



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 01:32 am BST

PDB ID : 8PJ4 / pdb_00008pj4
EMDB ID : EMD-17699
Title : Structure of human 48S translation initiation complex after eIF5 release (48S-4)
Authors : Petrychenko, V.; Yi, S.-H.; Liedtke, D.; Peng, B.Z.; Rodnina, M.V.; Fischer, N.
Deposited on : 2023-06-22
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
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

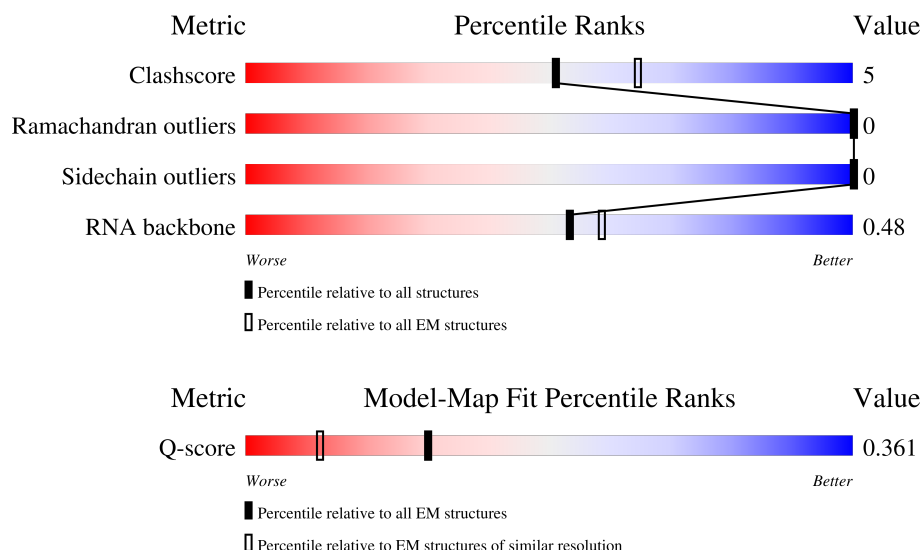
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	1220	 41% 10% 49%
2	1	814	 60% 68% 28%
3	2	325	 94% 94% 6%

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Mol	Chain	Length	Quality of chain
4	3	218	
5	4	357	
6	5	564	
7	6	374	
8	7	255	
9	8	352	
10	9	25	
11	A	1869	
12	B	158	
13	C	263	
14	D	194	
15	E	143	
16	F	133	
17	G	194	
18	H	84	
19	I	151	
20	J	130	
21	K	83	
22	L	293	
23	M	135	
24	N	295	
25	O	264	
26	P	151	
27	Q	115	
28	R	208	

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Mol	Chain	Length	Quality of chain
29	S	249	
30	T	133	
31	V	204	
32	Y	146	
33	Z	243	
34	a	165	
35	b	145	
36	c	317	
37	d	145	
38	e	125	
39	f	152	
40	h	119	
41	i	56	
42	k	156	
43	m	132	
44	n	69	
45	o	320	
46	q	144	
47	r	315	
48	t	472	
49	u	1382	
50	v	445	
51	w	75	
52	x	548	
53	y	913	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 121694 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	621	Total	C	N	O	S	0	0
			4920	3135	850	913	22		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	588	Total	C	N	O	S	0	0
			3258	1986	633	634	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	304	Total	C	N	O	0	0
			1493	885	304	304		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	213	Total	C	N	O	0	0
			1057	631	213	213		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	257	Total	C	N	O	0	0
			1272	757	257	258		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	520	Total	C	N	O	S	0	0
			4347	2814	721	793	19		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	362	Total	C	N	O	S	0	0
			2196	1348	414	427	7		

- Molecule 8 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	57	Total	C	N	O	P	0	0
			1218	547	231	383	57		

- Molecule 9 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	317	Total	C	N	O	0	0
			1574	937	318	319		

- Molecule 10 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 11 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1754	Total	C	N	O	P	0	0
			37429	16718	6714	12244	1753		

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 13 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 15 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 16 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	58	Total	C	N	O	S	0	0
			452	279	98	74	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	125	PRO	LYS	conflict	UNP P62861

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 19 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 20 is a protein called 40S ribosomal protein S15a.

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

- Molecule 21 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 22 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 23 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 25 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 26 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 28 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 29 is a protein called 40S ribosomal protein S6.

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

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 31 is a protein called 40S ribosomal protein S5.

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

- Molecule 32 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 33 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 34 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 35 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	131	Total	C	N	O	S	0	0
			1072	682	201	182	7		

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 37 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 38 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	81	Total	C	N	O	S	0	0
			649	420	119	109	1		

- Molecule 39 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	149	Total	C	N	O	S	0	0
			1227	770	249	207	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 41 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 42 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	68	Total	C	N	O	S	0	0
			554	349	103	95	7		

- Molecule 43 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 44 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	o	77	Total	C	N	O	0	0
			616	389	111	116		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	117	Total	C	N	O	S	1	0
			951	590	183	174	4		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	296	Total	C	N	O	S	0	0
			2138	1342	384	404	8		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	455	Total	C	N	O	S	0	0
			3439	2179	599	643	18		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	706	Total	C	N	O	S	1	0
			5383	3379	982	999	23		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	405	Total	C	N	O	S	0	0
			2740	1720	498	510	12		

- Molecule 51 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

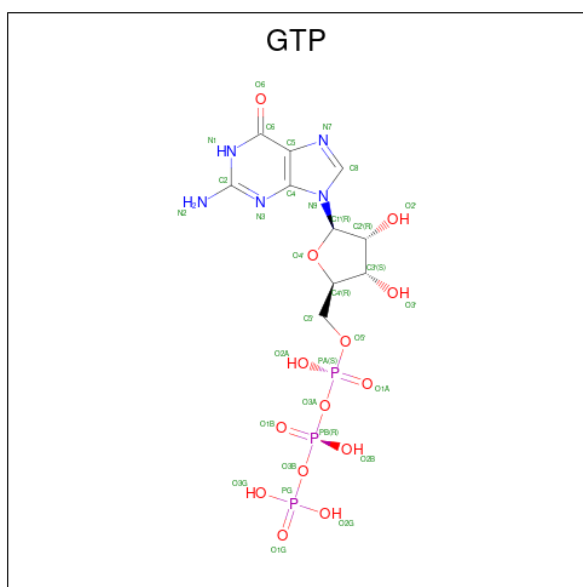
- Molecule 52 is a protein called Eukaryotic translation initiation factor 3 subunit D.

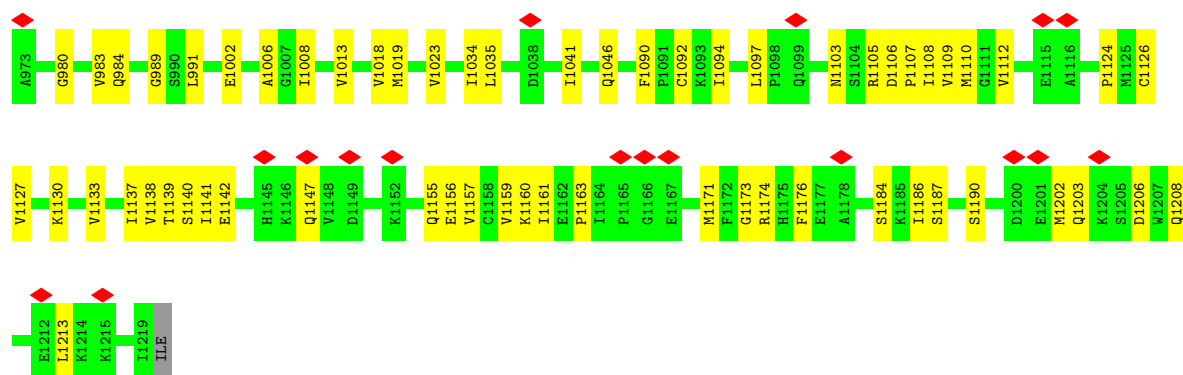
Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	423	Total	C	N	O	S	0	0
			2842	1752	523	557	10		

- Molecule 53 is a protein called Eukaryotic translation initiation factor 3 subunit C.

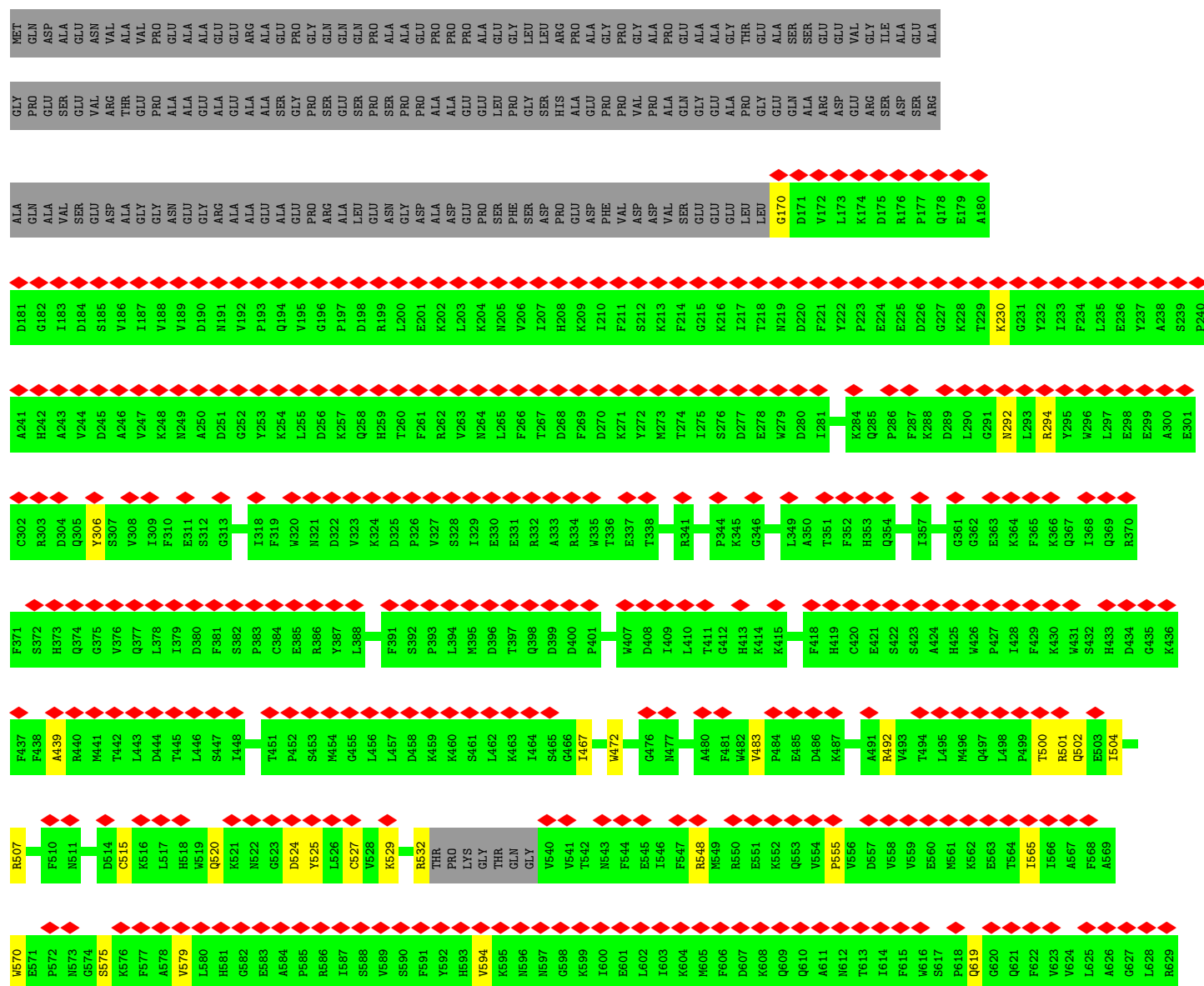
Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	543	Total	C	N	O	S	0	0
			4361	2743	776	809	33		

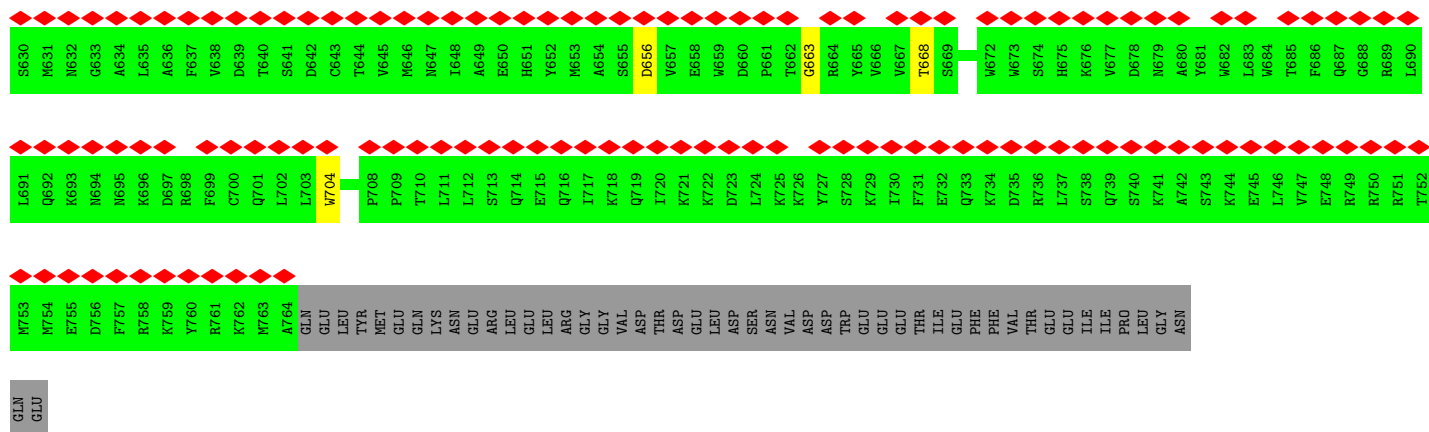
- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



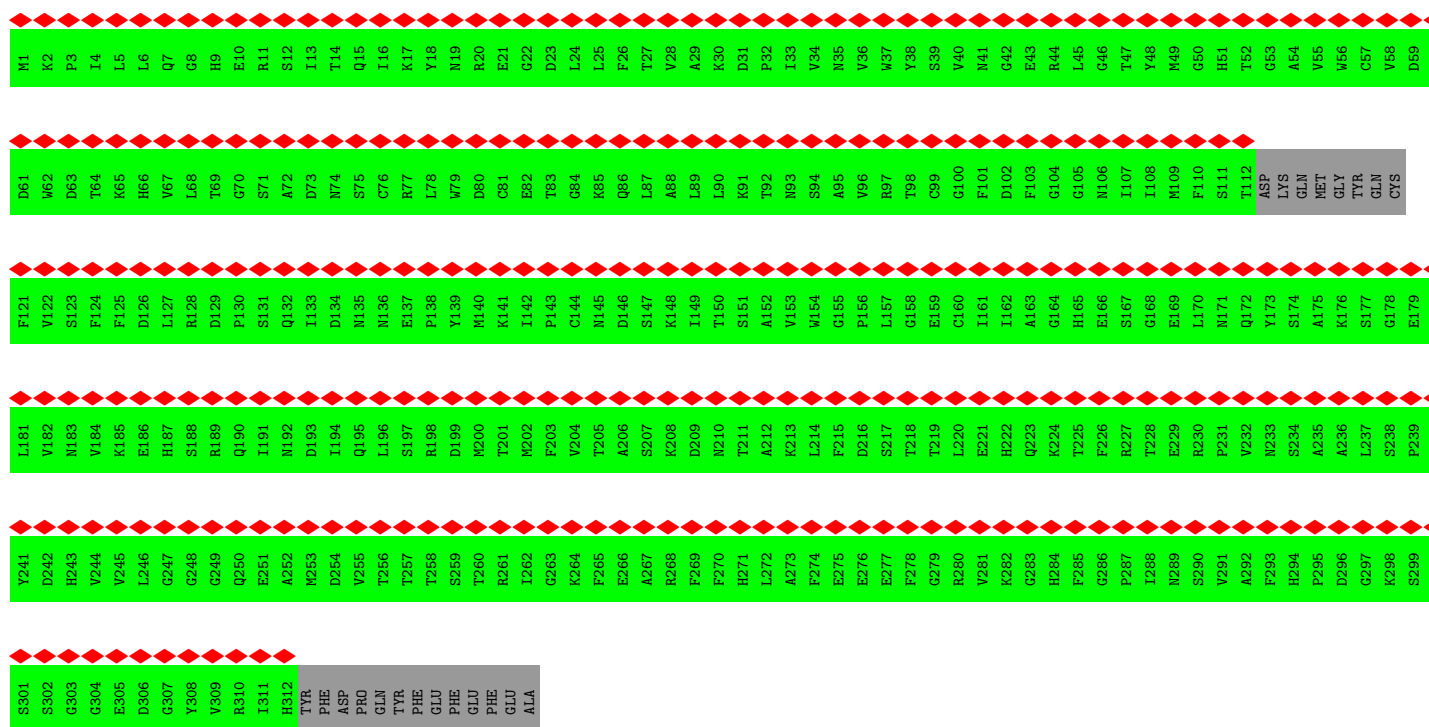


• Molecule 2: Eukaryotic translation initiation factor 3 subunit B

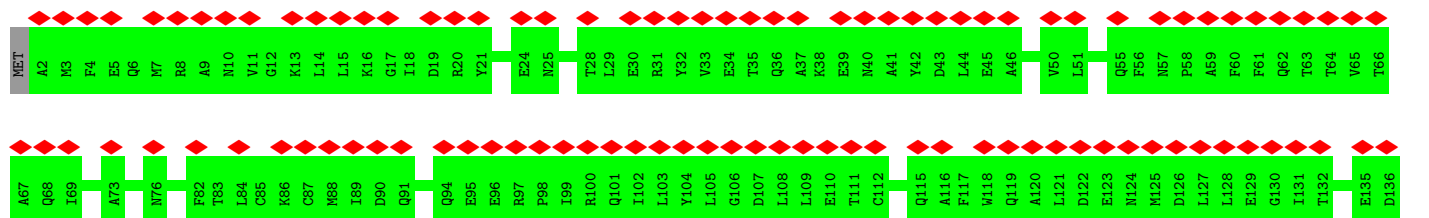


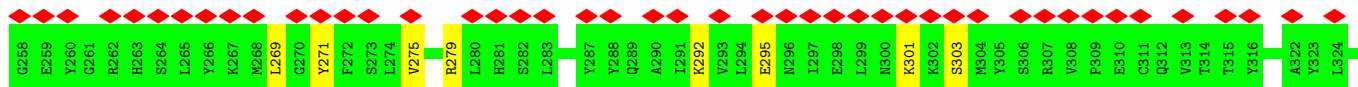


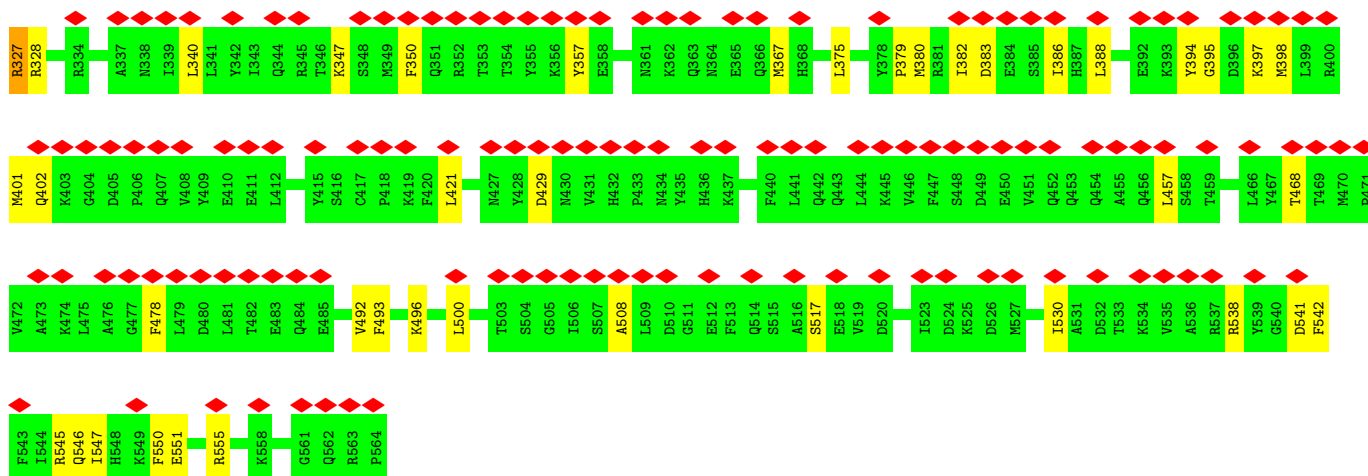
• Molecule 3: Eukaryotic translation initiation factor 3 subunit I



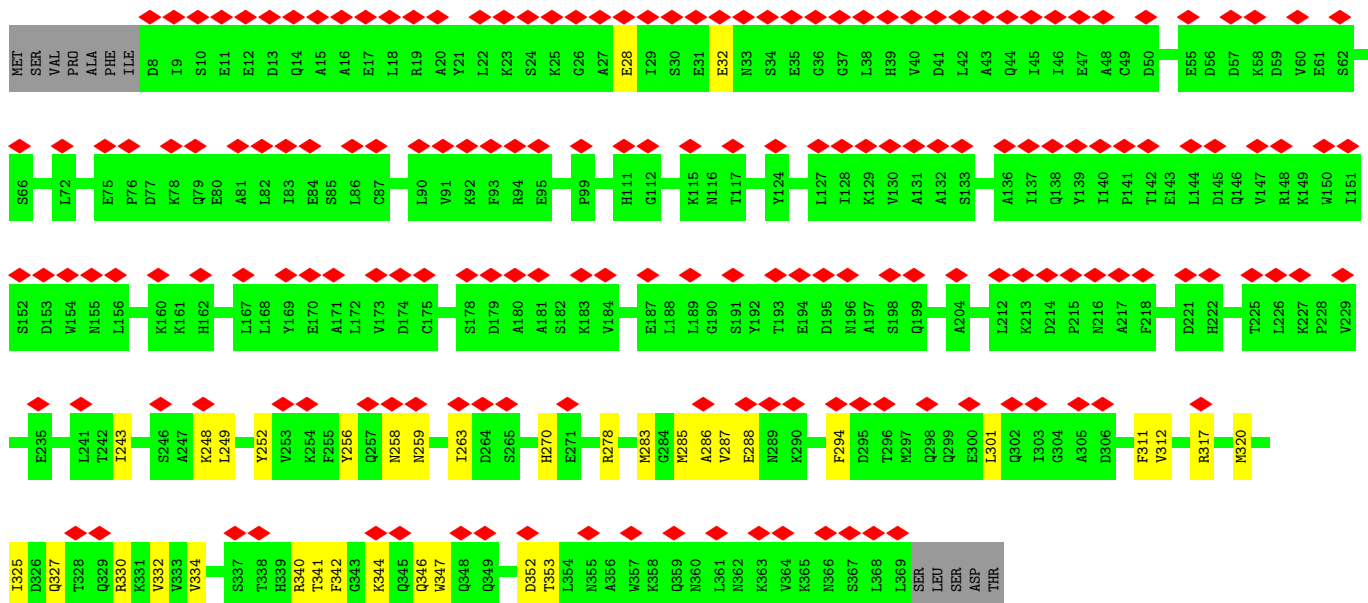
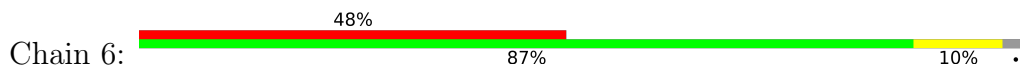
• Molecule 4: Eukaryotic translation initiation factor 3 subunit K



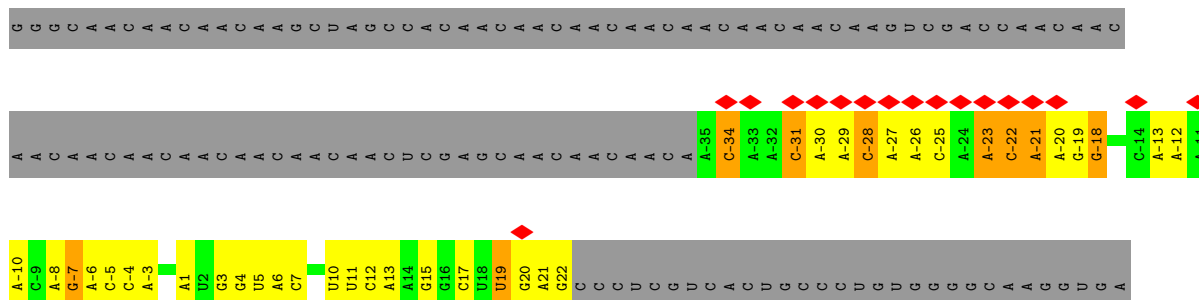




- Molecule 7: Eukaryotic translation initiation factor 3 subunit M

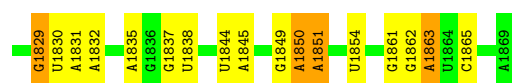


- Molecule 8: mRNA

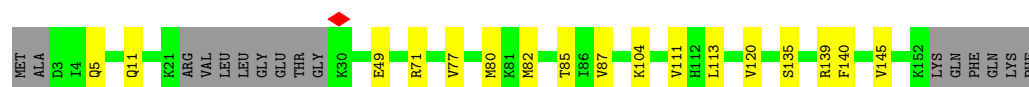




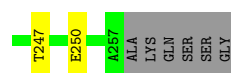
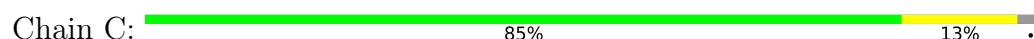




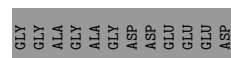
- Molecule 12: 40S ribosomal protein S11



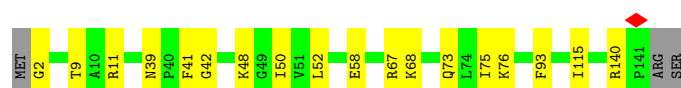
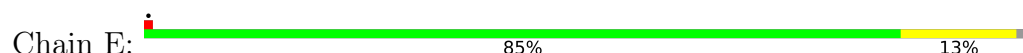
- Molecule 13: 40S ribosomal protein S4, X isoform



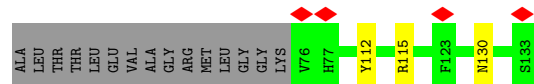
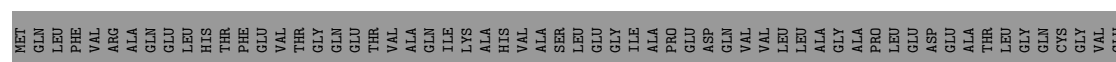
- Molecule 14: 40S ribosomal protein S9



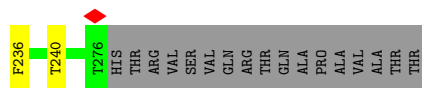
- Molecule 15: 40S ribosomal protein S23



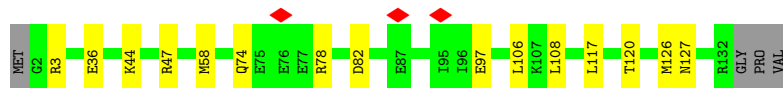
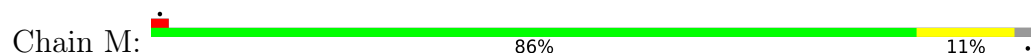
- Molecule 16: Small ribosomal subunit protein eS30



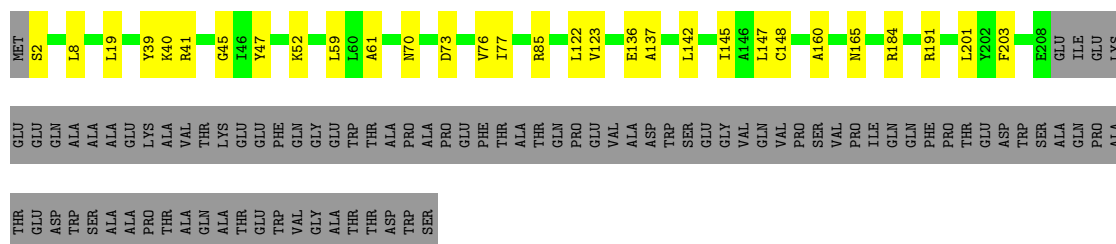
- Molecule 17: 40S ribosomal protein S7



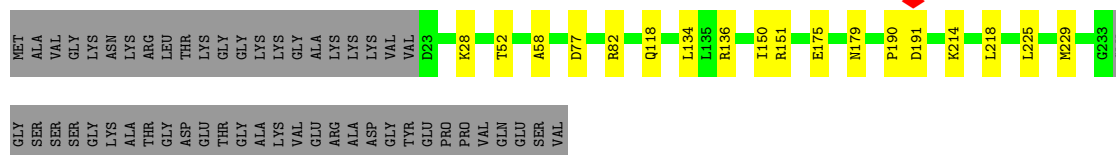
- Molecule 23: 40S ribosomal protein S17



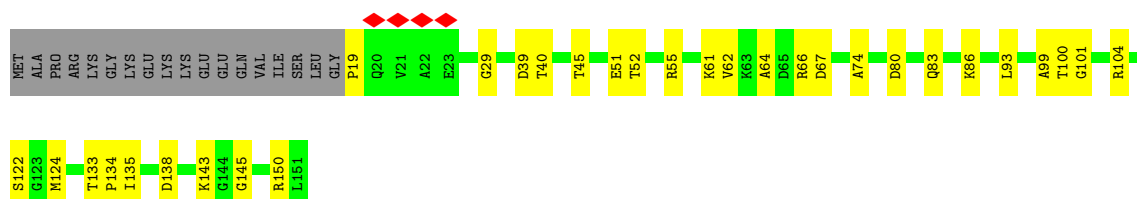
- Molecule 24: 40S ribosomal protein SA



- Molecule 25: 40S ribosomal protein S3a

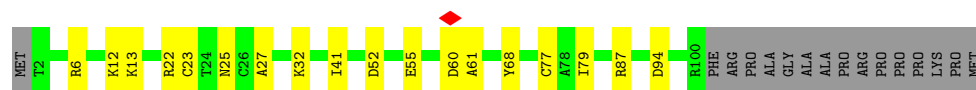


- Molecule 26: 40S ribosomal protein S14



- Molecule 27: 40S ribosomal protein S26





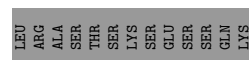
- Molecule 28: 40S ribosomal protein S8

Chain R: 82% 13% 5%



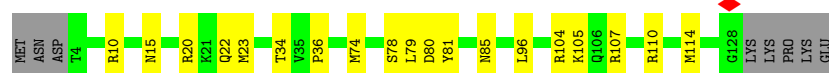
- Molecule 29: 40S ribosomal protein S6

Chain S: 81% 11% 8%



- Molecule 30: 40S ribosomal protein S24

Chain T: 80% 14% 6%



- Molecule 31: 40S ribosomal protein S5

Chain V: 78% 15% 7%



- Molecule 32: 40S ribosomal protein S16

Chain Y: 84% 12% 4%



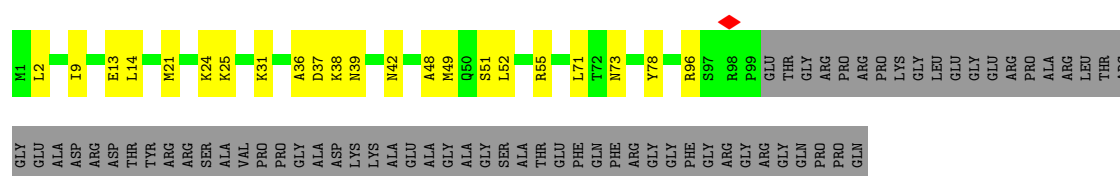
- Molecule 33: 40S ribosomal protein S3

Chain Z:  86% 7% 7%



- Molecule 34: 40S ribosomal protein S10

Chain a:  47% 13% 40%



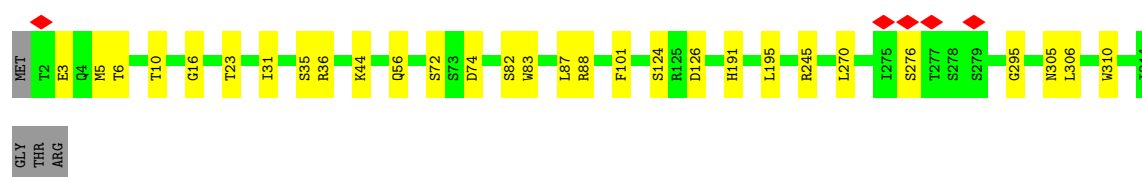
- Molecule 35: 40S ribosomal protein S15

Chain b:  74% 17% 10%



- Molecule 36: Receptor of activated protein C kinase 1

Chain c:  90% 9% .



