Full wwPDB EM Validation Report

Aug 8, 2026 – 08:21 am BST

PDB ID	:	9SCU / pdb_00009scu
EMDB ID	:	EMD-54774
Title	:	Cryo-EM structure of the Arabidopsis thaliana 60S ribosomal subunit
Authors	:	Karki, S.; Lu, X.; Paatero, A.O.; Ruonala, R.; Tranter, D.; Guryanov, S.; Rehan, S.; Hellmann, E.; Haakonsson, A.; Butcher, S.J.; Huiskonen, J.T.; Kajander, T.; Helariutta, Y.; Paavilainen, V.O.
Deposited on	:	2025-08-12
Resolution	:	2.90 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 (i) 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 (1)) were used in the production of this report:

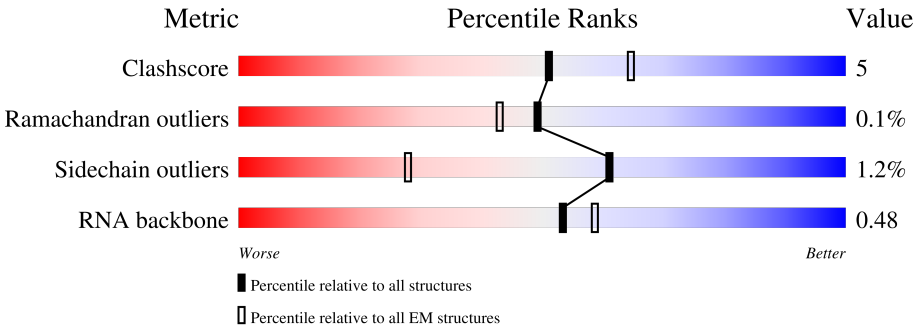
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

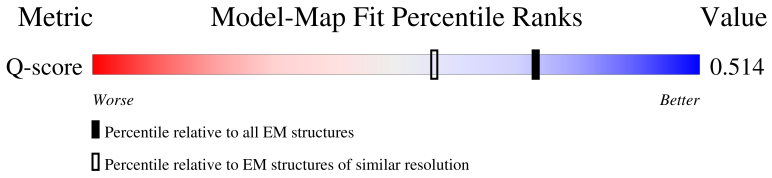
1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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 <=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	5	3381	56% 22% 9% 13%
2	Ck	69	75% 22% ••
3	CA	258	88% 5% •• 5%

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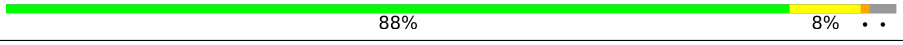
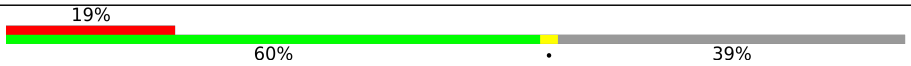
Mol	Chain	Length	Quality of chain
4	CK	105	
5	Cp	92	
6	Cl	51	
7	CY	146	
8	CL	206	
9	6	121	
10	Cm	128	
11	CZ	135	
12	CM	134	
13	7	164	
14	CN	204	
15	Ca	146	
16	w	124	
17	Cb	83	
18	CO	206	
19	CB	389	
20	CP	176	
21	Cc	112	
22	CQ	187	
23	CC	406	
24	CR	209	
25	Cd	119	
26	CS	217	
27	CD	301	
28	CT	164	

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Mol	Chain	Length	Quality of chain
29	Ce	133	
30	CV	140	
31	CE	233	
32	CW	164	
33	Cf	111	
34	CX	154	
35	CF	242	
36	Cg	120	
37	CG	257	
38	Ch	123	
39	CH	194	
40	Ci	112	
41	CI	221	
42	Cj	95	
43	CJ	182	

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 118119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	2953	63284	28258	11506	20567	2953	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein eL38z/eL38y.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Ck	68	561	359	103	97	2	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL2x.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CA	246	1891	1185	384	314	8	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein eL42z/eL42y.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CK	81	649	407	132	108	2	0	0

- Molecule 5 is a protein called (thale cress) hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Cp	89	697	437	134	120	6	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein eL39z/eL39x.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Cl	50	444	282	97	63	2	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CY	130	Total	C	N	O	S	0	0
			1062	656	217	186	3		

- Molecule 8 is a protein called Large ribosomal subunit protein eL13z.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CL	198	Total	C	N	O	S	0	0
			1607	1017	320	266	4		

- Molecule 9 is a RNA chain called RNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	6	119	Total	C	N	O	P	0	0
			2533	1132	454	829	118		

- Molecule 10 is a protein called Ubiquitin-ribosomal protein eL40z fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Cm	52	Total	C	N	O	S	0	0
			431	269	89	66	7		

- Molecule 11 is a protein called Large ribosomal subunit protein eL27x.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CZ	134	Total	C	N	O	S	0	0
			1092	706	200	183	3		

- Molecule 12 is a protein called Large ribosomal subunit protein eL14z.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CM	131	Total	C	N	O	S	0	0
			1071	685	199	183	4		

- Molecule 13 is a RNA chain called RNA (151-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	7	151	Total	C	N	O	P	0	0
			3218	1438	579	1051	150		

- Molecule 14 is a protein called Large ribosomal subunit protein eL15y.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CN	203	Total	C	N	O	S	0	0
			1705	1065	358	279	3		

- Molecule 15 is a protein called Large ribosomal subunit protein uL15x.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ca	145	Total	C	N	O	S	0	0
			1155	744	225	183	3		

- Molecule 16 is a protein called Large ribosomal subunit protein eL22z.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	w	76	Total	C	N	O	0	0
			475	306	79	90		

- Molecule 17 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Cb	49	Total	C	N	O	S	0	0
			346	208	73	64	1		

- Molecule 18 is a protein called Large ribosomal subunit protein uL13w.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CO	204	Total	C	N	O	S	0	0
			1640	1043	316	271	10		

- Molecule 19 is a protein called Large ribosomal subunit protein uL3z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CB	386	Total	C	N	O	S	0	0
			3110	1980	581	532	17		

- Molecule 20 is a protein called Large ribosomal subunit protein uL22z.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CP	156	Total	C	N	O	S	0	0
			1253	779	248	222	4		

- Molecule 21 is a protein called Large ribosomal subunit protein eL30x.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Cc	89	Total	C	N	O	S	0	0
			683	432	121	125	5		

- Molecule 22 is a protein called Large ribosomal subunit protein eL18y.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CQ	186	Total	C	N	O	S	0	0
			1465	931	282	248	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL4z.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CC	397	Total	C	N	O	S	0	0
			3087	1950	578	545	14		

- Molecule 24 is a protein called Large ribosomal subunit protein eL19z.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CR	169	Total	C	N	O	S	0	0
			1397	872	288	227	10		

- Molecule 25 is a protein called Large ribosomal subunit protein eL31x.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Cd	113	Total	C	N	O	S	0	0
			920	578	177	163	2		

- Molecule 26 is a protein called Ribosomal protein L18ae/LX family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CS	177	Total	C	N	O	S	0	0
			1493	965	275	245	8		

- Molecule 27 is a protein called Large ribosomal subunit protein uL18z.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CD	256	Total	C	N	O	S	0	0
			2078	1320	388	366	4		

- Molecule 28 is a protein called Large ribosomal subunit protein eL21x/eL21w.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CT	159	Total	C	N	O	S	0	0
			1281	810	251	216	4		

- Molecule 29 is a protein called Large ribosomal subunit protein eL32z.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ce	126	Total	C	N	O	S	0	0
			1028	649	204	171	4		

- Molecule 30 is a protein called Large ribosomal subunit protein uL14x/uL14z/uL14y.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CV	129	Total	C	N	O	S	0	0
			976	619	181	168	8		

- Molecule 31 is a protein called Large ribosomal subunit protein eL6x.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CE	180	Total	C	N	O	S	0	0
			1413	914	259	238	2		

- Molecule 32 is a protein called Large ribosomal subunit protein eL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CW	63	Total	C	N	O	S	0	0
			534	345	101	84	4		

- Molecule 33 is a protein called Large ribosomal subunit protein eL33z.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Cf	108	Total	C	N	O	S	0	0
			881	556	170	152	3		

- Molecule 34 is a protein called Large ribosomal subunit protein uL23y.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	CX	117	Total	C	N	O	S	0	0
			955	615	169	169	2		

- Molecule 35 is a protein called Large ribosomal subunit protein uL30y.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	CF	234	Total	C	N	O	S	0	0
			1928	1237	353	334	4		

- Molecule 36 is a protein called Large ribosomal subunit protein eL34z.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Cg	109	Total	C	N	O	S	0	0
			882	551	184	146	1		

- Molecule 37 is a protein called Large ribosomal subunit protein eL8z.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	CG	231	Total	C	N	O	S	0	0
			1854	1194	335	319	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL29x.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ch	121	Total	C	N	O	S	0	0
			983	622	192	168	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL6z/uL6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	CH	192	Total	C	N	O	S	0	0
			1528	971	272	279	6		

- Molecule 40 is a protein called Large ribosomal subunit protein eL36y.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ci	94	Total	C	N	O	S	0	0
			763	477	162	122	2		

- Molecule 41 is a protein called Large ribosomal subunit protein uL16y.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	CI	202	Total	C	N	O	S	0	0
			1627	1033	322	261	11		

- Molecule 42 is a protein called Large ribosomal subunit protein eL37z.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Cj	88	Total	C	N	O	S	0	0
			714	435	159	114	6		

- Molecule 43 is a protein called Large ribosomal subunit protein uL5z.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	CJ	170	Total	C	N	O	S	0	0
			1374	869	255	243	7		

- Molecule 44 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
44	5	18	Total	K	0
			18	18	

- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	5	32	Total	Mg	0
			32	32	

- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
46	Cp	1	Total	Zn	0
			1	1	

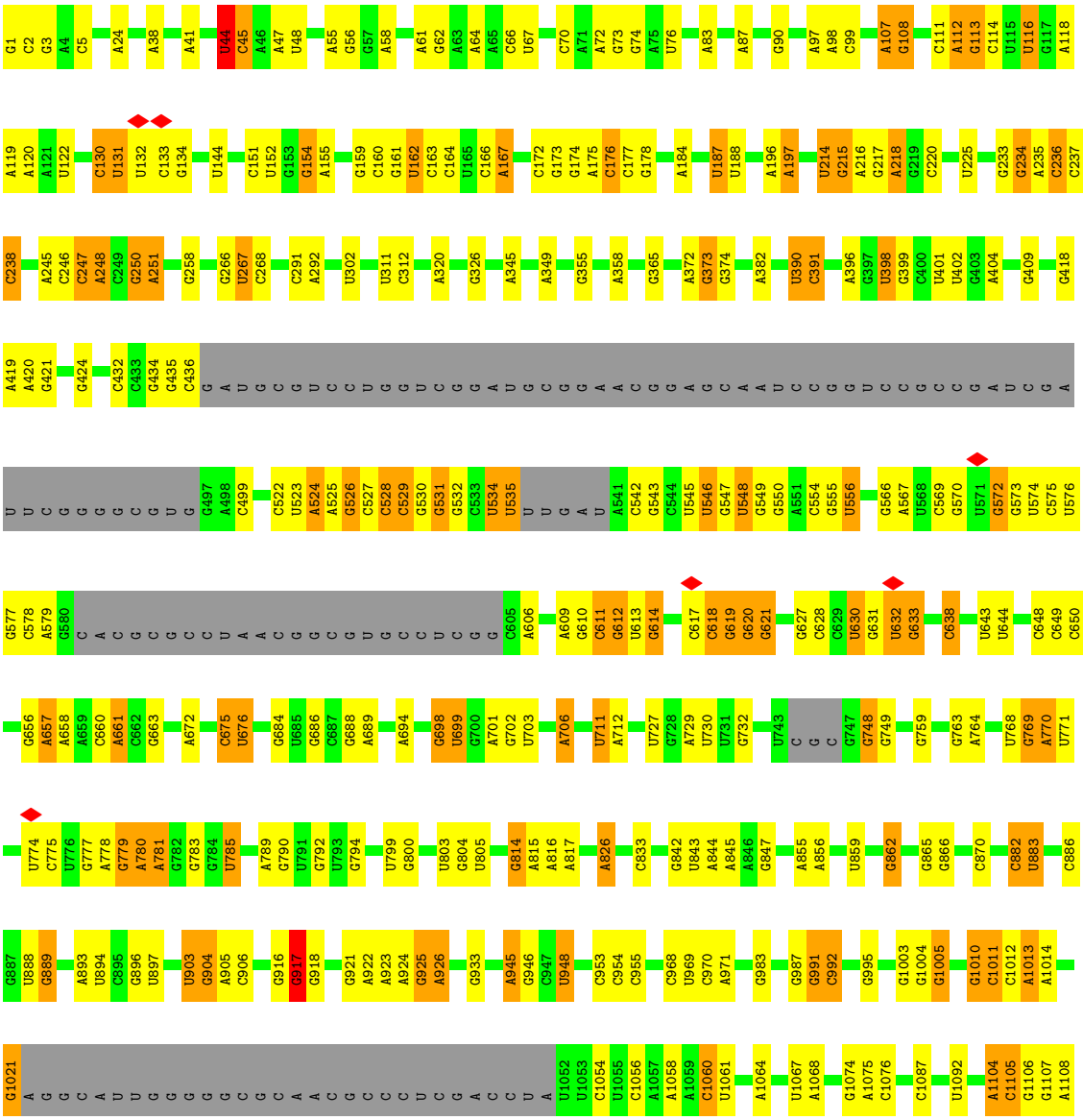
3 Residue-property plots (i)

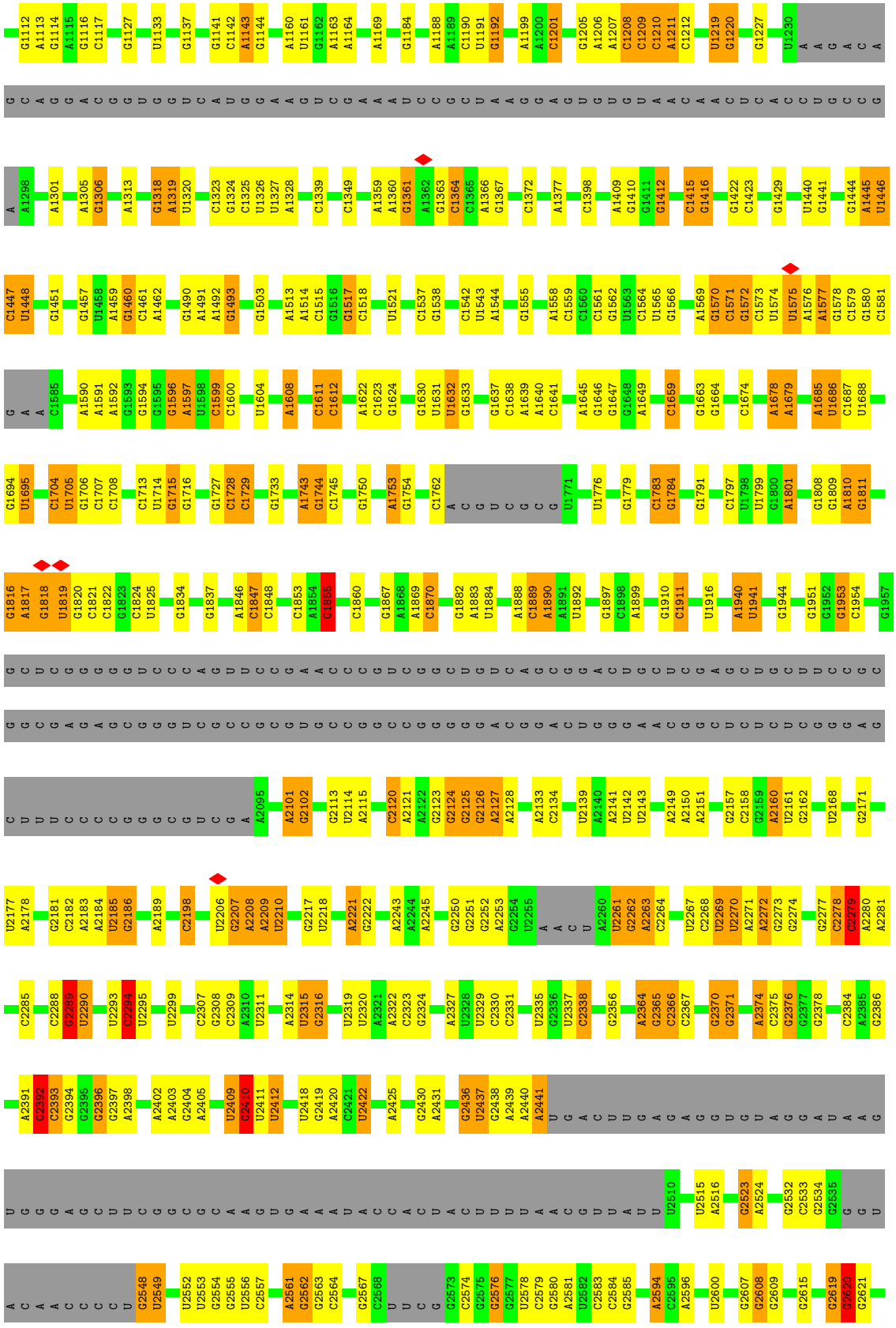
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

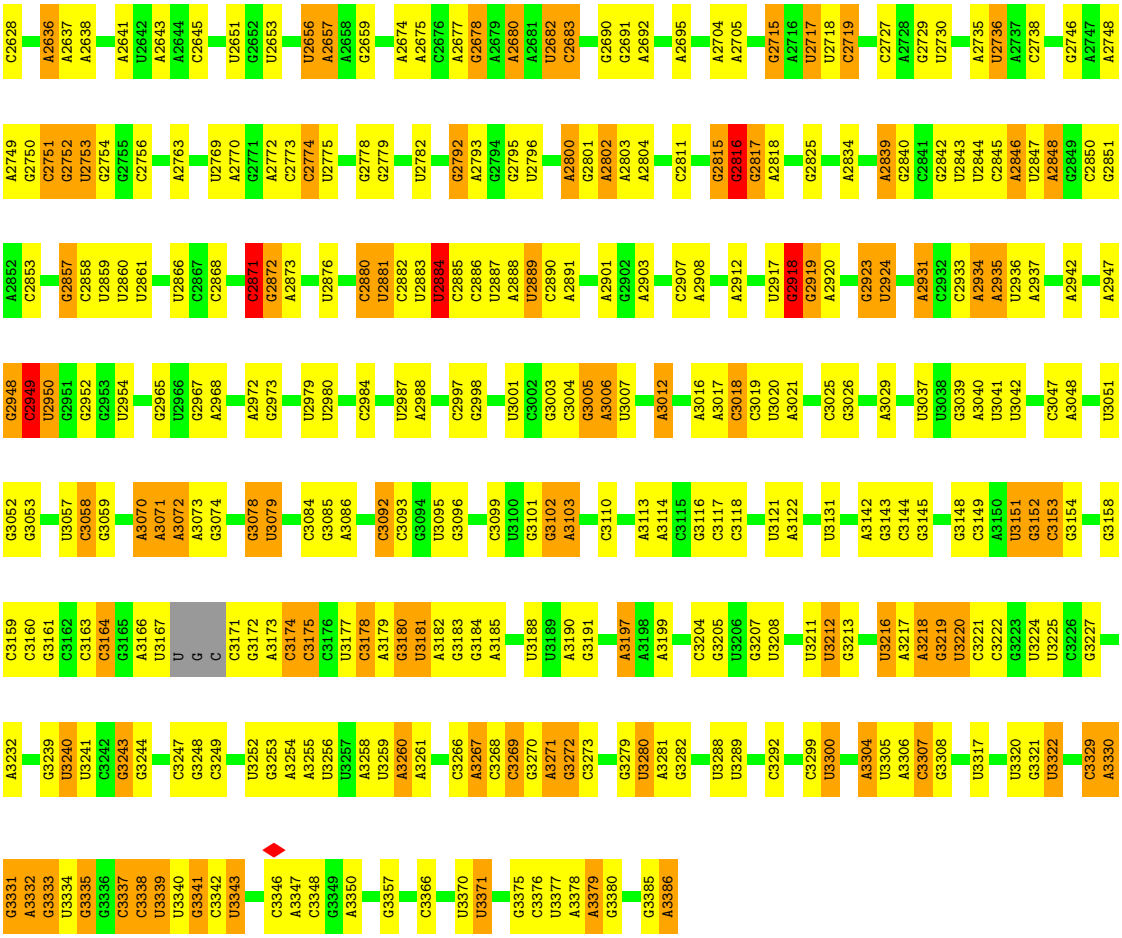
- Molecule 1: 25S RNA

Chain 5:





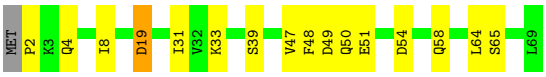




• Molecule 2: Large ribosomal subunit protein eL38z/eL38y

Chain Ck:





• Molecule 3: Large ribosomal subunit protein uL2x

Chain CA:

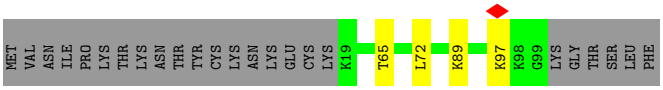




• Molecule 4: Large ribosomal subunit protein eL42z/eL42y

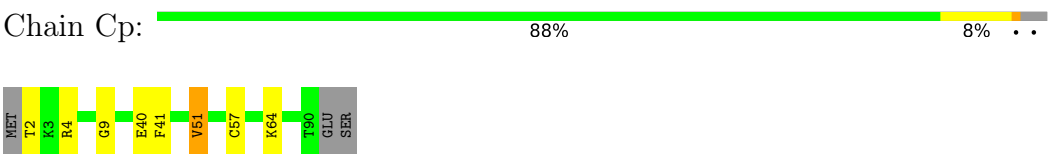
Chain CK:





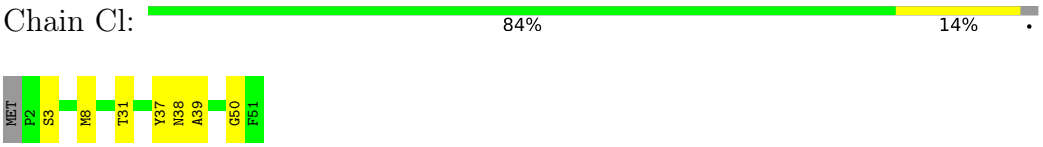
• Molecule 5: (thale cress) hypothetical protein

Chain Cp:



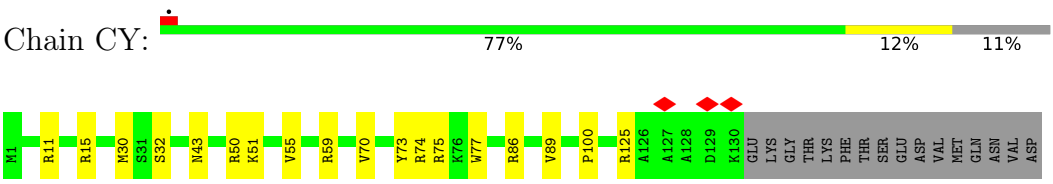
• Molecule 6: Large ribosomal subunit protein eL39z/eL39x

Chain Cl:



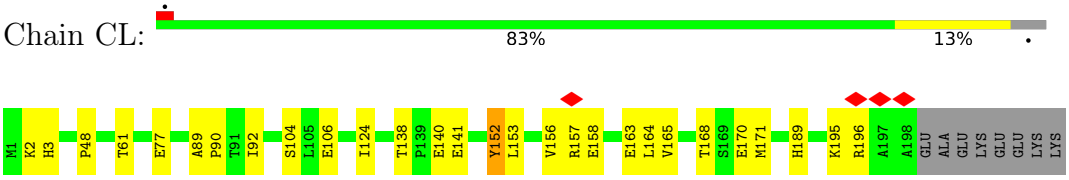
• Molecule 7: Large ribosomal subunit protein uL24z

Chain CY:



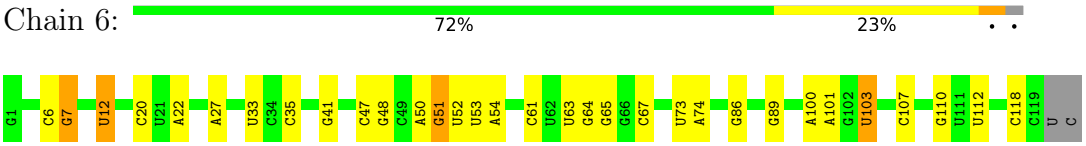
• Molecule 8: Large ribosomal subunit protein eL13z

Chain CL:



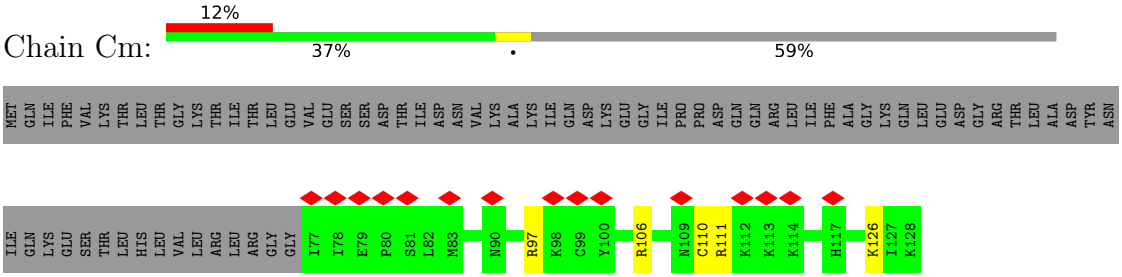
• Molecule 9: RNA (119-MER)

Chain 6:



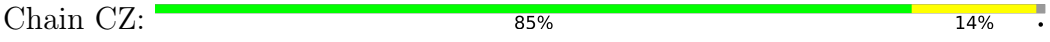
• Molecule 10: Ubiquitin-ribosomal protein eL40z fusion protein

Chain Cm:



• Molecule 11: Large ribosomal subunit protein eL27x

Chain CZ:

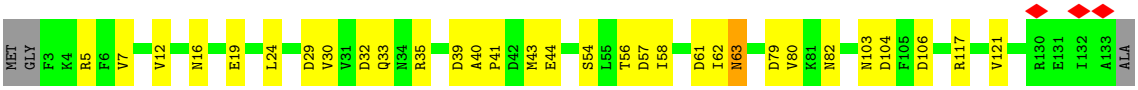




• Molecule 12: Large ribosomal subunit protein eL14z

Chain CM:

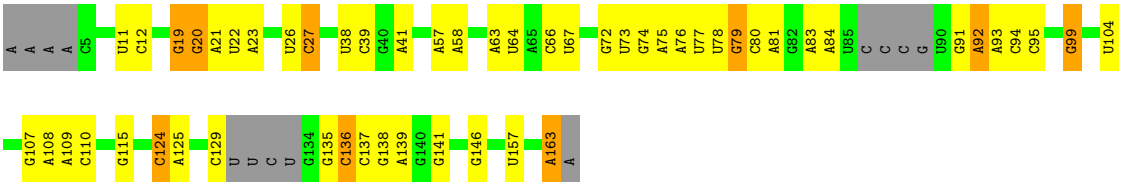




• Molecule 13: RNA (151-MER)

Chain 7:

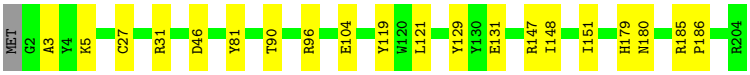




• Molecule 14: Large ribosomal subunit protein eL15y

Chain CN:

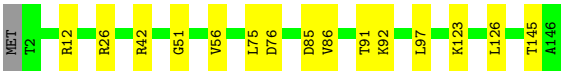




• Molecule 15: Large ribosomal subunit protein uL15x

Chain Ca:

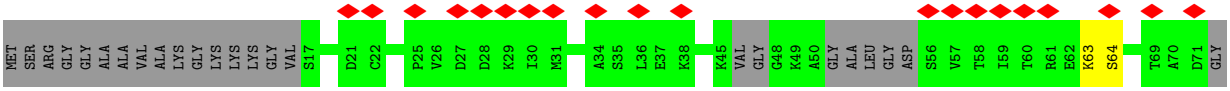


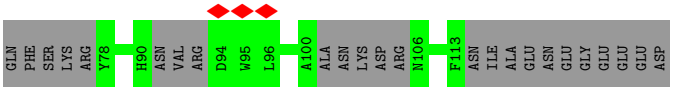


• Molecule 16: Large ribosomal subunit protein eL22z

Chain w:







• Molecule 17: 60S ribosomal protein L29

Chain Cb:



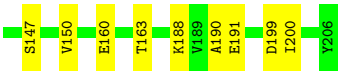


• Molecule 18: Large ribosomal subunit protein uL13w

Chain CO:



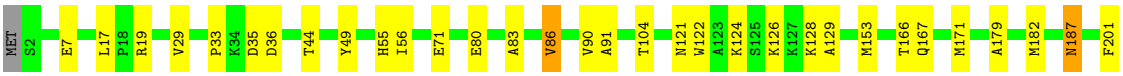




• Molecule 19: Large ribosomal subunit protein uL3z

Chain CB:



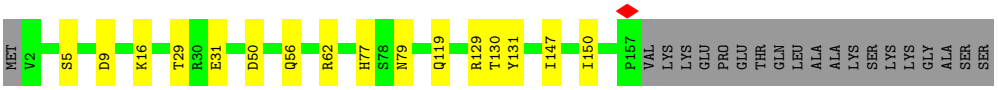




• Molecule 20: Large ribosomal subunit protein uL22z

Chain CP:





• Molecule 21: Large ribosomal subunit protein eL30x

Chain Cc:





• Molecule 22: Large ribosomal subunit protein eL18y

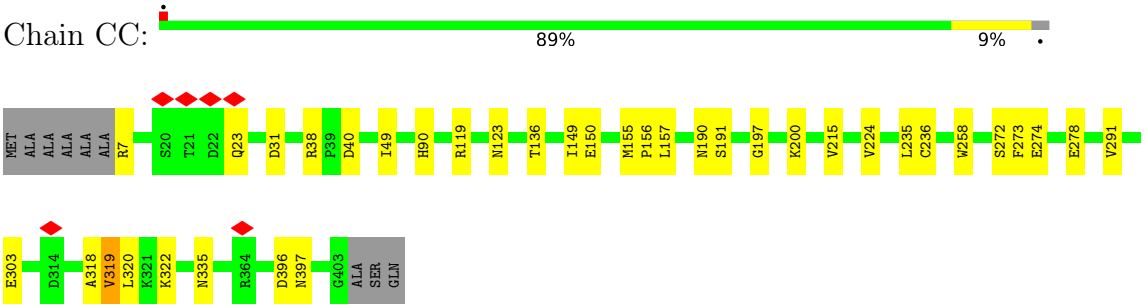
Chain CQ:





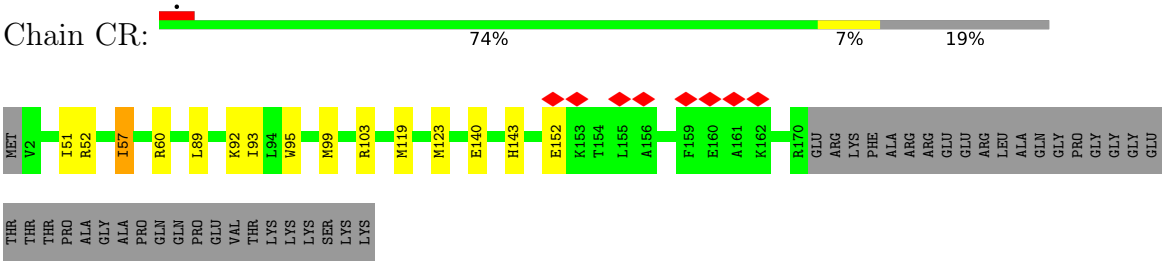
• Molecule 23: Large ribosomal subunit protein uL4z

Chain CC:



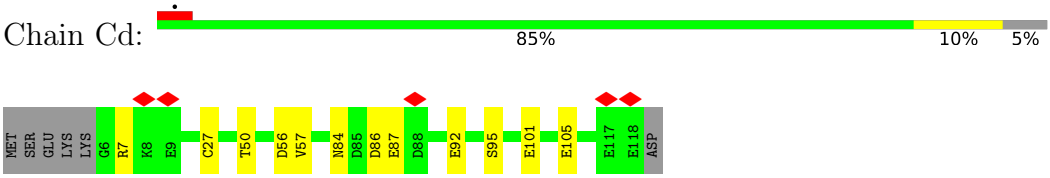
• Molecule 24: Large ribosomal subunit protein eL19z

Chain CR:



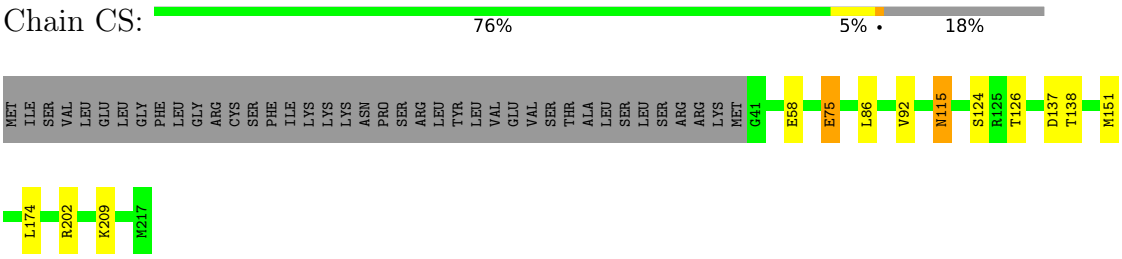
• Molecule 25: Large ribosomal subunit protein eL31x

Chain Cd:



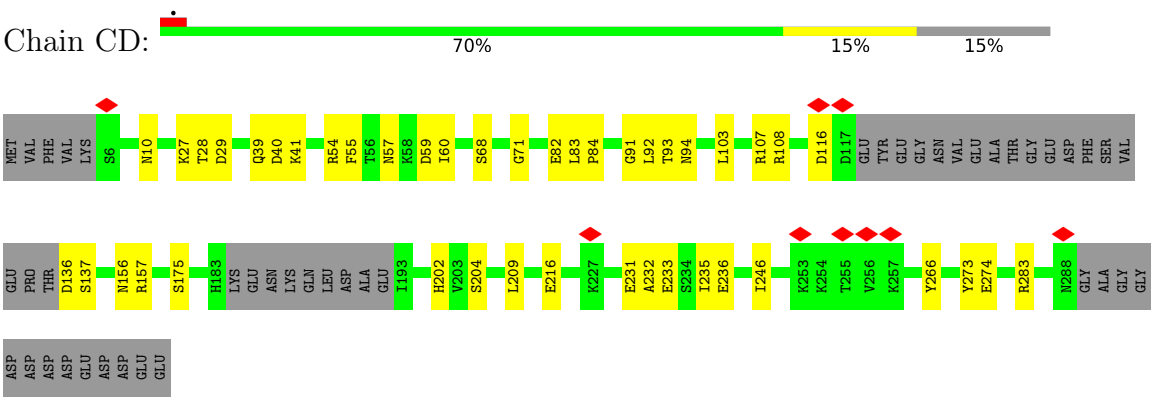
• Molecule 26: Ribosomal protein L18ae/LX family protein

Chain CS:



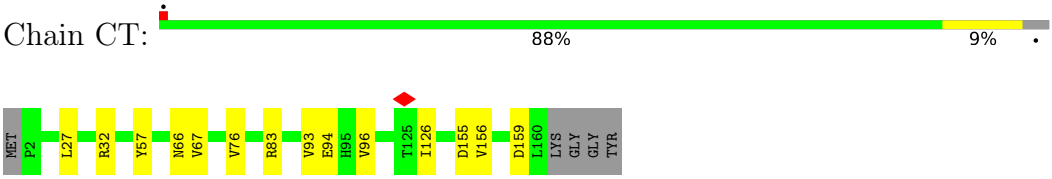
• Molecule 27: Large ribosomal subunit protein uL18z

Chain CD:



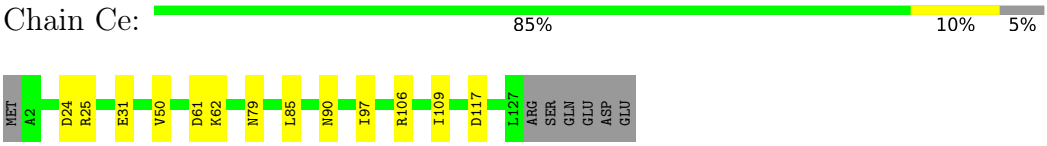
• Molecule 28: Large ribosomal subunit protein eL21x/eL21w

