



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 06:44 PM UTC

PDB ID : 6FYY / pdb_00006fyy
EMDB ID : EMD-4328
Title : Structure of a partial yeast 48S preinitiation complex with eIF5 N-terminal domain (model C2)
Authors : Llacer, J.L.; Hussain, T.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2018-03-12
Resolution : 3.02 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

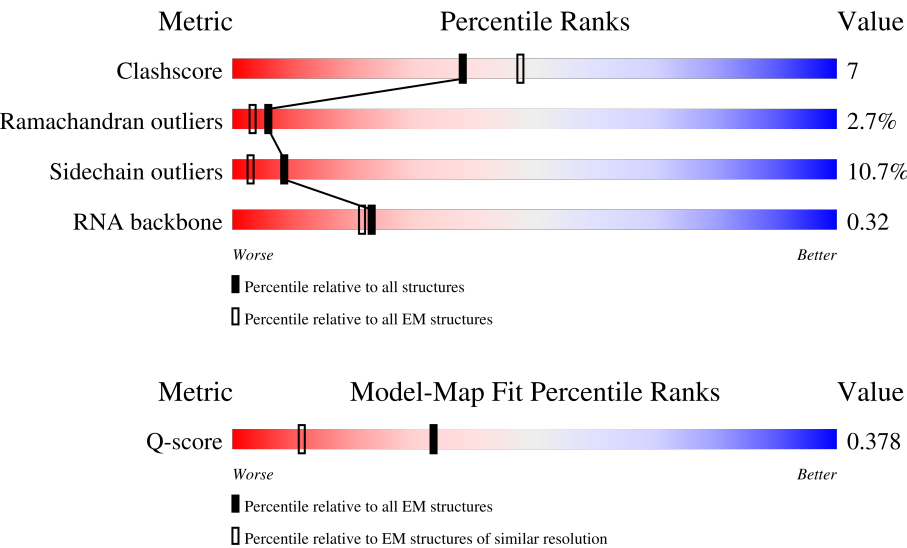
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.02 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	13913 (2.52 - 3.52)

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

Mol	Chain	Length	Quality of chain
1	1	76	67% 49%24%20%7% .
2	2	1798	12% 40%44%13% ..
3	3	49	49% 14%37%12%37%

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Mol	Chain	Length	Quality of chain
4	A	254	
5	B	255	
6	C	259	
7	D	237	
8	E	261	
9	F	227	
10	G	236	
11	H	190	
12	I	201	
13	J	188	
14	K	106	
15	L	156	
16	M	134	
17	N	151	
18	O	137	
19	P	142	
20	Q	143	
21	R	136	
22	S	146	
23	T	144	
24	U	117	
25	V	87	
26	W	130	
27	X	145	
28	Y	135	

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Mol	Chain	Length	Quality of chain
29	Z	108	
30	a	119	
31	b	82	
32	c	67	
33	d	56	
34	e	63	
35	f	150	
36	g	326	
37	h	25	
38	i	153	
39	j	304	
40	k	527	
41	l	285	
42	m	405	
43	o	964	
44	p	763	
45	q	812	
46	r	274	
47	s	347	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C4J	2	1190	X	-	-	-

2 Entry composition [i](#)

There are 51 unique types of molecules in this entry. The entry contains 104316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1780	Total	C	N	O	P	0	0
			37812	16904	6659	12469	1780		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	676	G	U	conflict	GB 49642208
2	678	U	G	conflict	GB 49642208
2	1190	C4J	U	conflict	GB 49642208

- Molecule 3 is a RNA chain called mRNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	31	Total	C	N	O	P	4	0
			719	324	108	252	35		

- Molecule 4 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	219	Total	C	N	O	S	0	0
			1702	1085	299	316	2		

- Molecule 5 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	225	Total	C	N	O	S	0	0
			1797	1135	330	329	3		

- Molecule 6 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	220	Total	C	N	O	S	0	0
			1648	1053	291	300	4		

- Molecule 7 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	227	Total	C	N	O	S	0	0
			1774	1126	320	323	5		

- Molecule 8 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 9 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 10 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	230	Total	C	N	O	S	0	0
			1832	1146	352	330	4		

- Molecule 11 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 14 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 15 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	M	117	Total	C	N	O	0	0
			885	553	161	171		

- Molecule 17 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	151	Total	C	N	O	S	0	0
			1195	761	224	207	3		

- Molecule 18 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	129	Total	C	N	O	S	0	0
			955	585	191	176	3		

- Molecule 19 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	117	Total	C	N	O	S	0	0
			923	592	165	161	5		

- Molecule 20 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Q	141	Total	C	N	O	0	0
			1105	709	204	192		

- Molecule 21 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	130	Total	C	N	O	S	0	0
			1033	643	194	193	3		

- Molecule 22 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	145	Total	C	N	O	S	0	0
			1189	739	239	209	2		

- Molecule 23 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 24 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 25 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 26 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 27 is a protein called KLLA0B11231p.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 28 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	134	Total	C	N	O	S	0	0
			1061	665	207	189			

- Molecule 29 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	78	Total	C	N	O	S	0	0
			594	376	111	106	1		

- Molecule 30 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	103	Total	C	N	O	S	0	0
			812	500	173	134	5		

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	64	Total	C	N	O	S	0	0
			499	308	99	91	1		

- Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	55	Total	C	N	O	S	0	0
			461	289	93	78	1		

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	60	Total	C	N	O	S	0	0
			472	295	96	80	1		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	74	Total	C	N	O	S	0	0
			584	374	111	95	4		

- Molecule 36 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	320	Total	C	N	O	S	0	0
			2469	1561	432	471	5		

- Molecule 37 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	121	Total	C	N	O	S	0	0
			958	587	183	183	5		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	147	Total	C	N	O	S	0	0
			1140	724	201	208	7		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	529	Total	C	N	O	S	0	0
			4070	2597	697	769	7		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	647	Total	C	N	O	S	0	0
			5114	3274	880	942	18		

- Molecule 45 is a protein called eIF3c, Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	621	Total	C	N	O	S	0	0
			4827	3076	813	926	12		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	r	49	Total	C	N	O	0	0
			392	240	76	76		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	330	Total	C	N	O	S	0	0
			2606	1661	429	507	9		

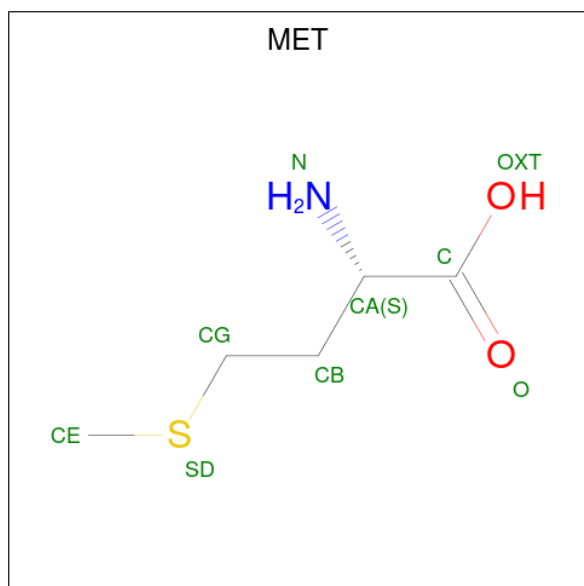
- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	116	Total	Mg	0
			116	116	
48	k	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

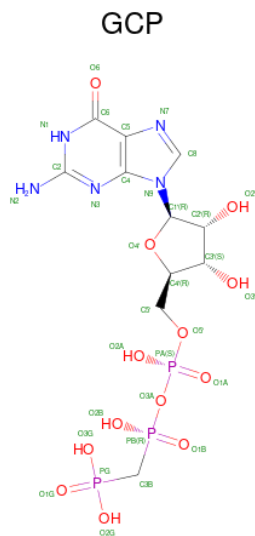
Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	Zn	0
			1	1	
49	b	1	Total	Zn	0
			1	1	
49	f	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	
49	m	1	Total	Zn	0
			1	1	

- Molecule 50 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
50	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

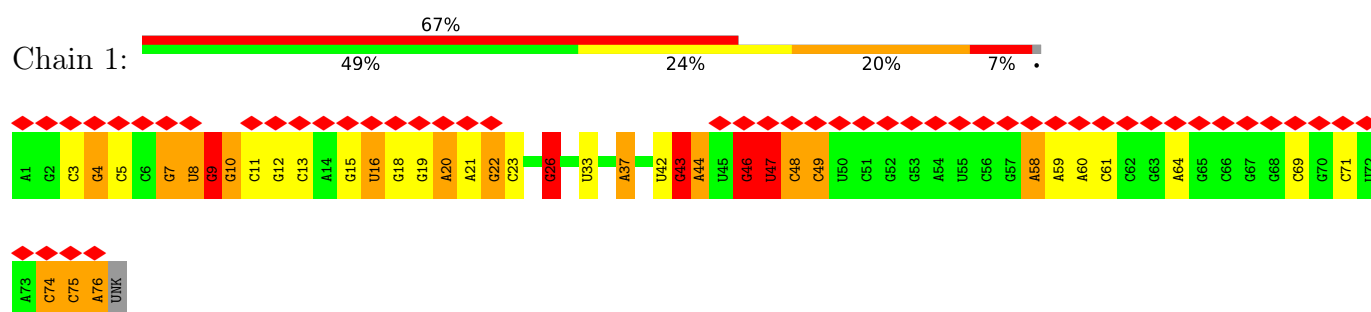


Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

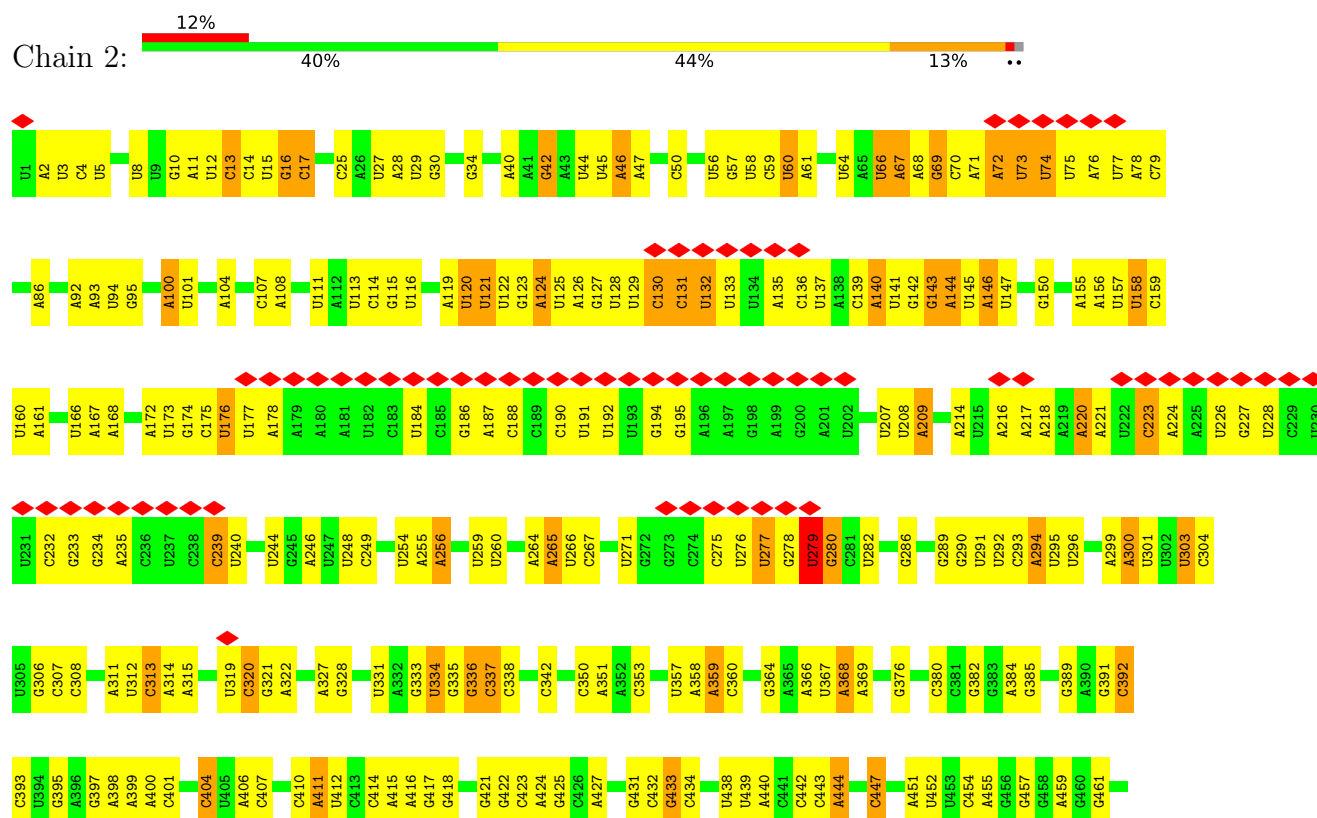
3 Residue-property plots

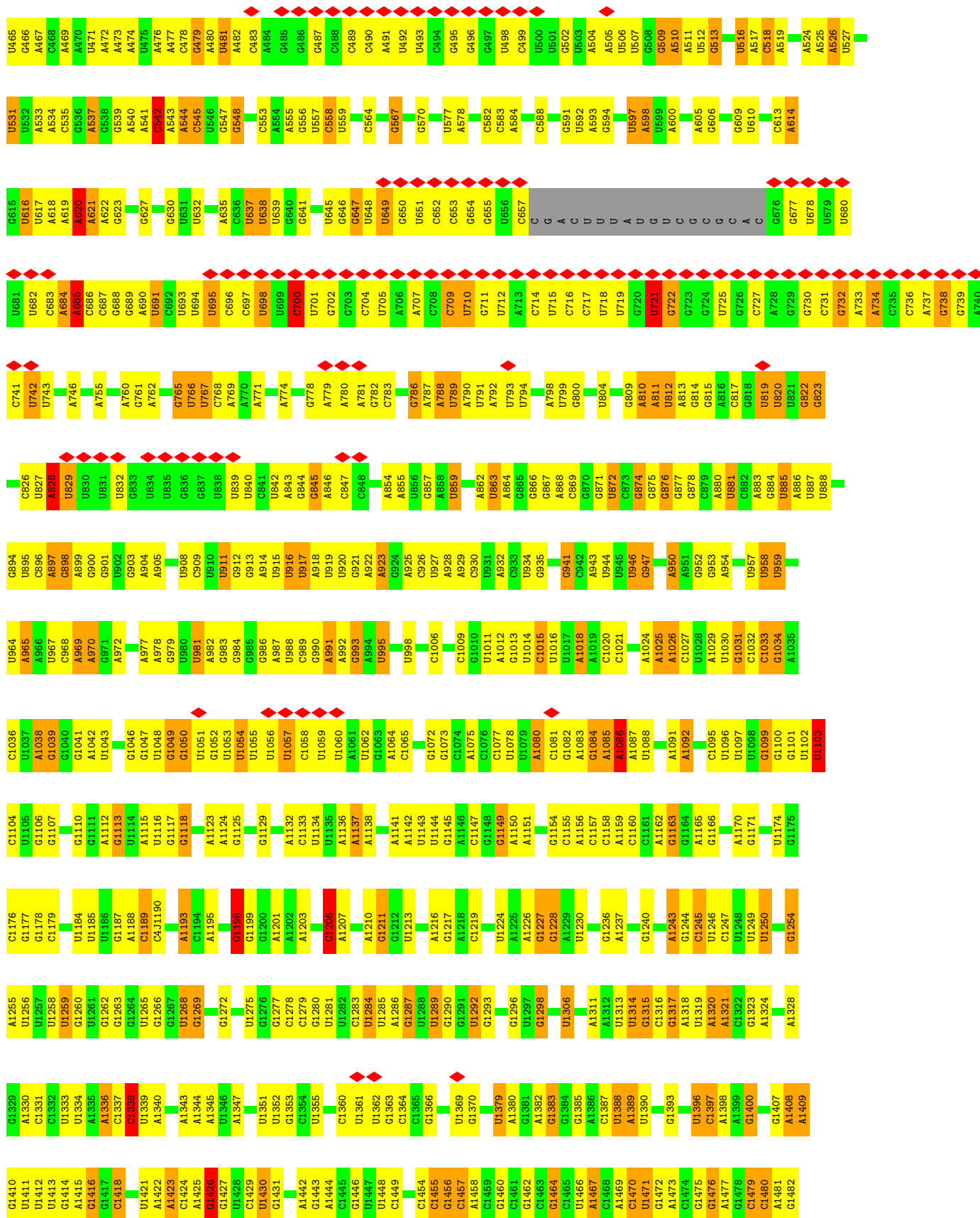
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

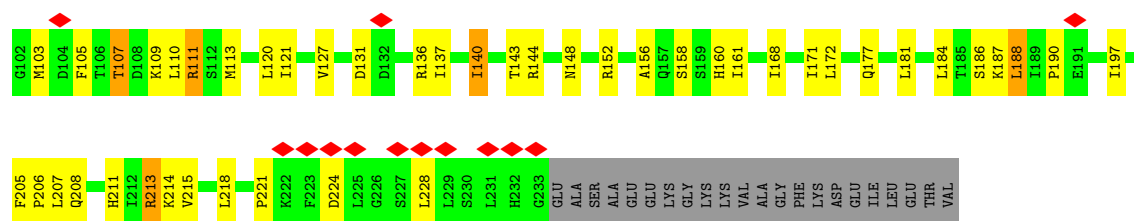
• Molecule 1: tRNAi



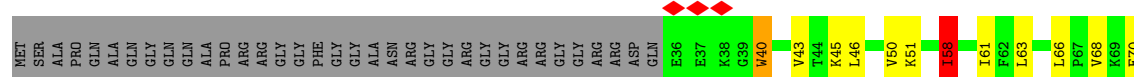
• Molecule 2: 18S ribosomal RNA



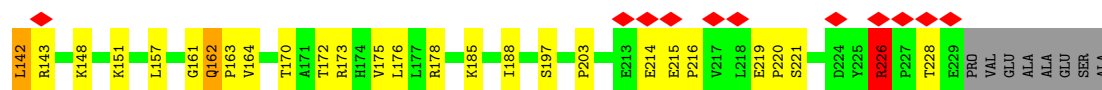
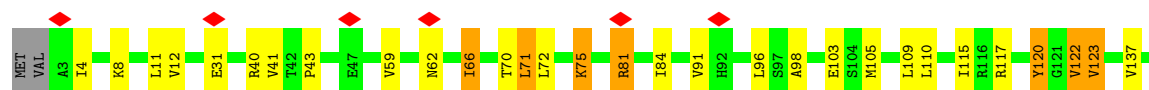




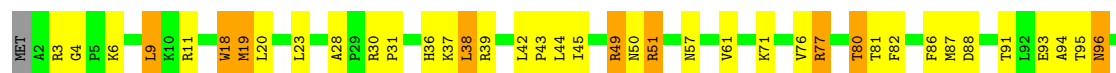
• Molecule 6: KLLA0F09812p



• Molecule 7: KLLA0D08305p

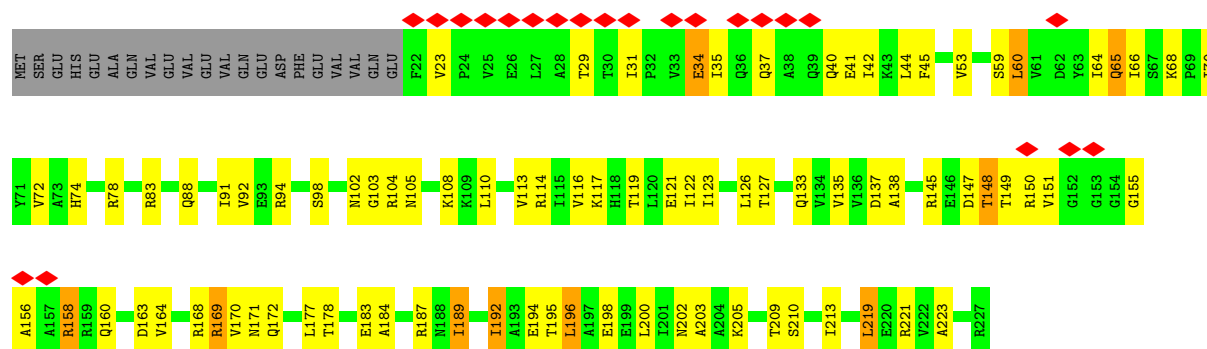


• Molecule 8: 40S ribosomal protein S4

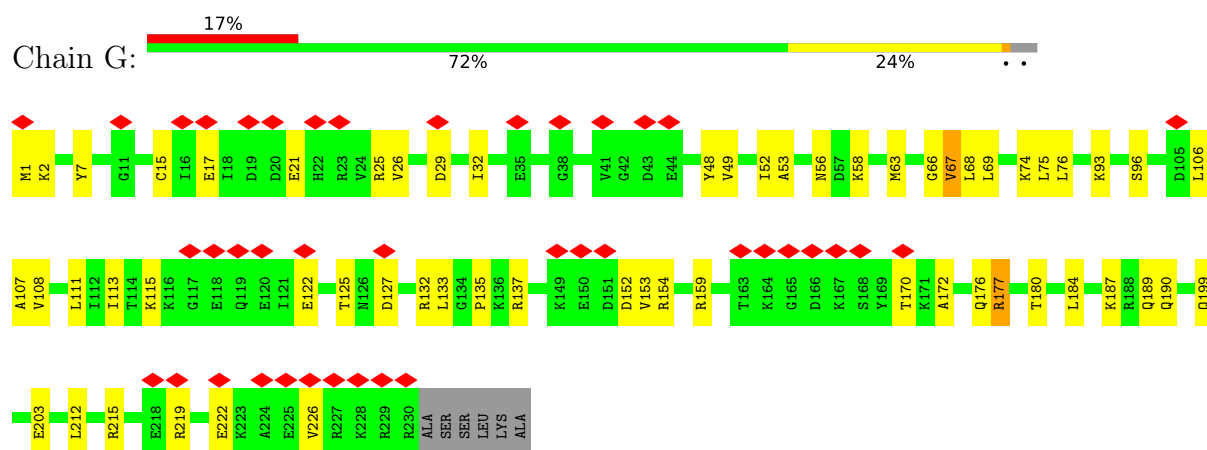


• Molecule 9: KLLA0D10659p

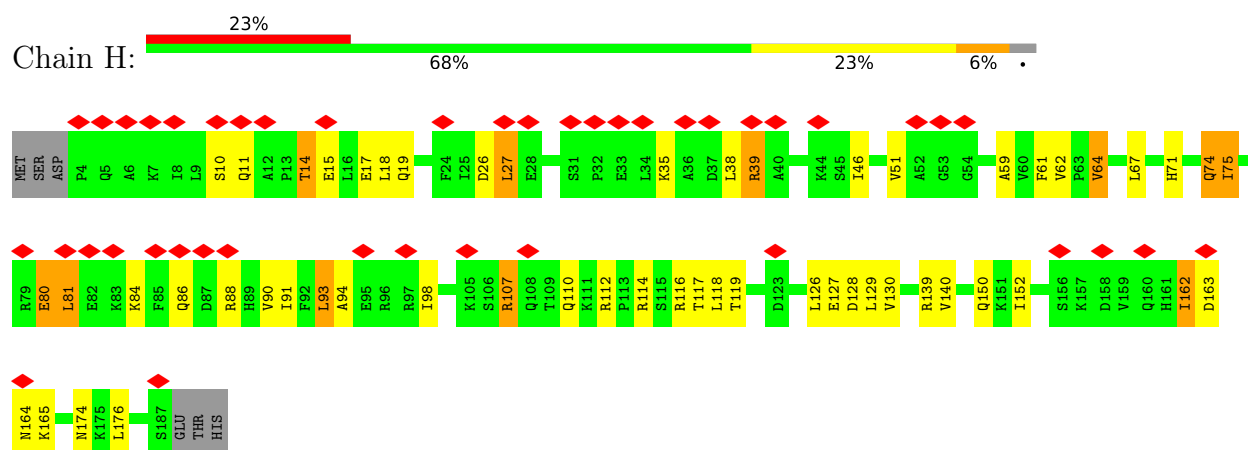




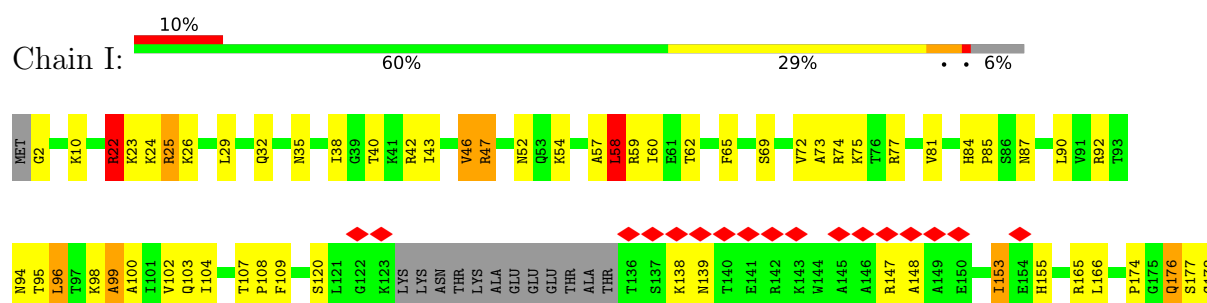
• Molecule 10: 40S ribosomal protein S6



• Molecule 11: 40S ribosomal protein S7



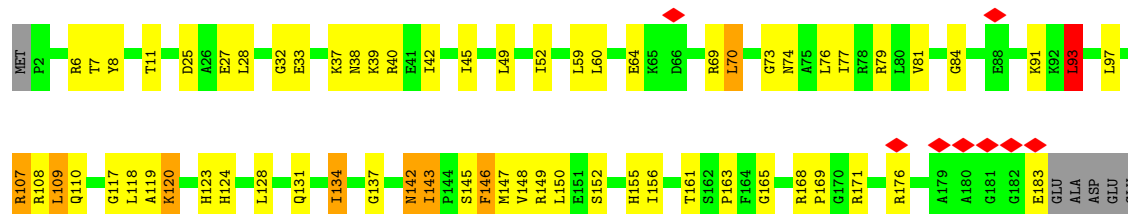
• Molecule 12: 40S ribosomal protein S8





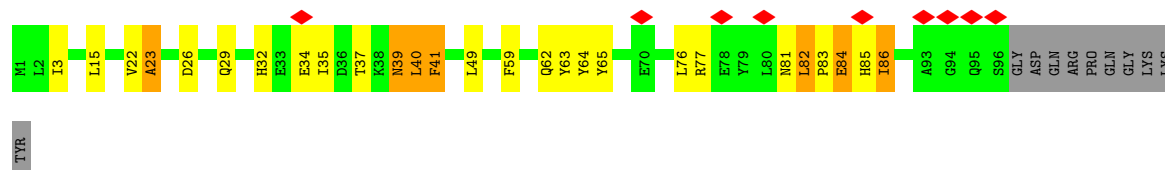
• Molecule 13: KLLA0E23673p

Chain J: 62% 30%



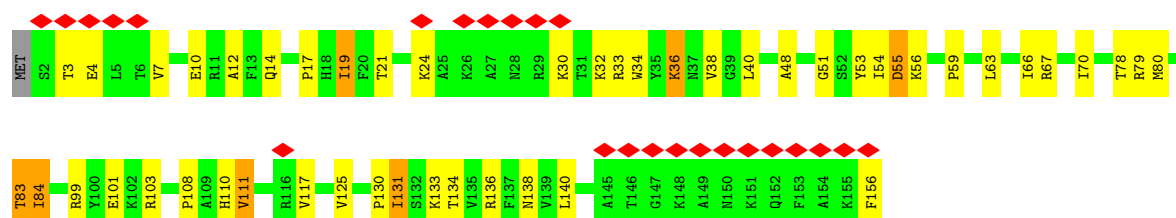
• Molecule 14: KLLA0B08173p

Chain K: 8% 65% 19% 7% 9%



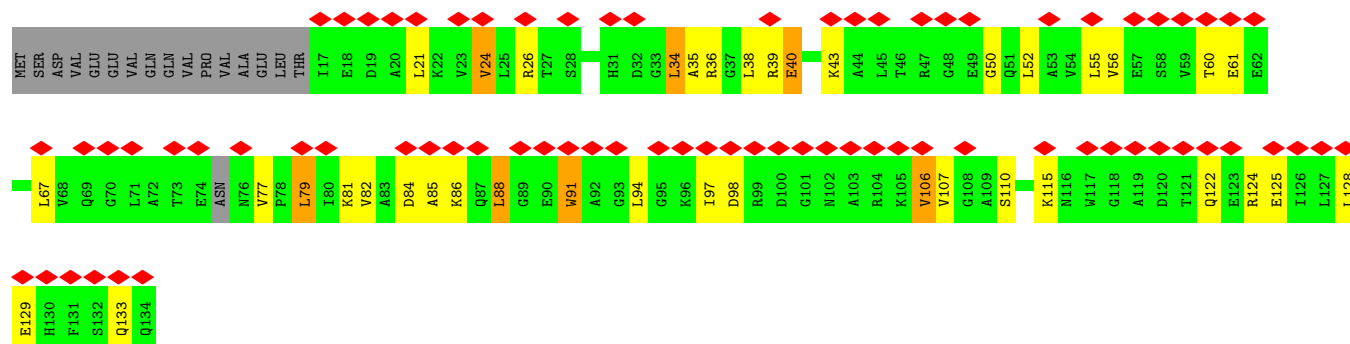
• Molecule 15: KLLA0A10483p

Chain L: 15% 68% 27%

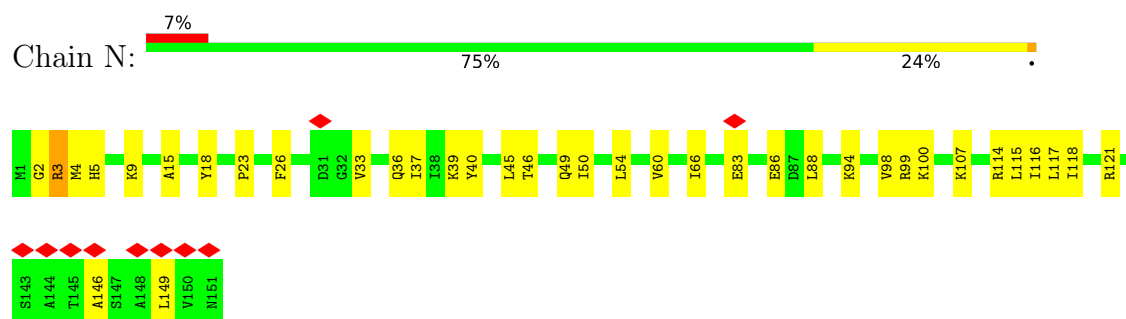


• Molecule 16: 40S ribosomal protein S12

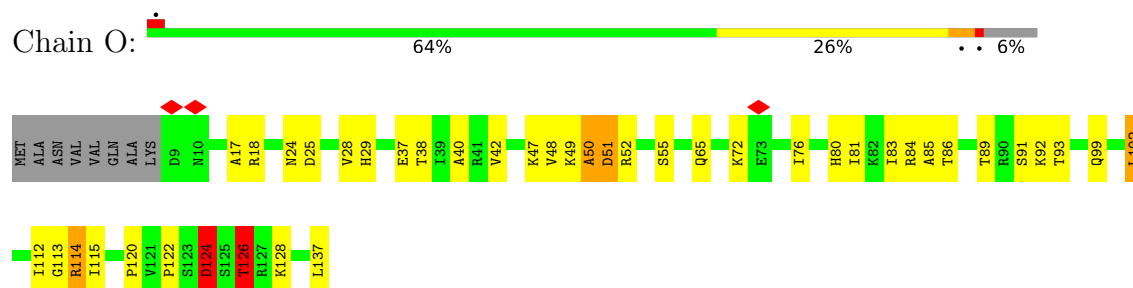
Chain M: 56% 58% 24% 5% 13%



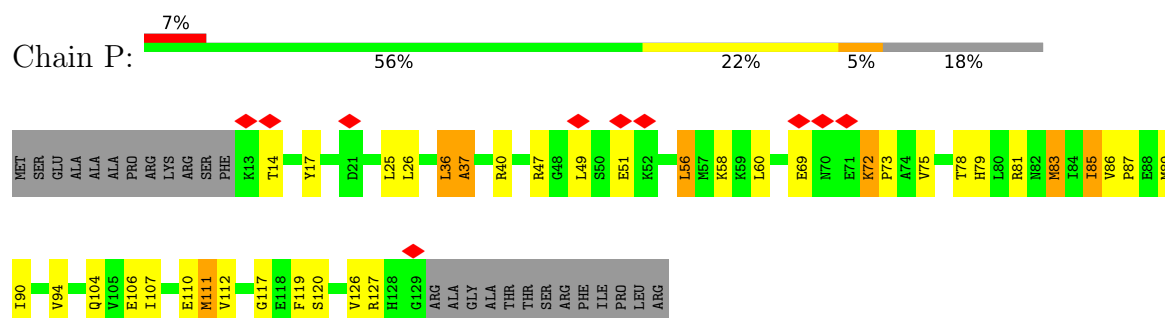
- Molecule 17: KLLA0F18040p



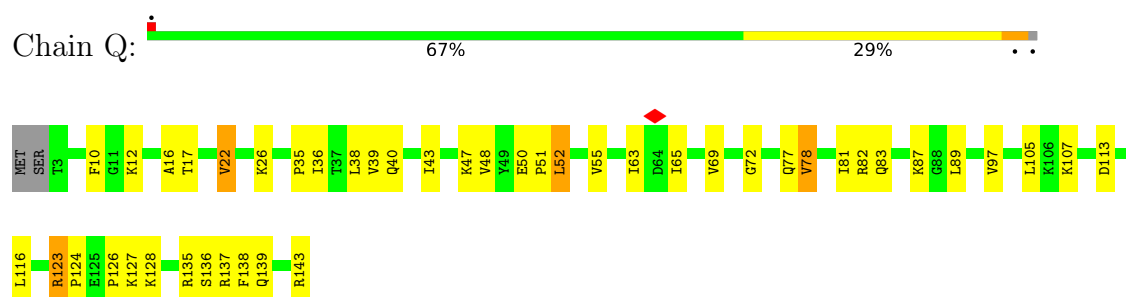
- Molecule 18: 40S ribosomal protein S14



- Molecule 19: KLLA0F07843p

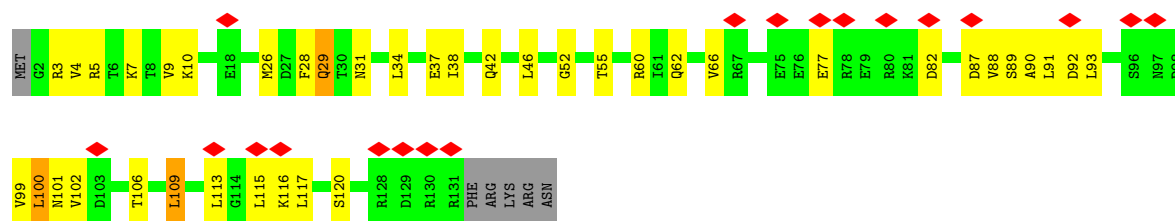


- Molecule 20: 40S ribosomal protein S16

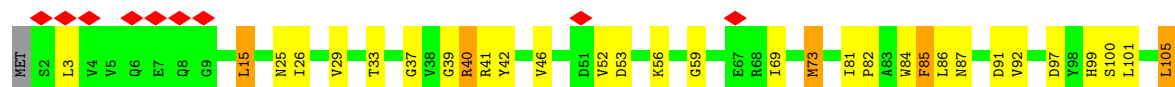


- Molecule 21: KLLA0B01474p

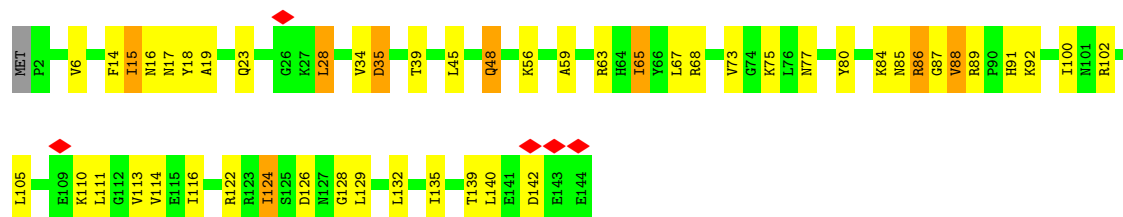




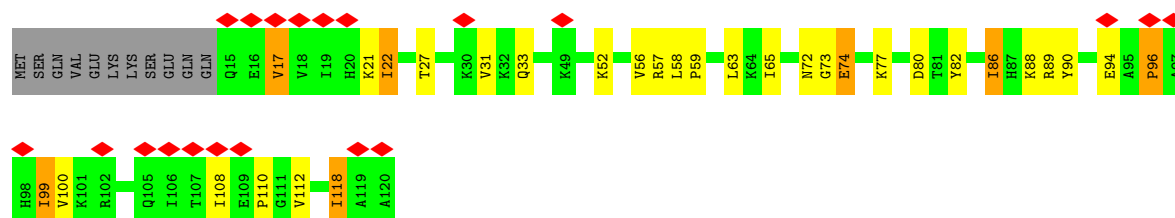
• Molecule 22: KLLA0B01562p



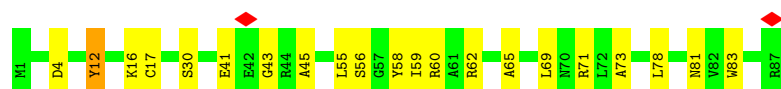
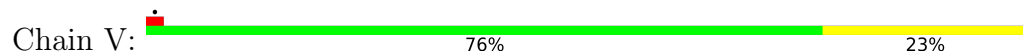
• Molecule 23: KLLA0A07194p