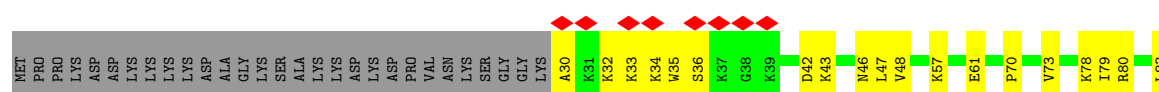
- Molecule 37: 40S ribosomal protein S19

Chain d:  86% 12% .



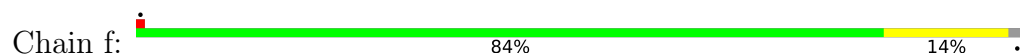
- Molecule 38: 40S ribosomal protein S25

Chain e:  6% 45% 20% 35%

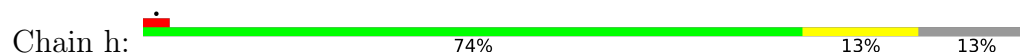




- Molecule 39: 40S ribosomal protein S18



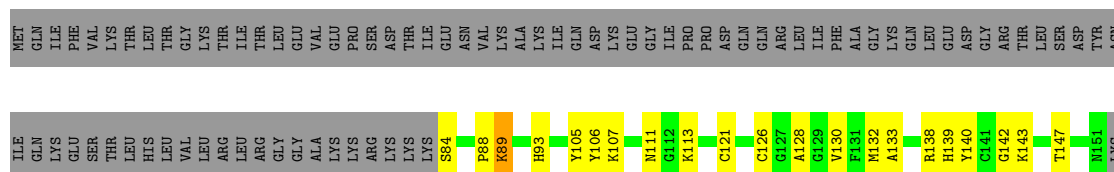
- Molecule 40: 40S ribosomal protein S20



- Molecule 41: 40S ribosomal protein S29



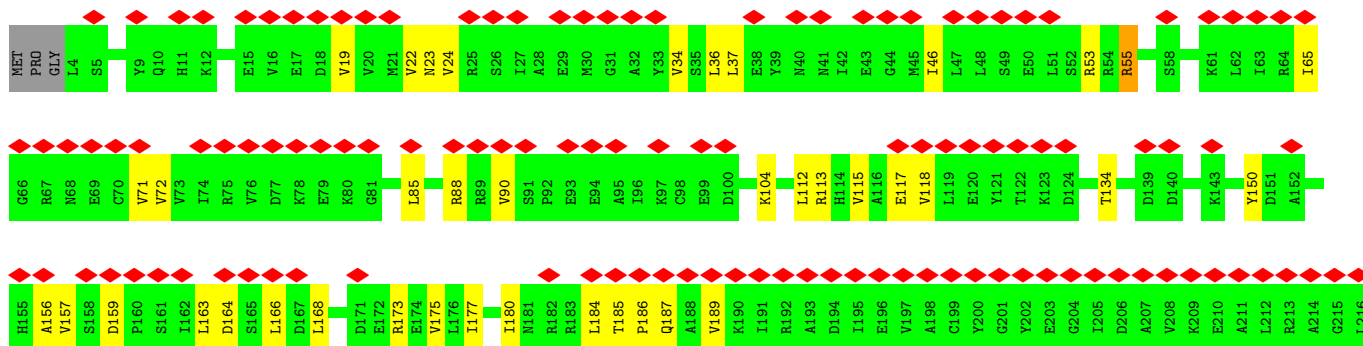
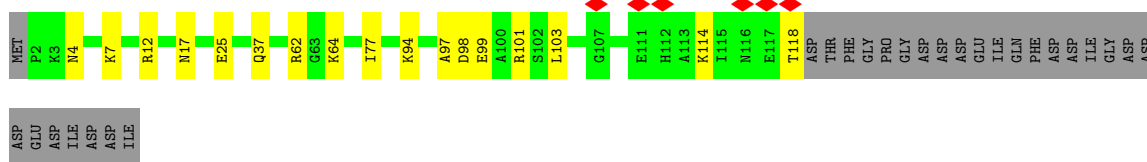
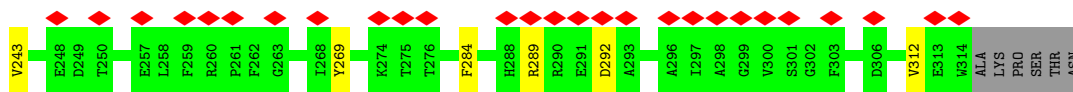
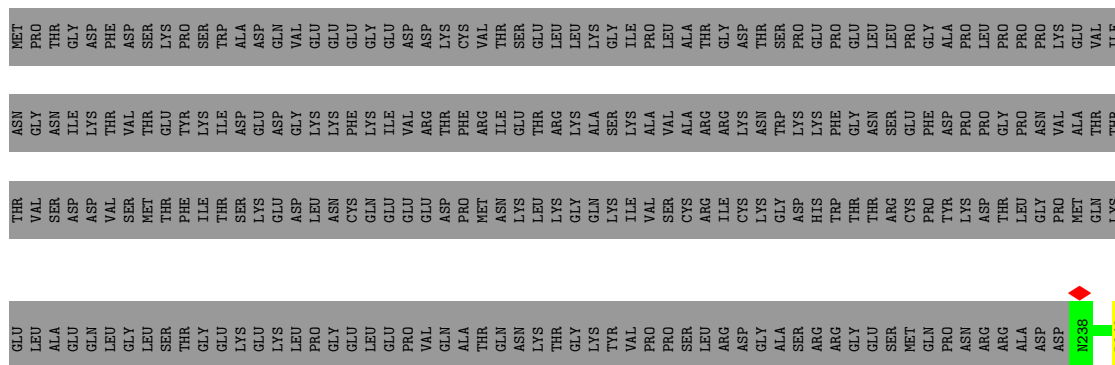
- Molecule 42: Ubiquitin

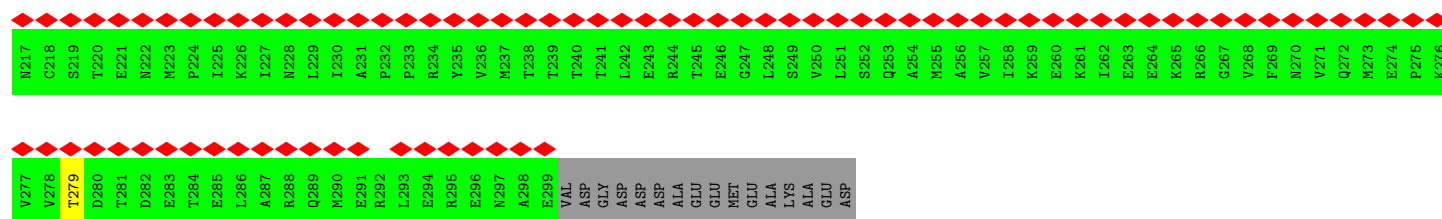


- Molecule 43: 40S ribosomal protein S12

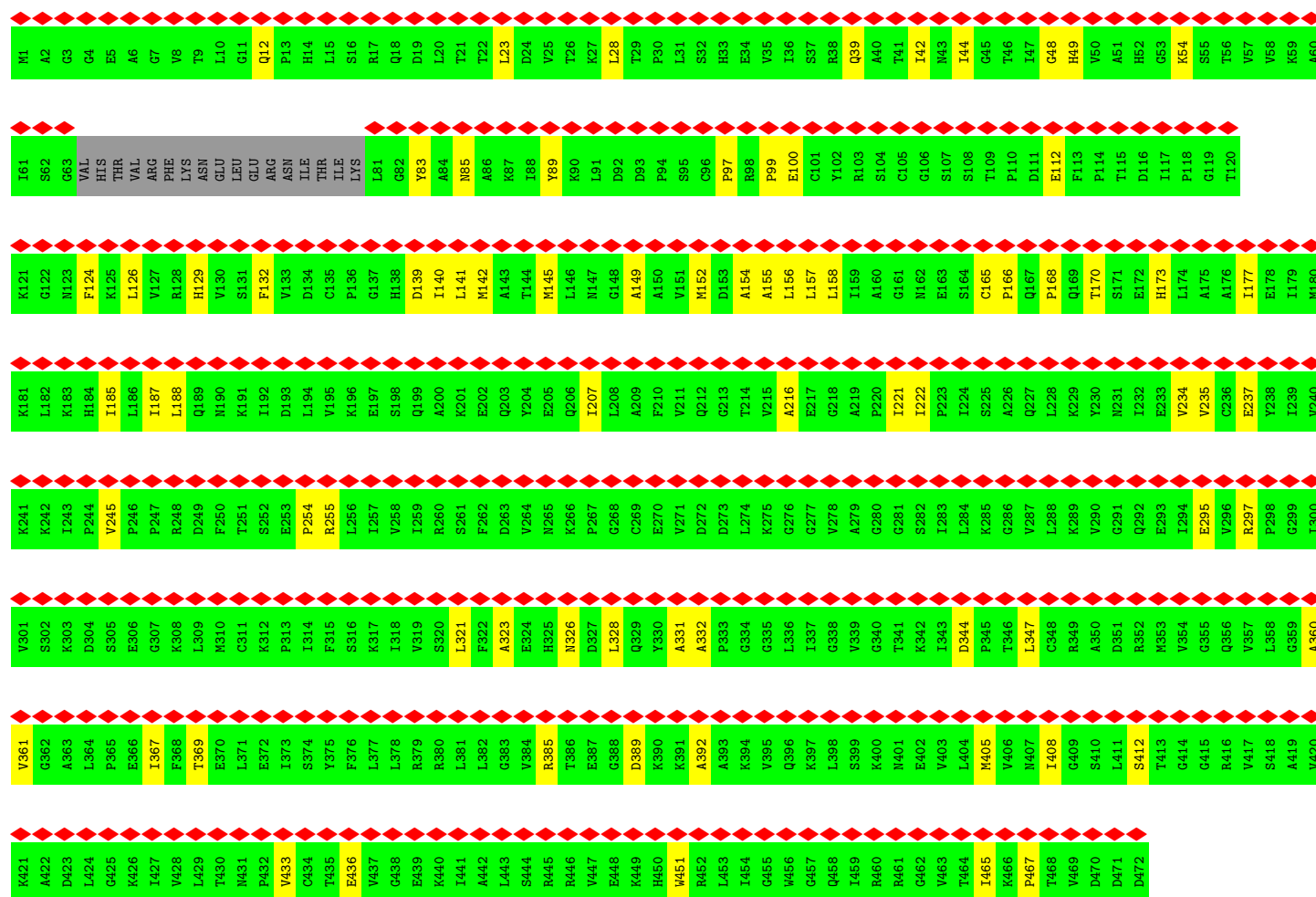
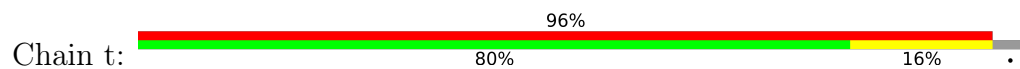


- Molecule 44: 40S ribosomal protein S28

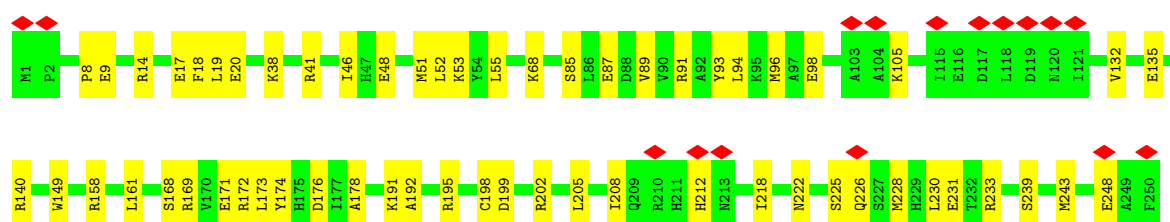




• Molecule 48: Eukaryotic translation initiation factor 2 subunit 3



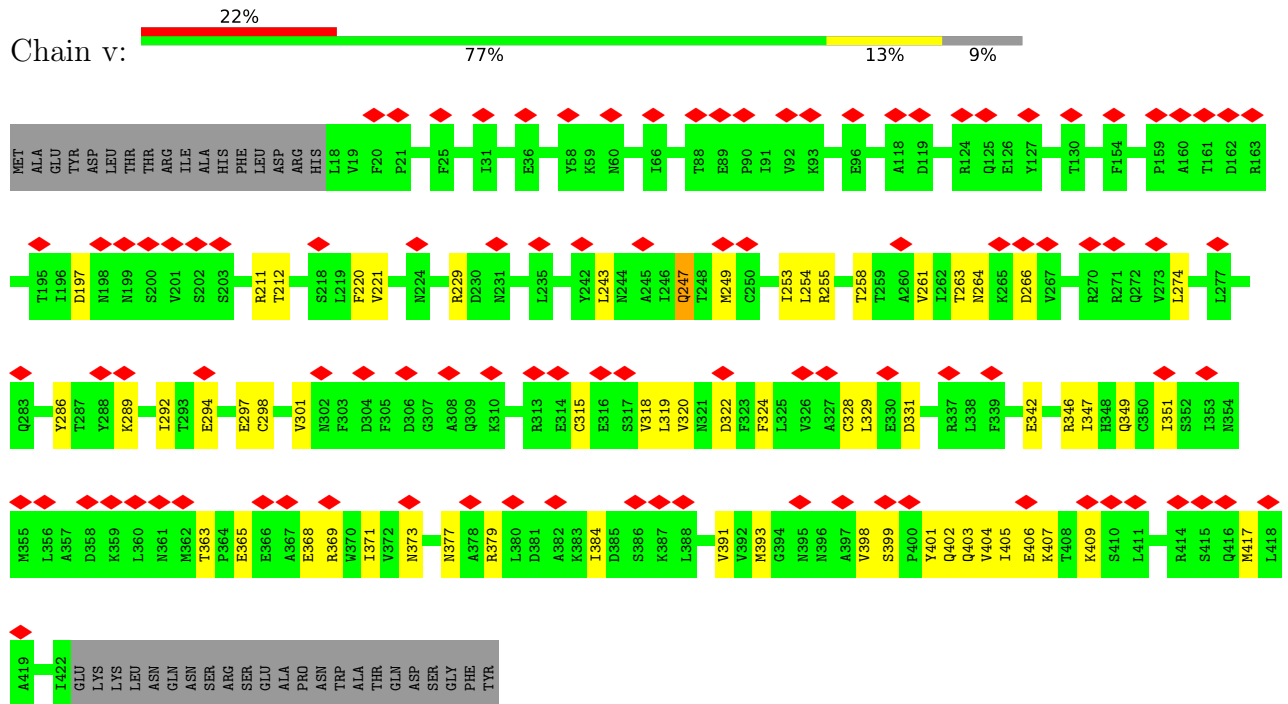
• Molecule 49: Eukaryotic translation initiation factor 3 subunit A



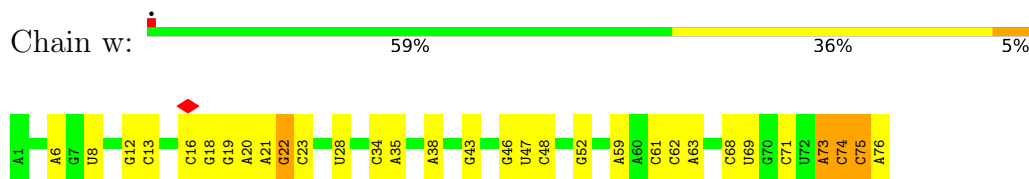


SER
LEU
ARG
ARG
THR
LYS
ASN
GLU
THR
ASP
GLU
ASP
GLY
TRP
THR
THR
VAL
ARG
ARG

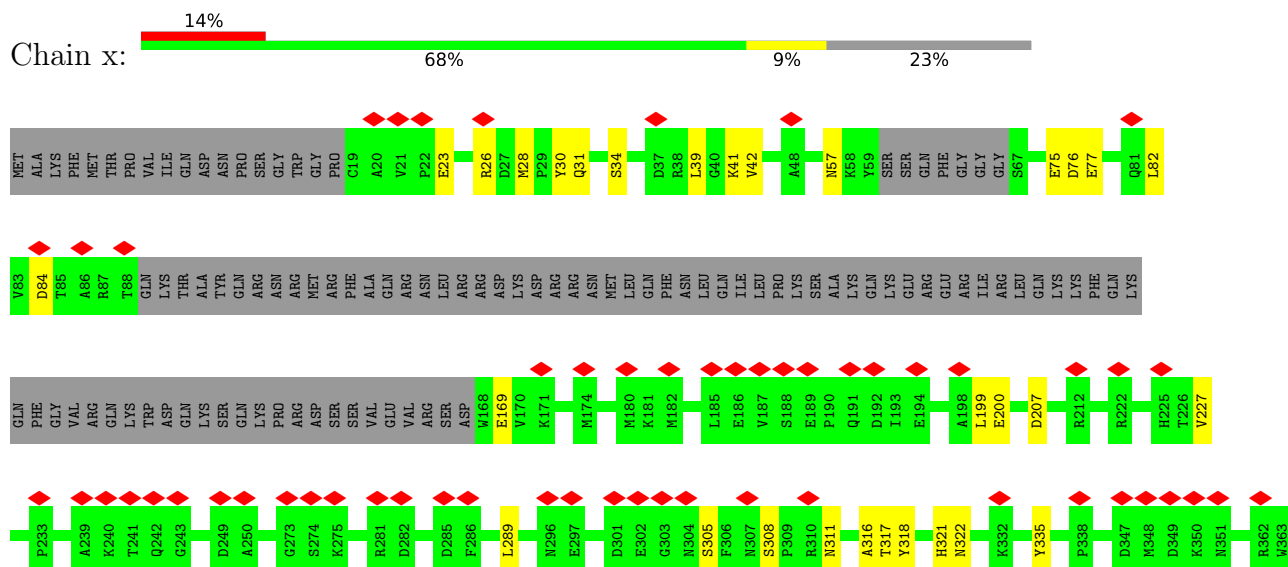
- Molecule 50: Eukaryotic translation initiation factor 3 subunit E



- Molecule 51: Initiator Met-tRNA-i



- Molecule 52: Eukaryotic translation initiation factor 3 subunit D



- Molecule 53: Eukaryotic translation initiation factor 3 subunit C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	22.337	Depositor
Minimum map value	-6.543	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size (Å)	417.74402, 417.74402, 417.74402	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96700007, 0.96700007, 0.96700007	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, 5MU, OMU, OMG, UR3, NA, JMH, MA6, 5MC, B8N, PSU, A2M, 6MZ, OMC, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.22	0/5002	0.57	1/6743 (0.0%)
2	1	0.21	0/3279	0.60	0/4534
3	2	0.15	0/1491	0.39	0/2068
4	3	0.15	0/1055	0.42	0/1469
5	4	0.15	0/1269	0.42	0/1762
6	5	0.20	0/4458	0.51	1/6027 (0.0%)
7	6	0.21	0/2212	0.58	0/3034
8	7	0.40	5/1365 (0.4%)	0.50	2/2124 (0.1%)
9	8	0.17	0/1572	0.47	0/2187
10	9	0.28	0/231	0.59	0/294
11	A	0.22	0/41130	0.41	3/64100 (0.0%)
12	B	0.18	0/1186	0.38	0/1585
13	C	0.19	0/2077	0.47	0/2796
14	D	0.24	0/1502	0.50	0/2008
15	E	0.22	0/1105	0.52	0/1476
16	F	0.19	0/459	0.55	0/607
17	G	0.23	0/1451	0.61	1/1942 (0.1%)
18	H	0.21	0/644	0.50	0/864
19	I	0.19	0/1232	0.44	0/1656
20	J	0.23	0/1051	0.54	0/1406
21	K	0.22	0/623	0.53	0/833
22	L	0.24	0/1743	0.56	0/2354
23	M	0.27	0/1078	0.65	0/1447
24	N	0.22	0/1670	0.54	0/2271
25	O	0.19	0/1742	0.54	0/2330
26	P	0.28	0/1010	0.66	1/1353 (0.1%)
27	Q	0.21	0/805	0.48	0/1079
28	R	0.17	0/1654	0.38	0/2203
29	S	0.18	0/1885	0.44	1/2510 (0.0%)
30	T	0.24	0/1032	0.51	0/1371
31	V	0.23	0/1516	0.53	0/2037
32	Y	0.23	0/1142	0.55	0/1528

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.20	0/1793	0.45	0/2414
34	a	0.23	0/859	0.57	0/1159
35	b	0.25	0/1094	0.67	1/1464 (0.1%)
36	c	0.19	0/2493	0.49	0/3394
37	d	0.20	0/1123	0.45	0/1504
38	e	0.49	1/657 (0.2%)	0.69	0/878
39	f	0.22	0/1245	0.54	0/1665
40	h	0.26	0/827	0.60	0/1110
41	i	0.26	0/429	0.48	0/568
42	k	0.48	1/566 (0.2%)	0.95	2/753 (0.3%)
43	m	0.25	0/960	0.67	0/1286
44	n	0.20	0/508	0.57	0/680
45	o	0.21	0/628	0.53	0/846
46	q	0.21	0/965	0.54	0/1282
47	r	0.27	1/2167 (0.0%)	0.57	0/2943
48	t	0.22	0/3494	0.56	0/4726
49	u	0.26	0/5475	0.67	1/7432 (0.0%)
50	v	0.26	0/2778	0.68	1/3797 (0.0%)
51	w	0.23	0/1795	0.50	1/2798 (0.0%)
52	x	0.17	0/2885	0.48	0/3940
53	y	0.26	0/4436	0.66	0/5989
All	All	0.23	8/126848 (0.0%)	0.51	16/180626 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	e	30	ALA	C-N	6.99	1.43	1.33
8	7	-31	C	C1'-N1	6.30	1.56	1.47
8	7	-34	C	C1'-N1	6.16	1.57	1.48
8	7	-25	C	C1'-N1	5.87	1.57	1.48
47	r	55	ARG	C-N	5.68	1.40	1.33
8	7	-28	C	C1'-N1	5.68	1.55	1.47
8	7	-22	C	C1'-N1	5.54	1.56	1.48
42	k	89	LYS	C-N	-5.08	1.24	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	68	PRO	CA-N-CD	-8.25	100.45	112.00
42	k	89	LYS	N-CA-C	7.92	121.79	109.52
11	A	644	OMG	O3'-P-O5'	7.55	115.32	104.00
26	P	19	PRO	CA-N-CD	-6.93	102.30	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	509	OMG	O3'-P-O5'	6.74	114.11	104.00
42	k	88	PRO	N-CA-C	-6.38	100.48	110.50
8	7	-31	C	C2'-C3'-O3'	5.62	117.93	109.50
11	A	731	G	P-O3'-C3'	5.47	128.40	120.20
6	5	327	ARG	CA-CB-CG	5.44	124.98	114.10
49	u	506	PRO	CA-N-CD	-5.44	104.38	112.00
29	S	122	PRO	CA-N-CD	-5.41	104.43	112.00
51	w	22	G	P-O3'-C3'	5.36	128.24	120.20
8	7	-31	C	P-O3'-C3'	5.36	128.23	120.20
50	v	247	GLN	CA-CB-CG	5.33	124.76	114.10
17	G	32	MET	CA-CB-CG	5.29	124.68	114.10
1	0	1002	GLU	CB-CG-CD	5.22	121.48	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4920	0	5100	83	0
2	1	3258	0	1917	20	0
3	2	1493	0	677	0	0
4	3	1057	0	475	1	0
5	4	1272	0	564	1	0
6	5	4347	0	4294	52	0
7	6	2196	0	1547	26	0
8	7	1218	0	620	8	0
9	8	1574	0	687	6	0
10	9	230	0	276	8	0
11	A	37429	0	18911	318	0
12	B	1166	0	1233	11	0
13	C	2035	0	2138	20	0
14	D	1477	0	1589	22	0
15	E	1087	0	1154	15	0
16	F	452	0	485	3	0
17	G	1430	0	1520	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	H	631	0	656	11	0
19	I	1208	0	1294	18	0
20	J	1034	0	1080	18	0
21	K	617	0	622	4	0
22	L	1707	0	1794	23	0
23	M	1064	0	1118	13	0
24	N	1633	0	1640	21	0
25	O	1715	0	1785	15	0
26	P	997	0	1021	21	0
27	Q	792	0	843	12	0
28	R	1627	0	1706	18	0
29	S	1862	0	2018	21	0
30	T	1015	0	1086	15	0
31	V	1495	0	1549	24	0
32	Y	1124	0	1193	12	0
33	Z	1765	0	1865	14	0
34	a	834	0	861	15	0
35	b	1072	0	1121	16	0
36	c	2436	0	2393	16	0
37	d	1105	0	1138	14	0
38	e	649	0	724	18	0
39	f	1227	0	1298	13	0
40	h	817	0	882	9	0
41	i	419	0	415	10	0
42	k	554	0	556	22	0
43	m	950	0	987	17	0
44	n	506	0	536	4	0
45	o	616	0	600	4	0
46	q	951	0	981	12	0
47	r	2138	0	1930	36	0
48	t	3439	0	3578	42	0
49	u	5383	0	5085	114	0
50	v	2740	0	2251	42	0
51	w	1604	0	816	4	0
52	x	2842	0	2209	35	0
53	y	4361	0	4334	102	0
54	0	32	0	12	2	0
55	0	1	0	0	0	0
56	0	1	0	0	0	0
56	A	87	0	0	0	0
56	f	1	0	0	0	0
57	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	k	1	0	0	0	0
All	All	121694	0	97164	1167	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 5.

