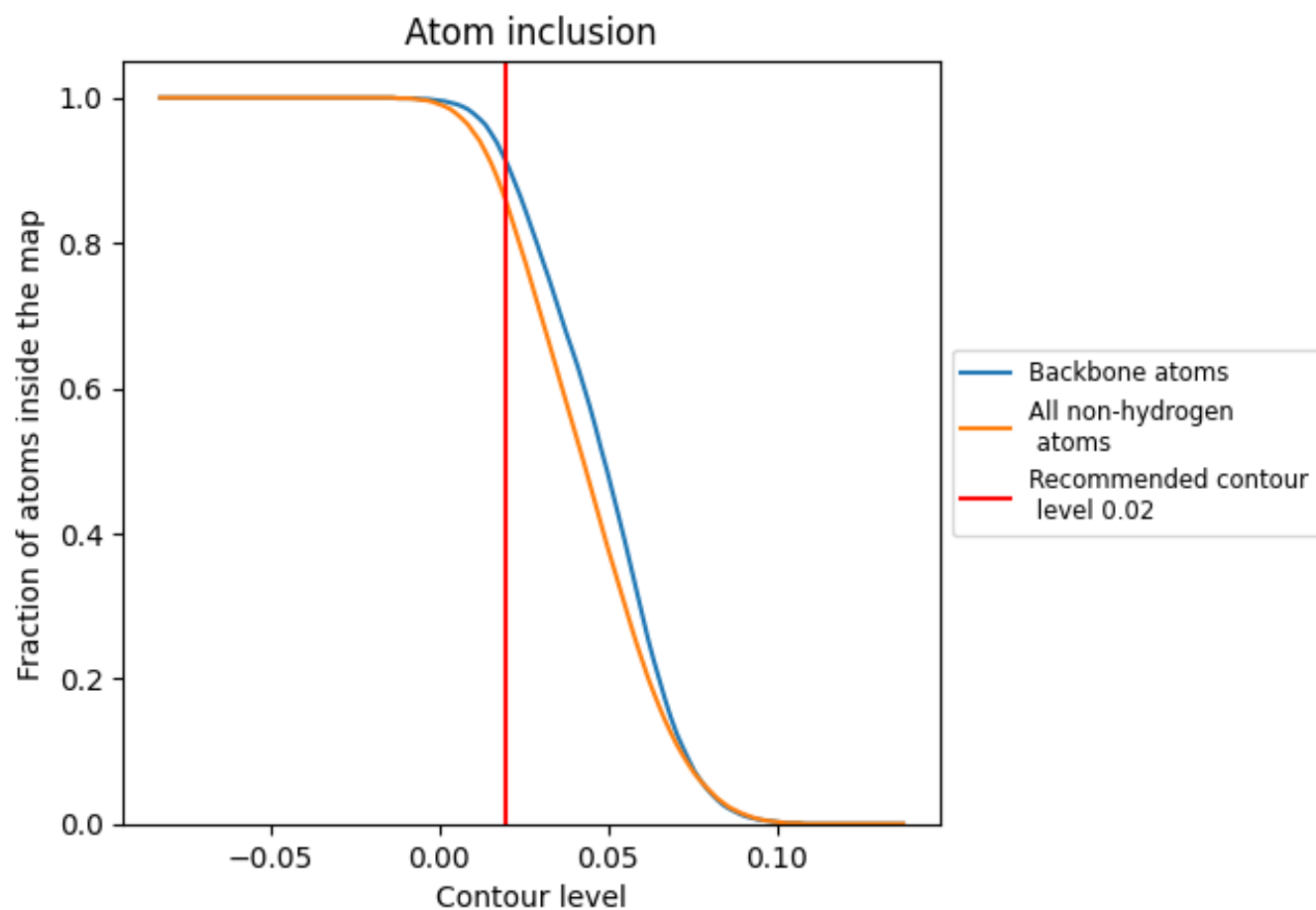
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.4650
1	 0.9120	 0.4690
2	 0.9560	 0.4720
3	 0.9480	 0.4930
A	 0.8520	 0.5170
B	 0.8510	 0.5000
C	 0.8380	 0.4970
D	 0.8080	 0.4310
E	 0.7870	 0.4630
F	 0.8250	 0.4810
G	 0.8300	 0.4720
H	 0.8030	 0.4680
I	 0.6730	 0.4530
J	 0.7590	 0.4110
L	 0.8490	 0.4860
M	 0.8250	 0.4750
N	 0.8590	 0.5200
O	 0.8470	 0.5050
P	 0.8220	 0.4990
Q	 0.8450	 0.4940
R	 0.8350	 0.4920
S	 0.8340	 0.4940
T	 0.7500	 0.4080
U	 0.7800	 0.4220
V	 0.7890	 0.5000
W	 0.5250	 0.2860
X	 0.8420	 0.5000
Y	 0.8460	 0.4980
Z	 0.8150	 0.4810
a	 0.8540	 0.4970
b	 0.5980	 0.3790
c	 0.8170	 0.4620
d	 0.8050	 0.4850
e	 0.8050	 0.5130
f	 0.8510	 0.5240



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Chain	Atom inclusion	Q-score
g	 0.7930	 0.5050
h	 0.8250	 0.4830
i	 0.8190	 0.4850
j	 0.8650	 0.5290
k	 0.7530	 0.4520
l	 0.8580	 0.5180
o	 0.7870	 0.4660
p	 0.8220	 0.4940
q	 0.3610	 0.1000
s	 0.8100	 0.3830
u	 0.7670	 0.4450
v	 0.6980	 0.4390
y	 0.7560	 0.4440
z	 0.5850	 0.4070