Chain CT:



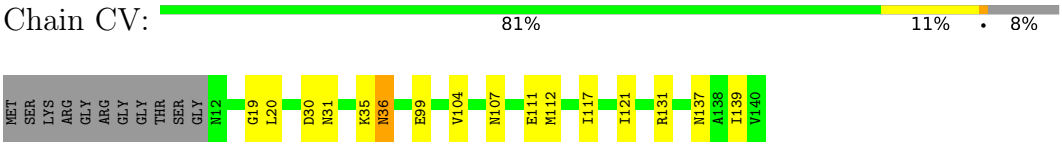
• Molecule 29: Large ribosomal subunit protein eL32z

Chain Ce:



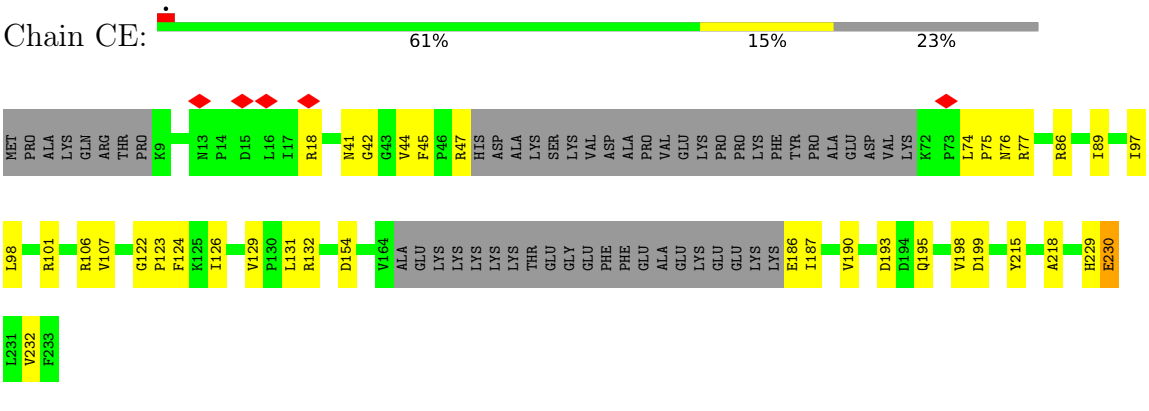
• Molecule 30: Large ribosomal subunit protein uL14x/uL14z/uL14y

Chain CV:



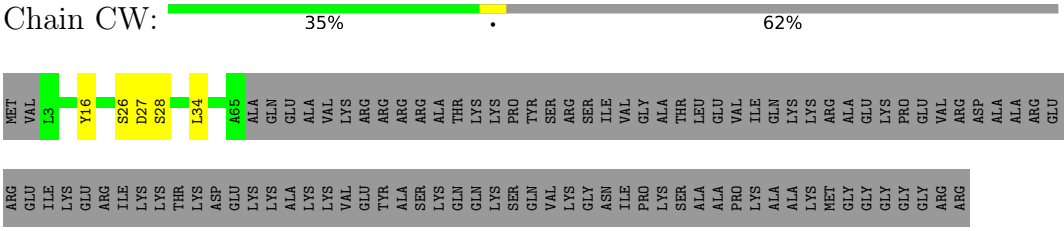
• Molecule 31: Large ribosomal subunit protein eL6x

Chain CE:



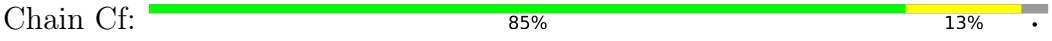
• Molecule 32: Large ribosomal subunit protein eL24z

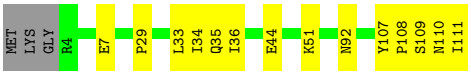
Chain CW:



• Molecule 33: Large ribosomal subunit protein eL33z

Chain Cf:





• Molecule 34: Large ribosomal subunit protein uL23y

Chain CX:

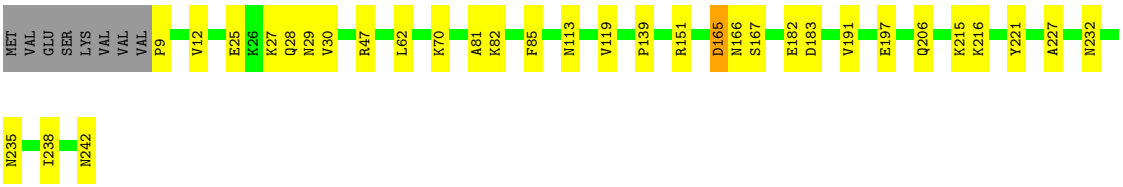




• Molecule 35: Large ribosomal subunit protein uL30y

Chain CF:





• Molecule 36: Large ribosomal subunit protein eL34z

Chain Cg:

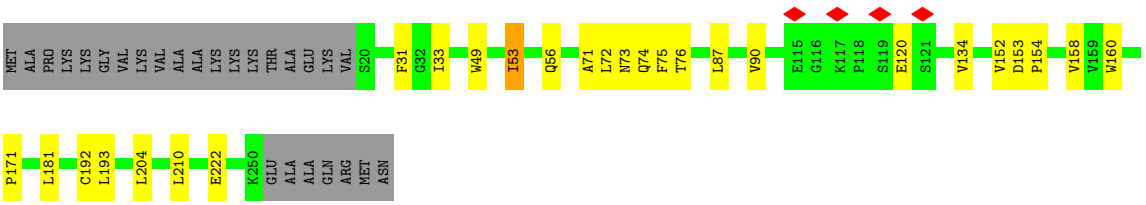




• Molecule 37: Large ribosomal subunit protein eL8z

Chain CG:

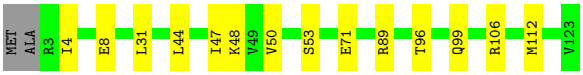




• Molecule 38: Large ribosomal subunit protein uL29x

Chain Ch:

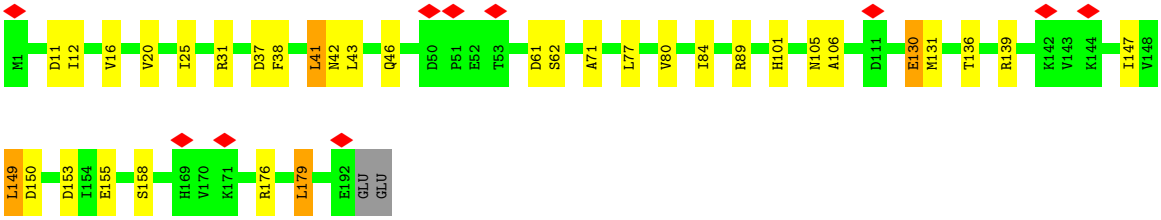




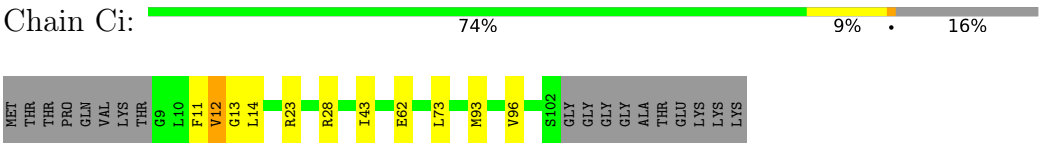
• Molecule 39: Large ribosomal subunit protein uL6z/uL6y

Chain CH:

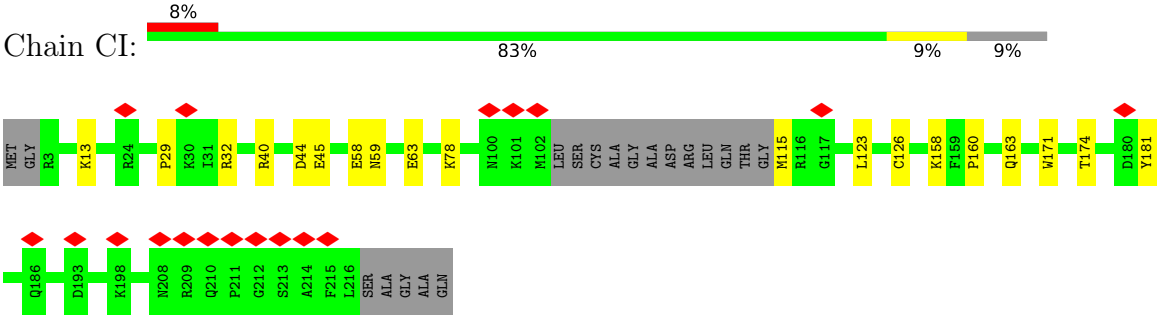




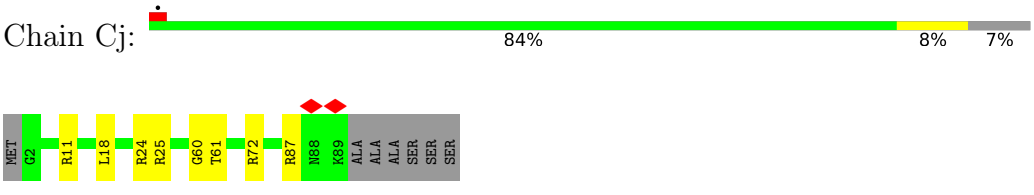
• Molecule 40: Large ribosomal subunit protein eL36y



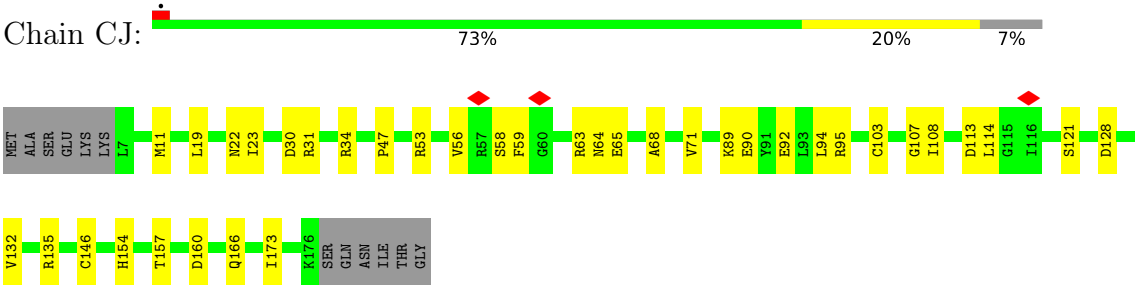
• Molecule 41: Large ribosomal subunit protein uL16y



• Molecule 42: Large ribosomal subunit protein eL37z



• Molecule 43: Large ribosomal subunit protein uL5z



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115070	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	24.512	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.481	Depositor
Minimum map value	-0.189	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, OMG, MG, 5MC, UR3, ZN, OMU, OMC, 1MA, K

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	5	0.22	0/69543	0.28	0/108431
2	Ck	0.13	0/569	0.25	0/758
3	CA	0.33	1/1936 (0.1%)	0.86	11/2601 (0.4%)
4	CK	0.16	0/661	0.27	0/874
5	Cp	0.40	0/706	0.74	1/936 (0.1%)
6	Cl	0.17	0/456	0.24	0/603
7	CY	0.18	0/1074	0.27	0/1433
8	CL	0.18	0/1639	0.31	0/2197
9	6	0.18	0/2831	0.24	0/4411
10	Cm	0.08	0/437	0.23	0/575
11	CZ	0.16	0/1110	0.25	0/1477
12	CM	0.15	0/1082	0.27	0/1446
13	7	0.21	0/3596	0.26	0/5599
14	CN	0.22	0/1743	0.29	0/2335
15	Ca	0.20	0/1186	0.27	0/1584
16	w	0.08	0/476	0.22	0/651
17	Cb	0.17	0/355	0.29	0/485
18	CO	0.18	0/1669	0.31	0/2232
19	CB	0.18	0/3177	0.29	0/4256
20	CP	0.20	0/1277	0.28	0/1717
21	Cc	0.18	0/693	0.34	0/930
22	CQ	0.20	0/1489	0.33	0/1989
23	CC	0.18	0/3144	0.27	0/4232
24	CR	0.16	0/1416	0.26	0/1869
25	Cd	0.18	0/932	0.28	0/1242
26	CS	0.18	0/1531	0.29	0/2054
27	CD	0.15	0/2117	0.27	0/2840
28	CT	0.18	0/1308	0.26	0/1756
29	Ce	0.17	0/1045	0.25	0/1399
30	CV	0.17	0/992	0.26	0/1334
31	CE	0.12	0/1438	0.26	0/1929
32	CW	0.14	0/547	0.27	0/726

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Cf	0.18	0/901	0.27	0/1209
34	CX	0.17	0/972	0.26	0/1309
35	CF	0.19	0/1962	0.30	0/2621
36	Cg	0.18	0/895	0.28	0/1196
37	CG	0.17	0/1888	0.31	0/2532
38	Ch	0.17	0/992	0.30	0/1316
39	CH	0.13	0/1549	0.29	0/2072
40	Ci	0.15	0/770	0.29	0/1016
41	CI	0.11	0/1665	0.24	0/2228
42	Cj	0.20	0/727	0.28	0/965
43	CJ	0.13	0/1396	0.26	0/1869
All	All	0.21	1/125892 (0.0%)	0.30	12/185234 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	CA	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CA	195	CYS	C-N	9.74	1.53	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CA	196	TRP	O-C-N	-28.23	88.86	121.32
3	CA	196	TRP	N-CA-C	11.88	136.06	109.81
3	CA	197	PRO	N-CA-C	-11.24	89.32	112.47
3	CA	196	TRP	CA-C-N	-10.82	106.31	119.84
3	CA	196	TRP	C-N-CA	-10.82	106.31	119.84
3	CA	197	PRO	CB-CA-C	9.59	127.38	111.56
3	CA	195	CYS	CA-C-N	-7.64	103.15	121.80
3	CA	195	CYS	C-N-CA	-7.64	103.15	121.80
3	CA	197	PRO	CA-N-CD	-7.42	101.61	112.00
3	CA	196	TRP	C-N-CD	6.60	152.04	125.00
3	CA	196	TRP	CB-CA-C	-5.22	99.88	110.17
5	Cp	41	PHE	CA-CB-CG	5.18	118.98	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	CA	195	CYS	Mainchain
3	CA	196	TRP	Mainchain