All (1167) 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)
11:A:191:A:H62	11:A:208:G:H21	0.99	0.99
11:A:961:G:N3	47:r:55:ARG:NH2	2.16	0.94
11:A:683:OMG:H1'	20:J:4:MET:HE1	1.47	0.93
11:A:191:A:N6	11:A:208:G:H21	1.65	0.93
11:A:191:A:H62	11:A:208:G:N2	1.66	0.92
11:A:683:OMG:C1'	20:J:4:MET:HE1	2.04	0.86
42:k:121:CYS:SG	42:k:126:CYS:HB2	2.19	0.83
22:L:178:HIS:HD1	22:L:179:THR:HG1	1.27	0.83
38:e:34:LYS:HE2	38:e:36:SER:OG	1.77	0.82
1:0:1140:SER:HB3	1:0:1160:LYS:HB3	1.61	0.82
49:u:340:ARG:HE	53:y:745:LYS:HD3	1.46	0.79
53:y:835:LEU:HB2	53:y:840:GLN:O	1.83	0.79
11:A:1507:G:N2	42:k:89:LYS:HB2	1.96	0.79
53:y:568:ALA:O	53:y:572:HIS:HB2	1.84	0.77
49:u:407:VAL:HG21	49:u:435:THR:HG21	1.67	0.76
48:t:39:GLN:HE22	48:t:332:ALA:H	1.33	0.76
49:u:172:ARG:HA	49:u:228:MET:HE1	1.67	0.75
53:y:698:MET:HA	53:y:702:GLU:HB2	1.68	0.75
11:A:961:G:H21	47:r:55:ARG:HH21	1.32	0.75
49:u:87:GLU:HG2	49:u:173:LEU:HD22	1.68	0.74
49:u:205:LEU:HD11	49:u:233:ARG:HH12	1.52	0.74
50:v:405:ILE:HG22	50:v:409:LYS:HE2	1.68	0.74
11:A:509:OMG:HM22	11:A:510:G:C8	2.23	0.73
11:A:1033:G:H1	11:A:1080:A:HO2'	1.32	0.73
50:v:342:GLU:HG3	50:v:346:ARG:HH22	1.55	0.72
11:A:925:G:H1	11:A:1017:U:H3	1.38	0.72
31:V:130:ARG:HH21	47:r:55:ARG:NH1	1.87	0.71
35:b:63:ALA:O	35:b:67:ALA:HB2	1.91	0.70
53:y:851:ALA:O	53:y:855:LEU:HB2	1.90	0.70
43:m:79:VAL:HG21	43:m:85:LEU:HB2	1.73	0.70
11:A:1091:C:HO2'	20:J:2:VAL:N	1.89	0.69
2:1:306:TYR:HA	2:1:704:TRP:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:v:406:GLU:HA	50:v:409:LYS:HD2	1.75	0.69
49:u:372:ASN:HA	49:u:375:VAL:HG22	1.74	0.69
50:v:243:LEU:HA	50:v:247:GLN:HB3	1.75	0.69
35:b:53:GLN:HG3	35:b:83:MET:HE1	1.75	0.69
11:A:1507:G:C2	42:k:89:LYS:HB2	2.28	0.68
1:0:634:ILE:HD11	1:0:724:ILE:HG13	1.76	0.68
1:0:1097:LEU:HD22	1:0:1156:GLU:HG3	1.76	0.68
20:J:111:MET:HE1	20:J:119:LYS:HD2	1.75	0.68
53:y:504:LEU:HD11	53:y:567:CYS:HB3	1.76	0.68
12:B:77:VAL:HG11	12:B:80:MET:HE3	1.76	0.68
37:d:85:ASN:HB2	37:d:88:MET:HB2	1.75	0.67
49:u:397:GLU:OE1	49:u:399:ASN:ND2	2.28	0.67
13:C:87:MET:HE1	13:C:236:ILE:HG21	1.76	0.67
14:D:71:LEU:O	14:D:75:ASN:ND2	2.23	0.67
12:B:104:LYS:O	15:E:11:ARG:NH2	2.28	0.66
53:y:683:GLU:HG3	53:y:733:MET:HE3	1.76	0.66
53:y:452:ASP:OD1	53:y:509:HIS:NE2	2.28	0.66
11:A:925:G:OP1	19:I:121:ARG:NH2	2.28	0.66
49:u:472:VAL:HG23	53:y:798:VAL:HG11	1.77	0.66
11:A:1497:G:N7	34:a:25:LYS:NZ	2.41	0.66
48:t:44:ILE:HG12	48:t:154:ALA:HB3	1.76	0.66
8:7:-21:A:H62	49:u:192:ALA:HB1	1.60	0.65
15:E:93:PHE:O	15:E:140:ARG:NH2	2.26	0.65
7:6:312:VAL:HG11	7:6:325:ILE:HD13	1.79	0.65
17:G:154:ILE:HB	17:G:185:VAL:HG12	1.77	0.65
49:u:132:VAL:O	53:y:678:ASN:ND2	2.29	0.65
53:y:393:MET:HE2	53:y:397:MET:HE3	1.78	0.65
13:C:45:ILE:HA	13:C:61:VAL:HG11	1.79	0.65
25:O:77:ASP:OD2	49:u:14[B]:ARG:NH1	2.30	0.65
6:5:183:LEU:HD22	6:5:269:LEU:HD13	1.79	0.65
26:P:80:ASP:HA	26:P:83:GLN:HG3	1.79	0.65
26:P:99:ALA:H	26:P:133:THR:HG22	1.61	0.65
11:A:528:A:N1	11:A:557:U:O2'	2.30	0.65
46:q:62:ARG:HE	46:q:64:LYS:HD2	1.62	0.65
14:D:21:GLU:OE1	14:D:24:ARG:NH1	2.29	0.65
49:u:335:ARG:NH2	49:u:352:GLN:OE1	2.30	0.64
52:x:31:GLN:NE2	53:y:591:MET:O	2.29	0.64
1:0:724:ILE:HD11	1:0:838:LEU:HD11	1.79	0.64
32:Y:110:ASP:O	32:Y:114:GLN:NE2	2.31	0.64
49:u:531:ALA:O	49:u:535:GLU:HB2	1.98	0.64
18:H:80:ARG:HH12	52:x:75:GLU:HG2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:64:ARG:NH1	34:a:73:ASN:OD1	2.30	0.63
24:N:77:ILE:HD12	24:N:122:LEU:HD11	1.79	0.63
49:u:17:GLU:HA	49:u:20:GLU:HG3	1.80	0.63
1:0:1155:GLN:NE2	1:0:1156:GLU:O	2.30	0.63
11:A:751:G:H22	11:A:789:G:H5''	1.62	0.63
53:y:394:LYS:HB3	53:y:397:MET:HG2	1.78	0.63
35:b:56:LEU:HD23	35:b:83:MET:HE3	1.80	0.63
53:y:687:LEU:HD12	53:y:733:MET:HE1	1.81	0.62
11:A:614:C:OP1	46:q:62:ARG:NH2	2.31	0.62
11:A:1016:U:OP2	18:H:20:LYS:NZ	2.33	0.62
11:A:922:A:OP2	20:J:28:ARG:NH1	2.33	0.62
11:A:961:G:N2	47:r:55:ARG:HH21	1.97	0.62
6:5:394:TYR:HB3	6:5:397:LYS:HB2	1.81	0.62
19:I:4:MET:SD	19:I:124:ARG:NH1	2.73	0.62
31:V:102:LEU:HD11	38:e:100:VAL:HG21	1.82	0.62
11:A:961:G:H21	47:r:55:ARG:HD2	1.65	0.62
11:A:1048:G:OP2	26:P:143:LYS:NZ	2.32	0.62
7:6:344:LYS:HA	7:6:347:TRP:HD1	1.63	0.62
15:E:39:ASN:ND2	15:E:42:GLY:O	2.33	0.62
31:V:71:ARG:NH2	31:V:148:ASN:OD1	2.33	0.62
49:u:172:ARG:HH21	49:u:176:ASP:HB2	1.63	0.62
13:C:100:ARG:HB2	13:C:114:ILE:HD13	1.81	0.62
29:S:159:ARG:NH2	29:S:171:THR:O	2.33	0.62
49:u:405:GLU:HA	49:u:408:THR:HG22	1.80	0.61
11:A:801:U:O4	17:G:106:ARG:NH1	2.32	0.61
11:A:1086:G:OP2	27:Q:12:LYS:NZ	2.33	0.61
27:Q:87:ARG:NH1	27:Q:94:ASP:OD1	2.33	0.61
6:5:478:PHE:O	50:v:369:ARG:NH1	2.33	0.61
11:A:643:A:OP1	14:D:38:ARG:NH1	2.33	0.61
49:u:414:VAL:O	49:u:425:GLN:NE2	2.32	0.61
11:A:973:C:N3	26:P:55:ARG:NH2	2.48	0.61
13:C:11:ARG:HA	13:C:28:ALA:HB2	1.82	0.61
11:A:1014:G:N2	18:H:51:GLN:OE1	2.34	0.61
26:P:101:GLY:HA3	26:P:134:PRO:HG2	1.83	0.61
53:y:758:ASN:HB3	53:y:761:MET:HG2	1.83	0.61
25:O:28:LYS:NZ	26:P:51:GLU:OE1	2.31	0.60
34:a:49:MET:HG2	34:a:52:LEU:HD12	1.83	0.60
11:A:926:A:H61	11:A:1015:U:H3	1.50	0.60
11:A:1674:G:H4'	31:V:77:MET:HE1	1.82	0.60
42:k:126:CYS:HB3	42:k:130:VAL:HG21	1.82	0.60
50:v:320:VAL:HG12	50:v:329:LEU:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:195:GLN:HG2	6:5:421:LEU:HD21	1.82	0.60
32:Y:53:GLU:OE2	32:Y:85:ARG:NH1	2.34	0.60
42:k:130:VAL:HA	43:m:36:ARG:HH22	1.66	0.60
11:A:1481:G:O3'	41:i:54:LYS:NZ	2.34	0.60
48:t:344:ASP:HB3	48:t:347:LEU:HG	1.83	0.60
49:u:191:LYS:HD2	49:u:243:MET:HE3	1.82	0.60
1:0:991:LEU:HD21	1:0:1008:ILE:HB	1.83	0.60
6:5:167:ILE:O	6:5:237:LYS:NZ	2.34	0.60
11:A:1829:G:H1'	11:A:1850:MA6:H2	1.82	0.60
30:T:110:ARG:HG2	30:T:114:MET:HE2	1.83	0.60
49:u:93:TYR:HA	49:u:96:MET:HE3	1.81	0.60
11:A:509:OMG:N3	11:A:509:OMG:HM23	2.17	0.60
11:A:1752:C:O2'	11:A:1782:G:N2	2.34	0.60
11:A:1780:G:O6	11:A:1782:G:N2	2.35	0.59
6:5:327:ARG:HH22	6:5:496:LYS:HG2	1.67	0.59
2:1:524:ASP:OD1	2:1:548:ARG:NH2	2.34	0.59
11:A:996:A:OP1	19:I:114:ARG:NH2	2.35	0.59
11:A:1854:U:OP1	26:P:150:ARG:NH1	2.34	0.59
49:u:329:ILE:O	49:u:367:ARG:NH1	2.36	0.59
50:v:263:THR:HG21	50:v:328:CYS:HB3	1.85	0.59
14:D:63:LEU:HD22	14:D:70:ARG:HB2	1.82	0.59
19:I:4:MET:HE3	19:I:121:ARG:HG2	1.84	0.59
22:L:64:THR:HG23	22:L:67:GLY:H	1.67	0.59
48:t:222:ILE:HD13	48:t:235:VAL:HA	1.85	0.59
53:y:410:ASP:OD1	53:y:485:ARG:NH2	2.35	0.59
49:u:337:ASP:HB2	53:y:746:MET:HE1	1.83	0.59
11:A:67:C:N4	29:S:168:LYS:O	2.36	0.59
11:A:1396:A:O2'	11:A:1398:G:N7	2.33	0.59
27:Q:25:ASN:ND2	27:Q:77:CYS:SG	2.76	0.59
11:A:1597:C:OP2	38:e:85:ARG:NH2	2.36	0.59
47:r:157:VAL:HB	47:r:186:PRO:HB3	1.84	0.59
33:Z:64:ARG:NH2	34:a:71:LEU:O	2.36	0.59
11:A:553:U:O4	11:A:555:A:N6	2.36	0.59
48:t:49:HIS:O	48:t:54:LYS:NZ	2.36	0.59
1:0:961:ASP:O	1:0:965:HIS:ND1	2.35	0.58
34:a:37:ASP:OD1	34:a:38:LYS:NZ	2.35	0.58
7:6:327:GLN:O	7:6:330:ARG:NH2	2.37	0.58
11:A:1669:G:OP1	40:h:79:ARG:NH1	2.36	0.58
42:k:84:SER:HB3	46:q:25:GLU:OE2	2.03	0.58
11:A:1416:C:OP1	37:d:133:ARG:NH2	2.37	0.58
47:r:180:ILE:HG13	47:r:184:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:104:ASP:HB3	13:C:110:ALA:HB2	1.85	0.58
11:A:1488:C:O2'	11:A:1490:G:OP2	2.19	0.58
11:A:1729:U:H3	11:A:1805:G:H1	1.49	0.58
53:y:679:LEU:HD13	53:y:682:LEU:HD23	1.85	0.58
44:n:13:ARG:HB3	52:x:426:LYS:HZ1	1.69	0.57
52:x:391:ILE:HG22	52:x:446:TYR:HB2	1.87	0.57
7:6:327:GLN:HE21	49:u:450:ILE:HA	1.69	0.57
11:A:830:A:OP2	11:A:846:G:N2	2.29	0.57
11:A:1310:U:H4'	42:k:143:LYS:HB2	1.87	0.57
53:y:673:PHE:HA	53:y:676:HIS:CD2	2.39	0.57
26:P:100:THR:HG21	26:P:104:ARG:HD2	1.85	0.57
26:P:86:LYS:NZ	26:P:122:SER:O	2.37	0.57
7:6:243:ILE:O	7:6:340:ARG:NH1	2.37	0.57
11:A:919:A:H5''	19:I:16:LEU:HD12	1.87	0.57
11:A:961:G:N2	47:r:55:ARG:HD2	2.20	0.57
6:5:148:PRO:HG2	6:5:153:ARG:HE	1.68	0.57
11:A:1024:A:OP2	19:I:124:ARG:NH1	2.36	0.57
1:0:712:LEU:HD21	1:0:989:GLY:HA3	1.87	0.56
11:A:688:U:OP1	17:G:116:ARG:NH1	2.37	0.56
12:B:135:SER:O	12:B:139:ARG:NH1	2.38	0.56
13:C:148:ARG:NH2	29:S:202:ASN:OD1	2.38	0.56
1:0:1142:GLU:HG2	1:0:1147:GLN:HA	1.87	0.56
7:6:249:LEU:HD11	7:6:301:LEU:HD23	1.86	0.56
11:A:752:G:N2	11:A:793:G:O2'	2.39	0.56
11:A:1656:G:H1	11:A:1668:U:H3	1.51	0.56
26:P:62:VAL:HG11	26:P:67:ASP:HB2	1.86	0.56
53:y:568:ALA:O	53:y:572:HIS:CB	2.52	0.56
7:6:278:ARG:HD3	7:6:311:PHE:HE2	1.70	0.56
11:A:919:A:OP2	19:I:64:ARG:NH2	2.38	0.56
11:A:1013:U:OP1	11:A:1129:G:O2'	2.22	0.56
11:A:1661:A:OP1	41:i:19:ARG:NH1	2.38	0.56
17:G:20:GLU:OE2	17:G:24:SER:OG	2.23	0.56
11:A:482:G:N1	11:A:485:A:OP2	2.39	0.56
11:A:1204:A:O2'	11:A:1700:C:OP2	2.21	0.56
18:H:23:ARG:O	20:J:60:LYS:NZ	2.39	0.56
26:P:64:ALA:O	47:r:88:ARG:NH2	2.39	0.56
29:S:121:ILE:HG21	29:S:124:LEU:HD12	1.87	0.56
50:v:373:ASN:O	50:v:377:ASN:ND2	2.37	0.56
11:A:1147:C:OP1	27:Q:6:ARG:NH1	2.36	0.56
43:m:32:ALA:HB1	43:m:37:GLU:HB3	1.87	0.56
53:y:700:ALA:HB2	53:y:793:PHE:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:u:208:ILE:O	49:u:212:HIS:ND1	2.35	0.56
49:u:340:ARG:HH22	53:y:742:LYS:HA	1.71	0.56
11:A:156:G:OP1	29:S:2:LYS:NZ	2.33	0.56
18:H:21:LYS:NZ	19:I:13:GLN:OE1	2.38	0.56
30:T:81:TYR:O	30:T:85:ASN:ND2	2.36	0.56
31:V:26:ASP:OD2	52:x:446:TYR:OH	2.24	0.56
11:A:379:C:O2	28:R:5:ARG:NE	2.36	0.56
53:y:422:GLU:OE2	53:y:433:ASN:ND2	2.39	0.56
11:A:163:U:OP2	29:S:87:ARG:NH2	2.39	0.55
13:C:54:TYR:O	30:T:15:ASN:ND2	2.39	0.55
30:T:80:ASP:OD1	30:T:81:TYR:N	2.40	0.55
49:u:135:GLU:OE2	53:y:465:HIS:ND1	2.37	0.55
6:5:457:LEU:HD11	6:5:492:VAL:HG12	1.88	0.55
53:y:788:LEU:HD11	53:y:818:VAL:HG23	1.89	0.55
38:e:46:ASN:HB3	38:e:79:ILE:C	2.31	0.55
2:1:527:CYS:SG	2:1:570:TRP:NE1	2.72	0.55
11:A:604:A:N3	11:A:639:C:O2'	2.34	0.55
11:A:1227:G:HO2'	38:e:35:TRP:CD1	2.24	0.55
11:A:838:G:O2'	11:A:840:C:OP2	2.24	0.55
46:q:101:ARG:HB3	46:q:118:THR:HB	1.89	0.55
11:A:494:C:H41	11:A:509:OMG:HN22	1.53	0.55
11:A:1304:U:O2'	42:k:93:HIS:NE2	2.39	0.55
19:I:63:VAL:HG11	19:I:71:ILE:HG13	1.89	0.55
23:M:82:ASP:O	24:N:85:ARG:NH2	2.39	0.55
43:m:82:ASN:ND2	43:m:107:SER:OG	2.36	0.55
49:u:171:GLU:HA	49:u:174:TYR:HB3	1.89	0.55
11:A:1550:G:O2'	11:A:1558:C:O2	2.21	0.55
22:L:77:SER:N	22:L:80:GLU:OE2	2.38	0.55
11:A:1639:G:C2	38:e:35:TRP:CZ3	2.95	0.55
9:8:311:PRO:O	9:8:315:ASP:N	2.35	0.55
11:A:1292:C:O2'	42:k:147:THR:OG1	2.22	0.55
47:r:24:VAL:HA	47:r:34:VAL:HG12	1.88	0.55
11:A:1094:C:O2	20:J:16:ASN:ND2	2.39	0.55
11:A:1825:A:O2'	35:b:145:LYS:O	2.23	0.55
26:P:86:LYS:HG3	26:P:124:MET:HE1	1.88	0.55
47:r:71:VAL:HG21	47:r:85:LEU:HD13	1.89	0.55
1:0:1138:VAL:HA	1:0:1161:ILE:HG12	1.89	0.54
11:A:1757:G:O2'	11:A:1776:G:N1	2.40	0.54
47:r:118:VAL:HG21	47:r:175:VAL:HG21	1.87	0.54
1:0:1138:VAL:H	1:0:1161:ILE:HG23	1.72	0.54
11:A:943:U:O2'	26:P:135:ILE:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:104:ASP:HB3	22:L:130:ILE:HG22	1.89	0.54
24:N:147:LEU:O	24:N:165:ASN:ND2	2.40	0.54
48:t:255:ARG:NH1	48:t:436:GLU:OE2	2.40	0.54
22:L:182:CYS:SG	22:L:183:LYS:N	2.80	0.54
47:r:72:VAL:HG23	47:r:90:VAL:HG22	1.90	0.54
49:u:485:ASP:OD1	53:y:801:SER:OG	2.25	0.54
52:x:289:LEU:HD23	52:x:316:ALA:HB1	1.90	0.54
53:y:476:GLU:OE2	53:y:509:HIS:ND1	2.41	0.54
6:5:216:ARG:NH2	6:5:429:ASP:OD1	2.41	0.54
7:6:28:GLU:O	7:6:32:GLU:N	2.39	0.54
11:A:1378:A:N6	24:N:136:GLU:OE2	2.41	0.54
33:Z:16:ILE:HD11	41:i:36:LEU:HD23	1.90	0.54
48:t:145:MET:HE3	48:t:173:HIS:CD2	2.43	0.54
49:u:233:ARG:NH1	49:u:255:ASP:OD2	2.40	0.54
1:0:983:VAL:HG12	1:0:1035:LEU:HB2	1.90	0.54
50:v:384:ILE:HG22	50:v:391:VAL:HG13	1.90	0.54
1:0:646:LYS:HD3	54:0:2001:GTP:C8	2.43	0.54
1:0:1126:CYS:HA	1:0:1133:VAL:O	2.08	0.54
47:r:189:VAL:HG23	47:r:279:THR:HA	1.88	0.54
1:0:707:GLU:OE1	1:0:736:GLN:NE2	2.40	0.54
1:0:1160:LYS:NZ	51:w:75:C:O2	2.41	0.54
24:N:85:ARG:NH1	24:N:203:PHE:O	2.40	0.54
45:o:289:ARG:NE	45:o:292:ASP:OD2	2.32	0.54
1:0:948:LEU:HD13	1:0:959:LEU:HD22	1.89	0.53
11:A:84:A:N3	11:A:150:A:O2'	2.39	0.53
11:A:350:C:O2'	11:A:383:G:N1	2.41	0.53
23:M:36:GLU:OE1	23:M:47:ARG:NH1	2.41	0.53
31:V:124:ASP:OD1	31:V:125:SER:N	2.41	0.53
36:c:124:SER:OG	36:c:126:ASP:OD1	2.25	0.53
49:u:321:ARG:HE	49:u:423:GLU:HG3	1.73	0.53
53:y:694:GLU:HG2	53:y:698:MET:SD	2.48	0.53
11:A:619:A:H61	15:E:115:ILE:HD11	1.73	0.53
11:A:1458:G:OP1	36:c:276:SER:OG	2.26	0.53
52:x:82:LEU:HG	52:x:84:ASP:H	1.73	0.53
11:A:60:G:H22	11:A:316:G:H21	1.56	0.53
1:0:670:ALA:HB3	1:0:913:LEU:HD12	1.91	0.53
11:A:1206:G:O2'	11:A:1208:A:OP1	2.23	0.53
28:R:11:ARG:NH1	28:R:15:GLY:O	2.40	0.53
53:y:698:MET:HA	53:y:702:GLU:CB	2.38	0.53
11:A:199:C:O2	11:A:200:G:N2	2.42	0.53
11:A:496:C:OP1	13:C:49:ARG:NH2	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:142:LEU:HD13	33:Z:150:MET:HE3	1.89	0.53
33:Z:193:ASP:OD1	33:Z:193:ASP:N	2.38	0.53
1:0:1103:ASN:ND2	1:0:1107:PRO:O	2.42	0.53
11:A:450:C:OP1	13:C:3:ARG:NH1	2.42	0.53
46:q:37:GLN:NE2	46:q:114:LYS:O	2.42	0.53
49:u:87:GLU:OE2	49:u:91:ARG:NH2	2.41	0.53
49:u:523:LEU:HG	49:u:527:SER:HB3	1.90	0.53
7:6:252:TYR:OH	7:6:270:HIS:ND1	2.39	0.53
11:A:520:A:O2'	11:A:825:A:N3	2.35	0.53
11:A:1133:A:O3'	27:Q:13:LYS:NZ	2.42	0.53
49:u:312:GLN:HA	49:u:315:MET:HG3	1.91	0.53
53:y:422:GLU:OE1	53:y:439:ARG:NH1	2.28	0.53
7:6:258:ASN:OD1	7:6:259:ASN:N	2.42	0.53
11:A:380:G:OP1	28:R:31:ARG:NH1	2.36	0.53
20:J:3:ARG:NH1	20:J:9:ASP:OD2	2.41	0.53
22:L:168:GLY:N	22:L:179:THR:O	2.40	0.53
25:O:82:ARG:NH2	25:O:191:ASP:OD1	2.42	0.53
53:y:373:LYS:O	53:y:377:ASN:ND2	2.42	0.53
11:A:65:C:N4	29:S:134:GLY:O	2.30	0.52
53:y:780:VAL:HA	53:y:783:ILE:HG12	1.91	0.52
1:0:630:ARG:NH1	1:0:721:ASP:OD2	2.42	0.52
1:0:1108:ILE:O	1:0:1160:LYS:HA	2.08	0.52
1:0:1141:ILE:HG23	1:0:1157:VAL:HG21	1.91	0.52
11:A:1252:C:N4	32:Y:146:ARG:O	2.43	0.52
29:S:57:ASP:OD1	29:S:58:LYS:N	2.41	0.52
35:b:24:GLN:O	35:b:28:MET:HB3	2.09	0.52
8:7:-7:G:N3	44:n:66:ARG:NH1	2.56	0.52
11:A:1598:G:OP1	38:e:80:ARG:NH1	2.41	0.52
22:L:70:VAL:HG11	22:L:93:ILE:HG23	1.91	0.52
23:M:106:LEU:HD11	24:N:19:LEU:HD11	1.91	0.52
33:Z:76:ARG:O	33:Z:76:ARG:NH1	2.42	0.52
20:J:87:GLU:OE2	20:J:117:ARG:NH1	2.42	0.52
31:V:130:ARG:HH21	47:r:55:ARG:HH11	1.56	0.52
52:x:42:VAL:HG11	53:y:636:ILE:HB	1.91	0.52
49:u:344:MET:HE1	53:y:719:ARG:HG3	1.91	0.52
11:A:570:C:H4'	30:T:36:PRO:HG3	1.92	0.52
11:A:641:A:OP1	14:D:40:LYS:NZ	2.33	0.52
13:C:44:LEU:HD21	13:C:70:ILE:HG21	1.90	0.52
1:0:984:GLN:HG3	1:0:1013:VAL:HG22	1.92	0.52
11:A:170:A:OP2	29:S:140:ARG:NH1	2.42	0.52
32:Y:40:GLU:O	32:Y:48:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:301:LYS:HE2	6:5:303:SER:HB2	1.92	0.52
27:Q:23:CYS:O	27:Q:27:ALA:HA	2.10	0.52
34:a:31:LYS:NZ	34:a:39:ASN:OD1	2.30	0.52
1:0:1187:SER:N	1:0:1190:SER:OG	2.42	0.52
32:Y:97:GLN:HB3	32:Y:105:LYS:HG3	1.90	0.52
52:x:207:ASP:O	52:x:468:THR:OG1	2.27	0.52
11:A:1563:G:OP1	37:d:121:ARG:NH1	2.43	0.52
1:0:1090:PHE:HE2	1:0:1202:MET:HA	1.75	0.51
6:5:48:ILE:HB	6:5:53:LYS:HE3	1.91	0.51
11:A:846:G:C4	13:C:19:MET:HE1	2.46	0.51
11:A:1604:G:OP2	39:f:38:ARG:NH2	2.43	0.51
11:A:1760:G:H21	11:A:1772:C:H5'	1.75	0.51
49:u:19:LEU:HD11	49:u:53:LYS:HD2	1.92	0.51
6:5:191:ILE:HG21	6:5:279:ARG:HE	1.76	0.51
11:A:823:PSU:N3	14:D:143:ASN:OD1	2.41	0.51
31:V:30:ILE:O	52:x:479:GLN:NE2	2.35	0.51
47:r:177:ILE:HA	47:r:180:ILE:HG22	1.91	0.51
48:t:23:LEU:HD11	48:t:28:LEU:HD11	1.91	0.51
49:u:340:ARG:HH12	53:y:742:LYS:HG3	1.75	0.51
50:v:261:VAL:HG11	50:v:274:LEU:HD13	1.91	0.51
52:x:445:GLU:OE2	52:x:472:LYS:NZ	2.43	0.51
1:0:896:PRO:HD3	1:0:964:ILE:HD11	1.92	0.51
11:A:544:G:H2'	11:A:545:A:C8	2.45	0.51
11:A:1403:C:N4	11:A:1433:C:OP1	2.44	0.51
17:G:69:LEU:HD22	17:G:96:ALA:HB2	1.92	0.51
49:u:135:GLU:OE1	49:u:140:ARG:NH1	2.43	0.51
52:x:381:MET:HG2	52:x:391:ILE:HD13	1.93	0.51
53:y:757:ILE:HD11	53:y:776:ARG:HD2	1.91	0.51
11:A:57:U:OP1	11:A:504:G:O2'	2.27	0.51
11:A:303:C:O2	28:R:184:ARG:NH1	2.43	0.51
11:A:1398:G:O2'	36:c:88:ARG:NH2	2.43	0.51
42:k:111:ASN:O	42:k:113:LYS:NZ	2.43	0.51
7:6:325:ILE:HG22	7:6:332:VAL:HG12	1.93	0.51
17:G:163:GLN:NE2	17:G:167:GLU:OE1	2.43	0.51
20:J:37:PHE:HD1	20:J:41:MET:HE2	1.75	0.51
26:P:145:GLY:O	27:Q:22:ARG:NH2	2.42	0.51
48:t:369:THR:HG21	48:t:465:ILE:HD12	1.91	0.51
49:u:468:GLU:HA	49:u:471:ILE:HD12	1.92	0.51
6:5:383:ASP:HA	6:5:545:ARG:HH21	1.75	0.51
10:9:15:ARG:NH1	11:A:1183:A:OP1	2.43	0.51
11:A:1228:A:H2'	11:A:1229:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:66:VAL:HG22	17:G:96:ALA:HB1	1.92	0.51
33:Z:167:TYR:OH	33:Z:202:LYS:O	2.27	0.51
48:t:142:MET:HA	48:t:145:MET:HG3	1.92	0.51
49:u:226:GLN:HG2	49:u:264:LYS:HE3	1.92	0.51
7:6:327:GLN:HE22	49:u:454:ARG:HG2	1.75	0.51
11:A:72:C:O2'	11:A:74:G:N2	2.43	0.51
11:A:98:C:OP2	11:A:426:A:O2'	2.26	0.51
11:A:484:A2M:O5'	11:A:484:A2M:H8	2.11	0.51
11:A:734:C:O2'	11:A:736:C:N4	2.43	0.51
11:A:1675:A:OP1	31:V:86:LYS:NZ	2.43	0.51
24:N:137:ALA:HB1	24:N:142:LEU:HB2	1.92	0.51
25:O:190:PRO:HA	49:u:14[B]:ARG:HH21	1.76	0.51
36:c:10:THR:HB	36:c:306:LEU:HD22	1.91	0.51
49:u:239:SER:O	49:u:243:MET:HG2	2.11	0.51
50:v:398:VAL:HA	53:y:846:ARG:HH21	1.75	0.51
7:6:286:ALA:HB1	7:6:334:VAL:HG21	1.93	0.51
24:N:76:VAL:HG12	24:N:123:VAL:HB	1.93	0.51
39:f:98:VAL:HG11	39:f:106:LYS:HG3	1.92	0.51
49:u:315:MET:HA	49:u:318:MET:HG3	1.92	0.51
1:0:660:GLU:OE2	1:0:914:ARG:NH1	2.43	0.51
31:V:27:ASP:OD1	31:V:27:ASP:N	2.42	0.51
6:5:220:LYS:O	6:5:223:ASN:ND2	2.33	0.51
10:9:17:ARG:NH1	11:A:1173:A:OP1	2.44	0.51
11:A:814:5MU:OP1	13:C:22:LYS:NZ	2.44	0.51
11:A:1550:G:H3'	11:A:1579:A:H61	1.76	0.51
24:N:85:ARG:NH2	24:N:201:LEU:O	2.43	0.51
27:Q:60:ASP:OD1	27:Q:61:ALA:N	2.43	0.51
37:d:9:VAL:HG21	37:d:138:VAL:HG13	1.91	0.51
48:t:157:LEU:HD11	48:t:170:THR:HB	1.93	0.51
1:0:1173:GLY:N	1:0:1176:PHE:O	2.39	0.50
11:A:545:A:O2'	11:A:546:G:O4'	2.28	0.50
11:A:546:G:N2	11:A:547:G:O6	2.42	0.50
11:A:1589:A:N3	11:A:1653:U:O2'	2.44	0.50
39:f:34:LYS:HG2	39:f:103:LEU:HD23	1.93	0.50
49:u:48:GLU:OE2	49:u:85:SER:OG	2.25	0.50
2:1:170:GLY:N	2:1:230:LYS:O	2.44	0.50
6:5:547:ILE:HA	6:5:550:PHE:CE1	2.46	0.50
11:A:1360:U:O2'	11:A:1379:A:OP2	2.26	0.50
11:A:1658:G:OP2	11:A:1660:C:N4	2.45	0.50
24:N:41:ARG:NH1	24:N:47:TYR:OH	2.44	0.50
49:u:336:THR:OG1	49:u:337:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:v:298:CYS:HA	50:v:301:VAL:HG12	1.93	0.50
53:y:745:LYS:HA	53:y:790:THR:HG21	1.93	0.50
11:A:70:G:OP2	29:S:167:LYS:NZ	2.44	0.50
11:A:319:C:N4	29:S:186:GLN:OE1	2.45	0.50
11:A:509:OMG:HM23	11:A:509:OMG:C4	2.47	0.50
17:G:145:ARG:NH1	20:J:51:GLU:OE2	2.37	0.50
18:H:46:VAL:HG22	18:H:54:VAL:HG11	1.94	0.50
19:I:5:HIS:HB3	19:I:117:LEU:HD13	1.91	0.50
29:S:18:VAL:HG21	29:S:24:LEU:HD21	1.93	0.50
34:a:31:LYS:NZ	34:a:36:ALA:O	2.35	0.50
48:t:156:LEU:HD13	48:t:188:LEU:HD11	1.93	0.50
53:y:697:TYR:O	53:y:701:HIS:HB2	2.10	0.50
10:9:11:ARG:NH2	11:A:1184:G:OP1	2.45	0.50
21:K:30:ALA:O	21:K:60:ARG:NH1	2.44	0.50
50:v:315:CYS:O	50:v:319:LEU:HB2	2.12	0.50
51:w:73:A:H3'	51:w:74:C:H6	1.77	0.50
11:A:637:U:O2	16:F:130:ASN:ND2	2.44	0.50
11:A:641:A:O2'	11:A:645:C:OP1	2.30	0.50
11:A:1292:C:N3	42:k:138:ARG:NH2	2.48	0.50
49:u:222:ASN:HB3	49:u:225:SER:HB3	1.93	0.50
11:A:987:A:OP1	27:Q:32:LYS:NZ	2.42	0.50
26:P:40:THR:HG21	26:P:74:ALA:HB2	1.93	0.50
38:e:57:LYS:O	38:e:61:GLU:HB3	2.12	0.50
49:u:502:ARG:HD2	53:y:850:THR:HG21	1.94	0.50
11:A:955:A:N1	11:A:968:U:O2'	2.42	0.50
11:A:1674:G:N7	32:Y:17:LYS:NZ	2.52	0.50
12:B:113:LEU:HD21	12:B:120:VAL:HG21	1.93	0.50
25:O:136:ARG:HB2	25:O:218:LEU:HD11	1.93	0.50
48:t:12:GLN:NE2	48:t:326:ASN:OD1	2.42	0.50
53:y:627:LYS:HA	53:y:693:LEU:HD21	1.93	0.50
6:5:68:ASP:HA	6:5:71:VAL:HG22	1.94	0.50
11:A:539:C:H2'	11:A:540:U:H3'	1.94	0.50
11:A:1454:A:O4'	23:M:3:ARG:NH1	2.45	0.50
11:A:1628:C:OP1	37:d:38:LYS:NZ	2.40	0.50
43:m:18:LEU:HD22	43:m:77:ILE:HG21	1.94	0.50
49:u:523:LEU:HD12	49:u:526:MET:HB2	1.93	0.50
6:5:340:LEU:HG	6:5:367:MET:HE1	1.93	0.50
39:f:114:LEU:HD11	39:f:121:ARG:HH21	1.75	0.50
43:m:108:CYS:SG	43:m:109:VAL:N	2.85	0.50
46:q:97:ALA:HB1	46:q:118:THR:HG22	1.94	0.50
53:y:664:LYS:HD2	53:y:667:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1018:VAL:HA	1:0:1034:ILE:HD11	1.94	0.49
10:9:11:ARG:NH2	11:A:1844:U:OP1	2.41	0.49
11:A:683:OMG:H4'	20:J:4:MET:HE3	1.93	0.49
11:A:1160:U:O4	15:E:2:GLY:N	2.45	0.49
11:A:1448:A:OP1	40:h:30:LYS:NZ	2.36	0.49
11:A:1605:G:OP1	37:d:84:ARG:NH2	2.45	0.49
28:R:3:ILE:O	28:R:30:GLY:N	2.44	0.49
49:u:198:CYS:HG	49:u:202:ARG:HH21	1.59	0.49
49:u:563:LYS:HA	49:u:567:ARG:HB2	1.93	0.49
2:1:565:ILE:HD11	2:1:579:VAL:HB	1.95	0.49
11:A:1232:U:OP2	39:f:135:HIS:ND1	2.45	0.49
18:H:14:GLU:OE1	18:H:17:ARG:NH1	2.45	0.49
21:K:78:ILE:O	24:N:2:SER:N	2.45	0.49
47:r:185:THR:HB	47:r:187:GLN:HG2	1.94	0.49
53:y:375:LYS:HA	53:y:378:ILE:HD12	1.94	0.49
11:A:1124:C:H5''	25:O:150:ILE:HG12	1.93	0.49
11:A:1231:C:O2'	11:A:1253:A:N6	2.45	0.49
11:A:1235:G:H5'	11:A:1247:C:H42	1.78	0.49
28:R:72:CYS:HG	28:R:112:TRP:CG	2.30	0.49
38:e:33:LYS:HE2	38:e:34:LYS:O	2.13	0.49
44:n:52:GLU:O	52:x:416:GLN:NE2	2.45	0.49
50:v:363:THR:OG1	50:v:365:GLU:OE1	2.28	0.49
1:0:948:LEU:HB3	1:0:959:LEU:HD13	1.94	0.49
35:b:85:ILE:HB	35:b:112:ILE:HA	1.93	0.49
48:t:405:MET:HE2	48:t:412:SER:HB3	1.95	0.49
52:x:381:MET:HG2	52:x:391:ILE:HG21	1.94	0.49
1:0:668:ILE:HG22	1:0:861:MET:HE3	1.94	0.49
6:5:382:ILE:O	6:5:538:ARG:NH1	2.45	0.49
11:A:1146:C:O2'	11:A:1150:A:N1	2.44	0.49
14:D:88:ASP:OD1	14:D:89:GLU:N	2.45	0.49
30:T:78:SER:OG	30:T:80:ASP:OD1	2.31	0.49
48:t:185:ILE:HD12	48:t:216:ALA:HB2	1.94	0.49
11:A:929:G:N2	11:A:1013:U:O2	2.45	0.49
36:c:5:MET:HG3	36:c:270:LEU:HD21	1.95	0.49
53:y:691:MET:O	53:y:695:ILE:HG12	2.12	0.49
53:y:804:MET:HE1	53:y:822:ILE:HD12	1.94	0.49
11:A:1010:G:H2'	11:A:1011:A:H8	1.77	0.49
31:V:29:GLN:N	31:V:110:GLN:OE1	2.45	0.49
31:V:77:MET:HG3	31:V:89:THR:HG21	1.94	0.49
33:Z:15:GLY:HA3	41:i:50:ILE:HG23	1.95	0.49
49:u:199:ASP:HA	49:u:202:ARG:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:755:LEU:HD22	1:0:794:ILE:HD13	1.93	0.49
10:9:19:LYS:O	10:9:23:ARG:HG3	2.12	0.49
11:A:158:A:H2'	11:A:159:A2M:H8	1.93	0.49
11:A:649:U:H2'	11:A:650:A:H8	1.78	0.49
11:A:930:C:O2'	11:A:1104:G:OP1	2.28	0.49
15:E:48:LYS:HB3	15:E:75:ILE:HD12	1.94	0.49
18:H:34:ASP:OD1	18:H:82:LYS:NZ	2.41	0.49
26:P:66:ARG:HH22	31:V:130:ARG:HH22	1.60	0.49
48:t:155:ALA:HB2	48:t:177:ILE:HD13	1.94	0.49
49:u:340:ARG:HH12	53:y:742:LYS:HA	1.78	0.49
49:u:384:VAL:O	49:u:388:LYS:N	2.43	0.49
50:v:292:ILE:HG13	50:v:315:CYS:HB2	1.95	0.49
53:y:405:ILE:HG21	53:y:451:MET:HE1	1.94	0.49
11:A:492:C:OP2	30:T:107:ARG:NH2	2.41	0.49
11:A:531:A:N1	11:A:552:G:C6	2.81	0.49
32:Y:116:ASP:OD1	32:Y:118:THR:OG1	2.29	0.49
53:y:504:LEU:HD12	53:y:507:ILE:HD11	1.94	0.49
6:5:154:PHE:HD1	6:5:221:ILE:HG21	1.78	0.49
11:A:1248:B8N:O2	11:A:1701:C:N4	2.44	0.49
11:A:1391:C:H4'	41:i:55:LEU:HD21	1.95	0.49
15:E:67:ARG:HG3	15:E:115:ILE:HG13	1.94	0.48
48:t:149:ALA:HA	48:t:152:MET:HG2	1.95	0.48
1:0:807:LEU:HD23	1:0:820:LEU:HB2	1.95	0.48
11:A:721:G:H21	11:A:723:C:H41	1.60	0.48
49:u:455:LEU:HD11	49:u:491:LEU:HD21	1.95	0.48
1:0:721:ASP:O	1:0:849:ARG:NH1	2.46	0.48
19:I:45:LEU:HD22	19:I:49:GLN:HG3	1.96	0.48
47:r:134:THR:HA	47:r:166:LEU:HD22	1.95	0.48
49:u:394:LEU:HD12	49:u:403:LEU:HD11	1.94	0.48
50:v:254:LEU:HB2	50:v:286:TYR:HE2	1.78	0.48
53:y:762:ASN:OD1	53:y:776:ARG:NH1	2.46	0.48
11:A:961:G:C2	47:r:55:ARG:NH2	2.80	0.48
14:D:89:GLU:N	14:D:89:GLU:OE1	2.42	0.48
47:r:23:ASN:HB2	47:r:37:LEU:HD11	1.95	0.48
49:u:384:VAL:HB	49:u:387:VAL:HG22	1.95	0.48
49:u:438:ARG:HD3	49:u:510:HIS:CE1	2.49	0.48
50:v:247:GLN:HE21	50:v:253:ILE:HD13	1.77	0.48
11:A:1171:G:O2'	11:A:1187:G:O6	2.27	0.48
47:r:34:VAL:HG11	47:r:46:ILE:HD12	1.95	0.48
53:y:788:LEU:HD12	53:y:813:LEU:HD12	1.96	0.48
1:0:1127:VAL:HB	1:0:1133:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:617:G:N7	15:E:67:ARG:NH1	2.61	0.48
11:A:1102:G:OP1	25:O:151:ARG:NH2	2.47	0.48
6:5:380:MET:HE1	6:5:517:SER:HA	1.96	0.48
6:5:457:LEU:HD13	6:5:493:PHE:HA	1.96	0.48
11:A:326:C:N4	11:A:327:G:N7	2.61	0.48
12:B:82:MET:HG3	12:B:85:THR:HB	1.95	0.48
14:D:110:LEU:O	14:D:111:GLN:C	2.55	0.48
34:a:48:ALA:O	34:a:51:SER:OG	2.24	0.48
38:e:42:ASP:O	38:e:43:LYS:C	2.54	0.48
49:u:462:VAL:HG13	49:u:466:GLN:HG2	1.96	0.48
52:x:452:VAL:HG22	52:x:465:ILE:HG22	1.95	0.48
53:y:691:MET:HE3	53:y:737:VAL:HB	1.94	0.48
6:5:340:LEU:HD13	6:5:386:ILE:HG12	1.96	0.48
11:A:878:G:H1	11:A:908:A:H61	1.61	0.48
24:N:70:ASN:ND2	24:N:73:ASP:OD1	2.47	0.48
40:h:107:GLU:OE2	40:h:110:VAL:HG23	2.13	0.48
48:t:187:ILE:HG21	48:t:207:ILE:HG21	1.96	0.48
1:0:964:ILE:O	1:0:968:LYS:HG3	2.14	0.48
6:5:328:ARG:NH1	6:5:508:ALA:O	2.47	0.48
11:A:1722:G:N2	11:A:1812:U:O2	2.43	0.48
48:t:83:TYR:HA	48:t:132:PHE:O	2.13	0.48
49:u:51:MET:HB3	49:u:89:VAL:HG21	1.96	0.48
1:0:651:LEU:O	1:0:681:GLN:NE2	2.47	0.48
1:0:764:TRP:HD1	1:0:766:LYS:HZ3	1.62	0.48
6:5:328:ARG:HH21	6:5:500:LEU:HD23	1.79	0.48
6:5:395:GLY:HA2	6:5:398:MET:HE3	1.96	0.48
11:A:317:C:OP2	29:S:183:ARG:NH2	2.46	0.48
11:A:712:G:H5'	11:A:712:G:H8	1.78	0.48
31:V:114:ASN:O	31:V:118:ASN:ND2	2.47	0.48
48:t:140:ILE:HG23	48:t:141:LEU:HD22	1.95	0.48
48:t:323:ALA:HB2	48:t:328:LEU:HD11	1.96	0.48
49:u:52:LEU:HD22	49:u:89:VAL:HG23	1.95	0.48
1:0:842:THR:HG22	1:0:846:LEU:HD12	1.96	0.47
11:A:516:A:N1	11:A:643:A:O2'	2.43	0.47
11:A:620:G:N2	11:A:647:U:OP1	2.47	0.47
11:A:683:OMG:H1'	11:A:683:OMG:HM23	1.61	0.47
25:O:52:THR:HG22	25:O:58:ALA:H	1.79	0.47
31:V:24:SER:OG	31:V:26:ASP:OD1	2.32	0.47
50:v:254:LEU:O	50:v:258:THR:HG23	2.13	0.47
2:1:467:ILE:HA	2:1:483:VAL:HG22	1.96	0.47
11:A:663:C:O2'	22:L:227:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:t:165:CYS:SG	48:t:166:PRO:HD3	2.54	0.47
49:u:465:PHE:CD1	53:y:810:MET:HB3	2.50	0.47
10:9:1:MET:HE2	10:9:1:MET:HB2	1.74	0.47
11:A:531:A:N1	11:A:552:G:O6	2.47	0.47
11:A:940:U:H3	11:A:1002:U:H3	1.63	0.47
14:D:30:LYS:HD2	16:F:112:TYR:HE1	1.80	0.47
36:c:3:GLU:OE1	36:c:245:ARG:NE	2.47	0.47
36:c:191:HIS:CG	36:c:195:LEU:HD21	2.49	0.47
48:t:168:PRO:HG3	48:t:385:ARG:H	1.79	0.47
11:A:570:C:O2'	30:T:34:THR:O	2.25	0.47
11:A:1310:U:OP1	43:m:36:ARG:NH2	2.46	0.47
49:u:55:LEU:HD13	49:u:93:TYR:HB2	1.96	0.47
49:u:559:LYS:O	49:u:562:ARG:NH1	2.47	0.47
50:v:347:ILE:HG23	53:y:826:ILE:HD11	1.95	0.47
8:7:-23:A:H4'	53:y:653:ARG:HH12	1.80	0.47
11:A:681:U:O2'	11:A:1160:U:OP1	2.31	0.47
11:A:719:G:H5''	11:A:719:G:H8	1.79	0.47
11:A:790:C:OP1	11:A:791:C:O2'	2.32	0.47
11:A:920:A:O2'	11:A:922:A:OP1	2.26	0.47
28:R:91:VAL:HG11	28:R:205:ARG:HH12	1.79	0.47
33:Z:62:LYS:O	33:Z:67:ARG:NH2	2.47	0.47
35:b:52:LYS:HG2	35:b:80:LEU:HD11	1.94	0.47
11:A:563:G:N7	14:D:172:ARG:NH1	2.63	0.47
11:A:588:G:OP2	11:A:588:G:N2	2.40	0.47
11:A:988:C:O2'	25:O:118:GLN:O	2.32	0.47
11:A:1275:G:N2	11:A:1506:A:OP2	2.39	0.47
18:H:80:ARG:NH1	52:x:75:GLU:HG2	2.28	0.47
1:0:891:PRO:HG3	1:0:963:LEU:HD22	1.97	0.47
1:0:1186:ILE:HD12	1:0:1213:LEU:HD11	1.97	0.47
6:5:56:ILE:HG23	6:5:128:PHE:HZ	1.80	0.47
7:6:342:PHE:HD2	7:6:346:GLN:HB2	1.79	0.47
11:A:617:G:OP2	15:E:68:LYS:NZ	2.47	0.47
11:A:734:C:O2	11:A:735:C:N4	2.31	0.47
11:A:1037:G:H4'	11:A:1845:A:H4'	1.97	0.47
11:A:1594:A:O2'	37:d:16:ARG:NH2	2.47	0.47
28:R:92:ARG:O	28:R:94:LYS:NZ	2.48	0.47
33:Z:28:GLU:HG2	33:Z:69:LEU:HD21	1.96	0.47
49:u:281:THR:OG1	49:u:285:LYS:NZ	2.47	0.47
50:v:401:TYR:H	53:y:846:ARG:HH22	1.61	0.47
52:x:41:LYS:HB2	53:y:595:GLN:HG3	1.96	0.47
11:A:511:U:O2'	11:A:576:A:N6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1017:U:H5'	19:I:55:ARG:HD3	1.97	0.47
43:m:33:ARG:N	43:m:37:GLU:OE1	2.44	0.47
53:y:651:LEU:HD11	53:y:667:ARG:HD2	1.97	0.47
1:0:1206:ASP:OD1	1:0:1208:GLN:NE2	2.47	0.47
46:q:4:ASN:OD1	46:q:12:ARG:NH1	2.48	0.47
6:5:82:ASP:OD1	6:5:83:VAL:N	2.48	0.47
6:5:327:ARG:NH2	6:5:496:LYS:HG2	2.29	0.47
8:7:19:U:OP2	45:o:242:ARG:NH1	2.48	0.47
11:A:681:U:H4'	15:E:9:THR:HG22	1.97	0.47
11:A:928:G:H2'	11:A:929:G:C8	2.50	0.47
13:C:112:HIS:NE2	13:C:237:SER:O	2.48	0.47
21:K:81:LYS:O	24:N:52:LYS:NZ	2.47	0.47
40:h:50:VAL:HG22	40:h:91:LEU:HD13	1.96	0.47
50:v:402:GLN:O	50:v:406:GLU:HG2	2.15	0.47
6:5:541:ASP:O	6:5:545:ARG:HG2	2.15	0.46
18:H:64:CYS:SG	18:H:65:GLN:N	2.87	0.46
31:V:122:ARG:N	31:V:197:GLU:OE2	2.48	0.46
31:V:123:GLU:N	31:V:197:GLU:OE2	2.46	0.46
36:c:35:SER:OG	36:c:36:ARG:N	2.48	0.46
47:r:19:VAL:HG22	47:r:72:VAL:HG22	1.96	0.46
49:u:161:LEU:HD11	49:u:178:ALA:HB2	1.96	0.46
11:A:205:G:N7	28:R:144:LYS:NZ	2.64	0.46
14:D:109:ARG:O	14:D:110:LEU:C	2.57	0.46
43:m:35:ILE:HB	43:m:61:TYR:HE1	1.80	0.46
52:x:317:THR:O	52:x:321:HIS:ND1	2.46	0.46
53:y:551:LEU:O	53:y:555:ILE:HG12	2.16	0.46
11:A:692:G:H2'	11:A:693:A:C4	2.50	0.46
11:A:839:C:H41	30:T:10:ARG:HA	1.80	0.46
11:A:943:U:OP1	25:O:214:LYS:NZ	2.47	0.46
25:O:134:LEU:HG	25:O:218:LEU:HD12	1.96	0.46
35:b:23:ASP:OD1	35:b:23:ASP:N	2.48	0.46
35:b:74:GLU:N	35:b:74:GLU:OE1	2.47	0.46