• Molecule 24: KLLA0F25542p

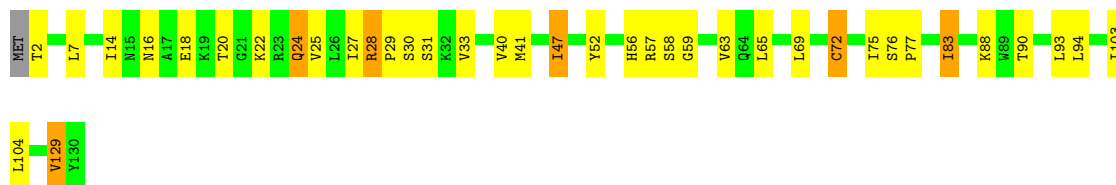


• Molecule 25: 40S ribosomal protein S21



• Molecule 26: 40S ribosomal protein S22

Chain W: 



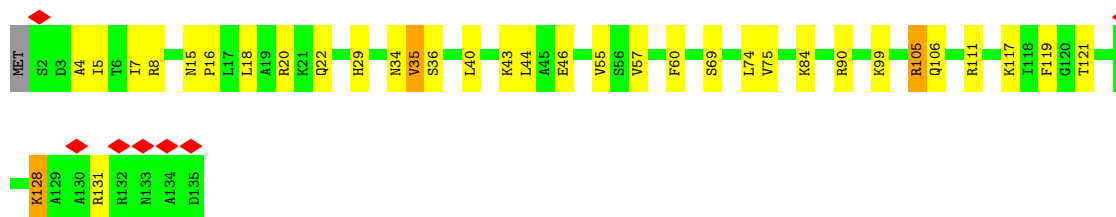
• Molecule 27: KLLA0B11231p

Chain X: 



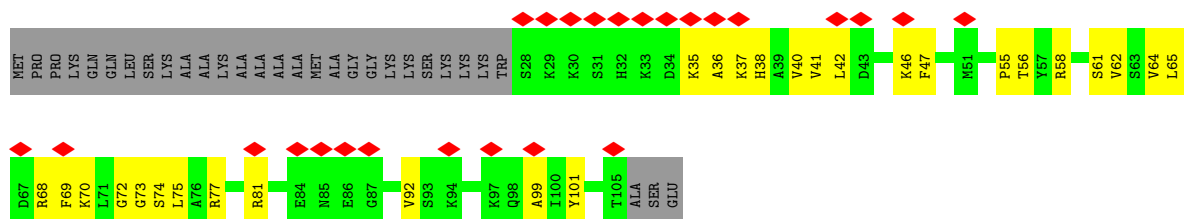
• Molecule 28: 40S ribosomal protein S24

Chain Y: 



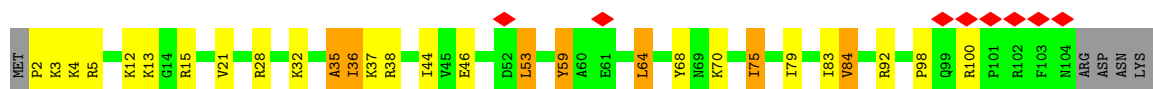
• Molecule 29: KLLA0B06182p

Chain Z: 



• Molecule 30: 40S ribosomal protein S26

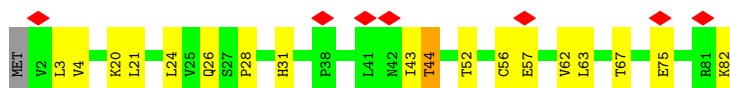
Chain a: 



SER
PRO
ALA
ASP
ALA
ALA
LYS
LYS
ALA
LEU

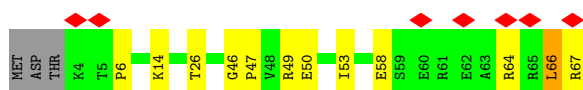
- Molecule 31: 40S ribosomal protein S27

Chain b: 



- Molecule 32: 40S ribosomal protein S28

Chain c: 



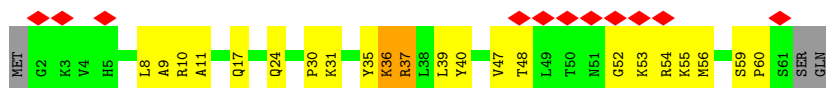
- Molecule 33: 40S ribosomal protein S29

Chain d: 



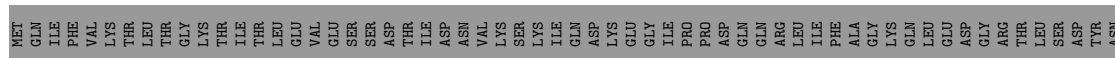
- Molecule 34: 40S ribosomal protein S30

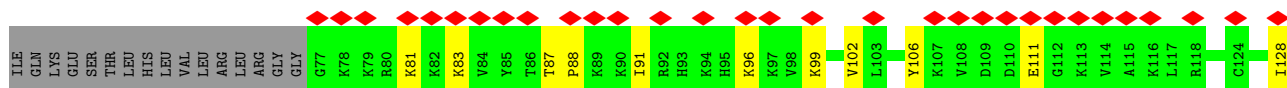
Chain e: 

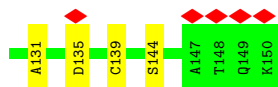


- Molecule 35: Ubiquitin-40S ribosomal protein S27a

Chain f: 

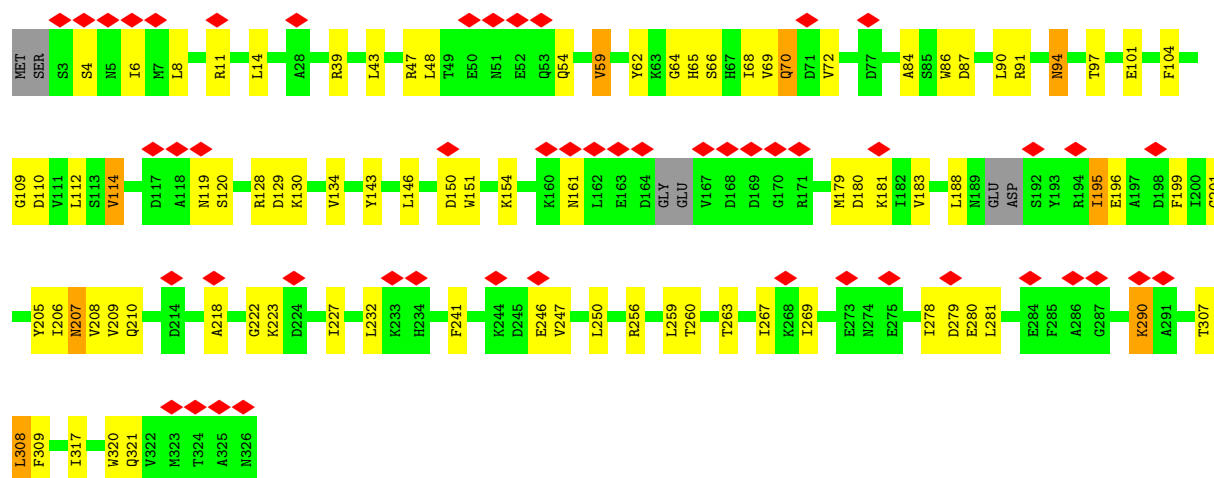




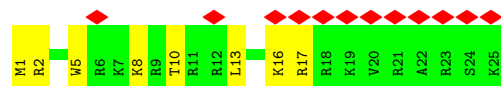


- Molecule 36: KLLA0E12277p

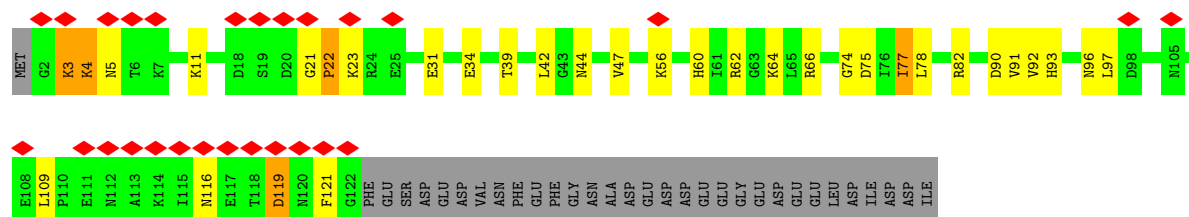
Chain g: 



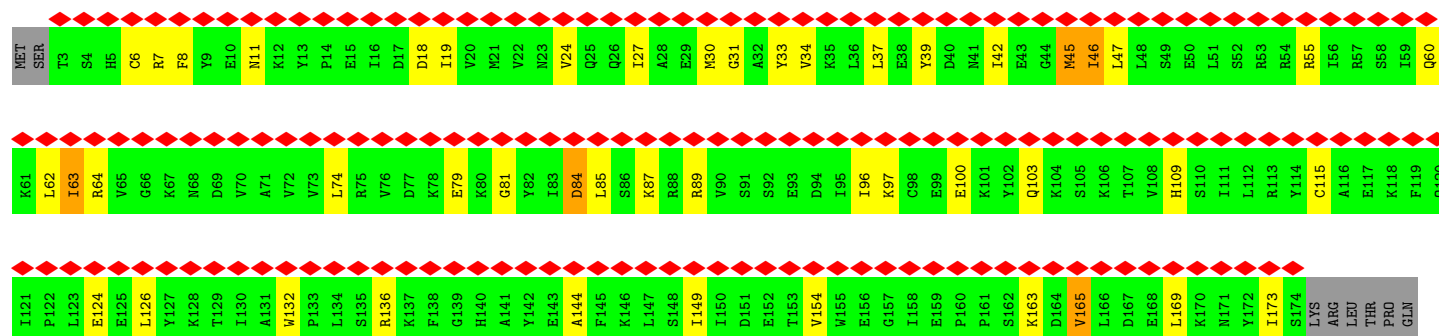
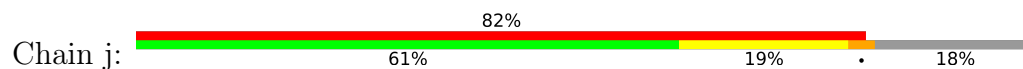
- Molecule 37: 60S ribosomal protein L41-A



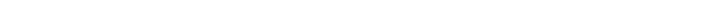
- Molecule 38: Eukaryotic translation initiation factor 1A



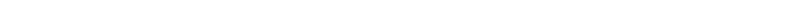
- Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha

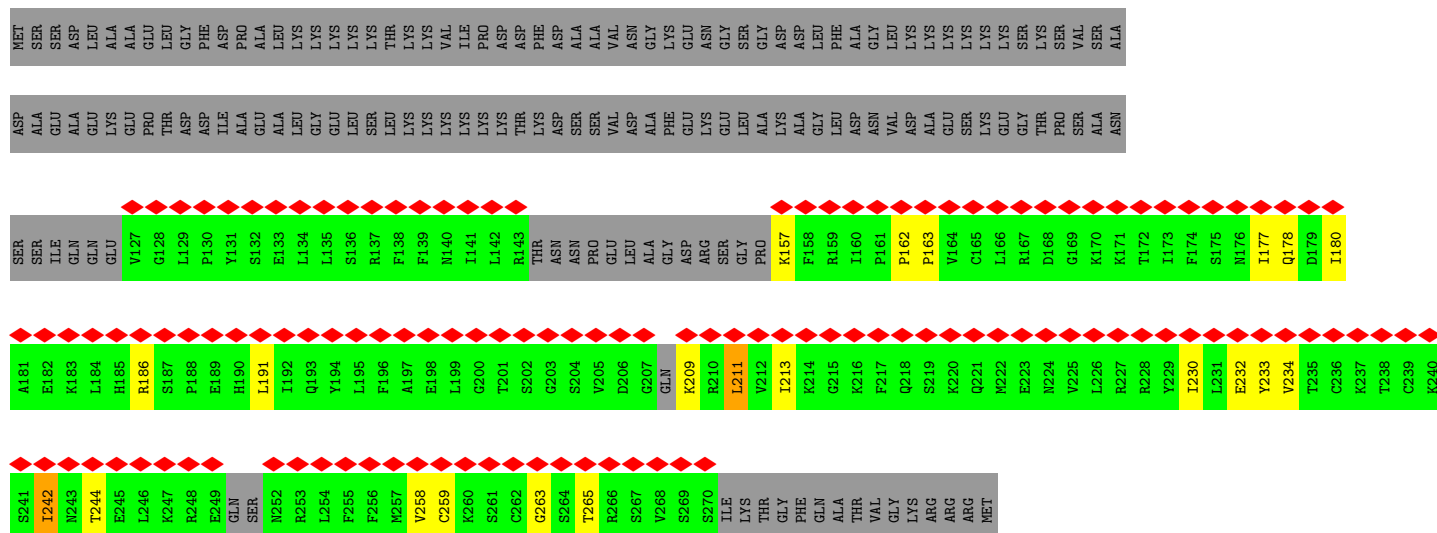




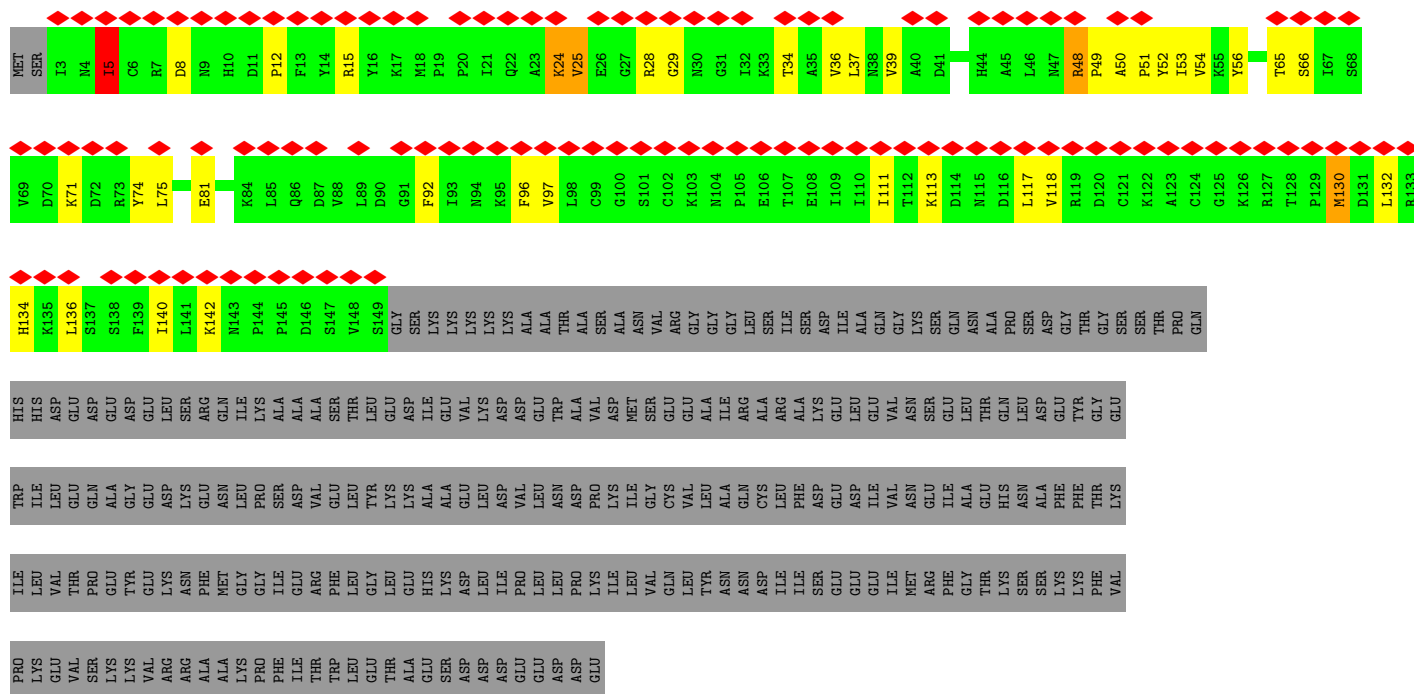
- Chain k:  75% 64% 10% 25%



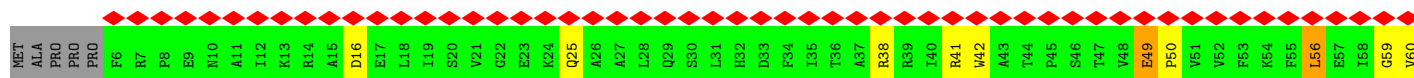
- Chain 1: 



• Molecule 42: Eukaryotic translation initiation factor 5



• Molecule 43: Eukaryotic translation initiation factor 3 subunit A

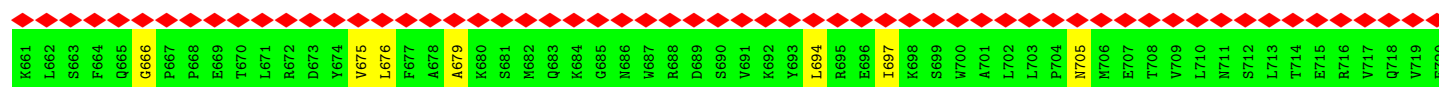
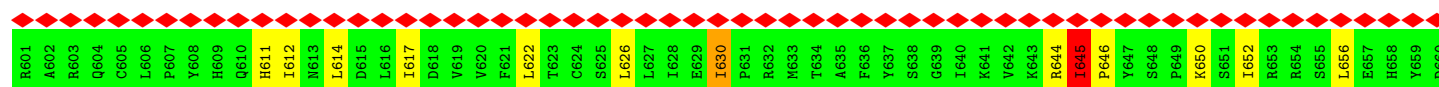
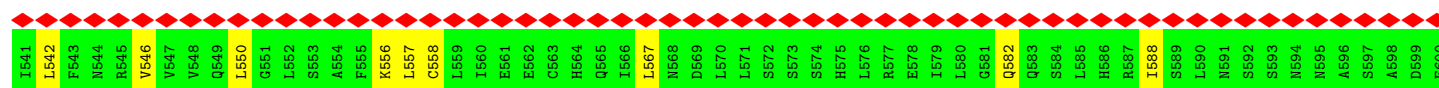
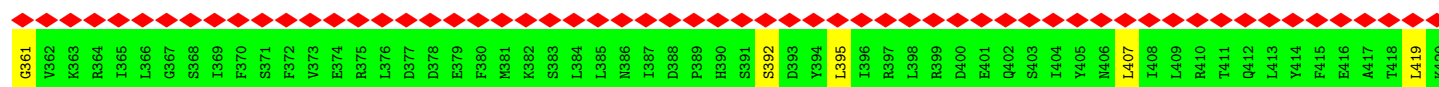
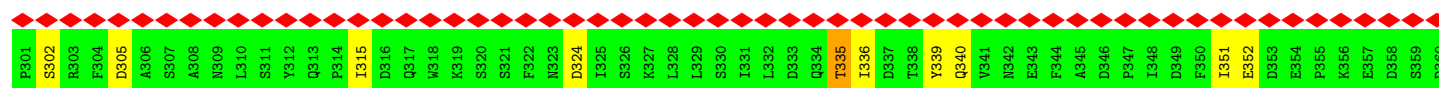
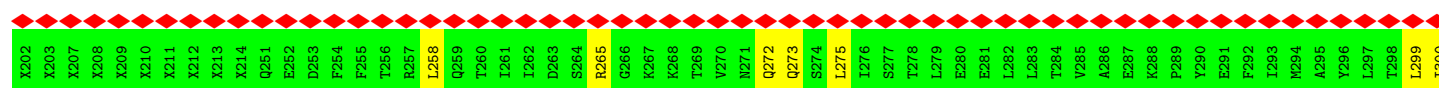
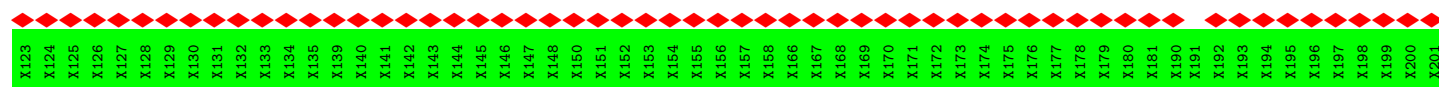
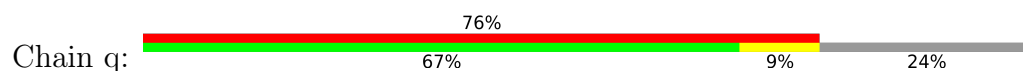


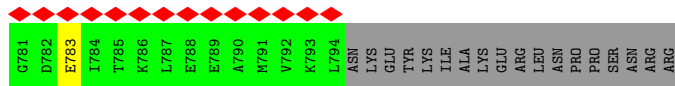




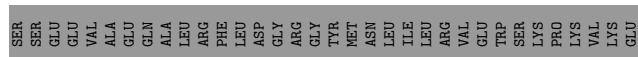
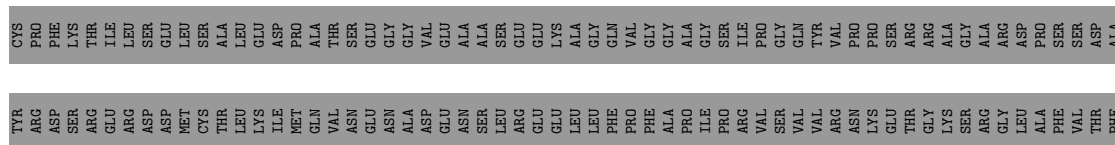
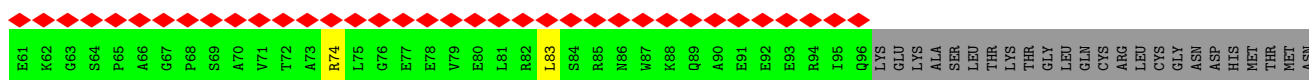


• Molecule 45: eIF3c, Eukaryotic translation initiation factor 3 subunit C

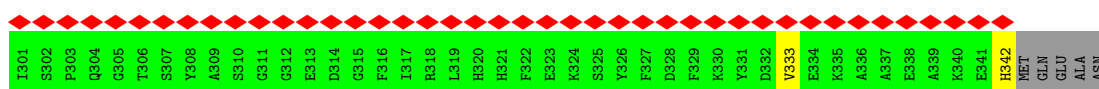
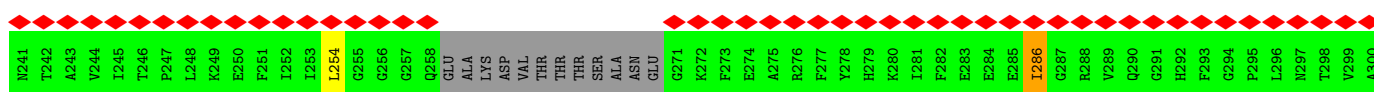
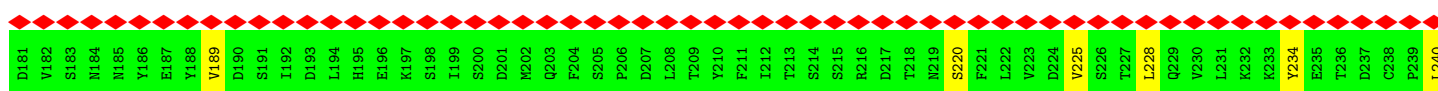
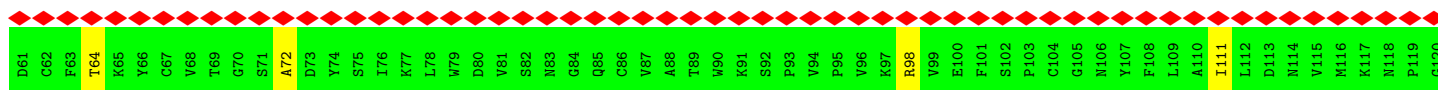




Chain r:



Chain s:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157868	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.157	Depositor
Minimum map value	-0.645	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, AYA, 2MG, 1MG, GCP, MG, M2G, 5MC, PSU, 1MA, H2U, C4J, ZN, T6A, RIA, MA6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.40	1/1529 (0.1%)	0.79	4/2376 (0.2%)
2	2	0.37	0/41987	0.76	42/65416 (0.1%)
3	3	0.39	0/797	0.77	0/1233
4	A	0.54	0/1742	1.05	0/2383
5	B	0.48	0/1813	0.98	2/2438 (0.1%)
6	C	0.51	0/1678	1.01	2/2277 (0.1%)
7	D	0.52	0/1800	1.01	2/2421 (0.1%)
8	E	0.48	0/2122	0.92	1/2861 (0.0%)
9	F	0.53	0/1628	1.08	0/2198
10	G	0.54	0/1855	0.98	2/2479 (0.1%)
11	H	0.56	0/1507	1.04	0/2028
12	I	0.47	0/1515	0.95	0/2029
13	J	0.51	0/1495	1.10	4/2001 (0.2%)
14	K	0.55	0/831	1.09	4/1123 (0.4%)
15	L	0.50	0/1276	0.85	1/1718 (0.1%)
16	M	0.63	0/891	1.04	1/1201 (0.1%)
17	N	0.51	0/1218	1.06	0/1638
18	O	0.53	0/966	1.02	2/1297 (0.2%)
19	P	0.52	0/942	1.05	2/1269 (0.2%)
20	Q	0.50	0/1125	0.99	0/1510
21	R	0.61	0/1044	1.08	0/1402
22	S	0.53	0/1208	1.03	0/1624
23	T	0.50	0/1129	1.08	0/1520
24	U	0.55	0/857	0.99	0/1158
25	V	0.48	0/696	0.92	1/938 (0.1%)
26	W	0.48	0/1039	1.03	0/1399
27	X	0.52	0/1137	0.92	1/1516 (0.1%)
28	Y	0.47	0/1075	0.93	0/1433
29	Z	0.51	0/603	0.98	0/814
30	a	0.53	0/825	0.98	1/1106 (0.1%)
31	b	0.48	0/619	0.84	0/837
32	c	0.52	0/501	0.91	2/673 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.43	0/473	0.90	0/629
34	e	0.53	0/480	0.98	0/640
35	f	0.53	0/597	0.88	0/795
36	g	0.49	0/2523	0.83	0/3434
37	h	0.42	0/234	1.10	0/300
38	i	0.50	0/969	0.96	0/1287
39	j	0.60	0/2034	1.01	0/2737
40	k	0.61	0/3079	0.94	0/4157
41	l	0.60	0/1051	0.92	0/1402
42	m	0.57	0/1164	0.99	0/1575
43	o	0.59	0/4140	1.13	6/5608 (0.1%)
44	p	0.61	0/5245	0.89	2/7115 (0.0%)
45	q	0.62	2/4523 (0.0%)	1.11	6/6114 (0.1%)
46	r	0.54	0/399	0.89	0/535
47	s	0.59	0/2669	0.85	0/3611
All	All	0.49	3/109030 (0.0%)	0.90	88/156255 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	1	0
20	Q	0	1
44	p	0	2
All	All	1	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	q	630	ILE	CA-CB	5.35	1.57	1.54
45	q	300	ILE	CA-CB	5.07	1.57	1.53
1	1	37	T6A	O3'-P	5.04	1.61	1.56

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1470	C	C2'-C3'-O3'	9.22	123.33	109.50
2	2	1206	C	C2'-C3'-O3'	8.99	122.98	109.50
2	2	1080	A	C4'-C3'-O3'	8.78	122.57	109.40
2	2	277	U	C2'-C3'-O3'	8.34	122.01	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	p	528	THR	N-CA-C	8.31	119.96	111.07
2	2	1455	C	C4'-C3'-O3'	8.07	121.50	109.40
2	2	542	C	C2'-C3'-O3'	7.93	121.39	109.50
2	2	685	A	C2'-C3'-O3'	7.76	125.34	113.70
2	2	1430	U	C4'-C3'-O3'	7.68	120.92	109.40
43	o	930	PRO	N-CA-CB	7.68	110.49	103.20
14	K	63	TYR	N-CA-C	7.29	122.88	113.18
44	p	633	VAL	N-CA-C	7.19	117.58	107.37
2	2	810	A	C4'-C3'-O3'	7.09	120.03	109.40
2	2	1765	G	C4'-C3'-O3'	7.08	120.02	109.40
2	2	279	U	C2'-C3'-O3'	7.06	120.09	109.50
19	P	86	VAL	CA-C-N	7.01	128.61	119.84
19	P	86	VAL	C-N-CA	7.01	128.61	119.84
43	o	933	PRO	N-CA-CB	6.98	110.58	103.25
2	2	1797	U	C4'-C3'-O3'	6.97	119.86	109.40
1	1	74	C	C2'-C3'-O3'	6.92	119.88	109.50
43	o	939	PRO	N-CA-CB	6.87	110.56	103.00
2	2	1765	G	C2'-C3'-O3'	6.86	119.79	109.50
2	2	239	C	C2'-C3'-O3'	6.77	119.66	109.50
2	2	1057	U	C4'-C3'-O3'	6.73	119.50	109.40
43	o	936	PRO	N-CA-CB	6.73	110.32	103.25
2	2	616	U	N1-C1'-C2'	6.68	122.03	112.00
45	q	666	GLY	CA-C-N	6.59	124.47	119.66
45	q	666	GLY	C-N-CA	6.59	124.47	119.66
43	o	927	PRO	N-CA-CB	6.55	110.06	102.33
43	o	397	VAL	N-CA-C	6.54	117.03	110.23
2	2	700	C	C2'-C3'-O3'	6.43	123.35	113.70
2	2	828	A	C4'-C3'-O3'	6.40	119.00	109.40
2	2	828	A	C2'-C3'-O3'	6.33	118.99	109.50
14	K	41	PHE	N-CA-CB	6.30	120.04	110.28
2	2	66	U	C4'-C3'-O3'	6.25	118.78	109.40
32	c	46	GLY	CA-C-N	6.17	127.55	119.84
32	c	46	GLY	C-N-CA	6.17	127.55	119.84
2	2	1430	U	C2'-C3'-O3'	6.16	118.74	109.50
1	1	74	C	C4'-C3'-O3'	6.14	118.61	109.40
8	E	76	VAL	N-CA-C	6.12	116.18	110.42
45	q	299	LEU	CA-C-N	6.12	124.10	120.24
45	q	299	LEU	C-N-CA	6.12	124.10	120.24
2	2	620	A	C4'-C3'-O3'	-6.09	103.86	113.00
13	J	168	ARG	CA-C-N	5.88	127.19	119.84
13	J	168	ARG	C-N-CA	5.88	127.19	119.84
2	2	130	C	C4'-C3'-O3'	5.85	118.17	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1198	G	C4'-C3'-O3'	5.82	121.73	113.00
2	2	1198	G	C2'-C3'-O3'	5.79	122.38	113.70
2	2	1571	A	C2'-C3'-O3'	5.76	118.15	109.50
2	2	542	C	C4'-C3'-O3'	5.76	118.04	109.40
13	J	143	ILE	CA-C-N	5.71	125.83	119.32
13	J	143	ILE	C-N-CA	5.71	125.83	119.32
2	2	130	C	C2'-C3'-O3'	5.70	118.04	109.50
18	O	28	VAL	N-CA-C	-5.67	101.50	109.21
25	V	41	GLU	N-CA-C	5.66	118.21	111.71
2	2	1571	A	C4'-C3'-O3'	5.63	117.84	109.40
30	a	35	ALA	N-CA-C	5.62	118.49	110.68
15	L	79	ARG	N-CA-C	5.61	118.11	111.33
2	2	1479	C	C4'-C3'-O3'	5.60	117.81	109.40
5	B	205	PHE	CA-C-N	5.51	126.73	119.84
5	B	205	PHE	C-N-CA	5.51	126.73	119.84
1	1	43	G	C4'-C3'-O3'	5.50	121.26	113.00
10	G	190	GLN	N-CA-C	-5.45	105.03	110.97
2	2	113	U	C4'-C3'-O3'	-5.43	104.85	113.00
2	2	74	U	C4'-C3'-O3'	5.38	117.46	109.40
7	D	226	ARG	CA-C-N	5.37	126.55	119.84
7	D	226	ARG	C-N-CA	5.37	126.55	119.84
2	2	1513	A	C2'-C3'-O3'	5.36	121.75	113.70
2	2	74	U	C2'-C3'-O3'	5.32	117.47	109.50
45	q	272	GLN	N-CA-C	5.30	116.87	111.14
16	M	24	VAL	N-CA-CB	5.30	117.75	110.54
2	2	1103	U	C1'-C2'-O2'	5.24	116.26	108.40
18	O	50	ALA	N-CA-C	5.24	116.80	111.14
45	q	441	TYR	N-CA-C	5.24	117.66	111.33
6	C	43	VAL	N-CA-C	-5.23	104.34	110.05
27	X	63	GLN	N-CA-C	5.19	121.28	109.81
1	1	7	G	C4'-C3'-O3'	5.17	117.15	109.40
6	C	58	ILE	CB-CA-C	-5.14	104.54	112.05
14	K	29	GLN	CA-C-N	5.12	124.30	118.97
14	K	29	GLN	C-N-CA	5.12	124.30	118.97
2	2	473	A	C4'-C3'-O3'	-5.11	105.33	113.00
2	2	1086	A	C4'-C3'-O3'	-5.11	105.34	113.00
2	2	1604	C	C3'-C2'-O2'	5.10	118.34	110.70
2	2	695	U	C4'-C3'-O3'	5.09	117.04	109.40
2	2	1298	G	C4'-C3'-O3'	-5.09	105.36	113.00
10	G	67	VAL	N-CA-C	-5.09	105.17	112.35
2	2	1338	C	C2'-C3'-O3'	5.04	117.06	109.50
2	2	721	U	C4'-C3'-O3'	5.03	116.94	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	1190	C4J	C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	Q	40	GLN	Peptide
44	p	336	TRP	Peptide
44	p	391	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1639	0	852	16	0
2	2	37812	0	19023	599	0
3	3	719	0	371	55	0
4	A	1702	0	1695	38	0
5	B	1797	0	1870	26	0
6	C	1648	0	1727	34	0
7	D	1774	0	1855	21	0
8	E	2078	0	2157	52	0
9	F	1609	0	1679	38	0
10	G	1832	0	1919	20	0
11	H	1483	0	1579	24	0
12	I	1489	0	1504	34	0
13	J	1471	0	1554	36	0
14	K	809	0	810	10	0
15	L	1248	0	1311	31	0
16	M	885	0	917	16	0
17	N	1195	0	1263	17	0
18	O	955	0	987	22	0
19	P	923	0	960	14	0
20	Q	1105	0	1170	18	0
21	R	1033	0	1082	19	0
22	S	1189	0	1211	27	0
23	T	1110	0	1124	31	0
24	U	845	0	913	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	V	687	0	682	12	0
26	W	1021	0	1056	25	0
27	X	1119	0	1198	20	0
28	Y	1061	0	1111	14	0
29	Z	594	0	590	12	0
30	a	812	0	855	22	0
31	b	609	0	630	6	0
32	c	499	0	536	4	0
33	d	461	0	448	13	0
34	e	472	0	508	8	0
35	f	584	0	601	4	0
36	g	2469	0	2403	34	0
37	h	233	0	284	8	0
38	i	958	0	957	10	0
39	j	2006	0	2066	27	0
40	k	3034	0	3195	25	0
41	l	1036	0	1079	9	0
42	m	1140	0	1141	15	0
43	o	4070	0	3936	75	0
44	p	5114	0	4934	47	0
45	q	4827	0	4561	26	0
46	r	392	0	382	1	0
47	s	2606	0	2528	16	0
48	2	116	0	0	0	0
48	k	1	0	0	0	0
49	a	1	0	0	0	0
49	b	1	0	0	0	0
49	f	1	0	0	0	0
49	l	1	0	0	0	0
49	m	1	0	0	0	0
50	k	8	0	8	0	0
51	k	32	0	14	0	0
All	All	104316	0	85236	1386	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 7.

