



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 02:28 am BST

PDB ID : 8A3D / pdb_00008a3d
EMDB ID : EMD-15113
Title : Human mature large subunit of the ribosome with eIF6 and homoharringtonine bound
Authors : Faille, A.; Warren, A.J.; Dent, K.C.
Deposited on : 2022-06-08
Resolution : 1.67 Å(reported)
Based on initial model : 6EK0

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

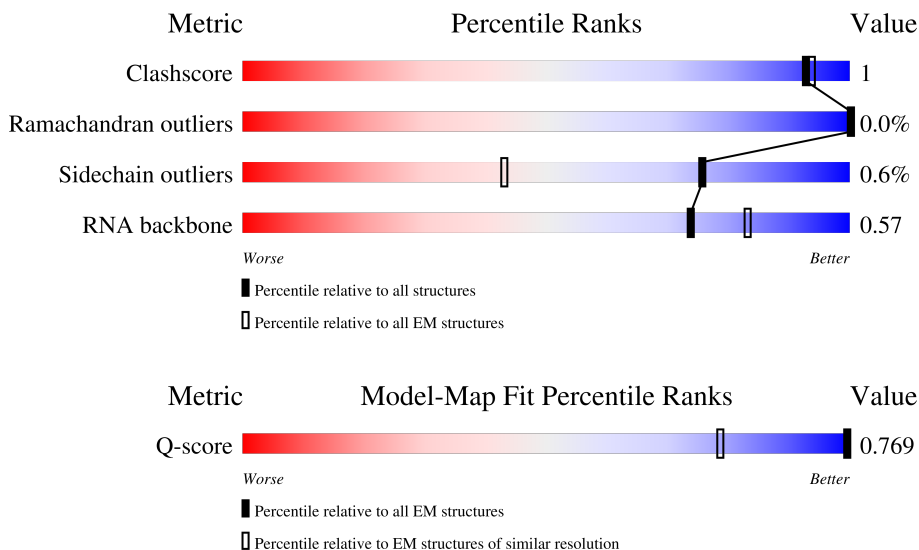
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.67 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	465 (1.19 - 2.17)

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

Mol	Chain	Length	Quality of chain
1	A	5069	
2	B	121	
3	C	157	

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Mol	Chain	Length	Quality of chain
4	D	257	5% 91%
5	E	403	20% 93% 5%
6	F	427	10% 81% 16%
7	G	297	45% 94%
8	H	288	37% 74% 24%
9	m	248	84% 15%
10	n	266	45% 80% 16%
11	o	192	34% 93% 6%
12	p	214	25% 89% 6% 5%
13	q	178	79% 94%
14	r	211	35% 95%
15	s	220	14% 59% 5% 37%
16	l	204	97%
17	I	203	11% 95%
18	J	184	11% 77% 6% 17%
19	K	188	97%
20	L	196	23% 79% 20%
21	M	176	6% 94% 6%
22	N	160	25% 96%
23	O	128	73% 74% 23%
24	P	140	18% 91% 6%
25	Q	157	10% 39% 61%
26	R	156	22% 72% 24%
27	S	145	23% 92% 8%
28	T	136	59% 96%

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Mol	Chain	Length	Quality of chain
29	U	148	
30	V	159	
31	W	115	
32	X	125	
33	Y	135	
34	Z	110	
35	a	117	
36	b	196	
37	c	105	
38	d	97	
39	e	70	
40	f	51	
41	g	99	
42	i	106	
43	j	92	
44	k	137	
45	h	245	

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 142233 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	3303	70928	31625	12983	23017	3303	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4910	A	G	conflict	GB 86475748

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2558	1141	456	842	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	148	3153	1408	563	1035	147	0	0

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	246	1887	1183	387	311	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	395	3194	2034	600	545	15	1	0

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	359	2855	1797	571	474	13	0	0

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	285	2308	1460	419	415	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	219	1757	1132	333	288	4	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	m	212	1755	1127	334	285	9	0	0

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	n	223	1809	1153	349	303	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	o	190	1518	956	284	272	6	0	0

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	p	204	1654	1051	318	272	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	q	170	Total	C	N	O	S	0	0
			1358	858	253	241	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	r	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	s	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	l	203	Total	C	N	O	S	1	0
			1708	1077	360	267	4		

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	152	Total	C	N	O	S	0	0
			1233	771	240	213	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	157	1304	813	280	202	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	176	1461	930	284	236	11	0	0

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	N	159	1298	823	252	217	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O	99	804	516	140	146	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	P	132	985	621	185	174	5	0	0

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	62	519	332	101	83	3	0	0

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	119	976	624	183	168	1	0	0

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	S	134	1115	700	226	186	3	0	0

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	135	1107	714	208	182	3	0	0

- Molecule 29 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	U	147	1162	736	237	186	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	V	94	773	480	171	119	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W	100	772	490	136	139	7	0	0

- Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	X	106	868	551	170	145	2	0	0

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Y	128	1053	667	216	165	5	0	0

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	109	Total	C	N	O	S	1	0
			879	557	174	144	4		

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	106	Total	C	N	O	S	0	0
			845	530	174	135	6		

- Molecule 36 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 38 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	86	Total	C	N	O	S	1	0
			713	442	155	111	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 43 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 44 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	124	Total	C	N	O	S	0	0
			992	615	206	167	4		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	h	225	Total	C	N	O	S	0	0
			1712	1065	295	340	12		

- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	A	214	Total	Mg	0
			214	214	
46	B	3	Total	Mg	0
			3	3	
46	C	6	Total	Mg	0
			6	6	
46	J	1	Total	Mg	0
			1	1	
46	L	2	Total	Mg	0
			2	2	
46	P	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
46	U	1	Total Mg 1 1	0
46	d	1	Total Mg 1 1	0

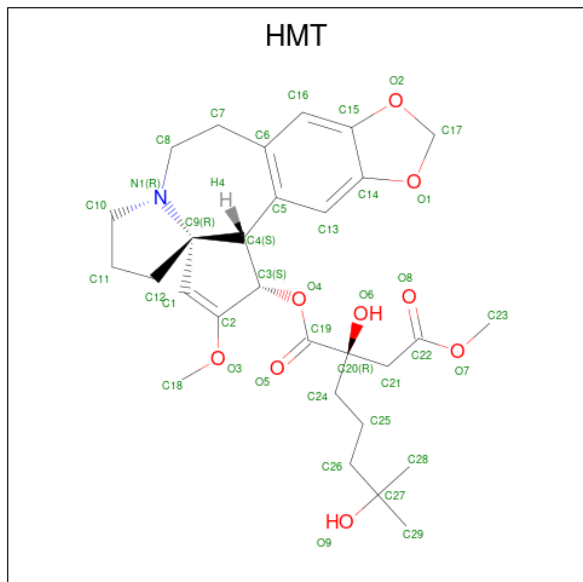
- Molecule 47 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
47	A	139	Total K 139 139	0
47	B	1	Total K 1 1	0
47	D	3	Total K 3 3	0
47	o	1	Total K 1 1	0
47	p	1	Total K 1 1	0
47	l	2	Total K 2 2	0
47	J	1	Total K 1 1	0
47	N	1	Total K 1 1	0
47	V	1	Total K 1 1	0
47	Y	1	Total K 1 1	0
47	Z	1	Total K 1 1	0
47	a	1	Total K 1 1	0
47	f	1	Total K 1 1	0
47	i	1	Total K 1 1	0

- Molecule 48 is SODIUM ION (CCD ID: NA) (formula: Na).

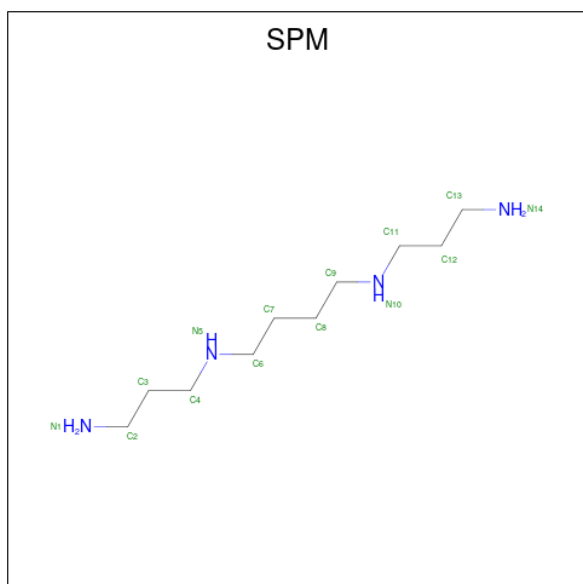
Mol	Chain	Residues	Atoms	AltConf
48	A	2	Total Na 2 2	0

- Molecule 49 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano yl]cephalotaxine (CCD ID: HMT) (formula: C₂₉H₃₉NO₉).



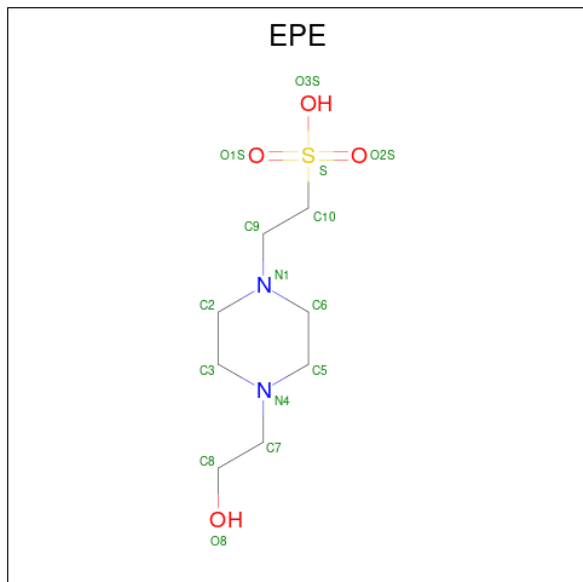
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
49	A	1	39	29	1	9	0

- Molecule 50 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
50	A	1	14	10	4	0

- Molecule 51 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
51	A	1	15	8	2	4	1	0

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
52	a	1	1	1	0
52	d	1	1	1	0
52	g	1	1	1	0
52	i	1	1	1	0
52	j	1	1	1	0

- Molecule 53 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
53	A	8641	8641	8641	0
53	B	261	261	261	0

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Mol	Chain	Residues	Atoms		AltConf
53	C	363	Total 363	O 363	0
53	D	131	Total 131	O 131	0
53	E	177	Total 177	O 177	0
53	F	202	Total 202	O 202	0
53	G	67	Total 67	O 67	0
53	H	49	Total 49	O 49	0
53	m	131	Total 131	O 131	0
53	n	46	Total 46	O 46	0
53	o	43	Total 43	O 43	0
53	p	81	Total 81	O 81	0
53	q	13	Total 13	O 13	0
53	r	101	Total 101	O 101	0
53	s	38	Total 38	O 38	0
53	l	155	Total 155	O 155	0
53	I	117	Total 117	O 117	0
53	J	63	Total 63	O 63	0
53	K	139	Total 139	O 139	0
53	L	57	Total 57	O 57	0
53	M	100	Total 100	O 100	0
53	N	87	Total 87	O 87	0
53	O	5	Total 5	O 5	0