52:x:34:SER:OG	52:x:57:ASN:OD1	2.28	0.46
1:0:1126:CYS:SG	1:0:1127:VAL:N	2.89	0.46
7:6:294:PHE:HB2	7:6:330:ARG:HB3	1.98	0.46
11:A:1142:G:OP1	22:L:187:ARG:NH1	2.47	0.46
34:a:24:LYS:O	34:a:42:ASN:ND2	2.43	0.46
47:r:113:ARG:NH1	47:r:117:GLU:OE2	2.48	0.46
48:t:295:GLU:HB2	48:t:361:VAL:HG22	1.97	0.46
50:v:404:VAL:HG13	50:v:407:LYS:HE3	1.97	0.46
1:0:807:LEU:O	1:0:811:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:863:VAL:HG12	1:0:873:ILE:HG22	1.97	0.46
1:0:1013:VAL:HB	1:0:1041:ILE:HG23	1.98	0.46
8:7:-23:A:N7	49:u:195:ARG:NH2	2.64	0.46
11:A:1217:A:H2'	11:A:1218:C:H6	1.80	0.46
27:Q:52:ASP:HA	27:Q:55:GLU:HG3	1.97	0.46
29:S:65:GLN:OE1	29:S:66:GLY:N	2.48	0.46
35:b:25:LEU:HA	35:b:28:MET:SD	2.56	0.46
35:b:93:MET:HE1	35:b:106:GLU:HG2	1.97	0.46
47:r:22:VAL:HG23	47:r:36:LEU:HD23	1.98	0.46
52:x:305:SER:O	52:x:308:SER:OG	2.24	0.46
53:y:643:LYS:HD2	53:y:650:LEU:HD21	1.97	0.46
1:0:1094:ILE:CG2	1:0:1112:VAL:HB	2.46	0.46
11:A:1032:C:H5''	19:I:109:LYS:HD2	1.98	0.46
11:A:1219:JMH:O2'	11:A:1220:A:OP1	2.32	0.46
42:k:132:MET:SD	42:k:139:HIS:HB3	2.56	0.46
47:r:46:ILE:HG12	47:r:85:LEU:HB2	1.98	0.46
50:v:255:ARG:NH2	50:v:322:ASP:OD2	2.48	0.46
52:x:28:MET:HE1	52:x:30:TYR:HD1	1.80	0.46
2:1:292:ASN:C	2:1:294:ARG:H	2.24	0.46
7:6:287:VAL:HG23	7:6:288:GLU:OE1	2.16	0.46
7:6:317:ARG:HH22	49:u:397:GLU:HB2	1.81	0.46
38:e:91:LEU:HD22	38:e:96:LEU:HD22	1.97	0.46
48:t:89:TYR:HE1	48:t:126:LEU:HD13	1.80	0.46
53:y:420:VAL:HG13	53:y:440:VAL:HG13	1.97	0.46
53:y:643:LYS:O	53:y:648:GLN:N	2.49	0.46
1:0:1137:ILE:HG13	1:0:1139:THR:HG22	1.97	0.46
11:A:116:OMU:HM23	11:A:116:OMU:H1'	1.67	0.46
11:A:919:A:O2'	11:A:1020:A:N1	2.45	0.46
11:A:1204:A:OP1	22:L:117:ARG:NE	2.48	0.46
11:A:1507:G:H1'	42:k:89:LYS:CE	2.46	0.46
11:A:1566:G:OP2	37:d:102:ARG:NH2	2.49	0.46
11:A:1752:C:H6	11:A:1779:G:H1	1.64	0.46
27:Q:41:ILE:HG12	27:Q:68:TYR:HD1	1.79	0.46
49:u:168:SER:OG	49:u:169:ARG:NH1	2.48	0.46
2:1:520:GLN:HG2	2:1:525:TYR:H	1.81	0.46
5:4:292:ASP:HA	7:6:344:LYS:HE2	1.98	0.46
6:5:468:THR:O	6:5:530:ILE:N	2.41	0.46
9:8:167:TYR:HA	9:8:200:GLU:HA	1.98	0.46
36:c:245:ARG:NH1	36:c:295:GLY:O	2.47	0.46
1:0:599:ARG:O	1:0:604:ARG:NH1	2.49	0.46
6:5:375:LEU:HD12	6:5:379:PRO:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:312:VAL:HG11	7:6:325:ILE:HG21	1.96	0.46
36:c:72:SER:OG	36:c:74:ASP:OD1	2.29	0.46
39:f:47:LYS:HA	39:f:47:LYS:HD3	1.72	0.46
49:u:38:LYS:HD3	49:u:41:ARG:HE	1.80	0.46
7:6:256:TYR:HD1	7:6:263:ILE:HG13	1.81	0.45
11:A:693:A:O2'	11:A:694:G:C8	2.51	0.45
41:i:46:TYR:O	41:i:50:ILE:HD12	2.16	0.45
11:A:1113:A:O2'	11:A:1114:U:O4'	2.23	0.45
13:C:151:ASP:OD2	29:S:216:ARG:NH2	2.49	0.45
37:d:41:LYS:HE3	37:d:93:SER:HB2	1.98	0.45
47:r:104:LYS:HD2	47:r:150:TYR:CZ	2.52	0.45
50:v:212:THR:OG1	50:v:247:GLN:OE1	2.27	0.45
50:v:220:PHE:O	50:v:229:ARG:NH2	2.50	0.45
52:x:428:ASN:HB3	52:x:431:LYS:HB3	1.98	0.45
53:y:739:ALA:HA	53:y:742:LYS:HE2	1.96	0.45
11:A:1007:C:O2'	19:I:104:ARG:NH2	2.50	0.45
22:L:191:VAL:HG11	22:L:236:PHE:HA	1.99	0.45
49:u:498:ASN:HA	49:u:518:GLN:HE22	1.82	0.45
50:v:351:ILE:HG12	50:v:393:MET:HE1	1.98	0.45
52:x:31:GLN:H	53:y:591:MET:HE1	1.81	0.45
53:y:753:HIS:O	53:y:757:ILE:HG22	2.15	0.45
53:y:754:SER:O	53:y:758:ASN:HB2	2.17	0.45
1:0:855:GLU:O	1:0:857:ARG:NH1	2.50	0.45
11:A:507:G:O6	30:T:105:LYS:NZ	2.37	0.45
12:B:82:MET:HE1	12:B:87:VAL:HG23	1.99	0.45
13:C:21:ASP:OD2	13:C:24:THR:OG1	2.34	0.45
46:q:77:ILE:HG22	46:q:94:LYS:HA	1.98	0.45
49:u:543:LEU:O	49:u:547:GLU:HB3	2.17	0.45
53:y:823:SER:O	53:y:827:ILE:HG12	2.17	0.45
1:0:1124:PRO:HA	1:0:1137:ILE:HA	1.99	0.45
11:A:476:A:O2'	11:A:487:U:O2'	2.34	0.45
11:A:1060:A:O2'	11:A:1062:A:N7	2.43	0.45
11:A:1507:G:C2	42:k:89:LYS:CB	2.99	0.45
11:A:1533:A:O2'	31:V:81:ARG:NH1	2.49	0.45
14:D:103:GLU:HA	14:D:106:LEU:HD12	1.98	0.45
17:G:159:ASP:OD1	17:G:161:ALA:N	2.46	0.45
24:N:61:ALA:HB1	24:N:145:ILE:HD13	1.97	0.45
28:R:162:LEU:HD11	28:R:191:GLU:HG2	1.97	0.45
48:t:112:GLU:HA	48:t:124:PHE:O	2.17	0.45
52:x:227:VAL:O	52:x:374:ARG:NH1	2.49	0.45
53:y:559:ASP:OD2	53:y:565:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:764:TRP:CD1	1:0:766:LYS:HZ3	2.34	0.45
1:0:1103:ASN:ND2	51:w:75:C:O4'	2.50	0.45
24:N:148:CYS:SG	24:N:160:ALA:HB1	2.56	0.45
37:d:130:ASP:O	37:d:134:ILE:HG12	2.16	0.45
48:t:48:GLY:HA2	48:t:170:THR:HG22	1.99	0.45
9:8:155:ILE:O	9:8:159:GLN:HA	2.17	0.45
11:A:550:C:O2'	11:A:551:U:O4'	2.27	0.45
11:A:1648:G:O2'	11:A:1674:G:O6	2.35	0.45
22:L:204:ILE:O	22:L:211:LYS:NZ	2.41	0.45
47:r:134:THR:HB	47:r:168:LEU:HD13	1.98	0.45
49:u:228:MET:HA	49:u:231:GLU:HG3	1.98	0.45
52:x:76:ASP:OD1	52:x:77:GLU:N	2.49	0.45
52:x:407:VAL:HG21	52:x:412:LYS:HD2	1.98	0.45
11:A:961:G:H21	47:r:55:ARG:CD	2.29	0.45
11:A:1512:C:O2'	41:i:7:TYR:O	2.26	0.45
29:S:106:LEU:HD13	29:S:109:LEU:HD13	1.99	0.45
33:Z:114:ALA:HB3	33:Z:117:ARG:HD3	1.99	0.45
53:y:822:ILE:HA	53:y:825:MET:HE2	1.99	0.45
11:A:453:C:O2'	29:S:92:ARG:O	2.28	0.45
11:A:639:C:OP1	16:F:115:ARG:NH2	2.50	0.45
11:A:682:U:H5'	11:A:1160:U:OP1	2.15	0.45
19:I:83:ASP:OD1	19:I:84:LEU:N	2.49	0.45
21:K:12:TYR:HB3	22:L:79:GLU:HB3	1.99	0.45
24:N:8:LEU:HB3	24:N:59:LEU:HD13	1.99	0.45
30:T:23:MET:SD	30:T:23:MET:N	2.90	0.45
47:r:156:ALA:HB1	47:r:163:LEU:HD22	1.99	0.45
49:u:465:PHE:HD1	53:y:810:MET:HB3	1.82	0.45
52:x:39:LEU:HD22	53:y:589:MET:HE2	1.99	0.45
53:y:329:VAL:HB	53:y:357:LEU:HD11	1.99	0.45
53:y:624:GLY:HA3	53:y:778:MET:HE2	1.98	0.45
53:y:628:ASP:OD1	53:y:629:ALA:N	2.49	0.45
53:y:804:MET:HE3	53:y:818:VAL:HG13	1.99	0.45
1:0:750:PRO:HG2	1:0:846:LEU:HD21	1.98	0.45
11:A:683:OMG:O4'	20:J:4:MET:HE1	2.16	0.45
11:A:863:U:O2'	20:J:78:ARG:NH1	2.50	0.45
11:A:1228:A:H2'	11:A:1229:G:H8	1.82	0.45
32:Y:41:MET:HE1	37:d:9:VAL:N	2.33	0.45
49:u:272:MET:SD	49:u:272:MET:N	2.90	0.45
53:y:704:ASP:OD2	53:y:856:ALA:HB3	2.17	0.45
11:A:26:U:H2'	11:A:27:A2M:H8	1.98	0.44
11:A:639:C:H2'	11:A:640:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1245:G:O2'	11:A:1492:U:OP1	2.26	0.44
11:A:1722:G:H1	11:A:1812:U:H3	1.64	0.44
31:V:34:SER:HA	44:n:55:VAL:HB	1.99	0.44
31:V:127:ARG:NH1	31:V:132:GLY:O	2.51	0.44
47:r:104:LYS:HB3	47:r:150:TYR:CG	2.52	0.44
52:x:397:ASN:HA	52:x:452:VAL:O	2.17	0.44
1:0:1110:MET:HG3	1:0:1112:VAL:HG13	1.98	0.44
6:5:59:PHE:HD1	6:5:94:ILE:HD13	1.83	0.44
11:A:166:A2M:H2'	11:A:167:G:H8	1.83	0.44
11:A:1543:U:OP1	37:d:62:ARG:NH1	2.45	0.44
13:C:37:LYS:HB2	13:C:40:GLU:CD	2.42	0.44
29:S:74:ARG:NH1	29:S:96:SER:OG	2.49	0.44
43:m:22:LEU:HD22	43:m:89:VAL:HG12	1.98	0.44
49:u:269:PRO:HB3	49:u:306:MET:HG3	1.99	0.44
11:A:203:G:O5'	28:R:147:LYS:NZ	2.51	0.44
11:A:1244:U:H2'	11:A:1245:G:H8	1.83	0.44
11:A:1446:A:H5''	40:h:58:THR:HG23	2.00	0.44
14:D:170:PRO:O	14:D:175:ARG:NH1	2.50	0.44
1:0:635:CYS:HB2	1:0:720:CYS:HB3	1.99	0.44
1:0:1023:VAL:HG21	15:E:50:ILE:HG12	1.99	0.44
6:5:347:LYS:HB3	50:v:417:MET:HE1	1.99	0.44
6:5:551:GLU:HB3	6:5:555:ARG:NH1	2.32	0.44
11:A:746:C:N4	11:A:797:C:O2	2.51	0.44
17:G:117:PRO:HB2	17:G:120:ARG:HG2	2.00	0.44
23:M:126:MET:HE2	23:M:126:MET:HB3	1.80	0.44
35:b:31:GLU:O	35:b:34:MET:HB2	2.17	0.44
47:r:112:LEU:HA	47:r:115:VAL:HG22	2.00	0.44
2:1:548:ARG:HB3	2:1:555:PRO:HD2	1.99	0.44
6:5:292:LYS:HA	6:5:295:GLU:HG2	1.99	0.44
6:5:457:LEU:HB3	6:5:493:PHE:HD1	1.83	0.44
11:A:17:C:O2'	11:A:1194:A:N1	2.45	0.44
36:c:44:LYS:HG2	36:c:56:GLN:HB2	1.99	0.44
6:5:228:LEU:O	6:5:232:HIS:ND1	2.51	0.44
11:A:962:A:N1	11:A:1055:A:O2'	2.49	0.44
11:A:1059:G:N2	11:A:1829:G:O3'	2.50	0.44
15:E:58:GLU:OE1	15:E:58:GLU:N	2.47	0.44
32:Y:53:GLU:HG3	32:Y:54:PRO:HD3	2.00	0.44
38:e:48:VAL:HG11	39:f:23:ARG:HA	1.99	0.44
40:h:46:LYS:HG3	40:h:101:ILE:HD11	2.00	0.44
43:m:18:LEU:HD21	43:m:51:VAL:HG21	1.99	0.44
50:v:404:VAL:O	50:v:407:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:536:A:H3'	11:A:537:C:H4'	2.00	0.44
11:A:701:G:H8	11:A:701:G:H5''	1.83	0.44
11:A:1010:G:H2'	11:A:1011:A:C8	2.52	0.44
23:M:117:LEU:HD12	23:M:117:LEU:HA	1.86	0.44
42:k:140:TYR:CZ	42:k:142:GLY:HA2	2.53	0.44
48:t:97:PRO:HG2	48:t:99:PRO:HD2	2.00	0.44
48:t:367:ILE:HD12	48:t:467:PRO:HG3	1.99	0.44
52:x:308:SER:OG	52:x:311:ASN:ND2	2.47	0.44
6:5:59:PHE:HD2	6:5:128:PHE:HE1	1.66	0.44
7:6:352:ASP:OD1	7:6:353:THR:N	2.51	0.44
14:D:95:ASP:OD1	14:D:96:TYR:N	2.51	0.44
25:O:175:GLU:O	25:O:179:ASN:ND2	2.51	0.44
34:a:9:ILE:O	34:a:13:GLU:HG3	2.18	0.44
42:k:133:ALA:N	42:k:140:TYR:O	2.51	0.44
48:t:254:PRO:HG2	48:t:360:ALA:HB2	1.99	0.44
53:y:445:LEU:HD22	53:y:501:ARG:CZ	2.48	0.44
1:0:644:LYS:N	54:0:2001:GTP:O1B	2.47	0.44
1:0:1105:ARG:HA	1:0:1105:ARG:HD2	1.69	0.44
2:1:500:THR:HG22	2:1:501:ARG:H	1.83	0.44
11:A:561:A:O2'	14:D:134:HIS:NE2	2.42	0.44
12:B:49:GLU:OE1	12:B:49:GLU:N	2.49	0.44
26:P:39:ASP:OD1	26:P:40:THR:N	2.48	0.44
1:0:980:GLY:H	1:0:1006:ALA:HB2	1.83	0.43
1:0:1103:ASN:HB3	1:0:1109:VAL:H	1.83	0.43
11:A:1256:G:N2	41:i:30:LEU:O	2.46	0.43
11:A:1304:U:HO2'	42:k:93:HIS:CE1	2.32	0.43
34:a:49:MET:HB3	34:a:49:MET:HE2	1.82	0.43
42:k:128:ALA:O	43:m:44:LYS:HD2	2.18	0.43
6:5:327:ARG:HH12	6:5:496:LYS:NZ	2.16	0.43
11:A:874:G:H2'	11:A:875:A:H8	1.83	0.43
11:A:1292:C:HO2'	42:k:147:THR:HG1	1.62	0.43
11:A:1358:U:OP2	22:L:123:ARG:NH2	2.51	0.43
11:A:1758:G:N1	11:A:1772:C:OP1	2.51	0.43
49:u:105:LYS:HE2	49:u:149:TRP:NE1	2.34	0.43
49:u:298:ARG:HA	49:u:301:HIS:CE1	2.53	0.43
4:3:180:SER:O	4:3:188:PHE:N	2.50	0.43
11:A:126:G:OP2	29:S:195:LYS:NZ	2.38	0.43
11:A:685:A:H5''	20:J:31:SER:HB3	2.00	0.43
13:C:212:ASP:OD1	13:C:216:ASN:N	2.51	0.43
14:D:54:ARG:NH2	22:L:200:ARG:O	2.46	0.43
26:P:45:THR:HG23	26:P:52:THR:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:t:187:ILE:HB	48:t:221:ILE:HG12	2.01	0.43
53:y:670:GLN:H	53:y:670:GLN:HG2	1.60	0.43
1:0:639:HIS:H	1:0:642:THR:HG21	1.83	0.43
17:G:46:THR:HG21	17:G:97:GLN:HG2	2.00	0.43
35:b:22:LEU:HA	35:b:25:LEU:HD12	1.99	0.43
53:y:326:HIS:HB2	53:y:366:LEU:HD13	1.99	0.43
53:y:801:SER:HA	53:y:842:VAL:HA	2.01	0.43
1:0:1202:MET:HE3	1:0:1203:GLN:HB2	2.00	0.43
2:1:656:ASP:O	2:1:668:THR:HA	2.18	0.43
6:5:402:GLN:OE1	50:v:379:ARG:NH1	2.37	0.43
11:A:45:A:N1	11:A:480:G:O2'	2.43	0.43
11:A:219:U:H1'	28:R:184:ARG:HD2	2.01	0.43
11:A:507:G:OP2	30:T:104:ARG:NH2	2.49	0.43
11:A:1255:G:OP1	11:A:1256:G:O2'	2.25	0.43
11:A:1678:A2M:HM'3	11:A:1678:A2M:H1'	1.77	0.43
49:u:292:HIS:HE2	49:u:427:TYR:HH	1.64	0.43
49:u:463:ASP:H	49:u:466:GLN:NE2	2.16	0.43
51:w:75:C:P	51:w:75:C:H3'	2.59	0.43
8:7:-19:G:O3'	49:u:158:ARG:NH2	2.52	0.43
11:A:517:OMC:H2'	11:A:518:G:O4'	2.19	0.43
11:A:1738:C:OP1	29:S:92:ARG:NH1	2.42	0.43
18:H:59:CYS:HB2	53:y:443:CYS:HB2	1.79	0.43
20:J:111:MET:HE3	20:J:115:GLU:HG3	2.00	0.43
31:V:89:THR:HA	31:V:92:ILE:HG12	2.01	0.43
34:a:55:ARG:NH1	34:a:78:TYR:OH	2.51	0.43
39:f:51:ASP:HB3	39:f:54:LYS:HG3	2.00	0.43
49:u:8:PRO:HG2	49:u:46:ILE:HG21	2.00	0.43
49:u:341:LEU:HD21	49:u:348:ILE:HA	2.00	0.43
50:v:255:ARG:HG3	50:v:292:ILE:HD13	1.99	0.43
53:y:469:TYR:OH	53:y:674:HIS:N	2.46	0.43
7:6:341:THR:O	7:6:341:THR:OG1	2.35	0.43
11:A:1233:G:N3	11:A:1252:C:O2'	2.43	0.43
23:M:108:LEU:HD13	24:N:39:TYR:HE2	1.84	0.43
53:y:856:ALA:N	53:y:859:LEU:HD13	2.34	0.43
1:0:725:LEU:HB3	1:0:753:VAL:HG22	2.01	0.43
1:0:1092:CYS:HB3	1:0:1184:SER:HB3	2.00	0.43
6:5:551:GLU:HB3	6:5:555:ARG:HH12	1.83	0.43
8:7:-23:A:H5''	49:u:192:ALA:HB2	2.01	0.43
11:A:681:U:HO2'	11:A:682:U:H5'	1.84	0.43
11:A:1536:G:P	31:V:88:MET:HE1	2.59	0.43
14:D:18:ARG:HB2	14:D:21:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:184:ARG:NH1	24:N:191:ARG:O	2.51	0.43
36:c:23:THR:HG22	36:c:31:ILE:HG22	2.01	0.43
39:f:60:THR:OG1	39:f:61:GLU:OE1	2.37	0.43
45:o:243:VAL:HG22	45:o:312:VAL:HG12	2.01	0.43
47:r:115:VAL:HA	47:r:118:VAL:HG22	2.00	0.43
48:t:408:ILE:HD13	48:t:433:VAL:HG21	2.01	0.43
49:u:385:PRO:HA	49:u:388:LYS:HB2	2.00	0.43
53:y:445:LEU:HA	53:y:448:VAL:HG22	2.01	0.43
11:A:1759:G:N2	11:A:1772:C:OP2	2.51	0.43
22:L:193:VAL:HG21	22:L:240:THR:HA	2.01	0.43
30:T:20:ARG:NH1	30:T:74:MET:SD	2.92	0.43
35:b:34:MET:HE1	35:b:46:ASN:HA	2.00	0.43
49:u:317:ARG:O	49:u:320:THR:OG1	2.34	0.43
50:v:399:SER:HA	50:v:403:GLN:HB2	2.01	0.43
53:y:504:LEU:HD22	53:y:564:ILE:HG12	2.00	0.43
1:0:1159:VAL:O	1:0:1161:ILE:HG13	2.19	0.43
11:A:60:G:N2	11:A:316:G:H21	2.17	0.43
38:e:32:LYS:HD3	38:e:32:LYS:HA	1.80	0.43
49:u:266:PRO:HA	49:u:267:PRO:HD3	1.90	0.43
49:u:292:HIS:O	49:u:295:THR:OG1	2.31	0.43
49:u:292:HIS:NE2	49:u:427:TYR:OH	2.45	0.43
49:u:403:LEU:HD23	49:u:439:LEU:HD13	2.01	0.43
53:y:468:GLU:O	53:y:472:HIS:ND1	2.51	0.43
53:y:667:ARG:HH22	53:y:668:ARG:NH2	2.17	0.43
2:1:529:LYS:HA	2:1:529:LYS:HD2	1.74	0.42
11:A:1017:U:OP2	19:I:55:ARG:NH1	2.46	0.42
36:c:16:GLY:N	36:c:305:ASN:OD1	2.52	0.42
42:k:106:TYR:CD2	42:k:107:LYS:HG2	2.53	0.42
47:r:159:ASP:OD1	47:r:159:ASP:N	2.52	0.42
50:v:368:GLU:HA	50:v:371:ILE:HB	2.00	0.42
52:x:23:GLU:O	52:x:26:ARG:NH1	2.52	0.42
11:A:1232:U:H2'	11:A:1233:G:C8	2.54	0.42
11:A:1277:C:H2'	11:A:1278:A:H8	1.83	0.42
11:A:1309:C:H5'	42:k:105:TYR:CE2	2.54	0.42
11:A:1513:C:H2'	11:A:1514:G:H8	1.84	0.42
23:M:74:GLN:HB3	23:M:78:ARG:NH1	2.34	0.42
24:N:19:LEU:HD23	24:N:19:LEU:HA	1.90	0.42
24:N:39:TYR:CD1	24:N:40:LYS:HG3	2.54	0.42
50:v:264:ASN:ND2	50:v:266:ASP:OD1	2.53	0.42
52:x:199:LEU:O	52:x:335:TYR:N	2.52	0.42
1:0:730:MET:HE3	1:0:730:MET:HB3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:145:G:H2'	11:A:146:G:C8	2.54	0.42
11:A:1273:C:O2	11:A:1508:A:N6	2.52	0.42
11:A:1512:C:H5''	41:i:8:TRP:HZ3	1.85	0.42
48:t:297:ARG:HA	48:t:297:ARG:HD3	1.90	0.42
11:A:640:A:H2'	11:A:641:A:C8	2.54	0.42
11:A:1247:C:OP1	46:q:17:ASN:ND2	2.53	0.42
11:A:1615:U:O4	35:b:40:ARG:NH2	2.52	0.42
11:A:1863:A:H1'	27:Q:79:ILE:HD11	2.01	0.42
28:R:119:LEU:HD21	28:R:153:LYS:HG2	2.02	0.42
45:o:269:TYR:HB3	45:o:284:PHE:HB2	2.01	0.42
1:0:882:LEU:HD21	1:0:949:VAL:HG21	2.01	0.42
11:A:535:G:N2	11:A:536:A:N7	2.68	0.42
11:A:1563:G:H5''	37:d:115:LYS:HE2	2.00	0.42
11:A:1652:G:H1	11:A:1672:U:H3	1.65	0.42
13:C:68:ARG:HE	13:C:76:VAL:HG11	1.85	0.42
13:C:197:ASN:ND2	13:C:199:GLU:OE2	2.50	0.42
17:G:164:ASN:OD1	17:G:165:ASN:N	2.52	0.42
22:L:178:HIS:CE1	22:L:179:THR:HG1	2.34	0.42
48:t:54:LYS:HG2	48:t:158:LEU:HD22	2.02	0.42
49:u:226:GLN:HE22	49:u:267:PRO:HB3	1.85	0.42
1:0:646:LYS:HG2	1:0:825:ALA:HB1	2.00	0.42
1:0:711:ASN:OD1	1:0:712:LEU:N	2.52	0.42
1:0:1171:MET:HB2	1:0:1174:ARG:HB2	2.00	0.42
6:5:136:TYR:CZ	6:5:140:ILE:HD11	2.54	0.42
11:A:1156:U:OP1	20:J:71:LYS:NZ	2.52	0.42
11:A:1236:G:O2'	35:b:131:PRO:O	2.22	0.42
11:A:1650:A:H5''	32:Y:139:ALA:HB2	2.02	0.42
11:A:1757:G:H8	11:A:1777:G:H22	1.67	0.42
14:D:54:ARG:HH22	22:L:202:THR:HG22	1.83	0.42
14:D:58:ARG:O	14:D:62:THR:HG23	2.18	0.42
39:f:82:TRP:O	39:f:87:GLN:NE2	2.53	0.42
43:m:52:LEU:HD13	43:m:65:VAL:HG11	2.00	0.42
49:u:432:GLN:O	49:u:436:ILE:HG12	2.19	0.42
49:u:441:GLN:OE1	49:u:510:HIS:NE2	2.53	0.42
49:u:688:LEU:O	49:u:692:GLU:N	2.51	0.42
11:A:562:U:H2'	11:A:563:G:C8	2.54	0.42
12:B:5:GLN:HE22	12:B:11:GLN:HB2	1.85	0.42
13:C:247:THR:OG1	13:C:250:GLU:OE1	2.24	0.42
33:Z:74:GLN:NE2	33:Z:79:PHE:O	2.41	0.42
38:e:47:LEU:N	38:e:78:LYS:O	2.49	0.42
43:m:49:LEU:HB3	43:m:111:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:q:98:ASP:OD1	46:q:99:GLU:N	2.53	0.42
48:t:85:ASN:HB3	48:t:129:HIS:NE2	2.34	0.42
48:t:100:GLU:HB3	48:t:234:VAL:HG22	2.01	0.42
49:u:542:ILE:HA	49:u:545:GLU:HG2	2.01	0.42
1:0:738:ILE:HA	1:0:741:ILE:HD12	2.02	0.42
11:A:701:G:H5''	11:A:701:G:C8	2.54	0.42
11:A:729:C:H5''	11:A:729:C:H6	1.85	0.42
11:A:943:U:H3	26:P:138:ASP:HB2	1.84	0.42
11:A:982:G:H2'	11:A:983:A:C8	2.54	0.42
32:Y:110:ASP:OD1	32:Y:111:ILE:N	2.53	0.42
43:m:18:LEU:HA	43:m:21:VAL:HG12	2.02	0.42
52:x:169:GLU:O	52:x:521:SER:N	2.52	0.42
53:y:788:LEU:HD23	53:y:792:LEU:HD23	2.01	0.42
9:8:213:VAL:HA	49:u:565:HIS:ND1	2.34	0.42
10:9:1:MET:HE2	10:9:6:ARG:HH11	1.85	0.42
11:A:28:U:H2'	11:A:29:G:H8	1.85	0.42
11:A:380:G:N1	11:A:383:G:OP2	2.45	0.42
11:A:897:U:N3	11:A:899:U:O4	2.53	0.42
11:A:1386:A:OP2	33:Z:160:SER:OG	2.29	0.42
30:T:20:ARG:NE	30:T:22:GLN:OE1	2.49	0.42
36:c:82:SER:OG	36:c:83:TRP:N	2.53	0.42
38:e:92:LEU:HD22	38:e:109:TYR:HE1	1.83	0.42
46:q:4:ASN:ND2	46:q:7:LYS:O	2.49	0.42
2:1:515:CYS:HA	2:1:529:LYS:O	2.19	0.42
2:1:532:ARG:HH22	14:D:118:GLY:HA3	1.84	0.42
6:5:398:MET:HA	6:5:401:MET:HG3	2.02	0.42
11:A:1285:G:N1	43:m:57:ASP:OD2	2.40	0.42
11:A:1617:G:N1	11:A:1620:A:OP2	2.53	0.42
15:E:41:PHE:O	15:E:76:LYS:NZ	2.38	0.42
39:f:114:LEU:HA	39:f:117:ILE:HG22	2.02	0.42
1:0:960:LYS:O	1:0:964:ILE:HG12	2.20	0.41
7:6:248:LYS:HZ2	7:6:285:MET:HE3	1.84	0.41
7:6:342:PHE:HB2	7:6:346:GLN:HG3	2.01	0.41
11:A:106:C:H2'	11:A:107:A:H8	1.85	0.41
11:A:522:A:N6	11:A:644:OMG:OP1	2.37	0.41
11:A:1587:G:C5	37:d:78:ILE:HD11	2.55	0.41
20:J:11:LEU:HD12	20:J:74:VAL:HG13	2.02	0.41
38:e:79:ILE:HB	38:e:83:LEU:HD23	2.02	0.41
48:t:139:ASP:HA	48:t:142:MET:HE3	2.02	0.41
50:v:349:GLN:OE1	50:v:393:MET:N	2.47	0.41
52:x:448:LYS:HG2	52:x:470:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:y:332:LYS:O	53:y:335:GLU:HG3	2.20	0.41
53:y:393:MET:SD	53:y:398:TRP:HB2	2.60	0.41
2:1:502:GLN:HE22	2:1:504:ILE:HG23	1.86	0.41
2:1:575:SER:OG	2:1:594:VAL:O	2.28	0.41
11:A:1114:U:O2'	11:A:1119:A:N6	2.53	0.41
11:A:1438:A:H2'	11:A:1439:A:C8	2.56	0.41
17:G:190:PRO:O	17:G:193:GLN:NE2	2.47	0.41
19:I:46:THR:H	19:I:49:GLN:NE2	2.18	0.41
28:R:113:TYR:OH	28:R:156:ALA:O	2.31	0.41
34:a:14:LEU:HD23	34:a:21:MET:HE1	2.02	0.41
49:u:198:CYS:SG	49:u:202:ARG:NH2	2.73	0.41
50:v:221:VAL:HB	50:v:324:PHE:HE1	1.85	0.41
53:y:603:PRO:HB2	53:y:669:ARG:HE	1.84	0.41
1:0:633:ILE:HG12	1:0:699:LEU:HD23	2.02	0.41
2:1:619:GLN:H	2:1:663:GLY:HA3	1.85	0.41
6:5:191:ILE:HG21	6:5:279:ARG:HH21	1.85	0.41
6:5:388:LEU:HD11	50:v:407:LYS:HB3	2.01	0.41
11:A:1345:G:OP1	11:A:1688:C:O2'	2.38	0.41
17:G:142:LYS:HE2	17:G:144:ILE:HD11	2.02	0.41
36:c:6:THR:O	36:c:310:TRP:HA	2.20	0.41
38:e:70:PRO:HA	38:e:73:VAL:HG12	2.01	0.41
39:f:109:GLU:HA	39:f:112:GLU:HG3	2.02	0.41
40:h:26:SER:OG	40:h:27:ARG:N	2.53	0.41
49:u:274:ASN:O	49:u:278:LYS:HG2	2.21	0.41
49:u:316:GLN:O	49:u:320:THR:HG23	2.19	0.41
50:v:294:GLU:HA	50:v:297:GLU:HG3	2.02	0.41
53:y:698:MET:HA	53:y:702:GLU:HG2	2.01	0.41
53:y:698:MET:HA	53:y:702:GLU:CG	2.49	0.41
11:A:159:A2M:H2	11:A:468:A:O4'	2.19	0.41
11:A:885:U:H3	11:A:901:G:H1	1.69	0.41
23:M:127:ASN:OD1	23:M:127:ASN:N	2.48	0.41
24:N:41:ARG:HE	24:N:45:GLY:HA2	1.84	0.41
25:O:190:PRO:HB2	49:u:18:PHE:CZ	2.56	0.41
26:P:61:LYS:HA	26:P:61:LYS:HD3	1.74	0.41
50:v:315:CYS:HA	50:v:318:VAL:HG12	2.01	0.41
7:6:283:MET:HE2	7:6:320:MET:HE2	2.02	0.41
7:6:325:ILE:HG12	49:u:446:ILE:HG13	2.02	0.41
11:A:29:G:H2'	11:A:30:C:C6	2.55	0.41
11:A:109:U:O2	12:B:71:ARG:NH2	2.53	0.41
11:A:1289:U:H4'	34:a:2:LEU:HD13	2.02	0.41
14:D:64:ASP:OD1	14:D:65:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:u:9:GLU:HB3	49:u:46:ILE:HD11	2.02	0.41
1:0:1106:ASP:OD1	1:0:1163:PRO:HD2	2.20	0.41
1:0:1130:LYS:HA	1:0:1130:LYS:HD3	1.93	0.41
6:5:350:PHE:HB3	6:5:357:TYR:HD1	1.86	0.41
11:A:16:G:H2'	11:A:17:C:C6	2.55	0.41
11:A:508:A:H2'	11:A:509:OMG:H5'	2.02	0.41
23:M:36:GLU:HB3	23:M:47:ARG:HH11	1.86	0.41
39:f:86:ARG:NH1	39:f:110:ASP:OD2	2.53	0.41
40:h:40:ILE:O	40:h:44:LYS:HG2	2.20	0.41
11:A:201:C:H5''	11:A:202:G:H21	1.86	0.41
11:A:796:G:N2	11:A:798:G:OP2	2.54	0.41
11:A:1190:A:N3	11:A:1714:U:O2'	2.48	0.41
11:A:1275:G:H22	11:A:1506:A:P	2.43	0.41
12:B:120:VAL:HG12	12:B:145:VAL:HG11	2.03	0.41
28:R:64:ASN:O	28:R:186:ASP:HA	2.20	0.41
30:T:79:LEU:HD11	30:T:96:LEU:HD21	2.03	0.41
48:t:42:ILE:HD12	48:t:245:VAL:HA	2.01	0.41
48:t:389:ASP:HB3	48:t:392:ALA:HB3	2.03	0.41
49:u:489:ARG:HH12	53:y:806:THR:HG21	1.85	0.41
50:v:331:ASP:OD1	50:v:331:ASP:N	2.53	0.41
53:y:636:ILE:O	53:y:639:SER:OG	2.35	0.41
1:0:1019:MET:HE1	15:E:75:ILE:HA	2.03	0.41
6:5:157:TYR:CD2	6:5:221:ILE:HG23	2.55	0.41
8:7:-18:G:H5'	49:u:68:LYS:NZ	2.35	0.41
11:A:17:C:H2'	11:A:18:C:C6	2.56	0.41
11:A:1015:U:O2'	11:A:1017:U:OP2	2.36	0.41
11:A:1228:A:H5''	38:e:32:LYS:HG3	2.03	0.41
22:L:147:VAL:O	22:L:151:ILE:HG12	2.21	0.41
49:u:172:ARG:NE	49:u:172:ARG:O	2.54	0.41
49:u:230:LEU:HB3	49:u:271:LEU:HD21	2.03	0.41
49:u:324:LEU:O	49:u:328:SER:OG	2.29	0.41
53:y:817:THR:O	53:y:821:ILE:HG12	2.21	0.41
1:0:1041:ILE:HB	1:0:1046:GLN:HE21	1.85	0.41
2:1:439:ALA:HB3	2:1:472:TRP:HE1	1.86	0.41
6:5:143:LYS:HA	6:5:143:LYS:HD2	1.89	0.41
6:5:163:LEU:HD12	6:5:163:LEU:HA	1.96	0.41
9:8:225:ALA:O	9:8:229:GLU:N	2.52	0.41
11:A:189:U:OP1	28:R:148:LYS:NZ	2.53	0.41
11:A:644:OMG:H2'	11:A:645:C:C6	2.56	0.41
11:A:1015:U:O2'	19:I:55:ARG:NH1	2.54	0.41
11:A:1357:A:H5''	22:L:112:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:39:GLN:OE1	17:G:39:GLN:N	2.49	0.41
22:L:204:ILE:HD13	22:L:214:LEU:HB3	2.03	0.41
25:O:225:LEU:HB3	25:O:229:MET:HE1	2.03	0.41
26:P:29:GLY:O	26:P:93:LEU:HA	2.21	0.41
28:R:101:ILE:HD12	28:R:190:LEU:HD11	2.03	0.41
31:V:35:LEU:HD12	31:V:117:ILE:HG12	2.02	0.41
32:Y:96:TYR:HA	32:Y:100:VAL:HG22	2.03	0.41
33:Z:67:ARG:NH1	34:a:96:ARG:H	2.18	0.41
40:h:21:ARG:HH11	40:h:88:LEU:HD23	1.85	0.41
49:u:228:MET:HE3	49:u:228:MET:HB2	1.92	0.41
49:u:316:GLN:HG2	49:u:382:TYR:O	2.21	0.41
53:y:635:ASP:OD1	53:y:636:ILE:N	2.53	0.41
53:y:712:LYS:HZ2	53:y:719:ARG:HH22	1.68	0.41
1:0:639:HIS:CG	1:0:640:VAL:H	2.39	0.41
6:5:271:TYR:O	6:5:275:VAL:HG23	2.21	0.41
11:A:1264:C:N4	11:A:1518:C:O2	2.54	0.41
11:A:1568:C:H2'	11:A:1569:A:C8	2.56	0.41
11:A:1745:A:O3'	29:S:31:ARG:NH1	2.48	0.41
15:E:52:LEU:HD11	15:E:73:GLN:HB2	2.03	0.41
1:0:966:GLU:O	1:0:970:THR:HG22	2.21	0.40
2:1:492:ARG:HA	2:1:507:ARG:O	2.20	0.40
2:1:575:SER:OG	2:1:575:SER:O	2.37	0.40
9:8:236:SER:O	9:8:241:LYS:N	2.54	0.40
11:A:913:A:OP1	17:G:99:ARG:NE	2.44	0.40
12:B:111:VAL:HG12	12:B:140:PHE:HB2	2.03	0.40
17:G:29:GLU:HA	17:G:32:MET:SD	2.61	0.40
47:r:164:ASP:OD1	47:r:173:ARG:NH2	2.54	0.40
48:t:405:MET:HB2	48:t:451:TRP:CZ3	2.56	0.40
49:u:191:LYS:NZ	49:u:248:GLU:OE2	2.40	0.40
53:y:347:ARG:HD2	53:y:385:TYR:HA	2.03	0.40
1:0:639:HIS:CD2	1:0:640:VAL:H	2.39	0.40
11:A:962:A:O2'	47:r:53:ARG:O	2.32	0.40
11:A:1451:G:N7	23:M:44:LYS:NZ	2.65	0.40
47:r:24:VAL:HB	47:r:65:ILE:HA	2.03	0.40
49:u:94:LEU:O	49:u:98:GLU:HG2	2.21	0.40
49:u:320:THR:HG22	49:u:383:VAL:HB	2.03	0.40
49:u:476:ARG:HG3	53:y:795:TYR:CE1	2.55	0.40
53:y:684:CYS:SG	53:y:765:VAL:HG21	2.61	0.40
1:0:724:ILE:HA	1:0:752:ILE:O	2.21	0.40
11:A:1304:U:HO2'	42:k:93:HIS:HE2	1.58	0.40
11:A:1756:C:H42	11:A:1776:G:H2'	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:O:190:PRO:HB3	49:u:17:GLU:OE2	2.21	0.40
43:m:14:VAL:HG21	43:m:126:GLU:HG3	2.04	0.40
48:t:321:LEU:HD13	48:t:331:ALA:HB2	2.04	0.40
50:v:401:TYR:H	53:y:846:ARG:NH2	2.19	0.40
52:x:200:GLU:O	52:x:380:VAL:N	2.51	0.40
1:0:882:LEU:HD23	1:0:882:LEU:HA	1.89	0.40
6:5:191:ILE:HD13	6:5:279:ARG:HE	1.86	0.40
6:5:542:PHE:O	6:5:546:GLN:HG2	2.21	0.40
11:A:725:C:H6	11:A:725:C:H5''	1.87	0.40
22:L:165:VAL:HG21	22:L:217:ALA:HB1	2.03	0.40
22:L:201:GLY:N	22:L:221:ASP:OD2	2.51	0.40
23:M:58:MET:HE3	23:M:58:MET:HB3	1.85	0.40
28:R:133:GLU:OE1	28:R:133:GLU:N	2.55	0.40
41:i:38:MET:HE3	41:i:38:MET:HB2	1.87	0.40
46:q:99:GLU:O	46:q:103:LEU:HG	2.22	0.40
50:v:197:ASP:HA	50:v:211:ARG:HH21	1.87	0.40
50:v:249:MET:O	50:v:289:LYS:NZ	2.41	0.40
52:x:318:TYR:O	52:x:322:ASN:ND2	2.54	0.40
53:y:844:MET:SD	53:y:844:MET:N	2.87	0.40
10:9:1:MET:SD	10:9:1:MET:N	2.72	0.40
11:A:484:A2M:H1'	11:A:484:A2M:HM'3	1.82	0.40
11:A:1232:U:H2'	11:A:1233:G:H8	1.87	0.40
23:M:97:GLU:OE2	23:M:120:THR:HB	2.21	0.40
31:V:40:ALA:HB1	31:V:45:TYR:CG	2.56	0.40
36:c:87:LEU:HB2	36:c:101:PHE:HB2	2.04	0.40
48:t:99:PRO:HA	48:t:237:GLU:OE1	2.22	0.40
49:u:205:LEU:O	49:u:208:ILE:HG22	2.21	0.40
49:u:208:ILE:HD11	49:u:218:ILE:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	619/1220 (51%)	587 (95%)	32 (5%)	0	100	100
2	1	584/814 (72%)	539 (92%)	45 (8%)	0	100	100
3	2	300/325 (92%)	291 (97%)	9 (3%)	0	100	100
4	3	209/218 (96%)	202 (97%)	7 (3%)	0	100	100
5	4	251/357 (70%)	238 (95%)	13 (5%)	0	100	100
6	5	518/564 (92%)	501 (97%)	17 (3%)	0	100	100
7	6	360/374 (96%)	338 (94%)	22 (6%)	0	100	100
9	8	313/352 (89%)	290 (93%)	23 (7%)	0	100	100
10	9	22/25 (88%)	22 (100%)	0	0	100	100
12	B	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
13	C	254/263 (97%)	248 (98%)	6 (2%)	0	100	100
14	D	175/194 (90%)	168 (96%)	7 (4%)	0	100	100
15	E	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
16	F	56/133 (42%)	47 (84%)	9 (16%)	0	100	100
17	G	171/194 (88%)	164 (96%)	7 (4%)	0	100	100
18	H	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
19	I	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
20	J	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
21	K	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
22	L	218/293 (74%)	210 (96%)	8 (4%)	0	100	100
23	M	129/135 (96%)	123 (95%)	6 (5%)	0	100	100
24	N	205/295 (70%)	197 (96%)	8 (4%)	0	100	100
25	O	209/264 (79%)	203 (97%)	6 (3%)	0	100	100
26	P	131/151 (87%)	123 (94%)	8 (6%)	0	100	100
27	Q	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
28	R	194/208 (93%)	190 (98%)	4 (2%)	0	100	100
29	S	228/249 (92%)	221 (97%)	7 (3%)	0	100	100
30	T	123/133 (92%)	123 (100%)	0	0	100	100
31	V	187/204 (92%)	178 (95%)	9 (5%)	0	100	100
32	Y	139/146 (95%)	132 (95%)	7 (5%)	0	100	100
33	Z	225/243 (93%)	222 (99%)	3 (1%)	0	100	100
34	a	97/165 (59%)	94 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	b	129/145 (89%)	122 (95%)	7 (5%)	0	100	100
36	c	311/317 (98%)	295 (95%)	16 (5%)	0	100	100
37	d	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
38	e	79/125 (63%)	73 (92%)	6 (8%)	0	100	100
39	f	147/152 (97%)	138 (94%)	9 (6%)	0	100	100
40	h	101/119 (85%)	92 (91%)	9 (9%)	0	100	100
41	i	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
42	k	66/156 (42%)	61 (92%)	5 (8%)	0	100	100
43	m	120/132 (91%)	114 (95%)	6 (5%)	0	100	100
44	n	62/69 (90%)	57 (92%)	5 (8%)	0	100	100
45	o	75/320 (23%)	72 (96%)	3 (4%)	0	100	100
46	q	116/144 (81%)	111 (96%)	5 (4%)	0	100	100
47	r	294/315 (93%)	275 (94%)	19 (6%)	0	100	100
48	t	451/472 (96%)	439 (97%)	12 (3%)	0	100	100
49	u	705/1382 (51%)	656 (93%)	49 (7%)	0	100	100
50	v	403/445 (91%)	369 (92%)	34 (8%)	0	100	100
52	x	417/548 (76%)	394 (94%)	23 (6%)	0	100	100
53	y	539/913 (59%)	514 (95%)	25 (5%)	0	100	100
All	All	10926/14338 (76%)	10398 (95%)	528 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	546/1081 (50%)	546 (100%)	0	100	100
2	1	97/702 (14%)	97 (100%)	0	100	100
6	5	477/515 (93%)	477 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	6	112/335 (33%)	112 (100%)	0	100	100
9	8	1/310 (0%)	1 (100%)	0	100	100
10	9	23/24 (96%)	23 (100%)	0	100	100
12	B	129/142 (91%)	129 (100%)	0	100	100
13	C	220/225 (98%)	220 (100%)	0	100	100
14	D	158/168 (94%)	158 (100%)	0	100	100
15	E	112/115 (97%)	112 (100%)	0	100	100
16	F	46/104 (44%)	46 (100%)	0	100	100
17	G	159/174 (91%)	159 (100%)	0	100	100
18	H	73/76 (96%)	73 (100%)	0	100	100
19	I	130/131 (99%)	130 (100%)	0	100	100
20	J	112/113 (99%)	112 (100%)	0	100	100
21	K	65/67 (97%)	65 (100%)	0	100	100
22	L	186/225 (83%)	186 (100%)	0	100	100
23	M	119/122 (98%)	119 (100%)	0	100	100
24	N	173/243 (71%)	173 (100%)	0	100	100
25	O	192/231 (83%)	192 (100%)	0	100	100
26	P	104/119 (87%)	104 (100%)	0	100	100
27	Q	86/98 (88%)	86 (100%)	0	100	100
28	R	172/180 (96%)	172 (100%)	0	100	100
29	S	200/218 (92%)	200 (100%)	0	100	100
30	T	107/115 (93%)	107 (100%)	0	100	100
31	V	159/170 (94%)	159 (100%)	0	100	100
32	Y	117/121 (97%)	117 (100%)	0	100	100
33	Z	190/202 (94%)	190 (100%)	0	100	100
34	a	90/136 (66%)	90 (100%)	0	100	100
35	b	117/130 (90%)	117 (100%)	0	100	100
36	c	272/275 (99%)	272 (100%)	0	100	100
37	d	112/115 (97%)	112 (100%)	0	100	100
38	e	71/103 (69%)	71 (100%)	0	100	100
39	f	129/132 (98%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	h	94/107 (88%)	94 (100%)	0	100	100
41	i	44/49 (90%)	44 (100%)	0	100	100
42	k	61/140 (44%)	61 (100%)	0	100	100
43	m	104/108 (96%)	104 (100%)	0	100	100
44	n	57/62 (92%)	57 (100%)	0	100	100
45	o	64/277 (23%)	64 (100%)	0	100	100
46	q	100/123 (81%)	100 (100%)	0	100	100
47	r	190/280 (68%)	190 (100%)	0	100	100
48	t	380/397 (96%)	380 (100%)	0	100	100
49	u	528/1259 (42%)	528 (100%)	0	100	100
50	v	206/406 (51%)	206 (100%)	0	100	100
52	x	207/494 (42%)	207 (100%)	0	100	100
53	y	472/811 (58%)	472 (100%)	0	100	100
All	All	7563/11730 (64%)	7563 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	639	HIS
1	0	655	HIS
1	0	679	ASN
1	0	859	GLN
1	0	1046	GLN
1	0	1103	ASN
2	1	497	GLN
2	1	502	GLN
2	1	511	ASN
6	5	225	HIS
6	5	427	ASN
12	B	11	GLN
12	B	18	GLN
12	B	19	ASN
12	B	100	ASN
13	C	50	ASN
13	C	142	HIS