All (1386) 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)
3:3:16[A]:U:O2	43:o:38:ARG:HA	1.17	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:28:A:N1	2:2:597:U:C4	2.08	1.21
2:2:760:A:N1	2:2:789:U:C4	2.13	1.16
2:2:28:A:N1	2:2:597:U:O4	1.82	1.13
2:2:760:A:N1	2:2:789:U:O4	1.82	1.11
2:2:617:U:C4	2:2:1086:A:C2	2.40	1.10
3:3:17[A]:C:C5	43:o:42:TRP:NE1	2.19	1.09
2:2:617:U:O4	2:2:1086:A:N1	1.85	1.09
3:3:16[A]:U:N3	43:o:41:ARG:HB2	1.46	1.05
2:2:28:A:C2	2:2:597:U:C5	2.45	1.05
3:3:17[A]:C:C4	43:o:42:TRP:NE1	2.24	1.05
3:3:16[A]:U:H3	43:o:41:ARG:HB2	0.99	1.04
3:3:17[A]:C:N4	43:o:41:ARG:HB3	1.71	1.04
3:3:16[A]:U:H1'	43:o:38:ARG:CB	1.89	1.02
2:2:1086:A:H2'	2:2:1087:A:C8	1.94	1.02
3:3:16[A]:U:O2	43:o:38:ARG:CA	2.06	1.02
2:2:617:U:C4	2:2:1086:A:N1	2.29	1.00
2:2:760:A:C2	2:2:789:U:C5	2.53	0.97
2:2:1290:G:H22	2:2:1323:G:N2	1.62	0.97
3:3:16[A]:U:N3	43:o:41:ARG:CB	2.28	0.95
2:2:760:A:C2	2:2:789:U:C4	2.54	0.95
2:2:28:A:C2	2:2:597:U:C4	2.55	0.94
2:2:293:C:H2'	2:2:294:A:H5''	1.49	0.94
3:3:17[A]:C:N3	43:o:38:ARG:O	2.01	0.94
2:2:984:G:H1	2:2:1015:C:H5	1.06	0.93
3:3:15[A]:C:O2	43:o:77:LYS:O	1.86	0.92
3:3:16[A]:U:C2'	43:o:38:ARG:HB3	1.99	0.92
2:2:989:C:H5	2:2:1013:G:H1	1.12	0.91
6:C:144:ILE:HG22	6:C:223:ILE:HG23	1.51	0.91
2:2:1290:G:H22	2:2:1323:G:H22	1.10	0.91
2:2:1188:A:H8	2:2:1193:A:HO2'	1.13	0.90
13:J:148:VAL:HG11	13:J:156:ILE:HD11	1.54	0.89
2:2:617:U:O4	2:2:1086:A:C6	2.26	0.87
2:2:1290:G:N2	2:2:1323:G:H22	1.72	0.87
2:2:548:G:H1	2:2:588:C:H5	0.89	0.87
2:2:946:U:HO2'	2:2:947:G:H8	0.88	0.87
2:2:28:A:H2	2:2:597:U:C5	1.88	0.86
2:2:1427:G:H1'	24:U:74:GLU:HG2	1.57	0.86
2:2:121:U:H2'	2:2:122:U:C6	2.10	0.86
3:3:37:U:O4	7:D:148:LYS:HD3	1.76	0.85
2:2:548:G:N1	2:2:588:C:H5	1.75	0.84
2:2:868:A:H61	2:2:957:U:H5	1.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:151:VAL:HG21	32:c:66:LEU:HB2	1.59	0.84
2:2:509:G:H5''	13:J:176:ARG:HH22	1.41	0.83
2:2:867:G:H1	2:2:959:U:H3	1.26	0.83
2:2:888:U:H3	2:2:922:A:H2	1.25	0.83
2:2:1115:A:H5''	37:h:17:ARG:HH12	1.43	0.83
4:A:124:THR:HG22	4:A:174:TRP:HE1	1.42	0.83
2:2:617:U:O4	2:2:1086:A:C2	2.28	0.83
2:2:617:U:C5	2:2:1086:A:C2	2.66	0.82
3:3:17[A]:C:C4	43:o:42:TRP:CD1	2.67	0.82
43:o:69:LYS:HB2	43:o:164:ALA:HB1	1.61	0.82
3:3:16[A]:U:H1'	43:o:38:ARG:HB3	1.62	0.81
3:3:15[A]:C:N3	43:o:80:GLN:NE2	2.28	0.81
3:3:16[A]:U:C1'	43:o:38:ARG:HB3	2.11	0.81
2:2:1170:A:H2'	2:2:1171:G:C8	2.15	0.80
2:2:760:A:H2	2:2:789:U:C5	1.98	0.80
2:2:1188:A:H8	2:2:1193:A:O2'	1.64	0.80
2:2:1143:U:H2'	2:2:1144:U:C6	2.18	0.78
45:q:622:LEU:HB3	45:q:675:VAL:HG11	1.65	0.78
7:D:105:MET:HG2	7:D:122:VAL:HG21	1.66	0.78
2:2:1033:C:HO2'	26:W:2:THR:N	1.81	0.78
13:J:123:HIS:CE1	34:e:37:ARG:HB2	2.19	0.77
31:b:21:LEU:HA	31:b:26:GLN:HG2	1.65	0.77
2:2:1418:C:H5''	2:2:1418:C:H6	1.49	0.77
36:g:70:GLN:HG2	36:g:86:TRP:HE1	1.50	0.77
2:2:1396:U:H3'	2:2:1397:C:H5'	1.65	0.76
3:3:17[A]:C:H41	43:o:41:ARG:HB3	1.49	0.76
2:2:1174:U:H5	2:2:1462:G:O6	1.68	0.76
2:2:1768:U:H2'	2:2:1769:U:C6	2.19	0.76
2:2:1171:G:H21	23:T:88:VAL:CG2	1.98	0.76
3:3:16[A]:U:N3	43:o:78:LEU:CD2	2.50	0.75
33:d:2:ALA:HA	33:d:7:TRP:HB2	1.69	0.75
39:j:74:LEU:HD22	39:j:89:ARG:HH21	1.50	0.75
2:2:291:U:H2'	2:2:292:U:C6	2.22	0.74
3:3:16[A]:U:O2'	43:o:38:ARG:HB3	1.87	0.74
2:2:815:G:H21	11:H:110:GLN:HE22	1.33	0.74
27:X:57:ILE:HD11	27:X:73:ARG:HB2	1.68	0.74
3:3:17[A]:C:H42	43:o:41:ARG:HB3	1.50	0.74
2:2:979:G:H4'	2:2:1774:A:H4'	1.69	0.74
29:Z:42:LEU:HD11	29:Z:47:PHE:HB2	1.69	0.74
44:p:650:ASP:HA	47:s:342:HIS:HB3	1.69	0.74
36:g:112:LEU:HD11	36:g:128:ARG:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:968:C:H4'	2:2:1103:U:O2'	1.88	0.73
28:Y:57:VAL:HB	28:Y:60:PHE:HE1	1.53	0.73
13:J:108:ARG:HH21	13:J:110:GLN:HE21	1.36	0.73
13:J:84:GLY:HA3	13:J:107:ARG:HH11	1.53	0.73
2:2:1206:C:H42	2:2:1454:C:H5	1.35	0.73
2:2:1408:A:O2'	2:2:1409:A:C8	2.41	0.73
2:2:946:U:O2'	2:2:947:G:H8	1.69	0.73
2:2:1289:PSU:H2'	2:2:1290:G:C8	2.23	0.72
2:2:760:A:C6	2:2:789:U:O4	2.41	0.72
2:2:1086:A:C2	2:2:1087:A:C6	2.77	0.72
2:2:28:A:C6	2:2:597:U:O4	2.43	0.72
2:2:452:U:O2	2:2:452:U:H2'	1.89	0.72
2:2:1085:A:H2'	2:2:1086:A:C8	2.24	0.72
3:3:16[A]:U:O2'	43:o:38:ARG:CB	2.38	0.71
3:3:16[A]:U:O2'	43:o:38:ARG:CG	2.37	0.71
22:S:84:TRP:O	22:S:85:PHE:HB2	1.88	0.71
2:2:140:A:H61	10:G:187:LYS:HB2	1.56	0.71
2:2:1679:A:H8	10:G:66:GLY:HA3	1.55	0.71
6:C:170:VAL:HG11	6:C:215:THR:HA	1.72	0.71
3:3:16[A]:U:C1'	43:o:38:ARG:CB	2.68	0.71
2:2:1679:A:H2	2:2:1718:G:H21	1.39	0.71
6:C:86:MET:HE3	6:C:191:LYS:HB3	1.71	0.71
2:2:984:G:N1	2:2:1015:C:H5	1.86	0.71
2:2:967:U:H1'	2:2:1102:U:O2'	1.89	0.70
12:I:57:ALA:HB2	12:I:178:GLY:HA2	1.72	0.70
36:g:109:GLY:H	36:g:129:ASP:HB3	1.56	0.70
2:2:684:A:H2'	2:2:685:A:C8	2.27	0.70
17:N:54:LEU:HB3	17:N:60:VAL:HB	1.73	0.70
2:2:1632:C:H1'	3:3:34:U:O4	1.91	0.70
2:2:1408:A:HO2'	2:2:1409:A:H8	1.34	0.70
21:R:28:PHE:HA	21:R:55:THR:HG21	1.74	0.70
2:2:1788:A:H2'	2:2:1789:A:C8	2.27	0.70
29:Z:38:HIS:HB2	29:Z:72:GLY:HA2	1.73	0.70
2:2:617:U:O4	2:2:1085:A:C6	2.44	0.70
3:3:16[A]:U:H3	43:o:78:LEU:CD2	2.05	0.70
44:p:78:TYR:O	44:p:159:THR:HG22	1.91	0.69
2:2:1025:A:N7	2:2:1770:C:O2'	2.21	0.69
15:L:54:ILE:HG23	15:L:55:ASP:H	1.56	0.69
43:o:97:ILE:HG22	43:o:185:LYS:HB2	1.75	0.69
2:2:328:G:H5''	12:I:98:LYS:HB3	1.74	0.69
7:D:172:THR:HG22	7:D:185:LYS:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:16[A]:U:H3	43:o:78:LEU:HD22	1.57	0.69
3:3:17[A]:C:C4	43:o:38:ARG:O	2.46	0.69
3:3:15[A]:C:C2	43:o:80:GLN:NE2	2.58	0.68
46:r:83:LEU:HD22	47:s:286:ILE:HD12	1.75	0.68
2:2:1427:G:C1'	24:U:74:GLU:HG2	2.22	0.68
43:o:97:ILE:HG21	43:o:182:VAL:HA	1.76	0.68
2:2:617:U:O4	2:2:1085:A:N6	2.26	0.68
3:3:16[A]:U:N3	43:o:78:LEU:HD23	2.08	0.68
2:2:1531:C:H4'	2:2:1537:G:O6	1.94	0.68
2:2:1579:C:H4'	20:Q:135:ARG:O	1.92	0.68
22:S:100:SER:HB3	22:S:105:LEU:HA	1.75	0.68
13:J:38:ASN:HB3	13:J:40:ARG:H	1.59	0.68
2:2:1086:A:O2'	2:2:1141:A:O2'	2.10	0.68
11:H:81:LEU:HB3	11:H:90:VAL:HG21	1.76	0.68
2:2:935:G:N7	30:a:15:ARG:NH1	2.42	0.67
24:U:58:LEU:HD21	24:U:90:TYR:HD2	1.59	0.67
2:2:1279:C:O2	2:2:1426:2MG:CM2	2.43	0.67
4:A:162:CYS:HB2	4:A:173:ILE:HD13	1.77	0.67
2:2:928:A:O4'	18:O:124:ASP:HB2	1.95	0.67
2:2:828:A:H4'	2:2:829:U:O5'	1.95	0.67
27:X:68:ILE:HD13	34:e:9:ALA:HB2	1.76	0.67
19:P:85:ILE:HB	19:P:112:VAL:HA	1.76	0.66
43:o:86:LEU:HD22	43:o:174:LEU:HB2	1.77	0.66
2:2:887:U:H2'	2:2:888:U:C6	2.30	0.66
2:2:131:C:H4'	2:2:132:U:H4'	1.77	0.66
11:H:162:ILE:HG23	11:H:165:LYS:HB3	1.78	0.66
2:2:1279:C:O2	2:2:1426:2MG:HM22	1.96	0.66
3:3:34:U:H2'	3:3:35:C:O4'	1.95	0.66
11:H:26:ASP:HB3	11:H:84:LYS:NZ	2.11	0.66
36:g:86:TRP:HA	36:g:110:ASP:HB2	1.77	0.66
2:2:1034:G:OP1	17:N:2:GLY:HA2	1.96	0.66
24:U:82:TYR:HB3	33:d:52:PHE:HB3	1.76	0.65
36:g:260:THR:HG22	36:g:269:ILE:HG12	1.78	0.65
2:2:12:U:H2'	2:2:13:C:C6	2.31	0.65
2:2:1314:U:H2'	2:2:1315:G:O4'	1.97	0.65
2:2:989:C:H5	2:2:1013:G:N1	1.91	0.65
2:2:1408:A:O2'	2:2:1409:A:H8	1.78	0.65
6:C:144:ILE:HD13	6:C:196:ALA:HB1	1.78	0.65
2:2:1338:C:OP1	20:Q:10:PHE:HZ	1.78	0.65
2:2:1564:U:H5''	22:S:39:GLY:H	1.61	0.65
13:J:77:ILE:HD11	13:J:93:LEU:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1198:G:N3	2:2:1198:G:H3'	2.12	0.65
15:L:78:THR:HG22	15:L:84:ILE:HD11	1.79	0.65
2:2:447:C:OP2	8:E:49:ARG:NH2	2.29	0.65
17:N:5:HIS:HB3	17:N:117:LEU:HD13	1.79	0.65
2:2:742:U:H1'	11:H:107:ARG:HH22	1.61	0.65
39:j:24:VAL:HG11	39:j:63:ILE:HG23	1.78	0.65
44:p:529:LYS:HG3	44:p:530:GLU:H	1.61	0.65
2:2:1400:G:H5'	21:R:4:VAL:HA	1.78	0.64
8:E:95:THR:HG22	28:Y:16:PRO:HD2	1.78	0.64
22:S:123:ARG:HG2	22:S:133:VAL:HG12	1.79	0.64
25:V:60:ARG:HA	25:V:65:ALA:HB2	1.78	0.64
15:L:14:GLN:HB3	15:L:54:ILE:HG21	1.79	0.64
26:W:90:THR:HG23	26:W:94:LEU:HD12	1.77	0.64
4:A:182:LEU:HB3	4:A:188:LEU:HB2	1.80	0.64
43:o:97:ILE:HG13	43:o:182:VAL:HG22	1.79	0.64
2:2:10:G:C6	2:2:1631:A:C2	2.85	0.64
2:2:1243:A:H2'	2:2:1243:A:N3	2.13	0.64
2:2:116:U:H3	2:2:299:A:H2	1.45	0.64
4:A:148:ASP:HB2	4:A:164:ASN:HB2	1.79	0.64
44:p:349:ALA:HB1	44:p:356:LEU:HD11	1.80	0.64
2:2:122:U:O2	2:2:294:A:H2	1.80	0.64
2:2:760:A:C2	2:2:761:G:H1'	2.33	0.64
2:2:886:A:H5''	18:O:120:PRO:HB3	1.79	0.64
2:2:1315:G:OP1	21:R:7:LYS:HB2	1.98	0.64
2:2:414:C:O2'	2:2:417:G:O6	2.15	0.64
2:2:760:A:C2	2:2:789:U:O4	2.48	0.64
3:3:17[A]:C:C5	43:o:42:TRP:CE2	2.85	0.64
45:q:523:LEU:HD11	45:q:550:LEU:HD22	1.79	0.63
2:2:406:A:H2'	2:2:407:C:C6	2.33	0.63
7:D:59:VAL:HA	7:D:66:ILE:HG12	1.79	0.63
8:E:182:TYR:HD2	8:E:228:ILE:HD12	1.63	0.63
44:p:649:GLU:HG3	47:s:342:HIS:HA	1.79	0.63
44:p:145:HIS:CE1	44:p:305:LYS:HD3	2.34	0.63
2:2:124:A:H2'	2:2:125:U:O4'	1.99	0.63
40:k:315:LEU:HD11	40:k:398:VAL:HG21	1.80	0.63
43:o:90:GLY:HA2	43:o:178:THR:HG23	1.79	0.63
47:s:98:ARG:HB3	47:s:111:ILE:HD12	1.81	0.63
2:2:1588:G:OP1	23:T:91:HIS:HB2	1.98	0.63
2:2:616:U:H2'	2:2:617:U:O2	1.98	0.63
22:S:123:ARG:HG2	22:S:133:VAL:CG1	2.29	0.63
2:2:1679:A:C8	10:G:66:GLY:HA3	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:98:ALA:HA	7:D:188:ILE:HD12	1.79	0.63
2:2:207:U:H2'	2:2:208:U:C6	2.34	0.62
42:m:96:PHE:HA	42:m:130:MET:HE1	1.81	0.62
2:2:168:A:C5'	10:G:176:GLN:HG2	2.29	0.62
2:2:958:U:H2'	2:2:958:U:O2	2.00	0.62
2:2:1085:A:H2'	2:2:1086:A:H8	1.64	0.62
2:2:567:G:N7	27:X:69:ARG:NH2	2.48	0.62
2:2:1471:U:OP1	9:F:192:ILE:N	2.30	0.62
2:2:1518:U:H5''	23:T:75:LYS:HE2	1.80	0.62
2:2:28:A:H2'	2:2:29:U:O4'	2.00	0.62
2:2:1456:G:H2'	2:2:1456:G:N3	2.15	0.62
3:3:16[A]:U:O2'	43:o:38:ARG:NE	2.23	0.62
2:2:404:C:H5'	10:G:93:LYS:HE2	1.82	0.62
2:2:1279:C:H5'	33:d:44:ARG:NH2	2.14	0.62
5:B:158:SER:HA	5:B:161:ILE:HD12	1.82	0.62
14:K:77:ARG:HD3	14:K:84:GLU:HA	1.81	0.62
22:S:136:GLN:H	22:S:136:GLN:HE21	1.47	0.62
3:3:17[A]:C:N3	43:o:38:ARG:C	2.58	0.61
2:2:922:A:N1	2:2:923:A:N6	2.48	0.61
6:C:86:MET:HG2	6:C:216:LEU:HD11	1.80	0.61
6:C:50:VAL:HG21	6:C:73:ILE:HG23	1.83	0.61
22:S:42:TYR:HA	22:S:85:PHE:HE1	1.65	0.61
2:2:1290:G:H1	2:2:1323:G:H1	1.47	0.61
8:E:18:TRP:HD1	8:E:20:LEU:HD11	1.66	0.61
13:J:39:LYS:HA	13:J:42:ILE:HD12	1.82	0.61
2:2:294:A:C2	2:2:295:U:C2	2.88	0.61
2:2:498:U:H2'	2:2:498:U:O2	2.00	0.61
28:Y:29:HIS:HE1	28:Y:69:SER:HB2	1.65	0.61
2:2:888:U:N3	2:2:922:A:H2	1.98	0.61
17:N:46:THR:HB	17:N:86:GLU:HG3	1.81	0.61
22:S:25:ASN:HB2	29:Z:40:VAL:HG21	1.82	0.60
2:2:122:U:N3	2:2:294:A:C2	2.65	0.60
2:2:1593:U:H3	2:2:1598:A:H2	1.47	0.60
8:E:128:LYS:HB3	8:E:140:VAL:HB	1.82	0.60
2:2:454:C:H3'	2:2:455:A:C8	2.36	0.60
13:J:59:LEU:HD13	13:J:73:GLY:HA2	1.83	0.60
23:T:113:VAL:HA	23:T:128:GLY:HA3	1.83	0.60
27:X:72:VAL:HG21	27:X:96:VAL:HG11	1.83	0.60
2:2:208:U:N3	2:2:255:A:C2	2.67	0.60
2:2:1554:A:H3'	19:P:40:ARG:HD3	1.84	0.60
42:m:134:HIS:HD2	42:m:136:LEU:H	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:98:SER:HB3	9:F:178:THR:HG21	1.84	0.60
2:2:384:A:H5''	12:I:22:ARG:HB3	1.83	0.60
2:2:894:G:H1	2:2:916:U:H3	1.49	0.60
8:E:11:ARG:NH1	8:E:20:LEU:HB3	2.16	0.60
22:S:87:ASN:H	22:S:99:HIS:CD2	2.20	0.60
5:B:87:ARG:HB2	5:B:101:HIS:HB2	1.83	0.60
1:1:33:U:OP2	20:Q:143:ARG:NH2	2.35	0.60
2:2:294:A:H2'	2:2:295:U:O4'	2.02	0.60
2:2:1171:G:H21	23:T:88:VAL:HG22	1.66	0.60
2:2:1670:G:H2'	2:2:1671:G:C8	2.37	0.60
8:E:45:ILE:HA	8:E:61:VAL:HG11	1.84	0.60
16:M:34:LEU:HD13	16:M:36:ARG:HE	1.65	0.59
33:d:38:ILE:HD11	33:d:43:PHE:HD1	1.68	0.59
2:2:1577:U:H2'	2:2:1578:C:C6	2.37	0.59
3:3:17[A]:C:N4	43:o:38:ARG:O	2.35	0.59
4:A:183:ARG:HG2	4:A:191:ARG:HB3	1.84	0.59
44:p:639:ILE:HD12	44:p:648:LYS:HB3	1.84	0.59
2:2:1292:U:C5	2:2:1321:A:N1	2.70	0.59
2:2:1788:A:C2	2:2:1789:A:C6	2.90	0.59
2:2:293:C:C2'	2:2:294:A:H5''	2.28	0.59
2:2:1053:U:H2'	2:2:1054:U:O4'	2.03	0.59
2:2:1792:A:OP2	30:a:4:LYS:NZ	2.33	0.59
8:E:31:PRO:HG3	8:E:43:PRO:HG3	1.84	0.59
2:2:10:G:H8	2:2:1631:A:HO2'	1.50	0.58
4:A:18:LEU:HD23	21:R:102:VAL:HG11	1.83	0.58
10:G:49:VAL:HG12	10:G:115:LYS:HB2	1.86	0.58
24:U:58:LEU:HD23	24:U:88:LYS:HB3	1.84	0.58
23:T:65:ILE:HG22	23:T:124:ILE:HG23	1.85	0.58
25:V:17:CYS:HB2	25:V:56:SER:HB3	1.86	0.58
2:2:209:A:H61	2:2:254:U:H3	1.50	0.58
44:p:391:GLN:HB3	44:p:392:PRO:CD	2.33	0.58
2:2:398:A:H4'	8:E:3:ARG:HB2	1.85	0.58
3:3:16[A]:U:O2'	43:o:38:ARG:HG3	2.03	0.58
36:g:307:THR:HG22	36:g:321:GLN:HG2	1.85	0.58
39:j:205:LEU:HG	40:k:330:ILE:HB	1.85	0.58
2:2:331:U:OP2	12:I:176:GLN:NE2	2.36	0.58
2:2:789:U:C5	2:2:790:A:C4	2.92	0.58
10:G:58:LYS:HA	10:G:107:ALA:HB2	1.86	0.58
2:2:336:G:H3'	15:L:133:LYS:HB2	1.86	0.58
2:2:925:A:H2'	2:2:926:C:C6	2.38	0.58
3:3:17[A]:C:N4	43:o:42:TRP:CD1	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:168:A:H5''	10:G:176:GLN:HG2	1.85	0.58
2:2:357:U:H2'	2:2:359:A:H5''	1.86	0.58
2:2:762:A:P	13:J:79:ARG:HH22	2.26	0.58
4:A:124:THR:HG22	4:A:174:TRP:NE1	2.17	0.58
8:E:141:THR:OG1	8:E:145:ARG:HB3	2.04	0.58
1:1:8:U:H3	1:1:13:C:H41	1.52	0.58
2:2:597:U:O4	2:2:598:A:C6	2.57	0.58
2:2:746:A:N1	2:2:804:U:H5	2.02	0.58
2:2:1532:G:O2'	29:Z:73:GLY:HA3	2.04	0.58
15:L:54:ILE:HG23	15:L:55:ASP:N	2.19	0.58
15:L:66:ILE:HG13	15:L:140:LEU:HD21	1.85	0.58
26:W:40:VAL:HG11	26:W:103:ILE:HD12	1.86	0.58
2:2:1170:A:H2'	2:2:1171:G:H8	1.67	0.57
3:3:18[A]:U:H6	3:3:18[A]:U:O5'	1.86	0.57
4:A:184:LEU:HD23	25:V:45:ALA:HB2	1.86	0.57
8:E:126:VAL:HG13	8:E:139:VAL:HG23	1.86	0.57
26:W:20:THR:HG21	26:W:22:LYS:HE2	1.86	0.57
4:A:48:ILE:HG21	4:A:161:PRO:HB2	1.87	0.57
20:Q:47:LYS:O	20:Q:50:GLU:HB2	2.04	0.57
2:2:886:A:N6	2:2:923:A:N6	2.52	0.57
15:L:19:ILE:HG12	15:L:34:TRP:HB2	1.85	0.57
2:2:155:A:H2'	2:2:156:A:O4'	2.04	0.57
40:k:313:PRO:HA	40:k:345:GLY:HA3	1.86	0.57
2:2:1227:G:H22	16:M:60:THR:HB	1.70	0.57
4:A:84:ARG:NH1	4:A:205:ARG:HG3	2.18	0.57
13:J:109:LEU:HB2	13:J:146:PHE:HB3	1.87	0.57
15:L:54:ILE:CG2	15:L:55:ASP:H	2.18	0.57
10:G:32:ILE:HD11	10:G:63:MET:HB3	1.86	0.57
43:o:104:ILE:HG23	43:o:193:TYR:HE1	1.69	0.57
2:2:1711:G:H3'	2:2:1712:A:C8	2.40	0.57
36:g:47:ARG:HB2	36:g:59:VAL:HG22	1.85	0.57
2:2:1454:C:OP1	2:2:1456:G:H8	1.88	0.57
2:2:1631:A:H8	2:2:1631:A:H5'	1.69	0.57
22:S:46:VAL:HG21	22:S:73:MET:HB3	1.86	0.57
2:2:1338:C:O2'	2:2:1340:A:N7	2.38	0.56
4:A:103:THR:O	4:A:106:SER:HB2	2.06	0.56
2:2:709:C:H2'	2:2:710:U:H4'	1.86	0.56
4:A:20:ALA:HB1	4:A:169:SER:HA	1.86	0.56
20:Q:78:VAL:HA	20:Q:81:ILE:HD12	1.88	0.56
28:Y:43:LYS:O	28:Y:46:GLU:HG2	2.05	0.56
33:d:36:LEU:HB3	33:d:38:ILE:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:112:THR:HG22	4:A:114:SER:H	1.70	0.56
11:H:64:VAL:HG22	11:H:94:ALA:HB1	1.86	0.56
27:X:19:ARG:O	27:X:23:ARG:HG2	2.06	0.56
28:Y:57:VAL:HB	28:Y:60:PHE:CE1	2.39	0.56
36:g:154:LYS:HD2	36:g:208:VAL:HG23	1.85	0.56
2:2:1540:G:N2	2:2:1566:C:H2'	2.20	0.56
4:A:7:PHE:HE2	25:V:43:GLY:HA2	1.71	0.56
14:K:3:ILE:HG12	14:K:41:PHE:HB2	1.87	0.56
38:i:21:GLY:N	38:i:22:PRO:HD3	2.21	0.56
39:j:33:TYR:HA	39:j:45:MET:HA	1.88	0.56
2:2:1471:U:H2'	2:2:1471:U:O2	2.05	0.56
2:2:1792:A:O2'	30:a:75:ILE:HD11	2.05	0.56
13:J:70:LEU:O	13:J:74:ASN:HB2	2.06	0.56
21:R:34:LEU:O	21:R:38:ILE:HG13	2.05	0.56
2:2:1640:G:H5'	37:h:1:MET:HB2	1.86	0.56
2:2:1791:G:O2'	30:a:5:ARG:NH2	2.39	0.56
7:D:71:LEU:HD22	7:D:75:LYS:HZ1	1.71	0.56
44:p:224:LEU:HD11	44:p:227:SER:HB2	1.86	0.56
2:2:452:U:O2	2:2:452:U:C2'	2.54	0.56
2:2:632:U:H3	2:2:965:A:H61	1.53	0.56
2:2:707:A:H61	2:2:730:G:H1	1.54	0.56
2:2:922:A:N1	2:2:923:A:C6	2.74	0.56
38:i:3:LYS:HG2	38:i:4:LYS:N	2.20	0.56
45:q:419:LEU:HD23	45:q:424:ASP:HB3	1.88	0.56
2:2:28:A:C2	2:2:597:U:O4	2.52	0.56
2:2:1630:C:N4	2:2:1631:A:H62	2.04	0.56
27:X:60:GLU:HG3	38:i:60:HIS:CD2	2.40	0.56
36:g:183:VAL:HB	36:g:199:PHE:HB2	1.86	0.56
43:o:56:LEU:HG	43:o:96:PHE:HB2	1.88	0.56
43:o:839:ALA:HB1	44:p:198:VAL:HG11	1.88	0.56
2:2:481:U:H3	2:2:504:A:H61	1.53	0.55
3:3:24:U:H5	32:c:67:ARG:HB2	1.70	0.55
2:2:1670:G:H2'	2:2:1671:G:H8	1.71	0.55
11:H:91:ILE:HG21	11:H:129:LEU:HD12	1.87	0.55
16:M:39:ARG:HE	16:M:43:LYS:HE3	1.72	0.55
18:O:17:ALA:HB3	18:O:81:ILE:HA	1.88	0.55
1:1:75:C:H5''	1:1:76:A:H5''	1.87	0.55
43:o:386:GLU:O	43:o:390:ILE:HG12	2.06	0.55
2:2:1639:C:H4'	37:h:1:MET:N	2.22	0.55
7:D:137:VAL:HG22	7:D:151:LYS:HG3	1.88	0.55
2:2:1733:U:H2'	2:2:1734:G:O4'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:45:ILE:HB	8:E:80:THR:HG22	1.88	0.55
40:k:353:ILE:HG12	40:k:417:VAL:HG12	1.89	0.55
2:2:511:A:H5''	13:J:163:PRO:HG3	1.87	0.55
2:2:922:A:C2	2:2:923:A:C6	2.95	0.55
2:2:1500:G:N7	23:T:102:ARG:NH2	2.55	0.55
2:2:1771:C:H2'	2:2:1772:G:C8	2.41	0.55
11:H:61:PHE:HA	11:H:93:LEU:O	2.07	0.55
45:q:614:LEU:HA	45:q:617:ILE:HD12	1.88	0.55
36:g:151:TRP:HB2	36:g:179:MET:HG2	1.89	0.55
43:o:240:ARG:O	43:o:244:VAL:HG23	2.07	0.55
2:2:1292:U:H5	2:2:1321:A:N1	2.05	0.55
26:W:24:GLN:HE22	31:b:4:VAL:HA	1.71	0.55
2:2:1292:U:H5	2:2:1321:A:C2	2.25	0.55
43:o:170:ARG:HD2	43:o:209:HIS:HD2	1.72	0.55
47:s:13:LEU:HD13	47:s:29:SER:HB2	1.89	0.55
2:2:1427:G:H1'	24:U:74:GLU:CG	2.35	0.55
2:2:1584:A:H2'	2:2:1585:A:O4'	2.07	0.55
13:J:120:LYS:HG3	44:p:434:VAL:HB	1.89	0.55
2:2:10:G:H8	2:2:1631:A:O2'	1.90	0.54
1:1:43:G:H4'	1:1:44:A:OP1	2.07	0.54
2:2:786:G:H4'	8:E:255:ARG:HH12	1.72	0.54
47:s:30:LYS:HA	47:s:54:THR:HG23	1.88	0.54
2:2:454:C:H3'	2:2:455:A:H8	1.72	0.54
9:F:64:ILE:HA	9:F:91:ILE:HD13	1.89	0.54
19:P:75:VAL:HG21	19:P:104:GLN:HE22	1.72	0.54
2:2:175:C:H2'	2:2:176:U:O4'	2.06	0.54
2:2:1717:A:H2'	2:2:1718:G:O4'	2.06	0.54
9:F:123:ILE:O	9:F:126:LEU:O	2.25	0.54
2:2:299:A:H2'	2:2:300:A:C8	2.42	0.54
2:2:637:U:H2'	2:2:637:U:O2	2.07	0.54
8:E:19:MET:SD	8:E:108:ARG:HG3	2.47	0.54
2:2:1086:A:HO2'	2:2:1141:A:HO2'	1.48	0.54
5:B:143:THR:HG21	5:B:156:ALA:HB2	1.89	0.54
9:F:94:ARG:HH21	9:F:170:VAL:HG12	1.73	0.54
16:M:55:LEU:HD21	16:M:79:LEU:HD23	1.90	0.54
43:o:97:ILE:CG2	43:o:185:LYS:HB2	2.38	0.54
2:2:648:U:O2	2:2:685:A:N1	2.41	0.54
3:3:16[A]:U:C2	43:o:78:LEU:CD2	2.91	0.54
2:2:1330:A:N6	7:D:161:GLY:HA3	2.23	0.54
8:E:156:VAL:O	8:E:157:ASN:HB2	2.08	0.54
2:2:397:G:P	12:I:47:ARG:HH22	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:323:MET:HB3	44:p:365:PHE:HE2	1.73	0.54
2:2:1320:A:H4'	2:2:1321:A:OP1	2.07	0.54
36:g:14:LEU:HB2	36:g:317:ILE:HB	1.90	0.54
45:q:645:ILE:HG13	45:q:646:PRO:HD3	1.90	0.54
2:2:1387:C:O2'	21:R:52:GLY:HA3	2.08	0.53
2:2:1557:A:O5'	22:S:135:GLY:HA3	2.09	0.53
8:E:18:TRP:HB3	8:E:20:LEU:HG	1.89	0.53
21:R:93:LEU:HD11	21:R:100:LEU:HD23	1.90	0.53
2:2:1613:C:H3'	9:F:83:ARG:HD3	1.89	0.53
9:F:155:GLY:HA2	39:j:55:ARG:HD2	1.90	0.53
45:q:582:GLN:HE22	45:q:612:ILE:H	1.55	0.53
2:2:885:U:H2'	2:2:886:A:O4'	2.09	0.53
5:B:121:ILE:HG12	5:B:161:ILE:HG23	1.89	0.53
13:J:27:GLU:HB3	13:J:39:LYS:HD2	1.90	0.53
7:D:162:GLN:N	7:D:163:PRO:HD2	2.24	0.53
2:2:867:G:H22	2:2:959:U:H3	1.55	0.53
2:2:1268:U:H4'	2:2:1269:G:O5'	2.08	0.53
2:2:1544:G:N2	22:S:87:ASN:O	2.41	0.53
2:2:1793:U:H1'	30:a:36:ILE:HD11	1.89	0.53
11:H:26:ASP:HB3	11:H:84:LYS:HZ3	1.74	0.53
2:2:868:A:H2'	2:2:869:C:O4'	2.08	0.53
7:D:40:ARG:HB3	24:U:110:PRO:HB3	1.90	0.53
44:p:285:VAL:HG22	44:p:314:ILE:HG12	1.90	0.53
2:2:875:G:O2'	2:2:943:A:H5'	2.09	0.53
3:3:16[A]:U:C2	43:o:38:ARG:HA	2.24	0.53
12:I:69:SER:HB3	15:L:24:LYS:HD3	1.89	0.53
26:W:14:ILE:HD11	26:W:27:ILE:HD11	1.91	0.53
26:W:76:SER:OG	26:W:77:PRO:HD3	2.09	0.53
2:2:1014:U:H3'	2:2:1015:C:O2	2.09	0.53
2:2:1351:U:H2'	2:2:1352:U:O4'	2.09	0.53
10:G:7:TYR:HD1	10:G:113:ILE:HG23	1.73	0.53
15:L:101:GLU:HG2	27:X:13:ARG:HB2	1.90	0.53
2:2:1177:G:H5'	2:2:1189:C:H42	1.73	0.53
2:2:1675:C:H2'	2:2:1676:A:O4'	2.09	0.53
8:E:11:ARG:HA	8:E:28:ALA:HB2	1.91	0.53
23:T:113:VAL:HA	23:T:128:GLY:CA	2.39	0.53
38:i:74:GLY:HA3	38:i:119:ASP:H	1.73	0.53
39:j:8:PHE:HE1	39:j:109:HIS:HB2	1.74	0.53
2:2:70:C:H2'	2:2:71:A:O4'	2.09	0.53
2:2:472:A:H4'	2:2:768:C:O2	2.09	0.53
2:2:1331:C:H4'	7:D:203:PRO:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:144:ALA:HB1	39:j:154:VAL:HG11	1.90	0.53
2:2:1141:A:H5''	30:a:2:PRO:HB3	1.92	0.52
6:C:87:ASN:HB3	6:C:212:LEU:HD22	1.91	0.52
28:Y:15:ASN:HD21	28:Y:18:LEU:HD12	1.74	0.52
40:k:349:LEU:HD12	40:k:388:LYS:HG2	1.91	0.52
44:p:368:LEU:HD13	44:p:373:LEU:HD13	1.91	0.52
2:2:597:U:C5	2:2:598:A:C4	2.96	0.52
2:2:1571:A:H4'	2:2:1572:G:O5'	2.09	0.52
44:p:553:SER:HB3	44:p:562:VAL:HB	1.90	0.52
44:p:706:GLN:HB3	47:s:333:VAL:HG21	1.90	0.52
2:2:157:U:O2'	2:2:158:U:H5'	2.09	0.52
2:2:391:G:O2'	2:2:1671:G:H1'	2.09	0.52
2:2:478:C:H2'	2:2:479:G:O4'	2.09	0.52
2:2:1769:U:O4	2:2:1788:A:N1	2.43	0.52
13:J:119:ALA:O	13:J:120:LYS:HB2	2.09	0.52
16:M:35:ALA:HB1	16:M:40:GLU:HB3	1.91	0.52
36:g:267:ILE:HB	36:g:281:LEU:HB2	1.90	0.52
2:2:1188:A:C8	2:2:1193:A:O2'	2.49	0.52
2:2:1396:U:C3'	2:2:1397:C:H5'	2.37	0.52
4:A:64:ILE:HG23	4:A:73:VAL:HG21	1.92	0.52
2:2:319:U:H5''	2:2:320:C:H3'	1.90	0.52
9:F:219:LEU:HG	39:j:30:MET:HE1	1.91	0.52
2:2:1250:U:O2'	35:f:131:ALA:HB1	2.09	0.52
6:C:121:LYS:HB2	6:C:136:ILE:HD12	1.92	0.52
17:N:36:GLN:O	17:N:39:LYS:HG2	2.09	0.52
2:2:479:G:H3'	2:2:480:A:H8	1.75	0.52
39:j:31:GLY:HA3	39:j:47:LEU:HA	1.89	0.52
2:2:597:U:C5	2:2:598:A:C5	2.97	0.52
2:2:859:U:H1'	11:H:114:ARG:HD2	1.90	0.52
2:2:1043:U:H5	2:2:1073:G:O6	1.93	0.52
8:E:45:ILE:HG13	8:E:61:VAL:HG21	1.91	0.52
2:2:28:A:C2	2:2:597:U:H5	2.20	0.52
2:2:1456:G:N3	2:2:1456:G:C2'	2.72	0.52
6:C:46:LEU:HB2	6:C:245:MET:HE3	1.90	0.52
16:M:35:ALA:HB2	16:M:115:LYS:HE2	1.92	0.52
22:S:84:TRP:O	22:S:85:PHE:CB	2.58	0.52
29:Z:68:ARG:HB2	29:Z:70:LYS:HD3	1.91	0.52
1:1:3:C:H2'	1:1:4:G:H8	1.75	0.52
6:C:153:LEU:HA	25:V:4:ASP:HB2	1.92	0.52
12:I:60:ILE:HG12	12:I:180:CYS:HB2	1.92	0.52
2:2:1388:U:H5''	21:R:3:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:120:TYR:O	7:D:123:VAL:HG12	2.09	0.51
11:H:17:GLU:HG2	11:H:46:ILE:HD12	1.92	0.51
12:I:96:LEU:HD11	12:I:180:CYS:SG	2.50	0.51
44:p:500:ARG:HG2	44:p:526:PRO:HD2	1.92	0.51
2:2:350:C:H5	2:2:630:G:H5''	1.76	0.51
2:2:700:C:H42	2:2:738:G:H1	1.58	0.51
8:E:9:LEU:HB2	8:E:30:ARG:HB2	1.91	0.51
11:H:112:ARG:CZ	11:H:117:THR:HG22	2.40	0.51
20:Q:35:PRO:HD2	20:Q:38:LEU:HD22	1.92	0.51
2:2:649:U:H2'	2:2:650:G:C8	2.45	0.51
2:2:864:A:N1	2:2:964:U:H5	2.08	0.51
42:m:24:LYS:HG3	42:m:37:LEU:HD11	1.92	0.51
2:2:1480:C:H5	2:2:1523:A:H62	1.58	0.51
9:F:158:ARG:HH21	9:F:158:ARG:HB2	1.76	0.51
41:l:157:LYS:HB2	41:l:242:ILE:HD13	1.92	0.51
2:2:1316:C:H2'	2:2:1317:G:O4'	2.10	0.51
5:B:188:LEU:HD21	5:B:215:VAL:HG21	1.93	0.51
9:F:60:LEU:HD11	9:F:169:ARG:HD2	1.93	0.51
24:U:80:ASP:HB2	33:d:54:LYS:HD3	1.92	0.51
43:o:202:LEU:HD23	43:o:243:GLN:HE22	1.75	0.51
44:p:592:ASN:HD22	44:p:595:VAL:HG13	1.76	0.51
2:2:8:U:H3	2:2:1138:A:H62	1.58	0.51
2:2:1292:U:O4'	2:2:1292:U:O2	2.28	0.51
2:2:498:U:O2	2:2:498:U:C2'	2.59	0.51
2:2:1245:C:O2	2:2:1245:C:O4'	2.25	0.51
7:D:72:LEU:HD22	14:K:65:TYR:HD1	1.74	0.51
45:q:533:ASN:HA	45:q:540:GLN:HE21	1.76	0.51
2:2:71:A:H3'	2:2:72:A:H5''	1.93	0.51
2:2:544:A:H2'	34:e:31:LYS:HE2	1.93	0.51
2:2:1421:U:H2'	2:2:1422:A:O4'	2.11	0.51
39:j:46:ILE:HG21	39:j:87:LYS:HB2	1.92	0.51
2:2:168:A:H5'	10:G:176:GLN:HG2	1.91	0.51
2:2:1382:A:H2'	2:2:1383:G:O4'	2.10	0.51
2:2:1530:U:H3'	29:Z:77:ARG:HH22	1.76	0.51
40:k:357:PRO:HB2	40:k:415:GLN:HE21	1.75	0.51
44:p:79:ILE:HG12	44:p:129:VAL:HB	1.92	0.51
2:2:1086:A:C2	2:2:1087:A:N1	2.79	0.51
2:2:1531:C:H4'	2:2:1537:G:C6	2.45	0.51
6:C:170:VAL:HA	6:C:206:THR:O	2.11	0.51
8:E:193:GLY:HA3	8:E:210:ILE:HG22	1.92	0.51
25:V:73:ALA:HB1	25:V:78:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:57:ARG:O	26:W:59:GLY:N	2.44	0.51
36:g:227:ILE:HB	36:g:241:PHE:HB2	1.91	0.51
36:g:247:VAL:HG22	36:g:263:THR:HG22	1.92	0.51
43:o:97:ILE:HA	43:o:100:VAL:HG22	1.93	0.51
47:s:179:LYS:HB2	47:s:228:LEU:HD11	1.93	0.51
2:2:174:G:H22	2:2:265:A:P	2.34	0.50
2:2:648:U:C2	2:2:685:A:N1	2.79	0.50
2:2:1219:C:H42	2:2:1262:G:H1	1.59	0.50
8:E:187:ARG:NH1	8:E:187:ARG:HB3	2.27	0.50
8:E:187:ARG:HB3	8:E:187:ARG:HH11	1.76	0.50
21:R:26:MET:HE2	21:R:62:GLN:HB2	1.91	0.50
22:S:132:ARG:HB3	22:S:136:GLN:NE2	2.27	0.50
43:o:303:TRP:HA	43:o:303:TRP:CE3	2.45	0.50
2:2:1781:C:H5	37:h:5:TRP:HB3	1.77	0.50
11:H:67:LEU:HD13	11:H:94:ALA:HB2	1.94	0.50
12:I:42:ARG:HD2	12:I:58:LEU:HD12	1.92	0.50
2:2:392:C:H2'	2:2:393:C:C6	2.46	0.50
4:A:34:GLU:HG3	4:A:36:TYR:HD2	1.76	0.50
9:F:164:VAL:HG13	9:F:168:ARG:HD3	1.92	0.50
33:d:21:CYS:O	33:d:38:ILE:HA	2.11	0.50
40:k:216:LEU:HD23	40:k:246:ILE:HG12	1.92	0.50
44:p:452:PHE:HB2	44:p:469:GLN:HB2	1.93	0.50
2:2:617:U:C5	2:2:1086:A:H2	2.27	0.50
12:I:109:PHE:CZ	12:I:184:ILE:HD11	2.47	0.50
14:K:22:VAL:HG23	14:K:23:ALA:H	1.76	0.50
41:l:230:ILE:HA	41:l:234:VAL:HB	1.94	0.50
2:2:684:A:C2	2:2:685:A:C6	2.99	0.50
3:3:16[A]:U:C2'	43:o:38:ARG:CB	2.81	0.50
11:H:35:LYS:HG2	11:H:39:ARG:HD2	1.94	0.50
15:L:34:TRP:CH2	15:L:36:LYS:HD2	2.46	0.50
15:L:66:ILE:HG21	15:L:140:LEU:HD11	1.92	0.50
2:2:804:U:H5''	26:W:33:VAL:HG22	1.93	0.50
3:3:16[A]:U:H1'	43:o:38:ARG:CA	2.41	0.50
27:X:50:LYS:HG3	27:X:103:LEU:HD23	1.93	0.50
40:k:320:SER:HB3	40:k:412:LEU:HB2	1.94	0.50
2:2:357:U:C2'	2:2:359:A:H5''	2.42	0.50
2:2:1279:C:O2	2:2:1426:2MG:HM23	2.12	0.50
2:2:1558:U:O2	2:2:1558:U:O4'	2.29	0.50
9:F:122:ILE:HD13	9:F:194:GLU:HA	1.93	0.50
15:L:33:ARG:HH21	15:L:51:GLY:C	2.20	0.50
44:p:323:MET:HB3	44:p:365:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:746:A:N1	2:2:804:U:C5	2.79	0.50
2:2:883:A:H5''	5:B:136:ARG:NE	2.27	0.50
14:K:37:THR:HB	14:K:41:PHE:HE1	1.76	0.50
2:2:592:U:OP1	13:J:40:ARG:HB2	2.10	0.50
9:F:202:ASN:CB	9:F:210:SER:HB2	2.42	0.50
36:g:179:MET:HA	36:g:205:TYR:HB2	1.94	0.50
2:2:635:A:H5''	26:W:31:SER:HB3	1.94	0.49
2:2:868:A:N6	2:2:957:U:H5	2.04	0.49
2:2:1087:A:C5	2:2:1088:U:H1'	2.47	0.49
7:D:109:LEU:HD12	7:D:175:VAL:HG21	1.94	0.49
23:T:19:ALA:HB2	23:T:56:LYS:HA	1.94	0.49
39:j:100:GLU:HA	39:j:103:GLN:HE21	1.77	0.49
43:o:90:GLY:HA2	43:o:178:THR:CG2	2.41	0.49
47:s:25:LEU:HB3	47:s:37:TRP:HB2	1.92	0.49
2:2:537:A:H5'	2:2:542:C:H41	1.76	0.49
2:2:789:U:H5	2:2:790:A:C4	2.30	0.49
5:B:111:ARG:HB3	30:a:68:TYR:HB2	1.94	0.49
6:C:58:ILE:HG12	6:C:78:LEU:HG	1.94	0.49
20:Q:39:VAL:HG21	20:Q:48:VAL:HG21	1.94	0.49
39:j:220:VAL:HG13	39:j:230:LEU:HB3	1.94	0.49
4:A:23:HIS:HB3	4:A:50:VAL:CG1	2.42	0.49
8:E:228:ILE:HD11	8:E:236:ILE:HD11	1.94	0.49
1:1:13:C:H42	1:1:22:G:H1	1.60	0.49
2:2:1038:A:O2'	2:2:1039:G:O5'	2.26	0.49
4:A:120:LEU:HD11	4:A:144:ILE:HD12	1.95	0.49
5:B:140:ILE:HD11	5:B:213:ARG:HB3	1.94	0.49
8:E:71:LYS:HB3	8:E:91:THR:HB	1.95	0.49
10:G:2:LYS:HG3	10:G:17:GLU:HG3	1.94	0.49
27:X:53:VAL:HG13	27:X:72:VAL:HG22	1.93	0.49
27:X:59:ILE:CG2	27:X:118:PRO:HD2	2.43	0.49
2:2:897:A:H2'	2:2:911:U:O4	2.13	0.49
12:I:166:LEU:HD13	12:I:184:ILE:HG12	1.95	0.49
36:g:134:VAL:HB	36:g:143:TYR:HB2	1.94	0.49
2:2:122:U:C2	2:2:294:A:H2	2.30	0.49
47:s:220:SER:HB3	47:s:234:TYR:HB2	1.95	0.49
1:1:43:G:H2'	1:1:44:A:C8	2.48	0.49
2:2:864:A:N1	2:2:964:U:C5	2.81	0.49
2:2:988:U:O2'	18:O:126:THR:HG23	2.12	0.49
2:2:1171:G:N2	23:T:88:VAL:HG22	2.28	0.49
2:2:1290:G:N2	2:2:1323:G:N2	2.38	0.49
2:2:1477:A:H4'	23:T:15:ILE:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:84:HIS:HD2	12:I:100:ALA:HB2	1.76	0.49
30:a:35:ALA:O	30:a:36:ILE:C	2.55	0.49
45:q:265:ARG:HH11	45:q:302:SER:HB2	1.77	0.49
2:2:223:C:H2'	2:2:224:A:H8	1.76	0.49
5:B:107:THR:HG22	5:B:111:ARG:HE	1.78	0.49
6:C:173:ARG:HB3	6:C:204:SER:HB3	1.95	0.49
11:H:14:THR:HB	11:H:17:GLU:HB2	1.94	0.49
22:S:52:VAL:HG11	22:S:69:ILE:HD11	1.93	0.49
24:U:96:PRO:HD2	24:U:99:ILE:HD11	1.94	0.49
44:p:417:ALA:HB3	44:p:431:VAL:HB	1.94	0.49
2:2:688:G:H2'	2:2:689:G:H8	1.76	0.49
2:2:811:A:N6	2:2:857:G:H2'	2.28	0.49
2:2:922:A:C6	2:2:923:A:N6	2.81	0.49
9:F:74:HIS:HB2	9:F:113:VAL:HG21	1.94	0.49
40:k:499:ILE:HD11	40:k:517:ILE:HG13	1.94	0.49
45:q:508:TYR:HB2	45:q:546:VAL:HG12	1.95	0.49
47:s:56:TRP:HE1	47:s:72:ALA:HB2	1.78	0.49
2:2:1100:G:H5''	26:W:76:SER:HB3	1.95	0.49
20:Q:123:ARG:HG3	20:Q:124:PRO:HD2	1.94	0.49
23:T:14:PHE:HA	23:T:139:THR:HG21	1.94	0.49
2:2:1780:MA6:H5'	37:h:1:MET:HE3	1.95	0.48
2:2:1788:A:H61	30:a:28:ARG:HH21	1.59	0.48
2:2:544:A:H4'	2:2:545:C:O5'	2.12	0.48
2:2:1262:G:H2'	2:2:1263:G:O4'	2.14	0.48
15:L:84:ILE:HB	15:L:111:VAL:HG22	1.96	0.48
29:Z:62:VAL:O	29:Z:66:VAL:HG23	2.13	0.48
39:j:149:ILE:HG21	39:j:173:ILE:HG21	1.96	0.48
2:2:364:G:N2	2:2:376:G:H1'	2.28	0.48
2:2:1574:A:H5'	39:j:60:GLN:HE22	1.79	0.48
13:J:52:ILE:HG23	13:J:76:LEU:HD11	1.95	0.48
39:j:225:ALA:HB1	40:k:404:PRO:HB2	1.95	0.48
44:p:141:ILE:HG12	44:p:157:LEU:HB3	1.96	0.48
2:2:10:G:C5	2:2:1631:A:C2	3.02	0.48
2:2:142:G:H2'	2:2:143:G:C8	2.48	0.48
2:2:395:G:O6	12:I:26:LYS:HE3	2.13	0.48
2:2:1757:C:H2'	2:2:1758:G:O4'	2.14	0.48
6:C:179:ARG:O	13:J:97:LEU:HB3	2.12	0.48
13:J:32:GLY:HA3	34:e:40:TYR:CG	2.49	0.48
22:S:37:GLY:O	22:S:99:HIS:HE1	1.96	0.48
47:s:179:LYS:HB3	47:s:189:VAL:HB	1.96	0.48
2:2:223:C:H2'	2:2:224:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:244:U:O2'	2:2:246:A:N7	2.47	0.48
2:2:1259:U:O2'	2:2:1260:G:H5''	2.12	0.48
22:S:86:LEU:HA	22:S:99:HIS:HD2	1.78	0.48
2:2:875:G:H1'	2:2:943:A:O4'	2.14	0.48
12:I:103:GLN:HB3	12:I:165:ARG:HB3	1.95	0.48
44:p:145:HIS:CE1	44:p:305:LYS:HB3	2.49	0.48
1:1:20:A:N3	1:1:20:A:H2'	2.27	0.48
2:2:279:U:H4'	2:2:280:G:O5'	2.13	0.48
2:2:433:G:OP1	27:X:78:LYS:HA	2.14	0.48
23:T:34:VAL:O	23:T:35:ASP:HB2	2.12	0.48
24:U:58:LEU:HB2	24:U:88:LYS:HB2	1.95	0.48
30:a:75:ILE:O	30:a:79:ILE:HG12	2.13	0.48
36:g:84:ALA:HB2	36:g:114:VAL:HG22	1.95	0.48
38:i:62:ARG:NH1	38:i:64:LYS:HD2	2.28	0.48
2:2:516:U:H3	2:2:534:A:H61	1.62	0.48
2:2:616:U:O2	2:2:617:U:C2	2.67	0.48
2:2:1769:U:H3	2:2:1788:A:H2	1.55	0.48
24:U:21:LYS:HG3	24:U:94:GLU:HG3	1.96	0.48
36:g:90:LEU:HB2	36:g:104:PHE:HB2	1.96	0.48
42:m:56:TYR:CE1	42:m:92:PHE:HB2	2.49	0.48
43:o:49:GLU:H	43:o:50:PRO:CD	2.27	0.48
2:2:107:C:H2'	2:2:108:A:C8	2.49	0.48
2:2:431:G:H2'	2:2:432:C:O4'	2.14	0.48
2:2:646:G:H1	2:2:687:C:H42	1.61	0.48
2:2:886:A:H1'	18:O:122:PRO:HB3	1.96	0.48
2:2:13:C:OP2	2:2:13:C:H6	1.97	0.47
2:2:293:C:C4	2:2:294:A:N7	2.82	0.47
2:2:1544:G:P	22:S:127:HIS:HE2	2.37	0.47
2:2:1472:G:H2'	2:2:1473:A:C8	2.49	0.47
3:3:18[A]:U:C6	3:3:18[A]:U:C5'	2.97	0.47
6:C:40:TRP:CD1	6:C:72:GLN:HG3	2.48	0.47
6:C:110:GLY:HA3	6:C:195:LEU:HB3	1.95	0.47
6:C:121:LYS:HG2	6:C:132:ALA:HB3	1.95	0.47
22:S:15:LEU:HD21	22:S:59:GLY:HA2	1.96	0.47
28:Y:20:ARG:HD2	28:Y:22:GLN:HE21	1.79	0.47
44:p:351:MET:HG3	44:p:381:PHE:HE1	1.80	0.47
6:C:88:ILE:HG21	6:C:126:VAL:HG13	1.95	0.47
6:C:108:VAL:HG12	6:C:195:LEU:HD13	1.96	0.47
10:G:159:ARG:HA	10:G:172:ALA:HB2	1.95	0.47
14:K:82:LEU:HD12	14:K:86:ILE:HG21	1.96	0.47
20:Q:12:LYS:HG2	20:Q:17:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:40:ARG:HD2	23:T:45:LEU:HD11	1.97	0.47
23:T:39:THR:HA	23:T:100:ILE:HD12	1.96	0.47
2:2:15:U:H2'	2:2:16:G:O4'	2.14	0.47
2:2:648:U:N3	2:2:685:A:N6	2.62	0.47
2:2:812:U:H4'	15:L:156:PHE:HA	1.96	0.47
2:2:1115:A:H2'	2:2:1116:U:O4'	2.15	0.47
11:H:27:LEU:HD11	11:H:80:GLU:HB3	1.95	0.47
26:W:20:THR:HB	26:W:22:LYS:HG2	1.96	0.47
40:k:359:ILE:HB	40:k:373:ILE:HD11	1.96	0.47
2:2:60:U:H5'	2:2:454:C:N4	2.30	0.47
2:2:1457:C:H5'	22:S:131:LEU:HD22	1.95	0.47
3:3:16[A]:U:O2	43:o:38:ARG:C	2.56	0.47
4:A:41:ARG:HD3	4:A:45:VAL:HB	1.94	0.47
5:B:61:LEU:HA	5:B:64:ARG:HD2	1.97	0.47
23:T:73:VAL:HG21	23:T:102:ARG:HG3	1.95	0.47
2:2:56:U:H2'	2:2:56:U:O2	2.14	0.47
2:2:100:A:H2'	2:2:101:U:O4'	2.14	0.47
2:2:122:U:C2	2:2:294:A:C2	3.02	0.47
2:2:1064:A:H2'	2:2:1065:C:O4'	2.14	0.47
2:2:1123:A:H2'	2:2:1124:A:C8	2.49	0.47
2:2:1333:U:H2'	2:2:1334:U:O4'	2.13	0.47
1:1:43:G:O2'	1:1:44:A:H5'	2.14	0.47
2:2:143:G:H2'	2:2:144:A:O4'	2.15	0.47