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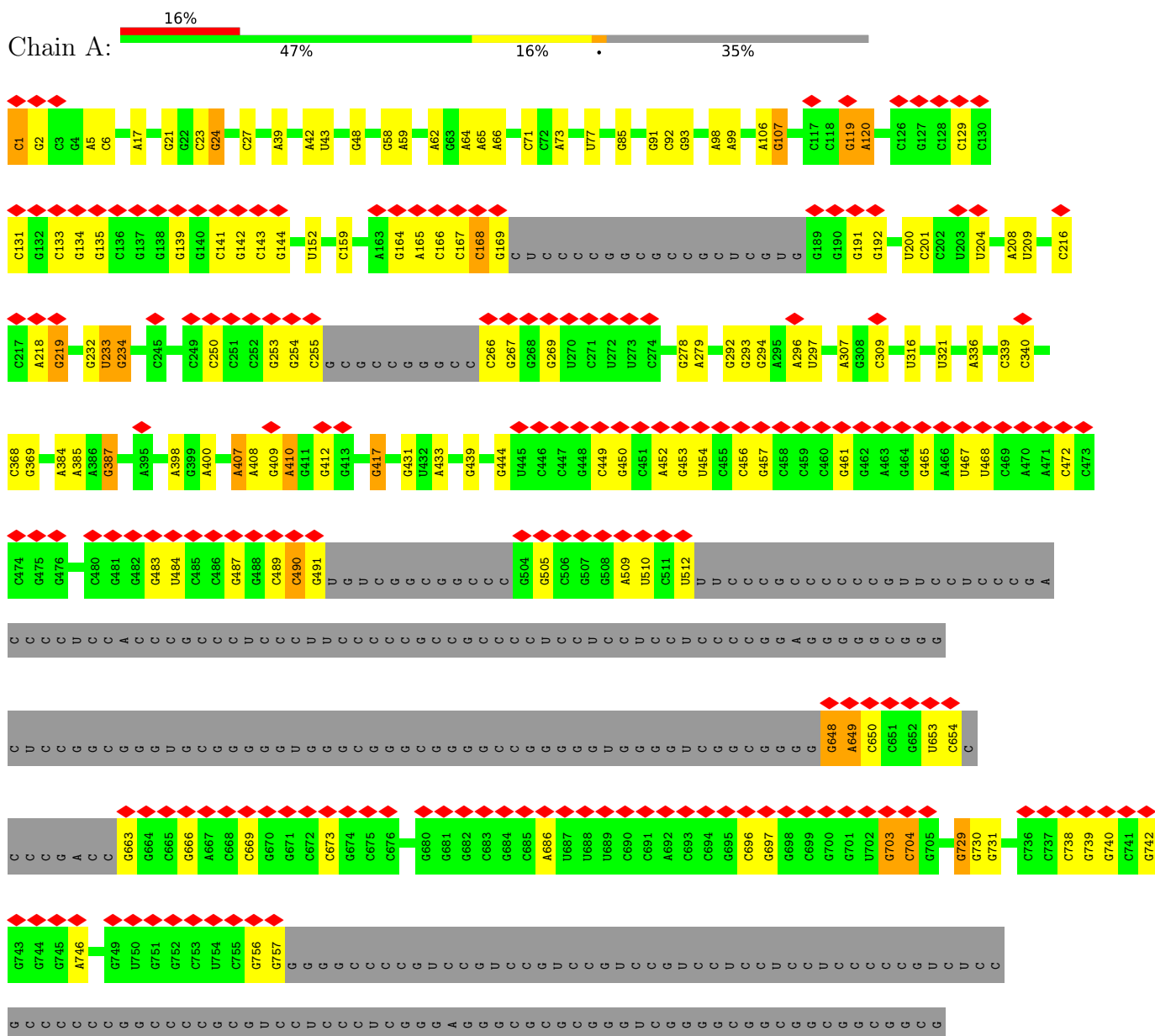
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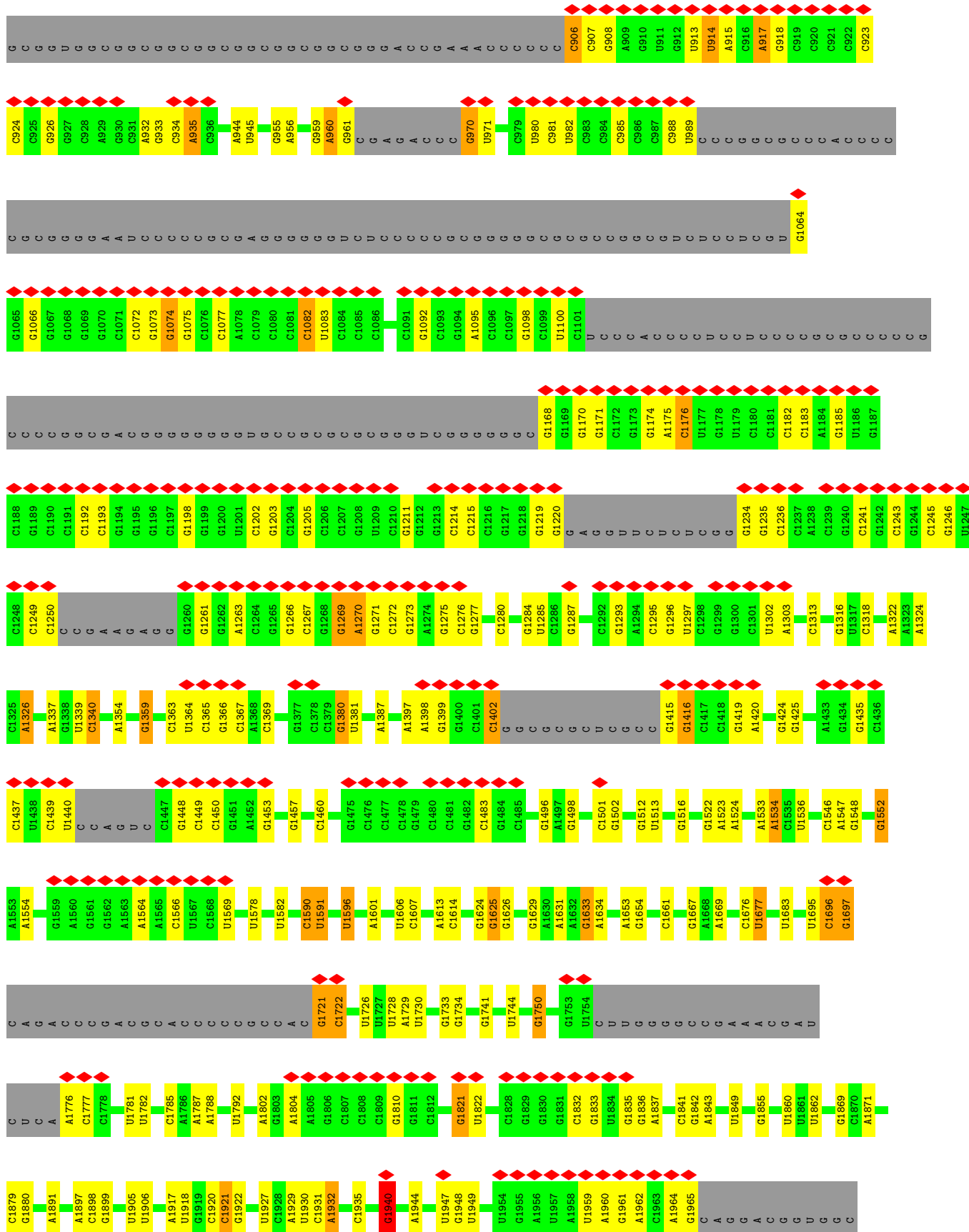
Mol	Chain	Residues	Atoms		AltConf
53	P	40	Total 40	O 40	0
53	Q	21	Total 21	O 21	0
53	R	35	Total 35	O 35	0
53	S	49	Total 49	O 49	0
53	T	13	Total 13	O 13	0
53	U	92	Total 92	O 92	0
53	V	39	Total 39	O 39	0
53	W	9	Total 9	O 9	0
53	X	37	Total 37	O 37	0
53	Y	112	Total 112	O 112	0
53	Z	72	Total 72	O 72	0
53	a	58	Total 58	O 58	0
53	b	29	Total 29	O 29	0
53	c	32	Total 32	O 32	0
53	d	62	Total 62	O 62	0
53	e	3	Total 3	O 3	0
53	f	19	Total 19	O 19	0
53	g	14	Total 14	O 14	0
53	i	52	Total 52	O 52	0
53	j	40	Total 40	O 40	0
53	k	78	Total 78	O 78	0