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Mol	Chain	Res	Type
13	C	188	ASN
16	F	132	ASN
19	I	58	HIS
21	K	33	GLN
22	L	115	GLN
22	L	235	ASN
23	M	31	ASN
23	M	83	ASN
25	O	186	ASN
27	Q	72	HIS
28	R	167	GLN
29	S	110	ASN
29	S	146	ASN
31	V	137	GLN
31	V	149	GLN
32	Y	24	HIS
32	Y	114	GLN
33	Z	145	GLN
34	a	66	HIS
40	h	85	HIS
46	q	44	ASN
48	t	39	GLN
49	u	110	GLN
49	u	270	GLN
49	u	442	GLN
49	u	551	GLN
49	u	560	ASN
50	v	239	GLN
50	v	377	ASN
50	v	396	ASN
52	x	51	GLN
52	x	68	GLN
52	x	411	GLN
53	y	334	ASN
53	y	520	GLN
53	y	597	ASN
53	y	600	HIS
53	y	631	ASN
53	y	659	ASN
53	y	670	GLN
53	y	701	HIS
53	y	758	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1746/1869 (93%)	411 (23%)	13 (0%)
51	w	74/75 (98%)	31 (41%)	0
8	7	56/255 (21%)	37 (66%)	3 (5%)
All	All	1876/2199 (85%)	479 (25%)	16 (0%)