2:2:742:U:C1'	11:H:107:ARG:HH22	2.26	0.47
2:2:876:G:H4'	2:2:941:G:N2	2.30	0.47
2:2:1016:U:O4'	2:2:1016:U:O2	2.30	0.47
2:2:1415:A:H2'	2:2:1416:G:O4'	2.15	0.47
2:2:1466:U:H2'	2:2:1467:A:O4'	2.15	0.47
3:3:16[A]:U:C2	43:o:38:ARG:O	2.68	0.47
3:3:24:U:C5	32:c:67:ARG:HB2	2.48	0.47
3:3:35:C:H4'	3:3:36:U:OP1	2.14	0.47
5:B:2:AYA:HB2	39:j:89:ARG:HH12	1.79	0.47
5:B:90:GLU:HB2	5:B:228:LEU:HD13	1.97	0.47
12:I:107:THR:N	12:I:108:PRO:HD2	2.29	0.47
15:L:55:ASP:OD2	15:L:110:HIS:HE1	1.96	0.47
17:N:114:ARG:O	17:N:118:ILE:HG12	2.14	0.47
18:O:89:THR:HB	18:O:128:LYS:HG3	1.97	0.47
38:i:78:LEU:HB3	38:i:93:HIS:HB3	1.96	0.47
2:2:1228:G:H1'	2:2:1254:G:H22	1.78	0.47
2:2:1379:U:H4'	24:U:59:PRO:HG3	1.96	0.47
2:2:1535:C:H5''	2:2:1570:2MG:HN1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:q:626:LEU:HD11	45:q:679:ALA:HB2	1.96	0.47
2:2:328:G:H5'	12:I:99:ALA:HB3	1.96	0.47
2:2:1087:A:N6	2:2:1092:A:C2	2.83	0.47
2:2:1418:C:H5''	2:2:1418:C:C6	2.38	0.47
2:2:1527:C:H2'	2:2:1528:C:C6	2.50	0.47
44:p:724:MET:HB3	44:p:730:PHE:HB3	1.97	0.47
45:q:542:LEU:O	45:q:546:VAL:HG13	2.15	0.47
2:2:92:A:H5''	2:2:93:A:H5''	1.97	0.47
2:2:1029:A:OP1	30:a:3:LYS:HD2	2.15	0.47
2:2:1203:A:H61	33:d:15:GLY:HA3	1.80	0.47
2:2:1476:G:H3'	2:2:1477:A:H8	1.80	0.47
12:I:185:LEU:HD22	12:I:189:GLU:HG2	1.97	0.47
21:R:109:LEU:O	21:R:113:LEU:HG	2.15	0.47
29:Z:74:SER:HA	29:Z:77:ARG:NH1	2.30	0.47
2:2:337:C:H2'	2:2:338:C:C6	2.50	0.46
2:2:767:U:H3	13:J:142:ASN:HD22	1.62	0.46
3:3:33:C:C5	38:i:11:LYS:HB3	2.50	0.46
9:F:59:SER:HA	32:c:53:ILE:HB	1.96	0.46
40:k:462:LEU:HD22	40:k:503:ARG:HG2	1.97	0.46
43:o:303:TRP:HA	43:o:303:TRP:HE3	1.79	0.46
44:p:341:TRP:HH2	44:p:365:PHE:HE1	1.63	0.46
44:p:409:GLU:HB2	44:p:415:CYS:HB2	1.97	0.46
2:2:917:U:H4'	18:O:18:ARG:HD3	1.97	0.46
2:2:977:A:H2'	2:2:978:A:O4'	2.15	0.46
2:2:1632:C:H6	2:2:1632:C:OP1	1.97	0.46
4:A:64:ILE:HA	4:A:67:ILE:HD12	1.97	0.46
5:B:109:LYS:HG3	5:B:113:MET:HE3	1.96	0.46
5:B:113:MET:HE1	5:B:211:HIS:CD2	2.49	0.46
13:J:120:LYS:O	13:J:124:HIS:HB3	2.15	0.46
39:j:24:VAL:HG13	39:j:34:VAL:HG11	1.97	0.46
2:2:1277:G:H2'	2:2:1278:C:O4'	2.16	0.46
2:2:1675:C:H5''	12:I:59:ARG:HH12	1.81	0.46
4:A:74:VAL:HG22	4:A:96:THR:HB	1.98	0.46
8:E:100:ARG:HH11	8:E:114:ILE:HD13	1.80	0.46
9:F:119:THR:HG21	9:F:196:LEU:HD13	1.97	0.46
9:F:156:ALA:HB1	18:O:52:ARG:HH12	1.80	0.46
17:N:94:LYS:O	17:N:98:VAL:HG23	2.14	0.46
43:o:445:GLN:HB2	43:o:487:ALA:HB1	1.97	0.46
1:1:9:IMG:O5'	1:1:46:7MG:H1'	2.16	0.46
2:2:220:A:H2'	2:2:221:A:H8	1.80	0.46
2:2:358:A:N3	2:2:358:A:H2'	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:647:G:O6	2:2:685:A:N6	2.49	0.46
2:2:988:U:H2'	2:2:989:C:O4'	2.16	0.46
2:2:1101:G:H2'	2:2:1102:U:O4'	2.15	0.46
4:A:126:PRO:HG2	4:A:147:THR:HG22	1.97	0.46
7:D:8:LYS:HD3	24:U:63:LEU:HD21	1.98	0.46
12:I:58:LEU:O	12:I:59:ARG:HB2	2.16	0.46
22:S:53:ASP:HB3	22:S:56:LYS:HB2	1.96	0.46
41:l:258:VAL:HG12	41:l:265:THR:HG22	1.96	0.46
44:p:641:ASN:HD21	44:p:645:ASN:HB2	1.80	0.46
2:2:767:U:H3	13:J:142:ASN:ND2	2.14	0.46
6:C:140:SER:O	6:C:141:VAL:C	2.58	0.46
8:E:181:VAL:HG21	8:E:225:VAL:HG22	1.98	0.46
9:F:184:ALA:HB3	9:F:195:THR:HB	1.97	0.46
1:1:37:T6A:N1	1:1:37:T6A:N11	2.40	0.46
2:2:1083:A:H2'	2:2:1084:G:O4'	2.16	0.46
4:A:162:CYS:HB2	4:A:173:ILE:CD1	2.44	0.46
6:C:175:ILE:HB	6:C:202:TYR:HB2	1.97	0.46
8:E:31:PRO:HD2	8:E:38:LEU:HD13	1.97	0.46
12:I:96:LEU:HD12	12:I:174:PRO:HG3	1.97	0.46
18:O:83:ILE:HD11	18:O:102:LEU:HD13	1.98	0.46
36:g:39:ARG:HA	36:g:68:ILE:HG23	1.97	0.46
39:j:248:ILE:HG12	39:j:264:ILE:HG21	1.97	0.46
2:2:124:A:H2	2:2:292:U:H3	1.58	0.46
2:2:313:C:O2	2:2:353:C:N3	2.48	0.46
2:2:1306:U:O2	2:2:1306:U:O4'	2.33	0.46
2:2:1671:G:H2'	2:2:1672:C:C6	2.51	0.46
18:O:29:HIS:HE1	18:O:38:THR:HG22	1.81	0.46
36:g:65:HIS:CE1	36:g:91:ARG:HB2	2.51	0.46
40:k:325:LYS:HA	40:k:326:PRO:HD3	1.79	0.46
40:k:353:ILE:HG13	40:k:419:ALA:HA	1.98	0.46
2:2:46:A:N6	2:2:432:C:H4'	2.31	0.46
2:2:555:A:H5'	34:e:56:MET:HE3	1.97	0.46
2:2:1629:A:H8	2:2:1629:A:OP1	1.98	0.46
14:K:59:PHE:CZ	14:K:62:GLN:HA	2.50	0.46
16:M:125:GLU:HA	16:M:128:LEU:HD12	1.98	0.46
34:e:30:PRO:O	34:e:35:TYR:HB2	2.15	0.46
40:k:263:GLN:HE22	40:k:280:ILE:HD13	1.81	0.46
41:l:186:ARG:HH22	41:l:244:THR:HG23	1.81	0.46
2:2:983:G:H1	2:2:1016:U:H5	1.63	0.46
2:2:1626:U:H2'	2:2:1627:G:C8	2.50	0.46
25:V:55:LEU:HB3	25:V:59:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:43:LEU:HB2	36:g:62:TYR:HB2	1.96	0.46
36:g:308:LEU:HB3	36:g:320:TRP:HB2	1.98	0.46
40:k:236:ILE:HG23	40:k:241:LEU:HB2	1.97	0.46
2:2:17:C:O2'	2:2:1136:A:N1	2.35	0.46
2:2:392:C:OP2	12:I:2:GLY:HA2	2.15	0.46
2:2:442:C:C5	28:Y:105:ARG:HD3	2.51	0.46
2:2:1586:G:H1	2:2:1606:U:H3	1.63	0.46
21:R:89:SER:C	21:R:91:LEU:H	2.23	0.46
2:2:67:A:O2'	2:2:69:G:OP1	2.33	0.45
2:2:1012:A:H2'	2:2:1013:G:O4'	2.16	0.45
2:2:1539:G:C6	2:2:1540:G:N1	2.84	0.45
2:2:1542:U:H2'	2:2:1543:A:O4'	2.15	0.45
2:2:1552:U:H5''	19:P:47:ARG:HH12	1.82	0.45
10:G:215:ARG:O	10:G:219:ARG:HG3	2.16	0.45
11:H:140:VAL:HB	26:W:52:TYR:HB3	1.98	0.45
26:W:24:GLN:HA	26:W:63:VAL:O	2.15	0.45
47:s:34:ALA:HB3	47:s:48:LEU:HB2	1.98	0.45
2:2:874:G:OP1	5:B:158:SER:N	2.49	0.45
2:2:1593:U:H3'	2:2:1594:C:O2	2.16	0.45
2:2:1778:G:H3'	2:2:1779:A:H8	1.80	0.45
4:A:55:GLU:O	4:A:58:VAL:HG12	2.16	0.45
6:C:83:ASP:HB3	6:C:109:VAL:HG23	1.97	0.45
19:P:17:TYR:HB2	19:P:25:LEU:HD11	1.98	0.45
30:a:21:VAL:HG22	30:a:32:LYS:HA	1.99	0.45
2:2:303:U:H2'	2:2:304:C:C6	2.51	0.45
2:2:621:A:O2'	2:2:1031:G:H5'	2.17	0.45
2:2:690:A:H2'	2:2:691:U:O4'	2.17	0.45
2:2:732:G:H1'	2:2:734:A:H61	1.81	0.45
6:C:144:ILE:HG22	6:C:223:ILE:CG2	2.35	0.45
21:R:29:GLN:HG2	36:g:68:ILE:HD11	1.99	0.45
2:2:1038:A:H5''	25:V:62:ARG:HH11	1.81	0.45
2:2:1085:A:H2'	2:2:1086:A:O4'	2.16	0.45
2:2:1286:A:H4'	2:2:1287:G:OP1	2.16	0.45
36:g:94:ASN:HD22	36:g:97:THR:H	1.63	0.45
44:p:356:LEU:HB3	44:p:375:PRO:HD2	1.98	0.45
2:2:1077:C:H2'	2:2:1078:U:C6	2.51	0.45
2:2:1086:A:C2	2:2:1087:A:C5	3.05	0.45
2:2:1423:A:H1'	6:C:97:ALA:HB1	1.99	0.45
2:2:1475:G:H1'	23:T:48:GLN:HB2	1.97	0.45
2:2:1716:A:H2'	2:2:1717:A:C8	2.52	0.45
2:2:511:A:H2'	2:2:512:U:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:614:A:C8	2:2:614:A:H5''	2.52	0.45
2:2:1043:U:O2	2:2:1043:U:O4'	2.34	0.45
2:2:1726:U:H2'	2:2:1727:C:C6	2.52	0.45
6:C:145:ARG:NH2	6:C:233:ASN:HD21	2.15	0.45
16:M:43:LYS:HZ3	35:f:128:ILE:HG12	1.82	0.45
18:O:84:ARG:HG2	18:O:85:ALA:O	2.17	0.45
24:U:86:ILE:HG13	24:U:86:ILE:O	2.17	0.45
36:g:48:LEU:HD21	36:g:309:PHE:HZ	1.82	0.45
2:2:487:G:H1	2:2:498:U:H3	1.64	0.45
2:2:871:G:H2'	2:2:872:U:O4'	2.15	0.45
2:2:941:G:O6	30:a:15:ARG:O	2.34	0.45
2:2:1165:A:O2'	2:2:1585:A:H4'	2.15	0.45
2:2:1601:U:H2'	2:2:1602:U:C6	2.52	0.45
2:2:1777:U:H2'	2:2:1779:A:OP2	2.17	0.45
2:2:119:A:H2'	2:2:120:PSU:O4'	2.17	0.45
2:2:335:G:H5'	15:L:130:PRO:O	2.17	0.45
2:2:366:A:H2'	2:2:367:U:O4'	2.16	0.45
2:2:1087:A:N7	2:2:1088:U:H1'	2.32	0.45
4:A:62:ARG:HA	4:A:184:LEU:HD22	1.99	0.45
18:O:25:ASP:H	18:O:55:SER:HB3	1.81	0.45
29:Z:35:LYS:C	29:Z:37:LYS:H	2.25	0.45
33:d:23:ILE:HD12	33:d:42:SER:HB3	1.99	0.45
47:s:169:ILE:HD11	47:s:225:VAL:HG13	1.99	0.45
2:2:531:U:H5''	2:2:531:U:H6	1.82	0.45
2:2:617:U:C6	2:2:1141:A:H5'	2.51	0.45
2:2:859:U:C1'	11:H:114:ARG:HD2	2.46	0.45
2:2:1088:U:O2'	2:2:1092:A:N1	2.47	0.45
2:2:1132:A:H2'	2:2:1133:C:O4'	2.16	0.45
2:2:1315:G:O2'	21:R:10:LYS:HE3	2.17	0.45
2:2:1336:A:N6	2:2:1385:G:H22	2.14	0.45
8:E:50:ASN:HB3	8:E:51:ARG:HH21	1.81	0.45
13:J:163:PRO:C	13:J:165:GLY:H	2.25	0.45
17:N:33:VAL:HG21	17:N:66:ILE:HG21	1.98	0.45
18:O:99:GLN:HE21	30:a:46:GLU:HG3	1.81	0.45
29:Z:61:SER:H	29:Z:64:VAL:HB	1.81	0.45
2:2:886:A:N6	2:2:923:A:H61	2.15	0.45
2:2:1086:A:C2	2:2:1087:A:C2	3.05	0.45
6:C:86:MET:CE	6:C:191:LYS:HB3	2.43	0.45
9:F:60:LEU:HB3	9:F:64:ILE:HD12	1.98	0.45
12:I:81:VAL:HA	12:I:102:VAL:HG12	1.99	0.45
24:U:22:ILE:HG13	24:U:118:ILE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:71:ARG:HG3	25:V:83:TRP:CE2	2.52	0.45
43:o:59:GLY:HA3	43:o:68:LEU:HD21	1.99	0.45
2:2:367:U:C2'	2:2:368:A:H5'	2.47	0.44
2:2:638:U:H5'	11:H:118:LEU:HB3	1.98	0.44
2:2:958:U:H5'	31:b:28:PRO:HB3	1.99	0.44
12:I:85:PRO:HB3	15:L:12:ALA:HB2	1.99	0.44
13:J:117:GLY:O	13:J:119:ALA:N	2.36	0.44
15:L:99:ARG:NH1	27:X:7:ARG:O	2.42	0.44
33:d:19:ARG:HG2	33:d:30:LEU:HD22	1.99	0.44
39:j:46:ILE:HG12	39:j:85:LEU:HD22	1.99	0.44
2:2:606:G:N2	2:2:613:C:H5''	2.32	0.44
2:2:698:U:H1'	11:H:107:ARG:HE	1.81	0.44
2:2:883:A:H5''	5:B:136:ARG:HE	1.83	0.44
2:2:1259:U:O2'	2:2:1260:G:H8	2.01	0.44
2:2:1533:U:H4'	2:2:1534:G:O5'	2.17	0.44
2:2:1637:5MC:H2'	2:2:1638:C:O4'	2.16	0.44
2:2:1637:5MC:O2	2:2:1761:A:N1	2.51	0.44
7:D:81:ARG:HH21	7:D:81:ARG:HB2	1.81	0.44
8:E:36:HIS:NE2	8:E:88:ASP:OD1	2.51	0.44
9:F:135:VAL:HG22	9:F:200:LEU:HD13	1.99	0.44
20:Q:16:ALA:HB2	20:Q:72:GLY:HA3	1.97	0.44
23:T:77:ASN:O	23:T:80:TYR:O	2.35	0.44
40:k:314:ARG:HE	40:k:494:GLU:HG2	1.82	0.44
40:k:314:ARG:HH11	40:k:344:ASN:HD21	1.64	0.44
43:o:296:PRO:HG2	43:o:335:THR:HA	1.99	0.44
1:1:47:H2U:H5''	1:1:47:H2U:H52	1.98	0.44
2:2:327:A:H2'	2:2:328:G:O4'	2.18	0.44
2:2:688:G:H2'	2:2:689:G:C8	2.52	0.44
2:2:1100:G:O3'	26:W:76:SER:HB2	2.17	0.44
9:F:53:VAL:HA	9:F:133:GLN:HG2	1.99	0.44
18:O:50:ALA:O	18:O:51:ASP:HB3	2.16	0.44
21:R:29:GLN:HB3	36:g:86:TRP:CZ3	2.52	0.44
23:T:18:TYR:CD1	23:T:135:ILE:HG13	2.53	0.44
27:X:86:PHE:HB2	27:X:120:VAL:HG11	1.99	0.44
33:d:21:CYS:O	33:d:22:ARG:HB3	2.16	0.44
36:g:218:ALA:HB2	36:g:232:LEU:HD11	1.99	0.44
45:q:510:THR:HG23	45:q:514:LYS:HD2	1.98	0.44
1:1:26:M2G:HM22	1:1:44:A:C2	2.52	0.44
2:2:614:A:H5''	2:2:614:A:H8	1.82	0.44
2:2:1015:C:O2	2:2:1015:C:O4'	2.35	0.44
2:2:1084:G:H2'	2:2:1086:A:N7	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1178:G:H2'	2:2:1179:C:O4'	2.17	0.44
3:3:29:A:H2'	3:3:30:U:O4'	2.18	0.44
20:Q:51:PRO:O	20:Q:55:VAL:HG23	2.17	0.44
36:g:70:GLN:HG2	36:g:86:TRP:NE1	2.26	0.44
39:j:198:ILE:HG13	40:k:404:PRO:HD3	1.98	0.44
2:2:1590:A:H2'	2:2:1591:A:C8	2.52	0.44
2:2:1788:A:C2	2:2:1789:A:N1	2.85	0.44
7:D:226:ARG:HD2	7:D:226:ARG:HA	1.53	0.44
9:F:189:ILE:HD13	29:Z:66:VAL:HG11	1.98	0.44
39:j:205:LEU:HD12	40:k:331:GLU:HG3	1.99	0.44
40:k:373:ILE:HD13	40:k:406:LEU:HD11	2.00	0.44
40:k:432:ILE:HD11	40:k:499:ILE:HD13	1.99	0.44
44:p:391:GLN:HB3	44:p:392:PRO:HD2	1.99	0.44
2:2:1134:U:O2'	2:2:1751:A:H5'	2.18	0.44
9:F:221:ARG:HD3	39:j:84:ASP:CG	2.43	0.44
13:J:155:HIS:HE1	44:p:477:ASP:HB2	1.83	0.44
15:L:38:VAL:HG11	15:L:59:PRO:HB2	2.00	0.44
16:M:56:VAL:HG21	16:M:85:ALA:HA	1.98	0.44
23:T:86:ARG:HH21	23:T:92:LYS:HG3	1.83	0.44
1:1:37:T6A:H5'	42:m:29:GLY:H	1.83	0.44
2:2:799:U:H2'	2:2:800:G:C8	2.53	0.44
2:2:863:U:C4	26:W:28:ARG:HD2	2.52	0.44
2:2:867:G:N2	2:2:959:U:H3	2.16	0.44
2:2:880:A:H2'	2:2:881:U:O4'	2.18	0.44
2:2:1540:G:N2	2:2:1566:C:C2'	2.81	0.44
2:2:1773:U:H2'	2:2:1774:A:C8	2.53	0.44
4:A:136:SER:HA	4:A:141:ILE:HD12	1.98	0.44
8:E:86:PHE:CZ	8:E:87:MET:HE2	2.53	0.44
8:E:234:PRO:HG3	8:E:238:LEU:HD11	2.00	0.44
18:O:83:ILE:HD12	30:a:44:ILE:HG12	1.99	0.44
43:o:395:PHE:HA	43:o:400:VAL:HG21	1.99	0.44
2:2:94:U:H2'	2:2:95:G:O4'	2.18	0.44
2:2:903:G:H4'	3:3:25:A:O5'	2.18	0.44
2:2:1266:G:HO2'	2:2:1446:G:HO2'	1.59	0.44
8:E:181:VAL:CG2	8:E:225:VAL:HG22	2.47	0.44
12:I:65:PHE:O	12:I:73:ALA:HA	2.17	0.44
12:I:87:ASN:HB3	12:I:90:LEU:HD13	1.99	0.44
13:J:59:LEU:HD22	13:J:69:ARG:HA	1.99	0.44
14:K:83:PRO:HB2	14:K:85:HIS:CD2	2.52	0.44
18:O:50:ALA:O	18:O:51:ASP:CB	2.66	0.44
27:X:51:GLY:HA3	27:X:74:VAL:CG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:55:VAL:HG22	28:Y:75:VAL:HG22	2.00	0.44
36:g:43:LEU:HD21	36:g:69:VAL:HG11	2.00	0.44
45:q:520:LYS:HA	45:q:523:LEU:HD12	1.99	0.44
2:2:93:A:O2'	8:E:4:GLY:HA3	2.18	0.44
2:2:294:A:H2'	2:2:295:U:C6	2.53	0.44
2:2:917:U:H2'	2:2:918:A:C8	2.52	0.44
2:2:1049:G:H5'	2:2:1050:G:OP2	2.18	0.44
5:B:68:VAL:HG23	5:B:73:LEU:HD11	2.00	0.44
9:F:34:GLU:HG2	9:F:35:ILE:HG13	2.00	0.44
16:M:67:LEU:HD11	35:f:106:TYR:HB2	1.99	0.44
17:N:15:ALA:H	31:b:20:LYS:HE3	1.83	0.44
27:X:103:LEU:HB3	27:X:126:LYS:HB2	1.99	0.44
38:i:77:ILE:HG12	38:i:91:VAL:HG13	2.00	0.44
2:2:597:U:H5	2:2:598:A:C4	2.36	0.43
8:E:136:ILE:HG23	8:E:149:TYR:CE1	2.53	0.43
9:F:72:VAL:C	9:F:74:HIS:H	2.26	0.43
15:L:99:ARG:HG2	27:X:9:LEU:HA	1.99	0.43
26:W:47:ILE:HD11	26:W:65:LEU:HD22	2.00	0.43
44:p:633:VAL:HA	44:p:635:HIS:CE1	2.52	0.43
2:2:874:G:H2'	2:2:876:G:OP2	2.18	0.43
2:2:1318:A:H2'	2:2:1319:U:O4'	2.17	0.43
2:2:1712:A:H2'	2:2:1713:G:H8	1.82	0.43
13:J:59:LEU:HD13	13:J:73:GLY:CA	2.47	0.43
16:M:21:LEU:O	16:M:24:VAL:HG22	2.18	0.43
26:W:41:MET:HG2	26:W:129:VAL:HG11	1.99	0.43
42:m:54:VAL:HG21	42:m:74:TYR:HB3	1.99	0.43
2:2:220:A:H2'	2:2:221:A:C8	2.53	0.43
2:2:472:A:O2'	13:J:143:ILE:HD12	2.17	0.43
2:2:627:G:O6	2:2:968:C:H5''	2.19	0.43
2:2:788:A:C2	2:2:789:U:H1'	2.53	0.43
7:D:137:VAL:HB	7:D:185:LYS:HB2	2.00	0.43
8:E:193:GLY:HA3	8:E:210:ILE:CG2	2.47	0.43
18:O:81:ILE:HG21	18:O:102:LEU:HD12	1.99	0.43
21:R:101:ASN:HA	21:R:120:SER:HB3	2.00	0.43
22:S:29:VAL:O	22:S:33:THR:HG23	2.17	0.43
45:q:493:GLN:HE22	45:q:495:ASN:HD22	1.66	0.43
2:2:385:G:P	12:I:25:ARG:HH22	2.40	0.43
2:2:789:U:C5	2:2:790:A:C8	3.07	0.43
2:2:884:G:H5''	2:2:885:U:OP2	2.18	0.43
2:2:897:A:N3	2:2:898:G:H1'	2.33	0.43
2:2:1159:A:H2'	2:2:1160:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:93:THR:HG22	4:A:94:GLY:H	1.83	0.43
14:K:40:LEU:HD12	14:K:40:LEU:H	1.82	0.43
15:L:108:PRO:HG2	15:L:134:THR:HB	2.00	0.43
42:m:66:SER:HB2	42:m:75:LEU:HB2	2.00	0.43
45:q:335:THR:HG21	45:q:339:TYR:HB3	2.00	0.43
2:2:296:U:H5''	8:E:37:LYS:HG2	1.99	0.43
2:2:472:A:P	13:J:11:THR:HG21	2.58	0.43
2:2:591:G:OP1	13:J:39:LYS:HG3	2.19	0.43
2:2:637:U:O2	2:2:637:U:C2'	2.67	0.43
2:2:1054:U:H2'	2:2:1055:U:O4'	2.19	0.43
2:2:1284:U:H4'	2:2:1285:U:O4'	2.19	0.43
3:3:16[A]:U:N3	43:o:78:LEU:HD22	2.25	0.43
9:F:202:ASN:HB2	9:F:210:SER:HB2	1.99	0.43
39:j:132:TRP:HD1	39:j:136:ARG:HE	1.65	0.43
41:l:177:ILE:HG21	41:l:211:LEU:HB2	2.00	0.43
2:2:86:A:H5''	28:Y:119:PHE:CE1	2.54	0.43
2:2:969:A:H2'	2:2:970:A:H5'	2.01	0.43
2:2:1582:G:O2'	2:2:1608:G:O6	2.35	0.43
6:C:121:LYS:HG3	6:C:122:THR:N	2.33	0.43
9:F:45:PHE:HB3	9:F:117:LYS:HE3	2.01	0.43
9:F:177:LEU:HD22	9:F:200:LEU:HD23	2.00	0.43
14:K:32:HIS:HB2	14:K:39:ASN:HA	2.00	0.43
16:M:86:LYS:HD2	16:M:106:VAL:HG22	2.00	0.43
41:l:232:GLU:HG3	41:l:233:TYR:CD1	2.54	0.43
44:p:85:PRO:HG2	44:p:95:LEU:HD21	2.00	0.43
2:2:472:A:H5'	2:2:769:A:H1'	1.99	0.43
2:2:597:U:C4	2:2:598:A:C5	3.06	0.43
2:2:617:U:H6	2:2:1141:A:H5'	1.82	0.43
2:2:789:U:O4	2:2:790:A:C6	2.71	0.43
2:2:876:G:H22	2:2:950:A:H2	1.67	0.43
2:2:927:U:H4'	18:O:124:ASP:HB3	2.00	0.43
2:2:1162:A:N6	2:2:1163:G:C6	2.87	0.43
2:2:1540:G:H22	2:2:1566:C:H2'	1.83	0.43
2:2:1639:C:H4'	37:h:1:MET:H1	1.82	0.43
10:G:21:GLU:HG2	10:G:25:ARG:HH12	1.83	0.43
12:I:62:THR:HG21	12:I:75:LYS:HE3	2.01	0.43
19:P:56:LEU:HD12	19:P:83:MET:HE2	2.00	0.43
19:P:90:ILE:HA	19:P:107:ILE:HG22	2.01	0.43
26:W:72:CYS:HA	26:W:129:VAL:HG12	2.01	0.43
2:2:1735:G:H2'	2:2:1736:U:O4'	2.19	0.43
2:2:1756:U:H2'	2:2:1757:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1769:U:N3	2:2:1788:A:C2	2.77	0.43
9:F:147:ASP:HB2	9:F:164:VAL:HG22	2.00	0.43
20:Q:22:VAL:HG12	20:Q:65:ILE:HG23	2.00	0.43
2:2:337:C:H5''	12:I:10:LYS:HG3	2.01	0.43
2:2:517:A:H2'	2:2:518:C:H5''	2.00	0.43
2:2:991:A:OP1	2:2:1784:G:H5'	2.19	0.43
2:2:995:U:H2'	2:2:995:U:O2	2.19	0.43
2:2:1581:A:N6	2:2:1610:U:H5	2.17	0.43
2:2:1660:G:H2'	2:2:1661:G:H8	1.83	0.43
13:J:145:SER:O	13:J:147:MET:N	2.41	0.43
16:M:94:LEU:HB3	16:M:107:VAL:HG21	2.01	0.43
29:Z:99:ALA:HB1	29:Z:101:TYR:HE2	1.84	0.43
44:p:637:TYR:CE1	44:p:650:ASP:HB2	2.54	0.43
2:2:209:A:N6	2:2:254:U:H3	2.14	0.43
2:2:790:A:C6	2:2:791:U:C4	3.07	0.43
2:2:1527:C:OP1	9:F:114:ARG:HD3	2.19	0.43
4:A:120:LEU:HD23	4:A:142:PRO:HG2	2.00	0.43
15:L:80:MET:HE3	15:L:83:THR:HB	2.00	0.43
16:M:129:GLU:HA	16:M:133:GLN:HB2	2.00	0.43
20:Q:36:ILE:HD13	20:Q:52:LEU:HD11	2.00	0.43
2:2:904:A:H5'	18:O:52:ARG:HB3	2.00	0.42
2:2:1781:C:H2'	2:2:1782:C:C6	2.53	0.42
4:A:198:MET:HE1	21:R:87:ASP:HA	2.00	0.42
5:B:171:ILE:HD13	5:B:197:ILE:HA	2.01	0.42
15:L:48:ALA:HA	15:L:53:TYR:HE1	1.82	0.42
20:Q:126:PRO:O	20:Q:128:LYS:HE3	2.19	0.42
37:h:2:ARG:HD3	37:h:5:TRP:NE1	2.34	0.42
45:q:392:SER:HA	45:q:395:LEU:HD12	2.02	0.42
2:2:845:G:H3'	2:2:846:A:H8	1.84	0.42
2:2:1794:C:C2	30:a:5:ARG:HG2	2.54	0.42
6:C:45:LYS:HB2	6:C:245:MET:HE2	2.00	0.42
6:C:237:VAL:HA	25:V:16:LYS:HZ1	1.83	0.42
8:E:108:ARG:CD	8:E:108:ARG:H	2.32	0.42
9:F:168:ARG:HA	9:F:171:ASN:HD22	1.83	0.42
42:m:5:ILE:HD13	42:m:5:ILE:H	1.85	0.42
43:o:263:VAL:HG12	43:o:267:MET:HE2	2.00	0.42
2:2:306:G:H5''	15:L:103:ARG:HH12	1.83	0.42
4:A:122:ILE:HA	4:A:144:ILE:O	2.19	0.42
5:B:136:ARG:HB2	5:B:218:LEU:HD11	2.01	0.42
11:H:62:VAL:HG12	11:H:64:VAL:H	1.84	0.42
21:R:31:ASN:HA	21:R:34:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:q:645:ILE:H	45:q:646:PRO:HD3	1.84	0.42
2:2:312:U:O4	2:2:1129:G:H1'	2.19	0.42
2:2:333:G:H2'	2:2:334:U:H6	1.84	0.42
2:2:1210:A:H2'	2:2:1211:G:O4'	2.19	0.42
2:2:1293:G:H21	2:2:1320:A:H8	1.67	0.42
2:2:1320:A:C8	2:2:1321:A:H1'	2.54	0.42
8:E:44:LEU:HD12	8:E:82:PHE:HB3	2.01	0.42
42:m:56:TYR:CD1	42:m:92:PHE:HB2	2.54	0.42
44:p:541:VAL:HG22	44:p:595:VAL:HG21	2.01	0.42
47:s:127:ILE:HG22	47:s:139:VAL:HG12	2.01	0.42
8:E:125:LYS:HA	8:E:159:THR:HG22	2.02	0.42
16:M:24:VAL:HG12	16:M:124:ARG:HD3	2.00	0.42
23:T:28:LEU:HD12	23:T:111:LEU:HD11	2.01	0.42
1:1:18:G:N3	1:1:18:G:H2'	2.34	0.42
2:2:471:U:O2'	2:2:769:A:N3	2.40	0.42
2:2:1240:G:H4'	19:P:78:THR:HA	2.01	0.42
3:3:16[A]:U:H2'	3:3:17[A]:C:C6	2.54	0.42
5:B:186:SER:O	5:B:190:PRO:HD3	2.18	0.42
25:V:58:TYR:HE2	26:W:20:THR:O	2.03	0.42
34:e:59:SER:HA	34:e:60:PRO:HD3	1.89	0.42
41:l:178:GLN:HB2	41:l:209:LYS:HA	2.02	0.42
41:l:259:CYS:HB3	41:l:263:GLY:H	1.83	0.42
43:o:94:ARG:HG2	43:o:181:GLY:HA3	2.01	0.42
43:o:333:ILE:HA	43:o:363:ARG:HH21	1.85	0.42
44:p:571:MET:HE3	44:p:571:MET:HA	2.01	0.42
45:q:626:LEU:HD12	45:q:652:ILE:HG21	2.00	0.42
2:2:442:C:O2'	2:2:444:A:C2	2.71	0.42
2:2:819:U:H2'	2:2:820:U:H4'	2.01	0.42
2:2:1024:A:H2'	2:2:1026:A:H5''	2.02	0.42
2:2:1523:A:OP2	2:2:1523:A:H8	2.03	0.42
4:A:49:ASN:HA	21:R:109:LEU:HD21	2.01	0.42
7:D:215:GLU:HA	7:D:216:PRO:HD3	1.88	0.42
8:E:203:GLY:HA3	15:L:40:LEU:HD21	2.02	0.42
33:d:41:GLN:NE2	33:d:41:GLN:H	2.17	0.42
36:g:43:LEU:CD2	36:g:69:VAL:HG11	2.50	0.42
42:m:52:TYR:CE2	42:m:140:ILE:HG12	2.55	0.42
2:2:145:U:H2'	2:2:146:A:H5''	2.01	0.42
2:2:478:C:O2	2:2:509:G:N2	2.52	0.42
2:2:682:U:H2'	2:2:683:C:O4'	2.20	0.42
2:2:1117:G:H2'	2:2:1118:G:O4'	2.18	0.42
2:2:1457:C:OP2	22:S:126:ARG:NH2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:32:ILE:HB	5:B:43:VAL:HB	2.02	0.42
5:B:144:ARG:HD3	5:B:208:GLN:HB3	2.01	0.42
8:E:18:TRP:CD1	8:E:20:LEU:HD11	2.50	0.42
8:E:94:ALA:HB1	28:Y:16:PRO:HB2	2.02	0.42
12:I:177:SER:C	12:I:179:ARG:H	2.28	0.42
34:e:36:LYS:HD3	34:e:39:LEU:HD12	2.01	0.42
39:j:203:ASP:HA	39:j:206:LYS:HD2	2.02	0.42
41:l:162:PRO:HA	41:l:163:PRO:HD3	1.85	0.42
42:m:50:ALA:N	42:m:51:PRO:HD2	2.34	0.42
44:p:735:VAL:HG13	44:p:737:PRO:HD3	2.02	0.42
2:2:645:U:H3	2:2:688:G:H1	1.68	0.42
2:2:649:U:H2'	2:2:650:G:H8	1.84	0.42
2:2:1775:G:O6	37:h:8:LYS:HE2	2.20	0.42
8:E:139:VAL:HG13	8:E:147:ILE:HB	2.00	0.42
10:G:74:LYS:HA	10:G:96:SER:HA	2.02	0.42
13:J:81:VAL:HG11	13:J:91:LYS:HG2	2.01	0.42
17:N:23:PRO:HG2	17:N:26:PHE:HB2	2.00	0.42
17:N:40:TYR:HB3	17:N:50:ILE:HG12	2.01	0.42
18:O:80:HIS:HA	18:O:113:GLY:O	2.19	0.42
19:P:81:ARG:HB3	19:P:117:GLY:HA3	2.01	0.42
23:T:85:ASN:C	23:T:87:GLY:H	2.28	0.42
26:W:18:GLU:HG2	26:W:69:LEU:O	2.19	0.42
39:j:84:ASP:OD1	39:j:84:ASP:N	2.53	0.42
40:k:458:PRO:HA	40:k:475:VAL:HB	2.01	0.42
44:p:343:TYR:HE1	44:p:401:VAL:HG22	1.84	0.42
45:q:556:LYS:HB3	45:q:705:ASN:HD21	1.85	0.42
2:2:588:C:O2	2:2:588:C:O4'	2.34	0.42
2:2:1021:C:O2'	2:2:1124:A:N1	2.52	0.42
2:2:1323:G:H4'	4:A:113:ARG:HH21	1.85	0.42
4:A:105:GLY:H	4:A:135:GLU:CD	2.28	0.42
8:E:94:ALA:C	8:E:96:ASN:H	2.27	0.42
13:J:107:ARG:HA	13:J:107:ARG:NE	2.34	0.42
23:T:65:ILE:HG21	23:T:114:VAL:HG22	2.00	0.42
23:T:135:ILE:O	23:T:139:THR:HG23	2.19	0.42
39:j:115:CYS:HB3	39:j:165:VAL:HG22	2.02	0.42
43:o:203:ALA:HA	43:o:240:ARG:HH22	1.85	0.42
43:o:236:TYR:HD1	43:o:266:LEU:HD11	1.84	0.42
45:q:440:ILE:HG12	45:q:448:ILE:HG23	2.00	0.42
45:q:694:LEU:HA	45:q:697:ILE:HD12	2.02	0.42
2:2:787:A:H3'	8:E:108:ARG:HH21	1.85	0.41
2:2:1147:C:O2'	2:2:1763:A:N1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:157:ASP:CG	25:V:60:ARG:HE	2.27	0.41
8:E:180:LEU:HD13	8:E:231:PRO:HA	2.01	0.41
19:P:72:LYS:HA	19:P:73:PRO:HD3	1.94	0.41
19:P:81:ARG:NH2	19:P:120:SER:O	2.53	0.41
26:W:75:ILE:HD11	26:W:93:LEU:HD21	2.02	0.41
39:j:7:ARG:HD3	39:j:7:ARG:H	1.85	0.41
44:p:81:VAL:HB	44:p:127:LEU:HG	2.01	0.41
2:2:444:A:N6	2:2:461:G:N3	2.67	0.41
2:2:842:U:H2'	2:2:843:A:C8	2.54	0.41
2:2:1113:G:O2'	2:2:1129:G:O6	2.34	0.41
2:2:1149:G:H22	3:3:29:A:P	2.43	0.41
9:F:65:GLN:HE22	9:F:68:LYS:H	1.67	0.41
15:L:17:PRO:HG3	15:L:63:LEU:HD11	2.03	0.41
19:P:111:MET:HG3	19:P:119:PHE:CZ	2.55	0.41
27:X:70:LYS:HB3	27:X:93:LEU:HG	2.01	0.41
47:s:240:LEU:HD22	47:s:254:LEU:HB3	2.01	0.41
2:2:477:A:H2	2:2:509:G:H22	1.68	0.41
2:2:1137:A:H2'	2:2:1138:A:C8	2.55	0.41
2:2:1427:G:N2	24:U:72:ASN:OD1	2.43	0.41
2:2:1597:C:H5''	2:2:1597:C:H6	1.85	0.41
2:2:1788:A:N1	2:2:1789:A:C6	2.88	0.41
10:G:32:ILE:HG23	10:G:53:ALA:HA	2.02	0.41
12:I:46:VAL:HG23	12:I:54:LYS:HB2	2.02	0.41
18:O:115:ILE:HD11	30:a:53:LEU:HD21	2.02	0.41
2:2:10:G:O6	2:2:1143:U:C2	2.74	0.41
2:2:40:A:N6	2:2:466:G:H1'	2.36	0.41
2:2:617:U:C4	2:2:1085:A:N6	2.89	0.41
2:2:632:U:H3	2:2:965:A:N6	2.17	0.41
2:2:765:G:O6	13:J:152:SER:OG	2.36	0.41
2:2:886:A:H61	2:2:923:A:N6	2.19	0.41
2:2:929:A:OP1	30:a:32:LYS:HE2	2.21	0.41
2:2:952:G:H2'	2:2:953:G:H8	1.85	0.41
2:2:1464:G:OP2	20:Q:139:GLN:HB3	2.21	0.41
2:2:1681:U:H2'	2:2:1682:U:O4'	2.20	0.41
2:2:1730:A:H2'	2:2:1731:C:C6	2.55	0.41
8:E:18:TRP:CZ2	8:E:43:PRO:HD3	2.55	0.41
43:o:931:ALA:HA	44:p:128:PHE:HZ	1.86	0.41
44:p:234:ASN:HD22	44:p:235:TYR:HD2	1.67	0.41
2:2:14:C:H5'	6:C:169:SER:OG	2.21	0.41
2:2:72:A:H1'	2:2:73:U:C5	2.56	0.41
2:2:630:G:H21	2:2:1103:U:P	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1176:C:H4'	2:2:1188:A:H62	1.85	0.41
2:2:1320:A:H8	2:2:1321:A:H1'	1.86	0.41
2:2:1506:U:H2'	2:2:1507:C:C6	2.55	0.41
2:2:1771:C:H2'	2:2:1772:G:H8	1.81	0.41
6:C:61:ILE:HA	6:C:66:LEU:HD12	2.02	0.41
10:G:48:TYR:CD1	10:G:113:ILE:HD11	2.54	0.41
17:N:146:ALA:HA	17:N:149:LEU:HD12	2.02	0.41
20:Q:77:GLN:O	20:Q:81:ILE:HG13	2.20	0.41
23:T:84:LYS:HG2	23:T:86:ARG:HG2	2.02	0.41
23:T:124:ILE:H	23:T:124:ILE:HG13	1.46	0.41
36:g:48:LEU:HD21	36:g:309:PHE:CZ	2.56	0.41
44:p:205:GLN:HE22	44:p:235:TYR:HA	1.85	0.41
2:2:866:G:H5'	17:N:4:MET:HE3	2.02	0.41
2:2:908:U:H2'	2:2:909:C:C6	2.56	0.41
2:2:1240:G:H1'	19:P:79:HIS:HB2	2.01	0.41
2:2:1486:G:H3'	2:2:1513:A:H61	1.86	0.41
2:2:1584:A:H5''	20:Q:136:SER:HB2	2.01	0.41
2:2:1645:U:H2'	2:2:1646:A:C8	2.55	0.41
3:3:17[A]:C:N4	43:o:41:ARG:CB	2.61	0.41
5:B:113:MET:HE2	5:B:113:MET:HB3	1.94	0.41
5:B:186:SER:O	5:B:190:PRO:CD	2.68	0.41
6:C:193:MET:HE3	6:C:198:VAL:HG21	2.02	0.41
9:F:105:ASN:HA	9:F:108:LYS:HD2	2.03	0.41
9:F:138:ALA:HB1	9:F:203:ALA:HB3	2.03	0.41
22:S:33:THR:HG22	22:S:40:ARG:HA	2.02	0.41
23:T:105:LEU:HD22	23:T:122:ARG:HD2	2.02	0.41
38:i:121:PHE:CZ	42:m:25:VAL:HG13	2.55	0.41
42:m:49:PRO:O	42:m:52:TYR:HB2	2.20	0.41
45:q:645:ILE:H	45:q:646:PRO:CD	2.34	0.41
2:2:410:C:H2'	2:2:411:A:O4'	2.21	0.41
2:2:477:A:C2	2:2:510:A:C2	3.09	0.41
2:2:822:G:H2'	2:2:823:G:O4'	2.20	0.41
2:2:1387:C:N4	2:2:1389:A:H1'	2.36	0.41
2:2:1793:U:H4'	30:a:84:VAL:HG13	2.02	0.41
7:D:105:MET:HE3	7:D:105:MET:HB3	1.99	0.41
8:E:126:VAL:HG22	8:E:139:VAL:HG21	2.03	0.41
10:G:137:ARG:HG3	10:G:177:ARG:HG3	2.02	0.41
31:b:44:THR:HG21	31:b:56:CYS:HA	2.02	0.41
40:k:371:LYS:HA	40:k:372:PRO:HD3	1.88	0.41
45:q:508:TYR:HD2	45:q:546:VAL:HG12	1.86	0.41
2:2:166:U:H5''	10:G:135:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:525:A:H2'	2:2:526:A:O4'	2.21	0.41
2:2:721:U:H4'	2:2:722:G:C8	2.55	0.41
2:2:954:A:H4'	2:2:1072:G:O2'	2.21	0.41
2:2:1581:A:H62	2:2:1610:U:H5	1.69	0.41
2:2:1598:A:HO2'	2:2:1599:G:P	2.42	0.41
8:E:101:LEU:HD23	8:E:101:LEU:HA	1.90	0.41
8:E:160:VAL:CG1	8:E:169:ILE:HG12	2.50	0.41
15:L:131:ILE:HD11	15:L:138:ASN:HD21	1.86	0.41
45:q:459:ILE:HA	45:q:460:PRO:HD3	1.89	0.41
1:1:11:C:H2'	1:1:12:G:H8	1.86	0.41
2:2:11:A:H1'	6:C:92:GLN:O	2.21	0.41
2:2:11:A:C2'	2:2:12:U:H5'	2.51	0.41
2:2:29:U:H2'	2:2:30:G:H8	1.86	0.41
2:2:42:G:H1	2:2:432:C:H42	1.67	0.41
2:2:256:A:H4'	12:I:74:ARG:HH22	1.85	0.41
2:2:843:A:H2'	2:2:844:G:C8	2.56	0.41
2:2:967:U:H5''	2:2:1032:C:O2'	2.21	0.41
2:2:1144:U:H2'	2:2:1145:G:O4'	2.21	0.41
2:2:1560:G:OP1	23:T:89:ARG:NH2	2.54	0.41
2:2:1589:C:H2'	2:2:1590:A:C8	2.56	0.41
2:2:1794:C:O2	30:a:92:ARG:HB3	2.21	0.41
5:B:187:LYS:O	5:B:190:PRO:HD2	2.21	0.41
9:F:114:ARG:HD2	20:Q:43:ILE:HD13	2.02	0.41
9:F:202:ASN:HB3	9:F:210:SER:HB2	2.03	0.41
13:J:128:LEU:HB3	13:J:134:ILE:HD12	2.02	0.41
15:L:21:THR:HG22	15:L:32:LYS:H	1.86	0.41
16:M:88:LEU:HD22	16:M:91:TRP:HE1	1.86	0.41
17:N:18:TYR:O	26:W:56:HIS:HD2	2.04	0.41
17:N:37:ILE:HG12	17:N:54:LEU:HD11	2.03	0.41
17:N:45:LEU:HD23	17:N:49:GLN:HB3	2.02	0.41
23:T:15:ILE:HG13	23:T:63:ARG:HD3	2.03	0.41
36:g:207:ASN:HB2	36:g:222:GLY:HA2	2.03	0.41
43:o:60:VAL:HG21	43:o:99:LEU:HB3	2.03	0.41
43:o:183:VAL:O	43:o:187:MET:HG2	2.21	0.41
43:o:295:ASP:HA	43:o:296:PRO:HD3	1.91	0.41
44:p:203:VAL:HB	44:p:238:PHE:HE2	1.86	0.41
44:p:472:ARG:HD2	44:p:479:PRO:HG2	2.02	0.41
2:2:188:C:H41	12:I:138:LYS:HD3	1.85	0.41
2:2:798:A:H4'	8:E:201:HIS:CD2	2.56	0.41
2:2:877:G:H2'	2:2:878:G:H8	1.86	0.41
2:2:1099:G:N3	2:2:1099:G:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1471:U:O2	2:2:1471:U:C2'	2.68	0.41
19:P:36:LEU:HB3	19:P:37:ALA:H	1.68	0.41
22:S:81:ILE:HA	22:S:82:PRO:HD3	1.97	0.41
40:k:314:ARG:HD2	40:k:344:ASN:HD21	1.86	0.41
43:o:325:SER:HA	43:o:328:ILE:HD12	2.02	0.41
44:p:548:PHE:HB3	44:p:565:ALA:HB2	2.03	0.41
2:2:290:G:H2'	2:2:291:U:C6	2.56	0.40
2:2:558:C:H2'	2:2:559:U:C6	2.55	0.40
2:2:632:U:H5'	27:X:8:GLY:HA3	2.02	0.40
2:2:1036:C:O2	26:W:16:ASN:ND2	2.54	0.40
2:2:1046:G:H2'	2:2:1047:G:O4'	2.20	0.40
2:2:1280:G:H2'	2:2:1281:U:O4'	2.20	0.40
2:2:1645:U:H2'	2:2:1646:A:H8	1.86	0.40
2:2:1742:A:H3'	2:2:1743:G:H8	1.85	0.40
4:A:67:ILE:HA	4:A:68:PRO:HD3	1.94	0.40
4:A:69:ASN:HA	4:A:70:PRO:HD3	1.87	0.40
5:B:168:ILE:O	5:B:172:LEU:HG	2.21	0.40
11:H:59:ALA:HB1	11:H:93:LEU:HD11	2.03	0.40
11:H:140:VAL:HG22	11:H:150:GLN:HG3	2.02	0.40
15:L:54:ILE:CG2	15:L:55:ASP:N	2.81	0.40
18:O:84:ARG:HH21	18:O:120:PRO:HG2	1.86	0.40
22:S:126:ARG:HG3	22:S:131:LEU:HB2	2.03	0.40
27:X:43:PHE:N	27:X:43:PHE:CD1	2.89	0.40
28:Y:7:ILE:HD12	28:Y:40:LEU:HD23	2.03	0.40
28:Y:44:LEU:HB2	28:Y:55:VAL:HG11	2.03	0.40
30:a:37:LYS:HB3	30:a:70:LYS:HE2	2.03	0.40
35:f:139:CYS:HB3	35:f:144:SER:H	1.85	0.40
36:g:278:ILE:HD12	36:g:279:ASP:HB2	2.03	0.40
45:q:340:GLN:HE22	45:q:361:GLY:HA3	1.86	0.40
45:q:483:ILE:HA	45:q:486:LEU:HD12	2.03	0.40
2:2:255:A:H2'	2:2:256:A:C1'	2.51	0.40
2:2:900:G:H2'	2:2:901:G:O4'	2.21	0.40
2:2:928:A:P	2:2:930:C:H42	2.44	0.40
2:2:1151:A:H5'	2:2:1764:A:H62	1.87	0.40
2:2:1540:G:N2	2:2:1566:C:O2'	2.54	0.40
2:2:1665:A:H2'	2:2:1666:G:O4'	2.21	0.40
2:2:1796:U:O2	2:2:1798:A:O2'	2.39	0.40
9:F:148:THR:HG23	9:F:223:ALA:HA	2.03	0.40
15:L:38:VAL:HG21	15:L:140:LEU:HD22	2.04	0.40
23:T:6:VAL:HG11	23:T:63:ARG:HG3	2.03	0.40
44:p:81:VAL:HG22	44:p:157:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:614:A:O2'	2:2:620:A:N1	2.51	0.40
2:2:1292:U:O4	2:2:1321:A:N1	2.54	0.40
4:A:34:GLU:HG3	4:A:36:TYR:CD2	2.55	0.40
8:E:139:VAL:HG11	8:E:169:ILE:HD11	2.03	0.40
12:I:98:LYS:C	12:I:100:ALA:H	2.30	0.40
38:i:21:GLY:N	38:i:22:PRO:CD	2.84	0.40
42:m:48:ARG:HD2	42:m:97:VAL:HG22	2.01	0.40
2:2:512:U:H2'	2:2:513:G:C8	2.56	0.40
2:2:789:U:C5	2:2:790:A:N9	2.90	0.40
2:2:925:A:H2'	2:2:926:C:H6	1.86	0.40
2:2:935:G:O6	30:a:15:ARG:HG3	2.22	0.40
2:2:992:A:H5'	2:2:993:G:OP2	2.22	0.40
2:2:1710:A:C6	2:2:1711:G:H1'	2.55	0.40
2:2:1712:A:H2'	2:2:1713:G:C8	2.56	0.40
4:A:177:LEU:O	4:A:181:VAL:HG23	2.20	0.40
6:C:159:LEU:HD22	6:C:226:THR:HG21	2.02	0.40
7:D:115:ILE:HG21	7:D:142:LEU:HD23	2.03	0.40
21:R:60:ARG:HB3	21:R:66:VAL:HG11	2.03	0.40
23:T:18:TYR:HB3	23:T:59:ALA:HB1	2.04	0.40
27:X:69:ARG:HD2	27:X:117:ILE:HG12	2.03	0.40
28:Y:128:LYS:HG2	28:Y:131:ARG:HH22	1.86	0.40
33:d:20:GLN:C	33:d:30:LEU:HD11	2.45	0.40
42:m:54:VAL:O	42:m:65:THR:HG21	2.21	0.40
2:2:768:C:H2'	2:2:769:A:O4'	2.22	0.40
2:2:789:U:C5	2:2:790:A:C5	3.09	0.40
2:2:981:U:H3	2:2:1018:A:H61	1.69	0.40
2:2:1286:A:N6	2:2:1328:A:H5'	2.36	0.40
2:2:1448:U:H2'	2:2:1449:C:C6	2.57	0.40
12:I:90:LEU:HG	12:I:95:THR:HB	2.03	0.40
17:N:54:LEU:HD22	17:N:60:VAL:HG21	2.03	0.40
26:W:57:ARG:HD2	31:b:26:GLN:NE2	2.36	0.40
36:g:150:ASP:HB3	36:g:179:MET:HB2	2.02	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	
4	A	217/254 (85%)	192 (88%)	16 (7%)	9 (4%)	2	12
5	B	220/255 (86%)	191 (87%)	19 (9%)	10 (4%)	2	11
6	C	218/259 (84%)	197 (90%)	16 (7%)	5 (2%)	5	23
7	D	225/237 (95%)	211 (94%)	8 (4%)	6 (3%)	4	20
8	E	258/261 (99%)	233 (90%)	21 (8%)	4 (2%)	7	32
9	F	204/227 (90%)	173 (85%)	21 (10%)	10 (5%)	1	10
10	G	228/236 (97%)	211 (92%)	15 (7%)	2 (1%)	14	46
11	H	182/190 (96%)	161 (88%)	14 (8%)	7 (4%)	2	13
12	I	184/201 (92%)	162 (88%)	12 (6%)	10 (5%)	1	8
13	J	180/188 (96%)	152 (84%)	20 (11%)	8 (4%)	2	11
14	K	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	3	17
15	L	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	4	21
16	M	113/134 (84%)	85 (75%)	20 (18%)	8 (7%)	1	4
17	N	149/151 (99%)	139 (93%)	9 (6%)	1 (1%)	18	51
18	O	127/137 (93%)	107 (84%)	13 (10%)	7 (6%)	1	8
19	P	115/142 (81%)	98 (85%)	11 (10%)	6 (5%)	1	9
20	Q	139/143 (97%)	125 (90%)	11 (8%)	3 (2%)	5	24
21	R	128/136 (94%)	110 (86%)	11 (9%)	7 (6%)	1	8
22	S	143/146 (98%)	127 (89%)	13 (9%)	3 (2%)	5	25
23	T	141/144 (98%)	132 (94%)	7 (5%)	2 (1%)	9	34
24	U	104/117 (89%)	90 (86%)	9 (9%)	5 (5%)	2	10
25	V	85/87 (98%)	80 (94%)	2 (2%)	3 (4%)	3	15
26	W	127/130 (98%)	115 (91%)	7 (6%)	5 (4%)	2	13
27	X	142/145 (98%)	126 (89%)	12 (8%)	4 (3%)	4	19
28	Y	132/135 (98%)	123 (93%)	5 (4%)	4 (3%)	3	18
29	Z	76/108 (70%)	62 (82%)	10 (13%)	4 (5%)	1	8
30	a	101/119 (85%)	84 (83%)	11 (11%)	6 (6%)	1	7
31	b	79/82 (96%)	68 (86%)	9 (11%)	2 (2%)	4	21
32	c	62/67 (92%)	55 (89%)	5 (8%)	2 (3%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	d	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
34	e	58/63 (92%)	44 (76%)	9 (16%)	5 (9%)	0	2
35	f	72/150 (48%)	57 (79%)	13 (18%)	2 (3%)	4	19
36	g	314/326 (96%)	276 (88%)	29 (9%)	9 (3%)	3	18
37	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	119/153 (78%)	102 (86%)	11 (9%)	6 (5%)	1	9
39	j	243/304 (80%)	213 (88%)	25 (10%)	5 (2%)	5	25
40	k	388/527 (74%)	333 (86%)	47 (12%)	8 (2%)	5	25
41	l	120/285 (42%)	109 (91%)	11 (9%)	0	100	100
42	m	145/405 (36%)	126 (87%)	17 (12%)	2 (1%)	9	34
43	o	519/964 (54%)	483 (93%)	30 (6%)	6 (1%)	10	38
44	p	637/763 (84%)	583 (92%)	43 (7%)	11 (2%)	7	30
45	q	538/812 (66%)	490 (91%)	39 (7%)	9 (2%)	7	30
46	r	47/274 (17%)	43 (92%)	4 (8%)	0	100	100
47	s	326/347 (94%)	311 (95%)	15 (5%)	0	100	100
All	All	7928/10147 (78%)	7065 (89%)	650 (8%)	213 (3%)	6	20