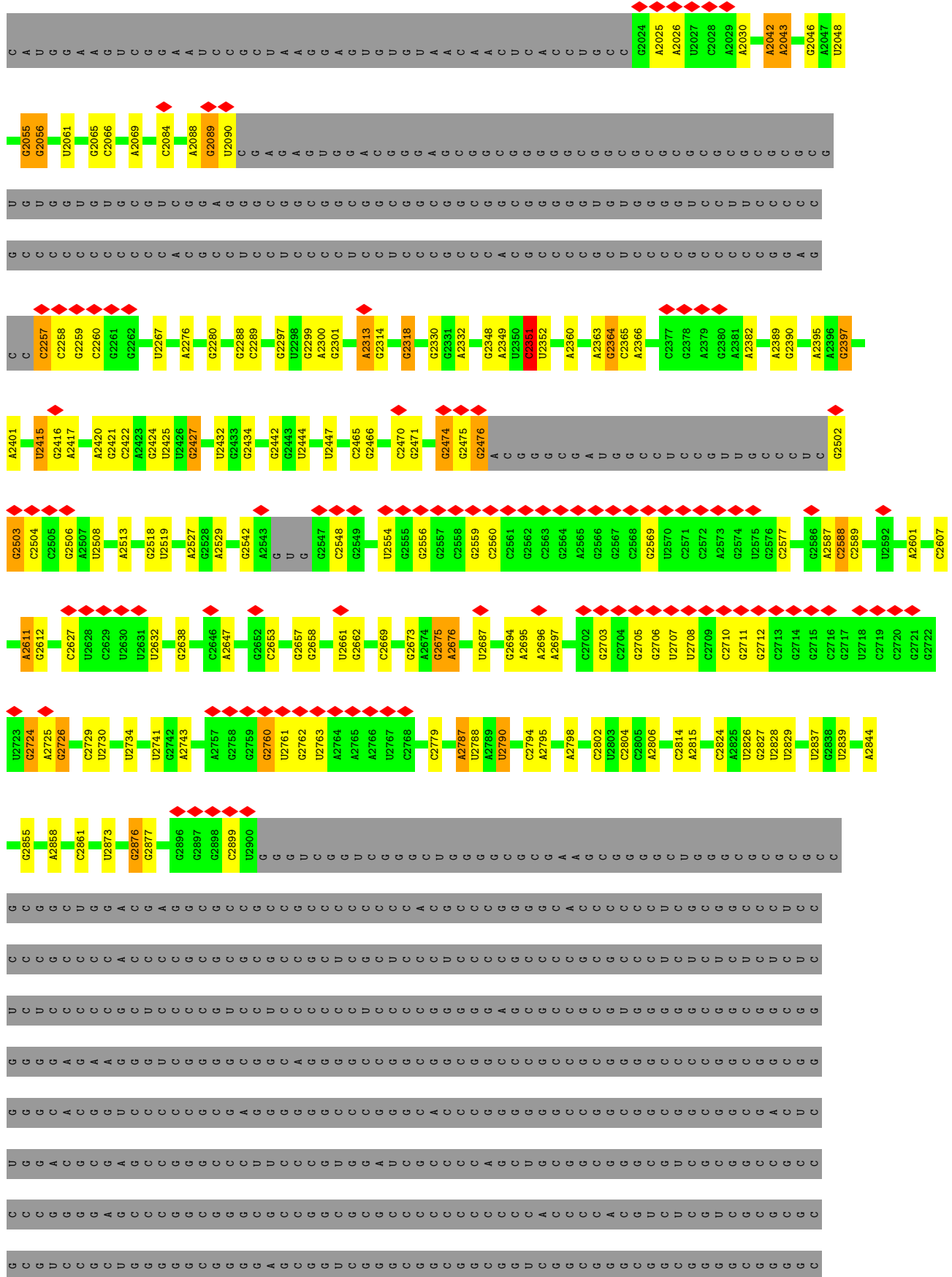
3 Residue-property plots [i](#)