All (479) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-34	C
8	7	-31	C
8	7	-30	A
8	7	-29	A
8	7	-28	C
8	7	-27	A
8	7	-26	A
8	7	-23	A
8	7	-22	C
8	7	-21	A
8	7	-20	A
8	7	-18	G
8	7	-13	A
8	7	-12	A
8	7	-10	A
8	7	-8	A
8	7	-7	G
8	7	-6	A
8	7	-5	C
8	7	-4	C
8	7	-3	A
8	7	1	A
8	7	3	G
8	7	4	G
8	7	5	U
8	7	6	A
8	7	7	C
8	7	10	U
8	7	11	U
8	7	12	C
8	7	13	A
8	7	15	G
8	7	17	C

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Mol	Chain	Res	Type
8	7	19	U
8	7	20	G
8	7	21	A
8	7	22	G
11	A	2	A
11	A	17	C
11	A	23	G
11	A	26	U
11	A	33	G
11	A	44	U
11	A	45	A
11	A	46	A
11	A	56	G
11	A	58	C
11	A	59	U
11	A	60	G
11	A	67	C
11	A	68	A
11	A	72	C
11	A	73	C
11	A	74	G
11	A	78	C
11	A	103	A
11	A	113	G
11	A	115	U
11	A	126	G
11	A	129	C
11	A	130	G
11	A	140	U
11	A	142	C
11	A	143	U
11	A	155	G
11	A	158	A
11	A	159	A2M
11	A	160	U
11	A	163	U
11	A	173	A
11	A	182	C
11	A	184	G
11	A	190	G
11	A	198	U
11	A	199	C

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Mol	Chain	Res	Type
11	A	200	G
11	A	202	G
11	A	203	G
11	A	204	G
11	A	206	G
11	A	208	G
11	A	291	G
11	A	292	A
11	A	294	U
11	A	295	C
11	A	306	C
11	A	307	G
11	A	308	G
11	A	318	A
11	A	319	C
11	A	321	C
11	A	323	C
11	A	324	C
11	A	325	C
11	A	326	C
11	A	327	G
11	A	329	G
11	A	347	G
11	A	351	G
11	A	362	C
11	A	364	A
11	A	368	U
11	A	369	C
11	A	370	G
11	A	381	C
11	A	384	U
11	A	385	G
11	A	386	C
11	A	409	C
11	A	418	A
11	A	421	G
11	A	448	A
11	A	450	C
11	A	452	G
11	A	465	A
11	A	471	G
11	A	472	C

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Mol	Chain	Res	Type
11	A	473	A
11	A	474	G
11	A	476	A
11	A	482	G
11	A	487	U
11	A	488	U
11	A	492	C
11	A	493	A
11	A	496	C
11	A	508	A
11	A	509	OMG
11	A	516	A
11	A	517	OMC
11	A	525	A
11	A	533	A
11	A	534	G
11	A	536	A
11	A	537	C
11	A	538	U
11	A	539	C
11	A	540	U
11	A	541	U
11	A	542	U
11	A	543	C
11	A	544	G
11	A	545	A
11	A	546	G
11	A	550	C
11	A	553	U
11	A	554	A
11	A	556	U
11	A	557	U
11	A	558	G
11	A	559	G
11	A	563	G
11	A	564	A
11	A	566	U
11	A	568	C
11	A	576	A
11	A	589	G
11	A	590	A
11	A	591	U

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Mol	Chain	Res	Type
11	A	598	G
11	A	604	A
11	A	607	U
11	A	608	C
11	A	614	C
11	A	617	G
11	A	626	G
11	A	628	A
11	A	631	U
11	A	643	A
11	A	644	OMG
11	A	645	C
11	A	655	A
11	A	660	C
11	A	662	G
11	A	668	A2M
11	A	669	A
11	A	671	A
11	A	672	A
11	A	673	G
11	A	683	OMG
11	A	688	U
11	A	689	U
11	A	690	G
11	A	691	G
11	A	692	G
11	A	694	G
11	A	695	C
11	A	696	G
11	A	697	G
11	A	698	G
11	A	699	C
11	A	700	G
11	A	705	G
11	A	707	C
11	A	712	G
11	A	713	C
11	A	715	A
11	A	717	G
11	A	719	G
11	A	720	A
11	A	721	G

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Mol	Chain	Res	Type
11	A	723	C
11	A	725	C
11	A	726	C
11	A	728	C
11	A	729	C
11	A	731	G
11	A	732	U
11	A	733	C
11	A	734	C
11	A	738	C
11	A	739	C
11	A	748	C
11	A	749	U
11	A	751	G
11	A	752	G
11	A	753	C
11	A	791	C
11	A	798	G
11	A	800	U
11	A	801	U
11	A	810	A
11	A	811	A
11	A	821	G
11	A	822	PSU
11	A	827	A
11	A	830	A
11	A	836	G
11	A	837	A
11	A	838	G
11	A	839	C
11	A	840	C
11	A	841	G
11	A	845	G
11	A	847	A
11	A	870	A
11	A	872	A
11	A	873	G
11	A	880	G
11	A	881	G
11	A	886	A
11	A	888	U
11	A	890	U

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Mol	Chain	Res	Type
11	A	891	G
11	A	892	U
11	A	895	G
11	A	896	U
11	A	897	U
11	A	898	U
11	A	899	U
11	A	900	C
11	A	903	A
11	A	908	A
11	A	909	G
11	A	913	A
11	A	920	A
11	A	922	A
11	A	930	C
11	A	933	G
11	A	934	G
11	A	954	U
11	A	956	G
11	A	963	A
11	A	970	G
11	A	972	A
11	A	990	A
11	A	992	A
11	A	999	G
11	A	1002	U
11	A	1017	U
11	A	1023	A
11	A	1045	U
11	A	1047	C
11	A	1061	U
11	A	1062	A
11	A	1083	A
11	A	1085	C
11	A	1089	G
11	A	1109	C
11	A	1113	A
11	A	1114	U
11	A	1115	U
11	A	1117	C
11	A	1119	A
11	A	1120	U

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Mol	Chain	Res	Type
11	A	1133	A
11	A	1138	C
11	A	1139	C
11	A	1143	A
11	A	1153	C
11	A	1154	U
11	A	1155	U
11	A	1183	A
11	A	1195	A
11	A	1207	G
11	A	1208	A
11	A	1209	A
11	A	1211	G
11	A	1215	C
11	A	1216	C
11	A	1217	A
11	A	1220	A
11	A	1224	G
11	A	1242	U
11	A	1247	C
11	A	1248	B8N
11	A	1251	A
11	A	1253	A
11	A	1256	G
11	A	1257	G
11	A	1259	A
11	A	1263	U
11	A	1274	G
11	A	1275	G
11	A	1283	C
11	A	1288	U
11	A	1290	G
11	A	1294	G
11	A	1295	A
11	A	1301	A
11	A	1302	G
11	A	1303	C
11	A	1308	U
11	A	1322	G
11	A	1326	U
11	A	1342	U
11	A	1355	C

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Mol	Chain	Res	Type
11	A	1356	G
11	A	1357	A
11	A	1371	U
11	A	1372	U
11	A	1378	A
11	A	1382	A
11	A	1397	U
11	A	1401	A
11	A	1402	A
11	A	1406	G
11	A	1417	C
11	A	1418	C
11	A	1419	C
11	A	1420	G
11	A	1421	A
11	A	1422	G
11	A	1423	C
11	A	1424	G
11	A	1433	C
11	A	1435	C
11	A	1436	C
11	A	1437	C
11	A	1438	A
11	A	1442	U
11	A	1454	A
11	A	1463	U
11	A	1487	A
11	A	1488	C
11	A	1489	A
11	A	1490	G
11	A	1497	G
11	A	1498	A
11	A	1507	G
11	A	1508	A
11	A	1520	G
11	A	1521	C
11	A	1531	A
11	A	1533	A
11	A	1534	C
11	A	1544	C
11	A	1552	G
11	A	1553	C

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Mol	Chain	Res	Type
11	A	1556	A
11	A	1558	C
11	A	1560	U
11	A	1570	G
11	A	1579	A
11	A	1580	A
11	A	1585	U
11	A	1587	G
11	A	1588	A
11	A	1594	A
11	A	1600	G
11	A	1601	A
11	A	1603	G
11	A	1619	A
11	A	1621	U
11	A	1623	A
11	A	1624	U
11	A	1639	G
11	A	1648	G
11	A	1654	G
11	A	1661	A
11	A	1663	A
11	A	1665	G
11	A	1671	G
11	A	1687	C
11	A	1695	A
11	A	1698	C
11	A	1706	G
11	A	1712	A
11	A	1715	A
11	A	1719	A
11	A	1721	U
11	A	1722	G
11	A	1729	U
11	A	1733	U
11	A	1749	G
11	A	1750	C
11	A	1752	C
11	A	1753	C
11	A	1754	G
11	A	1755	C
11	A	1756	C

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Mol	Chain	Res	Type
11	A	1757	G
11	A	1758	G
11	A	1759	G
11	A	1760	G
11	A	1772	C
11	A	1773	C
11	A	1774	C
11	A	1775	U
11	A	1776	G
11	A	1777	G
11	A	1778	C
11	A	1779	G
11	A	1780	G
11	A	1781	A
11	A	1782	G
11	A	1783	C
11	A	1784	G
11	A	1805	G
11	A	1808	U
11	A	1813	A
11	A	1819	A
11	A	1822	A
11	A	1823	A
11	A	1824	A
11	A	1825	A
11	A	1826	G
11	A	1829	G
11	A	1831	A
11	A	1835	A
11	A	1837	G
11	A	1838	U
11	A	1849	G
11	A	1851	MA6
11	A	1861	G
11	A	1862	G
11	A	1863	A
11	A	1865	C
51	w	6	A
51	w	8	U
51	w	12	G
51	w	13	C
51	w	16	C

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Mol	Chain	Res	Type
51	w	18	G
51	w	19	G
51	w	20	A
51	w	21	A
51	w	22	G
51	w	23	C
51	w	28	U
51	w	34	C
51	w	35	A
51	w	38	A
51	w	43	G
51	w	46	G
51	w	47	U
51	w	48	C
51	w	52	G
51	w	59	A
51	w	61	C
51	w	62	C
51	w	63	A
51	w	68	C
51	w	69	U
51	w	71	C
51	w	73	A
51	w	74	C
51	w	75	C
51	w	76	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-31	C
8	7	-21	A
8	7	-5	C
11	A	1	U
11	A	291	G
11	A	367	U
11	A	368	U
11	A	541	U
11	A	644	OMG
11	A	688	U
11	A	694	G
11	A	716	G

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Mol	Chain	Res	Type
11	A	731	G
11	A	797	C
11	A	912	C
11	A	1600	G

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

29 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
11	PSU	A	823	11	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
11	PSU	A	1081	11	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
11	UR3	A	1830	11	19,22,23	2.79	8 (42%)	26,32,35	1.51	4 (15%)
11	A2M	A	159	11	22,25,26	3.93	11 (50%)	31,36,39	3.39	16 (51%)
11	A2M	A	484	11	22,25,26	3.84	11 (50%)	31,36,39	3.32	13 (41%)
11	6MZ	A	1832	56,11	22,25,26	2.41	5 (22%)	30,36,39	2.43	10 (33%)
11	OMU	A	121	11	19,22,23	3.00	6 (31%)	26,31,34	1.71	5 (19%)
11	A2M	A	27	56,11	22,25,26	3.89	11 (50%)	31,36,39	3.34	13 (41%)
11	PSU	A	612	11	18,21,22	0.98	1 (5%)	22,30,33	1.78	5 (22%)
11	5MC	A	1374	11	18,22,23	0.56	0	26,32,35	0.53	0
11	A2M	A	668	56,11	22,25,26	3.88	11 (50%)	31,36,39	3.22	14 (45%)
11	OMG	A	683	11	23,26,27	1.30	4 (17%)	33,38,41	1.91	6 (18%)
11	PSU	A	1243	11	18,21,22	1.05	1 (5%)	22,30,33	1.79	4 (18%)
11	JMH	A	1219	56,11	18,22,23	2.93	5 (27%)	21,32,35	1.73	5 (23%)
11	B8N	A	1248	11	24,29,30	3.05	6 (25%)	29,42,45	1.83	6 (20%)
11	OMC	A	174	56,11	19,22,23	0.56	0	26,31,34	0.78	1 (3%)
11	PSU	A	822	11	18,21,22	1.07	1 (5%)	22,30,33	1.78	5 (22%)
11	A2M	A	1678	11	22,25,26	3.96	12 (54%)	31,36,39	3.38	14 (45%)
11	A2M	A	166	11	22,25,26	3.91	11 (50%)	31,36,39	3.25	13 (41%)
11	OMG	A	509	56,11	23,26,27	2.53	9 (39%)	33,38,41	3.36	14 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	A2M	A	1031	11	22,25,26	3.93	10 (45%)	31,36,39	3.26	12 (38%)
11	MA6	A	1850	11	23,26,27	1.56	2 (8%)	34,38,41	3.09	12 (35%)
11	OMG	A	644	11	23,26,27	2.37	7 (30%)	33,38,41	3.36	16 (48%)
11	PSU	A	119	11	18,21,22	1.00	1 (5%)	22,30,33	1.61	4 (18%)
11	MA6	A	1851	11	23,26,27	1.56	3 (13%)	34,38,41	3.17	12 (35%)
11	OMC	A	517	11	19,22,23	0.55	0	26,31,34	0.65	0
11	OMC	A	1703	11	19,22,23	0.57	0	26,31,34	0.66	0
11	5MU	A	814	11	19,22,23	0.47	0	28,32,35	1.15	2 (7%)
11	OMU	A	116	11	19,22,23	3.02	6 (31%)	26,31,34	1.64	5 (19%)

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
11	PSU	A	823	11	-	0/7/25/26	0/2/2/2
11	PSU	A	1081	11	-	1/7/25/26	0/2/2/2
11	UR3	A	1830	11	-	2/7/25/26	0/2/2/2
11	A2M	A	159	11	-	3/9/27/28	0/3/3/3
11	A2M	A	484	11	-	1/9/27/28	0/3/3/3
11	6MZ	A	1832	56,11	-	2/9/27/28	0/3/3/3
11	OMU	A	121	11	-	0/9/27/28	0/2/2/2
11	A2M	A	27	56,11	-	1/9/27/28	0/3/3/3
11	PSU	A	612	11	-	0/7/25/26	0/2/2/2
11	5MC	A	1374	11	-	0/7/25/26	0/2/2/2
11	A2M	A	668	56,11	-	2/9/27/28	0/3/3/3
11	OMG	A	683	11	-	3/9/27/28	0/3/3/3
11	PSU	A	1243	11	-	0/7/25/26	0/2/2/2
11	JMH	A	1219	56,11	-	1/7/25/26	0/2/2/2
11	B8N	A	1248	11	-	5/16/34/35	0/2/2/2
11	OMC	A	174	56,11	-	0/9/27/28	0/2/2/2
11	PSU	A	822	11	-	2/7/25/26	0/2/2/2
11	A2M	A	1678	11	-	1/9/27/28	0/3/3/3
11	A2M	A	166	11	-	1/9/27/28	0/3/3/3
11	OMG	A	509	56,11	-	3/9/27/28	0/3/3/3
11	A2M	A	1031	11	-	1/9/27/28	0/3/3/3
11	MA6	A	1850	11	-	3/11/29/30	0/3/3/3
11	OMG	A	644	11	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PSU	A	119	11	-	0/7/25/26	0/2/2/2
11	MA6	A	1851	11	-	4/11/29/30	0/3/3/3
11	OMC	A	517	11	-	2/9/27/28	0/2/2/2
11	OMC	A	1703	11	-	0/9/27/28	0/2/2/2
11	5MU	A	814	11	-	0/7/25/26	0/2/2/2
11	OMU	A	116	11	-	1/9/27/28	0/2/2/2

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1031	A2M	C3'-C2'	-12.89	1.24	1.52
11	A	1678	A2M	C3'-C2'	-12.79	1.24	1.52
11	A	27	A2M	C3'-C2'	-12.77	1.24	1.52
11	A	159	A2M	C3'-C2'	-12.73	1.24	1.52
11	A	166	A2M	C3'-C2'	-12.70	1.24	1.52
11	A	484	A2M	C3'-C2'	-12.32	1.25	1.52
11	A	668	A2M	C3'-C2'	-12.29	1.25	1.52
11	A	1832	6MZ	C6-N6	9.60	1.44	1.34
11	A	1219	JMH	C2-N1	8.35	1.50	1.38
11	A	1248	B8N	C4-N3	-8.13	1.25	1.40
11	A	1248	B8N	C6-N1	7.46	1.55	1.36
11	A	1830	UR3	C2-N1	7.38	1.49	1.38
11	A	116	OMU	C2-N1	7.12	1.49	1.38
11	A	116	OMU	C2-N3	7.11	1.50	1.38
11	A	121	OMU	C2-N3	7.02	1.50	1.38
11	A	121	OMU	C2-N1	6.94	1.49	1.38
11	A	668	A2M	O4'-C4'	-6.90	1.29	1.45
11	A	1678	A2M	O4'-C4'	-6.72	1.30	1.45
11	A	509	OMG	C4-N3	6.65	1.50	1.34
11	A	166	A2M	O4'-C4'	-6.47	1.30	1.45
11	A	1031	A2M	O4'-C4'	-6.41	1.30	1.45
11	A	159	A2M	O4'-C4'	-6.40	1.30	1.45
11	A	484	A2M	O4'-C4'	-6.33	1.30	1.45
11	A	27	A2M	O4'-C4'	-6.30	1.30	1.45
11	A	644	OMG	C4-N3	6.17	1.48	1.34
11	A	116	OMU	C6-C5	6.12	1.49	1.35
11	A	121	OMU	C6-C5	6.12	1.49	1.35
11	A	1830	UR3	C6-C5	6.09	1.49	1.35
11	A	1219	JMH	C6-C5	6.01	1.49	1.35
11	A	1248	B8N	C6-C5	5.49	1.42	1.34
11	A	1678	A2M	C3'-C4'	5.27	1.66	1.53
11	A	1219	JMH	C2-N3	5.23	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	509	OMG	C2-N3	5.19	1.45	1.33
11	A	159	A2M	C3'-C4'	5.16	1.66	1.53
11	A	1031	A2M	C3'-C4'	5.11	1.66	1.53
11	A	1830	UR3	C2-N3	5.08	1.48	1.39
11	A	484	A2M	C3'-C4'	5.07	1.66	1.53
11	A	1248	B8N	C2-N1	5.06	1.54	1.39
11	A	509	OMG	C2-N2	5.03	1.46	1.34
11	A	668	A2M	C3'-C4'	5.01	1.65	1.53
11	A	1851	MA6	C6-N6	4.98	1.51	1.36
11	A	27	A2M	C3'-C4'	4.97	1.65	1.53
11	A	1850	MA6	C6-N6	4.94	1.51	1.36
11	A	166	A2M	C3'-C4'	4.87	1.65	1.53
11	A	644	OMG	C2-N2	4.81	1.45	1.34
11	A	644	OMG	C2-N3	4.56	1.44	1.33
11	A	159	A2M	C6-N6	4.55	1.45	1.34
11	A	1678	A2M	C6-N6	4.53	1.45	1.34
11	A	484	A2M	C6-N6	4.51	1.45	1.34
11	A	166	A2M	C6-N6	4.51	1.45	1.34
11	A	668	A2M	C6-N6	4.50	1.45	1.34
11	A	27	A2M	C6-N6	4.50	1.45	1.34
11	A	1031	A2M	C6-N6	4.46	1.45	1.34
11	A	1678	A2M	C1'-N9	-4.45	1.33	1.46
11	A	159	A2M	C1'-N9	-4.37	1.33	1.46
11	A	166	A2M	C1'-N9	-4.33	1.34	1.46
11	A	159	A2M	O4'-C1'	4.32	1.52	1.42
11	A	27	A2M	C1'-N9	-4.23	1.34	1.46
11	A	1031	A2M	C1'-N9	-4.20	1.34	1.46
11	A	116	OMU	C4-N3	4.17	1.46	1.38
11	A	668	A2M	C1'-N9	-4.16	1.34	1.46
11	A	1031	A2M	O4'-C1'	4.10	1.51	1.42
11	A	121	OMU	C4-N3	4.10	1.45	1.38
11	A	1678	A2M	O4'-C1'	4.02	1.51	1.42
11	A	166	A2M	O4'-C1'	4.00	1.51	1.42
11	A	27	A2M	O4'-C1'	4.00	1.51	1.42
11	A	484	A2M	O4'-C1'	3.97	1.51	1.42
11	A	484	A2M	C1'-N9	-3.95	1.35	1.46
11	A	644	OMG	C5-N7	-3.86	1.31	1.39
11	A	1248	B8N	C1'-C5	3.71	1.58	1.50
11	A	668	A2M	O4'-C1'	3.67	1.50	1.42
11	A	509	OMG	C5-N7	-3.51	1.32	1.39
11	A	484	A2M	O2'-C2'	3.49	1.51	1.42
11	A	27	A2M	O2'-C2'	3.49	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1031	A2M	O2'-C2'	3.48	1.51	1.42
11	A	159	A2M	O2'-C2'	3.45	1.51	1.42
11	A	1248	B8N	O2-C2	-3.43	1.16	1.22
11	A	1243	PSU	C6-C5	3.42	1.39	1.35
11	A	668	A2M	O2'-C2'	3.38	1.51	1.42
11	A	166	A2M	O2'-C2'	3.37	1.51	1.42
11	A	1678	A2M	O2'-C2'	3.37	1.51	1.42
11	A	822	PSU	C6-C5	3.36	1.39	1.35
11	A	823	PSU	C6-C5	3.33	1.39	1.35
11	A	119	PSU	C6-C5	3.30	1.39	1.35
11	A	668	A2M	C2'-C1'	3.25	1.61	1.53
11	A	1081	PSU	C6-C5	3.24	1.39	1.35
11	A	484	A2M	C2'-C1'	3.22	1.61	1.53
11	A	1850	MA6	C5-C4	-3.03	1.33	1.39
11	A	1851	MA6	C5-C4	-3.02	1.33	1.39
11	A	612	PSU	C6-C5	3.02	1.38	1.35
11	A	1830	UR3	C6-N1	3.01	1.45	1.38
11	A	509	OMG	O6-C6	-3.01	1.17	1.23
11	A	166	A2M	C2'-C1'	3.01	1.60	1.53
11	A	1832	6MZ	C5-N7	-2.97	1.33	1.39
11	A	166	A2M	C5-C4	-2.96	1.33	1.39
11	A	1678	A2M	C5-C4	-2.95	1.33	1.39
11	A	27	A2M	C5-C4	-2.95	1.33	1.39
11	A	1031	A2M	C5-C4	-2.94	1.33	1.39
11	A	683	OMG	C6-N1	-2.89	1.33	1.38
11	A	668	A2M	C5-C4	-2.87	1.33	1.39
11	A	159	A2M	C5-C4	-2.82	1.33	1.39
11	A	1031	A2M	C2'-C1'	2.82	1.60	1.53
11	A	1219	JMH	C6-N1	2.80	1.44	1.38
11	A	644	OMG	O6-C6	-2.79	1.18	1.23
11	A	484	A2M	C5-C4	-2.79	1.33	1.39
11	A	27	A2M	C2'-C1'	2.74	1.60	1.53
11	A	159	A2M	C2'-C1'	2.74	1.60	1.53
11	A	484	A2M	C5-N7	-2.70	1.33	1.39
11	A	668	A2M	C5-N7	-2.63	1.34	1.39
11	A	121	OMU	C6-N1	2.61	1.44	1.38
11	A	116	OMU	C6-N1	2.58	1.44	1.38
11	A	683	OMG	C5-C4	2.58	1.45	1.38
11	A	27	A2M	C5-N7	-2.57	1.34	1.39
11	A	166	A2M	C5-N7	-2.56	1.34	1.39
11	A	1678	A2M	C2'-C1'	2.54	1.59	1.53
11	A	683	OMG	C5-N7	-2.53	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	159	A2M	C5-N7	-2.53	1.34	1.39
11	A	1031	A2M	C5-N7	-2.52	1.34	1.39
11	A	1219	JMH	C5-C4	2.52	1.48	1.42
11	A	1678	A2M	C5-N7	-2.47	1.34	1.39
11	A	509	OMG	C2-N1	2.32	1.43	1.37
11	A	509	OMG	C5-C6	2.31	1.53	1.44
11	A	1832	6MZ	C6-N1	-2.31	1.31	1.35
11	A	644	OMG	C5-C6	2.30	1.52	1.44
11	A	1830	UR3	O2-C2	-2.28	1.18	1.22
11	A	1830	UR3	O4-C4	-2.28	1.18	1.23
11	A	121	OMU	C5-C4	2.21	1.48	1.43
11	A	1830	UR3	C5-C4	2.18	1.49	1.43
11	A	116	OMU	C5-C4	2.15	1.48	1.43
11	A	644	OMG	C6-N1	2.14	1.42	1.38
11	A	159	A2M	C8-N9	-2.13	1.33	1.37
11	A	509	OMG	C6-N1	2.12	1.42	1.38
11	A	683	OMG	C4-N9	-2.12	1.32	1.38
11	A	484	A2M	O3'-C3'	2.11	1.47	1.43
11	A	1678	A2M	C8-N9	-2.11	1.33	1.37
11	A	1678	A2M	O3'-C3'	2.11	1.47	1.43
11	A	166	A2M	O3'-C3'	2.10	1.47	1.43
11	A	1830	UR3	C4-N3	2.10	1.45	1.40
11	A	1832	6MZ	C5-C4	-2.10	1.35	1.39
11	A	1832	6MZ	C8-N9	-2.10	1.33	1.37
11	A	668	A2M	O3'-C3'	2.08	1.47	1.43
11	A	509	OMG	O2'-C2'	-2.06	1.37	1.42
11	A	1851	MA6	C4-N3	2.06	1.38	1.34
11	A	27	A2M	O3'-C3'	2.01	1.47	1.43