All (213) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	C	141	VAL
7	D	220	PRO
9	F	104	ARG
11	H	64	VAL
11	H	74	GLN
12	I	22	ARG
12	I	153	ILE
13	J	169	PRO
16	M	82	VAL
16	M	84	ASP
18	O	91	SER
18	O	124	ASP
19	P	36	LEU
24	U	17	VAL
24	U	96	PRO
25	V	30	SER
26	W	58	SER

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Mol	Chain	Res	Type
27	X	63	GLN
30	a	36	ILE
34	e	54	ARG
38	i	31	GLU
38	i	66	ARG
38	i	116	ASN
44	p	337	PRO
44	p	392	PRO
4	A	206	ASN
5	B	19	ARG
5	B	214	LYS
7	D	221	SER
9	F	44	LEU
9	F	103	GLY
10	G	122	GLU
11	H	163	ASP
12	I	40	THR
12	I	147	ARG
13	J	118	LEU
15	L	3	THR
15	L	55	ASP
16	M	110	SER
17	N	3	ARG
18	O	51	ASP
18	O	114	ARG
19	P	89	MET
20	Q	138	PHE
21	R	99	VAL
21	R	117	LEU
22	S	85	PHE
25	V	12	TYR
27	X	3	LYS
28	Y	4	ALA
29	Z	55	PRO
29	Z	56	THR
34	e	47	VAL
34	e	48	THR
36	g	4	SER
36	g	195	ILE
38	i	4	LYS
39	j	81	GLY
40	k	122	GLY