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	5	63284	0	31955	631	0
2	Ck	561	0	606	12	0
3	CA	1891	0	1937	24	0
4	CK	649	0	676	3	0
5	Cp	697	0	737	4	0
6	Cl	444	0	477	5	0
7	CY	1062	0	1142	16	0
8	CL	1607	0	1719	21	0
9	6	2533	0	1286	12	0
10	Cm	431	0	476	5	0
11	CZ	1092	0	1182	13	0
12	CM	1071	0	1160	23	0
13	7	3218	0	1633	30	0
14	CN	1705	0	1765	15	0
15	Ca	1155	0	1207	12	0
16	w	475	0	363	1	0
17	Cb	346	0	281	3	0
18	CO	1640	0	1761	31	0
19	CB	3110	0	3221	30	0
20	CP	1253	0	1271	10	0
21	Cc	683	0	714	13	0
22	CQ	1465	0	1579	18	0
23	CC	3087	0	3239	28	0
24	CR	1397	0	1512	9	0
25	Cd	920	0	975	10	0
26	CS	1493	0	1555	9	0
27	CD	2078	0	2136	29	0
28	CT	1281	0	1335	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Ce	1028	0	1105	8	0
30	CV	976	0	1040	11	0
31	CE	1413	0	1524	32	0
32	CW	534	0	557	5	0
33	Cf	881	0	903	10	0
34	CX	955	0	1035	7	0
35	CF	1928	0	2028	20	0
36	Cg	882	0	957	11	0
37	CG	1854	0	1999	20	0
38	Ch	983	0	1109	11	0
39	CH	1528	0	1613	23	0
40	Ci	763	0	859	8	0
41	CI	1627	0	1684	16	0
42	Cj	714	0	743	7	0
43	CJ	1374	0	1418	25	0
44	5	18	0	0	0	0
45	5	32	0	0	0	0
46	Cp	1	0	0	0	0
All	All	118119	0	86474	1083	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 (1083) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CA:197:PRO:HD2	3:CA:198:LYS:H	1.00	1.12
1:5:2150:A:OP1	3:CA:197:PRO:O	1.72	1.05
3:CA:196:TRP:O	3:CA:197:PRO:C	1.82	1.00
1:5:3180:G:O2'	1:5:3181:U:O5'	1.78	1.00
3:CA:197:PRO:CD	3:CA:198:LYS:H	1.68	0.99
1:5:3341:G:O2'	1:5:3343:U:OP2	1.81	0.99
3:CA:197:PRO:HD2	3:CA:198:LYS:N	1.77	0.98
1:5:1727:G:O2'	1:5:1728:C:O5'	1.82	0.96
1:5:1415:C:O2'	1:5:1416:G:O5'	1.84	0.94
1:5:2871:5MC:O2'	1:5:2872:G:OP2	1.86	0.93
1:5:2208:A:O2'	1:5:2210:U:O2	1.86	0.92
1:5:768:U:O2	1:5:781:A:N6	2.02	0.91
1:5:948:U:OP2	15:Ca:26:ARG:NH2	2.04	0.91
1:5:2752:G:O2'	1:5:2753:U:OP1	1.88	0.90
1:5:197:A:OP1	7:CY:59:ARG:NH2	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1137:G:N7	41:CI:13:LYS:NZ	2.20	0.88
39:CH:31:ARG:NH1	39:CH:89:ARG:O	2.08	0.87
1:5:2901:A:OP1	1:5:2903:A:N6	2.08	0.87
13:7:124:C:O2	13:7:139:A:N6	2.08	0.87
1:5:2555:G:O2'	11:CZ:135:PHE:OXT	1.91	0.86
1:5:3181:U:O2'	1:5:3182:A:O4'	1.94	0.86
1:5:3188:U:O2'	1:5:3191:G:O6	1.93	0.86
1:5:3376:C:OP1	25:Cd:7:ARG:NH1	2.07	0.86
1:5:2795:G:O2'	1:5:2796:U:OP2	1.94	0.86
1:5:1199:A:N1	1:5:1326:U:O2'	2.09	0.85
1:5:1727:G:O2'	1:5:1728:C:O4'	1.94	0.85
1:5:528:C:O4'	1:5:550:G:N2	2.10	0.85
1:5:3331:G:N2	1:5:3333:G:O2'	2.09	0.85
1:5:3339:U:O2'	1:5:3341:G:N7	2.11	0.84
1:5:152:U:OP2	38:Ch:106:ARG:NH2	2.10	0.83
1:5:1571:C:O2'	1:5:1572:G:OP1	1.95	0.83
1:5:2608:G:OP1	3:CA:233:LYS:NZ	2.12	0.83
11:CZ:93:GLU:OE1	11:CZ:93:GLU:N	2.12	0.83
18:CO:79:ARG:O	18:CO:147:SER:OG	1.96	0.83
1:5:132:U:O2'	1:5:134:G:O6	1.96	0.83
1:5:418:G:N2	1:5:2384:C:O2	2.11	0.83
1:5:1659:C:O2'	1:5:1801:A:OP2	1.94	0.82
22:CQ:109:ARG:NH1	22:CQ:119:CYS:SG	2.53	0.81
26:CS:75:GLU:N	26:CS:75:GLU:OE1	2.14	0.81
9:6:63:U:OP2	27:CD:283:ARG:NH2	2.14	0.81
7:CY:50:ARG:NH1	13:7:75:A:OP2	2.14	0.80
7:CY:73:TYR:OH	13:7:79:G:OP2	1.97	0.80
1:5:2619:G:O2'	1:5:2866:U:OP1	1.99	0.80
12:CM:44:GLU:N	12:CM:44:GLU:OE1	2.14	0.80
21:Cc:39:ARG:O	21:Cc:40:SER:OG	1.98	0.80
1:5:530:G:N1	1:5:548:U:O4	2.15	0.80
1:5:1707:C:OP2	1:5:1708:C:N4	2.14	0.79
23:CC:150:GLU:N	23:CC:150:GLU:OE1	2.15	0.79
19:CB:71:GLU:N	19:CB:71:GLU:OE1	2.15	0.79
1:5:1716:G:O2'	1:5:1733:G:N2	2.15	0.79
1:5:643:U:OP1	18:CO:98:LYS:NZ	2.13	0.79
1:5:3219:G:O2'	1:5:3220:U:OP1	2.00	0.79
1:5:3114:A:N6	1:5:3118:C:O2	2.16	0.79
43:CJ:53:ARG:O	43:CJ:63:ARG:NH1	2.16	0.79
1:5:775:C:OP1	8:CL:196:ARG:NH1	2.16	0.79
1:5:2934:A:O2'	1:5:2935:A:O5'	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1819:U:O2'	1:5:1820:G:O4'	2.01	0.78
23:CC:274:GLU:N	23:CC:274:GLU:OE1	2.17	0.78
1:5:2186:G:O2'	1:5:2315:U:OP2	2.02	0.78
1:5:3026:G:N2	1:5:3029:A:OP2	2.14	0.78
1:5:3218:A:N6	1:5:3247:C:O2	2.16	0.78
12:CM:39:ASP:OD1	12:CM:40:ALA:N	2.17	0.77
1:5:1637:G:N2	1:5:1640:A:OP2	2.17	0.77
1:5:613:U:O4'	31:CE:47:ARG:NH2	2.18	0.77
9:6:51:G:H21	43:CJ:11:MET:HE1	1.49	0.77
1:5:2271:A:O2'	1:5:2272:A:O5'	2.02	0.76
1:5:2278:C:O2'	1:5:2279:5MC:OP1	2.02	0.76
14:CN:119:TYR:OH	14:CN:131:GLU:OE1	2.01	0.76
1:5:1889:C:O2'	1:5:1890:A:OP1	2.03	0.76
38:Ch:8:GLU:OE1	38:Ch:8:GLU:N	2.19	0.76
1:5:2746:G:N2	1:5:2749:A:OP2	2.19	0.76
1:5:3256:U:OP2	31:CE:101:ARG:NH2	2.18	0.76
8:CL:140:GLU:OE1	8:CL:140:GLU:N	2.18	0.76
1:5:865:G:OP1	24:CR:92:LYS:NZ	2.19	0.76
24:CR:152:GLU:N	24:CR:152:GLU:OE1	2.19	0.76
41:CI:63:GLU:N	41:CI:63:GLU:OE1	2.18	0.76
1:5:2552:U:OP1	36:Cg:104:LYS:NZ	2.19	0.75
1:5:196:A:O2'	1:5:197:A:OP2	2.03	0.75
1:5:1581:C:O3'	1:5:2523:G:N2	2.19	0.75
31:CE:229:HIS:NE2	33:Cf:44:GLU:OE1	2.18	0.75
8:CL:163:GLU:OE1	8:CL:163:GLU:N	2.19	0.75
1:5:2436:G:N2	1:5:2594:A:O2'	2.19	0.74
21:Cc:16:SER:OG	21:Cc:17:ARG:NH1	2.20	0.74
22:CQ:87:ASP:OD1	22:CQ:88:ASP:N	2.20	0.74
43:CJ:157:THR:OG1	43:CJ:160:ASP:OD1	2.04	0.74
12:CM:79:ASP:OD1	12:CM:82:ASN:ND2	2.20	0.74
41:CI:171:TRP:O	41:CI:174:THR:HG22	1.87	0.74
1:5:2567:G:N2	1:5:2576:G:N7	2.36	0.74
43:CJ:92:GLU:N	43:CJ:92:GLU:OE1	2.21	0.74
18:CO:73:HIS:ND1	18:CO:73:HIS:O	2.21	0.74
28:CT:94:GLU:OE1	28:CT:94:GLU:N	2.20	0.74
19:CB:7:GLU:OE1	19:CB:7:GLU:N	2.21	0.73
43:CJ:135:ARG:NH1	43:CJ:154:HIS:O	2.20	0.73
1:5:2842:G:N2	1:5:2847:U:OP1	2.21	0.73
8:CL:106:GLU:N	8:CL:106:GLU:OE1	2.22	0.73
1:5:1210:C:O2'	1:5:1211:A:OP2	2.07	0.73
1:5:2374:A:N3	1:5:2825:G:O2'	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CH:136:THR:OG1	39:CH:150:ASP:OD1	2.05	0.72
1:5:531:G:O2'	1:5:532:G:O4'	2.06	0.72
1:5:1575:U:O2'	1:5:1576:A:O4'	2.06	0.72
1:5:771:U:O4	1:5:779:G:N2	2.21	0.72
3:CA:197:PRO:CD	3:CA:198:LYS:N	2.34	0.72
15:Ca:56:VAL:HG23	22:CQ:176:ALA:HB2	1.70	0.72
12:CM:103:ASN:ND2	12:CM:106:ASP:OD1	2.23	0.72
22:CQ:65:SER:OG	22:CQ:88:ASP:OD2	2.05	0.72
1:5:618:C:OP1	23:CC:322:LYS:NZ	2.22	0.72
27:CD:136:ASP:OD1	27:CD:137:SER:N	2.23	0.72
1:5:3151:U:O2'	1:5:3152:G:OP1	2.07	0.72
1:5:2262:G:O2'	1:5:2263:A:OP2	2.06	0.72
1:5:530:G:O6	1:5:531:G:N2	2.23	0.71
2:Ck:51:GLU:OE1	2:Ck:51:GLU:N	2.22	0.71
1:5:921:G:OP2	3:CA:9:ARG:NH2	2.23	0.71
1:5:1596:G:O2'	1:5:1597:A:O5'	2.08	0.71
25:Cd:101:GLU:N	25:Cd:101:GLU:OE1	2.23	0.71
1:5:1011:C:H2'	1:5:1056:C:H41	1.54	0.71
26:CS:137:ASP:OD1	26:CS:138:THR:N	2.24	0.71
29:Ce:24:ASP:OD1	29:Ce:25:ARG:N	2.23	0.71
2:Ck:4:GLN:N	2:Ck:4:GLN:OE1	2.24	0.71
8:CL:158:GLU:N	8:CL:158:GLU:OE1	2.24	0.71
27:CD:59:ASP:OD1	27:CD:60:ILE:N	2.24	0.71
1:5:826:A:O2'	42:Cj:11:ARG:NH1	2.24	0.71
1:5:2815:G:O2'	1:5:2816:OMG:OP1	2.08	0.70
1:5:3078:G:O2'	1:5:3079:U:OP1	2.08	0.70
7:CY:32:SER:OG	7:CY:100:PRO:O	2.08	0.70
13:7:99:G:OP2	42:Cj:72:ARG:NH1	2.24	0.70
41:CI:45:GLU:N	41:CI:45:GLU:OE1	2.24	0.70
1:5:3180:G:HO2'	1:5:3181:U:P	2.13	0.70
1:5:3332:A:O3'	1:5:3333:G:N2	2.21	0.70
27:CD:236:GLU:N	27:CD:236:GLU:OE1	2.24	0.70
1:5:1490:G:O4'	1:5:1493:G:N2	2.24	0.70
31:CE:86:ARG:NH1	33:Cf:109:SER:OG	2.25	0.70
1:5:1817:A:O2'	1:5:1818:G:OP1	2.08	0.70
1:5:3148:G:O2'	19:CB:129:ALA:O	2.09	0.69
7:CY:43:ASN:OD1	7:CY:125:ARG:NH1	2.25	0.69
1:5:1021:G:OP1	41:CI:40:ARG:NH2	2.26	0.69
1:5:2704:A:N6	27:CD:28:THR:O	2.25	0.69
1:5:1361:G:N7	1:5:1364:C:N4	2.36	0.69
1:5:1695:U:HO2'	1:5:1776:U:HO2'	1.15	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2839:A:N6	1:5:2851:G:O2'	2.22	0.69
12:CM:121:VAL:HG22	18:CO:190:ALA:HB3	1.75	0.69
31:CE:86:ARG:NE	33:Cf:111:ILE:O	2.25	0.69
1:5:358:A:OP1	42:Cj:24:ARG:NH1	2.26	0.69
1:5:1820:G:O2'	1:5:1821:C:O4'	2.01	0.69
34:CX:89:GLU:N	34:CX:89:GLU:OE1	2.26	0.68
1:5:1664:G:N2	1:5:1791:G:H22	1.90	0.68
3:CA:197:PRO:O	3:CA:198:LYS:HB2	1.94	0.68
1:5:62:G:OP1	14:CN:185:ARG:NH1	2.26	0.68
10:Cm:126:LYS:O	39:CH:176:ARG:NH1	2.26	0.68
1:5:1014:A:N1	1:5:1060:C:O2'	2.25	0.68
32:CW:27:ASP:O	32:CW:28:SER:OG	2.09	0.68
1:5:434:G:O2'	1:5:630:U:O4	2.08	0.68
7:CY:11:ARG:NH1	13:7:26:U:OP1	2.27	0.68
3:CA:196:TRP:O	3:CA:196:TRP:CG	2.47	0.68
22:CQ:42:SER:OG	22:CQ:45:ASN:OD1	2.11	0.68
3:CA:5:ILE:HG22	3:CA:208:GLU:O	1.93	0.68
1:5:529:C:H42	1:5:549:G:H21	1.42	0.68
1:5:2261:U:O2'	1:5:2262:G:O5'	2.08	0.68
31:CE:186:GLU:OE1	31:CE:187:ILE:N	2.27	0.67
11:CZ:101:GLN:N	11:CZ:101:GLN:OE1	2.27	0.67
35:CF:232:ASN:O	35:CF:235:ASN:ND2	2.26	0.67
1:5:886:C:HO2'	1:5:889:G:HO2'	1.40	0.67
1:5:1646:G:OP1	1:5:1824:C:O2'	2.12	0.67
22:CQ:143:ASN:O	22:CQ:143:ASN:ND2	2.28	0.67
1:5:686:G:OP1	23:CC:38:ARG:NH1	2.28	0.67
10:Cm:110:CYS:SG	10:Cm:111:ARG:N	2.65	0.67
1:5:151:C:OP2	38:Ch:106:ARG:NH1	2.27	0.67
1:5:236:C:O2'	1:5:238:C:N4	2.26	0.67
39:CH:130:GLU:OE1	39:CH:131:MET:N	2.28	0.67
1:5:166:C:O2'	1:5:248:A:N7	2.25	0.67
30:CV:117:ILE:O	30:CV:137:ASN:ND2	2.26	0.67
1:5:844:A:O2'	1:5:866:G:N2	2.22	0.67
11:CZ:3:LYS:O	11:CZ:6:LYS:NZ	2.27	0.67
1:5:698:G:O2'	1:5:699:U:OP1	2.11	0.66
1:5:1632:U:O2'	1:5:1633:G:O4'	2.12	0.66
1:5:1707:C:OP2	1:5:1743:A:N6	2.28	0.66
3:CA:179:MET:O	3:CA:184:ASN:ND2	2.29	0.66
1:5:610:G:N2	31:CE:42:GLY:O	2.28	0.66
1:5:390:U:O2'	1:5:391:C:OP1	2.13	0.66
1:5:862:G:N7	5:Cp:2:THR:HG23	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ck:50:GLN:N	2:Ck:50:GLN:OE1	2.28	0.66
11:CZ:102:SER:OG	11:CZ:104:ASP:OD1	2.12	0.66
23:CC:197:GLY:O	23:CC:200:LYS:NZ	2.28	0.66
37:CG:222:GLU:OE1	37:CG:222:GLU:N	2.29	0.65
19:CB:209:GLU:N	19:CB:209:GLU:OE1	2.28	0.65
39:CH:46:GLN:N	39:CH:46:GLN:OE1	2.30	0.65
1:5:3110:C:O3'	39:CH:158:SER:OG	2.14	0.65
35:CF:47:ARG:NH2	35:CF:183:ASP:OD2	2.28	0.65
1:5:1750:G:H21	2:Ck:2:PRO:HA	1.62	0.65
1:5:2186:G:OP1	3:CA:211:HIS:ND1	2.28	0.64
1:5:2561:A:O2'	1:5:2562:G:O5'	2.15	0.64
25:Cd:50:THR:HG1	25:Cd:95:SER:HG	1.42	0.64
41:CI:29:PRO:O	41:CI:32:ARG:NH1	2.29	0.64
41:CI:44:ASP:OD1	41:CI:181:TYR:OH	2.11	0.64
1:5:1184:G:N2	18:CO:92:MET:SD	2.70	0.64
1:5:3334:U:N3	1:5:3335:G:O6	2.30	0.64
35:CF:151:ARG:NE	35:CF:242:ASN:O	2.30	0.64
36:Cg:110:GLN:OE1	36:Cg:110:GLN:N	2.31	0.64
1:5:163:C:O2	1:5:164:C:N4	2.30	0.64
27:CD:107:ARG:NH2	27:CD:116:ASP:OD1	2.31	0.64
1:5:3212:U:O2'	1:5:3213:G:O4'	2.10	0.64
1:5:1630:G:H21	1:5:1816:G:H21	1.46	0.64
13:7:41:A:OP2	38:Ch:89:ARG:NH1	2.30	0.64
1:5:3144:C:N3	1:5:3145:G:N2	2.46	0.64
26:CS:58:GLU:N	26:CS:58:GLU:OE1	2.29	0.63
12:CM:29:ASP:OD1	12:CM:30:VAL:N	2.31	0.63
31:CE:106:ARG:NH1	31:CE:218:ALA:O	2.30	0.63
1:5:3304:A:OP1	1:5:3377:U:O2'	2.12	0.63
13:7:125:A:N6	13:7:138:G:O2'	2.32	0.63
1:5:3102:G:O2'	1:5:3103:A:OP1	2.18	0.62
1:5:2178:A:C6	3:CA:125:VAL:HG13	2.34	0.62
23:CC:303:GLU:N	23:CC:303:GLU:OE1	2.29	0.62
22:CQ:146:GLU:OE2	22:CQ:163:LYS:NZ	2.32	0.62
41:CI:58:GLU:N	41:CI:58:GLU:OE1	2.32	0.62
1:5:161:G:O2'	1:5:162:U:O5'	2.17	0.62
9:6:12:U:OP2	9:6:67:C:O2'	2.17	0.62
33:Cf:110:ASN:ND2	33:Cf:110:ASN:O	2.32	0.62
23:CC:396:ASP:OD1	23:CC:397:ASN:N	2.33	0.62
25:Cd:92:GLU:OE1	25:Cd:92:GLU:N	2.32	0.62
27:CD:39:GLN:OE1	27:CD:40:ASP:N	2.33	0.62
1:5:886:C:O2'	1:5:889:G:O2'	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1664:G:H22	1:5:1791:G:H22	1.47	0.61
39:CH:41:LEU:HD12	39:CH:43:LEU:HD23	1.82	0.61
39:CH:105:ASN:OD1	39:CH:106:ALA:N	2.33	0.61
1:5:247:C:O2	1:5:248:A:N6	2.33	0.61
1:5:1576:A:O2'	1:5:1577:A:OP2	2.15	0.61
1:5:2270:U:N3	1:5:2272:A:OP2	2.33	0.61
1:5:2609:G:OP1	3:CA:2:GLY:N	2.33	0.61
1:5:1441:G:OP2	15:Ca:12:ARG:NH1	2.32	0.61
1:5:3117:C:O2	10:Cm:106:ARG:NH1	2.34	0.61
1:5:3254:A:OP1	1:5:3255:A:N6	2.34	0.61
8:CL:170:GLU:N	8:CL:170:GLU:OE1	2.33	0.61
1:5:3332:A:O2'	1:5:3333:G:OP1	2.12	0.61
21:Cc:61:GLU:OE2	21:Cc:73:ARG:NH2	2.34	0.61
20:CP:129:ARG:NH1	20:CP:131:TYR:OH	2.34	0.61
39:CH:42:ASN:C	39:CH:43:LEU:HD22	2.25	0.61
1:5:218:A:O2'	1:5:220:C:OP2	2.16	0.61
1:5:3224:U:O2	1:5:3225:U:N3	2.34	0.61
1:5:706:A:H5'	23:CC:49:ILE:HD11	1.83	0.61
1:5:992:C:H1'	1:5:1112:G:H22	1.66	0.61
27:CD:82:GLU:OE1	27:CD:108:ARG:NH2	2.34	0.61
19:CB:379:GLU:OE2	32:CW:16:TYR:OH	2.19	0.60
23:CC:278:GLU:N	23:CC:278:GLU:OE1	2.33	0.60
24:CR:89:LEU:HD11	24:CR:93:ILE:HD11	1.81	0.60
27:CD:55:PHE:CE2	27:CD:60:ILE:HD12	2.36	0.60
1:5:2409:U:O2'	1:5:2410:OMG:OP1	2.15	0.60
1:5:3260:A:OP2	31:CE:132:ARG:NH2	2.35	0.60
21:Cc:23:LYS:O	21:Cc:24:SER:OG	2.17	0.60
1:5:374:G:H4'	7:CY:89:VAL:HG11	1.83	0.60
1:5:3012:A:OP2	1:5:3099:C:N4	2.21	0.60
8:CL:77:GLU:OE2	40:Ci:23:ARG:NH2	2.32	0.60
27:CD:231:GLU:OE1	27:CD:233:GLU:N	2.31	0.59
1:5:214:U:O2'	1:5:215:G:OP1	2.16	0.59
1:5:620:G:N1	23:CC:320:LEU:O	2.34	0.59
1:5:1574:U:O2'	1:5:1577:A:N7	2.35	0.59
3:CA:196:TRP:O	3:CA:197:PRO:O	2.20	0.59
13:7:107:G:OP2	13:7:109:A:O2'	2.20	0.59
1:5:172:C:N4	1:5:237:C:OP2	2.36	0.59
29:Ce:31:GLU:OE1	29:Ce:31:GLU:N	2.36	0.59
1:5:1630:G:N2	1:5:1816:G:H21	2.01	0.58
1:5:1011:C:C2'	1:5:1056:C:H41	2.15	0.58
1:5:83:A:H62	1:5:98:A:H2	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:611:C:O2'	31:CE:45:PHE:O	2.13	0.58
1:5:921:G:N2	3:CA:208:GLU:OE2	2.34	0.58
1:5:688:G:N7	22:CQ:103:ARG:NH2	2.52	0.58
1:5:2364:A:O2'	1:5:2365:G:OP1	2.21	0.58
22:CQ:123:ASP:OD2	23:CC:291:VAL:N	2.36	0.58
1:5:176:C:H2'	1:5:177:C:C6	2.39	0.58
1:5:2674:A:O2'	43:CJ:128:ASP:OD1	2.21	0.58
1:5:418:G:O6	18:CO:73:HIS:NE2	2.33	0.58
25:Cd:56:ASP:OD1	25:Cd:57:VAL:N	2.36	0.58
27:CD:216:GLU:OE1	27:CD:216:GLU:N	2.34	0.58
1:5:2847:U:O2	1:5:2851:G:C6	2.57	0.58
1:5:3096:G:O2'	19:CB:283:LYS:NZ	2.36	0.58
1:5:3330:A:H2'	1:5:3331:G:O3'	2.03	0.58
1:5:816:A:N1	1:5:2412:U:O2'	2.32	0.57
1:5:1888:A:N6	25:Cd:27:CYS:SG	2.76	0.57
13:7:64:U:OP1	34:CX:66:ARG:NH2	2.37	0.57
28:CT:155:ASP:OD1	28:CT:156:VAL:N	2.36	0.57
12:CM:32:ASP:OD2	12:CM:35:ARG:NH1	2.38	0.57
1:5:72:A:OP1	8:CL:104:SER:OG	2.22	0.57
1:5:167:A:N6	1:5:245:A:O2'	2.37	0.57
1:5:526:G:O2'	1:5:527:C:O4'	2.21	0.57
1:5:3152:G:H21	1:5:3153:C:H42	1.52	0.57
1:5:1555:G:N2	1:5:1558:A:OP2	2.34	0.57
1:5:3199:A:OP1	26:CS:209:LYS:NZ	2.35	0.57
19:CB:80:GLU:OE1	19:CB:318:TYR:OH	2.17	0.57
1:5:2425:A:OP1	14:CN:90:THR:OG1	2.22	0.57
1:5:1808:G:OP1	36:Cg:72:ARG:NH1	2.38	0.56
1:5:2293:U:O2'	1:5:2294:OMC:O5'	2.20	0.56
1:5:2948:G:O2'	1:5:2949:OMC:O5'	2.21	0.56
15:Ca:91:THR:OG1	15:Ca:92:LYS:N	2.38	0.56
15:Ca:56:VAL:CG2	22:CQ:176:ALA:HB2	2.35	0.56
22:CQ:123:ASP:OD1	22:CQ:124:GLN:N	2.38	0.56
29:Ce:90:ASN:ND2	29:Ce:117:ASP:O	2.36	0.56
1:5:3020:U:OP2	1:5:3021:A:O2'	2.18	0.56
11:CZ:76:ASN:OD1	11:CZ:77:TYR:N	2.39	0.56
27:CD:91:GLY:O	27:CD:94:ASN:ND2	2.39	0.56
37:CG:192:CYS:O	37:CG:193:LEU:HD12	2.05	0.56
25:Cd:87:GLU:N	25:Cd:87:GLU:OE1	2.38	0.56
35:CF:113:ASN:ND2	35:CF:206:GLN:OE1	2.38	0.56
1:5:534:U:N3	1:5:543:G:O4'	2.38	0.56
1:5:610:G:H22	31:CE:44:VAL:HG23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1571:C:H1'	1:5:1572:G:P	2.46	0.56
19:CB:17:LEU:O	19:CB:19:ARG:N	2.39	0.56
1:5:2847:U:O2'	10:Cm:97:ARG:NH1	2.39	0.56
27:CD:204:SER:HB3	27:CD:235:ILE:HD11	1.88	0.56
1:5:2840:G:O6	1:5:2846:A:O2'	2.23	0.56
37:CG:134:VAL:HG11	37:CG:192:CYS:SG	2.45	0.56
33:Cf:33:LEU:C	33:Cf:34:ILE:HD12	2.32	0.55
1:5:2151:A:C2	1:5:2189:A:H4'	2.41	0.55
1:5:1695:U:O2'	1:5:1776:U:O2'	1.99	0.55
27:CD:231:GLU:OE1	27:CD:232:ALA:N	2.39	0.55
1:5:1816:G:C2	1:5:1817:A:C6	2.95	0.55
1:5:3151:U:HO2'	1:5:3152:G:P	2.28	0.55
1:5:711:U:O2	8:CL:157:ARG:N	2.37	0.55
1:5:1201:C:OP2	18:CO:54:ARG:NH1	2.33	0.55
1:5:698:G:HO2'	1:5:699:U:P	2.29	0.55
27:CD:156:ASN:OD1	27:CD:157:ARG:N	2.39	0.55
1:5:1707:C:P	1:5:1708:C:H41	2.30	0.55
14:CN:5:LYS:HG3	40:Ci:43:ILE:HG21	1.87	0.55
1:5:1820:G:H2'	1:5:1821:C:C6	2.42	0.55
1:5:2817:G:O4'	1:5:2871:5MC:HM53	2.07	0.55
12:CM:32:ASP:OD1	12:CM:33:GLN:N	2.37	0.54
9:6:27:A:OP2	27:CD:57:ASN:ND2	2.37	0.54
1:5:3179:A:C2'	1:5:3180:G:O5'	2.55	0.54
13:7:72:G:OP2	42:Cj:87:ARG:NH1	2.38	0.54
1:5:3163:C:O2	1:5:3272:G:N2	2.40	0.54
1:5:3174:C:O2'	1:5:3175:C:OP2	2.21	0.54
21:Cc:55:LEU:HD11	36:Cg:92:ILE:HG21	1.89	0.54
30:CV:19:GLY:C	30:CV:20:LEU:HD12	2.33	0.54
1:5:1611:C:HO2'	1:5:1612:C:P	2.31	0.54
1:5:2800:A:O2'	15:Ca:42:ARG:NH1	2.41	0.54
1:5:1633:G:OP1	11:CZ:69:LYS:NZ	2.34	0.54
1:5:1809:G:C2	1:5:1810:A:C2	2.95	0.54
1:5:2271:A:H2'	1:5:2272:A:C8	2.42	0.54
1:5:2678:G:O2'	1:5:2680:A:N7	2.30	0.54
1:5:638:C:N4	1:5:1412:G:N7	2.45	0.54
1:5:1611:C:O2'	1:5:1612:C:OP1	2.25	0.54
1:5:1799:U:N3	5:Cp:51:VAL:HG12	2.23	0.54
18:CO:74:GLY:O	18:CO:76:ILE:HD12	2.08	0.54
34:CX:80:THR:HG22	34:CX:153:ILE:HD12	1.89	0.54
1:5:372:A:O2'	7:CY:86:ARG:NH2	2.38	0.54
1:5:1326:U:OP1	18:CO:23:ARG:NE	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:112:A:O2'	1:5:113:G:OP1	2.25	0.53
1:5:845:A:H2	1:5:866:G:H21	1.56	0.53
23:CC:335:ASN:ND2	35:CF:182:GLU:OE2	2.42	0.53
1:5:3116:G:N2	1:5:3116:G:OP1	2.38	0.53
12:CM:121:VAL:HG22	18:CO:190:ALA:CB	2.38	0.53
20:CP:29:THR:HG21	20:CP:147:ILE:HD11	1.91	0.53
27:CD:92:LEU:O	27:CD:93:THR:OG1	2.16	0.53
1:5:173:G:OP2	1:5:236:C:N4	2.41	0.53
1:5:1191:U:OP1	26:CS:202:ARG:NH1	2.41	0.53
1:5:1570:G:H2'	1:5:1571:C:C6	2.43	0.53
1:5:2881:U:O2	19:CB:253:ALA:HB3	2.09	0.53
1:5:3163:C:H2'	1:5:3164:C:O4'	2.09	0.53
37:CG:75:PHE:O	37:CG:76:THR:OG1	2.24	0.53
1:5:111:C:OP1	14:CN:147:ARG:NH1	2.38	0.53
1:5:178:G:C6	1:5:233:G:O6	2.62	0.53
1:5:894:U:H5"	1:5:1855:OMG:HM23	1.91	0.53
7:CY:15:ARG:NH1	13:7:27:C:OP1	2.42	0.53
1:5:1817:A:HO2'	1:5:1818:G:P	2.32	0.53
1:5:1837:G:O2'	6:Cl:3:SER:O	2.26	0.53
1:5:3219:G:O2'	1:5:3220:U:P	2.67	0.53
6:Cl:31:THR:OG1	7:CY:75:ARG:NH1	2.42	0.53
18:CO:199:ASP:OD1	18:CO:200:ILE:N	2.42	0.53
23:CC:7:ARG:NH2	23:CC:31:ASP:OD1	2.42	0.53
37:CG:71:ALA:O	37:CG:74:GLN:NE2	2.42	0.53
1:5:1451:G:H4'	13:7:20:G:OP1	2.09	0.53
1:5:2848:A:OP1	10:Cm:97:ARG:NH1	2.42	0.53
1:5:2923:OMG:HM22	1:5:2952:G:N3	2.24	0.53
23:CC:215:VAL:HG21	23:CC:258:TRP:CE3	2.43	0.53
1:5:3073:A:H2'	1:5:3074:G:O4'	2.09	0.52
1:5:3102:G:HO2'	1:5:3103:A:P	2.31	0.52
1:5:1678:A:O2'	1:5:1679:A:P	2.68	0.52
1:5:2330:C:C5	1:5:2331:C:C5	2.98	0.52
1:5:2674:A:HO2'	43:CJ:128:ASP:CG	2.17	0.52
14:CN:27:CYS:SG	14:CN:31:ARG:NH2	2.83	0.52
15:Ca:85:ASP:OD1	15:Ca:86:VAL:N	2.42	0.52
20:CP:5:SER:HG	20:CP:119:GLN:CD	2.09	0.52
1:5:1219:U:O2'	1:5:1220:G:O5'	2.27	0.52
37:CG:120:GLU:N	37:CG:120:GLU:OE1	2.43	0.52
1:5:1664:G:H22	1:5:1791:G:H1	1.57	0.52
1:5:1867:G:N1	1:5:1870:C:OP2	2.32	0.52
28:CT:57:TYR:CD1	28:CT:76:VAL:HG21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CH:61:ASP:N	39:CH:61:ASP:OD1	2.41	0.52
19:CB:345:SER:OG	19:CB:349:GLN:NE2	2.41	0.52
20:CP:31:GLU:OE2	20:CP:62:ARG:N	2.42	0.52
36:Cg:2:VAL:HG22	36:Cg:3:GLN:H	1.73	0.52
1:5:3386:A:OP2	1:5:3386:A:O3'	2.28	0.52
22:CQ:16:ARG:O	22:CQ:17:THR:OG1	2.23	0.52
1:5:1728:C:O2'	1:5:1729:C:P	2.67	0.52
19:CB:91:ALA:HB2	19:CB:153:MET:HG3	1.92	0.52
26:CS:86:LEU:HD23	26:CS:92:VAL:HG21	1.92	0.52
1:5:748:G:C2	1:5:749:G:C8	2.97	0.52
1:5:1664:G:H22	1:5:1791:G:N2	2.08	0.52
1:5:1940:A:O2'	1:5:1941:U:P	2.68	0.52
1:5:2795:G:HO2'	1:5:2796:U:P	2.25	0.52
35:CF:165:ASP:OD1	35:CF:167:SER:N	2.43	0.52
1:5:67:U:OP1	14:CN:179:HIS:ND1	2.39	0.51
1:5:525:A:C2'	1:5:526:G:O5'	2.59	0.51
1:5:3018:C:H2'	1:5:3019:C:C6	2.46	0.51
1:5:3042:U:OP2	1:5:3092:C:N4	2.43	0.51
8:CL:92:ILE:HD11	8:CL:124:ILE:CD1	2.40	0.51
30:CV:35:LYS:C	30:CV:36:ASN:HD22	2.18	0.51
39:CH:149:LEU:HD12	39:CH:149:LEU:N	2.26	0.51
1:5:107:A:H4'	1:5:108:G:OP1	2.10	0.51
1:5:1576:A:O2'	1:5:1577:A:P	2.68	0.51
1:5:1889:C:HO2'	1:5:1890:A:P	2.34	0.51
1:5:2750:G:O2'	1:5:2751:C:O5'	2.29	0.51
21:Cc:18:LEU:O	21:Cc:21:VAL:HG12	2.10	0.51
1:5:409:G:OP1	20:CP:62:ARG:NH1	2.44	0.51
14:CN:185:ARG:HB3	14:CN:186:PRO:HD3	1.92	0.51
1:5:522:C:O5'	35:CF:70:LYS:NZ	2.43	0.51
28:CT:66:ASN:OD1	28:CT:67:VAL:N	2.43	0.51
1:5:524:A:N6	1:5:525:A:H62	2.09	0.51
1:5:1571:C:C2	1:5:1572:G:N7	2.79	0.51
1:5:2580:G:OP2	1:5:2581:A:O2'	2.26	0.51
7:CY:30:MET:HE2	7:CY:77:TRP:HA	1.92	0.51
1:5:345:A:N3	1:5:349:A:O2'	2.43	0.50
1:5:534:U:O2'	1:5:535:U:P	2.68	0.50
1:5:1005:G:O2'	1:5:1064:A:N6	2.41	0.50
35:CF:165:ASP:OD1	35:CF:166:ASN:N	2.44	0.50
1:5:845:A:O2'	5:Cp:9:GLY:O	2.27	0.50
1:5:1579:C:N4	1:5:1580:G:O6	2.45	0.50
3:CA:207:VAL:HG13	3:CA:208:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:137:C:H2'	13:7:138:G:O4'	2.11	0.50
1:5:613:U:H2'	1:5:614:G:C8	2.45	0.50
1:5:1728:C:HO2'	1:5:1729:C:P	2.34	0.50
30:CV:30:ASP:HB3	30:CV:104:VAL:HG23	1.93	0.50
37:CG:49:TRP:CB	37:CG:53:ILE:HD11	2.41	0.50
1:5:546:U:H2'	1:5:547:G:C4	2.47	0.50
1:5:1638:C:OP1	11:CZ:36:ARG:NH2	2.44	0.50
1:5:3171:C:H2'	1:5:3172:G:O4'	2.12	0.50
1:5:390:U:O2'	1:5:391:C:P	2.70	0.50
1:5:1704:C:O2'	1:5:1705:U:P	2.70	0.50
34:CX:151:ILE:HG22	34:CX:152:GLY:N	2.27	0.50
23:CC:155:MET:O	23:CC:157:LEU:N	2.45	0.50
30:CV:111:GLU:OE1	30:CV:131:ARG:NE	2.42	0.50
1:5:611:C:N4	1:5:612:G:O6	2.45	0.50
13:7:19:G:O2'	13:7:20:G:P	2.70	0.50
1:5:1753:A:OP2	2:Ck:33:LYS:NZ	2.42	0.50
1:5:2752:G:HO2'	1:5:2753:U:P	2.30	0.50
2:Ck:64:LEU:HD13	2:Ck:65:SER:N	2.27	0.50
1:5:686:G:O2'	23:CC:123:ASN:OD1	2.30	0.49
1:5:1415:C:O2'	1:5:1416:G:P	2.69	0.49
42:Cj:60:GLY:O	42:Cj:61:THR:OG1	2.26	0.49
1:5:2288:C:O2'	1:5:2289:OMG:OP1	2.23	0.49
7:CY:30:MET:HE1	7:CY:74:ARG:HA	1.93	0.49
38:Ch:50:VAL:O	38:Ch:53:SER:OG	2.28	0.49
43:CJ:64:ASN:ND2	43:CJ:64:ASN:O	2.45	0.49
1:5:111:C:H2'	1:5:112:A:H5'	1.93	0.49
1:5:175:A:C2'	1:5:176:C:H5'	2.42	0.49
1:5:759:G:H1	1:5:792:G:H22	1.60	0.49
1:5:3070:A:O2'	1:5:3071:A:OP1	2.30	0.49
43:CJ:56:VAL:HG22	43:CJ:58:SER:H	1.78	0.49
1:5:176:C:H2'	1:5:177:C:O4'	2.12	0.49
1:5:424:G:H22	1:5:644:U:H3	1.59	0.49
1:5:759:G:H22	1:5:792:G:N2	2.09	0.49
1:5:1305:A:C2	1:5:1306:G:N7	2.81	0.49
1:5:1674:C:OP1	24:CR:60:ARG:NH1	2.45	0.49
23:CC:90:HIS:O	23:CC:90:HIS:ND1	2.45	0.49
33:Cf:51:LYS:NZ	33:Cf:108:PRO:O	2.38	0.49
1:5:572:G:O6	31:CE:74:LEU:HD21	2.12	0.49
1:5:847:G:O6	5:Cp:4:ARG:NH2	2.43	0.49
1:5:2268:C:C2'	1:5:2269:U:O5'	2.60	0.49
1:5:2315:U:O2'	1:5:2316:G:OP1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2409:U:O2'	1:5:2410:OMG:P	2.71	0.49
24:CR:57:ILE:O	24:CR:57:ILE:HD12	2.12	0.49
24:CR:95:TRP:CZ2	24:CR:99:MET:HE3	2.47	0.49
1:5:176:C:O2'	1:5:177:C:O4'	2.30	0.49
1:5:1448:U:O2	1:5:1448:U:O4'	2.31	0.49
1:5:1632:U:C6	1:5:1816:G:C6	3.01	0.49
1:5:3102:G:O2'	1:5:3103:A:P	2.70	0.49
41:CI:160:PRO:O	41:CI:163:GLN:NE2	2.43	0.49
39:CH:37:ASP:OD1	39:CH:38:PHE:N	2.45	0.49
1:5:2251:G:C6	1:5:2268:C:N4	2.81	0.49
36:Cg:107:LEU:HD13	36:Cg:107:LEU:C	2.37	0.49
1:5:1623:C:H2'	1:5:1624:G:H8	1.77	0.49
1:5:2889:U:O4'	1:5:2912:A:N6	2.44	0.49
1:5:2933:C:H2'	1:5:2934:A:H2'	1.94	0.49
1:5:2364:A:O2'	1:5:2365:G:P	2.70	0.49
1:5:2578:U:H2'	1:5:2579:C:C6	2.48	0.49
14:CN:96:ARG:NH2	14:CN:104:GLU:OE1	2.45	0.49
1:5:390:U:HO2'	1:5:391:C:P	2.34	0.48
1:5:1630:G:H21	1:5:1816:G:N2	2.09	0.48
1:5:1632:U:C6	1:5:1816:G:O6	2.66	0.48
1:5:1104:A:OP2	1:5:1105:C:N4	2.43	0.48
1:5:1205:G:H2'	1:5:1206:A:C8	2.48	0.48
1:5:1422:G:OP1	29:Ce:106:ARG:NH2	2.45	0.48
1:5:1944:G:H21	1:5:3350:A:H8	1.60	0.48
1:5:2293:U:C2'	1:5:2294:OMC:O5'	2.61	0.48
16:w:63:LYS:O	16:w:64:SER:OG	2.29	0.48
35:CF:28:GLN:NE2	35:CF:29:ASN:OD1	2.46	0.48
1:5:1415:C:O2'	1:5:1416:G:C8	2.61	0.48
1:5:2802:A:O2'	1:5:2803:A:H2'	2.13	0.48
1:5:3379:A:H4'	1:5:3380:G:OP1	2.13	0.48
12:CM:58:ILE:HD12	12:CM:80:VAL:HG23	1.94	0.48
1:5:1538:G:O2'	1:5:1591:A:N3	2.42	0.48
1:5:2370:G:H2'	1:5:2371:G:C8	2.48	0.48
24:CR:119:MET:HE3	24:CR:123:MET:SD	2.53	0.48
43:CJ:103:CYS:SG	43:CJ:132:VAL:HG23	2.53	0.48
1:5:778:A:C5	1:5:779:G:H1'	2.47	0.48
1:5:2562:G:O2'	1:5:2563:G:H5'	2.13	0.48
1:5:2715:G:H2'	1:5:2752:G:H21	1.78	0.48
3:CA:143:ASN:OD1	3:CA:143:ASN:N	2.45	0.48
25:Cd:105:GLU:OE1	25:Cd:105:GLU:N	2.46	0.48
1:5:526:G:H2'	1:5:527:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:769:G:O2'	1:5:770:A:H8	1.95	0.48
9:6:6:C:OP1	27:CD:54:ARG:NE	2.41	0.48
35:CF:197:GLU:N	35:CF:197:GLU:OE1	2.44	0.48
37:CG:153:ASP:HB3	37:CG:154:PRO:HD3	1.96	0.48
40:Ci:93:MET:O	40:Ci:96:VAL:HG12	2.13	0.48
1:5:2891:A:O2'	1:5:2934:A:N3	2.43	0.48
1:5:3025:C:OP1	39:CH:101:HIS:NE2	2.45	0.48
1:5:3219:G:HO2'	1:5:3220:U:P	2.31	0.48
8:CL:92:ILE:HD11	8:CL:124:ILE:HD12	1.95	0.48
12:CM:16:ASN:ND2	12:CM:54:SER:OG	2.44	0.48
1:5:1594:G:OP2	36:Cg:17:SER:OG	2.31	0.48
1:5:3114:A:N7	1:5:3118:C:N3	2.61	0.48
19:CB:35:ASP:OD1	19:CB:36:ASP:N	2.47	0.48
37:CG:72:LEU:O	37:CG:73:ASN:HB3	2.13	0.48
43:CJ:113:ASP:OD1	43:CJ:114:LEU:N	2.47	0.48
1:5:3252:U:H2'	1:5:3253:G:C8	2.49	0.48
19:CB:56:ILE:HD12	19:CB:56:ILE:C	2.38	0.48
31:CE:229:HIS:NE2	31:CE:230:GLU:OE1	2.47	0.48
33:Cf:107:TYR:HB2	33:Cf:108:PRO:HD3	1.96	0.48
37:CG:53:ILE:O	37:CG:56:GLN:HG2	2.14	0.48
1:5:3071:A:H2'	1:5:3072:A:O4'	2.14	0.48
1:5:3183:G:H22	39:CH:62:SER:HA	1.78	0.48
1:5:3268:C:H3'	1:5:3269:C:H5"	1.96	0.48
1:5:3385:G:H21	1:5:3386:A:H62	1.61	0.48
12:CM:40:ALA:HB3	12:CM:43:MET:HG2	1.95	0.47
1:5:3040:A:H2'	1:5:3041:U:O2	2.14	0.47
13:7:22:U:C2	13:7:23:A:C8	3.02	0.47
43:CJ:47:PRO:HA	43:CJ:71:VAL:HG12	1.95	0.47
1:5:311:U:H2'	1:5:312:C:C6	2.49	0.47
1:5:2207:G:H5'	1:5:2209:A:H61	1.79	0.47
1:5:2834:A:C6	1:5:2857:G:C6	3.02	0.47
9:6:51:G:H21	43:CJ:11:MET:CE	2.22	0.47
12:CM:56:THR:OG1	12:CM:57:ASP:N	2.46	0.47
13:7:19:G:O2'	13:7:20:G:OP1	2.31	0.47
15:Ca:126:LEU:HD11	40:Ci:11:PHE:CD2	2.49	0.47
19:CB:90:VAL:HG22	19:CB:104:THR:HG22	1.96	0.47
1:5:1318:G:O2'	1:5:1319:A:OP2	2.26	0.47
8:CL:164:LEU:N	8:CL:164:LEU:HD12	2.29	0.47
12:CM:5:ARG:NE	12:CM:57:ASP:OD1	2.47	0.47
18:CO:111:GLU:OE1	18:CO:111:GLU:N	2.47	0.47
30:CV:31:ASN:O	30:CV:31:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Cf:35:GLN:OE1	33:Cf:36:ILE:N	2.47	0.47
43:CJ:30:ASP:OD1	43:CJ:31:ARG:N	2.48	0.47
1:5:621:G:OP2	1:5:621:G:H4'	2.14	0.47
43:CJ:34:ARG:NH1	43:CJ:121:SER:O	2.40	0.47
1:5:778:A:C4	1:5:779:G:H1'	2.49	0.47
1:5:2883:U:H2'	1:5:2884:OMU:H6	1.97	0.47
1:5:3152:G:N3	1:5:3153:C:N4	2.62	0.47
1:5:3178:C:N4	1:5:3179:A:H62	2.13	0.47
1:5:3331:G:H2'	1:5:3331:G:N3	2.30	0.47
18:CO:59:TYR:OH	18:CO:78:PHE:O	2.33	0.47
1:5:2182:C:C2	1:5:2183:A:C8	3.02	0.47
1:5:2278:C:O2'	1:5:2279:5MC:P	2.71	0.47
1:5:2748:A:OP1	27:CD:175:SER:OG	2.32	0.47
1:5:3006:A:H2'	1:5:3007:U:O4'	2.15	0.47
8:CL:168:THR:OG1	8:CL:171:MET:SD	2.72	0.47
19:CB:86:VAL:HG22	19:CB:201:PHE:O	2.14	0.47
27:CD:27:LYS:NZ	43:CJ:146:CYS:SG	2.68	0.47
37:CG:53:ILE:HD12	37:CG:53:ILE:C	2.39	0.47
1:5:112:A:HO2'	1:5:113:G:P	2.38	0.47
1:5:2285:C:N4	1:5:2309:C:O4'	2.48	0.47
6:Cl:38:ASN:OD1	6:Cl:39:ALA:N	2.48	0.47
1:5:1597:A:OP1	36:Cg:66:ARG:NH1	2.47	0.47
1:5:2168:U:O2	1:5:2168:U:O4'	2.32	0.47
1:5:2987:U:C2	1:5:2988:A:C8	3.03	0.47
1:5:3070:A:O2'	1:5:3071:A:P	2.73	0.47