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1851	MA6	N1-C6-N6	-12.13	103.82	117.08
11	A	1850	MA6	N1-C6-N6	-11.95	104.02	117.08
11	A	1678	A2M	C1'-N9-C8	-9.26	106.22	127.14
11	A	159	A2M	C1'-N9-C8	-9.13	106.52	127.14
11	A	27	A2M	C1'-N9-C8	-8.70	107.49	127.14
11	A	484	A2M	C1'-N9-C8	-8.70	107.50	127.14
11	A	1031	A2M	C1'-N9-C8	-8.40	108.16	127.14
11	A	166	A2M	C1'-N9-C8	-8.35	108.29	127.14
11	A	668	A2M	C1'-N9-C8	-8.28	108.44	127.14
11	A	509	OMG	C1'-N9-C8	-8.18	103.40	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	644	OMG	C1'-N9-C8	-8.16	103.46	126.70
11	A	509	OMG	C1'-N9-C4	8.03	150.36	126.50
11	A	159	A2M	C4-N9-C1'	7.78	145.12	126.59
11	A	484	A2M	C4-N9-C1'	7.70	144.95	126.59
11	A	1678	A2M	C4-N9-C1'	7.69	144.92	126.59
11	A	27	A2M	C4-N9-C1'	7.44	144.31	126.59
11	A	644	OMG	C5-C4-N3	-7.35	116.53	128.46
11	A	509	OMG	C5-C4-N3	-7.25	116.69	128.46
11	A	1031	A2M	C4-N9-C1'	7.19	143.71	126.59
11	A	668	A2M	C4-N9-C1'	7.10	143.51	126.59
11	A	166	A2M	C4-N9-C1'	7.05	143.38	126.59
11	A	644	OMG	C1'-N9-C4	6.74	146.53	126.50
11	A	1850	MA6	C5-C6-N6	6.44	136.51	125.30
11	A	1851	MA6	C5-C6-N6	6.42	136.48	125.30
11	A	644	OMG	O2'-C2'-C1'	6.34	121.44	109.08
11	A	644	OMG	C2-N3-C4	6.33	123.59	112.30
11	A	683	OMG	C5-C4-N3	-5.89	118.91	128.46
11	A	1832	6MZ	N1-C2-N3	-5.87	119.42	128.60
11	A	509	OMG	C2-N3-C4	5.85	122.72	112.30
11	A	166	A2M	N3-C2-N1	-5.82	119.50	128.60
11	A	27	A2M	N3-C2-N1	-5.70	119.69	128.60
11	A	1678	A2M	N3-C2-N1	-5.67	119.73	128.60
11	A	668	A2M	N6-C6-N1	-5.67	105.93	118.35
11	A	1851	MA6	N1-C2-N3	-5.60	119.84	128.60
11	A	1031	A2M	N6-C6-N1	-5.58	106.13	118.35
11	A	484	A2M	N3-C2-N1	-5.55	119.92	128.60
11	A	1678	A2M	N6-C6-N1	-5.54	106.23	118.35
11	A	1031	A2M	N3-C2-N1	-5.54	119.94	128.60
11	A	159	A2M	N6-C6-N1	-5.53	106.24	118.35
11	A	166	A2M	N6-C6-N1	-5.53	106.24	118.35
11	A	484	A2M	N6-C6-N1	-5.52	106.25	118.35
11	A	27	A2M	N6-C6-N1	-5.51	106.29	118.35
11	A	509	OMG	O2'-C2'-C1'	5.51	119.82	109.08
11	A	484	A2M	C5-C4-N3	-5.36	119.75	126.75
11	A	668	A2M	N3-C2-N1	-5.35	120.23	128.60
11	A	159	A2M	N3-C2-N1	-5.31	120.29	128.60
11	A	121	OMU	C4-N3-C2	-5.24	119.67	126.58
11	A	1832	6MZ	C5-C4-N3	-5.21	119.95	126.75
11	A	644	OMG	O3'-C3'-C4'	5.18	126.03	111.05
11	A	1850	MA6	N1-C2-N3	-5.12	120.60	128.60
11	A	159	A2M	C5-C4-N3	-5.09	120.11	126.75
11	A	27	A2M	C5-C4-N3	-5.08	120.12	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	668	A2M	C5-C6-N6	4.95	134.20	123.43
11	A	1031	A2M	C5-C4-N3	-4.93	120.32	126.75
11	A	116	OMU	C4-N3-C2	-4.93	120.08	126.58
11	A	509	OMG	N9-C4-N3	4.89	135.77	125.94
11	A	668	A2M	C5-C4-N3	-4.89	120.37	126.75
11	A	1851	MA6	C5-C4-N3	-4.86	120.41	126.75
11	A	1248	B8N	C5-C4-N3	4.86	125.17	116.17
11	A	1678	A2M	C5-C6-N6	4.85	133.97	123.43
11	A	166	A2M	C5-C6-N6	4.84	133.97	123.43
11	A	1031	A2M	C5-C6-N6	4.83	133.94	123.43
11	A	1832	6MZ	C9-N6-C6	4.78	126.99	122.87
11	A	683	OMG	C2-N3-C4	4.77	120.79	112.30
11	A	159	A2M	C5-C6-N6	4.74	133.75	123.43
11	A	484	A2M	C5-C6-N6	4.73	133.72	123.43
11	A	1243	PSU	N1-C2-N3	4.70	120.45	115.13
11	A	1678	A2M	C5-C4-N3	-4.67	120.65	126.75
11	A	1850	MA6	C5-C4-N3	-4.65	120.68	126.75
11	A	1678	A2M	N9-C8-N7	-4.64	107.56	113.91
11	A	166	A2M	C5-C4-N3	-4.64	120.70	126.75
11	A	27	A2M	C5-C6-N6	4.64	133.53	123.43
11	A	509	OMG	O3'-C3'-C4'	4.63	124.44	111.05
11	A	1851	MA6	N9-C8-N7	-4.62	107.60	113.91
11	A	683	OMG	N9-C4-N3	4.59	135.16	125.94
11	A	1850	MA6	N9-C8-N7	-4.56	107.68	113.91
11	A	1081	PSU	C4-N3-C2	-4.55	119.78	126.34
11	A	166	A2M	N9-C8-N7	-4.54	107.70	113.91
11	A	27	A2M	N9-C8-N7	-4.51	107.74	113.91
11	A	822	PSU	C4-N3-C2	-4.50	119.85	126.34
11	A	823	PSU	C4-N3-C2	-4.50	119.85	126.34
11	A	822	PSU	N1-C2-N3	4.50	120.23	115.13
11	A	1830	UR3	C4-N3-C2	-4.49	120.33	124.56
11	A	1243	PSU	C4-N3-C2	-4.49	119.87	126.34
11	A	612	PSU	N1-C2-N3	4.49	120.22	115.13
11	A	1081	PSU	N1-C2-N3	4.48	120.20	115.13
11	A	159	A2M	N9-C8-N7	-4.47	107.80	113.91
11	A	612	PSU	C4-N3-C2	-4.47	119.90	126.34
11	A	27	A2M	O4'-C1'-N9	4.47	116.86	108.06
11	A	1031	A2M	N9-C8-N7	-4.44	107.85	113.91
11	A	823	PSU	N1-C2-N3	4.42	120.14	115.13
11	A	1248	B8N	C4-N3-C2	-4.37	119.93	125.46
11	A	1832	6MZ	N9-C8-N7	-4.30	108.03	113.91
11	A	668	A2M	N9-C8-N7	-4.29	108.05	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	119	PSU	N1-C2-N3	4.18	119.86	115.13
11	A	1031	A2M	O4'-C1'-N9	4.15	116.23	108.06
11	A	119	PSU	C4-N3-C2	-4.12	120.40	126.34
11	A	166	A2M	O4'-C1'-N9	4.09	116.11	108.06
11	A	1219	JMH	C1'-N1-C2	4.01	123.77	116.99
11	A	484	A2M	N9-C8-N7	-3.96	108.50	113.91
11	A	1248	B8N	C31-N3-C4	3.95	123.13	117.31
11	A	159	A2M	O4'-C1'-N9	3.87	115.69	108.06
11	A	484	A2M	O4'-C1'-N9	3.85	115.65	108.06
11	A	1832	6MZ	C5-N7-C8	3.80	108.92	103.51
11	A	644	OMG	N9-C4-N3	3.75	133.46	125.94
11	A	121	OMU	N3-C2-N1	3.74	119.85	114.89
11	A	1832	6MZ	C2-N3-C4	3.69	120.48	111.75
11	A	1219	JMH	C6-N1-C2	-3.69	118.49	121.79
11	A	1851	MA6	C2-N1-C6	3.66	120.40	111.75
11	A	509	OMG	O3'-C3'-C2'	3.62	121.45	111.17
11	A	484	A2M	C2-N3-C4	3.60	120.26	111.75
11	A	644	OMG	O3'-C3'-C2'	3.60	121.39	111.17
11	A	1850	MA6	C4-C5-C6	3.59	119.90	115.88
11	A	1830	UR3	C1'-N1-C2	3.57	123.02	116.99
11	A	27	A2M	C2-N3-C4	3.57	120.19	111.75
11	A	116	OMU	N3-C2-N1	3.56	119.61	114.89
11	A	1850	MA6	C2-N1-C6	3.53	120.09	111.75
11	A	1678	A2M	O4'-C1'-N9	3.53	115.01	108.06
11	A	1219	JMH	O2-C2-N3	-3.48	116.44	121.34
11	A	1851	MA6	C2-N3-C4	3.47	119.95	111.75
11	A	1031	A2M	C2-N3-C4	3.46	119.92	111.75
11	A	509	OMG	C2-N1-C6	-3.45	118.81	125.10
11	A	166	A2M	C2-N3-C4	3.43	119.86	111.75
11	A	1851	MA6	C4-C5-C6	3.41	119.70	115.88
11	A	668	A2M	C2'-C1'-N9	3.41	119.27	113.53
11	A	159	A2M	C2-N3-C4	3.41	119.80	111.75
11	A	121	OMU	C5-C4-N3	3.38	119.90	114.84
11	A	1678	A2M	C2-N3-C4	3.37	119.72	111.75
11	A	1248	B8N	N3-C2-N1	3.34	121.47	116.76
11	A	668	A2M	C2-N3-C4	3.30	119.54	111.75
11	A	116	OMU	C5-C4-N3	3.27	119.73	114.84
11	A	159	A2M	C5-N7-C8	3.25	108.12	103.51
11	A	1832	6MZ	C4-C5-C6	3.23	119.31	116.81
11	A	27	A2M	C5-N7-C8	3.19	108.05	103.51
11	A	1850	MA6	C2-N3-C4	3.18	119.27	111.75
11	A	484	A2M	N3-C4-N9	3.15	132.26	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	159	A2M	N3-C4-N9	3.14	132.26	127.08
11	A	509	OMG	C5'-C4'-C3'	3.14	126.93	115.18
11	A	1851	MA6	C5-N7-C8	3.12	107.94	103.51
11	A	1678	A2M	C5-N7-C8	3.11	107.92	103.51
11	A	1031	A2M	C5-N7-C8	3.10	107.91	103.51
11	A	166	A2M	C5-N7-C8	3.04	107.82	103.51
11	A	27	A2M	N3-C4-N9	3.03	132.08	127.08
11	A	509	OMG	C5-C6-N1	3.02	120.87	113.19
11	A	668	A2M	C5-N7-C8	3.02	107.80	103.51
11	A	683	OMG	C6-C5-N7	3.02	135.87	130.25
11	A	1850	MA6	C5-N7-C8	3.00	107.78	103.51
11	A	484	A2M	C5-N7-C8	2.96	107.71	103.51
11	A	1678	A2M	N3-C4-N9	2.95	131.94	127.08
11	A	1851	MA6	N3-C4-N9	2.93	131.92	127.08
11	A	644	OMG	C2-N1-C6	-2.93	119.76	125.10
11	A	1832	6MZ	C4-C5-N7	-2.89	107.09	110.62
11	A	1830	UR3	C6-N1-C2	-2.88	119.21	121.79
11	A	612	PSU	O2-C2-N1	-2.87	119.63	122.79
11	A	121	OMU	O4-C4-C5	-2.86	120.12	125.16
11	A	116	OMU	O4-C4-C5	-2.86	120.13	125.16
11	A	1031	A2M	N3-C4-N9	2.85	131.78	127.08
11	A	668	A2M	N3-C4-N9	2.82	131.73	127.08
11	A	1832	6MZ	N3-C4-N9	2.82	131.72	127.08
11	A	814	5MU	C1'-N1-C2	2.81	122.65	117.57
11	A	1678	A2M	C4-N9-C8	2.78	108.74	105.73
11	A	1850	MA6	C4-N9-C8	2.76	108.72	105.73
11	A	509	OMG	O6-C6-C5	-2.76	119.29	126.60
11	A	1850	MA6	N3-C4-N9	2.73	131.59	127.08
11	A	814	5MU	O2-C2-N1	2.72	126.40	122.79
11	A	166	A2M	N3-C4-N9	2.69	131.52	127.08
11	A	1851	MA6	C4-N9-C8	2.67	108.62	105.73
11	A	1243	PSU	O2-C2-N1	-2.65	119.87	122.79
11	A	823	PSU	O2-C2-N1	-2.64	119.89	122.79
11	A	644	OMG	C5-C6-N1	2.63	119.86	113.19
11	A	159	A2M	C2'-C1'-N9	-2.60	109.15	113.53
11	A	822	PSU	O2-C2-N1	-2.53	120.00	122.79
11	A	644	OMG	N2-C2-N1	2.52	122.07	116.71
11	A	1219	JMH	O3'-C3'-C2'	2.46	119.79	111.82
11	A	644	OMG	O6-C6-C5	-2.44	120.13	126.60
11	A	159	A2M	C4-N9-C8	2.43	108.36	105.73
11	A	119	PSU	O2-C2-N1	-2.42	120.13	122.79
11	A	823	PSU	C6-N1-C2	-2.41	120.22	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	166	A2M	C4-N9-C8	2.40	108.33	105.73
11	A	644	OMG	N1-C2-N3	-2.40	118.85	123.32
11	A	1243	PSU	C6-N1-C2	-2.36	120.27	122.68
11	A	683	OMG	C4-C5-N7	-2.32	107.04	110.72
11	A	1678	A2M	C4'-O4'-C1'	-2.32	104.35	109.47
11	A	119	PSU	C6-N1-C2	-2.31	120.32	122.68
11	A	1081	PSU	O2-C2-N1	-2.31	120.25	122.79
11	A	27	A2M	C4-N9-C8	2.28	108.20	105.73
11	A	822	PSU	O4'-C1'-C2'	2.28	108.36	105.14
11	A	668	A2M	C3'-C2'-C1'	2.28	107.17	102.89
11	A	683	OMG	O6-C6-C5	-2.27	120.56	126.60
11	A	822	PSU	C6-N1-C2	-2.27	120.37	122.68
11	A	1248	B8N	O4'-C1'-C2'	2.24	108.30	105.14
11	A	174	OMC	C1'-N1-C2	2.24	123.42	118.42
11	A	612	PSU	O4'-C1'-C2'	2.22	108.27	105.14
11	A	1031	A2M	C4-N9-C8	2.21	108.12	105.73
11	A	1830	UR3	O2-C2-N3	-2.20	118.23	121.34
11	A	121	OMU	O2-C2-N1	-2.20	119.86	122.79
11	A	1832	6MZ	C5-C4-N9	2.19	108.33	105.78
11	A	612	PSU	C6-N1-C2	-2.18	120.45	122.68
11	A	668	A2M	C2'-C3'-C4'	2.16	106.69	101.99
11	A	509	OMG	O4'-C1'-N9	2.14	113.24	108.36
11	A	644	OMG	O5'-C5'-C4'	2.13	116.25	108.99
11	A	159	A2M	C2'-C3'-C4'	2.13	106.61	101.99
11	A	484	A2M	C3'-C2'-C1'	2.12	106.87	102.89
11	A	27	A2M	O4'-C1'-C2'	-2.11	102.86	106.57
11	A	1219	JMH	O3'-C3'-C4'	2.11	117.16	111.05
11	A	668	A2M	C4-N9-C8	2.10	108.00	105.73
11	A	484	A2M	C6-C5-C4	2.09	119.99	117.18
11	A	159	A2M	C4-C5-N7	-2.07	108.09	110.62
11	A	1850	MA6	C4-C5-N7	-2.07	108.10	110.62
11	A	1248	B8N	O2-C2-N3	-2.07	119.12	121.99
11	A	1081	PSU	C6-N1-C2	-2.07	120.57	122.68
11	A	644	OMG	C2'-C1'-N9	2.06	118.22	114.22
11	A	166	A2M	C4'-O4'-C1'	-2.05	104.95	109.47
11	A	509	OMG	N1-C2-N3	-2.04	119.51	123.32
11	A	1678	A2M	O2'-C2'-C1'	-2.04	105.09	109.08
11	A	644	OMG	C5'-C4'-C3'	2.04	122.82	115.18
11	A	1851	MA6	C4-C5-N7	-2.02	108.16	110.62
11	A	159	A2M	C6-C5-C4	2.01	119.89	117.18
11	A	116	OMU	O2-C2-N1	-2.00	120.12	122.79

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	27	A2M	C1'-C2'-O2'-CM'
11	A	116	OMU	C1'-C2'-O2'-CM2
11	A	159	A2M	C3'-C4'-C5'-O5'
11	A	159	A2M	C1'-C2'-O2'-CM'
11	A	166	A2M	C1'-C2'-O2'-CM'
11	A	484	A2M	C1'-C2'-O2'-CM'
11	A	509	OMG	C1'-C2'-O2'-CM2
11	A	644	OMG	C3'-C4'-C5'-O5'
11	A	644	OMG	C1'-C2'-O2'-CM2
11	A	668	A2M	O4'-C4'-C5'-O5'
11	A	822	PSU	C3'-C4'-C5'-O5'
11	A	1031	A2M	C1'-C2'-O2'-CM'
11	A	1678	A2M	C1'-C2'-O2'-CM'
11	A	1830	UR3	O4'-C1'-N1-C2
11	A	1832	6MZ	N1-C6-N6-C9
11	A	1850	MA6	C5-C6-N6-C10
11	A	1851	MA6	O4'-C4'-C5'-O5'
11	A	683	OMG	O4'-C4'-C5'-O5'
11	A	683	OMG	C3'-C4'-C5'-O5'
11	A	683	OMG	C1'-C2'-O2'-CM2
11	A	1248	B8N	O4'-C4'-C5'-O5'
11	A	1248	B8N	C3'-C4'-C5'-O5'
11	A	159	A2M	O4'-C4'-C5'-O5'
11	A	668	A2M	C3'-C4'-C5'-O5'
11	A	822	PSU	O4'-C4'-C5'-O5'
11	A	1851	MA6	C3'-C4'-C5'-O5'
11	A	1830	UR3	O4'-C1'-N1-C6
11	A	517	OMC	C3'-C4'-C5'-O5'
11	A	517	OMC	O4'-C4'-C5'-O5'
11	A	644	OMG	O4'-C4'-C5'-O5'
11	A	644	OMG	C4'-C5'-O5'-P
11	A	1850	MA6	C5-C6-N6-C9
11	A	1851	MA6	C5-C6-N6-C10
11	A	1850	MA6	N1-C6-N6-C10
11	A	509	OMG	C3'-C4'-C5'-O5'
11	A	1248	B8N	C31-C32-C33-C34
11	A	1248	B8N	N34-C33-C34-O36
11	A	1081	PSU	C4'-C5'-O5'-P
11	A	1851	MA6	C4'-C5'-O5'-P
11	A	1248	B8N	N34-C33-C34-O35
11	A	1832	6MZ	C5-C6-N6-C9
11	A	509	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
11	A	1219	JMH	C2'-C1'-N1-C2

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	823	PSU	1	0
11	A	159	A2M	2	0
11	A	484	A2M	2	0
11	A	27	A2M	1	0
11	A	683	OMG	5	0
11	A	1219	JMH	1	0
11	A	1248	B8N	1	0
11	A	1678	A2M	1	0
11	A	166	A2M	1	0
11	A	509	OMG	5	0
11	A	1850	MA6	1	0
11	A	644	OMG	2	0
11	A	517	OMC	1	0
11	A	814	5MU	1	0
11	A	116	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 92 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	GTP	0	2001	56,55	30,34,34	0.82	1 (3%)	46,54,54	1.87	12 (26%)

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
54	GTP	0	2001	56,55	-	2/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	0	2001	GTP	C2-N3	2.12	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	0	2001	GTP	PA-O3A-PB	-5.30	114.63	132.83
54	0	2001	GTP	C5-C4-N3	-4.97	120.40	128.46
54	0	2001	GTP	C2-N3-C4	4.52	120.36	112.30
54	0	2001	GTP	N9-C4-N3	3.08	132.13	125.94
54	0	2001	GTP	C2-N1-C6	-2.96	119.71	125.10
54	0	2001	GTP	N9-C8-N7	-2.75	108.21	113.39
54	0	2001	GTP	C8-N7-C5	2.67	109.06	104.24
54	0	2001	GTP	C5-C6-N1	2.58	119.75	113.19
54	0	2001	GTP	PB-O3B-PG	-2.53	124.15	132.83
54	0	2001	GTP	O6-C6-C5	-2.24	120.65	126.60
54	0	2001	GTP	C4-C5-N7	-2.03	107.51	110.72
54	0	2001	GTP	C3'-C2'-C1'	2.00	105.23	101.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	0	2001	GTP	PB-O3B-PG-O2G
54	0	2001	GTP	PG-O3B-PB-O2B

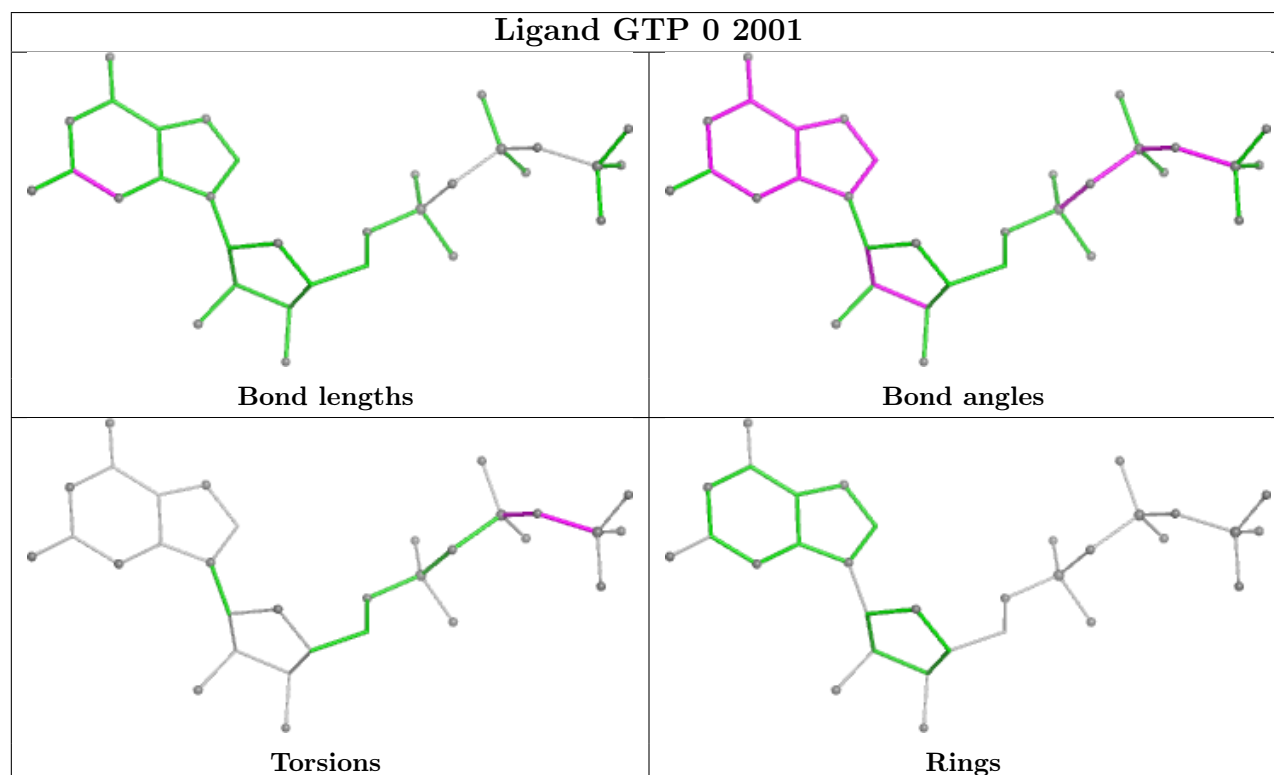
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	0	2001	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

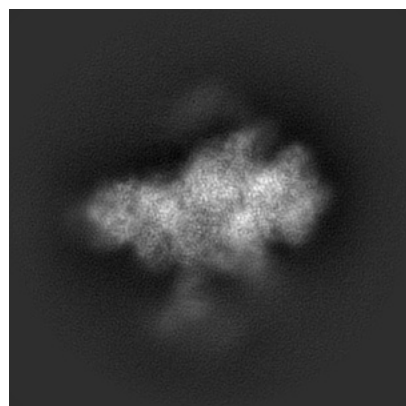
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17699. These allow visual inspection of the internal detail of the map and identification of artifacts.

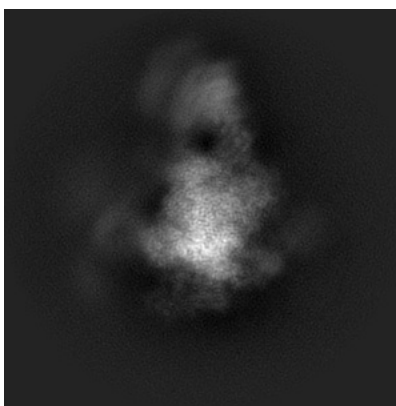
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

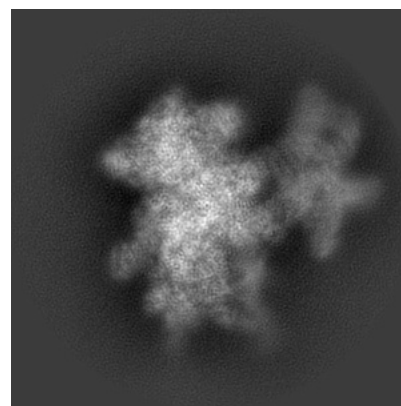
6.1.1 Primary map



X

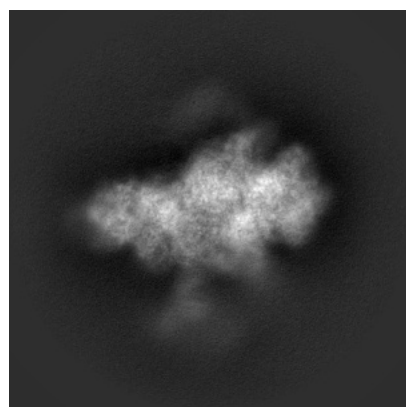


Y

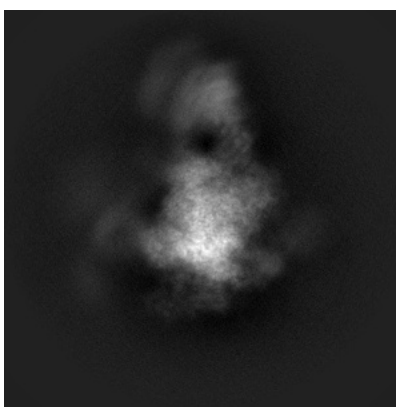


Z

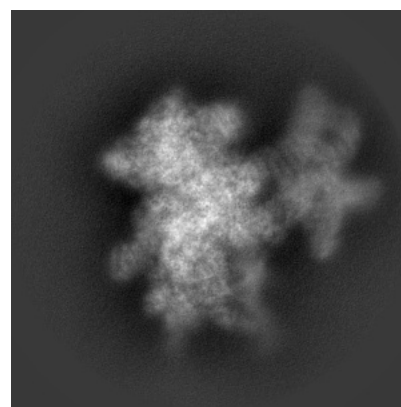
6.1.2 Raw map



X



Y

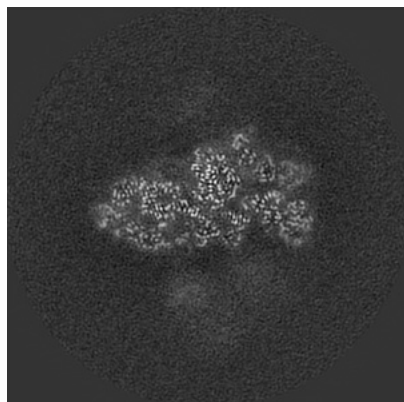


Z

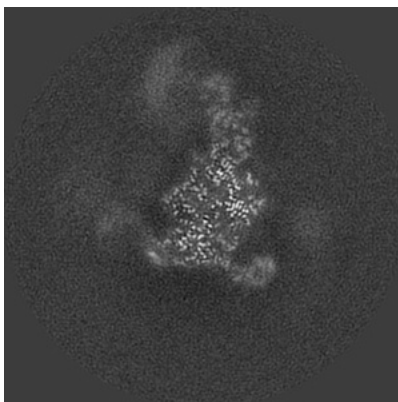
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

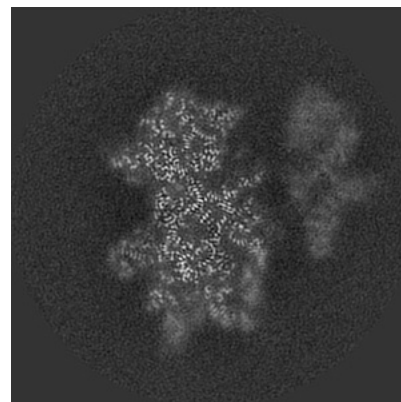
6.2.1 Primary map



X Index: 216

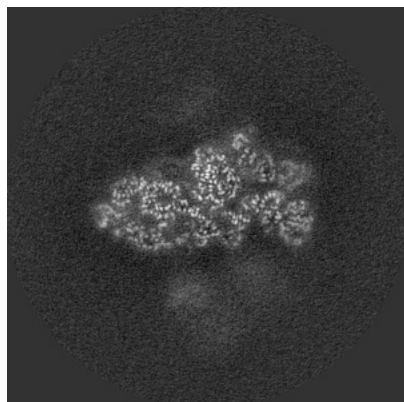


Y Index: 216

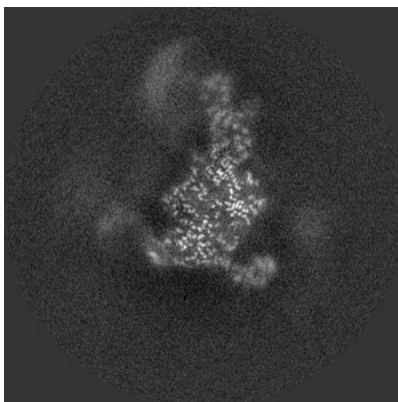


Z Index: 216

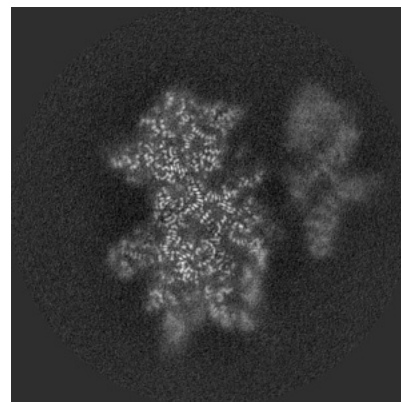
6.2.2 Raw map



X Index: 180



Y Index: 180

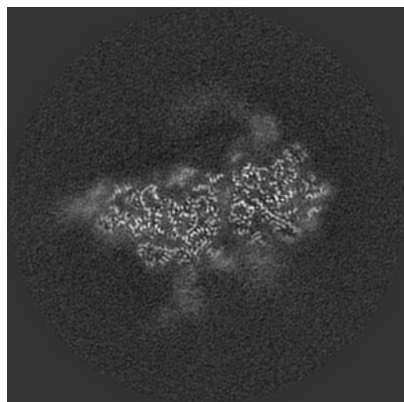


Z Index: 180

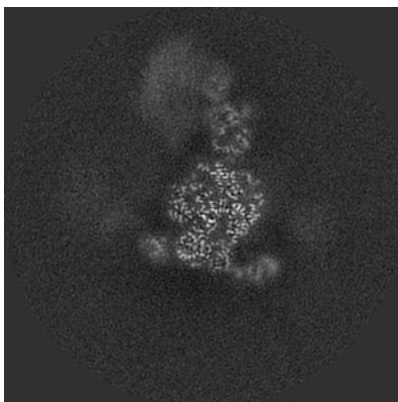
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

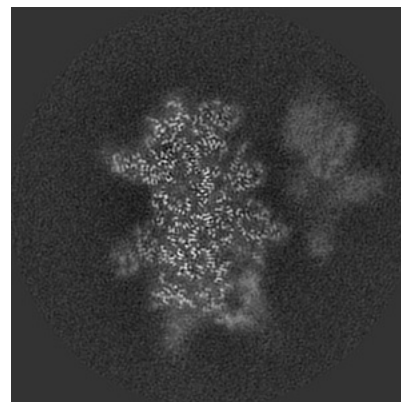
6.3.1 Primary map



X Index: 176

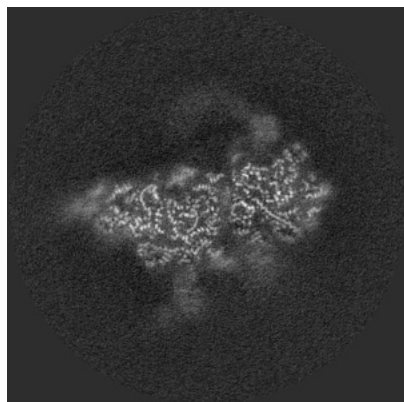


Y Index: 222

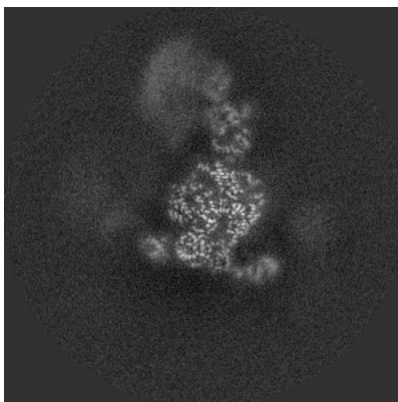


Z Index: 209

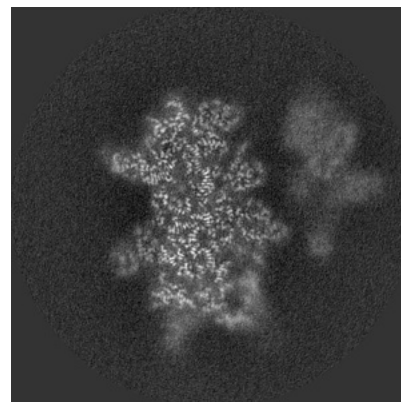
6.3.2 Raw map



X Index: 147



Y Index: 185

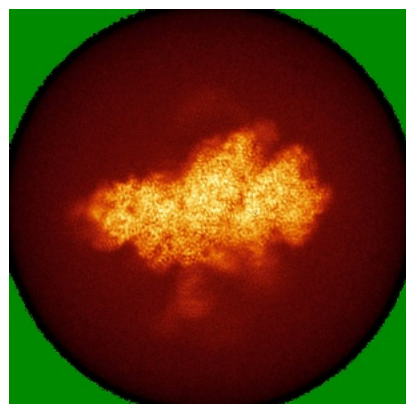


Z Index: 174

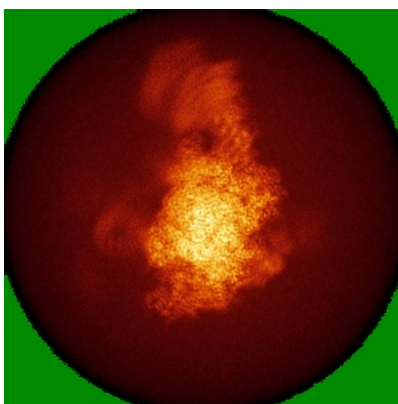
The images above show the largest variance slices of the map in three orthogonal directions.