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Mol	Chain	Res	Type
42	m	12	PRO
44	p	423	PRO
4	A	26	ALA
4	A	202	TYR
5	B	51	SER
5	B	131	ASP
5	B	148	ASN
7	D	197	SER
9	F	37	GLN
9	F	127	THR
11	H	10	SER
12	I	94	ASN
13	J	146	PHE
13	J	171	ARG
14	K	64	TYR
16	M	50	GLY
16	M	98	ASP
18	O	40	ALA
18	O	126	THR
19	P	69	GLU
20	Q	97	VAL
21	R	5	ARG
21	R	92	ASP
26	W	29	PRO
26	W	72	CYS
30	a	13	LYS
30	a	59	TYR
32	c	6	PRO
36	g	64	GLY
36	g	119	ASN
36	g	146	LEU
38	i	22	PRO
39	j	64	ARG
40	k	127	ARG
40	k	497	GLU
40	k	507	LYS
43	o	62	LEU
43	o	63	LYS
43	o	251	GLU
44	p	77	GLN
45	q	460	PRO
45	q	468	THR

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Mol	Chain	Res	Type
45	q	536	ASP
45	q	558	CYS
4	A	158	VAL
4	A	195	TRP
4	A	207	PRO
6	C	151	THR
6	C	253	THR
8	E	77	ARG
8	E	245	LYS
9	F	205	LYS
11	H	14	THR
11	H	98	ILE
12	I	99	ALA
12	I	120	SER
13	J	93	LEU
14	K	23	ALA
16	M	77	VAL
16	M	81	LYS
16	M	122	GLN
19	P	87	PRO
20	Q	113	ASP
21	R	90	ALA
21	R	116	LYS
23	T	28	LEU
23	T	35	ASP
24	U	77	LYS
25	V	81	ASN
27	X	41	SER
30	a	100	ARG
31	b	75	GLU
34	e	11	ALA
34	e	52	GLY
36	g	120	SER
36	g	161	ASN
36	g	290	LYS
38	i	97	LEU
44	p	634	GLU
45	q	645	ILE
45	q	650	LYS
4	A	93	THR
5	B	54	LEU
5	B	221	PRO

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Mol	Chain	Res	Type
5	B	224	ASP
6	C	40	TRP
8	E	195	ILE
10	G	152	ASP
12	I	52	ASN
12	I	148	ALA
13	J	134	ILE
14	K	26	ASP
15	L	4	GLU
15	L	7	VAL
18	O	42	VAL
21	R	88	VAL
22	S	91	ASP
24	U	73	GLY
24	U	89	ARG
26	W	30	SER
28	Y	36	SER
29	Z	36	ALA
30	a	64	LEU
35	f	111	GLU
40	k	383	GLU
40	k	408	ARG
42	m	5	ILE
43	o	49	GLU
43	o	394	ASN
44	p	207	ASP
44	p	569	PRO
45	q	514	LYS
45	q	779	GLU
4	A	68	PRO
5	B	207	LEU
6	C	155	GLN
7	D	219	GLU
9	F	42	ILE
9	F	66	ILE
9	F	102	ASN
12	I	58	LEU
13	J	120	LYS
13	J	137	GLY
19	P	14	THR
28	Y	5	ILE
29	Z	69	PHE

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Mol	Chain	Res	Type
31	b	62	VAL
39	j	6	CYS
39	j	197	GLY
44	p	198	VAL
44	p	536	LYS
45	q	351	ILE
5	B	206	PRO
27	X	4	GLY
36	g	201	GLY
40	k	225	PRO
43	o	933	PRO
44	p	422	VAL
4	A	103	THR
9	F	23	VAL
22	S	92	VAL
30	a	98	PRO
32	c	47	PRO
35	f	88	PRO
7	D	43	PRO
44	p	478	ILE
7	D	4	ILE
19	P	37	ALA
26	W	83	ILE
39	j	226	PRO
8	E	204	GLY
11	H	75	ILE
28	Y	35	VAL
40	k	282	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	180/211 (85%)	149 (83%)	31 (17%)	2	10
5	B	201/228 (88%)	178 (89%)	23 (11%)	5	22
6	C	177/203 (87%)	152 (86%)	25 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	188/196 (96%)	157 (84%)	31 (16%)	2	11
8	E	223/224 (100%)	182 (82%)	41 (18%)	1	8
9	F	174/194 (90%)	141 (81%)	33 (19%)	1	8
10	G	192/200 (96%)	162 (84%)	30 (16%)	2	12
11	H	164/170 (96%)	135 (82%)	29 (18%)	2	9
12	I	147/159 (92%)	123 (84%)	24 (16%)	2	11
13	J	153/158 (97%)	132 (86%)	21 (14%)	3	16
14	K	88/96 (92%)	77 (88%)	11 (12%)	4	19
15	L	136/137 (99%)	122 (90%)	14 (10%)	7	27
16	M	93/109 (85%)	82 (88%)	11 (12%)	5	21
17	N	128/128 (100%)	118 (92%)	10 (8%)	11	38
18	O	97/104 (93%)	80 (82%)	17 (18%)	2	9
19	P	99/119 (83%)	84 (85%)	15 (15%)	3	13
20	Q	117/119 (98%)	101 (86%)	16 (14%)	3	16
21	R	116/124 (94%)	105 (90%)	11 (10%)	8	30
22	S	127/129 (98%)	110 (87%)	17 (13%)	4	17
23	T	117/118 (99%)	99 (85%)	18 (15%)	2	13
24	U	96/107 (90%)	80 (83%)	16 (17%)	2	11
25	V	73/73 (100%)	71 (97%)	2 (3%)	39	70
26	W	110/111 (99%)	101 (92%)	9 (8%)	10	36
27	X	119/120 (99%)	104 (87%)	15 (13%)	4	19
28	Y	108/109 (99%)	95 (88%)	13 (12%)	5	20
29	Z	59/88 (67%)	52 (88%)	7 (12%)	5	21
30	a	85/100 (85%)	77 (91%)	8 (9%)	8	30
31	b	71/72 (99%)	61 (86%)	10 (14%)	3	15
32	c	55/59 (93%)	48 (87%)	7 (13%)	4	18
33	d	47/48 (98%)	40 (85%)	7 (15%)	3	14
34	e	51/55 (93%)	43 (84%)	8 (16%)	2	12
35	f	60/133 (45%)	52 (87%)	8 (13%)	4	17
36	g	264/272 (97%)	234 (89%)	30 (11%)	5	22
37	h	23/23 (100%)	20 (87%)	3 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	i	100/130 (77%)	83 (83%)	17 (17%)	2	10
39	j	224/274 (82%)	194 (87%)	30 (13%)	4	17
40	k	332/449 (74%)	311 (94%)	21 (6%)	16	46
41	l	119/246 (48%)	114 (96%)	5 (4%)	26	59
42	m	125/352 (36%)	105 (84%)	20 (16%)	2	12
43	o	406/846 (48%)	378 (93%)	28 (7%)	14	43
44	p	544/693 (78%)	533 (98%)	11 (2%)	48	75
45	q	506/523 (97%)	482 (95%)	24 (5%)	23	56
46	r	40/232 (17%)	39 (98%)	1 (2%)	42	71
47	s	287/301 (95%)	282 (98%)	5 (2%)	53	77
All	All	6821/8542 (80%)	6088 (89%)	733 (11%)	8	25

All (733) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	LEU
4	A	6	THR
4	A	17	LEU
4	A	18	LEU
4	A	24	LEU
4	A	33	GLN
4	A	34	GLU
4	A	37	VAL
4	A	54	TRP
4	A	55	GLU
4	A	58	VAL
4	A	80	THR
4	A	86	VAL
4	A	93	THR
4	A	108	THR
4	A	111	ILE
4	A	116	LYS
4	A	120	LEU
4	A	121	VAL
4	A	123	VAL
4	A	133	ILE
4	A	154	GLU
4	A	157	ASP

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Mol	Chain	Res	Type
4	A	162	CYS
4	A	172	LEU
4	A	182	LEU
4	A	184	LEU
4	A	185	ARG
4	A	188	LEU
4	A	191	ARG
4	A	212	GLN
5	B	26	ARG
5	B	32	ILE
5	B	37	THR
5	B	72	ASP
5	B	82	ARG
5	B	83	LYS
5	B	84	VAL
5	B	103	MET
5	B	105	PHE
5	B	107	THR
5	B	110	LEU
5	B	111	ARG
5	B	120	LEU
5	B	127	VAL
5	B	137	ILE
5	B	140	ILE
5	B	152	ARG
5	B	160	HIS
5	B	177	GLN
5	B	181	LEU
5	B	184	LEU
5	B	188	LEU
5	B	213	ARG
6	C	51	LYS
6	C	58	ILE
6	C	63	LEU
6	C	68	VAL
6	C	70	GLU
6	C	72	GLN
6	C	91	VAL
6	C	95	THR
6	C	99	GLN
6	C	102	ARG
6	C	109	VAL

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Mol	Chain	Res	Type
6	C	116	VAL
6	C	118	LEU
6	C	131	ARG
6	C	141	VAL
6	C	145	ARG
6	C	146	ARG
6	C	153	LEU
6	C	159	LEU
6	C	206	THR
6	C	223	ILE
6	C	230	LEU
6	C	238	GLN
6	C	240	LEU
6	C	241	THR
7	D	11	LEU
7	D	12	VAL
7	D	31	GLU
7	D	41	VAL
7	D	62	ASN
7	D	66	ILE
7	D	70	THR
7	D	71	LEU
7	D	75	LYS
7	D	81	ARG
7	D	84	ILE
7	D	91	VAL
7	D	96	LEU
7	D	103	GLU
7	D	110	LEU
7	D	117	ARG
7	D	120	TYR
7	D	122	VAL
7	D	123	VAL
7	D	142	LEU
7	D	143	ARG
7	D	157	LEU
7	D	162	GLN
7	D	164	VAL
7	D	170	THR
7	D	173	ARG
7	D	176	LEU
7	D	178	ARG

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Mol	Chain	Res	Type
7	D	214	GLU
7	D	226	ARG
7	D	228	THR
8	E	6	LYS
8	E	9	LEU
8	E	18	TRP
8	E	19	MET
8	E	23	LEU
8	E	38	LEU
8	E	39	ARG
8	E	42	LEU
8	E	49	ARG
8	E	51	ARG
8	E	57	ASN
8	E	77	ARG
8	E	80	THR
8	E	81	THR
8	E	93	GLU
8	E	96	ASN
8	E	100	ARG
8	E	106	LYS
8	E	108	ARG
8	E	111	VAL
8	E	113	ARG
8	E	114	ILE
8	E	123	LEU
8	E	128	LYS
8	E	130	GLN
8	E	155	LYS
8	E	160	VAL
8	E	163	ASP
8	E	173	ILE
8	E	181	VAL
8	E	198	ARG
8	E	200	ARG
8	E	206	ASP
8	E	208	VAL
8	E	220	THR
8	E	221	ARG
8	E	225	VAL
8	E	238	LEU
8	E	248	ILE

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Mol	Chain	Res	Type
8	E	254	ARG
8	E	259	HIS
9	F	29	THR
9	F	31	ILE
9	F	34	GLU
9	F	40	GLN
9	F	41	GLU
9	F	60	LEU
9	F	65	GLN
9	F	70	ILE
9	F	78	ARG
9	F	88	GLN
9	F	92	VAL
9	F	110	LEU
9	F	116	VAL
9	F	121	GLU
9	F	137	ASP
9	F	145	ARG
9	F	148	THR
9	F	149	THR
9	F	150	ARG
9	F	158	ARG
9	F	160	GLN
9	F	163	ASP
9	F	169	ARG
9	F	172	GLN
9	F	183	GLU
9	F	187	ARG
9	F	189	ILE
9	F	192	ILE
9	F	196	LEU
9	F	198	GLU
9	F	209	THR
9	F	213	ILE
9	F	219	LEU
10	G	1	MET
10	G	15	CYS
10	G	26	VAL
10	G	29	ASP
10	G	52	ILE
10	G	56	ASN
10	G	67	VAL

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Mol	Chain	Res	Type
10	G	68	LEU
10	G	69	LEU
10	G	75	LEU
10	G	76	LEU
10	G	106	LEU
10	G	108	VAL
10	G	111	LEU
10	G	125	THR
10	G	127	ASP
10	G	132	ARG
10	G	133	LEU
10	G	153	VAL
10	G	154	ARG
10	G	170	THR
10	G	177	ARG
10	G	180	THR
10	G	184	LEU
10	G	189	GLN
10	G	199	GLN
10	G	203	GLU
10	G	212	LEU
10	G	222	GLU
10	G	226	VAL
11	H	11	GLN
11	H	15	GLU
11	H	18	LEU
11	H	19	GLN
11	H	27	LEU
11	H	38	LEU
11	H	39	ARG
11	H	51	VAL
11	H	71	HIS
11	H	74	GLN
11	H	75	ILE
11	H	80	GLU
11	H	81	LEU
11	H	86	GLN
11	H	88	ARG
11	H	93	LEU
11	H	107	ARG
11	H	116	ARG
11	H	119	THR

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Mol	Chain	Res	Type
11	H	126	LEU
11	H	127	GLU
11	H	128	ASP
11	H	130	VAL
11	H	139	ARG
11	H	152	ILE
11	H	162	ILE
11	H	164	ASN
11	H	174	ASN
11	H	176	LEU
12	I	22	ARG
12	I	23	LYS
12	I	24	LYS
12	I	25	ARG
12	I	29	LEU
12	I	32	GLN
12	I	35	ASN
12	I	38	ILE
12	I	43	ILE
12	I	46	VAL
12	I	47	ARG
12	I	58	LEU
12	I	72	VAL
12	I	77	ARG
12	I	92	ARG
12	I	96	LEU
12	I	104	ILE
12	I	139	ASN
12	I	153	ILE
12	I	155	HIS
12	I	176	GLN
12	I	179	ARG
12	I	190	LEU
12	I	196	ARG
13	J	6	ARG
13	J	7	THR
13	J	8	TYR
13	J	25	ASP
13	J	28	LEU
13	J	33	GLU
13	J	37	LYS
13	J	45	ILE

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Mol	Chain	Res	Type
13	J	49	LEU
13	J	60	LEU
13	J	64	GLU
13	J	70	LEU
13	J	93	LEU
13	J	107	ARG
13	J	109	LEU
13	J	131	GLN
13	J	142	ASN
13	J	149	ARG
13	J	150	LEU
13	J	161	THR
13	J	183	GLU
14	K	15	LEU
14	K	34	GLU
14	K	35	ILE
14	K	39	ASN
14	K	40	LEU
14	K	49	LEU
14	K	76	LEU
14	K	81	ASN
14	K	82	LEU
14	K	84	GLU
14	K	86	ILE
15	L	10	GLU
15	L	19	ILE
15	L	30	LYS
15	L	36	LYS
15	L	56	LYS
15	L	67	ARG
15	L	70	ILE
15	L	83	THR
15	L	84	ILE
15	L	111	VAL
15	L	117	VAL
15	L	125	VAL
15	L	131	ILE
15	L	136	ARG
16	M	26	ARG
16	M	34	LEU
16	M	38	LEU
16	M	40	GLU

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Mol	Chain	Res	Type
16	M	52	LEU
16	M	61	GLU
16	M	79	LEU
16	M	88	LEU
16	M	91	TRP
16	M	97	ILE
16	M	106	VAL
17	N	3	ARG
17	N	9	LYS
17	N	83	GLU
17	N	88	LEU
17	N	99	ARG
17	N	100	LYS
17	N	107	LYS
17	N	115	LEU
17	N	116	ILE
17	N	121	ARG
18	O	24	ASN
18	O	37	GLU
18	O	47	LYS
18	O	48	VAL
18	O	49	LYS
18	O	65	GLN
18	O	72	LYS
18	O	76	ILE
18	O	86	THR
18	O	92	LYS
18	O	93	THR
18	O	102	LEU
18	O	112	ILE
18	O	114	ARG
18	O	124	ASP
18	O	126	THR
18	O	137	LEU
19	P	26	LEU
19	P	49	LEU
19	P	51	GLU
19	P	56	LEU
19	P	58	LYS
19	P	60	LEU
19	P	72	LYS
19	P	83	MET

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Mol	Chain	Res	Type
19	P	85	ILE
19	P	94	VAL
19	P	106	GLU
19	P	110	GLU
19	P	111	MET
19	P	126	VAL
19	P	127	ARG
20	Q	22	VAL
20	Q	26	LYS
20	Q	52	LEU
20	Q	63	ILE
20	Q	69	VAL
20	Q	78	VAL
20	Q	82	ARG
20	Q	83	GLN
20	Q	87	LYS
20	Q	89	LEU
20	Q	105	LEU
20	Q	107	LYS
20	Q	116	LEU
20	Q	123	ARG
20	Q	127	LYS
20	Q	137	ARG
21	R	9	VAL
21	R	29	GLN
21	R	37	GLU
21	R	42	GLN
21	R	46	LEU
21	R	77	GLU
21	R	82	ASP
21	R	100	LEU
21	R	106	THR
21	R	109	LEU
21	R	115	LEU
22	S	3	LEU
22	S	15	LEU
22	S	26	ILE
22	S	40	ARG
22	S	41	ARG
22	S	73	MET
22	S	97	ASP
22	S	101	LEU

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Mol	Chain	Res	Type
22	S	105	LEU
22	S	106	GLU
22	S	108	LYS
22	S	111	ASP
22	S	114	GLU
22	S	117	LYS
22	S	123	ARG
22	S	133	VAL
22	S	136	GLN
23	T	15	ILE
23	T	16	ASN
23	T	17	ASN
23	T	23	GLN
23	T	48	GLN
23	T	65	ILE
23	T	67	LEU
23	T	68	ARG
23	T	86	ARG
23	T	88	VAL
23	T	110	LYS
23	T	116	ILE
23	T	124	ILE
23	T	126	ASP
23	T	129	LEU
23	T	132	LEU
23	T	140	LEU
23	T	142	ASP
24	U	17	VAL
24	U	22	ILE
24	U	27	THR
24	U	31	VAL
24	U	33	GLN
24	U	52	LYS
24	U	56	VAL
24	U	57	ARG
24	U	65	ILE
24	U	74	GLU
24	U	86	ILE
24	U	99	ILE
24	U	100	VAL
24	U	108	ILE
24	U	112	VAL

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Mol	Chain	Res	Type
24	U	118	ILE
25	V	12	TYR
25	V	69	LEU
26	W	7	LEU
26	W	24	GLN
26	W	25	VAL
26	W	28	ARG
26	W	47	ILE
26	W	83	ILE
26	W	88	LYS
26	W	104	LEU
26	W	129	VAL
27	X	16	ARG
27	X	57	ILE
27	X	59	ILE
27	X	62	LYS
27	X	72	VAL
27	X	79	ASN
27	X	93	LEU
27	X	94	ASN
27	X	100	ASP
27	X	103	LEU
27	X	107	PHE
27	X	117	ILE
27	X	127	VAL
27	X	141	GLU
27	X	144	ARG
28	Y	8	ARG
28	Y	34	ASN
28	Y	35	VAL
28	Y	74	LEU
28	Y	84	LYS
28	Y	90	ARG
28	Y	99	LYS
28	Y	105	ARG
28	Y	106	GLN
28	Y	111	ARG
28	Y	117	LYS
28	Y	121	THR
28	Y	128	LYS
29	Z	41	VAL
29	Z	46	LYS

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Mol	Chain	Res	Type
29	Z	58	ARG
29	Z	65	LEU
29	Z	75	LEU
29	Z	81	ARG
29	Z	92	VAL
30	a	12	LYS
30	a	38	ARG
30	a	53	LEU
30	a	59	TYR
30	a	64	LEU
30	a	75	ILE
30	a	83	ILE
30	a	84	VAL
31	b	3	LEU
31	b	24	LEU
31	b	31	HIS
31	b	43	ILE
31	b	44	THR
31	b	52	THR
31	b	57	GLU
31	b	63	LEU
31	b	67	THR
31	b	82	LYS
32	c	14	LYS
32	c	26	THR
32	c	49	ARG
32	c	50	GLU
32	c	58	GLU
32	c	64	ARG
32	c	66	LEU
33	d	16	LYS
33	d	19	ARG
33	d	20	GLN
33	d	30	LEU
33	d	38	ILE
33	d	39	ASP
33	d	41	GLN
34	e	8	LEU
34	e	10	ARG
34	e	17	GLN
34	e	24	GLN
34	e	36	LYS

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Mol	Chain	Res	Type
34	e	37	ARG
34	e	53	LYS
34	e	55	LYS
35	f	81	LYS
35	f	83	LYS
35	f	87	THR
35	f	91	ILE
35	f	96	LYS
35	f	99	LYS
35	f	102	VAL
35	f	135	ASP
36	g	6	ILE
36	g	8	LEU
36	g	11	ARG
36	g	54	GLN
36	g	59	VAL
36	g	66	SER
36	g	70	GLN
36	g	72	VAL
36	g	87	ASP
36	g	94	ASN
36	g	101	GLU
36	g	114	VAL
36	g	130	LYS
36	g	180	ASP
36	g	181	LYS
36	g	188	LEU
36	g	195	ILE
36	g	196	GLU
36	g	206	ILE
36	g	207	ASN
36	g	209	VAL
36	g	210	GLN
36	g	223	LYS
36	g	246	GLU
36	g	250	LEU
36	g	256	ARG
36	g	259	LEU
36	g	280	GLU
36	g	290	LYS
36	g	308	LEU
37	h	10	THR

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Mol	Chain	Res	Type
37	h	13	LEU
37	h	16	LYS
38	i	3	LYS
38	i	5	ASN
38	i	23	LYS
38	i	34	GLU
38	i	39	THR
38	i	42	LEU
38	i	44	ASN
38	i	47	VAL
38	i	56	LYS
38	i	75	ASP
38	i	77	ILE
38	i	82	ARG
38	i	90	ASP
38	i	92	VAL
38	i	96	ASN
38	i	109	LEU
38	i	119	ASP
39	j	11	ASN
39	j	18	ASP
39	j	19	ILE
39	j	27	ILE
39	j	37	LEU
39	j	39	TYR
39	j	42	ILE
39	j	45	MET
39	j	46	ILE
39	j	62	LEU
39	j	63	ILE
39	j	79	GLU
39	j	84	ASP
39	j	96	ILE
39	j	97	LYS
39	j	124	GLU
39	j	126	LEU
39	j	163	LYS
39	j	165	VAL
39	j	169	LEU
39	j	187	ASP
39	j	195	TYR
39	j	198	ILE

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Mol	Chain	Res	Type
39	j	203	ASP
39	j	230	LEU
39	j	235	LEU
39	j	241	ILE
39	j	244	LEU
39	j	251	ILE
39	j	255	ILE
40	k	105	THR
40	k	136	ILE
40	k	228	GLN
40	k	236	ILE
40	k	311	ILE
40	k	315	LEU
40	k	318	ILE
40	k	352	GLU
40	k	359	ILE
40	k	395	LEU
40	k	402	VAL
40	k	403	ASP
40	k	406	LEU
40	k	426	ILE
40	k	432	ILE
40	k	437	LEU
40	k	475	VAL
40	k	494	GLU
40	k	495	ILE
40	k	508	HIS
40	k	511	LEU
41	l	180	ILE
41	l	191	LEU
41	l	211	LEU
41	l	213	ILE
41	l	242	ILE
42	m	5	ILE
42	m	8	ASP
42	m	15	ARG
42	m	24	LYS
42	m	25	VAL
42	m	28	ARG
42	m	34	THR
42	m	36	VAL
42	m	39	VAL

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Mol	Chain	Res	Type
42	m	48	ARG
42	m	53	ILE
42	m	71	LYS
42	m	81	GLU
42	m	111	ILE
42	m	113	LYS
42	m	117	LEU
42	m	118	VAL
42	m	130	MET
42	m	132	LEU
42	m	142	LYS
43	o	16	ASP
43	o	25	GLN
43	o	56	LEU
43	o	72	LEU
43	o	84	GLU
43	o	104	ILE
43	o	152	THR
43	o	172	ASN
43	o	178	THR
43	o	183	VAL
43	o	217	GLN
43	o	229	ASP
43	o	239	GLN
43	o	248	VAL
43	o	278	THR
43	o	292	VAL
43	o	303	TRP
43	o	309	LEU
43	o	330	LEU
43	o	346	ASP
43	o	355	LEU
43	o	356	ASN
43	o	381	ASP
43	o	384	LEU
43	o	397	VAL
43	o	421	ILE
43	o	476	ASP
43	o	480	ILE
44	p	77	GLN
44	p	79	ILE
44	p	158	TYR

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Mol	Chain	Res	Type
44	p	277	VAL
44	p	418	THR
44	p	422	VAL
44	p	470	ILE
44	p	485	LEU
44	p	489	VAL
44	p	599	LEU
44	p	616	ASP
45	q	258	LEU
45	q	273	GLN
45	q	275	LEU
45	q	305	ASP
45	q	315	ILE
45	q	324	ASP
45	q	335	THR
45	q	336	ILE
45	q	352	GLU
45	q	407	LEU
45	q	438	ASP
45	q	490	LEU
45	q	532	ILE
45	q	557	LEU
45	q	567	LEU
45	q	588	ILE
45	q	611	HIS
45	q	630	ILE
45	q	644	ARG
45	q	645	ILE
45	q	656	LEU
45	q	676	LEU
45	q	754	GLU
45	q	783	GLU
46	r	74	ARG
47	s	64	THR
47	s	147	ILE
47	s	157	THR
47	s	158	VAL
47	s	286	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (167) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	69	ASN
4	A	83	GLN
4	A	109	ASN
4	A	168	HIS
5	B	92	GLN
5	B	95	ASN
5	B	124	ASN
5	B	163	GLN
5	B	194	ASN
5	B	211	HIS
6	C	64	HIS
6	C	233	ASN
7	D	111	ASN
7	D	159	HIS
7	D	179	GLN
8	E	50	ASN
8	E	112	HIS
8	E	130	GLN
8	E	142	HIS
9	F	37	GLN
9	F	39	GLN
9	F	65	GLN
9	F	102	ASN
9	F	133	GLN
9	F	188	ASN
10	G	10	ASN
10	G	139	ASN
10	G	197	ASN
10	G	201	GLN
11	H	22	GLN
11	H	74	GLN
11	H	110	GLN
11	H	150	GLN
11	H	170	GLN
12	I	64	ASN
12	I	116	HIS
12	I	119	GLN
13	J	110	GLN
13	J	112	GLN
13	J	142	ASN
13	J	155	HIS
14	K	13	GLN
14	K	39	ASN

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Mol	Chain	Res	Type
14	K	81	ASN
14	K	85	HIS
15	L	8	GLN
15	L	138	ASN
16	M	69	GLN
16	M	116	ASN
17	N	49	GLN
17	N	62	GLN
17	N	69	ASN
17	N	105	ASN
18	O	10	ASN
18	O	29	HIS
18	O	99	GLN
19	P	82	ASN
19	P	104	GLN
20	Q	8	GLN
20	Q	74	HIS
20	Q	83	GLN
21	R	101	ASN
21	R	105	GLN
22	S	44	ASN
22	S	71	GLN
22	S	87	ASN
22	S	89	GLN
22	S	99	HIS
22	S	136	GLN
23	T	43	ASN
23	T	64	HIS
23	T	70	GLN
23	T	85	ASN
23	T	101	ASN
24	U	36	ASN
24	U	105	GLN
25	V	21	ASN
26	W	24	GLN
26	W	42	GLN
26	W	64	GLN
26	W	66	ASN
26	W	80	ASN
26	W	92	ASN
27	X	10	ASN
28	Y	15	ASN

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Mol	Chain	Res	Type
28	Y	22	GLN
28	Y	29	HIS
28	Y	106	GLN
29	Z	85	ASN
30	a	11	ASN
30	a	17	HIS
30	a	80	HIS
31	b	26	GLN
31	b	49	HIS
32	c	43	ASN
33	d	41	GLN
34	e	46	ASN
35	f	132	ASN
36	g	94	ASN
36	g	189	ASN
36	g	203	ASN
36	g	226	GLN
36	g	295	HIS
36	g	321	GLN
38	i	85	GLN
38	i	116	ASN
39	j	23	ASN
39	j	26	GLN
39	j	41	ASN
39	j	60	GLN
39	j	103	GLN
39	j	109	HIS
40	k	98	GLN
40	k	243	HIS
40	k	248	GLN
40	k	286	GLN
40	k	295	ASN
40	k	344	ASN
40	k	376	ASN
40	k	384	GLN
40	k	415	GLN
40	k	433	ASN
40	k	465	ASN
41	l	140	ASN
41	l	178	GLN
41	l	193	GLN
41	l	218	GLN

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Mol	Chain	Res	Type
41	l	252	ASN
42	m	44	HIS
42	m	64	GLN
42	m	134	HIS
43	o	25	GLN
43	o	194	GLN
43	o	216	GLN
43	o	243	GLN
43	o	254	HIS
43	o	281	ASN
43	o	299	HIS
43	o	356	ASN
43	o	394	ASN
43	o	403	GLN
44	p	135	ASN
44	p	145	HIS
44	p	215	ASN
44	p	230	ASN
44	p	234	ASN
44	p	311	GLN
44	p	412	ASN
44	p	570	ASN
44	p	592	ASN
44	p	712	GLN
45	q	309	ASN
45	q	340	GLN
45	q	406	ASN
45	q	412	GLN
45	q	457	ASN
45	q	495	ASN
45	q	506	ASN
45	q	529	GLN
45	q	540	GLN
45	q	582	GLN
45	q	586	HIS
45	q	595	ASN
45	q	686	ASN
47	s	145	HIS
47	s	150	HIS
47	s	219	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	72/76 (94%)	29 (40%)	8 (11%)
2	2	1777/1798 (98%)	659 (37%)	72 (4%)
3	3	27/49 (55%)	16 (59%)	4 (14%)
All	All	1876/1923 (97%)	704 (37%)	84 (4%)

All (704) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	G
1	1	5	C
1	1	8	U
1	1	9	1MG
1	1	10	2MG
1	1	15	G
1	1	16	H2U
1	1	19	G
1	1	20	A
1	1	21	A
1	1	22	G
1	1	23	C
1	1	26	M2G
1	1	42	U
1	1	44	A
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	49	5MC
1	1	58	1MA
1	1	59	A
1	1	60	A
1	1	61	C
1	1	64	RIA
1	1	69	C
1	1	71	C
1	1	74	C
1	1	75	C
1	1	76	A
2	2	2	A
2	2	3	U
2	2	4	C
2	2	5	U
2	2	13	C
2	2	16	G

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Mol	Chain	Res	Type
2	2	17	C
2	2	25	C
2	2	27	U
2	2	34	G
2	2	42	G
2	2	44	U
2	2	45	U
2	2	46	A
2	2	47	A
2	2	50	C
2	2	57	G
2	2	58	U
2	2	59	C
2	2	60	U
2	2	61	A
2	2	64	U
2	2	66	U
2	2	67	A
2	2	68	A
2	2	69	G
2	2	72	A
2	2	73	U
2	2	74	U
2	2	75	U
2	2	76	A
2	2	77	U
2	2	78	A
2	2	79	C
2	2	100	A
2	2	104	A
2	2	111	U
2	2	114	C
2	2	115	G
2	2	121	U
2	2	123	G
2	2	124	A
2	2	126	A
2	2	127	G
2	2	128	U
2	2	129	U
2	2	130	C
2	2	131	C

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Mol	Chain	Res	Type
2	2	132	U
2	2	133	U
2	2	135	A
2	2	136	C
2	2	137	U
2	2	139	C
2	2	140	A
2	2	141	U
2	2	143	G
2	2	144	A
2	2	146	A
2	2	147	U
2	2	150	G
2	2	158	U
2	2	159	C
2	2	160	U
2	2	161	A
2	2	167	A
2	2	172	A
2	2	173	U
2	2	176	U
2	2	177	U
2	2	178	A
2	2	184	U
2	2	186	G
2	2	187	A
2	2	190	C
2	2	191	U
2	2	192	U
2	2	194	G
2	2	195	G
2	2	209	A
2	2	214	A
2	2	217	A
2	2	218	A
2	2	220	A
2	2	223	C
2	2	226	U
2	2	227	G
2	2	228	U
2	2	232	C
2	2	233	G

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Mol	Chain	Res	Type
2	2	234	G
2	2	235	A
2	2	239	C
2	2	240	U
2	2	248	U
2	2	249	C
2	2	256	A
2	2	259	U
2	2	260	U
2	2	264	A
2	2	265	A
2	2	266	U
2	2	267	C
2	2	271	U
2	2	275	C
2	2	276	U
2	2	277	U
2	2	278	G
2	2	279	U
2	2	280	G
2	2	282	U
2	2	286	G
2	2	289	G
2	2	294	A
2	2	300	A
2	2	301	U
2	2	303	U
2	2	307	C
2	2	308	C
2	2	311	A
2	2	313	C
2	2	314	A
2	2	315	A
2	2	320	C
2	2	321	G
2	2	322	A
2	2	334	U
2	2	336	G
2	2	337	C
2	2	342	C
2	2	351	A
2	2	359	A

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Mol	Chain	Res	Type
2	2	360	C
2	2	368	A
2	2	369	A
2	2	380	C
2	2	382	G
2	2	389	G
2	2	392	C
2	2	399	A
2	2	400	A
2	2	401	C
2	2	404	C
2	2	411	A
2	2	412	U
2	2	415	A
2	2	416	A
2	2	418	G
2	2	421	G
2	2	422	G
2	2	423	C
2	2	424	A
2	2	425	G
2	2	427	A
2	2	433	G
2	2	434	C
2	2	438	U
2	2	439	U
2	2	440	A
2	2	443	C
2	2	444	A
2	2	447	C
2	2	457	G
2	2	459	A
2	2	469	A
2	2	474	A
2	2	476	A
2	2	479	G
2	2	481	U
2	2	482	A
2	2	483	C
2	2	489	C
2	2	490	C
2	2	491	A

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Mol	Chain	Res	Type
2	2	492	U
2	2	493	U
2	2	495	G
2	2	496	G
2	2	499	C
2	2	502	G
2	2	505	A
2	2	506	U
2	2	507	U
2	2	509	G
2	2	510	A
2	2	513	G
2	2	516	U
2	2	518	C
2	2	519	A
2	2	524	A
2	2	526	A
2	2	527	U
2	2	531	U
2	2	533	A
2	2	535	C
2	2	537	A
2	2	539	G
2	2	540	A
2	2	541	A
2	2	542	C
2	2	543	A
2	2	544	A
2	2	545	C
2	2	547	G
2	2	548	G
2	2	553	C
2	2	556	G
2	2	557	U
2	2	558	C
2	2	564	C
2	2	567	G
2	2	570	G
2	2	577	U
2	2	578	A
2	2	582	C
2	2	583	C

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Mol	Chain	Res	Type
2	2	584	A
2	2	593	A
2	2	594	G
2	2	597	U
2	2	598	A
2	2	600	A
2	2	605	A
2	2	609	G
2	2	610	U
2	2	614	A
2	2	618	A
2	2	619	A
2	2	620	A
2	2	621	A
2	2	622	A
2	2	623	G
2	2	637	U
2	2	638	U
2	2	639	U
2	2	641	G
2	2	647	G
2	2	649	U
2	2	651	U
2	2	652	C
2	2	653	C
2	2	654	G
2	2	655	G
2	2	657	C
2	2	677	G
2	2	678	U
2	2	680	U
2	2	684	A
2	2	686	C
2	2	691	U
2	2	693	U
2	2	694	U
2	2	695	U
2	2	696	C
2	2	697	C
2	2	698	U
2	2	701	U
2	2	702	G

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Mol	Chain	Res	Type
2	2	704	C
2	2	705	U
2	2	709	C
2	2	710	U
2	2	711	G
2	2	712	U
2	2	714	C
2	2	715	U
2	2	716	C
2	2	717	C
2	2	718	U
2	2	719	U
2	2	721	U
2	2	722	G
2	2	725	U
2	2	727	C
2	2	731	C
2	2	732	G
2	2	733	A
2	2	734	A
2	2	736	C
2	2	737	A
2	2	738	G
2	2	739	G
2	2	741	C
2	2	742	U
2	2	743	U
2	2	755	A
2	2	765	G
2	2	766	PSU
2	2	767	U
2	2	771	A
2	2	774	A
2	2	778	G
2	2	779	A
2	2	780	A
2	2	781	A
2	2	782	G
2	2	783	C
2	2	786	G
2	2	788	A
2	2	789	U

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Mol	Chain	Res	Type
2	2	792	A
2	2	793	U
2	2	794	U
2	2	809	G
2	2	811	A
2	2	812	U
2	2	813	A
2	2	814	G
2	2	817	C
2	2	819	U
2	2	820	U
2	2	822	G
2	2	823	G
2	2	826	C
2	2	827	U
2	2	828	A
2	2	829	U
2	2	832	U
2	2	839	U
2	2	840	U
2	2	845	G
2	2	847	C
2	2	854	A
2	2	855	A
2	2	859	U
2	2	862	A
2	2	863	U
2	2	872	U
2	2	874	G
2	2	876	G
2	2	881	U
2	2	885	U
2	2	895	U
2	2	896	C
2	2	897	A
2	2	898	G
2	2	899	A
2	2	905	A
2	2	911	U
2	2	912	G
2	2	913	G
2	2	914	A