11:CZ:75:VAL:HG11	11:CZ:80:LEU:HD21	1.97	0.47
19:CB:121:ASN:OD1	19:CB:124:LYS:N	2.39	0.47
1:5:785:U:OP1	17:Cb:63:ARG:NH1	2.48	0.47
1:5:1133:U:O2	1:5:1133:U:O4'	2.33	0.47
2:Ck:8:ILE:H	2:Ck:8:ILE:HD12	1.80	0.47
18:CO:26:SER:N	18:CO:92:MET:HE1	2.30	0.47
43:CJ:19:LEU:HD23	43:CJ:19:LEU:C	2.40	0.47
1:5:2289:OMG:H2'	1:5:2290:U:C6	2.50	0.46
1:5:2561:A:O2'	1:5:2562:G:H8	1.98	0.46
43:CJ:22:ASN:OD1	43:CJ:23:ILE:N	2.48	0.46
1:5:1911:C:O4'	1:5:1911:C:O2	2.33	0.46
1:5:2150:A:H2'	1:5:2151:A:C8	2.50	0.46
21:Cc:34:VAL:HG23	21:Cc:95:SER:HB2	1.96	0.46
1:5:2436:G:H22	1:5:2594:A:C2'	2.28	0.46
1:5:3179:A:O2'	1:5:3180:G:O5'	2.33	0.46
1:5:3240:U:H2'	1:5:3241:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CQ:75:GLU:OE1	22:CQ:75:GLU:N	2.35	0.46
31:CE:107:VAL:HG12	31:CE:129:VAL:HG21	1.98	0.46
1:5:1916:U:N3	1:5:2124:G:OP2	2.46	0.46
1:5:2315:U:HO2'	1:5:2316:G:P	2.37	0.46
1:5:2430:G:H2'	1:5:2431:A:H8	1.81	0.46
1:5:3172:G:H1'	33:Cf:7:GLU:HG2	1.98	0.46
1:5:3321:G:O2'	1:5:3322:U:OP2	2.27	0.46
19:CB:49:TYR:CD1	19:CB:171:MET:HE1	2.51	0.46
19:CB:187:ASN:OD1	19:CB:187:ASN:N	2.47	0.46
1:5:2437:U:H2'	1:5:2438:G:H5"	1.97	0.46
1:5:3152:G:N2	1:5:3153:C:H42	2.13	0.46
19:CB:17:LEU:C	19:CB:17:LEU:HD13	2.40	0.46
1:5:174:G:H2'	1:5:175:A:O4'	2.16	0.46
1:5:1596:G:O2'	1:5:1597:A:P	2.74	0.46
1:5:2552:U:O2'	1:5:2553:U:C6	2.69	0.46
1:5:3266:C:H2'	1:5:3267:A:C4	2.51	0.46
13:7:76:A:C5	13:7:77:U:C5	3.04	0.46
24:CR:99:MET:SD	24:CR:103:ARG:NH1	2.89	0.46
1:5:1713:C:C2	1:5:1714:U:C5	3.04	0.46
1:5:2718:U:H2'	1:5:2719:C:H5'	1.98	0.46
1:5:3070:A:HO2'	1:5:3071:A:P	2.39	0.46
1:5:3266:C:O3'	1:5:3267:A:O4'	2.34	0.46
13:7:136:C:H2'	13:7:137:C:C1'	2.46	0.46
20:CP:16:LYS:HG2	20:CP:150:ILE:HG22	1.98	0.46
27:CD:83:LEU:N	27:CD:84:PRO:HD2	2.31	0.46
30:CV:104:VAL:HG21	30:CV:112:MET:HE3	1.98	0.46
1:5:1372:C:H5"	23:CC:318:ALA:HB2	1.98	0.46
1:5:2370:G:O2'	1:5:2371:G:P	2.74	0.46
1:5:3041:U:O2	1:5:3041:U:O4'	2.32	0.46
12:CM:12:VAL:O	12:CM:56:THR:HG22	2.16	0.46
35:CF:62:LEU:HD23	35:CF:62:LEU:O	2.16	0.46
1:5:187:U:C2'	1:5:188:U:OP2	2.64	0.46
1:5:2949:OMC:H2'	1:5:2950:U:C6	2.51	0.46
1:5:3197:A:O2'	1:5:3199:A:OP1	2.26	0.46
13:7:136:C:H2'	13:7:137:C:N1	2.30	0.46
18:CO:57:MET:SD	18:CO:60:MET:HE2	2.55	0.46
20:CP:50:ASP:OD2	20:CP:56:GLN:NE2	2.47	0.46
22:CQ:166:VAL:HG11	22:CQ:174:GLU:HG3	1.97	0.46
31:CE:122:GLY:H	31:CE:129:VAL:HG23	1.80	0.46
1:5:233:G:O2'	1:5:234:G:OP2	2.20	0.45
1:5:1318:G:H1'	1:5:1319:A:OP2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3057:U:H3'	1:5:3058:C:H4'	1.98	0.45
1:5:3218:A:H3'	1:5:3219:G:H8	1.81	0.45
9:6:107:C:OP1	27:CD:273:TYR:OH	2.33	0.45
41:CI:163:GLN:OE1	41:CI:163:GLN:N	2.49	0.45
43:CJ:94:LEU:N	43:CJ:94:LEU:HD12	2.31	0.45
1:5:525:A:H2'	1:5:526:G:O5'	2.17	0.45
1:5:1611:C:O2'	1:5:1612:C:P	2.73	0.45
1:5:2268:C:H2'	1:5:2269:U:O5'	2.16	0.45
1:5:3227:G:C6	1:5:3239:G:O6	2.69	0.45
31:CE:74:LEU:HD23	31:CE:75:PRO:N	2.31	0.45
36:Cg:2:VAL:HG22	36:Cg:3:GLN:N	2.30	0.45
1:5:917:OMG:H3'	14:CN:81:TYR:OH	2.16	0.45
1:5:2749:A:H2'	1:5:2750:G:H5'	1.98	0.45
1:5:2752:G:O2'	1:5:2753:U:P	2.73	0.45
18:CO:115:THR:HG23	18:CO:116:PRO:HD3	1.98	0.45
23:CC:224:VAL:HA	23:CC:235:LEU:HD22	1.99	0.45
39:CH:153:ASP:OD1	39:CH:155:GLU:N	2.48	0.45
1:5:529:C:H2'	1:5:530:G:C1'	2.46	0.45
1:5:531:G:O4'	1:5:547:G:N2	2.50	0.45
1:5:1190:C:C2	1:5:1192:G:C8	3.05	0.45
31:CE:190:VAL:O	31:CE:193:ASP:OD1	2.34	0.45
35:CF:25:GLU:O	35:CF:28:GLN:NE2	2.49	0.45
38:Ch:31:LEU:HD23	38:Ch:47:ILE:HA	1.98	0.45
1:5:627:G:H2'	1:5:628:C:C6	2.51	0.45
1:5:2149:A:H2'	1:5:2150:A:O4'	2.16	0.45
1:5:2208:A:H2'	1:5:2208:A:N3	2.30	0.45
1:5:2364:A:HO2'	1:5:2365:G:P	2.38	0.45
1:5:3051:U:C2	1:5:3052:G:C8	3.04	0.45
1:5:3084:C:H2'	1:5:3085:G:O4'	2.15	0.45
18:CO:28:THR:HG23	18:CO:38:VAL:HG21	1.98	0.45
19:CB:55:HIS:NE2	19:CB:364:ASP:OD2	2.48	0.45
37:CG:152:VAL:HG21	37:CG:158:VAL:HG22	1.99	0.45
1:5:116:U:O2	1:5:116:U:O4'	2.34	0.45
1:5:698:G:H2'	1:5:699:U:O4'	2.16	0.45
1:5:2871:5MC:HO2'	1:5:2872:G:P	2.34	0.45
1:5:2917:U:C2'	1:5:2918:OMG:O5'	2.64	0.45
1:5:2919:G:C2	1:5:2920:A:N7	2.85	0.45
1:5:2965:G:N2	1:5:2968:A:OP2	2.43	0.45
1:5:3017:A:C2'	1:5:3018:C:H5'	2.45	0.45
2:Ck:19:ASP:OD1	2:Ck:39:SER:N	2.50	0.45
6:Cl:50:GLY:O	42:Cj:25:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CV:117:ILE:HG21	30:CV:121:ILE:HD11	1.98	0.45
37:CG:153:ASP:CB	37:CG:154:PRO:HD3	2.47	0.45
43:CJ:95:ARG:N	43:CJ:173:ILE:HD11	2.32	0.45
11:CZ:104:ASP:OD1	11:CZ:105:LYS:N	2.49	0.45
35:CF:85:PHE:CD2	35:CF:238:ILE:HD11	2.52	0.45
1:5:1323:C:H2'	1:5:1324:G:O4'	2.17	0.45
1:5:1423:C:O4'	1:5:1423:C:O2	2.34	0.45
1:5:2149:A:H4'	3:CA:197:PRO:HB2	1.98	0.45
1:5:2751:C:O2'	1:5:2752:G:H5'	2.16	0.45
1:5:3047:C:O2'	1:5:3048:A:H5'	2.16	0.45
1:5:3220:U:H2'	1:5:3221:C:C6	2.51	0.45
1:5:3371:U:O2	1:5:3371:U:O4'	2.34	0.45
30:CV:107:ASN:OD1	30:CV:111:GLU:N	2.49	0.45
1:5:233:G:C6	1:5:234:G:C6	3.04	0.45
1:5:2431:A:N1	1:5:2600:U:H5	2.15	0.45
1:5:2853:C:N3	41:CI:158:LYS:NZ	2.63	0.45
1:5:2923:OMG:H2'	1:5:2924:U:O4'	2.16	0.45
17:Cb:43:ILE:HG22	17:Cb:43:ILE:O	2.17	0.45
18:CO:8:CYS:SG	18:CO:9:SER:N	2.90	0.45
43:CJ:107:GLY:C	43:CJ:108:ILE:HD12	2.42	0.45
1:5:617:C:H41	31:CE:18:ARG:HB2	1.82	0.45
35:CF:27:LYS:O	35:CF:30:VAL:HG22	2.17	0.45
39:CH:16:VAL:HG21	39:CH:84:ILE:HD12	1.99	0.45
1:5:161:G:HO2'	1:5:162:U:P	2.39	0.44
1:5:663:G:O2'	1:5:1445:A:OP1	2.35	0.44
1:5:1855:OMG:HM22	1:5:1855:OMG:H1'	1.78	0.44
1:5:3260:A:O2'	1:5:3261:A:O5'	2.22	0.44
8:CL:138:THR:HG1	8:CL:141:GLU:CD	2.25	0.44
23:CC:272:SER:OG	23:CC:274:GLU:OE1	2.36	0.44
27:CD:68:SER:OG	27:CD:71:GLY:O	2.31	0.44
28:CT:32:ARG:NH2	28:CT:96:VAL:O	2.49	0.44
34:CX:38:ILE:C	34:CX:38:ILE:HD12	2.42	0.44
41:CI:115:MET:HE2	41:CI:115:MET:HA	1.98	0.44
1:5:44:OMU:O2'	1:5:45:C:P	2.75	0.44
1:5:3331:G:H1	1:5:3334:U:C1'	2.31	0.44
18:CO:94:PRO:O	18:CO:97:THR:HG22	2.17	0.44
19:CB:259:HIS:C	19:CB:261:ALA:N	2.75	0.44
32:CW:27:ASP:C	32:CW:28:SER:HG	2.18	0.44
1:5:1714:U:C2'	1:5:1715:G:O5'	2.64	0.44
4:CK:65:THR:HG22	4:CK:89:LYS:HB3	1.98	0.44
9:6:6:C:H3'	9:6:7:G:H5"	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CO:160:GLU:O	18:CO:163:THR:OG1	2.36	0.44
1:5:112:A:O2'	1:5:113:G:P	2.76	0.44
1:5:833:C:O2'	1:5:1544:A:N3	2.49	0.44
12:CM:19:GLU:OE1	12:CM:19:GLU:N	2.43	0.44
15:Ca:123:LYS:HD2	15:Ca:145:THR:HG21	1.99	0.44
18:CO:73:HIS:O	18:CO:73:HIS:CG	2.70	0.44
35:CF:85:PHE:HB2	35:CF:139:PRO:HG3	2.00	0.44
1:5:61:A:N3	1:5:76:U:O2'	2.43	0.44
1:5:534:U:HO2'	1:5:535:U:P	2.41	0.44
1:5:859:U:O2	1:5:859:U:O4'	2.35	0.44
1:5:1821:C:H2'	1:5:1822:C:H6	1.83	0.44
1:5:2556:U:O5'	1:5:2556:U:O2	2.36	0.44
1:5:2750:G:O2'	1:5:2751:C:H6	1.99	0.44
18:CO:20:MET:HE2	18:CO:130:LYS:HG3	2.00	0.44
31:CE:97:ILE:C	31:CE:98:LEU:HD12	2.42	0.44
34:CX:99:ASP:OD1	34:CX:100:ILE:N	2.50	0.44
41:CI:59:ASN:ND2	41:CI:126:CYS:SG	2.84	0.44
1:5:175:A:H2'	1:5:176:C:H5'	2.00	0.44
1:5:3183:G:N2	39:CH:61:ASP:O	2.51	0.44
7:CY:75:ARG:NH2	13:7:78:U:OP1	2.51	0.44
28:CT:126:ILE:HD12	28:CT:126:ILE:C	2.42	0.44
1:5:528:C:H5'	1:5:529:C:OP2	2.17	0.44
1:5:1517:G:H22	20:CP:130:THR:HA	1.82	0.44
1:5:2184:A:H2'	1:5:2185:U:H5"	1.99	0.44
3:CA:33:ASP:N	3:CA:33:ASP:OD1	2.49	0.44
8:CL:152:TYR:N	8:CL:152:TYR:CD1	2.84	0.44
11:CZ:22:LYS:NZ	11:CZ:131:THR:O	2.50	0.44
18:CO:97:THR:HG23	18:CO:100:GLY:H	1.82	0.44
27:CD:274:GLU:OE1	27:CD:274:GLU:N	2.43	0.44
31:CE:74:LEU:HD22	31:CE:76:ASN:HA	1.99	0.44
1:5:418:G:N3	1:5:418:G:O2'	2.47	0.44
1:5:1021:G:OP2	41:CI:40:ARG:NE	2.51	0.44
1:5:2319:U:H2'	1:5:2320:U:O4'	2.18	0.44
1:5:2918:OMG:O6	1:5:2931:A:N6	2.50	0.44
1:5:2934:A:O2'	1:5:2935:A:C8	2.71	0.44
1:5:3217:A:H61	1:5:3248:G:H1'	1.83	0.44
13:7:92:A:H2'	13:7:93:A:O4'	2.18	0.44
31:CE:123:PRO:HB2	31:CE:126:ILE:HG22	1.99	0.44
31:CE:154:ASP:OD1	31:CE:154:ASP:N	2.51	0.44
1:5:903:U:H4'	1:5:904:G:H5'	1.99	0.43
1:5:1144:G:O2'	1:5:2643:A:N3	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2330:C:O2	1:5:2330:C:O4'	2.33	0.43
1:5:2886:C:O2'	1:5:2887:U:H5'	2.18	0.43
1:5:3270:G:H3'	1:5:3271:A:H4'	1.99	0.43
19:CB:166:THR:O	19:CB:179:ALA:HB1	2.18	0.43
21:Cc:104:ILE:HD12	21:Cc:104:ILE:C	2.42	0.43
23:CC:190:ASN:O	23:CC:191:SER:OG	2.22	0.43
38:Ch:47:ILE:O	38:Ch:50:VAL:HG12	2.18	0.43
1:5:770:A:H62	1:5:779:G:H21	1.65	0.43
12:CM:7:VAL:O	12:CM:7:VAL:HG23	2.18	0.43
12:CM:117:ARG:O	12:CM:121:VAL:HG23	2.17	0.43
31:CE:41:ASN:ND2	31:CE:44:VAL:HG22	2.33	0.43
37:CG:33:ILE:N	37:CG:33:ILE:HD12	2.33	0.43
1:5:1:G:OP1	13:7:163:A:O2'	2.36	0.43
1:5:1678:A:HO2'	1:5:1679:A:P	2.41	0.43
1:5:2548:G:H1'	1:5:2549:U:P	2.58	0.43
1:5:3018:C:H2'	1:5:3019:C:O4'	2.18	0.43
1:5:3149:C:H4'	19:CB:128:LYS:O	2.19	0.43
2:Ck:8:ILE:HD12	2:Ck:8:ILE:N	2.33	0.43
18:CO:59:TYR:CD1	18:CO:150:VAL:HG21	2.52	0.43
1:5:267:U:O2	1:5:268:C:C6	2.72	0.43
1:5:924:A:O2'	1:5:926:A:OP1	2.30	0.43
1:5:987:G:N3	1:5:987:G:H3'	2.33	0.43
1:5:1514:A:C5	1:5:1515:C:C5	3.07	0.43
1:5:2376:G:O2'	1:5:2378:G:OP2	2.36	0.43
1:5:2549:U:N3	37:CG:31:PHE:O	2.51	0.43
1:5:2782:U:H4'	8:CL:195:LYS:HD3	2.00	0.43
23:CC:40:ASP:OD1	23:CC:40:ASP:N	2.51	0.43
31:CE:122:GLY:O	31:CE:123:PRO:C	2.61	0.43
33:Cf:29:PRO:O	33:Cf:92:ASN:ND2	2.41	0.43
40:Ci:73:LEU:HD13	40:Ci:73:LEU:C	2.44	0.43
1:5:925:G:H5'	1:5:926:A:OP1	2.18	0.43
1:5:1783:C:H4'	1:5:1784:G:OP1	2.19	0.43
1:5:2436:G:H1	1:5:2594:A:H2'	1.81	0.43
1:5:2678:G:N3	1:5:2678:G:H2'	2.34	0.43
1:5:2847:U:O2	1:5:2850:C:N4	2.51	0.43
1:5:3227:G:N1	1:5:3239:G:C6	2.85	0.43
1:5:3337:C:N4	1:5:3338:C:N3	2.66	0.43
15:Ca:51:GLY:HA2	22:CQ:177:ARG:H	1.84	0.43
18:CO:93:ILE:HG23	18:CO:94:PRO:HD2	2.00	0.43
22:CQ:176:ALA:O	22:CQ:183:ARG:HB3	2.18	0.43
1:5:176:C:C2'	1:5:177:C:O4'	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:355:G:N2	1:5:358:A:OP2	2.50	0.43
1:5:566:G:H2'	1:5:567:A:H8	1.83	0.43
1:5:569:C:O2'	1:5:570:G:H5'	2.18	0.43
1:5:1899:A:O2'	1:5:3053:G:H4'	2.18	0.43
1:5:2600:U:O2	1:5:2600:U:O5'	2.36	0.43
11:CZ:98:ASP:OD1	11:CZ:99:ALA:N	2.51	0.43
28:CT:159:ASP:OD1	28:CT:159:ASP:N	2.52	0.43
1:5:130:C:C4	1:5:131:U:H1'	2.53	0.43
1:5:555:G:H2'	1:5:556:U:C6	2.54	0.43
1:5:1663:G:H2'	1:5:1664:G:C8	2.53	0.43
1:5:1809:G:C2'	1:5:1810:A:H5"	2.49	0.43
1:5:2288:C:O2'	1:5:2289:OMG:P	2.77	0.43
1:5:2329:U:H2'	1:5:2330:C:O2	2.18	0.43
1:5:3216:U:H4'	1:5:3217:A:C8	2.53	0.43
8:CL:2:LYS:O	8:CL:3:HIS:CG	2.71	0.43
17:Cb:43:ILE:O	28:CT:83:ARG:HA	2.18	0.43
21:Cc:28:THR:C	21:Cc:29:LEU:HD12	2.44	0.43
21:Cc:55:LEU:HD11	36:Cg:92:ILE:CG2	2.49	0.43
29:Ce:97:ILE:CD1	29:Ce:109:ILE:HG21	2.49	0.43
32:CW:34:LEU:HD13	32:CW:34:LEU:C	2.43	0.43
1:5:1608:A:N3	1:5:1608:A:H2'	2.34	0.43
1:5:2847:U:O2	1:5:2847:U:O4'	2.37	0.43
15:Ca:75:LEU:O	15:Ca:76:ASP:CG	2.62	0.43
1:5:2556:U:C2'	1:5:2557:C:O5'	2.66	0.43
1:5:3163:C:O2	1:5:3272:G:C2	2.72	0.43
12:CM:61:ASP:O	12:CM:62:ILE:HG23	2.19	0.43
13:7:73:U:H2'	13:7:74:G:O4'	2.18	0.43
18:CO:21:LEU:HD22	18:CO:48:LEU:HD21	2.01	0.43
21:Cc:49:SER:OG	21:Cc:50:SER:N	2.52	0.43
1:5:525:A:C6	1:5:526:G:C2	3.07	0.43
1:5:2185:U:O2'	1:5:2186:G:P	2.76	0.43
1:5:2198:OMC:N4	1:5:2243:A:O4'	2.52	0.43
1:5:3071:A:O2'	1:5:3072:A:OP1	2.31	0.43
1:5:3304:A:C8	1:5:3379:A:N1	2.87	0.43
24:CR:51:ILE:HG22	24:CR:52:ARG:N	2.34	0.43
1:5:534:U:O2'	1:5:535:U:O5'	2.26	0.42
1:5:577:G:H2'	1:5:577:G:N3	2.34	0.42
1:5:2858:C:H2'	1:5:2859:U:C6	2.54	0.42
1:5:3221:C:H2'	1:5:3222:C:C6	2.53	0.42
1:5:3272:G:H2'	1:5:3273:C:O4'	2.19	0.42
1:5:3279:G:C2'	1:5:3280:U:O5'	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CM:40:ALA:HB1	12:CM:41:PRO:HD2	2.01	0.42
23:CC:272:SER:OG	23:CC:273:PHE:N	2.51	0.42
26:CS:124:SER:O	26:CS:126:THR:N	2.52	0.42
1:5:291:C:O2'	1:5:292:A:O5'	2.32	0.42
1:5:1694:G:H2'	1:5:1695:U:H5'	2.00	0.42
1:5:2750:G:O2'	1:5:2751:C:P	2.77	0.42
37:CG:171:PRO:HB2	37:CG:210:LEU:HD11	2.00	0.42
39:CH:20:VAL:HG12	39:CH:25:ILE:HG22	2.00	0.42
1:5:769:G:HO2'	1:5:770:A:H8	1.66	0.42
1:5:896:G:H2'	1:5:897:U:C6	2.54	0.42
1:5:1561:C:H2'	1:5:1562:G:O4'	2.20	0.42
1:5:1817:A:O2'	1:5:1818:G:P	2.77	0.42
1:5:2185:U:O2'	1:5:2186:G:H8	2.02	0.42
1:5:2769:U:H2'	1:5:2770:A:H8	1.83	0.42
1:5:3282:G:OP2	19:CB:126:LYS:NZ	2.52	0.42
7:CY:50:ARG:HG2	7:CY:51:LYS:H	1.83	0.42
22:CQ:174:GLU:HA	22:CQ:174:GLU:OE1	2.20	0.42
29:Ce:85:LEU:C	29:Ce:85:LEU:HD12	2.45	0.42
31:CE:124:PHE:N	31:CE:199:ASP:OD2	2.46	0.42
38:Ch:47:ILE:HG23	38:Ch:48:LYS:N	2.35	0.42
1:5:611:C:H2'	1:5:612:G:OP1	2.20	0.42
1:5:804:G:H2'	1:5:805:U:H6	1.83	0.42
1:5:842:G:H2'	1:5:843:U:C6	2.53	0.42
1:5:1445:A:O2'	1:5:1446:U:P	2.77	0.42
1:5:2120:C:H2'	1:5:2121:A:O4'	2.20	0.42
1:5:2619:G:C4'	1:5:2620:OMG:OP2	2.67	0.42
12:CM:104:ASP:OD2	31:CE:215:TYR:OH	2.34	0.42
21:Cc:21:VAL:O	21:Cc:22:MET:C	2.61	0.42
23:CC:149:ILE:N	23:CC:150:GLU:OE1	2.52	0.42
37:CG:181:LEU:HB3	37:CG:193:LEU:HD13	2.01	0.42
1:5:55:A:O2'	1:5:56:G:H5'	2.19	0.42
1:5:250:G:H2'	1:5:251:A:O4'	2.19	0.42
1:5:1649:A:N6	1:5:1811:G:H21	2.17	0.42
1:5:1940:A:HO2'	1:5:1941:U:P	2.42	0.42
1:5:2267:U:H2'	1:5:2268:C:C6	2.54	0.42
1:5:3329:C:H2'	1:5:3330:A:H5'	2.02	0.42
9:6:65:G:O2'	27:CD:10:ASN:OD1	2.37	0.42
12:CM:24:LEU:HD22	12:CM:24:LEU:N	2.34	0.42
20:CP:9:ASP:OD1	20:CP:9:ASP:N	2.53	0.42
40:Ci:14:LEU:HD13	40:Ci:14:LEU:O	2.19	0.42
1:5:99:C:O2	1:5:99:C:O4'	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:111:C:C2'	1:5:112:A:H5'	2.49	0.42
1:5:373:G:OP2	7:CY:89:VAL:HG12	2.20	0.42
1:5:777:G:O5'	8:CL:189:HIS:NE2	2.47	0.42
1:5:893:A:N7	1:5:2141:A:C4	2.87	0.42
1:5:2657:A:C5	1:5:2659:G:C8	3.08	0.42
1:5:2727:C:O5'	1:5:2727:C:O2	2.38	0.42
1:5:2839:A:H2'	1:5:2840:G:O4'	2.20	0.42
1:5:2871:5MC:O2'	1:5:2872:G:P	2.76	0.42
1:5:3070:A:H2'	1:5:3071:A:H8	1.84	0.42
1:5:3307:C:H2'	1:5:3308:G:N9	2.33	0.42
1:5:3385:G:N2	1:5:3386:A:H62	2.16	0.42
14:CN:148:ILE:O	14:CN:151:ILE:HG22	2.20	0.42
19:CB:122:TRP:O	19:CB:122:TRP:CG	2.73	0.42
19:CB:364:ASP:OD1	19:CB:365:THR:N	2.53	0.42
38:Ch:96:THR:HG23	38:Ch:99:GLN:H	1.84	0.42
1:5:3016:A:H2'	1:5:3017:A:H8	1.84	0.42
1:5:3288:U:C4	1:5:3289:U:C5	3.07	0.42
1:5:3386:A:HO3'	1:5:3386:A:P	2.43	0.42
2:Ck:31:ILE:HD12	2:Ck:48:PHE:CD2	2.55	0.42
14:CN:46:ASP:OD1	14:CN:46:ASP:N	2.52	0.42
23:CC:155:MET:HB3	23:CC:156:PRO:HD3	2.02	0.42
35:CF:191:VAL:O	35:CF:191:VAL:HG22	2.18	0.42
39:CH:179:LEU:HD23	39:CH:179:LEU:N	2.35	0.42
1:5:1599:C:H2'	1:5:1600:C:C6	2.54	0.42
1:5:2150:A:C3'	1:5:2151:A:C8	3.03	0.42
1:5:2181:G:H2'	1:5:2182:C:C6	2.54	0.42
1:5:2209:A:H4'	1:5:2210:U:OP1	2.20	0.42
1:5:2636:A:H4'	1:5:2637:A:O5'	2.20	0.42
1:5:2774:C:C2	1:5:2775:U:C5	3.07	0.42
14:CN:3:ALA:HB1	37:CG:160:TRP:HZ2	1.85	0.42
40:Ci:12:VAL:HG23	40:Ci:13:GLY:H	1.85	0.42
1:5:373:G:O2'	1:5:398:U:O4	2.30	0.42
1:5:1003:G:O2'	1:5:1004:G:H5'	2.20	0.42
1:5:1010:G:O2'	1:5:1011:C:C6	2.68	0.42
1:5:1604:U:O2	1:5:1604:U:O4'	2.38	0.42
1:5:2102:G:C8	1:5:2102:G:OP2	2.72	0.42
1:5:2126:G:H22	1:5:2330:C:H5	1.67	0.42
1:5:3181:U:O2	1:5:3185:A:H4'	2.19	0.42
8:CL:165:VAL:HG11	15:Ca:97:LEU:HD22	2.02	0.42
13:7:136:C:H2'	13:7:137:C:C6	2.55	0.42
14:CN:121:LEU:HB3	14:CN:129:TYR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CP:77:HIS:NE2	20:CP:79:ASN:OD1	2.53	0.42
23:CC:23:GLN:N	23:CC:23:GLN:OE1	2.53	0.42
35:CF:221:TYR:N	35:CF:227:ALA:O	2.52	0.42
1:5:248:A:N1	38:Ch:112:MET:HE1	2.35	0.42
1:5:922:A:O4'	3:CA:197:PRO:HG2	2.20	0.42
1:5:1207:A:O2'	1:5:1209:C:N4	2.52	0.42
1:5:1398:C:OP1	29:Ce:79:ASN:ND2	2.52	0.42
1:5:2907:C:C2	1:5:2908:A:C8	3.07	0.42
1:5:3084:C:O2'	1:5:3320:U:OP1	2.30	0.42
31:CE:131:LEU:HD11	31:CE:198:VAL:HG11	2.02	0.42
41:CI:123:LEU:H	41:CI:123:LEU:HD23	1.85	0.42
1:5:130:C:H3'	1:5:131:U:O4'	2.20	0.41
1:5:527:C:C6	1:5:550:G:C2	3.08	0.41
1:5:610:G:N2	31:CE:44:VAL:HG23	2.35	0.41
1:5:1743:A:O2'	1:5:1744:G:O4'	2.36	0.41
1:5:2846:A:N3	1:5:2846:A:H2'	2.35	0.41
1:5:3113:A:O2'	39:CH:71:ALA:O	2.38	0.41
1:5:3239:G:C5	1:5:3240:U:C4	3.08	0.41
21:Cc:51:ASN:OD1	21:Cc:78:ASN:N	2.50	0.41
31:CE:89:ILE:N	31:CE:89:ILE:HD12	2.34	0.41
38:Ch:44:LEU:O	38:Ch:47:ILE:HG22	2.19	0.41
1:5:575:C:N3	1:5:619:G:N2	2.68	0.41
1:5:632:U:H1'	1:5:633:G:OP1	2.20	0.41
1:5:987:G:H2'	1:5:991:G:O4'	2.20	0.41
1:5:1188:A:N3	1:5:1339:C:O2'	2.53	0.41
1:5:1810:A:H2'	1:5:1811:G:C5'	2.50	0.41
1:5:2391:A:H2'	1:5:2392:OMG:O4'	2.21	0.41
1:5:2682:U:OP1	43:CJ:53:ARG:N	2.46	0.41
1:5:2782:U:O2	1:5:2782:U:O4'	2.37	0.41
1:5:2847:U:C2	1:5:2851:G:O6	2.73	0.41
6:Cl:8:MET:HE2	42:Cj:18:LEU:HD12	2.02	0.41
13:7:104:U:O2	13:7:104:U:O4'	2.38	0.41
35:CF:81:ALA:O	35:CF:82:LYS:HB2	2.20	0.41
1:5:162:U:H2'	1:5:163:C:O4'	2.20	0.41
1:5:1326:U:OP1	18:CO:23:ARG:NH2	2.49	0.41
1:5:2208:A:H2'	1:5:2209:A:C2	2.55	0.41
1:5:2882:C:H2'	1:5:2883:U:C6	2.55	0.41
1:5:3017:A:H2'	1:5:3018:C:H5'	2.02	0.41
8:CL:48:PRO:HB2	8:CL:152:TYR:CE1	2.56	0.41
9:6:52:U:H1'	43:CJ:11:MET:HE3	2.01	0.41
27:CD:41:LYS:HE2	28:CT:93:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Ce:61:ASP:OD1	29:Ce:62:LYS:N	2.53	0.41
1:5:620:G:O6	23:CC:319:VAL:HG13	2.21	0.41
1:5:1809:G:H2'	1:5:1810:A:H5"	2.02	0.41
1:5:2718:U:O2	1:5:2718:U:O4'	2.35	0.41
1:5:3239:G:C2'	1:5:3240:U:O5'	2.69	0.41
3:CA:196:TRP:CD2	3:CA:196:TRP:C	2.93	0.41
4:CK:72:LEU:HD12	4:CK:72:LEU:N	2.35	0.41
9:6:73:U:OP2	9:6:74:A:O2'	2.30	0.41
25:Cd:86:ASP:OD1	25:Cd:87:GLU:N	2.54	0.41
31:CE:97:ILE:O	31:CE:98:LEU:HD12	2.19	0.41
1:5:154:G:OP2	40:Ci:28:ARG:NH1	2.54	0.41
1:5:532:G:H21	1:5:546:U:H3	1.68	0.41
1:5:954:C:H2'	1:5:955:C:C6	2.56	0.41
1:5:1160:A:C2	1:5:1161:U:C5	3.09	0.41
1:5:1596:G:H4'	1:5:1597:A:OP1	2.20	0.41
1:5:1704:C:O2'	1:5:1705:U:O5'	2.38	0.41
1:5:2949:OMC:HM22	1:5:2949:OMC:H1'	1.91	0.41
1:5:3004:C:O2'	1:5:3005:G:H5'	2.21	0.41
1:5:3266:C:H5"	1:5:3267:A:OP1	2.21	0.41
12:CM:63:ASN:N	12:CM:63:ASN:OD1	2.53	0.41
13:7:80:C:H2'	13:7:81:A:O4'	2.20	0.41
22:CQ:175:LYS:O	22:CQ:176:ALA:HB3	2.20	0.41
35:CF:215:LYS:O	35:CF:216:LYS:HG3	2.20	0.41
1:5:727:U:O2'	1:5:763:G:OP1	2.34	0.41
1:5:2392:OMG:HM22	1:5:2392:OMG:H1'	1.89	0.41
1:5:2392:OMG:H2'	1:5:2393:C:C6	2.56	0.41
1:5:2717:U:C2	1:5:2718:U:O2	2.74	0.41
1:5:2839:A:H61	1:5:2851:G:C2'	2.30	0.41
1:5:44:OMU:HM23	1:5:44:OMU:H1'	1.77	0.41
1:5:159:G:C5	1:5:160:C:C5	3.09	0.41
1:5:404:A:C2	13:7:21:A:H1'	2.55	0.41
1:5:531:G:HO2'	1:5:532:G:C1'	2.30	0.41
1:5:799:U:OP1	23:CC:119:ARG:NH2	2.52	0.41
1:5:2750:G:C4	1:5:2751:C:C5	3.08	0.41
11:CZ:42:LEU:C	11:CZ:42:LEU:HD23	2.46	0.41
1:5:161:G:C4	1:5:162:U:C5	3.08	0.41
1:5:1728:C:O2'	1:5:1729:C:O5'	2.38	0.41
1:5:1951:G:O6	1:5:2101:A:C2	2.74	0.41
1:5:3159:C:C2	1:5:3160:C:C5	3.08	0.41
2:Ck:47:VAL:HG22	2:Ck:49:ASP:H	1.85	0.41
26:CS:174:LEU:N	26:CS:174:LEU:HD22	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CH:77:LEU:O	39:CH:80:VAL:HG12	2.21	0.41
43:CJ:23:ILE:O	43:CJ:68:ALA:HB1	2.19	0.41
1:5:763:G:H2'	1:5:764:A:H8	1.85	0.41
1:5:882:C:H3'	1:5:883:U:H4'	2.02	0.41
1:5:1013:A:N1	1:5:1061:U:O2'	2.47	0.41
1:5:1116:G:O2'	1:5:1117:C:H5'	2.21	0.41
1:5:1457:G:O2'	1:5:2356:G:O6	2.37	0.41
1:5:1940:A:H2'	1:5:1941:U:C6	2.56	0.41
1:5:1953:G:N3	1:5:1953:G:H2'	2.35	0.41
1:5:2561:A:O2'	1:5:2562:G:O4'	2.39	0.41
1:5:2583:C:O2'	1:5:2584:C:H5'	2.21	0.41
1:5:2735:A:H2'	1:5:2736:OMU:H6	2.03	0.41
1:5:2840:G:OP1	41:CI:78:LYS:NZ	2.54	0.41
1:5:2847:U:O2	1:5:2851:G:O6	2.39	0.41
1:5:3307:C:H2'	1:5:3308:G:C1'	2.51	0.41
8:CL:89:ALA:HB3	8:CL:90:PRO:HD3	2.03	0.41
18:CO:17:ARG:NH1	18:CO:45:GLU:OE1	2.46	0.41
35:CF:9:PRO:O	35:CF:12:VAL:HG22	2.20	0.41
37:CG:204:LEU:HD23	37:CG:204:LEU:H	1.85	0.41
1:5:391:C:OP1	7:CY:86:ARG:NH1	2.44	0.41
1:5:1054:C:O2	1:5:1054:C:O4'	2.37	0.41
1:5:1208:C:H2'	1:5:1209:C:O5'	2.21	0.41
1:5:1572:G:C6	1:5:1573:C:C4	3.09	0.41
1:5:1573:C:C4	1:5:1574:U:C2	3.09	0.41
1:5:2288:C:HO2'	1:5:2289:OMG:P	2.39	0.41
1:5:2772:A:C5	1:5:2774:C:C5	3.08	0.41
26:CS:115:ASN:OD1	26:CS:115:ASN:N	2.53	0.41
1:5:401:U:N3	1:5:402:U:C5	2.89	0.40
1:5:631:G:C2'	1:5:632:U:H3'	2.51	0.40
1:5:2134:C:O2	1:5:2134:C:H2'	2.21	0.40
1:5:2139:U:C6	1:5:2143:U:C4	3.09	0.40
1:5:2815:G:O2'	1:5:2816:OMG:P	2.78	0.40
13:7:57:A:C4	13:7:58:A:C8	3.10	0.40
13:7:135:G:C2	13:7:136:C:C4	3.09	0.40
14:CN:148:ILE:O	14:CN:148:ILE:HG13	2.22	0.40
19:CB:33:PRO:HD2	19:CB:44:THR:HG21	2.02	0.40
19:CB:83:ALA:O	19:CB:167:GLN:NE2	2.54	0.40
27:CD:28:THR:HG22	27:CD:29:ASP:N	2.36	0.40
30:CV:139:ILE:N	30:CV:139:ILE:HD12	2.36	0.40
36:Cg:25:THR:OG1	36:Cg:26:PRO:HD2	2.21	0.40
37:CG:87:LEU:O	37:CG:90:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:648:C:O2	1:5:2378:G:O2'	2.29	0.40
1:5:769:G:C2'	1:5:770:A:OP2	2.70	0.40
1:5:779:G:H2'	1:5:780:A:C8	2.56	0.40
1:5:1810:A:H2'	1:5:1811:G:O5'	2.22	0.40
1:5:2160:A:H5'	1:5:2162:G:O4'	2.21	0.40
1:5:2268:C:H2'	1:5:2269:U:C6	2.56	0.40
1:5:2323:C:O2'	1:5:2324:G:H5'	2.21	0.40
1:5:2440:A:C2	1:5:2441:A:H1'	2.56	0.40
3:CA:36:GLU:OE2	3:CA:163:ARG:NH1	2.45	0.40
9:6:103:U:O2	9:6:103:U:H2'	2.21	0.40
13:7:125:A:H62	13:7:138:G:C2'	2.35	0.40
18:CO:147:SER:HA	18:CO:150:VAL:HG12	2.03	0.40
19:CB:220:ILE:HD12	19:CB:220:ILE:N	2.35	0.40
19:CB:288:LEU:HD23	19:CB:288:LEU:C	2.46	0.40
25:Cd:84:ASN:N	25:Cd:92:GLU:O	2.47	0.40
1:5:532:G:H1'	1:5:545:U:O4	2.22	0.40
1:5:619:G:H21	31:CE:77:ARG:HH22	1.68	0.40
1:5:1821:C:H2'	1:5:1822:C:C6	2.57	0.40
1:5:2150:A:O3'	1:5:2151:A:H8	2.03	0.40
1:5:2620:OMG:N3	1:5:2620:OMG:H2'	2.37	0.40
1:5:3243:G:H2'	1:5:3244:G:O4'	2.21	0.40
18:CO:32:LEU:HD21	18:CO:38:VAL:HG22	2.03	0.40
34:CX:103:ASP:N	34:CX:103:ASP:OD1	2.53	0.40
39:CH:11:ASP:OD1	39:CH:12:ILE:N	2.54	0.40
39:CH:139:ARG:HA	39:CH:147:ILE:HA	2.03	0.40
1:5:1503:G:OP2	1:5:1503:G:N2	2.48	0.40
1:5:1542:C:H2'	1:5:1543:U:C6	2.56	0.40
1:5:2251:G:O6	1:5:2268:C:N4	2.54	0.40
1:5:2271:A:C2'	1:5:2272:A:O5'	2.69	0.40
2:Ck:54:ASP:O	2:Ck:58:GLN:HG2	2.22	0.40
18:CO:188:LYS:O	18:CO:191:GLU:HG3	2.22	0.40
27:CD:103:LEU:HD23	27:CD:246:ILE:HD11	2.02	0.40
27:CD:209:LEU:HD13	27:CD:209:LEU:C	2.46	0.40
30:CV:99:GLU:OE1	32:CW:26:SER:N	2.52	0.40
31:CE:195:GLN:NE2	31:CE:199:ASP:OD1	2.55	0.40
43:CJ:89:LYS:O	43:CJ:90:GLU:HB2	2.21	0.40
1:5:420:A:H2'	1:5:421:G:O4'	2.21	0.40
1:5:684:G:C6	1:5:800:G:C6	3.10	0.40
1:5:1513:A:C4	1:5:1514:A:C8	3.10	0.40
1:5:1571:C:C1'	1:5:1572:G:P	3.08	0.40
1:5:1685:A:H2'	1:5:1686:U:H5'	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2656:U:H2'	4:CK:97:LYS:O	2.21	0.40
1:5:3113:A:H2'	1:5:3114:A:O4'	2.22	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	
2	Ck	66/69 (96%)	62 (94%)	4 (6%)	0	100	100
3	CA	244/258 (95%)	230 (94%)	11 (4%)	3 (1%)	10	34
4	CK	79/105 (75%)	75 (95%)	4 (5%)	0	100	100
5	Cp	87/92 (95%)	81 (93%)	6 (7%)	0	100	100
6	Cl	48/51 (94%)	40 (83%)	8 (17%)	0	100	100
7	CY	128/146 (88%)	124 (97%)	4 (3%)	0	100	100
8	CL	196/206 (95%)	184 (94%)	12 (6%)	0	100	100
10	Cm	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
11	CZ	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
12	CM	129/134 (96%)	124 (96%)	5 (4%)	0	100	100
14	CN	201/204 (98%)	185 (92%)	16 (8%)	0	100	100
15	Ca	143/146 (98%)	133 (93%)	10 (7%)	0	100	100
16	w	64/124 (52%)	62 (97%)	2 (3%)	0	100	100
17	Cb	47/83 (57%)	38 (81%)	9 (19%)	0	100	100
18	CO	202/206 (98%)	197 (98%)	5 (2%)	0	100	100
19	CB	384/389 (99%)	362 (94%)	22 (6%)	0	100	100
20	CP	154/176 (88%)	148 (96%)	6 (4%)	0	100	100
21	Cc	87/112 (78%)	76 (87%)	9 (10%)	2 (2%)	5	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	CQ	184/187 (98%)	172 (94%)	12 (6%)	0	100	100
23	CC	395/406 (97%)	369 (93%)	26 (7%)	0	100	100
24	CR	167/209 (80%)	160 (96%)	7 (4%)	0	100	100
25	Cd	111/119 (93%)	101 (91%)	10 (9%)	0	100	100
26	CS	175/217 (81%)	167 (95%)	8 (5%)	0	100	100
27	CD	250/301 (83%)	240 (96%)	10 (4%)	0	100	100
28	CT	157/164 (96%)	147 (94%)	10 (6%)	0	100	100
29	Ce	124/133 (93%)	121 (98%)	3 (2%)	0	100	100
30	CV	127/140 (91%)	125 (98%)	2 (2%)	0	100	100
31	CE	174/233 (75%)	165 (95%)	9 (5%)	0	100	100
32	CW	61/164 (37%)	59 (97%)	2 (3%)	0	100	100
33	Cf	106/111 (96%)	102 (96%)	4 (4%)	0	100	100
34	CX	115/154 (75%)	112 (97%)	3 (3%)	0	100	100
35	CF	232/242 (96%)	222 (96%)	10 (4%)	0	100	100
36	Cg	107/120 (89%)	105 (98%)	2 (2%)	0	100	100
37	CG	229/257 (89%)	215 (94%)	14 (6%)	0	100	100
38	Ch	119/123 (97%)	114 (96%)	5 (4%)	0	100	100
39	CH	190/194 (98%)	176 (93%)	14 (7%)	0	100	100
40	Ci	92/112 (82%)	89 (97%)	3 (3%)	0	100	100
41	CI	198/221 (90%)	191 (96%)	7 (4%)	0	100	100
42	Cj	86/95 (90%)	78 (91%)	8 (9%)	0	100	100
43	CJ	168/182 (92%)	163 (97%)	5 (3%)	0	100	100
All	All	6008/6848 (88%)	5686 (95%)	317 (5%)	5 (0%)	49	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	Cc	91	VAL
3	CA	196	TRP
3	CA	198	LYS
21	Cc	46	ILE
3	CA	197	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Ck	64/65 (98%)	63 (98%)	1 (2%)	55 83
3	CA	191/197 (97%)	189 (99%)	2 (1%)	68 89
4	CK	67/93 (72%)	67 (100%)	0	100 100
5	Cp	73/76 (96%)	69 (94%)	4 (6%)	19 50
6	Cl	47/48 (98%)	46 (98%)	1 (2%)	47 77
7	CY	118/133 (89%)	116 (98%)	2 (2%)	53 82
8	CL	170/177 (96%)	166 (98%)	4 (2%)	43 75
10	Cm	48/115 (42%)	48 (100%)	0	100 100
11	CZ	116/117 (99%)	116 (100%)	0	100 100
12	CM	115/116 (99%)	114 (99%)	1 (1%)	70 90
14	CN	179/180 (99%)	178 (99%)	1 (1%)	78 93
15	Ca	120/121 (99%)	120 (100%)	0	100 100
16	w	31/104 (30%)	31 (100%)	0	100 100
17	Cb	29/71 (41%)	28 (97%)	1 (3%)	32 66
18	CO	175/177 (99%)	172 (98%)	3 (2%)	53 82
19	CB	327/330 (99%)	321 (98%)	6 (2%)	51 80
20	CP	132/148 (89%)	132 (100%)	0	100 100
21	Cc	77/96 (80%)	75 (97%)	2 (3%)	40 73
22	CQ	156/157 (99%)	155 (99%)	1 (1%)	78 93
23	CC	328/331 (99%)	325 (99%)	3 (1%)	70 90
24	CR	148/179 (83%)	145 (98%)	3 (2%)	48 78
25	Cd	98/104 (94%)	98 (100%)	0	100 100
26	CS	161/198 (81%)	158 (98%)	3 (2%)	50 79
27	CD	217/254 (85%)	215 (99%)	2 (1%)	70 90
28	CT	136/139 (98%)	135 (99%)	1 (1%)	76 92
29	Ce	114/121 (94%)	113 (99%)	1 (1%)	70 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	CV	103/110 (94%)	102 (99%)	1 (1%)	68 89
31	CE	151/197 (77%)	149 (99%)	2 (1%)	61 86
32	CW	58/137 (42%)	58 (100%)	0	100 100
33	Cf	95/97 (98%)	95 (100%)	0	100 100
34	CX	108/136 (79%)	106 (98%)	2 (2%)	50 79
35	CF	204/212 (96%)	202 (99%)	2 (1%)	68 89
36	Cg	96/104 (92%)	94 (98%)	2 (2%)	47 77
37	CG	202/221 (91%)	201 (100%)	1 (0%)	81 93
38	Ch	109/110 (99%)	107 (98%)	2 (2%)	51 80
39	CH	173/175 (99%)	169 (98%)	4 (2%)	44 76
40	Ci	81/94 (86%)	79 (98%)	2 (2%)	42 74
41	CI	168/179 (94%)	168 (100%)	0	100 100
42	Cj	74/78 (95%)	74 (100%)	0	100 100
43	CJ	148/158 (94%)	145 (98%)	3 (2%)	48 78
All	All	5207/5855 (89%)	5144 (99%)	63 (1%)	61 86