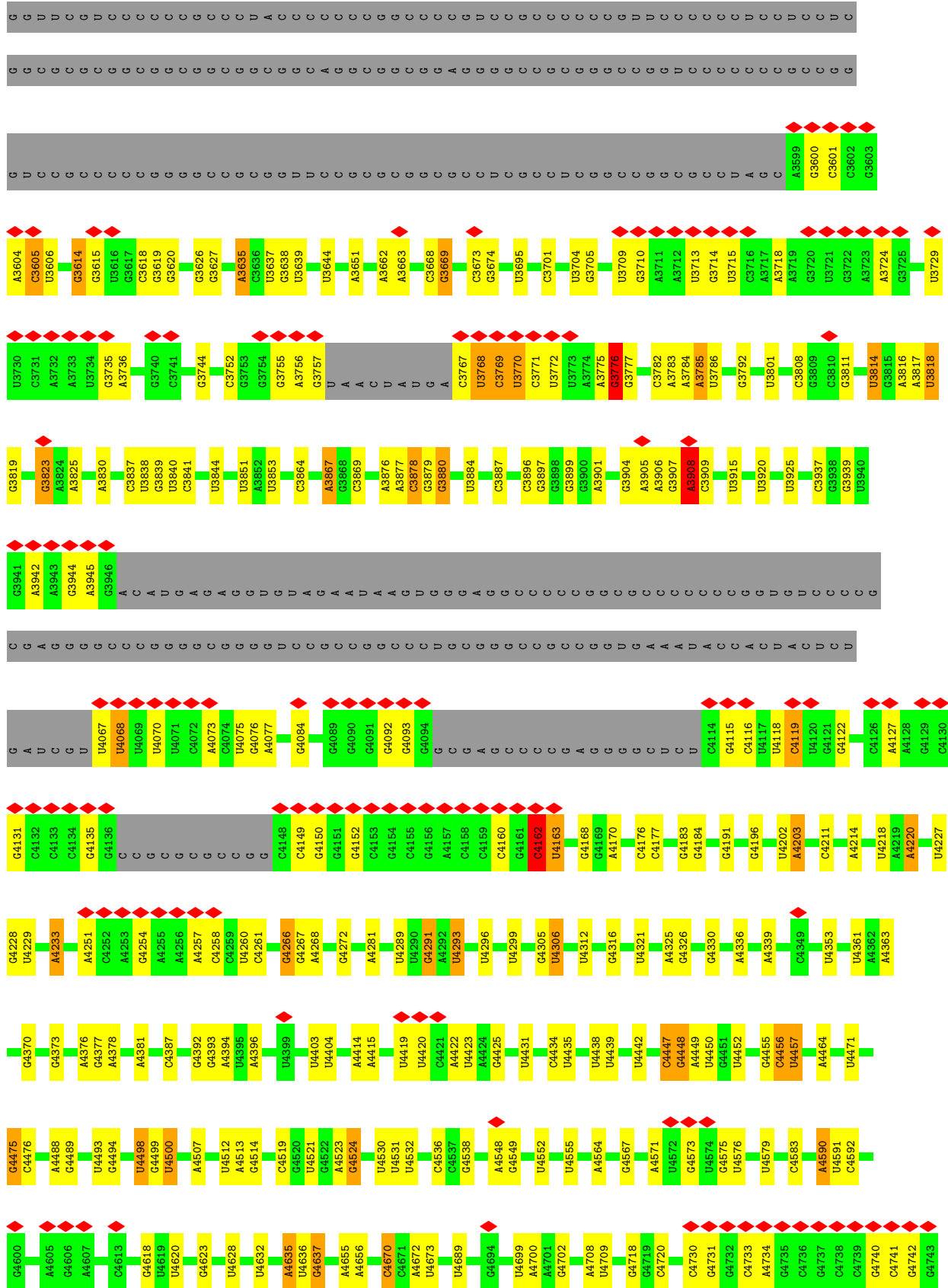
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