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Mol	Chain	Res	Type
2	2	915	U
2	2	916	U
2	2	917	U
2	2	919	U
2	2	920	U
2	2	921	G
2	2	923	A
2	2	932	A
2	2	934	U
2	2	941	G
2	2	944	U
2	2	947	G
2	2	950	A
2	2	958	U
2	2	959	U
2	2	965	A
2	2	969	A
2	2	970	A
2	2	972	A
2	2	981	U
2	2	982	A
2	2	986	G
2	2	987	A
2	2	990	G
2	2	991	A
2	2	993	G
2	2	995	U
2	2	1009	C
2	2	1011	U
2	2	1015	C
2	2	1018	A
2	2	1020	C
2	2	1025	A
2	2	1026	A
2	2	1027	C
2	2	1030	U
2	2	1031	G
2	2	1033	C
2	2	1034	G
2	2	1038	A
2	2	1039	G
2	2	1041	G

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Mol	Chain	Res	Type
2	2	1042	A
2	2	1048	U
2	2	1049	G
2	2	1050	G
2	2	1051	U
2	2	1052	G
2	2	1054	U
2	2	1056	U
2	2	1057	U
2	2	1058	C
2	2	1059	U
2	2	1060	U
2	2	1062	U
2	2	1075	A
2	2	1081	C
2	2	1082	G
2	2	1084	G
2	2	1085	A
2	2	1086	A
2	2	1091	A
2	2	1092	A
2	2	1095	C
2	2	1096	U
2	2	1097	U
2	2	1099	G
2	2	1103	U
2	2	1104	C
2	2	1106	G
2	2	1110	G
2	2	1112	A
2	2	1113	G
2	2	1118	G
2	2	1125	G
2	2	1137	A
2	2	1142	A
2	2	1149	G
2	2	1150	A
2	2	1154	G
2	2	1155	C
2	2	1156	A
2	2	1157	C
2	2	1158	C

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Mol	Chain	Res	Type
2	2	1163	G
2	2	1166	G
2	2	1184	U
2	2	1185	U
2	2	1187	G
2	2	1189	C
2	2	1193	A
2	2	1195	A
2	2	1198	G
2	2	1199	G
2	2	1201	A
2	2	1206	C
2	2	1207	A
2	2	1211	G
2	2	1213	U
2	2	1216	A
2	2	1217	G
2	2	1224	U
2	2	1226	A
2	2	1227	G
2	2	1228	G
2	2	1230	U
2	2	1236	G
2	2	1237	A
2	2	1243	A
2	2	1244	G
2	2	1245	C
2	2	1246	U
2	2	1247	C
2	2	1249	U
2	2	1250	U
2	2	1254	G
2	2	1255	A
2	2	1256	U
2	2	1258	U
2	2	1259	U
2	2	1265	U
2	2	1268	U
2	2	1269	G
2	2	1272	G
2	2	1275	U
2	2	1283	C

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Mol	Chain	Res	Type
2	2	1284	U
2	2	1287	G
2	2	1292	U
2	2	1296	G
2	2	1298	G
2	2	1306	U
2	2	1311	A
2	2	1313	U
2	2	1314	U
2	2	1315	G
2	2	1317	G
2	2	1320	A
2	2	1321	A
2	2	1324	A
2	2	1336	A
2	2	1337	C
2	2	1338	C
2	2	1339	U
2	2	1343	A
2	2	1344	A
2	2	1345	A
2	2	1347	A
2	2	1353	G
2	2	1355	U
2	2	1360	C
2	2	1361	U
2	2	1362	U
2	2	1363	G
2	2	1364	C
2	2	1366	G
2	2	1369	U
2	2	1370	G
2	2	1379	U
2	2	1380	A
2	2	1383	G
2	2	1388	U
2	2	1389	A
2	2	1390	U
2	2	1393	G
2	2	1396	U
2	2	1397	C
2	2	1398	A

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Mol	Chain	Res	Type
2	2	1400	G
2	2	1407	G
2	2	1408	A
2	2	1409	A
2	2	1410	G
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1414	G
2	2	1416	G
2	2	1418	C
2	2	1423	A
2	2	1424	C
2	2	1425	A
2	2	1426	2MG
2	2	1429	C
2	2	1430	U
2	2	1431	G
2	2	1442	A
2	2	1443	G
2	2	1444	A
2	2	1455	C
2	2	1456	G
2	2	1457	C
2	2	1458	A
2	2	1460	G
2	2	1464	G
2	2	1467	A
2	2	1469	A
2	2	1471	U
2	2	1476	G
2	2	1479	C
2	2	1480	C
2	2	1481	A
2	2	1482	G
2	2	1483	C
2	2	1484	G
2	2	1488	A
2	2	1489	C
2	2	1490	A
2	2	1491	A
2	2	1494	U

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Mol	Chain	Res	Type
2	2	1499	C
2	2	1504	G
2	2	1510	G
2	2	1512	U
2	2	1513	A
2	2	1514	A
2	2	1515	U
2	2	1516	C
2	2	1519	G
2	2	1520	U
2	2	1521	G
2	2	1522	A
2	2	1532	G
2	2	1533	U
2	2	1534	G
2	2	1535	C
2	2	1536	U
2	2	1538	G
2	2	1544	G
2	2	1548	A
2	2	1555	U
2	2	1557	A
2	2	1558	U
2	2	1566	C
2	2	1570	2MG
2	2	1571	A
2	2	1572	G
2	2	1581	A
2	2	1588	G
2	2	1595	A
2	2	1597	C
2	2	1598	A
2	2	1599	G
2	2	1600	C
2	2	1605	G
2	2	1614	G
2	2	1616	C
2	2	1617	C
2	2	1620	G
2	2	1632	C
2	2	1633	A
2	2	1634	C

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Mol	Chain	Res	Type
2	2	1644	C
2	2	1647	G
2	2	1648	U
2	2	1655	U
2	2	1656	G
2	2	1662	C
2	2	1666	G
2	2	1667	U
2	2	1676	A
2	2	1678	G
2	2	1679	A
2	2	1682	U
2	2	1685	U
2	2	1686	U
2	2	1687	A
2	2	1688	G
2	2	1692	A
2	2	1693	G
2	2	1694	G
2	2	1695	G
2	2	1696	G
2	2	1697	G
2	2	1698	C
2	2	1699	A
2	2	1700	A
2	2	1702	U
2	2	1703	C
2	2	1705	A
2	2	1706	U
2	2	1707	C
2	2	1709	C
2	2	1710	A
2	2	1711	G
2	2	1712	A
2	2	1715	G
2	2	1725	G
2	2	1730	A
2	2	1734	G
2	2	1742	A
2	2	1743	G
2	2	1748	A
2	2	1750	U

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Mol	Chain	Res	Type
2	2	1753	A
2	2	1755	G
2	2	1758	G
2	2	1760	A
2	2	1763	A
2	2	1764	A
2	2	1766	G
2	2	1767	U
2	2	1768	U
2	2	1769	U
2	2	1778	G
2	2	1780	MA6
2	2	1781	C
2	2	1787	G
2	2	1788	A
2	2	1790	G
2	2	1791	G
2	2	1792	A
2	2	1793	U
2	2	1794	C
2	2	1796	U
2	2	1797	U
2	2	1798	A
3	3	19	A
3	3	20	A
3	3	22	U
3	3	23	A
3	3	24	U
3	3	25	A
3	3	26	A
3	3	33	C
3	3	34	U
3	3	36	U
3	3	38	C
3	3	39	U
3	3	40	C
3	3	43	U
3	3	44	C
3	3	45	U

All (84) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	7	G
1	1	8	U
1	1	43	G
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	58	1MA
1	1	74	C
2	2	3	U
2	2	16	G
2	2	44	U
2	2	66	U
2	2	74	U
2	2	126	A
2	2	128	U
2	2	130	C
2	2	131	C
2	2	176	U
2	2	190	C
2	2	216	A
2	2	217	A
2	2	239	C
2	2	275	C
2	2	277	U
2	2	279	U
2	2	321	G
2	2	336	G
2	2	399	A
2	2	451	A
2	2	467	A
2	2	542	C
2	2	544	A
2	2	597	U
2	2	685	A
2	2	693	U
2	2	695	U
2	2	700	C
2	2	710	U
2	2	721	U
2	2	780	A
2	2	781	A
2	2	810	A
2	2	826	C

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Mol	Chain	Res	Type
2	2	828	A
2	2	854	A
2	2	896	C
2	2	912	G
2	2	914	A
2	2	946	U
2	2	1057	U
2	2	1058	C
2	2	1080	A
2	2	1107	G
2	2	1198	G
2	2	1206	C
2	2	1226	A
2	2	1284	U
2	2	1320	A
2	2	1338	C
2	2	1343	A
2	2	1430	U
2	2	1455	C
2	2	1456	G
2	2	1470	C
2	2	1479	C
2	2	1513	A
2	2	1515	U
2	2	1533	U
2	2	1545	A
2	2	1570	2MG
2	2	1571	A
2	2	1599	G
2	2	1613	C
2	2	1648	U
2	2	1655	U
2	2	1678	G
2	2	1765	G
2	2	1766	G
2	2	1796	U
2	2	1797	U
3	3	22	U
3	3	33	C
3	3	35	C
3	3	38	C

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	T6A	1	37	1	31,34,35	1.41	4 (12%)	43,49,52	2.53	17 (39%)
2	7MG	2	1573	2,1	23,26,27	1.52	7 (30%)	27,39,42	2.75	6 (22%)
1	M2G	1	26	1	24,27,28	1.43	4 (16%)	33,40,43	2.06	7 (21%)
1	5MC	1	49	1	19,22,23	2.02	2 (10%)	26,32,35	1.37	4 (15%)
1	RIA	1	64	1	35,38,39	0.33	0	50,57,60	0.69	0
1	H2U	1	47	1	18,21,22	0.85	0	19,30,33	1.37	3 (15%)
2	2MG	2	1570	2	23,26,27	1.27	3 (13%)	33,38,41	2.28	7 (21%)
2	PSU	2	465	2	18,21,22	1.55	3 (16%)	21,30,33	2.04	5 (23%)
1	7MG	1	46	1	23,26,27	1.43	4 (17%)	27,39,42	2.73	9 (33%)
1	H2U	1	16	1	18,21,22	0.84	1 (5%)	19,30,33	1.68	3 (15%)
1	5MC	1	48	1	19,22,23	1.70	2 (10%)	26,32,35	1.27	3 (11%)
1	1MG	1	9	1	23,26,27	1.41	3 (13%)	33,39,42	2.09	8 (24%)
1	1MA	1	58	1	21,25,26	1.55	5 (23%)	30,37,40	1.96	5 (16%)
2	PSU	2	120	2	18,21,22	1.42	2 (11%)	21,30,33	2.08	4 (19%)
2	C4J	2	1190	2	25,29,30	0.88	1 (4%)	28,42,45	1.04	1 (3%)
1	2MG	1	10	1	23,26,27	1.29	3 (13%)	33,38,41	2.25	7 (21%)
2	2MG	2	1426	2,48	23,26,27	1.19	3 (13%)	33,38,41	3.38	12 (36%)
5	AYA	B	2	-	6,7,8	0.67	0	6,8,10	0.96	0
2	PSU	2	998	2	18,21,22	1.45	3 (16%)	21,30,33	2.08	4 (19%)
2	5MC	2	1637	2	19,22,23	1.85	2 (10%)	26,32,35	1.39	6 (23%)
2	MA6	2	1780	2	23,26,27	1.68	6 (26%)	33,38,41	2.36	10 (30%)
2	PSU	2	1289	2	18,21,22	1.51	3 (16%)	21,30,33	2.05	4 (19%)
2	5MC	2	1006	2	19,22,23	1.38	2 (10%)	26,32,35	1.70	6 (23%)
2	PSU	2	766	2	18,21,22	1.40	2 (11%)	21,30,33	2.27	5 (23%)

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
1	T6A	1	37	1	-	5/23/41/42	0/3/3/3
2	7MG	2	1573	2,1	-	2/7/37/38	0/3/3/3
1	M2G	1	26	1	-	2/11/29/30	0/3/3/3
1	5MC	1	49	1	-	2/7/25/26	0/2/2/2
1	RIA	1	64	1	-	3/17/51/52	0/4/4/4
1	H2U	1	47	1	-	4/7/38/39	0/2/2/2
2	2MG	2	1570	2	-	0/9/27/28	0/3/3/3
2	PSU	2	465	2	-	0/7/25/26	0/2/2/2
1	7MG	1	46	1	-	1/7/37/38	0/3/3/3
1	H2U	1	16	1	-	2/7/38/39	0/2/2/2
1	5MC	1	48	1	-	3/7/25/26	0/2/2/2
1	1MG	1	9	1	-	3/7/25/26	0/3/3/3
1	1MA	1	58	1	-	0/7/25/26	0/3/3/3
2	PSU	2	120	2	-	0/7/25/26	0/2/2/2
2	C4J	2	1190	2	1/1/7/7	0/16/34/35	0/2/2/2
1	2MG	1	10	1	-	2/9/27/28	0/3/3/3
2	2MG	2	1426	2,48	-	3/9/27/28	0/3/3/3
5	AYA	B	2	-	-	0/5/6/8	-
2	PSU	2	998	2	-	0/7/25/26	0/2/2/2
2	5MC	2	1637	2	-	1/7/25/26	0/2/2/2
2	MA6	2	1780	2	-	5/11/29/30	0/3/3/3
2	PSU	2	1289	2	-	0/7/25/26	0/2/2/2
2	5MC	2	1006	2	-	0/7/25/26	0/2/2/2
2	PSU	2	766	2	-	1/7/25/26	0/2/2/2

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	49	5MC	C5-C4	7.46	1.49	1.44
2	2	1637	5MC	C5-C4	6.77	1.49	1.44
1	1	48	5MC	C5-C4	5.95	1.48	1.44
2	2	1780	MA6	C5-C4	4.82	1.47	1.39
1	1	37	T6A	C5-C4	4.73	1.47	1.39
2	2	465	PSU	C6-C5	4.47	1.40	1.35
2	2	1006	5MC	C5-C4	4.46	1.47	1.44
2	2	1289	PSU	C6-C5	4.46	1.40	1.35
2	2	120	PSU	C6-C5	4.12	1.39	1.35
2	2	998	PSU	C6-C5	4.11	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	766	PSU	C6-C5	3.96	1.39	1.35
1	1	26	M2G	C2-N2	3.89	1.42	1.35
2	2	1190	C4J	C4-C5	-3.57	1.39	1.47
1	1	58	1MA	C5-C4	3.56	1.48	1.38
1	1	46	7MG	C5-C4	3.55	1.48	1.37
1	1	58	1MA	C6-N6	3.45	1.36	1.28
2	2	1780	MA6	C5-C6	3.44	1.50	1.41
1	1	9	1MG	C2-N1	3.42	1.43	1.37
1	1	9	1MG	C5-C4	3.41	1.48	1.38
2	2	1573	7MG	C5-C4	3.38	1.48	1.37
1	1	49	5MC	C6-C5	3.34	1.40	1.34
1	1	10	2MG	C5-C4	3.33	1.47	1.38
2	2	1637	5MC	C6-C5	3.31	1.40	1.34
1	1	26	M2G	C5-C4	3.24	1.47	1.38
2	2	1570	2MG	C5-C4	3.23	1.47	1.38
1	1	48	5MC	C6-C5	3.09	1.39	1.34
1	1	58	1MA	C2-N3	2.90	1.35	1.30
1	1	37	T6A	C5-C6	2.76	1.48	1.41
2	2	1573	7MG	C4-N9	-2.74	1.34	1.37
2	2	465	PSU	C4-N3	-2.73	1.33	1.38
2	2	1426	2MG	C5-C4	2.72	1.46	1.38
2	2	1573	7MG	C8-N9	2.72	1.47	1.45
2	2	1289	PSU	C4-N3	-2.63	1.33	1.38
1	1	46	7MG	C4-N9	-2.61	1.34	1.37
2	2	766	PSU	C4-N3	-2.59	1.34	1.38
2	2	1006	5MC	C6-N1	-2.53	1.33	1.38
1	1	46	7MG	C8-N9	2.46	1.47	1.45
1	1	58	1MA	C5-N7	-2.45	1.34	1.39
2	2	465	PSU	C2-N3	-2.36	1.33	1.37
2	2	1780	MA6	C5-N7	-2.34	1.34	1.39
2	2	1780	MA6	C8-N7	2.33	1.36	1.31
1	1	37	T6A	C5-N7	-2.32	1.34	1.39
1	1	46	7MG	C5-C6	2.30	1.49	1.43
2	2	998	PSU	C4-N3	-2.29	1.34	1.38
2	2	1570	2MG	C2-N3	2.29	1.36	1.32
1	1	37	T6A	C8-N7	2.29	1.36	1.31
1	1	10	2MG	C2-N3	2.28	1.36	1.32
2	2	1573	7MG	C1'-N9	2.23	1.50	1.46
1	1	10	2MG	C5-N7	-2.21	1.34	1.39
2	2	1573	7MG	C6-N1	-2.21	1.34	1.38
2	2	120	PSU	C4-N3	-2.19	1.34	1.38
1	1	26	M2G	C5-N7	-2.19	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1780	MA6	C6-N6	2.15	1.42	1.36
1	1	26	M2G	C2-N3	2.14	1.37	1.32
2	2	998	PSU	C4-C5	2.14	1.50	1.44
2	2	1573	7MG	C5-C6	2.13	1.48	1.43
2	2	1426	2MG	C5-N7	-2.10	1.34	1.39
2	2	1570	2MG	C4-N9	-2.06	1.32	1.38
2	2	1573	7MG	C5-N7	-2.05	1.33	1.35
1	1	16	H2U	C2-N3	-2.04	1.34	1.38
1	1	58	1MA	C5-C6	2.04	1.49	1.43
2	2	1289	PSU	C4-C5	2.03	1.50	1.44
1	1	9	1MG	C5-N7	-2.03	1.35	1.39
2	2	1426	2MG	C4-N9	-2.01	1.32	1.38
2	2	1780	MA6	C4-N9	-2.00	1.33	1.37

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1426	2MG	N1-C2-N2	10.66	127.44	116.56
2	2	1573	7MG	N9-C4-N3	9.04	138.71	125.46
2	2	1426	2MG	C2-N3-C4	8.92	123.16	112.00
1	1	46	7MG	N9-C4-N3	8.92	138.53	125.46
1	1	37	T6A	C12-N11-C10	8.57	136.24	121.99
1	1	10	2MG	C2-N3-C4	7.87	121.84	112.00
2	2	1570	2MG	C2-N3-C4	7.59	121.49	112.00
2	2	1426	2MG	N2-C2-N3	-7.56	110.89	120.51
2	2	1289	PSU	N1-C2-N3	6.52	122.04	115.17
1	1	26	M2G	C5-C4-N3	-6.42	118.17	128.39
2	2	465	PSU	N1-C2-N3	6.34	121.85	115.17
2	2	998	PSU	N1-C2-N3	6.34	121.85	115.17
2	2	766	PSU	N1-C2-N3	6.33	121.84	115.17
1	1	58	1MA	C5-C4-N3	-6.28	118.02	127.27
2	2	1426	2MG	C5-C4-N3	-6.12	118.65	128.39
1	1	10	2MG	C5-C4-N3	-6.06	118.75	128.39
2	2	120	PSU	N1-C2-N3	5.93	121.42	115.17
2	2	1573	7MG	C5-C4-N3	-5.86	117.14	128.13
1	1	9	1MG	C5-C4-N3	-5.59	119.50	128.39
2	2	1780	MA6	C5-C4-N3	-5.56	119.06	126.72
1	1	46	7MG	C5-C4-N3	-5.48	117.85	128.13
1	1	26	M2G	C2-N3-C4	5.46	122.60	112.51
2	2	1570	2MG	C5-C4-N3	-5.45	119.72	128.39
1	1	37	T6A	C5-C4-N3	-5.37	119.32	126.72
2	2	1573	7MG	N9-C8-N7	-5.04	96.24	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	16	H2U	O4'-C1'-N1	5.03	116.15	109.30
1	1	37	T6A	C14-C12-C13	4.98	118.72	110.03
1	1	46	7MG	N9-C8-N7	-4.96	96.35	103.37
1	1	9	1MG	C2-N3-C4	4.88	122.95	111.98
1	1	46	7MG	C2-N3-C4	4.84	120.64	112.30
2	2	1573	7MG	C2-N3-C4	4.79	120.55	112.30
1	1	26	M2G	N9-C4-N3	4.78	135.52	125.95
2	2	1780	MA6	C4-C5-N7	-4.75	105.16	110.58
1	1	58	1MA	C2-N3-C4	4.70	121.75	112.53
2	2	1780	MA6	C2-N1-C6	4.62	123.11	111.83
2	2	1426	2MG	C6-C5-N7	4.51	138.49	130.29
1	1	37	T6A	N3-C4-N9	4.35	134.56	127.17
2	2	766	PSU	C4-N3-C2	-4.28	120.47	126.37
2	2	1780	MA6	C10-N6-C6	-4.14	109.98	120.52
1	1	9	1MG	N9-C4-N3	4.13	134.21	125.95
1	1	10	2MG	N9-C4-N3	4.12	134.18	125.95
1	1	37	T6A	C2'-C1'-N9	-4.03	103.28	113.30
2	2	1006	5MC	C5-C4-N3	-4.02	117.63	121.75
2	2	1570	2MG	C6-C5-N7	3.97	137.51	130.29
2	2	120	PSU	C4-N3-C2	-3.97	120.91	126.37
2	2	1289	PSU	C4-N3-C2	-3.94	120.94	126.37
2	2	998	PSU	C4-N3-C2	-3.91	120.98	126.37
1	1	58	1MA	N9-C4-N3	3.90	135.79	126.90
1	1	37	T6A	N3-C2-N1	-3.84	122.77	128.58
2	2	1780	MA6	C2-N3-C4	3.81	121.14	111.83
2	2	120	PSU	O2-C2-N1	-3.77	118.91	122.79
2	2	1573	7MG	O4'-C1'-N9	3.73	114.38	109.30
2	2	1570	2MG	N9-C4-N3	3.73	133.41	125.95
1	1	37	T6A	C2-N3-C4	3.71	120.89	111.83
2	2	766	PSU	O2-C2-N1	-3.63	119.05	122.79
2	2	1190	C4J	C4-N3-C2	-3.61	121.17	125.62
2	2	465	PSU	C4-N3-C2	-3.61	121.40	126.37
2	2	1006	5MC	CM5-C5-C6	-3.59	117.99	122.85
2	2	998	PSU	O2-C2-N1	-3.56	119.12	122.79
1	1	10	2MG	C6-C5-N7	3.51	136.68	130.29
2	2	1780	MA6	N1-C2-N3	-3.51	123.27	128.58
1	1	37	T6A	C6-C5-N7	3.51	136.25	132.43
2	2	1780	MA6	N3-C4-N9	3.49	133.10	127.17
2	2	1426	2MG	C4-C5-N7	-3.46	105.19	110.67
2	2	1426	2MG	N9-C4-N3	3.41	132.78	125.95
1	1	9	1MG	O4'-C1'-N9	3.40	116.06	108.36
1	1	37	T6A	C4-C5-N7	-3.39	106.70	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	47	H2U	C3'-C2'-C1'	3.22	107.56	101.46
1	1	49	5MC	O2-C2-N3	-3.15	117.36	122.33
2	2	465	PSU	C6-C5-C4	-3.13	116.06	118.17
1	1	26	M2G	C6-C5-N7	3.12	135.97	130.29
1	1	49	5MC	C5-C4-N3	-3.12	118.56	121.75
2	2	1637	5MC	C5-C4-N3	-3.11	118.57	121.75
1	1	46	7MG	C5-C6-N1	3.02	116.26	110.94
1	1	48	5MC	O2-C2-N3	-3.00	117.60	122.33
2	2	1780	MA6	C5-N7-C8	2.96	108.11	103.45
2	2	1289	PSU	O2-C2-N1	-2.92	119.78	122.79
2	2	1780	MA6	C10-N6-C9	-2.85	107.03	116.18
2	2	766	PSU	C3'-C2'-C1'	2.81	105.01	101.69
2	2	1573	7MG	C5-C6-N1	2.80	115.88	110.94
1	1	58	1MA	C3'-C2'-C1'	2.80	106.76	101.46
2	2	1570	2MG	N1-C2-N2	2.80	119.42	116.56
1	1	26	M2G	O6-C6-C5	-2.79	119.16	126.53
1	1	37	T6A	C4-N9-C8	2.78	108.65	105.74
1	1	46	7MG	O4'-C1'-N9	2.74	113.03	109.30
2	2	1006	5MC	O2-C2-N3	-2.74	118.01	122.33
1	1	10	2MG	C4-C5-N7	-2.74	106.33	110.67
1	1	16	H2U	C5-C4-N3	2.73	119.59	116.69
1	1	9	1MG	N2-C2-N1	2.71	120.97	118.79
1	1	9	1MG	C6-C5-N7	2.70	135.36	129.36
2	2	1637	5MC	O4'-C1'-N1	2.70	114.47	108.36
2	2	1570	2MG	C4-C5-N7	-2.68	106.42	110.67
2	2	1426	2MG	C2-N1-C6	-2.66	121.34	124.55
2	2	1780	MA6	C6-C5-N7	2.62	137.61	133.43
2	2	766	PSU	C6-C5-C4	-2.61	116.41	118.17
2	2	998	PSU	C6-C5-C4	-2.61	116.41	118.17
2	2	1637	5MC	O2-C2-N3	-2.61	118.21	122.33
2	2	1426	2MG	O6-C6-C5	-2.59	119.70	126.53
1	1	58	1MA	C4-C5-N7	-2.58	106.58	110.67
2	2	465	PSU	O2-C2-N1	-2.57	120.14	122.79
1	1	48	5MC	C5-C6-N1	-2.56	120.53	123.31
1	1	37	T6A	C5-N7-C8	2.55	107.46	103.45
1	1	48	5MC	O4'-C1'-N1	2.52	114.07	108.36
2	2	1426	2MG	CM2-N2-C2	2.48	128.97	123.65
1	1	9	1MG	C4-C5-N7	-2.47	106.75	110.67
2	2	1006	5MC	C5-C6-N1	-2.47	120.63	123.31
2	2	1637	5MC	C5-C6-N1	-2.46	120.65	123.31
1	1	10	2MG	N1-C2-N2	2.44	119.05	116.56
1	1	37	T6A	O4'-C1'-N9	2.44	112.77	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	49	5MC	O4'-C1'-N1	2.43	113.87	108.36
2	2	120	PSU	C6-C5-C4	-2.38	116.57	118.17
1	1	9	1MG	O6-C6-C5	-2.33	118.58	124.59
2	2	1006	5MC	N4-C4-N3	2.33	122.73	118.51
1	1	37	T6A	C2-N1-C6	2.33	122.96	115.24
1	1	26	M2G	C4-C5-N7	-2.32	106.99	110.67
1	1	47	H2U	C5-C4-N3	2.31	119.14	116.69
2	2	1006	5MC	C2'-C1'-N1	-2.29	106.89	113.25
1	1	37	T6A	O10-C10-N6	-2.26	119.62	123.64
2	2	1570	2MG	O6-C6-C5	-2.24	120.62	126.53
2	2	1637	5MC	N1-C2-N3	2.23	122.68	118.80
1	1	37	T6A	C14-C12-N11	2.22	117.60	111.70
2	2	1426	2MG	C5-C6-N1	2.20	118.86	113.25
2	2	1637	5MC	CM5-C5-C6	-2.17	119.91	122.85
2	2	465	PSU	O2-C2-N3	-2.17	118.00	121.86
1	1	26	M2G	C5-C6-N1	2.14	118.69	113.25
1	1	46	7MG	C5-C4-N9	-2.12	103.62	106.33
1	1	16	H2U	C4'-O4'-C1'	-2.09	104.85	109.47
1	1	47	H2U	C5-C6-N1	-2.09	105.21	111.52
1	1	37	T6A	C15-C14-C12	2.09	116.41	112.29
1	1	10	2MG	O6-C6-C5	-2.08	121.03	126.53
2	2	1289	PSU	O2-C2-N3	-2.07	118.18	121.86
1	1	46	7MG	O3'-C3'-C4'	-2.06	105.17	111.08
1	1	46	7MG	O6-C6-C5	-2.05	122.59	127.62
2	2	1426	2MG	C8-N7-C5	2.04	107.89	104.26
1	1	37	T6A	N9-C8-N7	-2.03	111.06	113.94
1	1	49	5MC	C3'-C2'-C1'	2.01	105.27	101.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	1190	C4J	C4'

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	1780	MA6	O4'-C4'-C5'-O5'
2	2	1780	MA6	C5-C6-N6-C10
2	2	1780	MA6	N1-C6-N6-C10
1	1	9	1MG	O4'-C4'-C5'-O5'
1	1	10	2MG	O4'-C4'-C5'-O5'
1	1	16	H2U	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	1	37	T6A	C14-C12-N11-C10
1	1	37	T6A	N11-C12-C14-O14
1	1	47	H2U	O4'-C4'-C5'-O5'
1	1	48	5MC	C4'-C5'-O5'-P
1	1	64	RIA	C3'-C4'-C5'-O5'
1	1	9	1MG	C3'-C4'-C5'-O5'
1	1	26	M2G	C3'-C4'-C5'-O5'
1	1	47	H2U	C3'-C4'-C5'-O5'
1	1	47	H2U	C2'-C1'-N1-C2
2	2	1426	2MG	O4'-C4'-C5'-O5'
2	2	1780	MA6	C3'-C4'-C5'-O5'
1	1	10	2MG	C3'-C4'-C5'-O5'
1	1	26	M2G	O4'-C4'-C5'-O5'
1	1	64	RIA	O1'-C4'-C5'-O5'
1	1	48	5MC	O4'-C4'-C5'-O5'
1	1	48	5MC	C3'-C4'-C5'-O5'
1	1	37	T6A	N11-C12-C14-C15
1	1	47	H2U	C2'-C1'-N1-C6
1	1	37	T6A	N11-C12-C13-ODA
2	2	1573	7MG	O4'-C4'-C5'-O5'
2	2	1573	7MG	C3'-C4'-C5'-O5'
1	1	49	5MC	O4'-C4'-C5'-O5'
1	1	37	T6A	N11-C12-C13-ODB
1	1	46	7MG	C4'-C5'-O5'-P
1	1	64	RIA	C4A-C5A-O5A-P
1	1	9	1MG	C4'-C5'-O5'-P
2	2	1426	2MG	C4'-C5'-O5'-P
2	2	1780	MA6	C4'-C5'-O5'-P
2	2	766	PSU	C3'-C4'-C5'-O5'
2	2	1637	5MC	O4'-C4'-C5'-O5'
1	1	16	H2U	C3'-C4'-C5'-O5'
2	2	1426	2MG	C3'-C4'-C5'-O5'
1	1	49	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	37	T6A	2	0
1	1	26	M2G	1	0
1	1	47	H2U	1	0
2	2	1570	2MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	46	7MG	1	0
1	1	9	1MG	1	0
2	2	120	PSU	1	0
2	2	1426	2MG	3	0
5	B	2	AYA	1	0
2	2	1637	5MC	2	0
2	2	1780	MA6	1	0
2	2	1289	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 124 ligands modelled in this entry, 122 are monoatomic - leaving 2 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	$\# Z > 2$
51	GCP	k	603	-	32,34,34	1.79	9 (28%)	49,54,54	1.78	8 (16%)
50	MET	k	601	-	6,7,8	0.48	0	2,7,9	0.06	0

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
51	GCP	k	603	-	-	1/19/38/38	0/3/3/3
50	MET	k	601	-	-	1/5/6/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O1G	5.54	1.61	1.50
51	k	603	GCP	C5-C4	3.46	1.48	1.38
51	k	603	GCP	PB-O3A	2.95	1.61	1.58
51	k	603	GCP	PG-O3G	-2.93	1.48	1.55
51	k	603	GCP	PG-O2G	2.88	1.61	1.55
51	k	603	GCP	PA-O3A	2.12	1.61	1.59
51	k	603	GCP	PB-O2B	2.09	1.61	1.56
51	k	603	GCP	C5-N7	-2.04	1.35	1.39
51	k	603	GCP	C6-N1	-2.02	1.35	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C5-C4-N3	-6.33	118.31	128.39
51	k	603	GCP	C2-N3-C4	5.27	121.38	112.30
51	k	603	GCP	N9-C4-N3	4.68	135.31	125.95
51	k	603	GCP	C6-C5-N7	3.25	136.20	130.29
51	k	603	GCP	PB-O3A-PA	-2.89	122.93	132.37
51	k	603	GCP	C4-C5-N7	-2.57	106.60	110.67
51	k	603	GCP	C3'-C2'-C1'	2.24	105.69	101.46
51	k	603	GCP	O6-C6-C5	-2.13	120.91	126.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

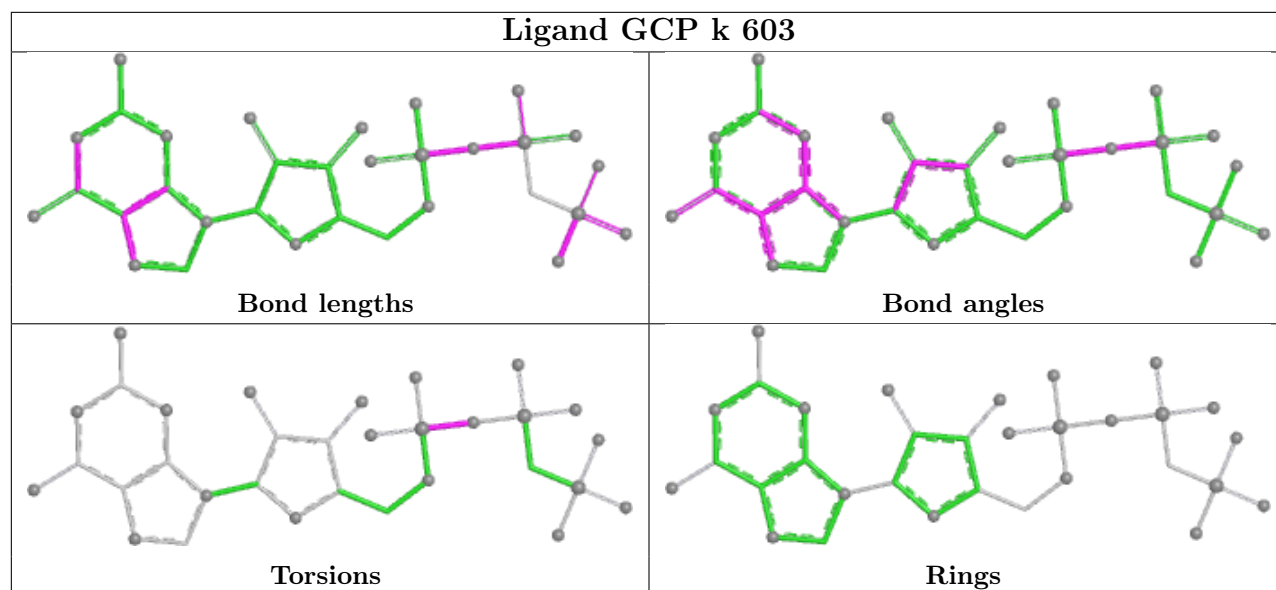
Mol	Chain	Res	Type	Atoms
50	k	601	MET	CA-CB-CG-SD
51	k	603	GCP	PB-O3A-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
45	q	8
2	2	1
1	1	1
44	p	1
5	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	214:UNK	C	251:GLN	N	50.55
1	q	158:UNK	C	166:UNK	N	17.71
1	q	181:UNK	C	190:UNK	N	14.31
1	q	135:UNK	C	139:UNK	N	7.79
1	q	203:UNK	C	207:UNK	N	6.84
1	2	224:A	O3'	225:A	P	4.58
1	1	16:H2U	O3'	18:G	P	4.54
1	q	582:GLN	C	583:GLN	N	3.87

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	148:UNK	C	150:UNK	N	3.60
1	q	605:CYS	C	606:LEU	N	3.34
1	p	688:GLU	C	689:GLU	N	3.29
1	B	2:AYA	C	3:VAL	N	3.09

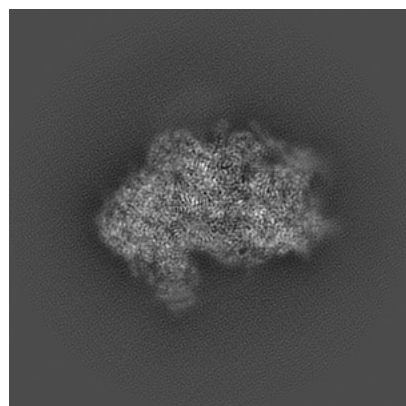
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4328. These allow visual inspection of the internal detail of the map and identification of artifacts.