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Ck	19	ASP
3	CA	119	HIS
3	CA	143	ASN
5	Cp	40	GLU
5	Cp	51	VAL
5	Cp	57	CYS
5	Cp	64	LYS
6	Cl	37	TYR
7	CY	55	VAL
7	CY	70	VAL
8	CL	61	THR
8	CL	152	TYR
8	CL	153	LEU
8	CL	156	VAL
12	CM	63	ASN
14	CN	180	ASN
17	Cb	65	GLN
18	CO	76	ILE

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Mol	Chain	Res	Type
18	CO	115	THR
18	CO	129	LEU
19	CB	29	VAL
19	CB	86	VAL
19	CB	182	MET
19	CB	187	ASN
19	CB	202	PHE
19	CB	259	HIS
21	Cc	88	TYR
21	Cc	91	VAL
22	CQ	187	VAL
23	CC	136	THR
23	CC	236	CYS
23	CC	319	VAL
24	CR	57	ILE
24	CR	140	GLU
24	CR	143	HIS
26	CS	75	GLU
26	CS	115	ASN
26	CS	151	MET
27	CD	202	HIS
27	CD	266	TYR
28	CT	27	LEU
29	Ce	50	VAL
30	CV	36	ASN
31	CE	230	GLU
31	CE	232	VAL
34	CX	103	ASP
34	CX	116	ASP
35	CF	119	VAL
35	CF	165	ASP
36	Cg	89	GLU
36	Cg	109	LEU
37	CG	53	ILE
38	Ch	4	ILE
38	Ch	71	GLU
39	CH	41	LEU
39	CH	130	GLU
39	CH	149	LEU
39	CH	179	LEU
40	Ci	12	VAL
40	Ci	62	GLU

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Mol	Chain	Res	Type
43	CJ	59	PHE
43	CJ	65	GLU
43	CJ	166	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	CA	119	HIS
8	CL	102	ASN
10	Cm	91	GLN
11	CZ	33	ASN
12	CM	34	ASN
15	Ca	14	HIS
15	Ca	41	HIS
15	Ca	113	HIS
16	w	106	ASN
17	Cb	34	GLN
18	CO	170	HIS
19	CB	193	GLN
20	CP	90	GLN
22	CQ	58	ASN
23	CC	43	ASN
23	CC	46	HIS
23	CC	48	GLN
23	CC	94	GLN
23	CC	117	HIS
26	CS	103	ASN
26	CS	130	ASN
29	Ce	79	ASN
33	Cf	81	ASN
35	CF	110	GLN
35	CF	113	ASN
35	CF	159	GLN
35	CF	166	ASN
35	CF	206	GLN
35	CF	232	ASN
36	Cg	70	ASN
37	CG	74	GLN
41	CI	177	ASN
42	Cj	30	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	2939/3381 (86%)	609 (20%)	72 (2%)
13	7	148/164 (90%)	28 (18%)	1 (0%)
9	6	118/121 (97%)	23 (19%)	0
All	All	3205/3666 (87%)	660 (20%)	73 (2%)

All (660) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	2	C
1	5	3	G
1	5	5	C
1	5	24	A
1	5	38	A
1	5	41	A
1	5	44	OMU
1	5	45	C
1	5	47	A
1	5	58	A
1	5	64	A
1	5	66	C
1	5	70	C
1	5	73	G
1	5	74	G
1	5	87	A
1	5	90	G
1	5	97	A
1	5	107	A
1	5	108	G
1	5	112	A
1	5	113	G
1	5	114	C
1	5	116	U
1	5	118	A
1	5	119	A
1	5	120	A
1	5	122	U
1	5	130	C
1	5	131	U
1	5	133	C
1	5	154	G
1	5	155	A

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Mol	Chain	Res	Type
1	5	162	U
1	5	167	A
1	5	176	C
1	5	184	A
1	5	187	U
1	5	197	A
1	5	215	G
1	5	216	A
1	5	217	G
1	5	218	A
1	5	225	U
1	5	234	G
1	5	235	A
1	5	236	C
1	5	238	C
1	5	246	C
1	5	247	C
1	5	248	A
1	5	250	G
1	5	251	A
1	5	258	G
1	5	266	G
1	5	267	U
1	5	302	U
1	5	320	A
1	5	326	G
1	5	365	G
1	5	373	G
1	5	382	A
1	5	391	C
1	5	396	A
1	5	398	U
1	5	399	G
1	5	419	A
1	5	432	C
1	5	435	G
1	5	436	C
1	5	499	C
1	5	523	U
1	5	524	A
1	5	526	G
1	5	528	C

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Mol	Chain	Res	Type
1	5	529	C
1	5	531	G
1	5	535	U
1	5	542	C
1	5	546	U
1	5	548	U
1	5	554	C
1	5	556	U
1	5	572	G
1	5	573	G
1	5	574	U
1	5	576	U
1	5	578	C
1	5	579	A
1	5	606	A
1	5	609	A
1	5	611	C
1	5	612	G
1	5	614	G
1	5	618	C
1	5	619	G
1	5	620	G
1	5	621	G
1	5	630	U
1	5	633	G
1	5	638	C
1	5	649	C
1	5	650	C
1	5	656	G
1	5	657	1MA
1	5	658	A
1	5	660	C
1	5	661	A2M
1	5	672	A
1	5	675	OMC
1	5	676	OMU
1	5	689	A
1	5	694	A
1	5	699	U
1	5	701	A
1	5	702	G
1	5	703	U

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Mol	Chain	Res	Type
1	5	706	A
1	5	711	U
1	5	712	A
1	5	729	A
1	5	730	U
1	5	732	G
1	5	748	G
1	5	769	G
1	5	770	A
1	5	774	U
1	5	779	G
1	5	780	A
1	5	781	A
1	5	783	G
1	5	785	U
1	5	789	A
1	5	790	G
1	5	794	G
1	5	814	OMG
1	5	815	A
1	5	817	A
1	5	826	A
1	5	855	A
1	5	856	A
1	5	862	G
1	5	870	C
1	5	883	U
1	5	888	U
1	5	889	G
1	5	903	U
1	5	904	G
1	5	905	A
1	5	906	C
1	5	916	G
1	5	917	OMG
1	5	918	G
1	5	923	A
1	5	925	G
1	5	926	A
1	5	933	G
1	5	945	A2M
1	5	946	G

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Mol	Chain	Res	Type
1	5	948	U
1	5	953	C
1	5	968	C
1	5	969	U
1	5	971	A
1	5	983	G
1	5	991	G
1	5	992	C
1	5	995	G
1	5	1005	G
1	5	1011	C
1	5	1012	C
1	5	1013	A
1	5	1021	G
1	5	1058	A
1	5	1060	C
1	5	1068	A
1	5	1074	G
1	5	1075	A
1	5	1076	C
1	5	1087	C
1	5	1092	U
1	5	1104	A
1	5	1105	C
1	5	1106	G
1	5	1107	G
1	5	1108	A
1	5	1113	A
1	5	1114	G
1	5	1127	G
1	5	1141	G
1	5	1142	C
1	5	1143	A2M
1	5	1163	A
1	5	1164	A
1	5	1169	A
1	5	1192	G
1	5	1201	C
1	5	1208	C
1	5	1209	C
1	5	1210	C
1	5	1211	A

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Mol	Chain	Res	Type
1	5	1212	C
1	5	1220	G
1	5	1227	G
1	5	1301	A
1	5	1306	G
1	5	1313	A
1	5	1318	G
1	5	1319	A
1	5	1320	U
1	5	1325	C
1	5	1327	U
1	5	1328	A
1	5	1349	C
1	5	1359	A
1	5	1360	A
1	5	1361	G
1	5	1363	G
1	5	1364	C
1	5	1366	A
1	5	1367	G
1	5	1409	A
1	5	1410	G
1	5	1412	G
1	5	1415	C
1	5	1416	G
1	5	1429	G
1	5	1440	U
1	5	1444	G
1	5	1445	A
1	5	1446	U
1	5	1447	OMC
1	5	1448	U
1	5	1460	OMG
1	5	1461	C
1	5	1462	A
1	5	1491	A
1	5	1492	A
1	5	1493	G
1	5	1517	G
1	5	1518	C
1	5	1521	U
1	5	1537	C

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Mol	Chain	Res	Type
1	5	1559	C
1	5	1564	C
1	5	1565	U
1	5	1566	G
1	5	1569	A
1	5	1570	G
1	5	1571	C
1	5	1572	G
1	5	1575	U
1	5	1577	A
1	5	1578	G
1	5	1590	A
1	5	1592	A
1	5	1597	A
1	5	1599	C
1	5	1608	A
1	5	1612	C
1	5	1622	A
1	5	1631	U
1	5	1632	U
1	5	1639	A
1	5	1641	C
1	5	1645	A
1	5	1647	G
1	5	1659	C
1	5	1679	A
1	5	1685	A
1	5	1686	U
1	5	1687	C
1	5	1688	U
1	5	1695	U
1	5	1705	U
1	5	1706	G
1	5	1715	G
1	5	1728	C
1	5	1729	C
1	5	1743	A
1	5	1744	G
1	5	1745	C
1	5	1753	A
1	5	1754	G
1	5	1762	C

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Mol	Chain	Res	Type
1	5	1779	G
1	5	1783	C
1	5	1784	G
1	5	1797	C
1	5	1801	A
1	5	1810	A
1	5	1811	G
1	5	1816	G
1	5	1818	G
1	5	1819	U
1	5	1825	U
1	5	1834	G
1	5	1846	A
1	5	1847	OMC
1	5	1848	C
1	5	1853	C
1	5	1855	OMG
1	5	1869	A
1	5	1870	C
1	5	1882	G
1	5	1883	A
1	5	1884	U
1	5	1889	C
1	5	1890	A
1	5	1897	G
1	5	1910	G
1	5	1911	C
1	5	1941	U
1	5	1953	G
1	5	1954	C
1	5	2101	A
1	5	2102	G
1	5	2113	G
1	5	2114	U
1	5	2115	A
1	5	2120	C
1	5	2123	G
1	5	2124	G
1	5	2125	OMG
1	5	2126	G
1	5	2127	A2M
1	5	2128	A

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Mol	Chain	Res	Type
1	5	2133	A
1	5	2142	U
1	5	2157	G
1	5	2158	C
1	5	2160	A
1	5	2161	U
1	5	2171	G
1	5	2177	U
1	5	2185	U
1	5	2186	G
1	5	2206	U
1	5	2207	G
1	5	2208	A
1	5	2209	A
1	5	2210	U
1	5	2217	G
1	5	2218	U
1	5	2221	A2M
1	5	2222	G
1	5	2245	A
1	5	2250	G
1	5	2252	G
1	5	2253	A
1	5	2262	G
1	5	2263	A
1	5	2264	C
1	5	2269	U
1	5	2270	U
1	5	2272	A
1	5	2273	G
1	5	2274	G
1	5	2277	G
1	5	2279	5MC
1	5	2280	A
1	5	2281	A
1	5	2289	OMG
1	5	2290	U
1	5	2294	OMC
1	5	2295	U
1	5	2299	U
1	5	2308	G
1	5	2311	U

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Mol	Chain	Res	Type
1	5	2314	A
1	5	2315	U
1	5	2316	G
1	5	2327	A
1	5	2335	U
1	5	2337	U
1	5	2338	OMC
1	5	2365	G
1	5	2366	OMC
1	5	2367	C
1	5	2371	G
1	5	2374	A
1	5	2375	C
1	5	2376	G
1	5	2386	G
1	5	2392	OMG
1	5	2393	C
1	5	2394	G
1	5	2396	OMG
1	5	2397	G
1	5	2398	A
1	5	2402	A
1	5	2403	A
1	5	2404	G
1	5	2405	A
1	5	2410	OMG
1	5	2411	U
1	5	2412	U
1	5	2418	U
1	5	2419	G
1	5	2420	A
1	5	2422	OMU
1	5	2436	G
1	5	2437	U
1	5	2439	A
1	5	2441	A
1	5	2515	U
1	5	2516	A
1	5	2523	G
1	5	2524	A
1	5	2532	G
1	5	2533	C

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Mol	Chain	Res	Type
1	5	2534	G
1	5	2549	U
1	5	2554	G
1	5	2561	A
1	5	2562	G
1	5	2564	C
1	5	2574	C
1	5	2576	G
1	5	2585	G
1	5	2594	A
1	5	2596	A
1	5	2607	G
1	5	2608	G
1	5	2615	G
1	5	2620	OMG
1	5	2621	G
1	5	2628	C
1	5	2636	A
1	5	2638	A
1	5	2645	C
1	5	2653	U
1	5	2656	U
1	5	2657	A
1	5	2675	A
1	5	2678	G
1	5	2680	A
1	5	2682	U
1	5	2683	OMC
1	5	2690	G
1	5	2691	G
1	5	2692	A
1	5	2695	A
1	5	2705	A
1	5	2715	G
1	5	2717	U
1	5	2719	C
1	5	2729	G
1	5	2730	U
1	5	2738	C
1	5	2751	C
1	5	2753	U
1	5	2754	G

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Mol	Chain	Res	Type
1	5	2756	C
1	5	2763	A
1	5	2773	C
1	5	2774	C
1	5	2778	G
1	5	2779	G
1	5	2792	OMG
1	5	2793	A
1	5	2800	A
1	5	2801	G
1	5	2802	A
1	5	2804	A
1	5	2811	C
1	5	2815	G
1	5	2816	OMG
1	5	2817	G
1	5	2818	A
1	5	2839	A
1	5	2843	U
1	5	2844	U
1	5	2845	C
1	5	2846	A
1	5	2848	A
1	5	2857	G
1	5	2860	U
1	5	2861	U
1	5	2868	C
1	5	2871	5MC
1	5	2872	G
1	5	2873	A
1	5	2876	U
1	5	2880	OMC
1	5	2881	U
1	5	2884	OMU
1	5	2885	C
1	5	2888	A
1	5	2889	U
1	5	2890	C
1	5	2918	OMG
1	5	2919	G
1	5	2924	U
1	5	2931	A

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Mol	Chain	Res	Type
1	5	2934	A
1	5	2935	A
1	5	2936	U
1	5	2937	A
1	5	2942	A
1	5	2948	G
1	5	2949	OMC
1	5	2950	U
1	5	2967	G
1	5	2972	A
1	5	2973	G
1	5	2979	U
1	5	2980	U
1	5	2984	C
1	5	2997	C
1	5	2998	G
1	5	3001	U
1	5	3003	G
1	5	3005	G
1	5	3006	A
1	5	3012	A
1	5	3018	C
1	5	3037	U
1	5	3039	G
1	5	3058	C
1	5	3059	G
1	5	3071	A
1	5	3072	A
1	5	3078	G
1	5	3079	U
1	5	3086	A
1	5	3092	C
1	5	3093	C
1	5	3095	U
1	5	3101	G
1	5	3103	A
1	5	3121	U
1	5	3122	A
1	5	3131	U
1	5	3142	A
1	5	3143	G
1	5	3151	U

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Mol	Chain	Res	Type
1	5	3152	G
1	5	3153	C
1	5	3154	G
1	5	3158	G
1	5	3161	G
1	5	3164	C
1	5	3166	A
1	5	3167	U
1	5	3173	A
1	5	3174	C
1	5	3175	C
1	5	3177	U
1	5	3178	C
1	5	3180	G
1	5	3181	U
1	5	3184	G
1	5	3190	A
1	5	3197	A
1	5	3204	C
1	5	3205	G
1	5	3207	G
1	5	3208	U
1	5	3211	U
1	5	3212	U
1	5	3216	U
1	5	3218	A
1	5	3220	U
1	5	3232	A
1	5	3240	U
1	5	3243	G
1	5	3249	C
1	5	3258	A
1	5	3259	U
1	5	3260	A
1	5	3267	A
1	5	3269	C
1	5	3271	A
1	5	3272	G
1	5	3280	U
1	5	3281	A
1	5	3292	C
1	5	3299	C

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Mol	Chain	Res	Type
1	5	3300	OMU
1	5	3305	U
1	5	3306	A
1	5	3307	C
1	5	3317	U
1	5	3322	U
1	5	3329	C
1	5	3330	A
1	5	3331	G
1	5	3332	A
1	5	3333	G
1	5	3335	G
1	5	3337	C
1	5	3338	C
1	5	3339	U
1	5	3340	U
1	5	3341	G
1	5	3342	C
1	5	3343	U
1	5	3346	C
1	5	3347	A
1	5	3348	C
1	5	3357	G
1	5	3366	C
1	5	3370	U
1	5	3371	U
1	5	3375	G
1	5	3378	A
1	5	3379	A
1	5	3386	A
9	6	7	G
9	6	12	U
9	6	20	C
9	6	22	A
9	6	33	U
9	6	35	C
9	6	41	G
9	6	47	C
9	6	48	G
9	6	50	A
9	6	51	G
9	6	53	U

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Mol	Chain	Res	Type
9	6	54	A
9	6	61	C
9	6	64	G
9	6	86	G
9	6	89	G
9	6	100	A
9	6	101	A
9	6	103	U
9	6	110	G
9	6	112	U
9	6	118	C
13	7	11	U
13	7	12	C
13	7	19	G
13	7	20	G
13	7	27	C
13	7	38	U
13	7	39	C
13	7	63	A
13	7	66	C
13	7	67	U
13	7	79	G
13	7	83	A
13	7	84	A
13	7	91	G
13	7	92	A
13	7	94	C
13	7	95	C
13	7	99	G
13	7	108	A
13	7	110	C
13	7	115	G
13	7	124	C
13	7	129	C
13	7	136	C
13	7	141	G
13	7	146	G
13	7	157	U
13	7	163	A

All (73) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	112	A
1	5	113	G
1	5	130	C
1	5	214	U
1	5	390	U
1	5	534	U
1	5	620	G
1	5	632	U
1	5	656	G
1	5	698	G
1	5	814	OMG
1	5	882	C
1	5	917	OMG
1	5	925	G
1	5	970	C
1	5	1010	G
1	5	1208	C
1	5	1219	U
1	5	1318	G
1	5	1415	C
1	5	1445	A
1	5	1447	OMC
1	5	1460	OMG
1	5	1571	C
1	5	1596	G
1	5	1611	C
1	5	1678	A
1	5	1704	C
1	5	1728	C
1	5	1783	C
1	5	1817	A
1	5	1847	OMC
1	5	1855	OMG
1	5	1940	A
1	5	2125	OMG
1	5	2160	A
1	5	2209	A
1	5	2261	U
1	5	2278	C
1	5	2279	5MC
1	5	2294	OMC
1	5	2307	C
1	5	2338	OMC

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Mol	Chain	Res	Type
1	5	2364	A
1	5	2366	OMC
1	5	2370	G
1	5	2392	OMG
1	5	2396	OMG
1	5	2409	U
1	5	2410	OMG
1	5	2548	G
1	5	2619	G
1	5	2620	OMG
1	5	2677	A
1	5	2683	OMC
1	5	2752	G
1	5	2792	OMG
1	5	2815	G
1	5	2816	OMG
1	5	2871	5MC
1	5	2880	OMC
1	5	2918	OMG
1	5	2934	A
1	5	2949	OMC
1	5	3070	A
1	5	3071	A
1	5	3102	G
1	5	3174	C
1	5	3180	G
1	5	3219	G
1	5	3304	A
1	5	3332	A
13	7	19	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMU	5	144	1	19,22,23	2.83	6 (31%)	26,31,34	1.76	5 (19%)
1	OMG	5	2792	1	23,26,27	2.40	8 (34%)	33,38,41	2.46	15 (45%)
1	1MA	5	657	1	21,25,26	2.81	5 (23%)	31,37,40	3.19	12 (38%)
1	OMG	5	2289	1	23,26,27	2.41	8 (34%)	33,38,41	2.52	16 (48%)
1	5MC	5	2279	1	18,22,23	3.67	7 (38%)	26,32,35	1.63	6 (23%)
1	OMG	5	2816	1	23,26,27	2.40	8 (34%)	33,38,41	2.45	16 (48%)
1	OMG	5	2396	1,45	23,26,27	2.37	9 (39%)	33,38,41	2.47	15 (45%)
1	OMC	5	675	1	19,22,23	2.91	8 (42%)	26,31,34	1.61	5 (19%)
1	OMC	5	2338	1	19,22,23	2.92	8 (42%)	26,31,34	1.62	6 (23%)
1	A2M	5	2221	1	22,25,26	3.44	9 (40%)	31,36,39	2.63	12 (38%)
1	A2M	5	661	1	22,25,26	3.44	9 (40%)	31,36,39	2.68	11 (35%)
1	OMG	5	1460	1	23,26,27	2.38	9 (39%)	33,38,41	2.35	15 (45%)
1	OMG	5	1855	1	23,26,27	2.39	9 (39%)	33,38,41	2.41	16 (48%)
1	OMU	5	48	1	19,22,23	2.79	6 (31%)	26,31,34	1.74	5 (19%)
1	OMG	5	2923	1	23,26,27	2.42	9 (39%)	33,38,41	2.52	16 (48%)
1	A2M	5	1459	1	22,25,26	3.46	9 (40%)	31,36,39	2.69	11 (35%)
1	A2M	5	2947	1	22,25,26	3.48	9 (40%)	31,36,39	2.71	12 (38%)
1	A2M	5	1377	1	22,25,26	3.45	9 (40%)	31,36,39	2.70	11 (35%)
1	OMU	5	803	1	19,22,23	2.80	6 (31%)	26,31,34	1.75	5 (19%)
1	5MC	5	2871	1	18,22,23	3.70	8 (44%)	26,32,35	1.62	6 (23%)
1	OMU	5	44	1	19,22,23	2.84	6 (31%)	26,31,34	1.83	6 (23%)
1	OMU	5	2884	1	19,22,23	2.83	7 (36%)	26,31,34	1.95	8 (30%)
1	A2M	5	1143	1	22,25,26	3.44	9 (40%)	31,36,39	2.65	10 (32%)
1	OMC	5	2366	1	19,22,23	2.93	8 (42%)	26,31,34	1.75	6 (23%)
1	OMU	5	1067	1	19,22,23	2.85	6 (31%)	26,31,34	1.84	7 (26%)
1	A2M	5	2322	1	22,25,26	3.45	9 (40%)	31,36,39	2.61	11 (35%)
1	OMG	5	2392	1	23,26,27	2.40	8 (34%)	33,38,41	2.41	16 (48%)
1	OMC	5	2294	1	19,22,23	2.98	8 (42%)	26,31,34	1.72	6 (23%)
1	OMG	5	2918	1	23,26,27	2.40	9 (39%)	33,38,41	2.45	16 (48%)
1	A2M	5	2127	1	22,25,26	3.42	9 (40%)	31,36,39	2.64	11 (35%)
1	OMU	5	1892	1	19,22,23	2.84	6 (31%)	26,31,34	1.77	5 (19%)
1	OMU	5	2422	1	19,22,23	2.84	6 (31%)	26,31,34	1.75	5 (19%)
1	OMC	5	2683	1	19,22,23	2.98	8 (42%)	26,31,34	1.78	6 (23%)
1	OMC	5	2949	1	19,22,23	2.93	8 (42%)	26,31,34	1.84	6 (23%)
1	OMG	5	2620	1	23,26,27	2.39	8 (34%)	33,38,41	2.45	16 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMG	5	917	1	23,26,27	2.44	8 (34%)	33,38,41	2.26	14 (42%)
1	OMC	5	1847	1	19,22,23	2.93	8 (42%)	26,31,34	1.48	4 (15%)
1	OMG	5	2125	1	23,26,27	2.41	8 (34%)	33,38,41	2.47	15 (45%)
1	OMG	5	814	1	23,26,27	2.39	9 (39%)	33,38,41	2.52	16 (48%)
1	UR3	5	2954	1	19,22,23	2.71	8 (42%)	26,32,35	1.31	1 (3%)
1	OMU	5	2736	1	19,22,23	2.83	6 (31%)	26,31,34	1.72	5 (19%)
1	OMU	5	676	1	19,22,23	2.84	6 (31%)	26,31,34	1.75	5 (19%)
1	OMC	5	1860	1	19,22,23	2.92	8 (42%)	26,31,34	1.77	6 (23%)
1	OMU	5	2651	1	19,22,23	2.87	6 (31%)	26,31,34	1.75	5 (19%)
1	OMC	5	2198	44,1	19,22,23	2.95	8 (42%)	26,31,34	1.79	3 (11%)
1	OMG	5	2410	1	23,26,27	2.40	8 (34%)	33,38,41	2.26	13 (39%)
1	OMC	5	2880	1	19,22,23	2.91	8 (42%)	26,31,34	1.69	6 (23%)
1	A2M	5	2641	1	22,25,26	3.45	9 (40%)	31,36,39	2.64	10 (32%)
1	OMU	5	3300	1	19,22,23	2.83	6 (31%)	26,31,34	1.74	5 (19%)
1	OMC	5	1447	1	19,22,23	2.90	8 (42%)	26,31,34	1.75	6 (23%)
1	A2M	5	945	1	22,25,26	3.48	9 (40%)	31,36,39	2.66	10 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	5	144	1	-	3/9/27/28	0/2/2/2
1	OMG	5	2792	1	-	3/9/27/28	0/3/3/3
1	1MA	5	657	1	-	2/7/25/26	0/3/3/3
1	OMG	5	2289	1	-	4/9/27/28	0/3/3/3
1	5MC	5	2279	1	-	2/7/25/26	0/2/2/2
1	OMG	5	2816	1	-	2/9/27/28	0/3/3/3
1	OMG	5	2396	1,45	-	4/9/27/28	0/3/3/3
1	OMC	5	675	1	-	4/9/27/28	0/2/2/2
1	OMC	5	2338	1	-	3/9/27/28	0/2/2/2
1	A2M	5	2221	1	-	3/9/27/28	0/3/3/3
1	A2M	5	661	1	-	3/9/27/28	0/3/3/3
1	OMG	5	1460	1	-	4/9/27/28	0/3/3/3
1	OMG	5	1855	1	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	5	48	1	-	0/9/27/28	0/2/2/2
1	OMG	5	2923	1	-	3/9/27/28	0/3/3/3
1	A2M	5	1459	1	-	0/9/27/28	0/3/3/3
1	A2M	5	2947	1	-	1/9/27/28	0/3/3/3
1	A2M	5	1377	1	-	0/9/27/28	0/3/3/3
1	OMU	5	803	1	-	2/9/27/28	0/2/2/2
1	5MC	5	2871	1	-	6/7/25/26	0/2/2/2
1	OMU	5	44	1	-	3/9/27/28	0/2/2/2
1	OMU	5	2884	1	-	1/9/27/28	0/2/2/2
1	A2M	5	1143	1	-	2/9/27/28	0/3/3/3
1	OMC	5	2366	1	-	1/9/27/28	0/2/2/2
1	OMU	5	1067	1	-	0/9/27/28	0/2/2/2
1	A2M	5	2322	1	-	0/9/27/28	0/3/3/3
1	OMG	5	2392	1	-	3/9/27/28	0/3/3/3
1	OMC	5	2294	1	-	3/9/27/28	0/2/2/2
1	OMG	5	2918	1	-	3/9/27/28	0/3/3/3
1	A2M	5	2127	1	-	2/9/27/28	0/3/3/3
1	OMU	5	1892	1	-	0/9/27/28	0/2/2/2
1	OMU	5	2422	1	-	2/9/27/28	0/2/2/2
1	OMC	5	2683	1	-	3/9/27/28	0/2/2/2
1	OMC	5	2949	1	-	4/9/27/28	0/2/2/2
1	OMG	5	2620	1	-	4/9/27/28	0/3/3/3
1	OMG	5	917	1	-	1/9/27/28	0/3/3/3
1	OMC	5	1847	1	-	4/9/27/28	0/2/2/2
1	OMG	5	2125	1	-	4/9/27/28	0/3/3/3
1	OMG	5	814	1	-	2/9/27/28	0/3/3/3
1	UR3	5	2954	1	-	0/7/25/26	0/2/2/2
1	OMU	5	2736	1	-	1/9/27/28	0/2/2/2
1	OMU	5	676	1	-	2/9/27/28	0/2/2/2
1	OMC	5	1860	1	-	1/9/27/28	0/2/2/2
1	OMU	5	2651	1	-	0/9/27/28	0/2/2/2
1	OMC	5	2198	44,1	-	3/9/27/28	0/2/2/2
1	OMG	5	2410	1	-	1/9/27/28	0/3/3/3
1	OMC	5	2880	1	-	3/9/27/28	0/2/2/2
1	A2M	5	2641	1	-	0/9/27/28	0/3/3/3
1	OMU	5	3300	1	-	2/9/27/28	0/2/2/2
1	OMC	5	1447	1	-	5/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	5	945	1	-	3/9/27/28	0/3/3/3