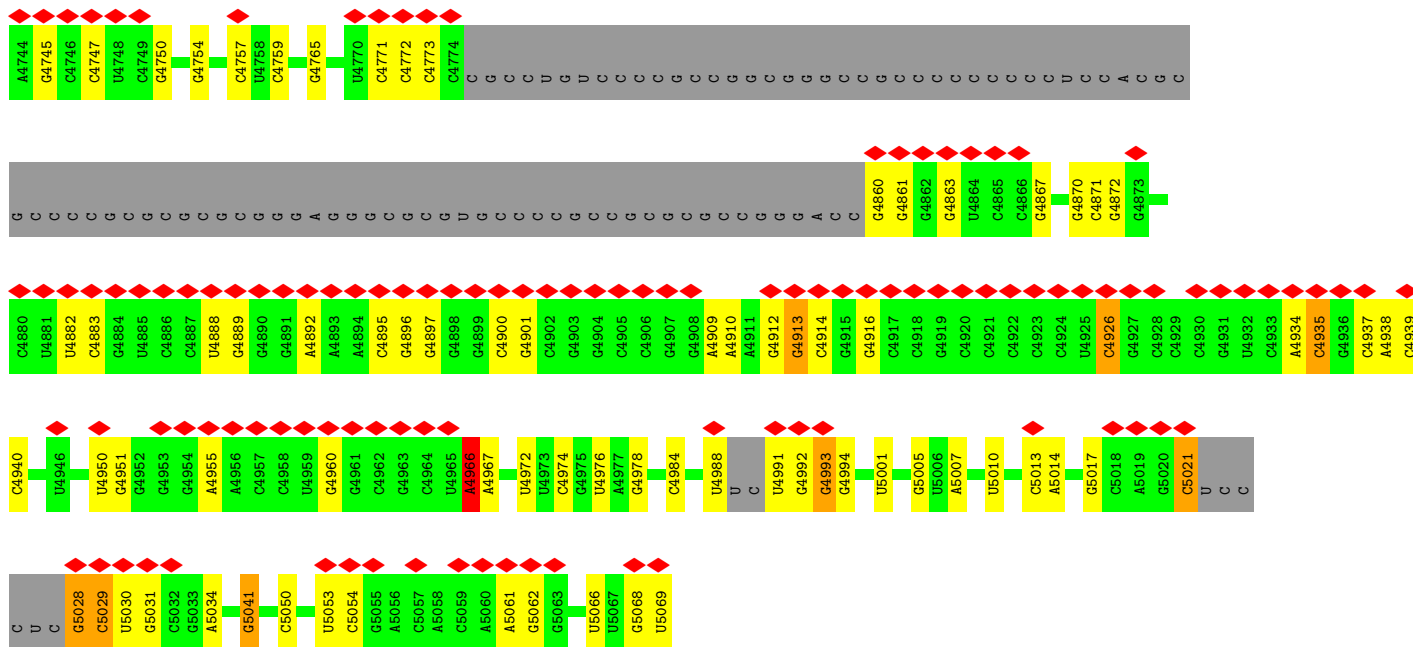
- Molecule 1: 28S ribosomal RNA



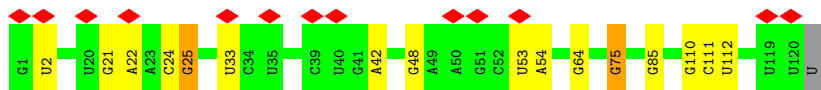
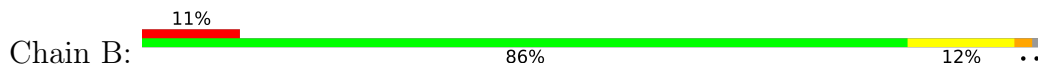




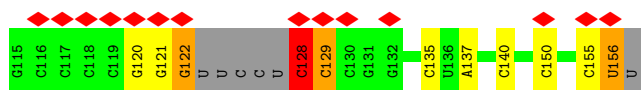
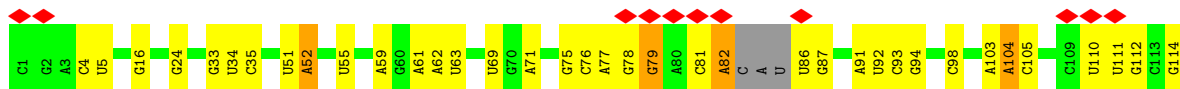




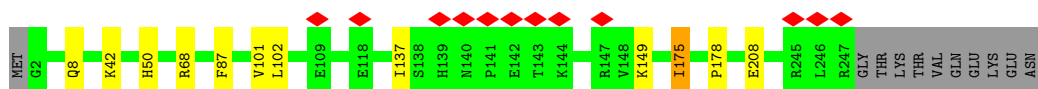
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA