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

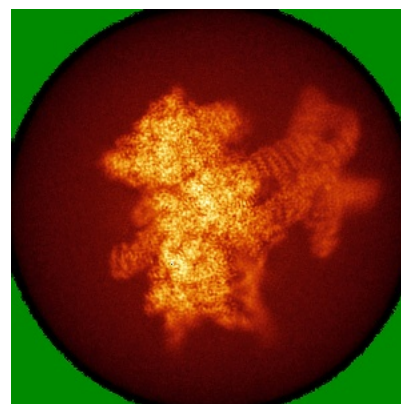
6.4.1 Primary map



X

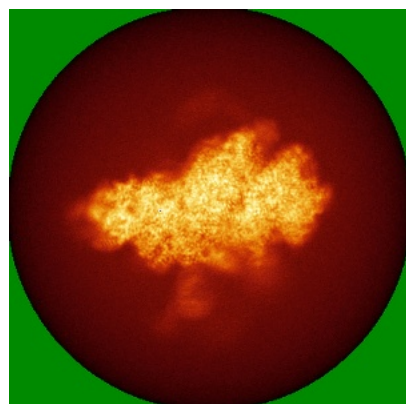


Y

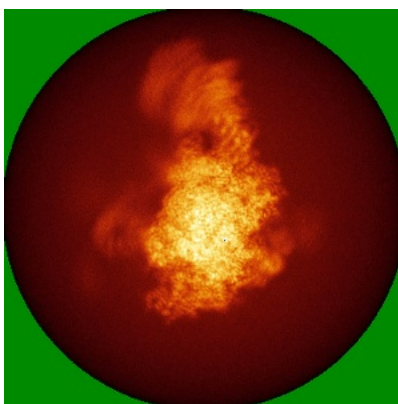


Z

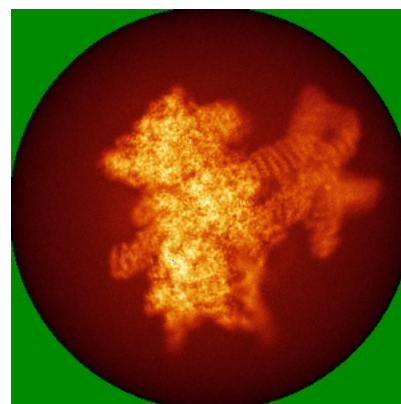
6.4.2 Raw map



X



Y

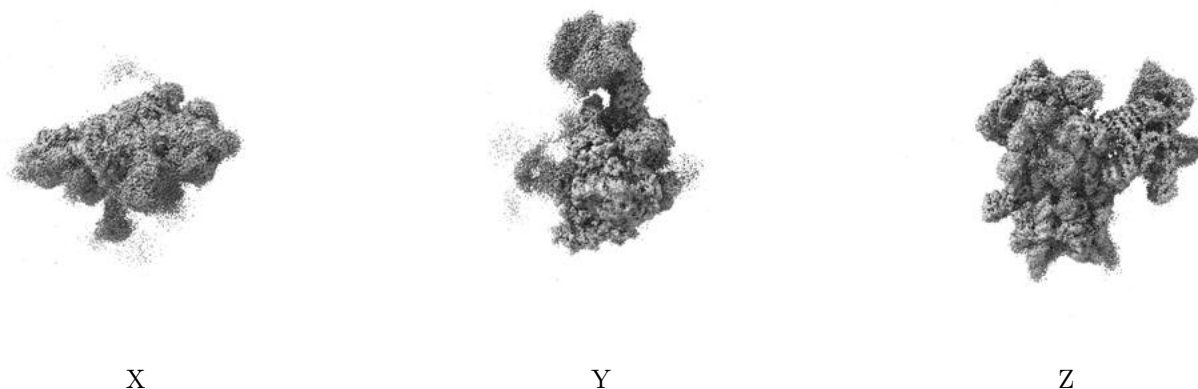


Z

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 3.0. 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.

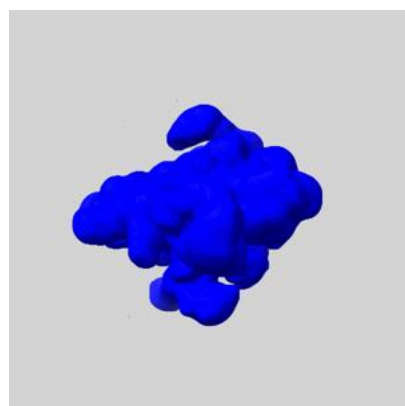
6.6 Mask visualisation [i](#)

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

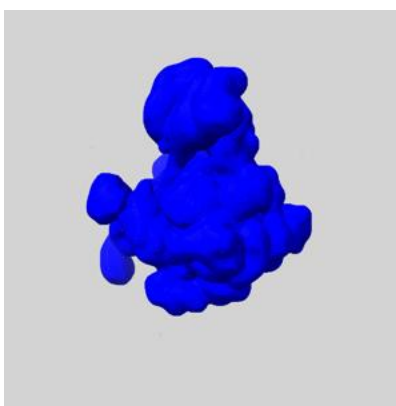
A mask typically either:

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

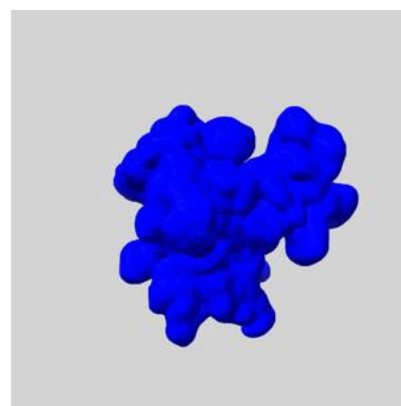
6.6.1 emd_17699_msk_1.map [i](#)



X



Y

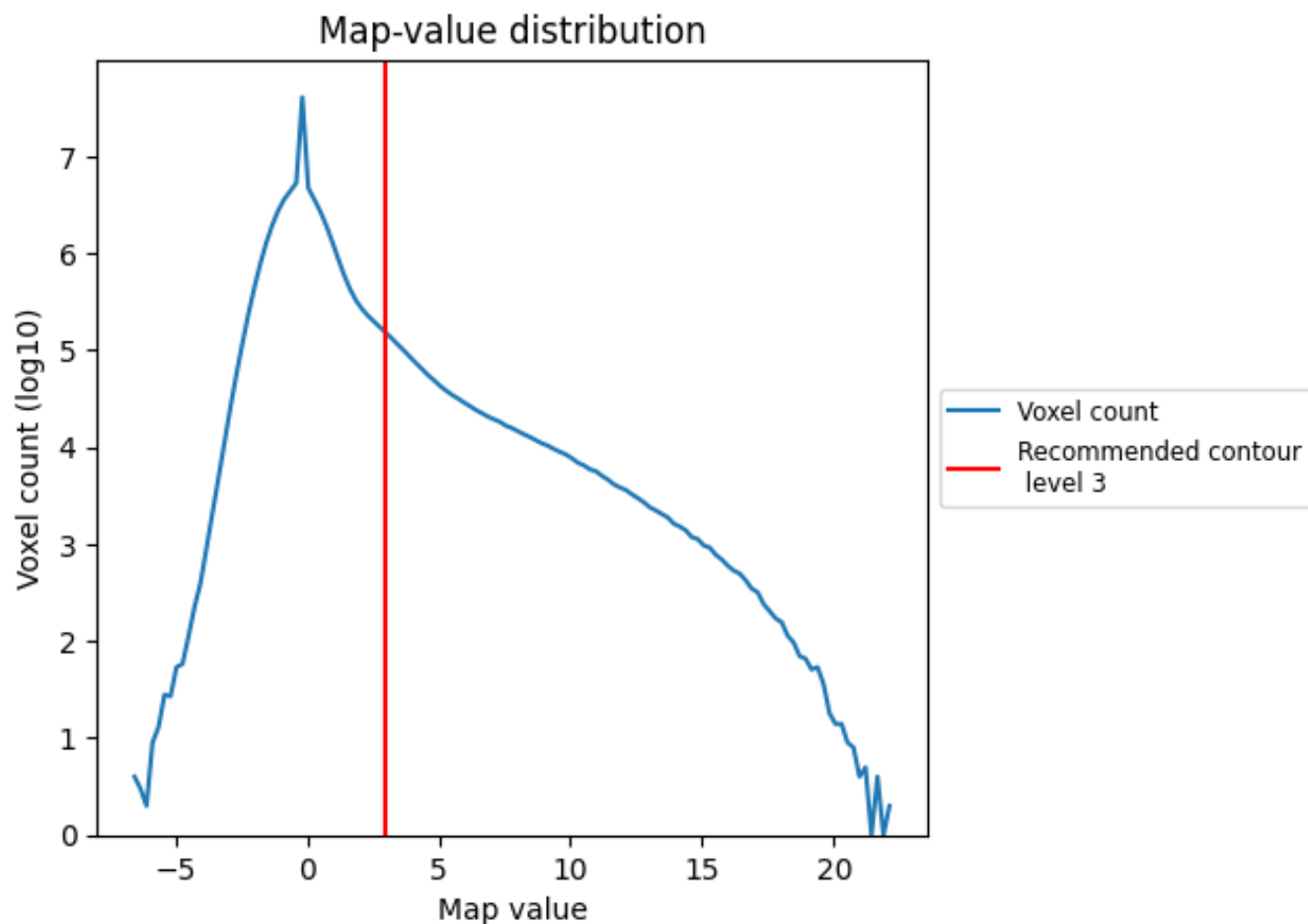


Z

7 Map analysis [i](#)

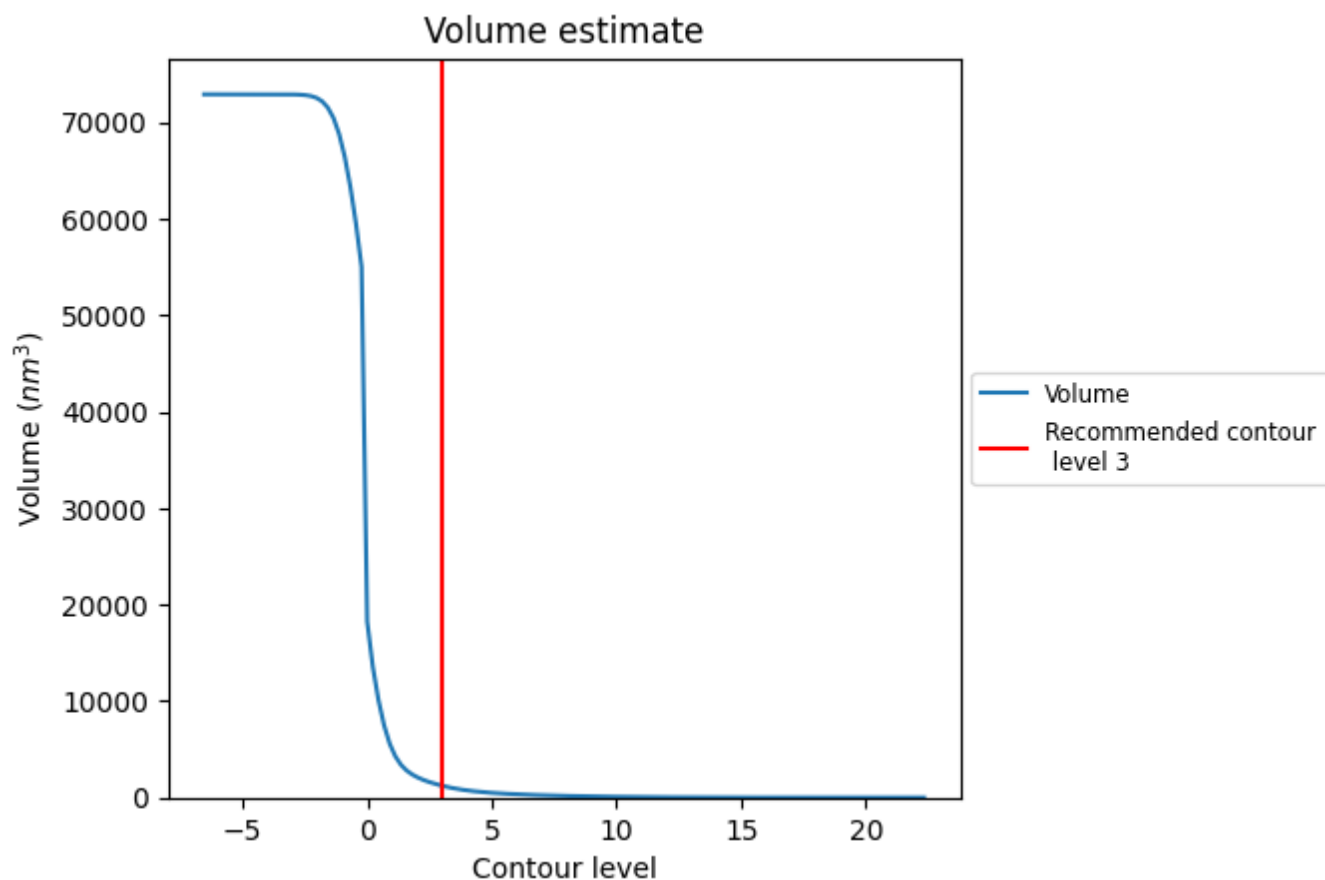
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

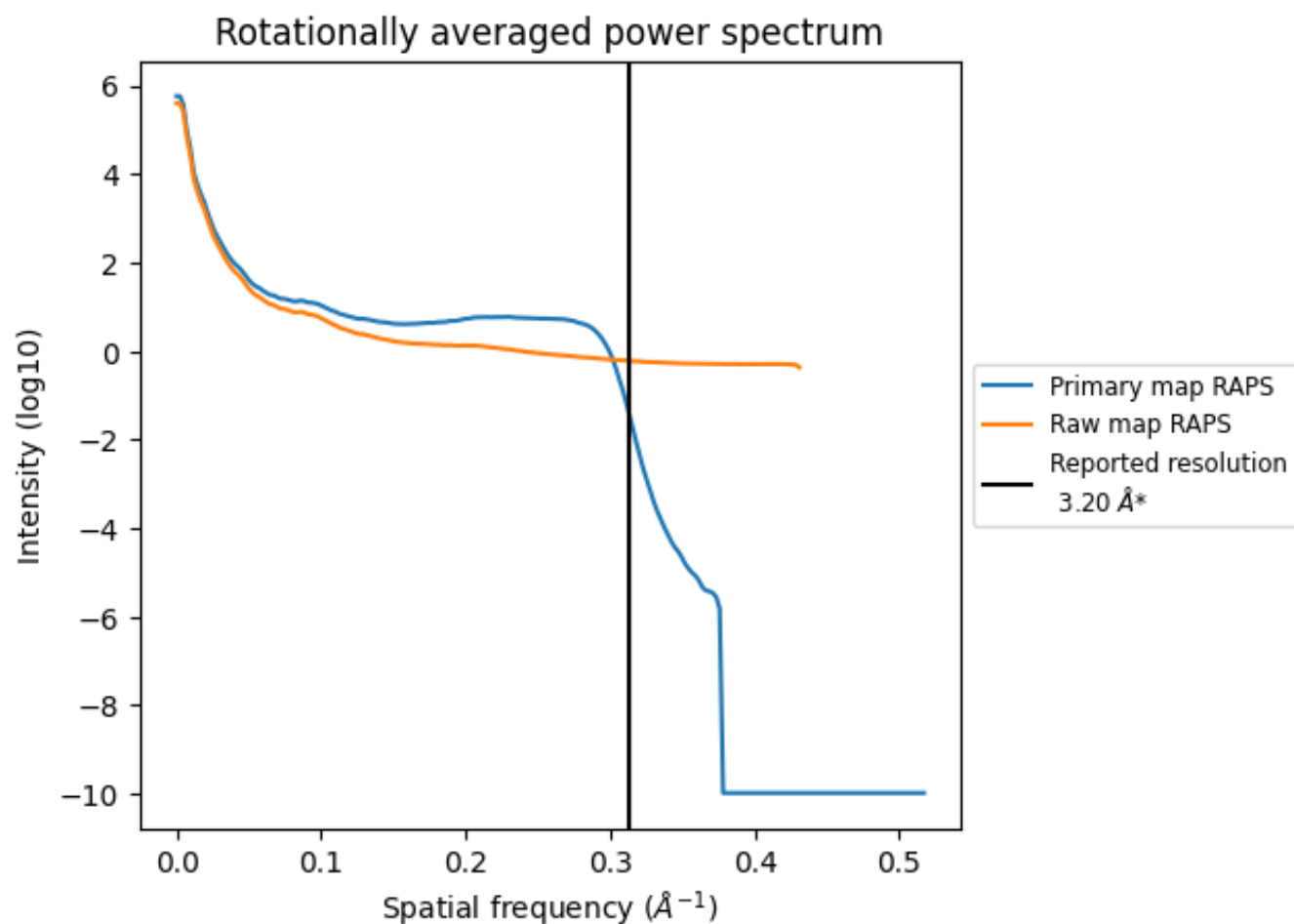
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1228 nm³; this corresponds to an approximate mass of 1109 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

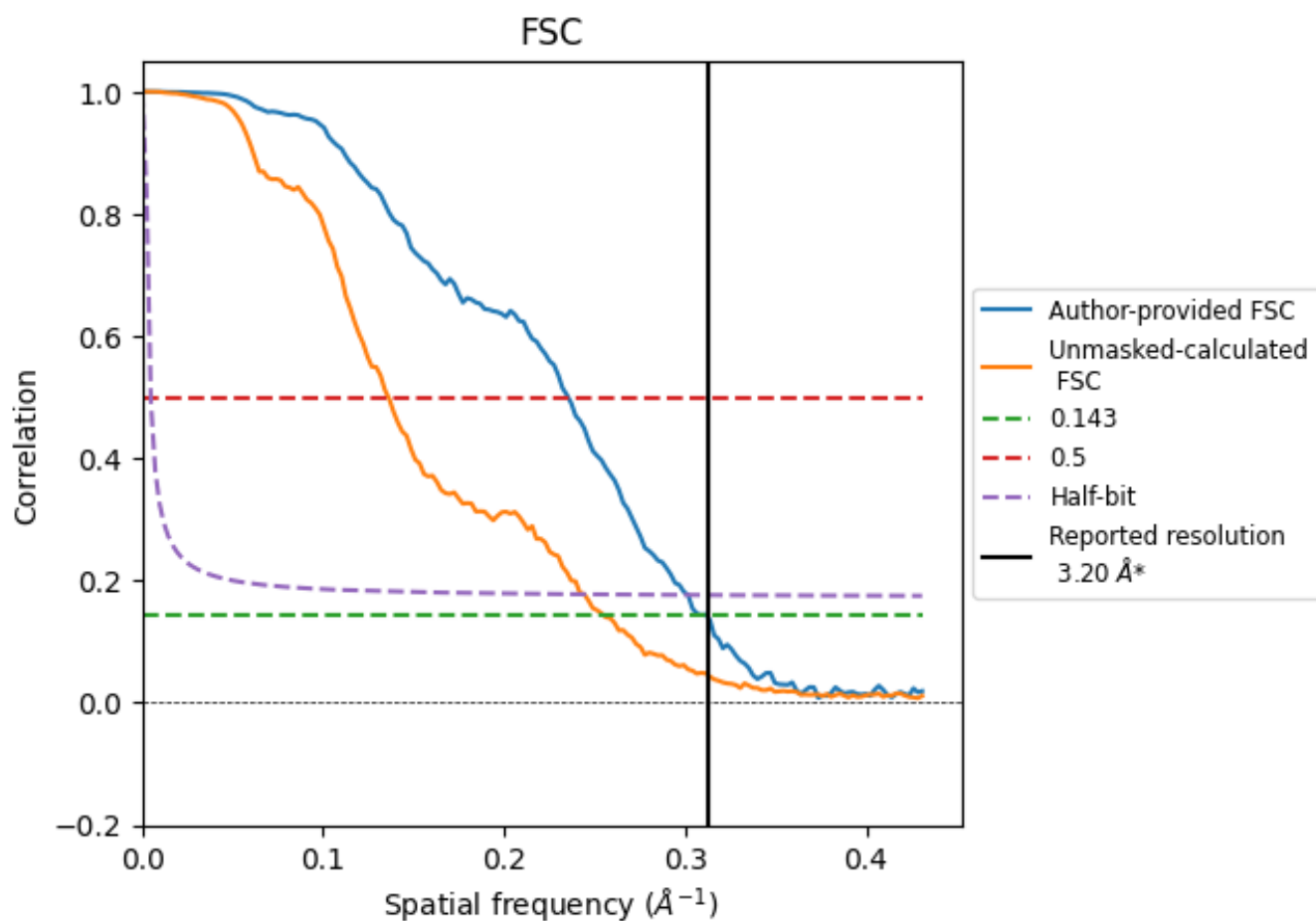


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

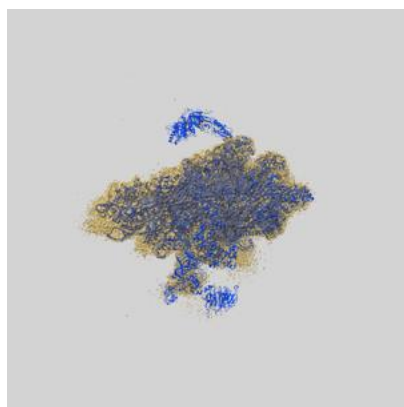
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	4.25	3.32
Unmasked-calculated*	3.92	7.35	4.09

*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 3.92 differs from the reported value 3.2 by more than 10 %

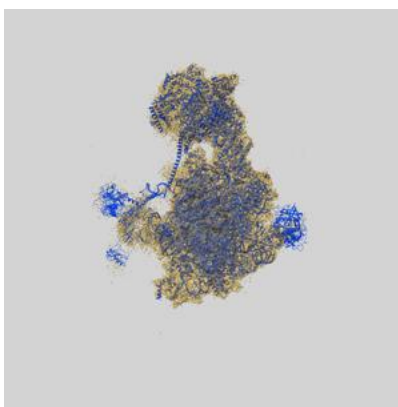
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17699 and PDB model 8PJ4. Per-residue inclusion information can be found in section 3 on page 14.

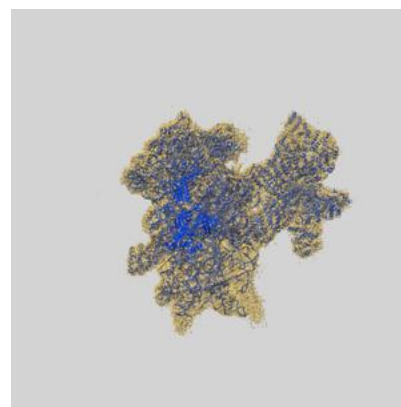
9.1 Map-model overlay [i](#)



X



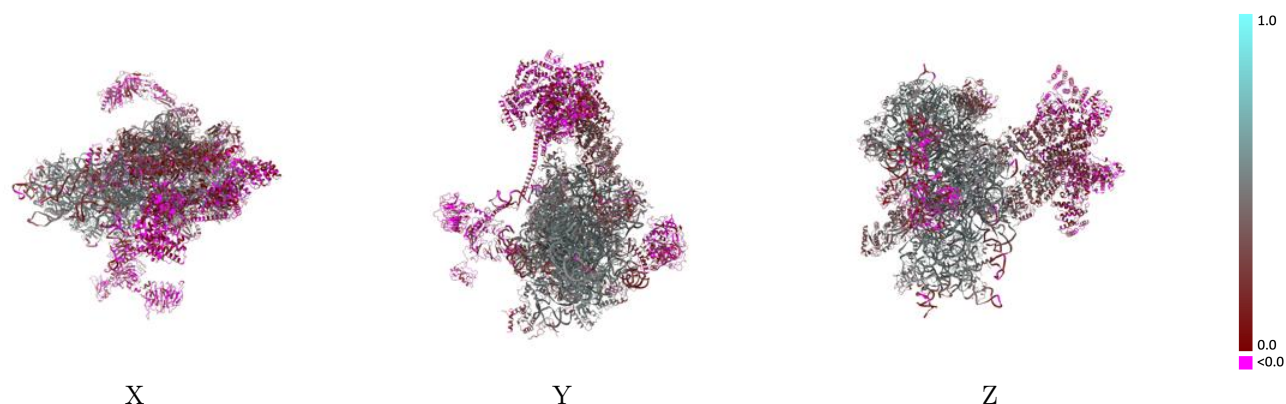
Y



Z

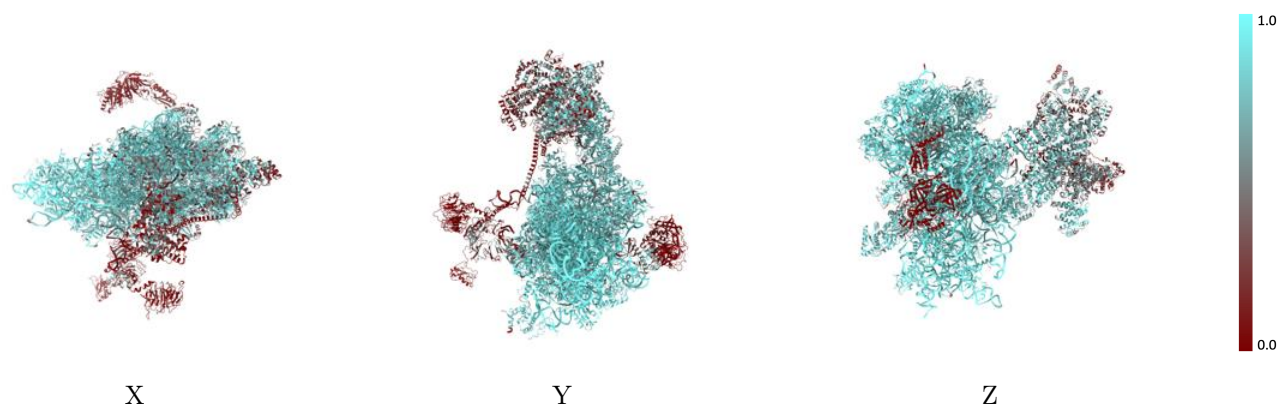
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



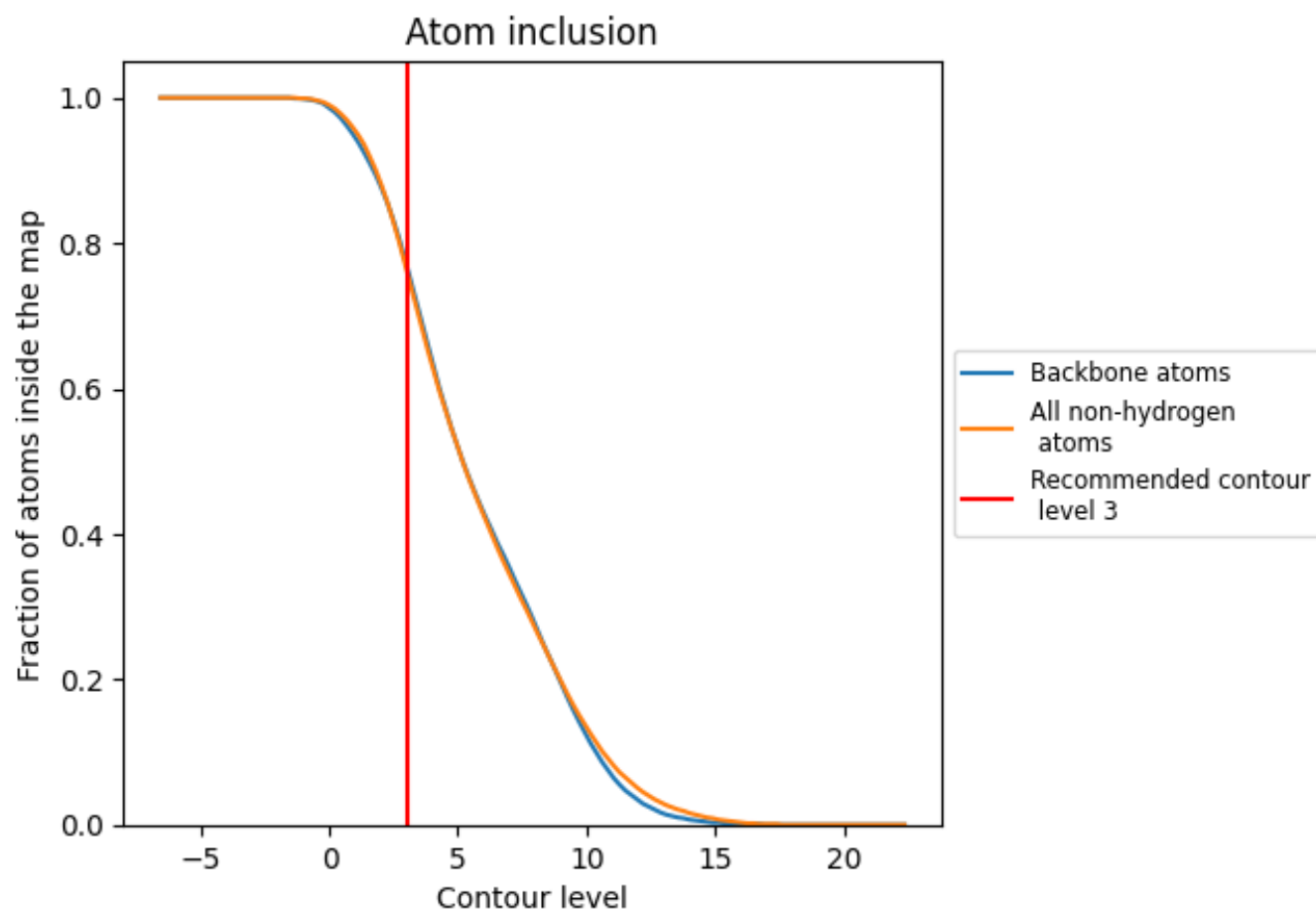
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.3610
0	 0.7650	 0.3440
1	 0.2110	 0.0910
2	 0.0010	 0.0010
3	 0.3310	 0.0280
4	 0.5490	 0.0800
5	 0.3200	 0.0380
6	 0.4880	 0.0730
7	 0.6010	 0.2300
8	 0.5060	 0.1010
9	 0.8760	 0.4570
A	 0.9590	 0.4670
B	 0.9120	 0.5040
C	 0.9280	 0.5060
D	 0.8950	 0.4980
E	 0.9010	 0.5150
F	 0.8240	 0.4430
G	 0.8150	 0.4210
H	 0.8600	 0.4650
I	 0.8920	 0.4920
J	 0.9090	 0.5130
K	 0.8510	 0.4850
L	 0.8710	 0.4990
M	 0.8260	 0.4620
N	 0.8870	 0.4920
O	 0.8780	 0.4770
P	 0.8780	 0.4810
Q	 0.9260	 0.5000
R	 0.9320	 0.4780
S	 0.9140	 0.4380
T	 0.9100	 0.4710
V	 0.8800	 0.4870
Y	 0.9430	 0.5120
Z	 0.8300	 0.4710
a	 0.9010	 0.4730



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Chain	Atom inclusion	Q-score
b	 0.9010	 0.4820
c	 0.8820	 0.4550
d	 0.9380	 0.5060
e	 0.8020	 0.4720
f	 0.8900	 0.4670
h	 0.8670	 0.4520
i	 0.9530	 0.5260
k	 0.8430	 0.3240
m	 0.7320	 0.2900
n	 0.7880	 0.4440
o	 0.5260	 0.2060
q	 0.7930	 0.4620
r	 0.3250	 0.1750
t	 0.0050	 0.0630
u	 0.6040	 0.2230
v	 0.6110	 0.1290
w	 0.9170	 0.2640
x	 0.6870	 0.2840
y	 0.7280	 0.2830