All (397) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2871	5MC	C6-C5	9.53	1.50	1.34
1	5	2279	5MC	C6-C5	9.15	1.49	1.34
1	5	2947	A2M	C2'-C1'	-8.84	1.30	1.53
1	5	1459	A2M	C2'-C1'	-8.78	1.30	1.53
1	5	1143	A2M	C2'-C1'	-8.69	1.30	1.53
1	5	1377	A2M	C2'-C1'	-8.68	1.30	1.53
1	5	661	A2M	C2'-C1'	-8.68	1.30	1.53
1	5	2322	A2M	C2'-C1'	-8.65	1.30	1.53
1	5	2641	A2M	C2'-C1'	-8.64	1.30	1.53
1	5	2221	A2M	C2'-C1'	-8.64	1.30	1.53
1	5	945	A2M	C2'-C1'	-8.64	1.30	1.53
1	5	2947	A2M	O4'-C1'	8.62	1.62	1.42
1	5	2127	A2M	C2'-C1'	-8.62	1.30	1.53
1	5	2221	A2M	O4'-C1'	8.59	1.62	1.42
1	5	945	A2M	O4'-C1'	8.53	1.62	1.42
1	5	1377	A2M	O4'-C1'	8.51	1.62	1.42
1	5	1143	A2M	O4'-C1'	8.50	1.62	1.42
1	5	2322	A2M	O4'-C1'	8.48	1.62	1.42
1	5	657	1MA	C2-N3	8.47	1.46	1.30
1	5	2641	A2M	O4'-C1'	8.46	1.62	1.42
1	5	661	A2M	O4'-C1'	8.42	1.62	1.42
1	5	2127	A2M	O4'-C1'	8.42	1.61	1.42
1	5	1459	A2M	O4'-C1'	8.38	1.61	1.42
1	5	2954	UR3	C2-N1	6.88	1.48	1.38
1	5	2651	OMU	C2-N1	6.84	1.49	1.38
1	5	1067	OMU	C2-N1	6.75	1.49	1.38
1	5	144	OMU	C2-N1	6.70	1.49	1.38
1	5	2884	OMU	C2-N1	6.69	1.49	1.38
1	5	2736	OMU	C2-N1	6.68	1.49	1.38
1	5	44	OMU	C2-N1	6.67	1.49	1.38
1	5	2422	OMU	C2-N1	6.66	1.49	1.38
1	5	676	OMU	C2-N1	6.63	1.49	1.38
1	5	945	A2M	O4'-C4'	-6.61	1.30	1.45
1	5	1892	OMU	C2-N1	6.60	1.49	1.38
1	5	3300	OMU	C2-N1	6.59	1.49	1.38
1	5	2279	5MC	C2-N3	6.55	1.49	1.36
1	5	657	1MA	C4-N3	6.51	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	48	OMU	C2-N1	6.49	1.48	1.38
1	5	1377	A2M	O4'-C4'	-6.47	1.30	1.45
1	5	3300	OMU	C2-N3	6.47	1.49	1.38
1	5	803	OMU	C2-N1	6.46	1.48	1.38
1	5	2641	A2M	O4'-C4'	-6.46	1.30	1.45
1	5	661	A2M	O4'-C4'	-6.46	1.30	1.45
1	5	2736	OMU	C2-N3	6.46	1.49	1.38
1	5	2322	A2M	O4'-C4'	-6.46	1.30	1.45
1	5	2651	OMU	C2-N3	6.45	1.49	1.38
1	5	2884	OMU	C2-N3	6.45	1.49	1.38
1	5	1067	OMU	C2-N3	6.45	1.49	1.38
1	5	1459	A2M	O4'-C4'	-6.44	1.30	1.45
1	5	44	OMU	C2-N3	6.42	1.49	1.38
1	5	2422	OMU	C2-N3	6.42	1.49	1.38
1	5	803	OMU	C2-N3	6.41	1.49	1.38
1	5	676	OMU	C2-N3	6.41	1.49	1.38
1	5	1892	OMU	C2-N3	6.38	1.49	1.38
1	5	675	OMC	C2-N3	6.36	1.49	1.36
1	5	2949	OMC	C2-N3	6.35	1.49	1.36
1	5	2871	5MC	C2-N3	6.35	1.49	1.36
1	5	48	OMU	C2-N3	6.35	1.49	1.38
1	5	144	OMU	C2-N3	6.34	1.49	1.38
1	5	2620	OMG	C4-N3	6.34	1.49	1.34
1	5	2947	A2M	O4'-C4'	-6.33	1.30	1.45
1	5	1143	A2M	O4'-C4'	-6.33	1.30	1.45
1	5	917	OMG	C4-N3	6.31	1.49	1.34
1	5	2221	A2M	O4'-C4'	-6.30	1.30	1.45
1	5	2923	OMG	C4-N3	6.28	1.49	1.34
1	5	2127	A2M	O4'-C4'	-6.27	1.31	1.45
1	5	2125	OMG	C4-N3	6.26	1.49	1.34
1	5	2279	5MC	C4-N3	6.26	1.44	1.34
1	5	2792	OMG	C4-N3	6.26	1.49	1.34
1	5	2289	OMG	C4-N3	6.24	1.49	1.34
1	5	2410	OMG	C4-N3	6.24	1.49	1.34
1	5	2816	OMG	C4-N3	6.24	1.49	1.34
1	5	2392	OMG	C4-N3	6.22	1.49	1.34
1	5	2198	OMC	C2-N3	6.22	1.49	1.36
1	5	2338	OMC	C2-N3	6.21	1.49	1.36
1	5	2918	OMG	C4-N3	6.19	1.49	1.34
1	5	1855	OMG	C4-N3	6.19	1.49	1.34
1	5	2683	OMC	C2-N3	6.18	1.48	1.36
1	5	1460	OMG	C4-N3	6.17	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2294	OMC	C2-N3	6.17	1.48	1.36
1	5	814	OMG	C4-N3	6.16	1.48	1.34
1	5	2880	OMC	C2-N3	6.14	1.48	1.36
1	5	1860	OMC	C2-N3	6.13	1.48	1.36
1	5	2954	UR3	C6-C5	6.12	1.49	1.35
1	5	1847	OMC	C2-N3	6.08	1.48	1.36
1	5	2396	OMG	C4-N3	6.07	1.48	1.34
1	5	2366	OMC	C2-N3	6.07	1.48	1.36
1	5	2294	OMC	C6-C5	6.04	1.49	1.35
1	5	1447	OMC	C2-N3	6.02	1.48	1.36
1	5	2683	OMC	C6-C5	6.02	1.49	1.35
1	5	2366	OMC	C6-C5	6.01	1.49	1.35
1	5	1847	OMC	C6-C5	5.97	1.48	1.35
1	5	1860	OMC	C6-C5	5.94	1.48	1.35
1	5	2871	5MC	C4-N3	5.94	1.44	1.34
1	5	2880	OMC	C6-C5	5.93	1.48	1.35
1	5	2198	OMC	C6-C5	5.92	1.48	1.35
1	5	2338	OMC	C6-C5	5.92	1.48	1.35
1	5	1447	OMC	C6-C5	5.84	1.48	1.35
1	5	2949	OMC	C6-C5	5.82	1.48	1.35
1	5	1892	OMU	C6-C5	5.80	1.48	1.35
1	5	2651	OMU	C6-C5	5.77	1.48	1.35
1	5	44	OMU	C6-C5	5.74	1.48	1.35
1	5	3300	OMU	C6-C5	5.73	1.48	1.35
1	5	1067	OMU	C6-C5	5.73	1.48	1.35
1	5	2736	OMU	C6-C5	5.71	1.48	1.35
1	5	144	OMU	C6-C5	5.70	1.48	1.35
1	5	803	OMU	C6-C5	5.69	1.48	1.35
1	5	675	OMC	C6-C5	5.69	1.48	1.35
1	5	2422	OMU	C6-C5	5.68	1.48	1.35
1	5	676	OMU	C6-C5	5.67	1.48	1.35
1	5	48	OMU	C6-C5	5.64	1.48	1.35
1	5	2884	OMU	C6-C5	5.60	1.48	1.35
1	5	917	OMG	C2-N3	5.51	1.46	1.33
1	5	2289	OMG	C2-N3	5.44	1.46	1.33
1	5	2125	OMG	C2-N3	5.43	1.46	1.33
1	5	2918	OMG	C2-N3	5.42	1.46	1.33
1	5	2410	OMG	C2-N3	5.41	1.46	1.33
1	5	2792	OMG	C2-N3	5.41	1.46	1.33
1	5	2923	OMG	C2-N3	5.40	1.46	1.33
1	5	2392	OMG	C2-N3	5.39	1.46	1.33
1	5	2620	OMG	C2-N3	5.37	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2816	OMG	C2-N3	5.37	1.46	1.33
1	5	1855	OMG	C2-N3	5.35	1.46	1.33
1	5	1460	OMG	C2-N3	5.30	1.46	1.33
1	5	814	OMG	C2-N3	5.29	1.45	1.33
1	5	2396	OMG	C2-N3	5.28	1.45	1.33
1	5	2279	5MC	C2-N1	5.16	1.51	1.40
1	5	2683	OMC	C4-N3	5.13	1.44	1.34
1	5	675	OMC	C4-N3	5.11	1.44	1.34
1	5	2294	OMC	C4-N3	5.06	1.44	1.34
1	5	2871	5MC	C2-N1	5.06	1.51	1.40
1	5	2954	UR3	C2-N3	5.04	1.48	1.39
1	5	2949	OMC	C4-N3	4.99	1.44	1.34
1	5	2683	OMC	C4-N4	4.98	1.45	1.33
1	5	2198	OMC	C4-N3	4.97	1.44	1.34
1	5	1860	OMC	C4-N3	4.94	1.44	1.34
1	5	2366	OMC	C4-N4	4.93	1.45	1.33
1	5	1847	OMC	C4-N4	4.92	1.45	1.33
1	5	2338	OMC	C4-N3	4.91	1.44	1.34
1	5	2294	OMC	C4-N4	4.91	1.45	1.33
1	5	2366	OMC	C4-N3	4.90	1.44	1.34
1	5	1847	OMC	C4-N3	4.88	1.44	1.34
1	5	1860	OMC	C4-N4	4.88	1.45	1.33
1	5	2949	OMC	C4-N4	4.86	1.45	1.33
1	5	2198	OMC	C4-N4	4.86	1.45	1.33
1	5	2871	5MC	C6-N1	4.85	1.46	1.38
1	5	2880	OMC	C4-N4	4.84	1.45	1.33
1	5	2338	OMC	C4-N4	4.83	1.45	1.33
1	5	2880	OMC	C4-N3	4.81	1.44	1.34
1	5	675	OMC	C4-N4	4.78	1.45	1.33
1	5	2125	OMG	C2-N2	4.75	1.45	1.34
1	5	1447	OMC	C4-N3	4.74	1.44	1.34
1	5	1447	OMC	C4-N4	4.74	1.45	1.33
1	5	2923	OMG	C2-N2	4.70	1.45	1.34
1	5	2918	OMG	C2-N2	4.67	1.45	1.34
1	5	2792	OMG	C2-N2	4.66	1.45	1.34
1	5	917	OMG	C2-N2	4.65	1.45	1.34
1	5	2410	OMG	C2-N2	4.65	1.45	1.34
1	5	2289	OMG	C2-N2	4.64	1.45	1.34
1	5	814	OMG	C2-N2	4.63	1.45	1.34
1	5	1855	OMG	C2-N2	4.63	1.45	1.34
1	5	2620	OMG	C2-N2	4.62	1.45	1.34
1	5	2392	OMG	C2-N2	4.62	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2816	OMG	C2-N2	4.60	1.45	1.34
1	5	2396	OMG	C2-N2	4.60	1.45	1.34
1	5	1460	OMG	C2-N2	4.59	1.45	1.34
1	5	657	1MA	C2-N1	4.53	1.44	1.35
1	5	2279	5MC	C6-N1	4.53	1.45	1.38
1	5	2221	A2M	C6-N6	4.47	1.45	1.34
1	5	1377	A2M	C6-N6	4.44	1.45	1.34
1	5	2641	A2M	C6-N6	4.44	1.45	1.34
1	5	1459	A2M	C6-N6	4.43	1.45	1.34
1	5	2127	A2M	C6-N6	4.42	1.45	1.34
1	5	1447	OMC	C2-N1	4.42	1.49	1.40
1	5	2279	5MC	C4-N4	4.42	1.45	1.34
1	5	1143	A2M	C6-N6	4.41	1.45	1.34
1	5	2322	A2M	C6-N6	4.40	1.45	1.34
1	5	2947	A2M	C6-N6	4.38	1.45	1.34
1	5	661	A2M	C6-N6	4.37	1.45	1.34
1	5	945	A2M	C6-N6	4.36	1.45	1.34
1	5	2871	5MC	C4-N4	4.33	1.45	1.34
1	5	2294	OMC	C2-N1	4.30	1.49	1.40
1	5	2683	OMC	C2-N1	4.24	1.49	1.40
1	5	2198	OMC	C2-N1	4.20	1.49	1.40
1	5	2880	OMC	C2-N1	4.18	1.49	1.40
1	5	2366	OMC	C2-N1	4.18	1.49	1.40
1	5	2949	OMC	C2-N1	4.16	1.49	1.40
1	5	1860	OMC	C2-N1	4.14	1.49	1.40
1	5	2338	OMC	C2-N1	4.10	1.48	1.40
1	5	1847	OMC	C2-N1	4.07	1.48	1.40
1	5	675	OMC	C2-N1	3.99	1.48	1.40
1	5	657	1MA	C5-C6	3.74	1.53	1.43
1	5	676	OMU	C4-N3	3.33	1.44	1.38
1	5	1067	OMU	C4-N3	3.30	1.44	1.38
1	5	945	A2M	O3'-C3'	-3.29	1.35	1.43
1	5	1892	OMU	C4-N3	3.29	1.44	1.38
1	5	2947	A2M	O3'-C3'	-3.28	1.35	1.43
1	5	2816	OMG	C5-N7	-3.27	1.32	1.39
1	5	2392	OMG	C5-N7	-3.27	1.32	1.39
1	5	2422	OMU	C4-N3	3.26	1.44	1.38
1	5	2736	OMU	C4-N3	3.23	1.44	1.38
1	5	814	OMG	C5-N7	-3.22	1.32	1.39
1	5	3300	OMU	C4-N3	3.21	1.44	1.38
1	5	917	OMG	C5-N7	-3.21	1.32	1.39
1	5	2198	OMC	C6-N1	3.21	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1460	OMG	C5-N7	-3.20	1.32	1.39
1	5	2651	OMU	C4-N3	3.19	1.44	1.38
1	5	2410	OMG	C5-N7	-3.19	1.32	1.39
1	5	1855	OMG	C5-N7	-3.19	1.32	1.39
1	5	2792	OMG	C5-N7	-3.18	1.32	1.39
1	5	2884	OMU	C4-N3	3.18	1.44	1.38
1	5	803	OMU	C4-N3	3.17	1.44	1.38
1	5	2947	A2M	C5-C4	-3.16	1.33	1.39
1	5	2289	OMG	C5-N7	-3.15	1.33	1.39
1	5	1459	A2M	C5-C4	-3.15	1.33	1.39
1	5	44	OMU	C4-N3	3.15	1.44	1.38
1	5	144	OMU	C4-N3	3.14	1.44	1.38
1	5	1143	A2M	O3'-C3'	-3.14	1.35	1.43
1	5	2620	OMG	C5-N7	-3.12	1.33	1.39
1	5	48	OMU	C4-N3	3.12	1.44	1.38
1	5	2127	A2M	O3'-C3'	-3.12	1.35	1.43
1	5	1847	OMC	C6-N1	3.11	1.45	1.38
1	5	2918	OMG	C5-N7	-3.10	1.33	1.39
1	5	2683	OMC	C6-N1	3.09	1.45	1.38
1	5	2396	OMG	C5-N7	-3.09	1.33	1.39
1	5	2221	A2M	O3'-C3'	-3.09	1.35	1.43
1	5	1860	OMC	C6-N1	3.08	1.45	1.38
1	5	2127	A2M	C5-C4	-3.08	1.33	1.39
1	5	1377	A2M	C5-C4	-3.07	1.33	1.39
1	5	661	A2M	C5-C4	-3.06	1.33	1.39
1	5	2125	OMG	C5-N7	-3.06	1.33	1.39
1	5	2923	OMG	C5-N7	-3.06	1.33	1.39
1	5	2322	A2M	O3'-C3'	-3.05	1.35	1.43
1	5	945	A2M	C5-C4	-3.04	1.33	1.39
1	5	2294	OMC	C6-N1	3.03	1.45	1.38
1	5	2641	A2M	C5-C4	-3.03	1.33	1.39
1	5	2322	A2M	C5-C4	-3.03	1.33	1.39
1	5	1447	OMC	C6-N1	3.01	1.45	1.38
1	5	2338	OMC	C6-N1	3.01	1.45	1.38
1	5	2366	OMC	C6-N1	3.01	1.45	1.38
1	5	2641	A2M	O3'-C3'	-3.00	1.35	1.43
1	5	2221	A2M	C5-C4	-2.99	1.33	1.39
1	5	1377	A2M	O3'-C3'	-2.98	1.36	1.43
1	5	1143	A2M	C5-C4	-2.97	1.33	1.39
1	5	2880	OMC	C6-N1	2.97	1.45	1.38
1	5	657	1MA	C5-N7	-2.94	1.33	1.39
1	5	1459	A2M	O3'-C3'	-2.93	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	661	A2M	O3'-C3'	-2.93	1.36	1.43
1	5	675	OMC	O2-C2	-2.92	1.18	1.23
1	5	1447	OMC	O2-C2	-2.89	1.18	1.23
1	5	2949	OMC	C6-N1	2.89	1.45	1.38
1	5	2294	OMC	O2-C2	-2.89	1.18	1.23
1	5	48	OMU	O4-C4	-2.88	1.18	1.24
1	5	2954	UR3	C6-N1	2.87	1.44	1.38
1	5	661	A2M	C5-N7	-2.87	1.33	1.39
1	5	44	OMU	O2-C2	-2.86	1.17	1.23
1	5	1847	OMC	O2-C2	-2.86	1.18	1.23
1	5	2949	OMC	O2-C2	-2.86	1.18	1.23
1	5	1459	A2M	C5-N7	-2.86	1.33	1.39
1	5	945	A2M	C5-N7	-2.86	1.33	1.39
1	5	2338	OMC	O2-C2	-2.85	1.18	1.23
1	5	144	OMU	O4-C4	-2.85	1.19	1.24
1	5	2880	OMC	O2-C2	-2.85	1.18	1.23
1	5	2366	OMC	O2-C2	-2.84	1.18	1.23
1	5	1860	OMC	O2-C2	-2.84	1.18	1.23
1	5	2422	OMU	O4-C4	-2.83	1.19	1.24
1	5	803	OMU	O2-C2	-2.82	1.17	1.23
1	5	44	OMU	O4-C4	-2.82	1.19	1.24
1	5	2422	OMU	O2-C2	-2.81	1.17	1.23
1	5	2641	A2M	C5-N7	-2.81	1.33	1.39
1	5	2884	OMU	O4-C4	-2.80	1.19	1.24
1	5	144	OMU	O2-C2	-2.80	1.17	1.23
1	5	2127	A2M	C5-N7	-2.80	1.33	1.39
1	5	48	OMU	O2-C2	-2.79	1.17	1.23
1	5	2884	OMU	O2-C2	-2.79	1.17	1.23
1	5	2322	A2M	C5-N7	-2.79	1.33	1.39
1	5	1143	A2M	C5-N7	-2.79	1.33	1.39
1	5	675	OMC	C6-N1	2.78	1.44	1.38
1	5	3300	OMU	O4-C4	-2.78	1.19	1.24
1	5	945	A2M	O2'-C2'	2.78	1.49	1.42
1	5	3300	OMU	O2-C2	-2.78	1.18	1.23
1	5	2641	A2M	O2'-C2'	2.78	1.49	1.42
1	5	2736	OMU	O4-C4	-2.77	1.19	1.24
1	5	2651	OMU	O4-C4	-2.75	1.19	1.24
1	5	1892	OMU	O2-C2	-2.75	1.18	1.23
1	5	676	OMU	O4-C4	-2.75	1.19	1.24
1	5	676	OMU	O2-C2	-2.75	1.18	1.23
1	5	2322	A2M	O2'-C2'	2.74	1.49	1.42
1	5	2221	A2M	O2'-C2'	2.74	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2198	OMC	O2-C2	-2.74	1.18	1.23
1	5	2651	OMU	O2-C2	-2.73	1.18	1.23
1	5	2736	OMU	O2-C2	-2.72	1.18	1.23
1	5	1377	A2M	C5-N7	-2.72	1.33	1.39
1	5	1067	OMU	O2-C2	-2.72	1.18	1.23
1	5	2127	A2M	O2'-C2'	2.72	1.49	1.42
1	5	2221	A2M	C5-N7	-2.72	1.33	1.39
1	5	1892	OMU	O4-C4	-2.72	1.19	1.24
1	5	803	OMU	O4-C4	-2.72	1.19	1.24
1	5	1067	OMU	O4-C4	-2.71	1.19	1.24
1	5	1459	A2M	O2'-C2'	2.70	1.49	1.42
1	5	661	A2M	O2'-C2'	2.69	1.49	1.42
1	5	2947	A2M	C5-N7	-2.68	1.34	1.39
1	5	2683	OMC	O2-C2	-2.67	1.18	1.23
1	5	2947	A2M	O2'-C2'	2.66	1.49	1.42
1	5	2125	OMG	O6-C6	-2.65	1.18	1.23
1	5	2392	OMG	O6-C6	-2.65	1.18	1.23
1	5	814	OMG	O6-C6	-2.63	1.18	1.23
1	5	2816	OMG	O6-C6	-2.63	1.18	1.23
1	5	2923	OMG	C2-N1	2.63	1.44	1.37
1	5	1143	A2M	O2'-C2'	2.62	1.49	1.42
1	5	2396	OMG	O6-C6	-2.62	1.18	1.23
1	5	917	OMG	O6-C6	-2.62	1.18	1.23
1	5	2792	OMG	O6-C6	-2.61	1.18	1.23
1	5	1855	OMG	O6-C6	-2.61	1.18	1.23
1	5	2410	OMG	O6-C6	-2.60	1.18	1.23
1	5	1377	A2M	O2'-C2'	2.60	1.49	1.42
1	5	2918	OMG	C2-N1	2.57	1.44	1.37
1	5	917	OMG	C2-N1	2.57	1.44	1.37
1	5	2289	OMG	C2-N1	2.57	1.44	1.37
1	5	2918	OMG	O6-C6	-2.56	1.18	1.23
1	5	2125	OMG	C2-N1	2.54	1.44	1.37
1	5	1855	OMG	C2-N1	2.53	1.43	1.37
1	5	2923	OMG	O6-C6	-2.53	1.18	1.23
1	5	2620	OMG	C2-N1	2.53	1.43	1.37
1	5	1460	OMG	O6-C6	-2.52	1.18	1.23
1	5	2392	OMG	C2-N1	2.52	1.43	1.37
1	5	2289	OMG	O6-C6	-2.52	1.18	1.23
1	5	2620	OMG	O6-C6	-2.50	1.18	1.23
1	5	2816	OMG	C2-N1	2.50	1.43	1.37
1	5	2683	OMC	C5-C4	2.49	1.48	1.42
1	5	1460	OMG	C2-N1	2.48	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2396	OMG	C2-N1	2.48	1.43	1.37
1	5	2923	OMG	C6-N1	2.47	1.43	1.38
1	5	2410	OMG	C2-N1	2.47	1.43	1.37
1	5	2620	OMG	C5-C6	2.47	1.53	1.44
1	5	814	OMG	C2-N1	2.47	1.43	1.37
1	5	2294	OMC	C5-C4	2.47	1.48	1.42
1	5	2792	OMG	C2-N1	2.47	1.43	1.37
1	5	1459	A2M	C8-N9	-2.46	1.33	1.37
1	5	2923	OMG	C5-C6	2.46	1.53	1.44
1	5	2289	OMG	C5-C6	2.42	1.53	1.44
1	5	2198	OMC	C5-C4	2.41	1.48	1.42
1	5	2918	OMG	C5-C6	2.41	1.53	1.44
1	5	2366	OMC	C5-C4	2.41	1.48	1.42
1	5	2792	OMG	C5-C6	2.40	1.53	1.44
1	5	2125	OMG	C5-C6	2.40	1.53	1.44
1	5	2289	OMG	C6-N1	2.39	1.43	1.38
1	5	917	OMG	C5-C6	2.38	1.53	1.44
1	5	2396	OMG	C5-C6	2.38	1.53	1.44
1	5	2641	A2M	C8-N9	-2.38	1.33	1.37
1	5	2322	A2M	C8-N9	-2.37	1.33	1.37
1	5	2410	OMG	C5-C6	2.37	1.53	1.44
1	5	1847	OMC	C5-C4	2.36	1.48	1.42
1	5	945	A2M	C8-N9	-2.35	1.33	1.37
1	5	814	OMG	C5-C6	2.35	1.53	1.44
1	5	661	A2M	C8-N9	-2.35	1.33	1.37
1	5	1855	OMG	C5-C6	2.34	1.53	1.44
1	5	2392	OMG	C5-C6	2.34	1.53	1.44
1	5	2880	OMC	C5-C4	2.34	1.48	1.42
1	5	1447	OMC	C5-C4	2.34	1.48	1.42
1	5	2918	OMG	C6-N1	2.34	1.43	1.38
1	5	2816	OMG	C5-C6	2.33	1.53	1.44
1	5	1460	OMG	C5-C6	2.33	1.53	1.44
1	5	2947	A2M	C8-N9	-2.31	1.33	1.37
1	5	917	OMG	C6-N1	2.30	1.43	1.38
1	5	1143	A2M	C8-N9	-2.29	1.33	1.37
1	5	2620	OMG	C6-N1	2.26	1.43	1.38
1	5	2127	A2M	C8-N9	-2.26	1.33	1.37
1	5	2954	UR3	O4-C4	-2.26	1.18	1.23
1	5	1377	A2M	C8-N9	-2.26	1.33	1.37
1	5	2816	OMG	C6-N1	2.26	1.43	1.38
1	5	2125	OMG	C6-N1	2.25	1.43	1.38
1	5	1860	OMC	C5-C4	2.25	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1855	OMG	C6-N1	2.25	1.43	1.38
1	5	2949	OMC	C5-C4	2.23	1.48	1.42
1	5	2338	OMC	C5-C4	2.23	1.48	1.42
1	5	2279	5MC	CM5-C5	2.22	1.56	1.50
1	5	2396	OMG	C6-N1	2.21	1.42	1.38
1	5	814	OMG	C6-N1	2.21	1.42	1.38
1	5	2954	UR3	O2-C2	-2.21	1.18	1.22
1	5	1460	OMG	C6-N1	2.21	1.42	1.38
1	5	2871	5MC	CM5-C5	2.20	1.56	1.50
1	5	2410	OMG	C6-N1	2.20	1.42	1.38
1	5	2954	UR3	C5-C4	2.17	1.49	1.43
1	5	1460	OMG	C4-N9	-2.17	1.32	1.38
1	5	2396	OMG	C4-N9	-2.17	1.32	1.38
1	5	2871	5MC	O2-C2	-2.16	1.19	1.23
1	5	2392	OMG	C6-N1	2.14	1.42	1.38
1	5	2792	OMG	C6-N1	2.12	1.42	1.38
1	5	2221	A2M	C8-N9	-2.10	1.33	1.37
1	5	675	OMC	C5-C4	2.09	1.47	1.42
1	5	2954	UR3	C4-N3	2.08	1.45	1.40
1	5	2918	OMG	C4-N9	-2.07	1.32	1.38
1	5	1855	OMG	C4-N9	-2.06	1.32	1.38
1	5	2923	OMG	C4-N9	-2.03	1.32	1.38
1	5	814	OMG	C4-N9	-2.01	1.32	1.38
1	5	2884	OMU	C6-N1	2.00	1.42	1.38