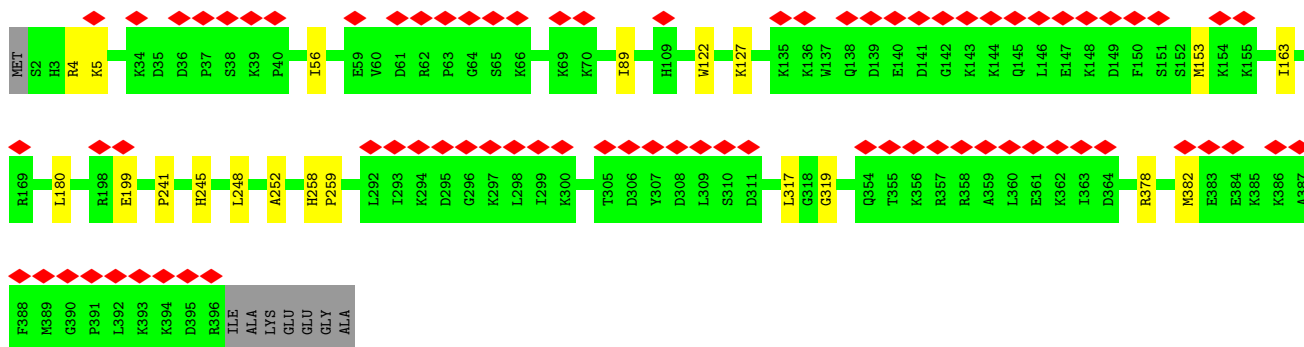


• Molecule 4: 60S ribosomal protein L8

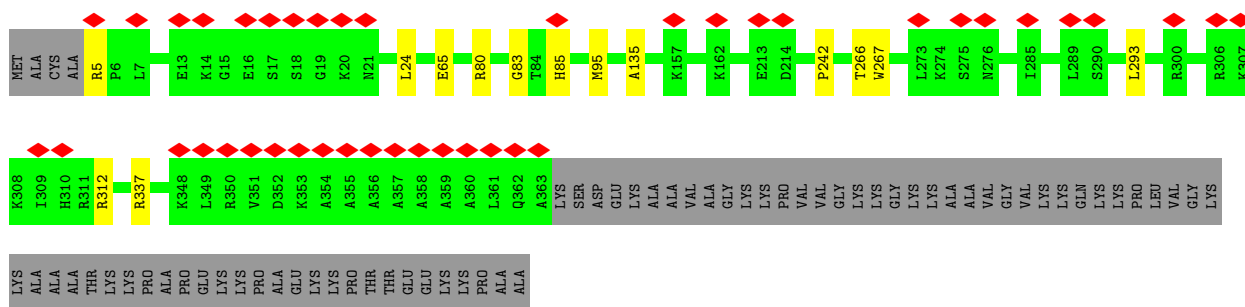
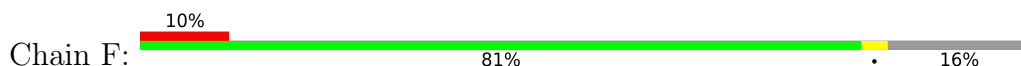


• Molecule 5: 60S ribosomal protein L3

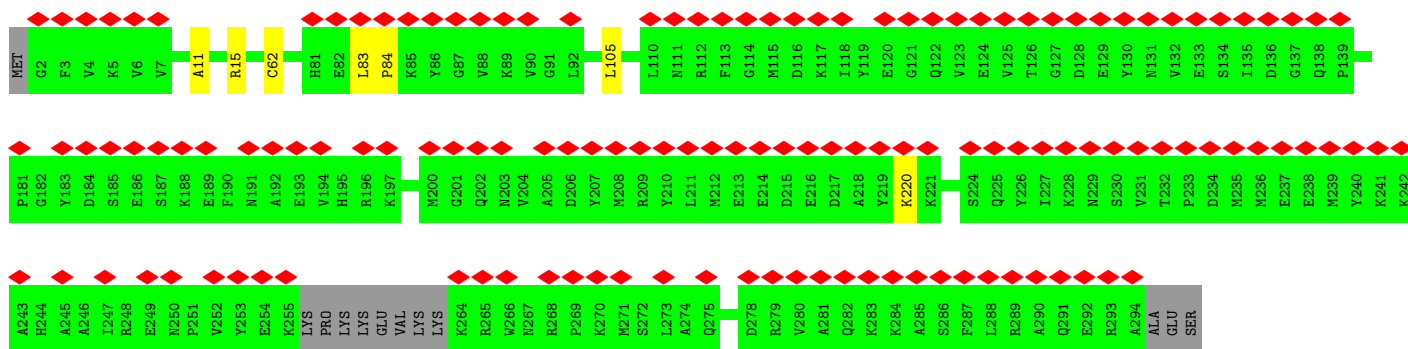




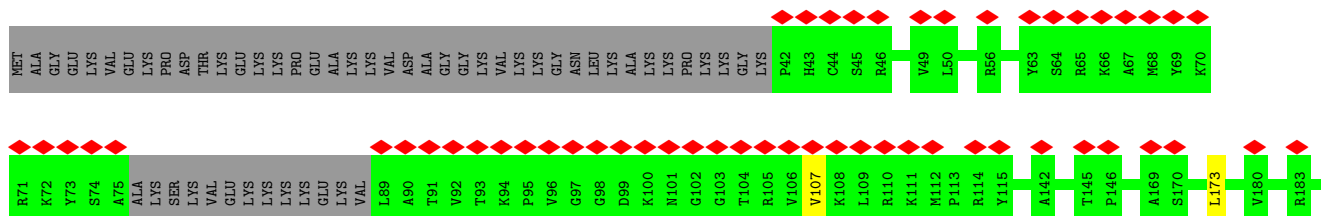
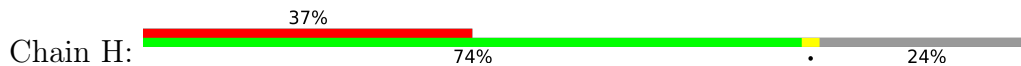
• Molecule 6: 60S ribosomal protein L4