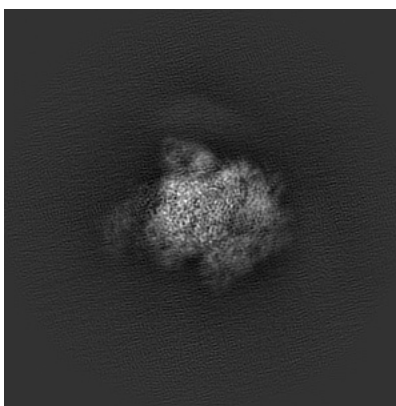
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

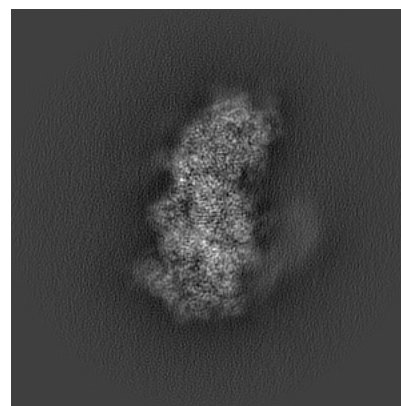
6.1.1 Primary map



X

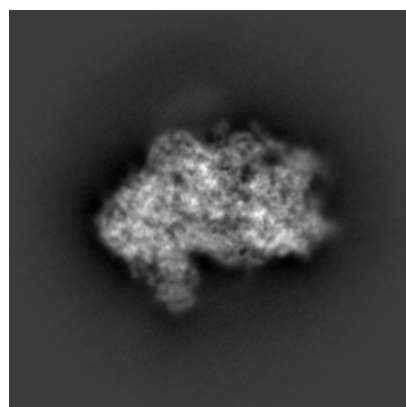


Y

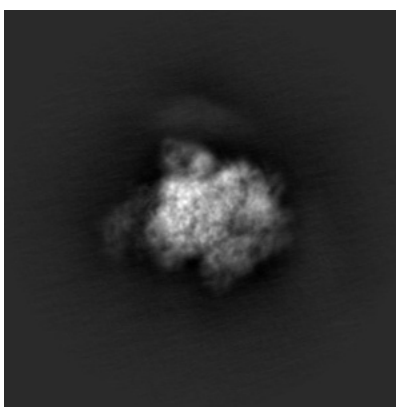


Z

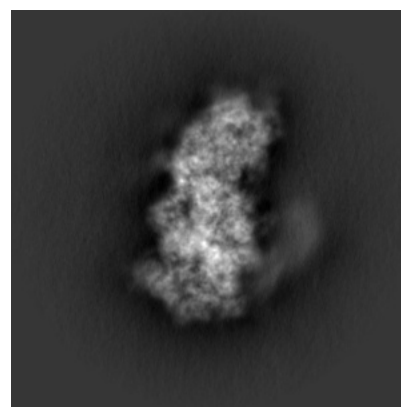
6.1.2 Raw map



X



Y

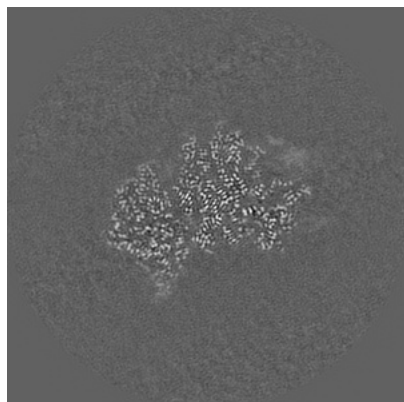


Z

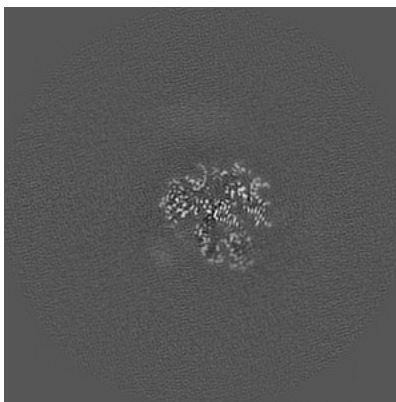
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

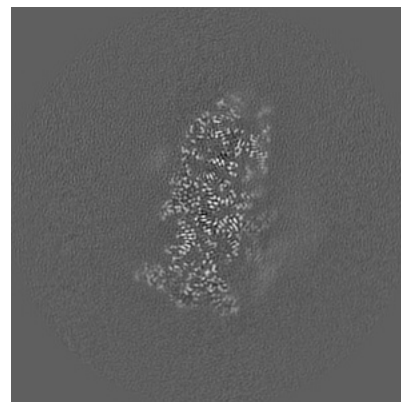
6.2.1 Primary map



X Index: 150

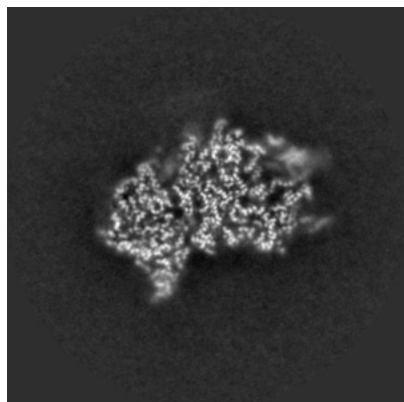


Y Index: 150

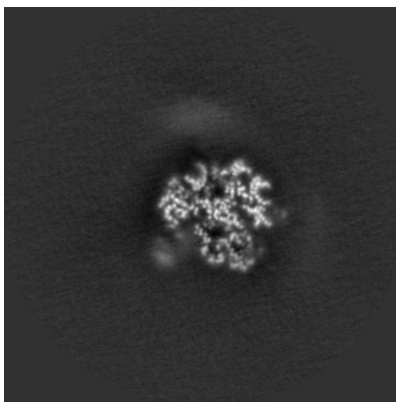


Z Index: 150

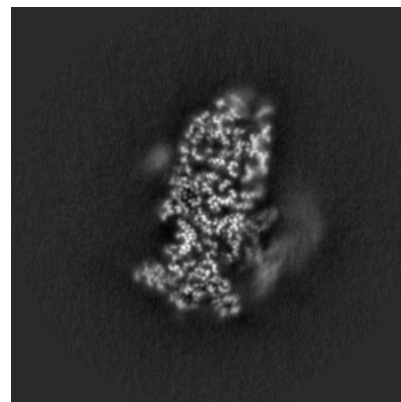
6.2.2 Raw map



X Index: 150



Y Index: 150

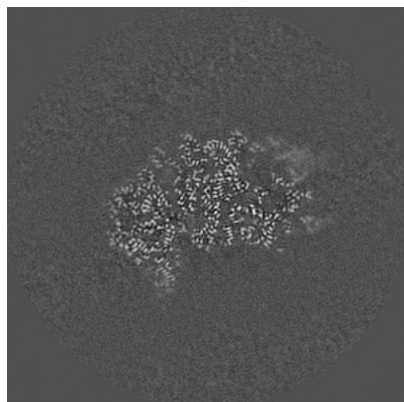


Z Index: 150

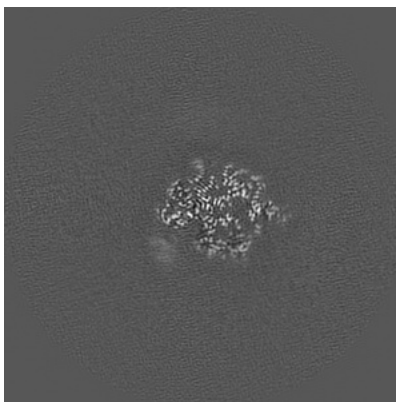
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

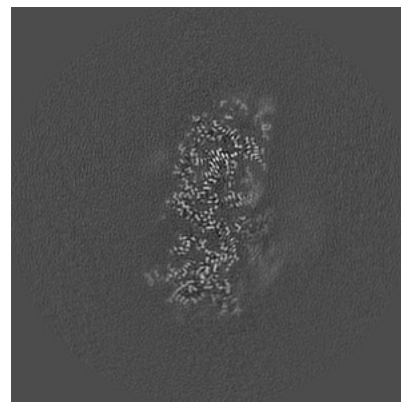
6.3.1 Primary map



X Index: 152

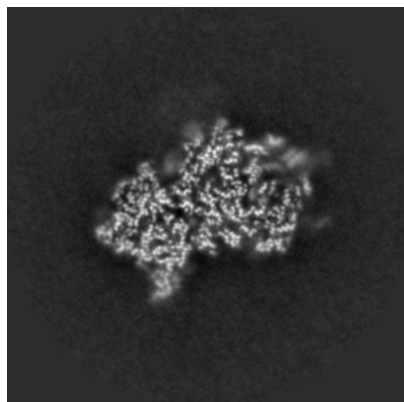


Y Index: 155

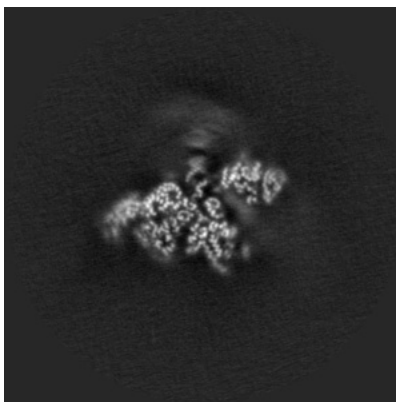


Z Index: 147

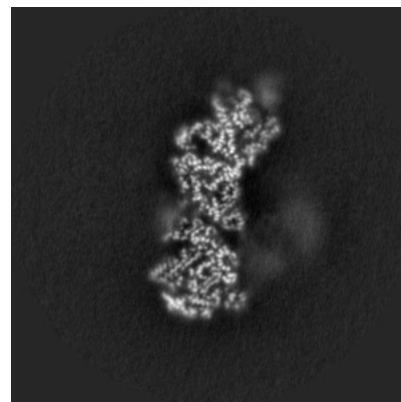
6.3.2 Raw map



X Index: 148



Y Index: 119

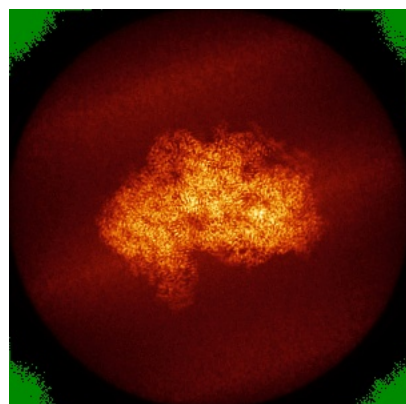


Z Index: 132

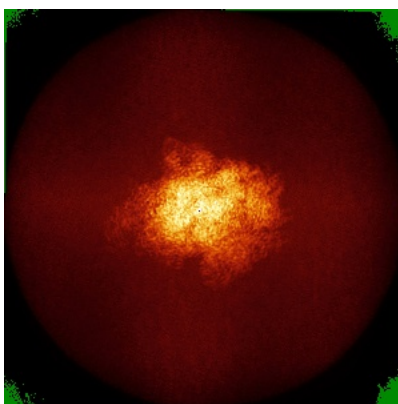
The images above show the largest variance slices of the map in three orthogonal directions.

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

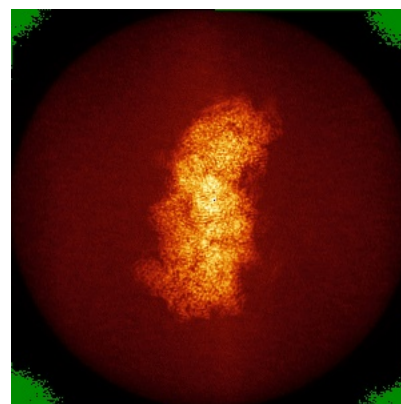
6.4.1 Primary map



X



Y

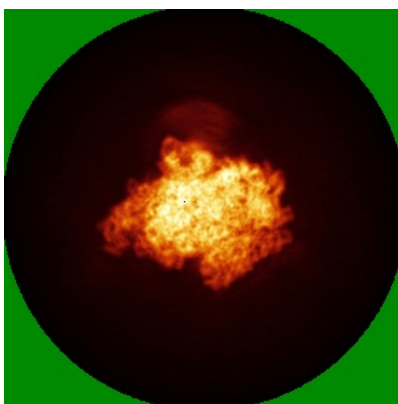


Z

6.4.2 Raw map



X



Y

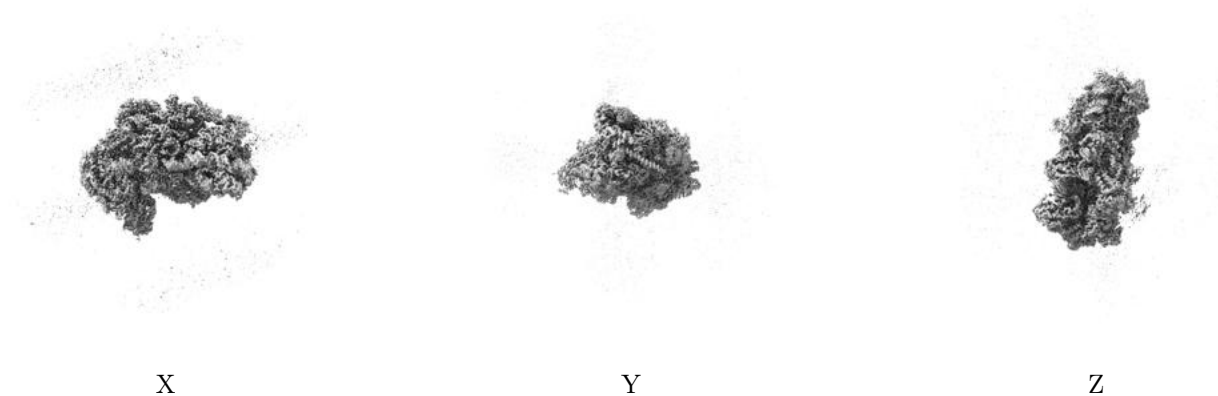


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

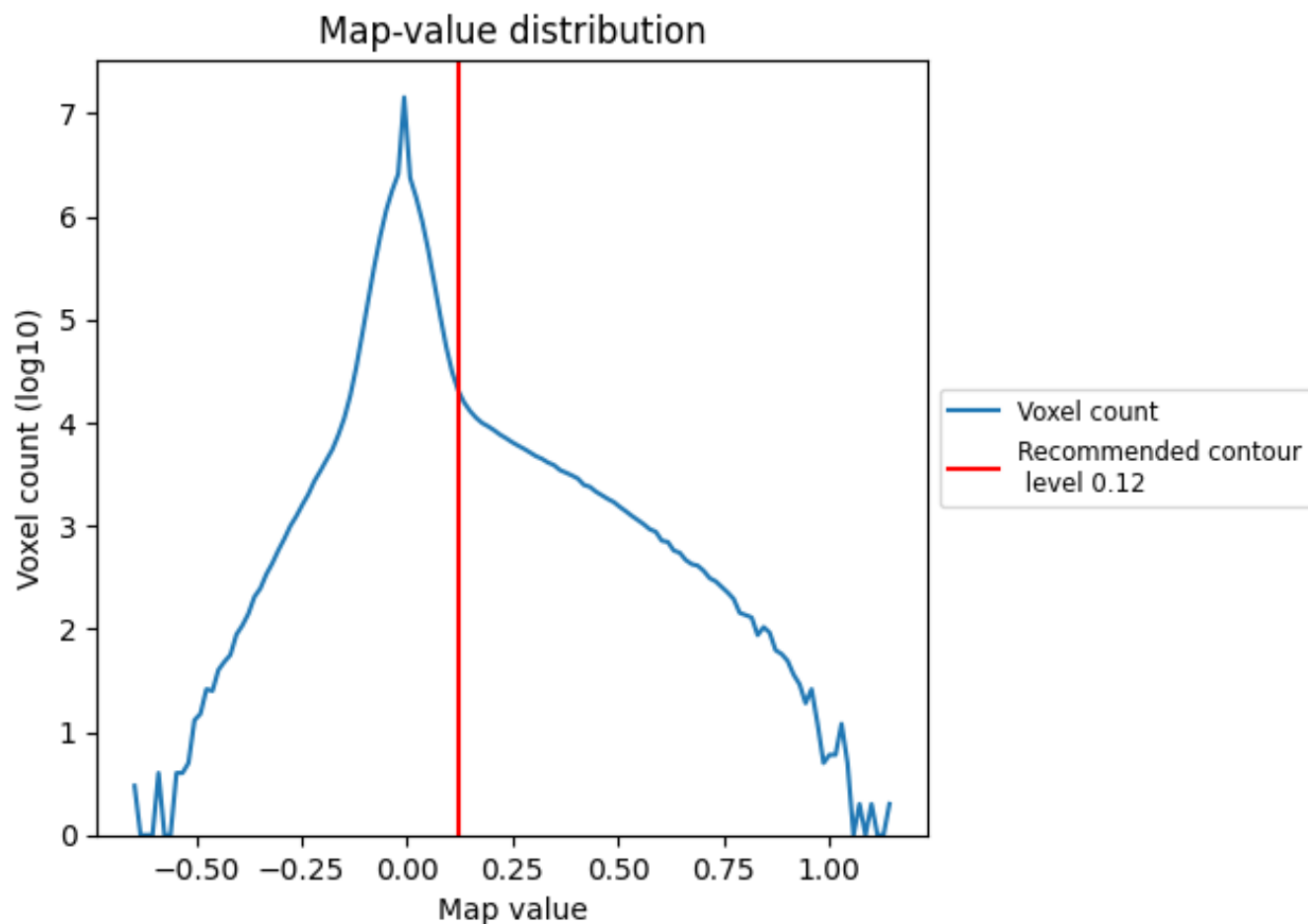
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

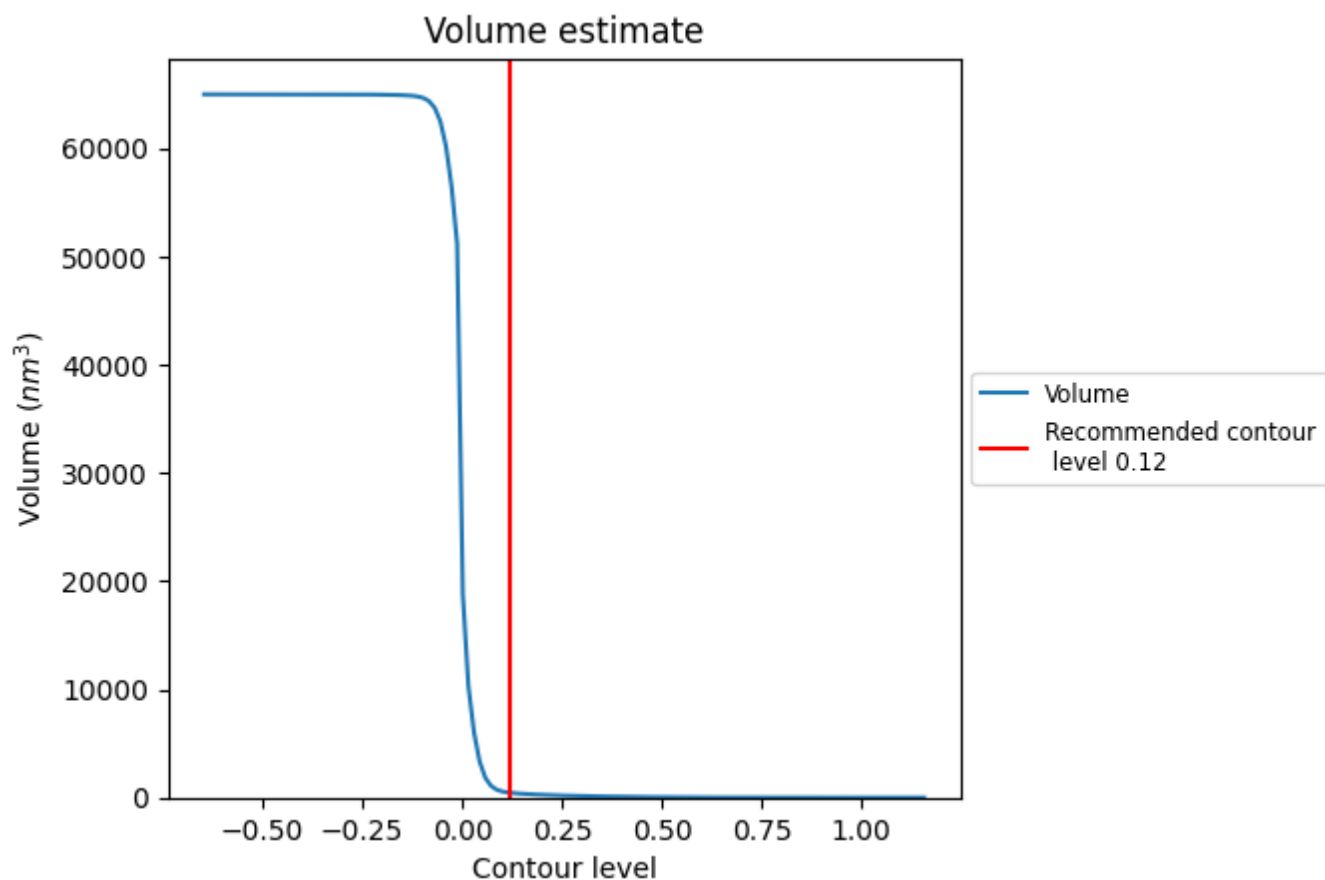
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

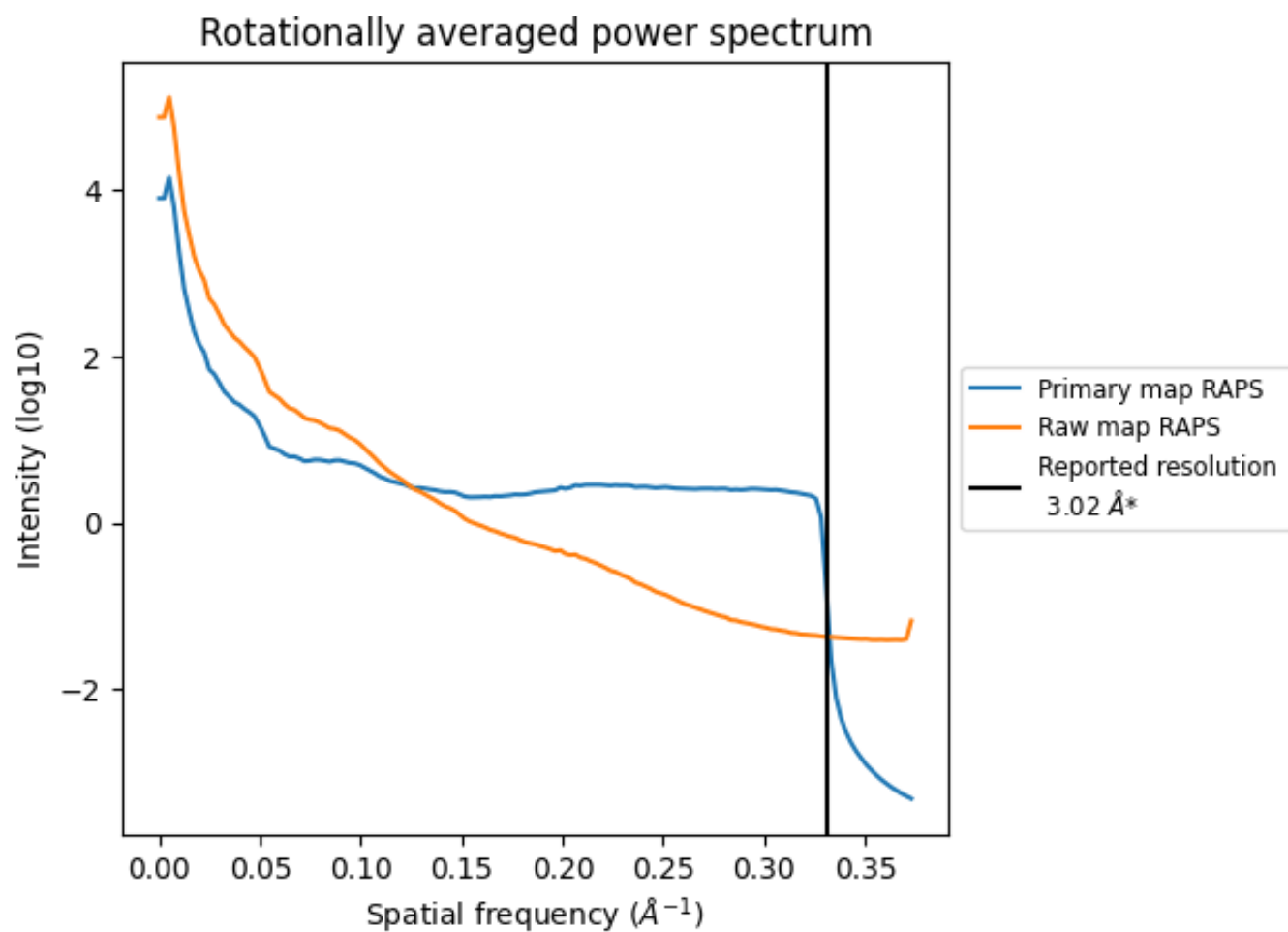
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 447 nm³; this corresponds to an approximate mass of 404 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 ⓘ

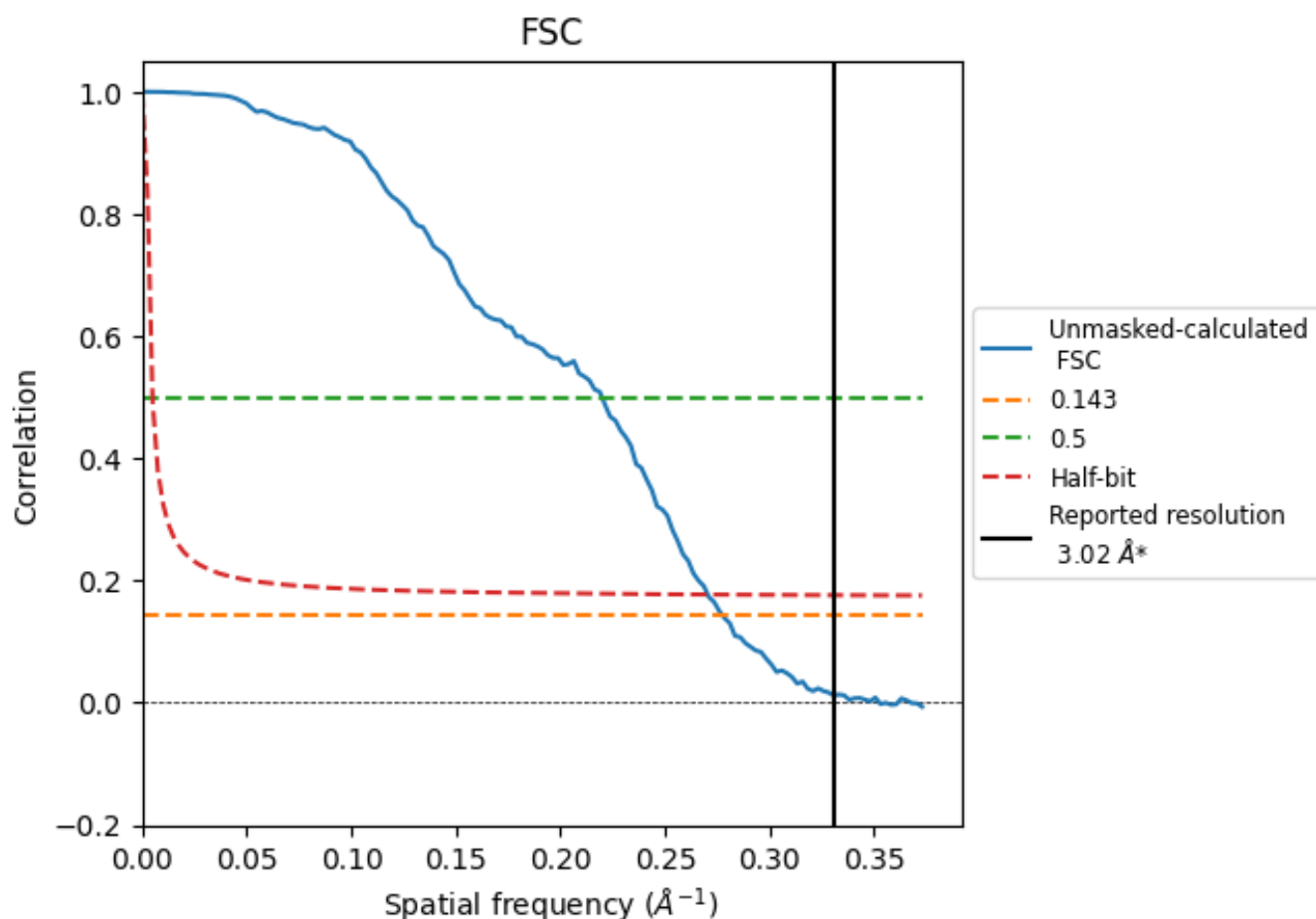


*Reported resolution corresponds to spatial frequency of 0.331 $\text{\AA}^{-1}$

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 0.331 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

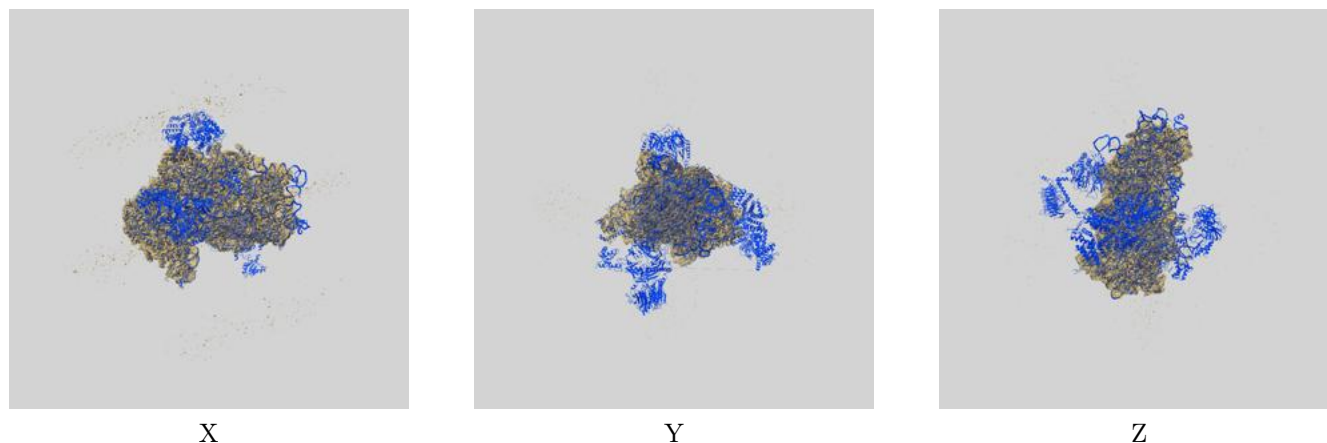
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.60	4.55	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 3.02 by more than 10 %

9 Map-model fit [i](#)

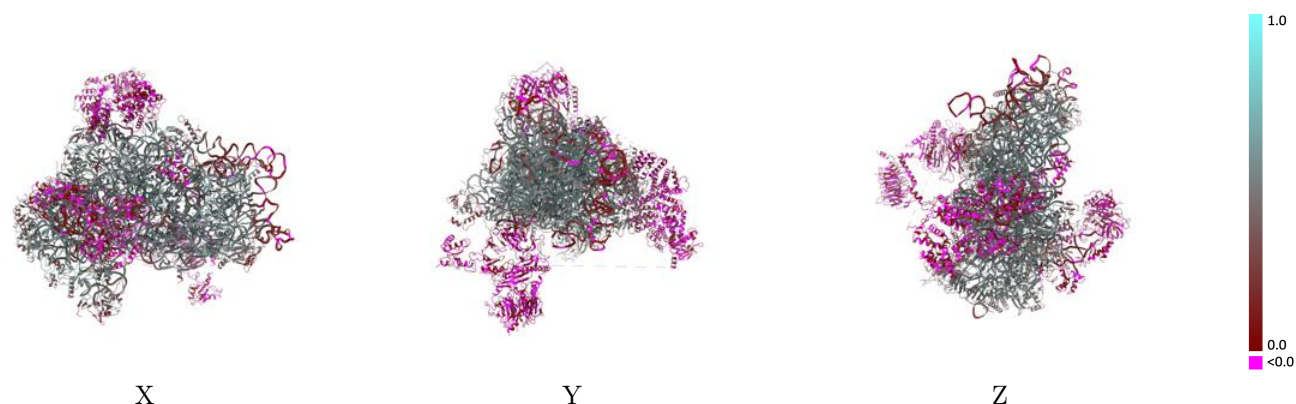
This section contains information regarding the fit between EMDB map EMD-4328 and PDB model 6FYY. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



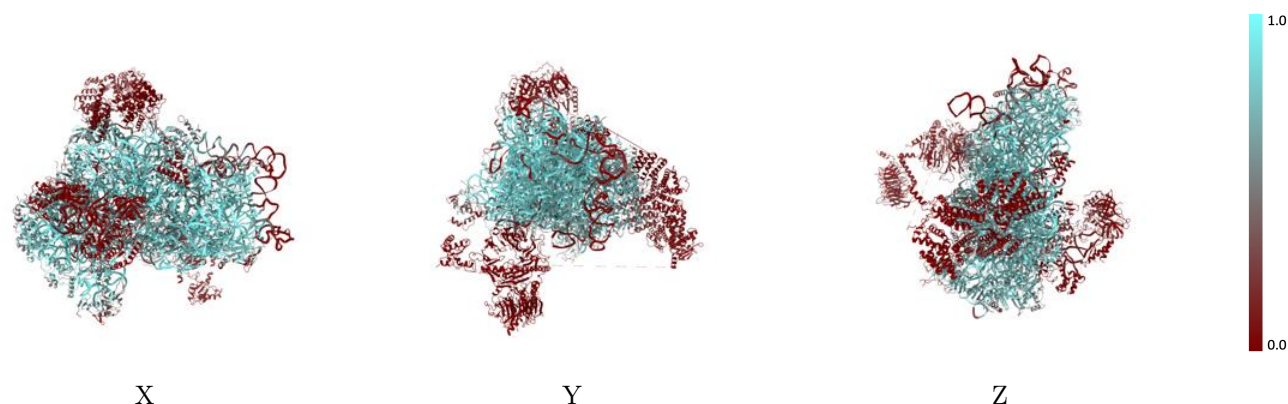
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



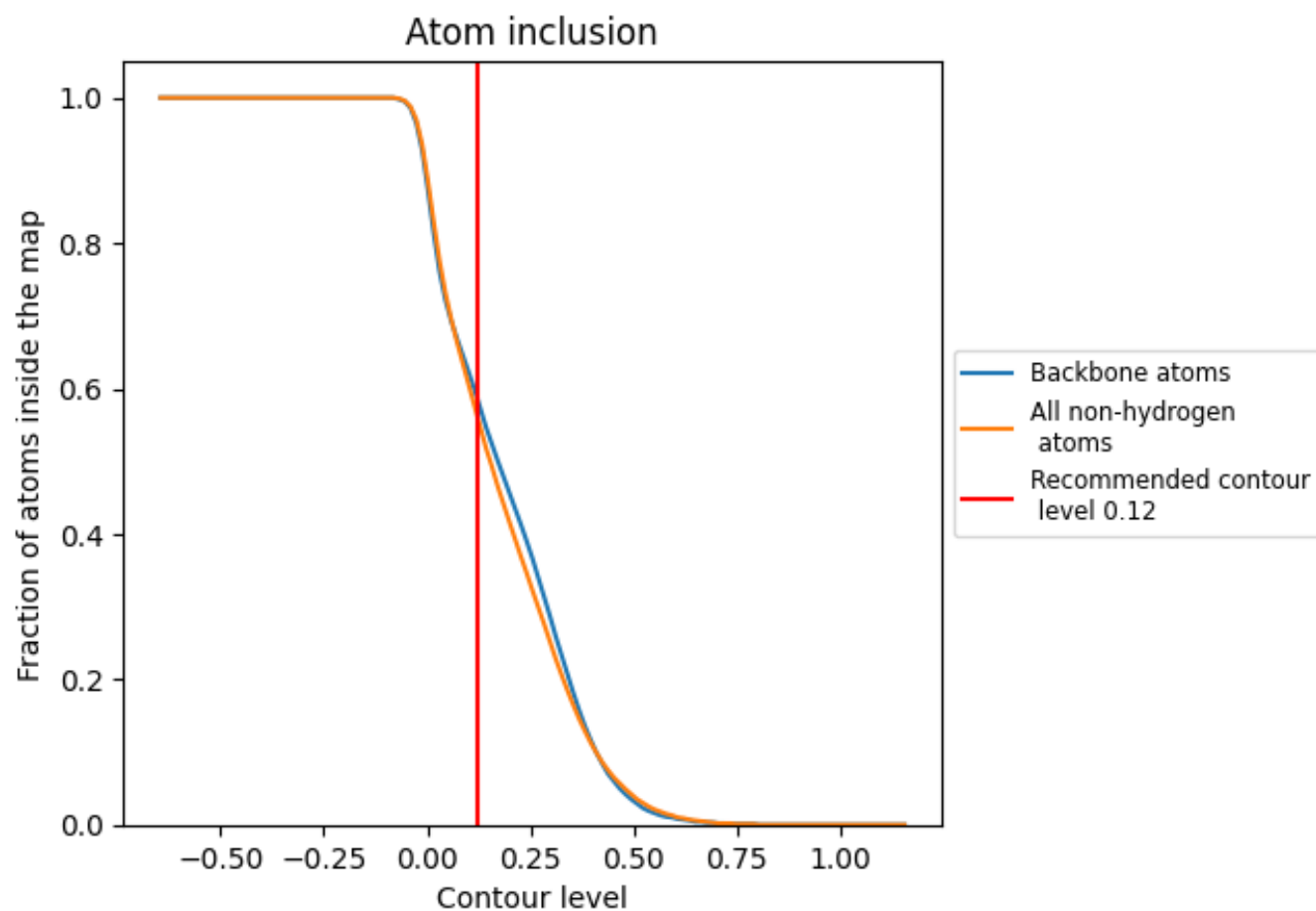
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 57% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5660	 0.3780
1	 0.3120	 0.2600
2	 0.8100	 0.4820
3	 0.2570	 0.2510
A	 0.7070	 0.4840
B	 0.6630	 0.4590
C	 0.7640	 0.5220
D	 0.6750	 0.4700
E	 0.7960	 0.5310
F	 0.6620	 0.4770
G	 0.6330	 0.4360
H	 0.5630	 0.4250
I	 0.7200	 0.4870
J	 0.7650	 0.5110
K	 0.6910	 0.4620
L	 0.6960	 0.4930
M	 0.2850	 0.2570
N	 0.7520	 0.5110
O	 0.7400	 0.5100
P	 0.7040	 0.4800
Q	 0.7480	 0.5120
R	 0.6330	 0.4600
S	 0.7000	 0.4680
T	 0.7690	 0.5010
U	 0.5920	 0.4170
V	 0.7360	 0.5000
W	 0.8000	 0.5420
X	 0.8050	 0.5470
Y	 0.7550	 0.5010
Z	 0.4990	 0.3820
a	 0.7570	 0.5150
b	 0.6890	 0.4940
c	 0.6620	 0.4980
d	 0.8580	 0.5620
e	 0.6790	 0.4730



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Chain	Atom inclusion	Q-score
f	 0.4190	 0.3750
g	 0.6160	 0.4590
h	 0.4720	 0.4180
i	 0.6140	 0.4750
j	 0.0030	 0.1410
k	 0.0010	 0.0430
l	 0.0010	 0.0530
m	 0.2220	 0.3860
o	 0.0000	 0.0240
p	 0.0000	 0.0450
q	 0.0010	 0.0430
r	 0.0000	 0.0090
s	 0.0000	 0.0250