All (475) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	657	1MA	C1'-N9-C8	-9.46	99.78	126.70
1	5	657	1MA	C1'-N9-C4	8.41	151.50	126.50
1	5	1377	A2M	N6-C6-N1	-7.14	102.71	118.35
1	5	1459	A2M	N6-C6-N1	-7.11	102.78	118.35
1	5	661	A2M	N6-C6-N1	-7.08	102.85	118.35
1	5	2127	A2M	N6-C6-N1	-6.94	103.16	118.35
1	5	2322	A2M	N6-C6-N1	-6.94	103.16	118.35
1	5	2641	A2M	N6-C6-N1	-6.93	103.17	118.35
1	5	1143	A2M	N6-C6-N1	-6.92	103.19	118.35
1	5	2947	A2M	N6-C6-N1	-6.92	103.19	118.35
1	5	2221	A2M	N6-C6-N1	-6.81	103.43	118.35
1	5	945	A2M	N6-C6-N1	-6.72	103.63	118.35
1	5	1459	A2M	C5-C6-N6	6.36	137.27	123.43
1	5	661	A2M	C5-C6-N6	6.25	137.04	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1377	A2M	C5-C6-N6	6.24	137.01	123.43
1	5	2322	A2M	C5-C6-N6	6.19	136.89	123.43
1	5	1143	A2M	C5-C6-N6	6.17	136.86	123.43
1	5	2641	A2M	C5-C6-N6	6.15	136.82	123.43
1	5	2127	A2M	C5-C6-N6	6.15	136.80	123.43
1	5	2221	A2M	C5-C6-N6	6.12	136.76	123.43
1	5	2947	A2M	C5-C6-N6	6.09	136.67	123.43
1	5	945	A2M	C5-C6-N6	5.99	136.46	123.43
1	5	2620	OMG	C5-C4-N3	-5.64	119.31	128.46
1	5	2198	OMC	O2'-C2'-C1'	5.61	120.02	109.08
1	5	945	A2M	C5-C4-N3	-5.60	119.45	126.75
1	5	2947	A2M	N3-C2-N1	-5.51	119.97	128.60
1	5	1377	A2M	C5-C4-N3	-5.50	119.58	126.75
1	5	2641	A2M	C5-C4-N3	-5.47	119.61	126.75
1	5	1143	A2M	N3-C2-N1	-5.47	120.05	128.60
1	5	661	A2M	C5-C4-N3	-5.46	119.62	126.75
1	5	144	OMU	C4-N3-C2	-5.46	119.38	126.58
1	5	2651	OMU	C4-N3-C2	-5.46	119.38	126.58
1	5	2221	A2M	N3-C2-N1	-5.45	120.07	128.60
1	5	2127	A2M	N3-C2-N1	-5.43	120.11	128.60
1	5	2422	OMU	C4-N3-C2	-5.41	119.45	126.58
1	5	1892	OMU	C4-N3-C2	-5.40	119.46	126.58
1	5	661	A2M	N3-C2-N1	-5.39	120.18	128.60
1	5	48	OMU	C4-N3-C2	-5.37	119.50	126.58
1	5	2410	OMG	C5-C4-N3	-5.36	119.76	128.46
1	5	2792	OMG	C5-C4-N3	-5.36	119.77	128.46
1	5	3300	OMU	C4-N3-C2	-5.36	119.51	126.58
1	5	676	OMU	C4-N3-C2	-5.36	119.51	126.58
1	5	2322	A2M	C5-C4-N3	-5.36	119.76	126.75
1	5	1377	A2M	N3-C2-N1	-5.35	120.23	128.60
1	5	44	OMU	C4-N3-C2	-5.33	119.54	126.58
1	5	1459	A2M	C5-C4-N3	-5.33	119.79	126.75
1	5	803	OMU	C4-N3-C2	-5.33	119.55	126.58
1	5	1459	A2M	N3-C2-N1	-5.28	120.34	128.60
1	5	2641	A2M	N3-C2-N1	-5.28	120.35	128.60
1	5	2392	OMG	C5-C4-N3	-5.27	119.91	128.46
1	5	945	A2M	N3-C2-N1	-5.26	120.38	128.60
1	5	1067	OMU	C4-N3-C2	-5.25	119.66	126.58
1	5	2736	OMU	C4-N3-C2	-5.24	119.67	126.58
1	5	917	OMG	C5-C4-N3	-5.22	119.99	128.46
1	5	2947	A2M	C5-C4-N3	-5.21	119.95	126.75
1	5	2127	A2M	C5-C4-N3	-5.21	119.95	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2322	A2M	N3-C2-N1	-5.20	120.47	128.60
1	5	1855	OMG	C5-C4-N3	-5.19	120.04	128.46
1	5	2816	OMG	C5-C4-N3	-5.19	120.05	128.46
1	5	2125	OMG	C5-C4-N3	-5.18	120.06	128.46
1	5	2221	A2M	C5-C4-N3	-5.16	120.01	126.75
1	5	1143	A2M	C5-C4-N3	-5.14	120.05	126.75
1	5	2289	OMG	C5-C4-N3	-5.10	120.19	128.46
1	5	814	OMG	C5-C4-N3	-5.08	120.22	128.46
1	5	2918	OMG	C5-C4-N3	-5.04	120.29	128.46
1	5	1460	OMG	C5-C4-N3	-5.03	120.30	128.46
1	5	2884	OMU	C4-N3-C2	-5.01	119.97	126.58
1	5	2923	OMG	C5-C4-N3	-5.00	120.36	128.46
1	5	657	1MA	N1-C2-N3	-4.95	120.11	126.00
1	5	2954	UR3	C4-N3-C2	-4.93	119.92	124.56
1	5	2396	OMG	C5-C4-N3	-4.90	120.52	128.46
1	5	657	1MA	C5-C4-N3	-4.79	120.12	127.26
1	5	2198	OMC	C2'-C1'-N1	4.75	123.46	114.22
1	5	2923	OMG	C1'-N9-C4	-4.74	112.41	126.50
1	5	2620	OMG	C2-N3-C4	4.70	120.67	112.30
1	5	2396	OMG	C1'-N9-C4	-4.60	112.83	126.50
1	5	2289	OMG	C1'-N9-C4	-4.55	112.98	126.50
1	5	2923	OMG	C1'-N9-C8	4.54	139.62	126.70
1	5	2410	OMG	C2-N3-C4	4.51	120.34	112.30
1	5	2918	OMG	C1'-N9-C4	-4.50	113.14	126.50
1	5	675	OMC	O3'-C3'-C2'	4.46	123.84	111.17
1	5	814	OMG	C1'-N9-C4	-4.45	113.27	126.50
1	5	2289	OMG	C2-N3-C4	4.45	120.23	112.30
1	5	2125	OMG	C2-N3-C4	4.45	120.22	112.30
1	5	2923	OMG	C2-N3-C4	4.43	120.19	112.30
1	5	1855	OMG	C2-N3-C4	4.42	120.17	112.30
1	5	2792	OMG	C2-N3-C4	4.41	120.16	112.30
1	5	2918	OMG	C2-N3-C4	4.40	120.15	112.30
1	5	2947	A2M	N9-C8-N7	-4.40	107.89	113.91
1	5	917	OMG	C2-N3-C4	4.38	120.11	112.30
1	5	814	OMG	C2-N3-C4	4.37	120.08	112.30
1	5	2816	OMG	C2-N3-C4	4.35	120.06	112.30
1	5	2392	OMG	C2-N3-C4	4.32	120.00	112.30
1	5	2396	OMG	C1'-N9-C8	4.32	138.99	126.70
1	5	2289	OMG	C1'-N9-C8	4.31	138.97	126.70
1	5	2918	OMG	C1'-N9-C8	4.28	138.89	126.70
1	5	2125	OMG	C1'-N9-C4	-4.28	113.78	126.50
1	5	1460	OMG	C2-N3-C4	4.25	119.87	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2396	OMG	C2-N3-C4	4.25	119.87	112.30
1	5	2949	OMC	O3'-C3'-C2'	4.24	123.21	111.17
1	5	1459	A2M	N9-C8-N7	-4.23	108.12	113.91
1	5	1860	OMC	O3'-C3'-C4'	4.23	123.29	111.05
1	5	2949	OMC	O3'-C3'-C4'	4.22	123.26	111.05
1	5	1855	OMG	C1'-N9-C4	-4.22	113.98	126.50
1	5	814	OMG	O3'-C3'-C2'	4.21	123.13	111.17
1	5	2816	OMG	C1'-N9-C4	-4.20	114.03	126.50
1	5	814	OMG	C1'-N9-C8	4.16	138.55	126.70
1	5	1143	A2M	N9-C8-N7	-4.16	108.22	113.91
1	5	661	A2M	N9-C8-N7	-4.16	108.22	113.91
1	5	44	OMU	N3-C2-N1	4.16	120.41	114.89
1	5	657	1MA	O4'-C1'-N9	4.15	117.85	108.36
1	5	1377	A2M	N9-C8-N7	-4.15	108.24	113.91
1	5	2683	OMC	O3'-C3'-C2'	4.13	122.89	111.17
1	5	2125	OMG	O3'-C3'-C2'	4.12	122.88	111.17
1	5	2127	A2M	N9-C8-N7	-4.12	108.28	113.91
1	5	2884	OMU	N3-C2-N1	4.09	120.31	114.89
1	5	2683	OMC	O3'-C3'-C4'	4.08	122.86	111.05
1	5	2410	OMG	C1'-N9-C4	-4.08	114.39	126.50
1	5	657	1MA	C2'-C1'-N9	4.08	124.77	113.22
1	5	2125	OMG	C1'-N9-C8	4.08	138.30	126.70
1	5	2641	A2M	N9-C8-N7	-4.07	108.35	113.91
1	5	2366	OMC	CM2-O2'-C2'	4.07	125.20	114.52
1	5	945	A2M	N9-C8-N7	-4.06	108.36	113.91
1	5	2792	OMG	O3'-C3'-C2'	4.06	122.69	111.17
1	5	2396	OMG	O3'-C3'-C2'	4.04	122.65	111.17
1	5	2289	OMG	O3'-C3'-C4'	4.04	122.74	111.05
1	5	2792	OMG	C1'-N9-C4	-4.03	114.54	126.50
1	5	2620	OMG	O3'-C3'-C2'	4.02	122.60	111.17
1	5	2294	OMC	O3'-C3'-C2'	4.02	122.59	111.17
1	5	2392	OMG	O3'-C3'-C2'	4.02	122.59	111.17
1	5	803	OMU	N3-C2-N1	4.01	120.21	114.89
1	5	1855	OMG	C1'-N9-C8	4.01	138.10	126.70
1	5	1892	OMU	N3-C2-N1	4.01	120.21	114.89
1	5	144	OMU	N3-C2-N1	4.00	120.21	114.89
1	5	2322	A2M	N9-C8-N7	-3.98	108.47	113.91
1	5	2816	OMG	C1'-N9-C8	3.97	138.00	126.70
1	5	657	1MA	C2-N3-C4	3.96	120.19	112.41
1	5	2366	OMC	O3'-C3'-C2'	3.95	122.39	111.17
1	5	1847	OMC	O3'-C3'-C2'	3.95	122.38	111.17
1	5	2918	OMG	O3'-C3'-C2'	3.93	122.32	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2651	OMU	N3-C2-N1	3.92	120.10	114.89
1	5	2422	OMU	N3-C2-N1	3.92	120.09	114.89
1	5	2221	A2M	N9-C8-N7	-3.91	108.56	113.91
1	5	2198	OMC	O4'-C1'-N1	3.91	117.31	108.36
1	5	1860	OMC	O3'-C3'-C2'	3.91	122.26	111.17
1	5	2736	OMU	N3-C2-N1	3.89	120.05	114.89
1	5	2410	OMG	C1'-N9-C8	3.89	137.76	126.70
1	5	3300	OMU	N3-C2-N1	3.88	120.04	114.89
1	5	1067	OMU	N3-C2-N1	3.86	120.01	114.89
1	5	2880	OMC	O3'-C3'-C2'	3.86	122.12	111.17
1	5	917	OMG	C1'-N9-C4	-3.85	115.07	126.50
1	5	2289	OMG	O3'-C3'-C2'	3.85	122.10	111.17
1	5	2949	OMC	CM2-O2'-C2'	3.85	124.62	114.52
1	5	1460	OMG	O3'-C3'-C2'	3.83	122.03	111.17
1	5	1460	OMG	O3'-C3'-C4'	3.82	122.11	111.05
1	5	2338	OMC	O3'-C3'-C2'	3.82	122.02	111.17
1	5	2923	OMG	O3'-C3'-C4'	3.82	122.08	111.05
1	5	2816	OMG	O3'-C3'-C2'	3.81	122.00	111.17
1	5	1447	OMC	O3'-C3'-C2'	3.81	121.99	111.17
1	5	2792	OMG	C1'-N9-C8	3.81	137.54	126.70
1	5	2396	OMG	O3'-C3'-C4'	3.81	122.05	111.05
1	5	2392	OMG	O3'-C3'-C4'	3.80	122.03	111.05
1	5	48	OMU	N3-C2-N1	3.80	119.93	114.89
1	5	2294	OMC	O3'-C3'-C4'	3.78	121.97	111.05
1	5	2294	OMC	CM2-O2'-C2'	3.77	124.41	114.52
1	5	1460	OMG	C1'-N9-C4	-3.77	115.31	126.50
1	5	676	OMU	N3-C2-N1	3.76	119.88	114.89
1	5	2923	OMG	O3'-C3'-C2'	3.76	121.84	111.17
1	5	1855	OMG	O3'-C3'-C2'	3.76	121.83	111.17
1	5	2683	OMC	CM2-O2'-C2'	3.75	124.36	114.52
1	5	1447	OMC	O3'-C3'-C4'	3.75	121.88	111.05
1	5	2392	OMG	C1'-N9-C4	-3.74	115.39	126.50
1	5	2125	OMG	O3'-C3'-C4'	3.74	121.87	111.05
1	5	2366	OMC	O3'-C3'-C4'	3.73	121.84	111.05
1	5	814	OMG	O3'-C3'-C4'	3.72	121.81	111.05
1	5	2279	5MC	O3'-C3'-C4'	3.72	121.81	111.05
1	5	1447	OMC	CM2-O2'-C2'	3.69	124.21	114.52
1	5	675	OMC	O3'-C3'-C4'	3.69	121.71	111.05
1	5	2792	OMG	O3'-C3'-C4'	3.68	121.69	111.05
1	5	2880	OMC	O3'-C3'-C4'	3.67	121.67	111.05
1	5	2880	OMC	CM2-O2'-C2'	3.67	124.15	114.52
1	5	2918	OMG	O3'-C3'-C4'	3.65	121.59	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1377	A2M	C2-N3-C4	3.64	120.35	111.75
1	5	2620	OMG	O3'-C3'-C4'	3.63	121.54	111.05
1	5	917	OMG	C1'-N9-C8	3.60	136.96	126.70
1	5	2816	OMG	O3'-C3'-C4'	3.57	121.38	111.05
1	5	2947	A2M	C2-N3-C4	3.56	120.17	111.75
1	5	1847	OMC	O3'-C3'-C4'	3.55	121.32	111.05
1	5	2338	OMC	O3'-C3'-C4'	3.55	121.31	111.05
1	5	661	A2M	C2-N3-C4	3.55	120.13	111.75
1	5	945	A2M	C2-N3-C4	3.50	120.02	111.75
1	5	1460	OMG	C1'-N9-C8	3.49	136.64	126.70
1	5	2392	OMG	C1'-N9-C8	3.49	136.62	126.70
1	5	2641	A2M	C2-N3-C4	3.49	119.99	111.75
1	5	1855	OMG	O3'-C3'-C4'	3.48	121.12	111.05
1	5	2127	A2M	C2-N3-C4	3.48	119.97	111.75
1	5	2221	A2M	C2-N3-C4	3.47	119.96	111.75
1	5	1143	A2M	C2-N3-C4	3.47	119.94	111.75
1	5	48	OMU	C5-C4-N3	3.46	120.02	114.84
1	5	1459	A2M	C2-N3-C4	3.46	119.93	111.75
1	5	2322	A2M	C2-N3-C4	3.44	119.88	111.75
1	5	144	OMU	C5-C4-N3	3.42	119.96	114.84
1	5	2422	OMU	C5-C4-N3	3.41	119.95	114.84
1	5	657	1MA	O2'-C2'-C3'	3.40	122.82	111.82
1	5	2651	OMU	C5-C4-N3	3.39	119.92	114.84
1	5	676	OMU	C5-C4-N3	3.39	119.91	114.84
1	5	2620	OMG	C1'-N9-C4	-3.39	116.44	126.50
1	5	1860	OMC	CM2-O2'-C2'	3.37	123.38	114.52
1	5	945	A2M	N3-C4-N9	3.37	132.63	127.08
1	5	3300	OMU	C5-C4-N3	3.36	119.86	114.84
1	5	2620	OMG	N9-C4-N3	3.33	132.62	125.94
1	5	2279	5MC	O3'-C3'-C2'	3.30	122.51	111.82
1	5	2279	5MC	C5-C6-N1	-3.30	119.94	123.34
1	5	1067	OMU	C5-C4-N3	3.29	119.75	114.84
1	5	2620	OMG	C1'-N9-C8	3.28	136.03	126.70
1	5	1892	OMU	C5-C4-N3	3.27	119.74	114.84
1	5	657	1MA	N9-C8-N7	-3.27	107.23	113.39
1	5	2736	OMU	C5-C4-N3	3.25	119.70	114.84
1	5	2871	5MC	C5-C6-N1	-3.24	120.00	123.34
1	5	803	OMU	C5-C4-N3	3.22	119.66	114.84
1	5	2620	OMG	C2-N1-C6	-3.22	119.23	125.10
1	5	2410	OMG	C2-N1-C6	-3.22	119.23	125.10
1	5	44	OMU	C5-C4-N3	3.21	119.65	114.84
1	5	2392	OMG	C2-N1-C6	-3.21	119.24	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2792	OMG	C2-N1-C6	-3.21	119.25	125.10
1	5	2816	OMG	C2-N1-C6	-3.19	119.28	125.10
1	5	2641	A2M	N3-C4-N9	3.19	132.34	127.08
1	5	1459	A2M	C5-N7-C8	3.18	108.03	103.51
1	5	661	A2M	C5-N7-C8	3.17	108.02	103.51
1	5	1855	OMG	C2-N1-C6	-3.16	119.34	125.10
1	5	2947	A2M	C5-N7-C8	3.16	108.00	103.51
1	5	657	1MA	O2'-C2'-C1'	3.16	120.58	110.02
1	5	2396	OMG	C2-N1-C6	-3.16	119.34	125.10
1	5	1377	A2M	C5-N7-C8	3.16	107.99	103.51
1	5	917	OMG	C2-N1-C6	-3.13	119.40	125.10
1	5	2289	OMG	C2-N1-C6	-3.12	119.41	125.10
1	5	814	OMG	C2-N1-C6	-3.10	119.44	125.10
1	5	2125	OMG	C2-N1-C6	-3.10	119.44	125.10
1	5	2884	OMU	C5-C4-N3	3.09	119.46	114.84
1	5	2792	OMG	N9-C4-N3	3.09	132.13	125.94
1	5	2392	OMG	N9-C4-N3	3.08	132.13	125.94
1	5	2641	A2M	C5-N7-C8	3.08	107.89	103.51
1	5	2918	OMG	C2-N1-C6	-3.08	119.48	125.10
1	5	2338	OMC	CM2-O2'-C2'	3.08	122.61	114.52
1	5	675	OMC	O4'-C4'-C5'	3.08	119.49	109.37
1	5	676	OMU	O4-C4-C5	-3.07	119.76	125.16
1	5	2410	OMG	N9-C4-N3	3.07	132.11	125.94
1	5	917	OMG	N9-C4-N3	3.07	132.11	125.94
1	5	2923	OMG	C2-N1-C6	-3.06	119.52	125.10
1	5	1460	OMG	C2-N1-C6	-3.03	119.56	125.10
1	5	2322	A2M	N3-C4-N9	3.03	132.08	127.08
1	5	2127	A2M	C5-N7-C8	3.03	107.81	103.51
1	5	945	A2M	C5-N7-C8	3.02	107.80	103.51
1	5	661	A2M	N3-C4-N9	3.02	132.06	127.08
1	5	2947	A2M	N3-C4-N9	3.02	132.05	127.08
1	5	48	OMU	O4-C4-C5	-3.02	119.86	125.16
1	5	1143	A2M	N3-C4-N9	3.01	132.04	127.08
1	5	2396	OMG	CM2-O2'-C2'	3.01	122.42	114.52
1	5	1377	A2M	N3-C4-N9	3.00	132.02	127.08
1	5	2392	OMG	CM2-O2'-C2'	2.99	122.38	114.52
1	5	144	OMU	O4-C4-C5	-2.98	119.92	125.16
1	5	1143	A2M	C5-N7-C8	2.97	107.73	103.51
1	5	814	OMG	N9-C8-N7	-2.97	107.80	113.39
1	5	2736	OMU	O4-C4-C5	-2.97	119.94	125.16
1	5	2396	OMG	N9-C8-N7	-2.97	107.81	113.39
1	5	2816	OMG	N9-C4-N3	2.96	131.89	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	3300	OMU	O4-C4-C5	-2.96	119.95	125.16
1	5	2322	A2M	C5-N7-C8	2.96	107.71	103.51
1	5	2792	OMG	O4'-C4'-C5'	2.95	119.09	109.37
1	5	1459	A2M	N3-C4-N9	2.94	131.93	127.08
1	5	2127	A2M	N3-C4-N9	2.94	131.93	127.08
1	5	44	OMU	O4-C4-C5	-2.94	119.99	125.16
1	5	1460	OMG	CM2-O2'-C2'	2.92	122.20	114.52
1	5	1460	OMG	N9-C4-N3	2.92	131.81	125.94
1	5	1067	OMU	O4-C4-C5	-2.92	120.02	125.16
1	5	2289	OMG	N9-C8-N7	-2.92	107.90	113.39
1	5	2620	OMG	CM2-O2'-C2'	2.92	122.17	114.52
1	5	2125	OMG	N9-C4-N3	2.91	131.78	125.94
1	5	2923	OMG	N9-C8-N7	-2.90	107.92	113.39
1	5	1855	OMG	N9-C4-N3	2.90	131.77	125.94
1	5	2422	OMU	O4-C4-C5	-2.90	120.06	125.16
1	5	803	OMU	O4-C4-C5	-2.90	120.06	125.16
1	5	2125	OMG	CM2-O2'-C2'	2.90	122.13	114.52
1	5	2816	OMG	CM2-O2'-C2'	2.90	122.12	114.52
1	5	2221	A2M	C5-N7-C8	2.89	107.61	103.51
1	5	814	OMG	N9-C4-N3	2.89	131.74	125.94
1	5	2884	OMU	O4-C4-C5	-2.88	120.10	125.16
1	5	2396	OMG	O4'-C4'-C5'	2.88	118.84	109.37
1	5	2125	OMG	O4'-C4'-C5'	2.88	118.84	109.37
1	5	2792	OMG	CM2-O2'-C2'	2.87	122.05	114.52
1	5	2620	OMG	O4'-C4'-C5'	2.86	118.78	109.37
1	5	814	OMG	CM2-O2'-C2'	2.86	122.02	114.52
1	5	2289	OMG	N9-C4-N3	2.85	131.66	125.94
1	5	2651	OMU	O4-C4-C5	-2.85	120.15	125.16
1	5	2816	OMG	N9-C8-N7	-2.84	108.04	113.39
1	5	2221	A2M	N3-C4-N9	2.84	131.76	127.08
1	5	2392	OMG	N9-C8-N7	-2.84	108.05	113.39
1	5	2125	OMG	N9-C8-N7	-2.83	108.05	113.39
1	5	2410	OMG	N9-C8-N7	-2.83	108.07	113.39
1	5	2792	OMG	N9-C8-N7	-2.82	108.07	113.39
1	5	2816	OMG	O4'-C4'-C5'	2.82	118.66	109.37
1	5	2918	OMG	N9-C8-N7	-2.82	108.08	113.39
1	5	2410	OMG	C5-C6-N1	2.81	120.33	113.19
1	5	1855	OMG	N9-C8-N7	-2.80	108.12	113.39
1	5	917	OMG	N9-C8-N7	-2.79	108.13	113.39
1	5	2792	OMG	C5-C6-N1	2.78	120.25	113.19
1	5	2125	OMG	C5-C6-N1	2.78	120.25	113.19
1	5	2620	OMG	C5-C6-N1	2.77	120.24	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2918	OMG	N9-C4-N3	2.77	131.51	125.94
1	5	2289	OMG	CM2-O2'-C2'	2.77	121.79	114.52
1	5	1892	OMU	O4-C4-C5	-2.77	120.29	125.16
1	5	2289	OMG	C5-C6-N1	2.76	120.21	113.19
1	5	2816	OMG	C5-C6-N1	2.76	120.20	113.19
1	5	917	OMG	C5-C6-N1	2.76	120.19	113.19
1	5	1855	OMG	C5-C6-N1	2.75	120.18	113.19
1	5	1447	OMC	O4'-C4'-C5'	2.75	118.42	109.37
1	5	917	OMG	O3'-C3'-C2'	2.75	118.96	111.17
1	5	2396	OMG	C5-C6-N1	2.74	120.16	113.19
1	5	2918	OMG	C5-C6-N1	2.74	120.16	113.19
1	5	2923	OMG	C5-C6-N1	2.74	120.14	113.19
1	5	2392	OMG	C5-C6-N1	2.74	120.14	113.19
1	5	1460	OMG	N9-C8-N7	-2.74	108.24	113.39
1	5	1855	OMG	O4'-C4'-C5'	2.73	118.35	109.37
1	5	814	OMG	C5-C6-N1	2.73	120.11	113.19
1	5	2923	OMG	C5'-C4'-C3'	2.72	125.37	115.18
1	5	2871	5MC	O3'-C3'-C4'	2.71	118.89	111.05
1	5	2923	OMG	CM2-O2'-C2'	2.71	121.63	114.52
1	5	2918	OMG	O4'-C4'-C5'	2.70	118.26	109.37
1	5	2366	OMC	O4'-C4'-C5'	2.69	118.23	109.37
1	5	1855	OMG	C5'-C4'-C3'	2.68	125.23	115.18
1	5	2923	OMG	N9-C4-N3	2.68	131.32	125.94
1	5	2871	5MC	O3'-C3'-C2'	2.68	120.48	111.82
1	5	2396	OMG	C5'-C4'-C3'	2.67	125.20	115.18
1	5	2396	OMG	N9-C4-N3	2.67	131.31	125.94
1	5	814	OMG	O4'-C4'-C5'	2.67	118.17	109.37
1	5	1460	OMG	C5-C6-N1	2.67	119.97	113.19
1	5	2289	OMG	C5'-C4'-C3'	2.66	125.17	115.18
1	5	2871	5MC	C1'-N1-C6	2.66	125.56	121.12
1	5	675	OMC	C5'-C4'-C3'	2.65	125.11	115.18
1	5	2947	A2M	C2'-C1'-N9	-2.64	109.09	113.53
1	5	2884	OMU	O4'-C4'-C5'	2.63	118.04	109.37
1	5	917	OMG	O4'-C4'-C5'	2.63	118.02	109.37
1	5	2816	OMG	O6-C6-C5	-2.63	119.64	126.60
1	5	2289	OMG	O4'-C4'-C5'	2.62	117.99	109.37
1	5	2620	OMG	N9-C8-N7	-2.62	108.46	113.39
1	5	2125	OMG	C5'-C4'-C3'	2.62	124.99	115.18
1	5	1847	OMC	C5'-C4'-C3'	2.60	124.93	115.18
1	5	2392	OMG	O4'-C4'-C5'	2.60	117.93	109.37
1	5	2816	OMG	C5'-C4'-C3'	2.60	124.91	115.18
1	5	917	OMG	O6-C6-C5	-2.59	119.72	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1447	OMC	C5'-C4'-C3'	2.58	124.86	115.18
1	5	917	OMG	O3'-C3'-C4'	2.58	118.52	111.05
1	5	814	OMG	O6-C6-C5	-2.57	119.78	126.60
1	5	2338	OMC	O4'-C4'-C5'	2.56	117.81	109.37
1	5	2949	OMC	O4'-C4'-C5'	2.56	117.81	109.37
1	5	2880	OMC	O4'-C4'-C5'	2.56	117.80	109.37
1	5	2279	5MC	O4'-C4'-C5'	2.56	117.79	109.37
1	5	2289	OMG	O6-C6-C5	-2.56	119.81	126.60
1	5	2392	OMG	C5'-C4'-C3'	2.55	124.74	115.18
1	5	2923	OMG	O6-C6-C5	-2.55	119.84	126.60
1	5	1860	OMC	C5'-C4'-C3'	2.55	124.73	115.18
1	5	1892	OMU	O2-C2-N1	-2.55	119.40	122.79
1	5	2923	OMG	O4'-C4'-C5'	2.55	117.75	109.37
1	5	2410	OMG	O3'-C3'-C4'	2.54	118.39	111.05
1	5	2392	OMG	O6-C6-C5	-2.54	119.87	126.60
1	5	2338	OMC	C5'-C4'-C3'	2.54	124.69	115.18
1	5	2410	OMG	O6-C6-C5	-2.54	119.87	126.60
1	5	2880	OMC	C5'-C4'-C3'	2.53	124.68	115.18
1	5	1460	OMG	C5'-C4'-C3'	2.53	124.67	115.18
1	5	2918	OMG	CM2-O2'-C2'	2.53	121.17	114.52
1	5	945	A2M	C6-C5-C4	2.52	120.58	117.18
1	5	2884	OMU	C5'-C4'-C3'	2.51	124.59	115.18
1	5	2792	OMG	C5'-C4'-C3'	2.51	124.59	115.18
1	5	1067	OMU	O4'-C4'-C5'	2.50	117.61	109.37
1	5	2683	OMC	C2'-C3'-C4'	2.50	107.43	101.99
1	5	2871	5MC	O4'-C4'-C5'	2.50	117.61	109.37
1	5	2125	OMG	O6-C6-C5	-2.50	119.97	126.60
1	5	2294	OMC	O4'-C4'-C5'	2.50	117.58	109.37
1	5	1860	OMC	O4'-C4'-C5'	2.49	117.57	109.37
1	5	2620	OMG	O6-C6-C5	-2.49	119.99	126.60
1	5	1860	OMC	C2'-C3'-C4'	2.48	107.39	101.99
1	5	2918	OMG	O6-C6-C5	-2.48	120.02	126.60
1	5	803	OMU	O2-C2-N1	-2.48	119.49	122.79
1	5	1855	OMG	O6-C6-C5	-2.48	120.03	126.60
1	5	814	OMG	C2'-C3'-C4'	2.48	107.37	101.99
1	5	2366	OMC	C5'-C4'-C3'	2.47	124.43	115.18
1	5	2396	OMG	O6-C6-C5	-2.46	120.07	126.60
1	5	2683	OMC	O4'-C4'-C5'	2.46	117.47	109.37
1	5	1460	OMG	O6-C6-C5	-2.46	120.08	126.60
1	5	2918	OMG	C5'-C4'-C3'	2.45	124.38	115.18
1	5	2949	OMC	C5'-C4'-C3'	2.44	124.33	115.18
1	5	2884	OMU	O3'-C3'-C2'	2.44	118.08	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2792	OMG	O6-C6-C5	-2.43	120.15	126.60
1	5	2279	5MC	C5'-C4'-C3'	2.42	124.27	115.18
1	5	2683	OMC	C5'-C4'-C3'	2.42	124.26	115.18
1	5	2294	OMC	C5'-C4'-C3'	2.42	124.26	115.18
1	5	2620	OMG	C5'-C4'-C3'	2.42	124.24	115.18
1	5	1067	OMU	C5'-C4'-C3'	2.41	124.23	115.18
1	5	44	OMU	O2-C2-N1	-2.38	119.62	122.79
1	5	814	OMG	C5'-C4'-C3'	2.37	124.05	115.18
1	5	2641	A2M	C6-C5-C4	2.36	120.36	117.18
1	5	2871	5MC	C5'-C4'-C3'	2.34	123.97	115.18
1	5	3300	OMU	O2-C2-N1	-2.33	119.69	122.79
1	5	2923	OMG	C2'-C3'-C4'	2.32	107.04	101.99
1	5	1847	OMC	O4'-C4'-C5'	2.32	117.02	109.37
1	5	1377	A2M	C4-C5-N7	-2.32	107.79	110.62
1	5	2410	OMG	O3'-C3'-C2'	2.32	117.74	111.17
1	5	2422	OMU	O2-C2-N1	-2.31	119.72	122.79
1	5	1459	A2M	C4-C5-N7	-2.30	107.81	110.62
1	5	2322	A2M	C6-C5-C4	2.30	120.28	117.18
1	5	661	A2M	C4-C5-N7	-2.29	107.83	110.62
1	5	657	1MA	C8-N7-C5	2.29	108.39	104.24
1	5	1067	OMU	O2-C2-N1	-2.29	119.74	122.79
1	5	1459	A2M	C6-C5-C4	2.29	120.26	117.18
1	5	917	OMG	C5'-C4'-C3'	2.28	123.71	115.18
1	5	2651	OMU	O2-C2-N1	-2.28	119.76	122.79
1	5	2949	OMC	C2'-C3'-C4'	2.28	106.94	101.99
1	5	657	1MA	N9-C4-N3	2.26	132.22	126.94
1	5	2289	OMG	C2'-C3'-C4'	2.26	106.91	101.99
1	5	1460	OMG	O4'-C4'-C5'	2.26	116.79	109.37
1	5	1377	A2M	C5-C4-N9	2.26	108.41	105.78
1	5	2366	OMC	C2'-C3'-C4'	2.25	106.88	101.99
1	5	661	A2M	C6-C5-C4	2.23	120.18	117.18
1	5	2736	OMU	O2-C2-N1	-2.23	119.83	122.79
1	5	1460	OMG	C2'-C3'-C4'	2.23	106.83	101.99
1	5	2620	OMG	C2'-C3'-C4'	2.22	106.82	101.99
1	5	2338	OMC	C2'-C3'-C4'	2.21	106.80	101.99
1	5	2947	A2M	C4-N9-C8	2.21	108.12	105.73
1	5	48	OMU	O2-C2-N1	-2.20	119.86	122.79
1	5	2221	A2M	C2'-C3'-C4'	2.20	106.77	101.99
1	5	661	A2M	C5-C4-N9	2.18	108.32	105.78
1	5	2884	OMU	O2-C2-N1	-2.17	119.90	122.79
1	5	44	OMU	O3'-C3'-C2'	2.17	117.32	111.17
1	5	2947	A2M	C4-C5-N7	-2.16	107.99	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2641	A2M	C4-C5-N7	-2.15	108.00	110.62
1	5	2221	A2M	C6-C5-C4	2.15	120.07	117.18
1	5	814	OMG	C8-N7-C5	2.15	108.12	104.24
1	5	2289	OMG	C8-N7-C5	2.15	108.12	104.24
1	5	1459	A2M	C5-C4-N9	2.14	108.27	105.78
1	5	676	OMU	O2-C2-N1	-2.14	119.94	122.79
1	5	2816	OMG	C2'-C3'-C4'	2.14	106.64	101.99
1	5	2410	OMG	O4'-C4'-C5'	2.12	116.35	109.37
1	5	2880	OMC	C2'-C3'-C4'	2.12	106.60	101.99
1	5	2410	OMG	C8-N7-C5	2.12	108.07	104.24
1	5	2918	OMG	C2'-C3'-C4'	2.12	106.59	101.99
1	5	2923	OMG	C8-N7-C5	2.11	108.06	104.24
1	5	1377	A2M	C6-C5-C4	2.11	120.02	117.18
1	5	2322	A2M	C4-C5-N7	-2.11	108.05	110.62
1	5	2792	OMG	C8-N7-C5	2.10	108.04	104.24
1	5	1855	OMG	C2'-C3'-C4'	2.10	106.55	101.99
1	5	2279	5MC	C2'-C3'-C4'	2.09	106.71	102.64
1	5	2221	A2M	C5-C4-N9	2.09	108.22	105.78
1	5	2127	A2M	C6-C5-C4	2.09	120.00	117.18
1	5	2392	OMG	C2'-C3'-C4'	2.08	106.52	101.99
1	5	1447	OMC	O2-C2-N3	-2.07	118.96	122.33
1	5	2127	A2M	C4-C5-N7	-2.07	108.09	110.62
1	5	2392	OMG	C8-N7-C5	2.07	107.98	104.24
1	5	1143	A2M	C6-C5-C4	2.05	119.94	117.18
1	5	2620	OMG	C8-N7-C5	2.05	107.94	104.24
1	5	2816	OMG	C8-N7-C5	2.05	107.94	104.24
1	5	144	OMU	O2-C2-N1	-2.04	120.07	122.79
1	5	2322	A2M	C5-C4-N9	2.04	108.15	105.78
1	5	2125	OMG	C8-N7-C5	2.04	107.92	104.24
1	5	2294	OMC	C2'-C3'-C4'	2.03	106.41	101.99
1	5	1143	A2M	C4-N9-C8	2.03	107.93	105.73
1	5	2396	OMG	C8-N7-C5	2.03	107.92	104.24
1	5	675	OMC	N4-C4-N3	2.02	121.52	117.97
1	5	2221	A2M	C4-C5-N7	-2.02	108.16	110.62
1	5	917	OMG	C8-N7-C5	2.02	107.89	104.24
1	5	1855	OMG	C8-N7-C5	2.01	107.88	104.24
1	5	945	A2M	C4-C5-N7	-2.01	108.17	110.62
1	5	1855	OMG	CM2-O2'-C2'	2.01	119.80	114.52
1	5	2127	A2M	C5-C4-N9	2.00	108.11	105.78
1	5	2918	OMG	C8-N7-C5	2.00	107.86	104.24
1	5	2947	A2M	C6-C5-C4	2.00	119.87	117.18

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	5	44	OMU	C1'-C2'-O2'-CM2
1	5	661	A2M	O4'-C4'-C5'-O5'
1	5	661	A2M	C3'-C4'-C5'-O5'
1	5	675	OMC	O4'-C4'-C5'-O5'
1	5	814	OMG	C1'-C2'-O2'-CM2
1	5	945	A2M	O4'-C4'-C5'-O5'
1	5	945	A2M	C3'-C4'-C5'-O5'
1	5	1143	A2M	O4'-C4'-C5'-O5'
1	5	1143	A2M	C3'-C4'-C5'-O5'
1	5	1447	OMC	C1'-C2'-O2'-CM2
1	5	1460	OMG	C3'-C4'-C5'-O5'
1	5	1460	OMG	C1'-C2'-O2'-CM2
1	5	1847	OMC	C3'-C4'-C5'-O5'
1	5	1847	OMC	O4'-C4'-C5'-O5'
1	5	1855	OMG	C1'-C2'-O2'-CM2
1	5	1860	OMC	C1'-C2'-O2'-CM2
1	5	2125	OMG	O4'-C4'-C5'-O5'
1	5	2125	OMG	C3'-C4'-C5'-O5'
1	5	2125	OMG	C1'-C2'-O2'-CM2
1	5	2221	A2M	C3'-C4'-C5'-O5'
1	5	2279	5MC	O4'-C4'-C5'-O5'
1	5	2279	5MC	C3'-C4'-C5'-O5'
1	5	2289	OMG	C1'-C2'-O2'-CM2
1	5	2294	OMC	C1'-C2'-O2'-CM2
1	5	2294	OMC	C3'-C4'-C5'-O5'
1	5	2338	OMC	C1'-C2'-O2'-CM2
1	5	2366	OMC	C1'-C2'-O2'-CM2
1	5	2392	OMG	C1'-C2'-O2'-CM2
1	5	2396	OMG	O4'-C4'-C5'-O5'
1	5	2396	OMG	C3'-C4'-C5'-O5'
1	5	2396	OMG	C1'-C2'-O2'-CM2
1	5	2422	OMU	C3'-C4'-C5'-O5'
1	5	2422	OMU	O4'-C4'-C5'-O5'
1	5	2620	OMG	C1'-C2'-O2'-CM2
1	5	2683	OMC	C1'-C2'-O2'-CM2
1	5	2792	OMG	O4'-C4'-C5'-O5'
1	5	2792	OMG	C1'-C2'-O2'-CM2
1	5	2816	OMG	C1'-C2'-O2'-CM2
1	5	2871	5MC	O4'-C4'-C5'-O5'
1	5	2871	5MC	C2'-C1'-N1-C6
1	5	2880	OMC	C1'-C2'-O2'-CM2
1	5	2884	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
1	5	2918	OMG	C1'-C2'-O2'-CM2
1	5	2923	OMG	C1'-C2'-O2'-CM2
1	5	2949	OMC	C1'-C2'-O2'-CM2
1	5	2949	OMC	C3'-C4'-C5'-O5'
1	5	2949	OMC	O4'-C4'-C5'-O5'
1	5	676	OMU	C3'-C4'-C5'-O5'
1	5	1460	OMG	O4'-C4'-C5'-O5'
1	5	2294	OMC	O4'-C4'-C5'-O5'
1	5	2338	OMC	C3'-C4'-C5'-O5'
1	5	2392	OMG	O4'-C4'-C5'-O5'
1	5	2392	OMG	C3'-C4'-C5'-O5'
1	5	2620	OMG	C3'-C4'-C5'-O5'
1	5	2683	OMC	C3'-C4'-C5'-O5'
1	5	2792	OMG	C3'-C4'-C5'-O5'
1	5	2880	OMC	C3'-C4'-C5'-O5'
1	5	2918	OMG	C3'-C4'-C5'-O5'
1	5	44	OMU	C3'-C4'-C5'-O5'
1	5	44	OMU	O4'-C4'-C5'-O5'
1	5	676	OMU	O4'-C4'-C5'-O5'
1	5	814	OMG	C3'-C4'-C5'-O5'
1	5	917	OMG	C3'-C4'-C5'-O5'
1	5	1447	OMC	O4'-C4'-C5'-O5'
1	5	1855	OMG	O4'-C4'-C5'-O5'
1	5	2221	A2M	O4'-C4'-C5'-O5'
1	5	2338	OMC	O4'-C4'-C5'-O5'
1	5	2620	OMG	O4'-C4'-C5'-O5'
1	5	2816	OMG	C3'-C4'-C5'-O5'
1	5	2871	5MC	C3'-C4'-C5'-O5'
1	5	1460	OMG	C3'-C2'-O2'-CM2
1	5	2198	OMC	C3'-C2'-O2'-CM2
1	5	2683	OMC	C3'-C2'-O2'-CM2
1	5	2923	OMG	C3'-C2'-O2'-CM2
1	5	2871	5MC	C2'-C1'-N1-C2
1	5	2410	OMG	C3'-C4'-C5'-O5'
1	5	657	1MA	O4'-C4'-C5'-O5'
1	5	2289	OMG	C3'-C4'-C5'-O5'
1	5	2923	OMG	O4'-C4'-C5'-O5'
1	5	144	OMU	O4'-C4'-C5'-O5'
1	5	2880	OMC	O4'-C4'-C5'-O5'
1	5	675	OMC	C3'-C4'-C5'-O5'
1	5	3300	OMU	O4'-C4'-C5'-O5'
1	5	675	OMC	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	5	803	OMU	O4'-C4'-C5'-O5'
1	5	3300	OMU	C3'-C4'-C5'-O5'
1	5	2198	OMC	O4'-C1'-N1-C2
1	5	2198	OMC	O4'-C1'-N1-C6
1	5	2396	OMG	C4'-C5'-O5'-P
1	5	2949	OMC	C4'-C5'-O5'-P
1	5	657	1MA	C3'-C4'-C5'-O5'
1	5	2289	OMG	O4'-C4'-C5'-O5'
1	5	2947	A2M	O4'-C4'-C5'-O5'
1	5	661	A2M	C4'-C5'-O5'-P
1	5	2127	A2M	C3'-C4'-C5'-O5'
1	5	2125	OMG	C4'-C5'-O5'-P
1	5	2620	OMG	C4'-C5'-O5'-P
1	5	2871	5MC	O4'-C1'-N1-C6
1	5	1447	OMC	C2'-C1'-N1-C2
1	5	1447	OMC	C2'-C1'-N1-C6
1	5	2871	5MC	O4'-C1'-N1-C2
1	5	2918	OMG	C4'-C5'-O5'-P
1	5	144	OMU	C3'-C2'-O2'-CM2
1	5	144	OMU	C3'-C4'-C5'-O5'
1	5	1847	OMC	C2'-C1'-N1-C6
1	5	945	A2M	C4'-C5'-O5'-P
1	5	1447	OMC	C3'-C4'-C5'-O5'
1	5	2736	OMU	O4'-C4'-C5'-O5'
1	5	675	OMC	C2'-C1'-N1-C2
1	5	2289	OMG	C4'-C5'-O5'-P
1	5	2127	A2M	O4'-C4'-C5'-O5'
1	5	1847	OMC	C2'-C1'-N1-C2
1	5	2221	A2M	C4'-C5'-O5'-P
1	5	803	OMU	C3'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5	2289	OMG	4	0
1	5	2279	5MC	2	0
1	5	2816	OMG	2	0
1	5	1855	OMG	2	0
1	5	2923	OMG	2	0
1	5	2871	5MC	4	0
1	5	44	OMU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5	2884	OMU	1	0
1	5	2392	OMG	3	0
1	5	2294	OMC	2	0
1	5	2918	OMG	2	0
1	5	2949	OMC	3	0
1	5	2620	OMG	2	0
1	5	917	OMG	1	0
1	5	2736	OMU	1	0
1	5	2198	OMC	1	0
1	5	2410	OMG	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 51 ligands modelled in this entry, 51 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

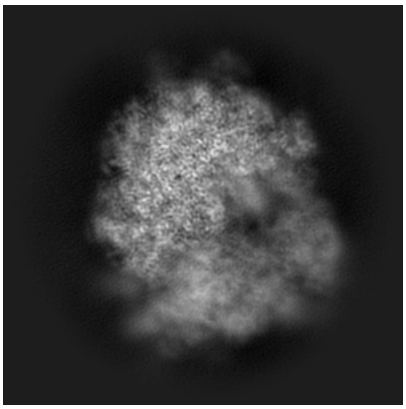
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54774. These allow visual inspection of the internal detail of the map and identification of artifacts.

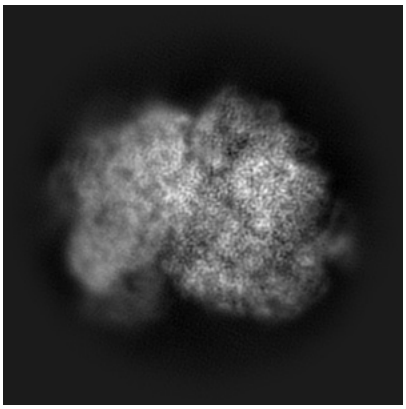
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

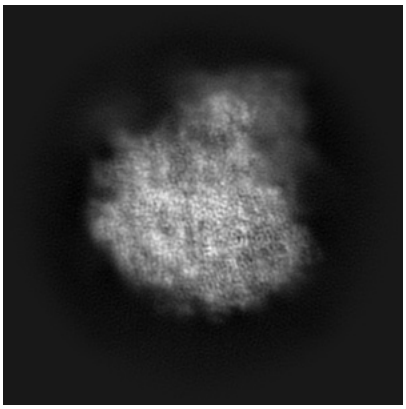
6.1.1 Primary map



X

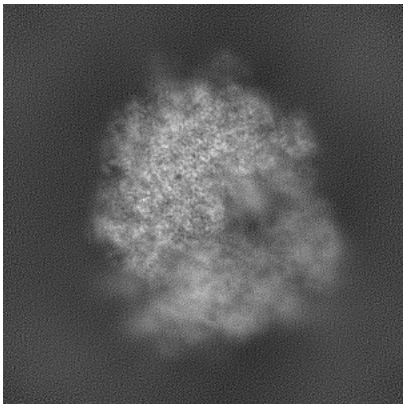


Y

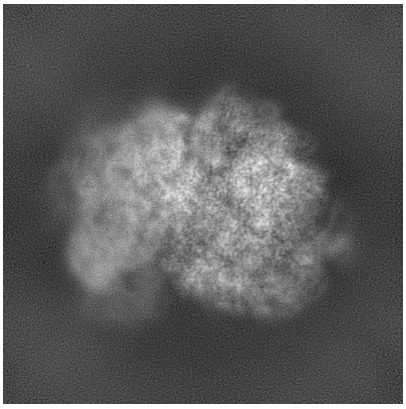


Z

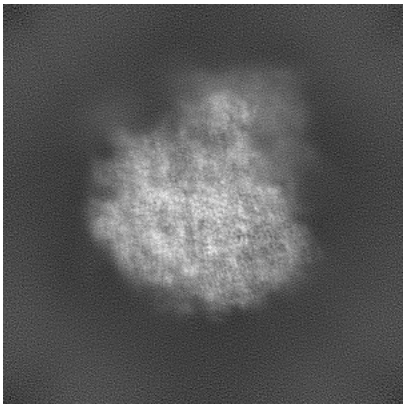
6.1.2 Raw map



X



Y

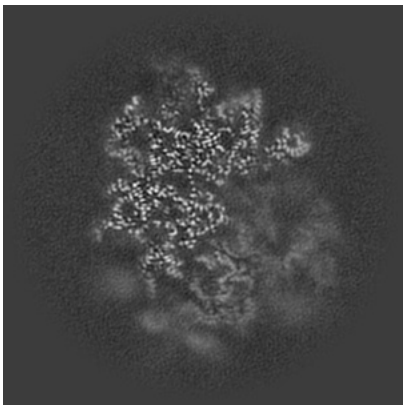


Z

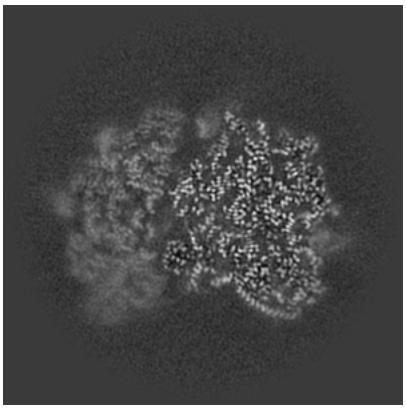
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

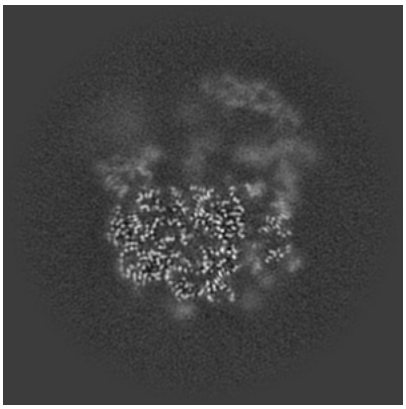
6.2.1 Primary map



X Index: 225

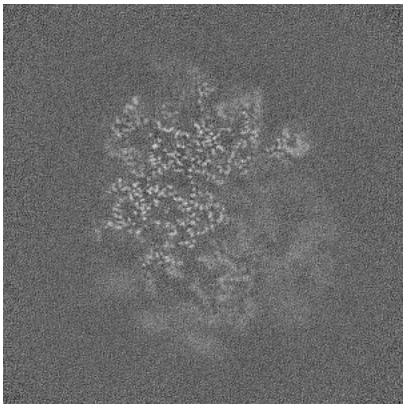


Y Index: 225

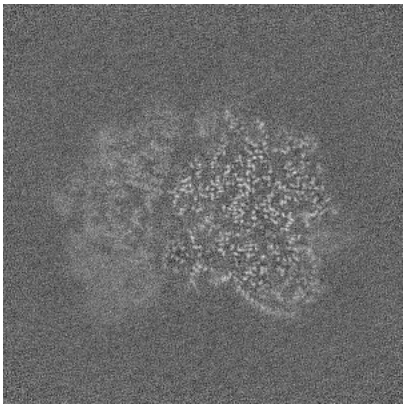


Z Index: 225

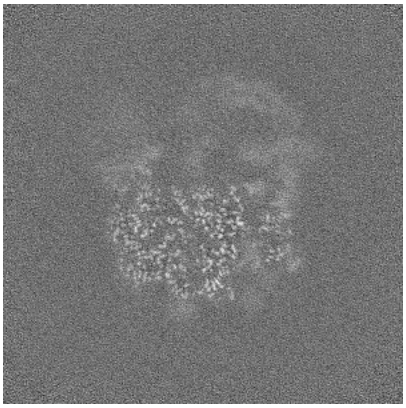
6.2.2 Raw map



X Index: 225



Y Index: 225

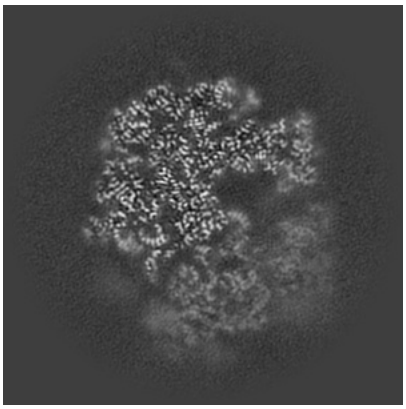


Z Index: 225

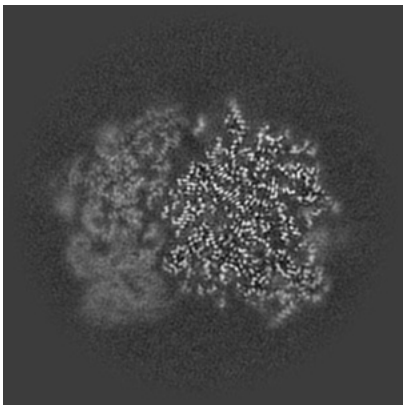
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

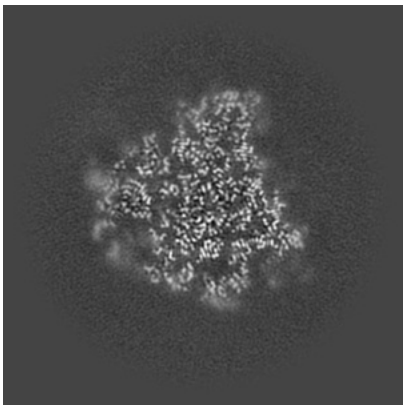
6.3.1 Primary map



X Index: 241

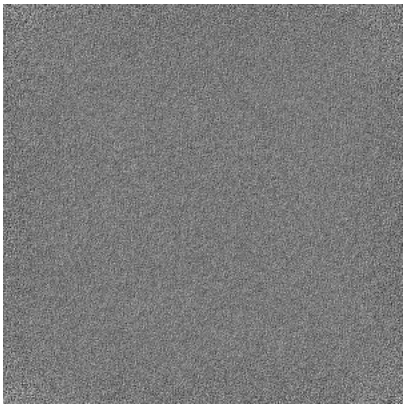


Y Index: 218

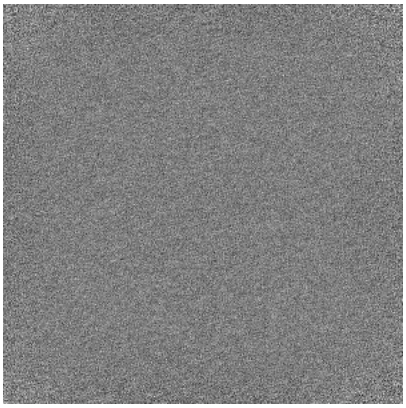


Z Index: 290

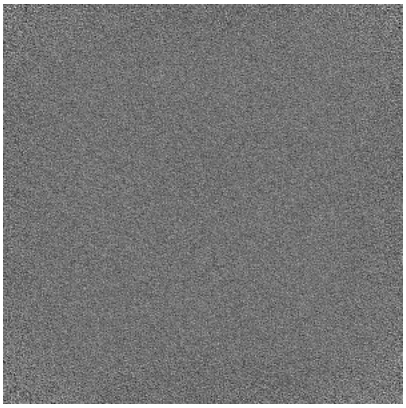
6.3.2 Raw map



X Index: 0



Y Index: 0

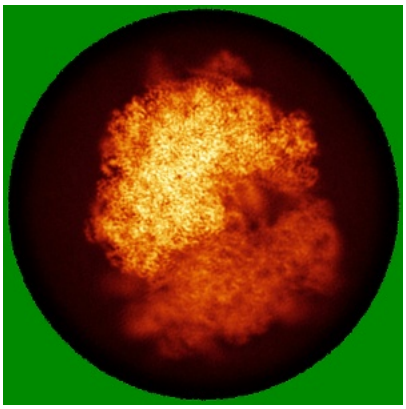


Z Index: 449

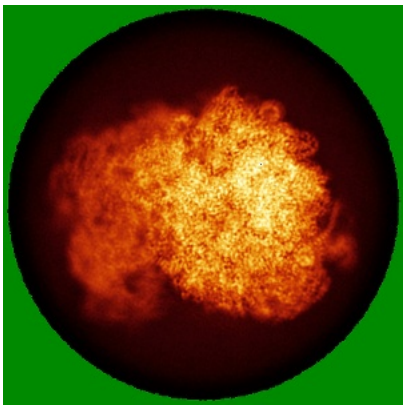
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

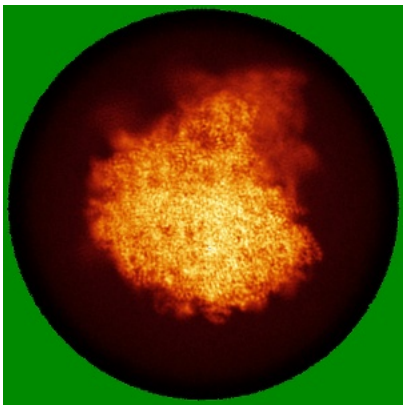
6.4.1 Primary map



X

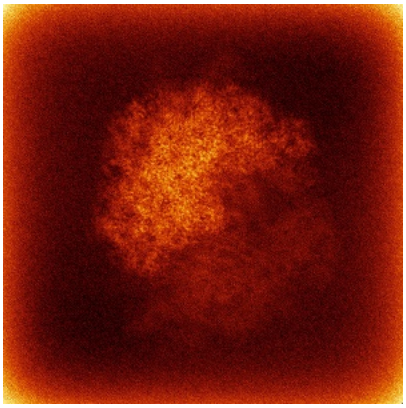


Y

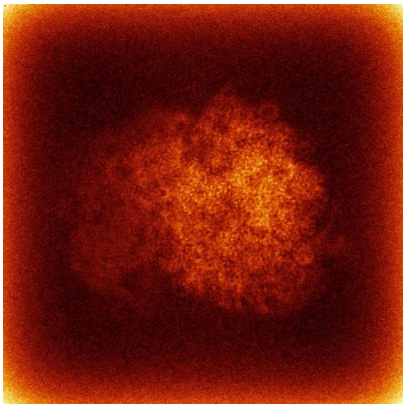


Z

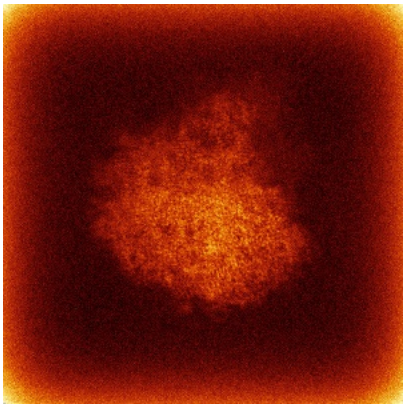
6.4.2 Raw map



X



Y

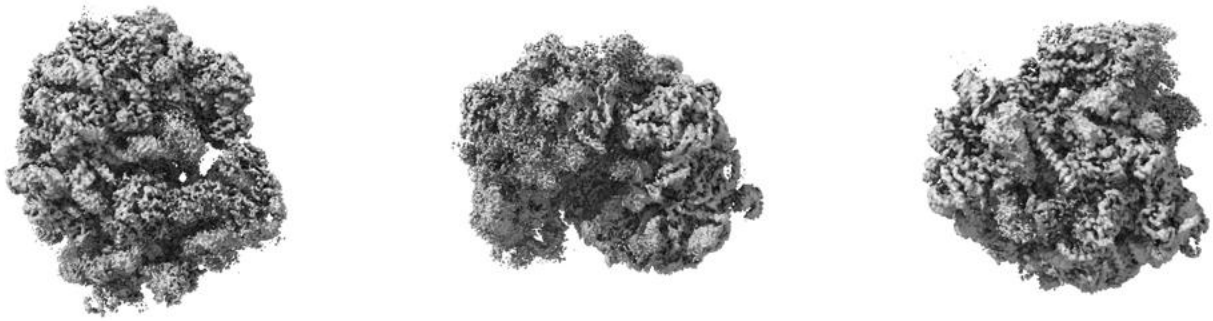


Z

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)

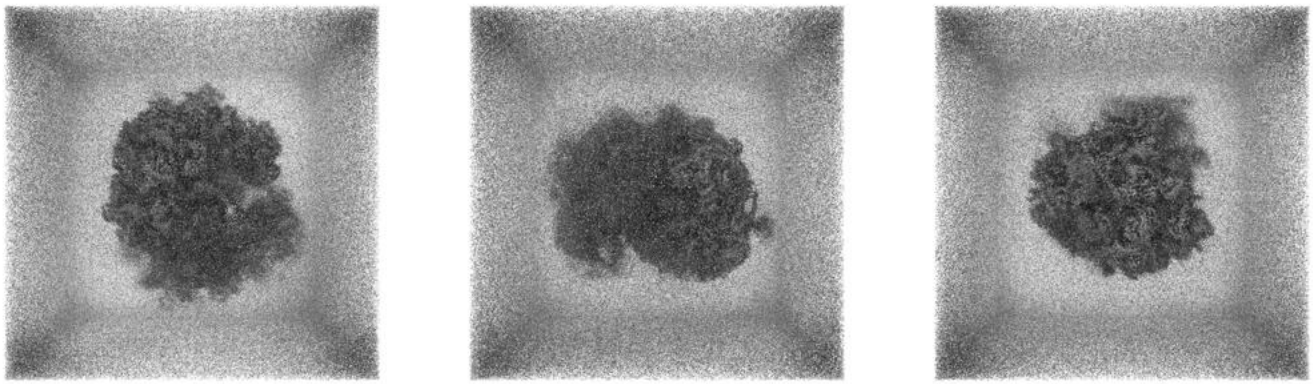
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. 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



X Y Z

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

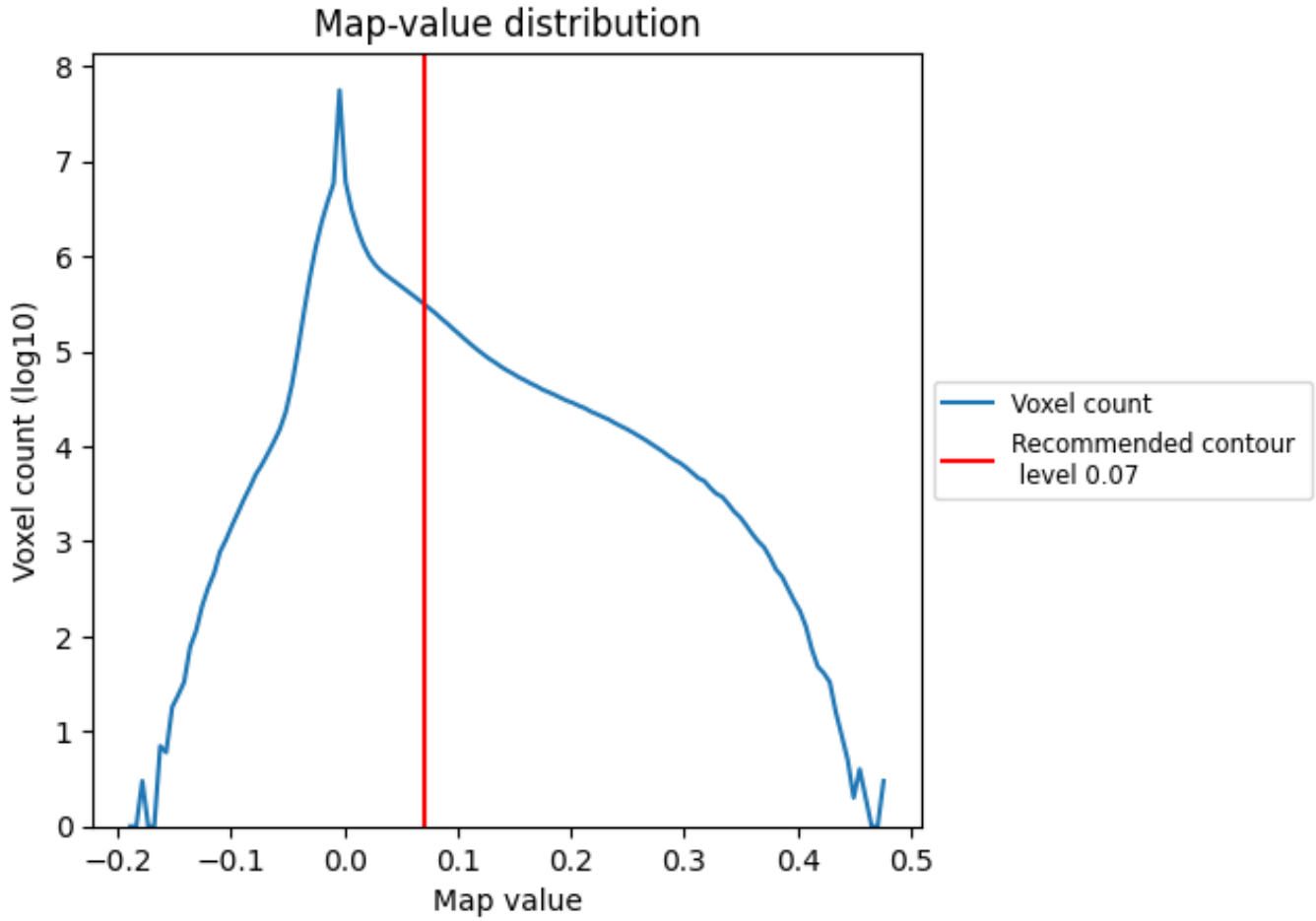
6.6 Mask visualisation (i)

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

7 Map analysis

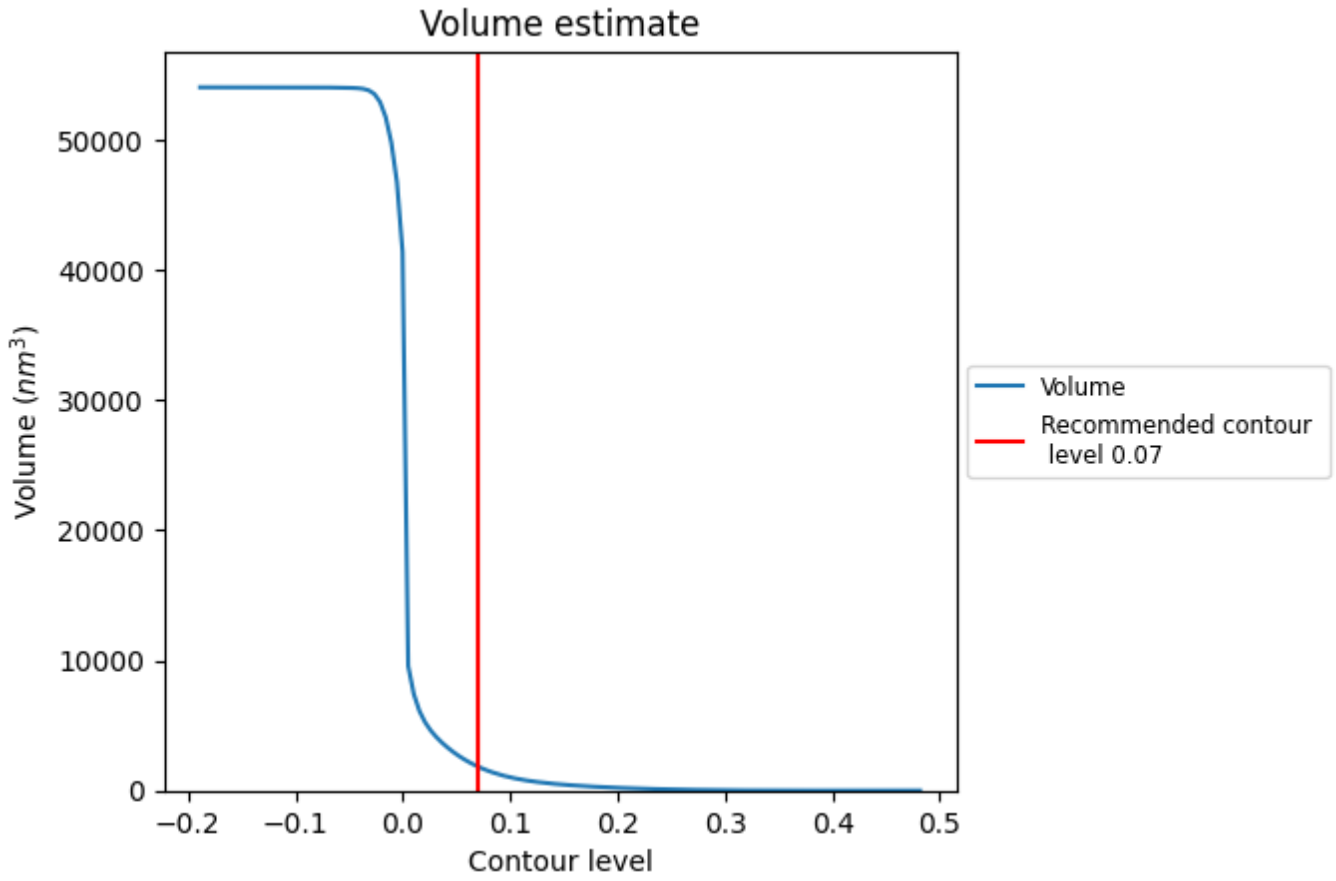
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

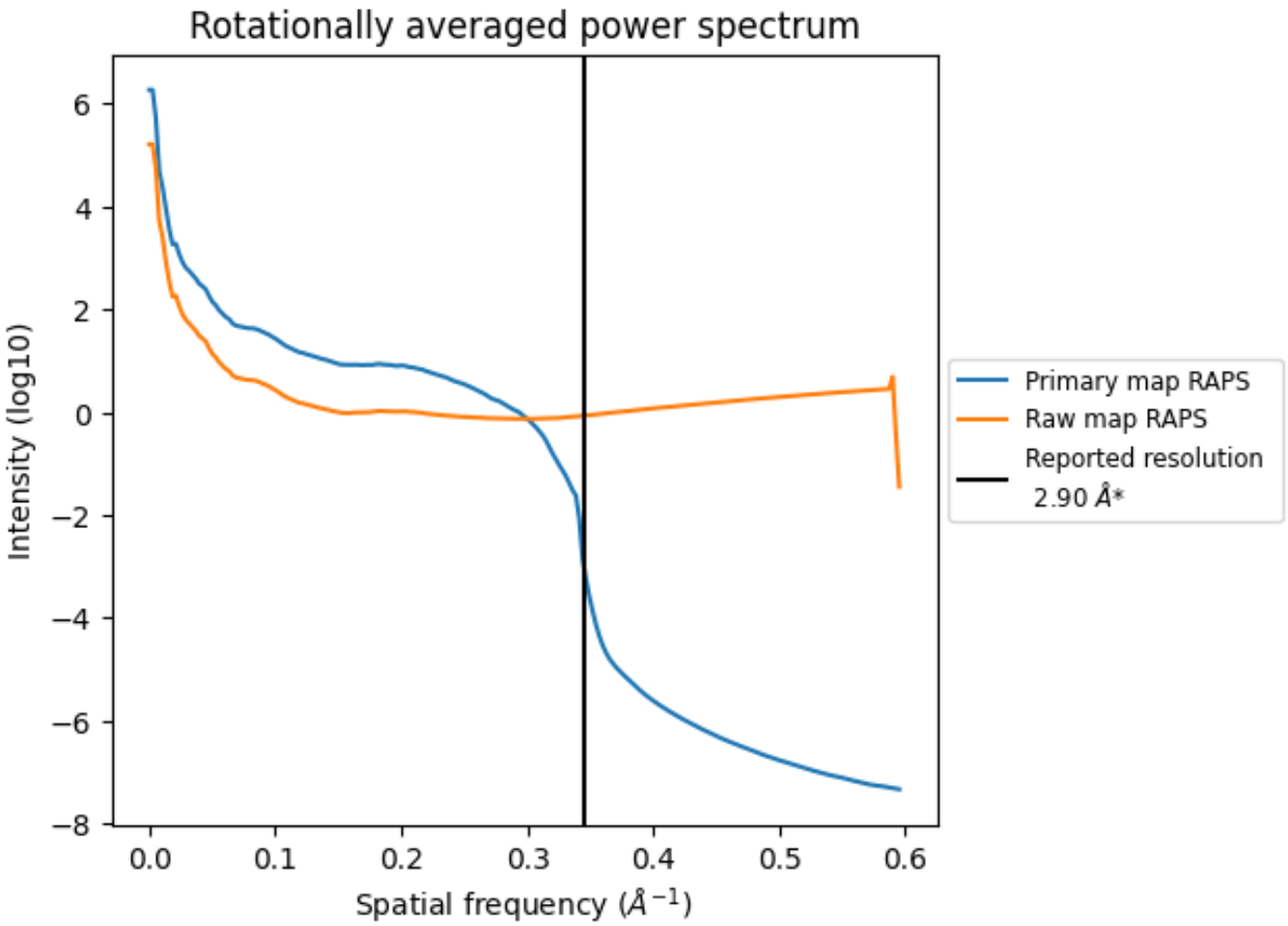
7.2 Volume estimate



The volume at the recommended contour level is 1842 nm^3; this corresponds to an approximate mass of 1664 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 (i)

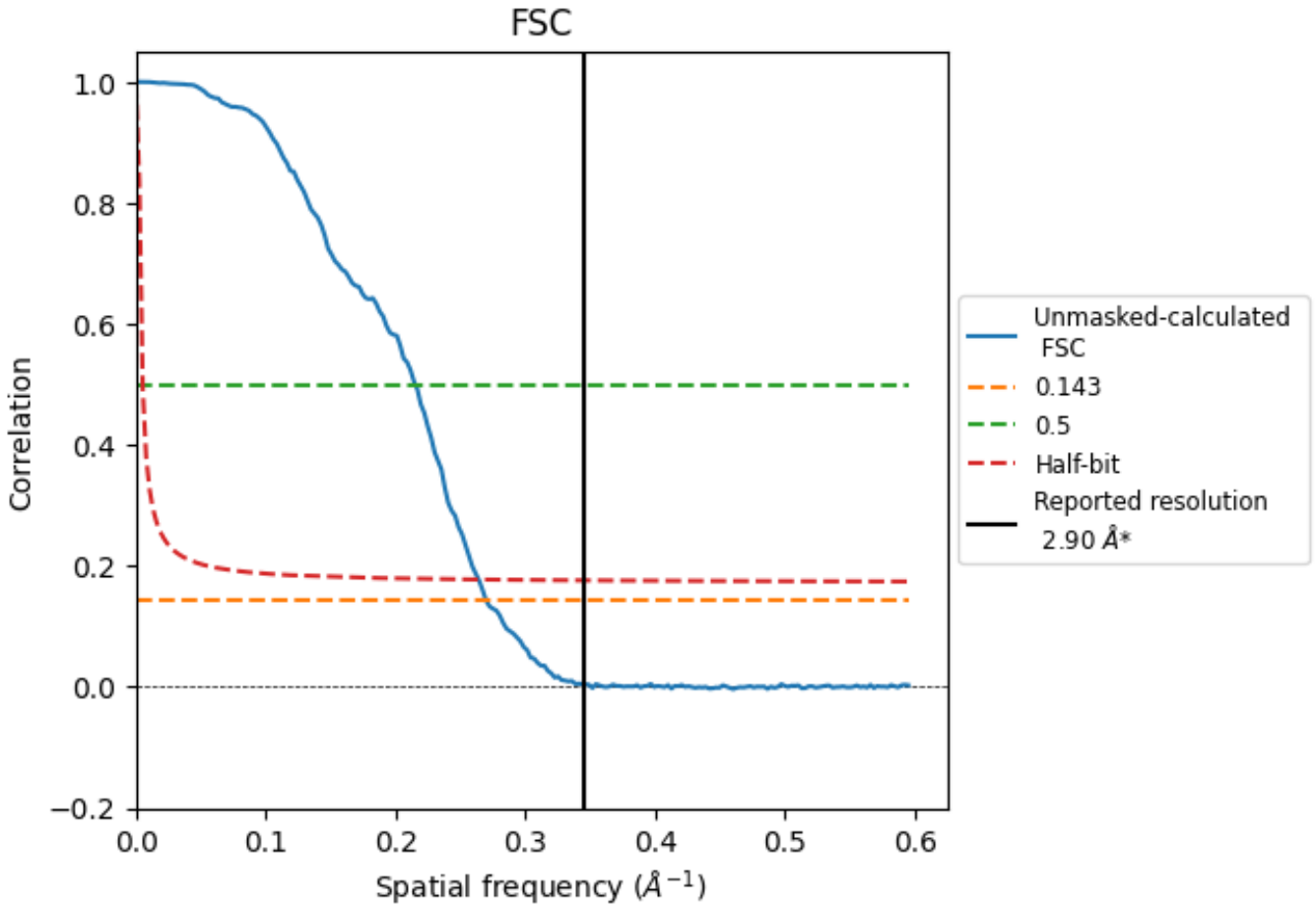


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

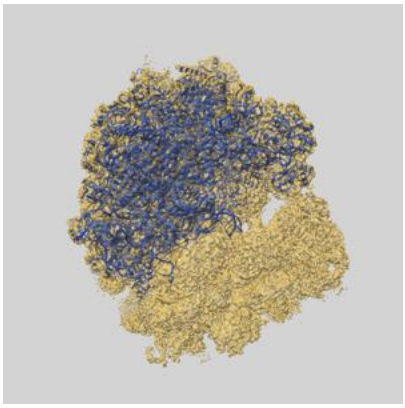
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.71	4.64	3.79

*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 3.71 differs from the reported value 2.9 by more than 10 %

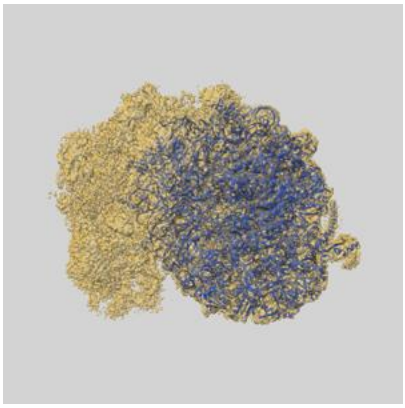
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54774 and PDB model 9SCU. Per-residue inclusion information can be found in section 3 on page 12.

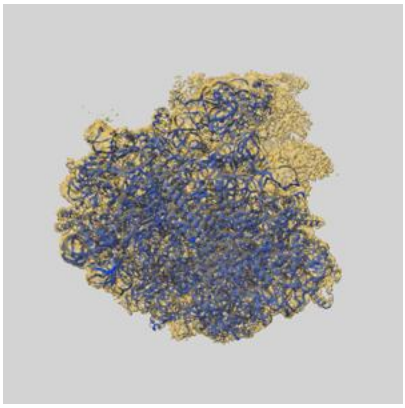
9.1 Map-model overlay



X



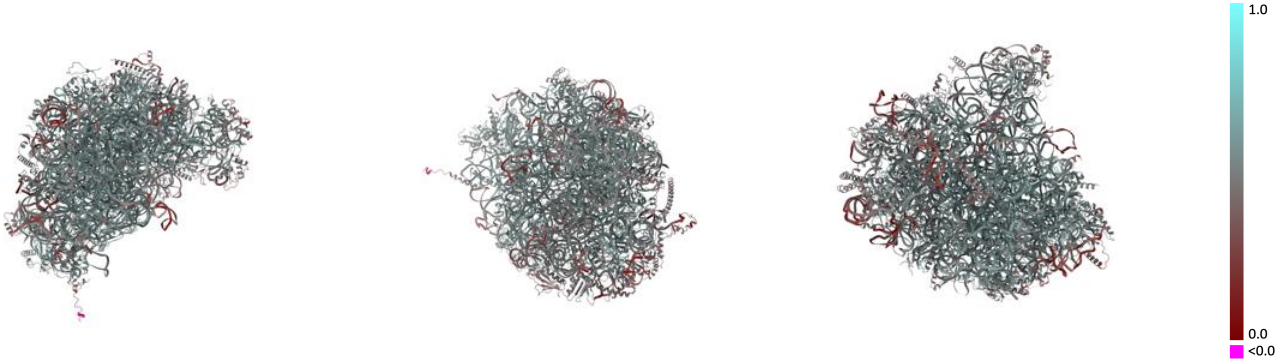
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

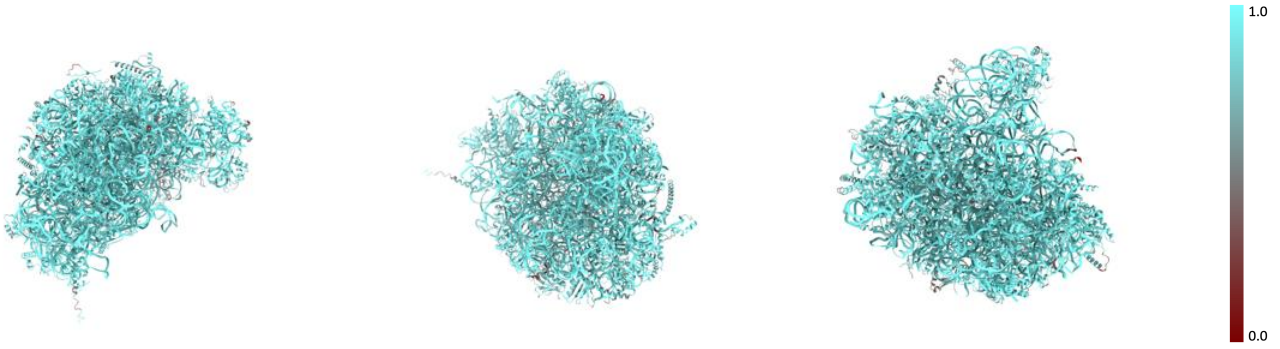
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

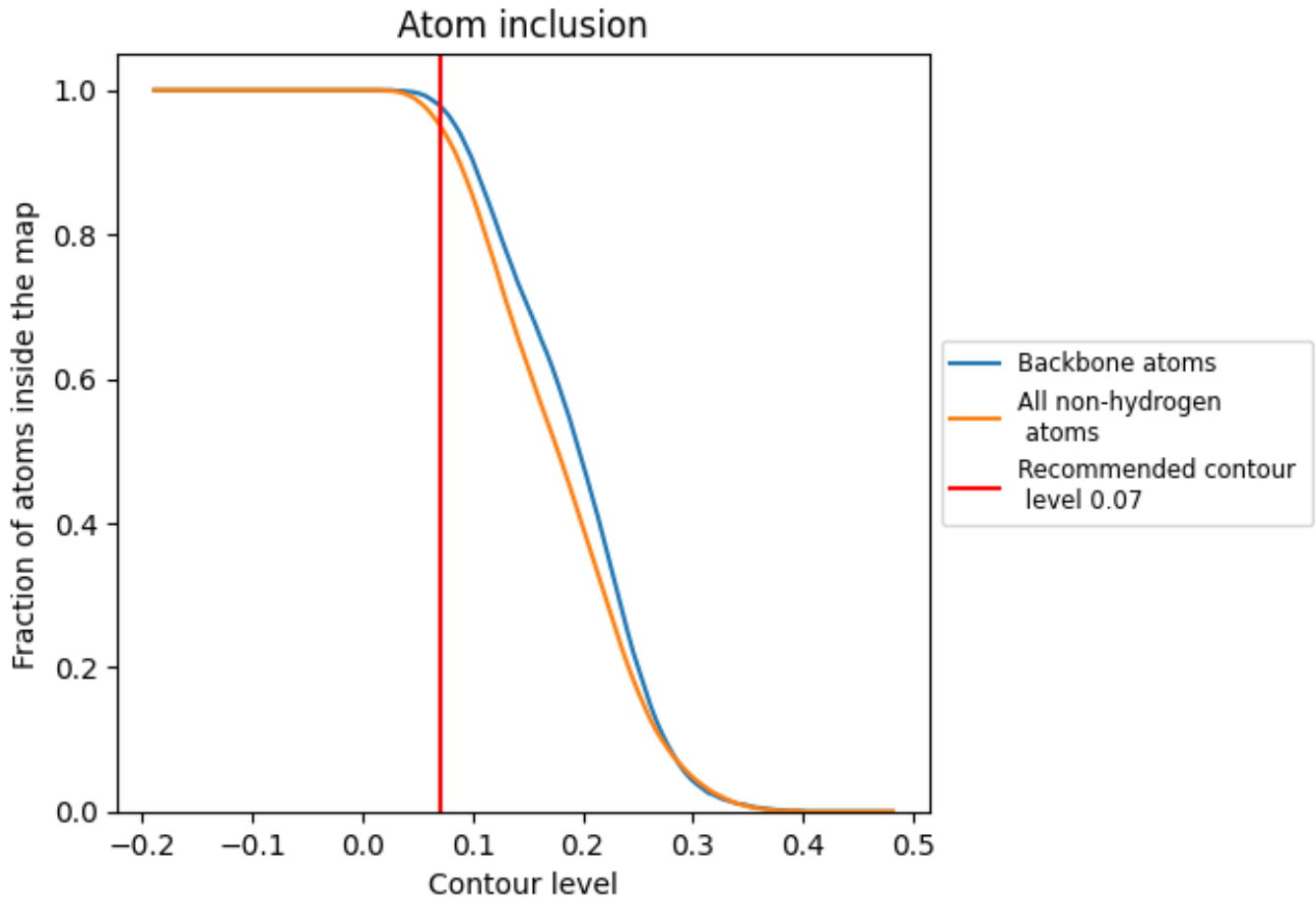
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.5140
5	0.9820	0.5080
6	0.9980	0.5150
7	0.9890	0.5140
CA	0.9590	0.5740
CB	0.9470	0.5510
CC	0.9170	0.5300
CD	0.8800	0.4750
CE	0.8610	0.4400
CF	0.9130	0.5310
CG	0.8990	0.5030
CH	0.7950	0.4250
CI	0.8000	0.4620
CJ	0.8500	0.4480
CK	0.9200	0.5270
CL	0.9320	0.5280
CM	0.8890	0.4960
CN	0.9780	0.5810
CO	0.9110	0.5250
CP	0.9400	0.5550
CQ	0.9620	0.5620
CR	0.8850	0.4860
CS	0.9430	0.5390
CT	0.9290	0.5380
CV	0.9210	0.5540
CW	0.8980	0.5280
CX	0.9230	0.5410
CY	0.9400	0.5380
CZ	0.9330	0.5260
Ca	0.9550	0.5610
Cb	0.9680	0.5430
Cc	0.9500	0.5000
Cd	0.9000	0.5210
Ce	0.9370	0.5510
Cf	0.9410	0.5430



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Cg	0.9520	0.5580
Ch	0.9200	0.5150
Ci	0.9280	0.5200
Cj	0.9540	0.5670
Ck	0.8990	0.4830
Cl	0.9150	0.5320
Cm	0.5300	0.4150
Cp	0.9250	0.5260
w	0.5760	0.3990