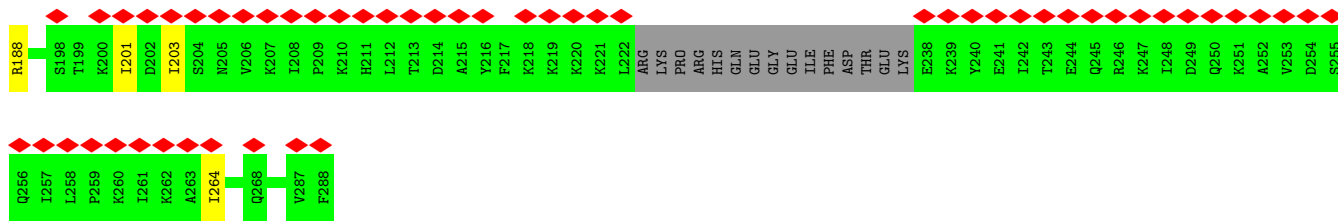


• Molecule 7: 60S ribosomal protein L5

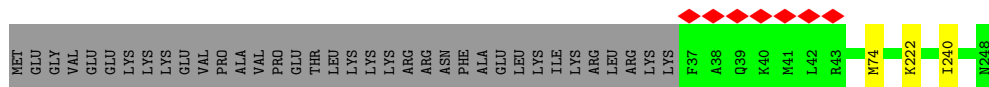
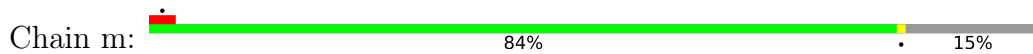


• Molecule 8: 60S ribosomal protein L6

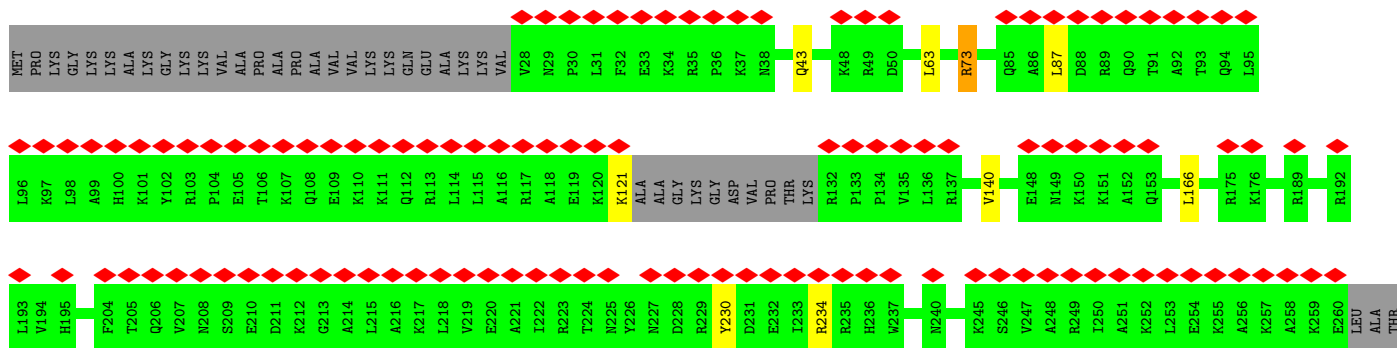
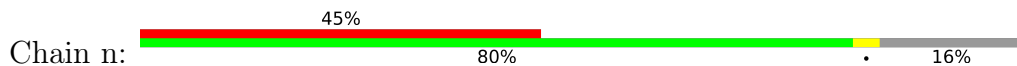




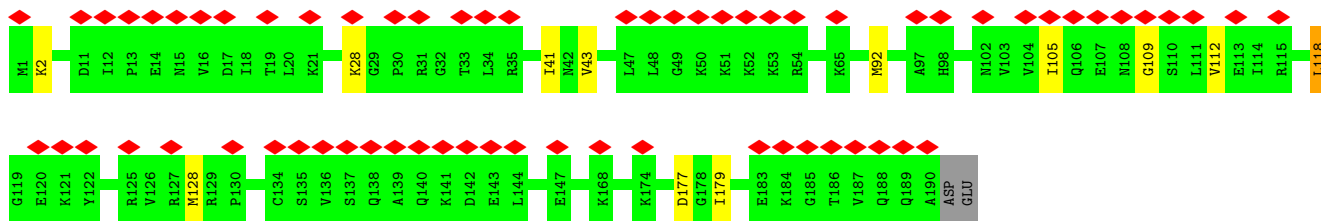
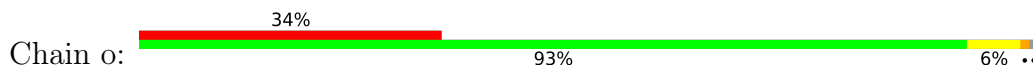
• Molecule 9: 60S ribosomal protein L7



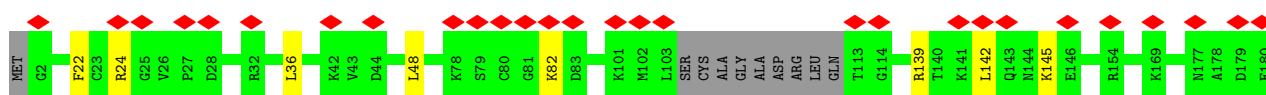
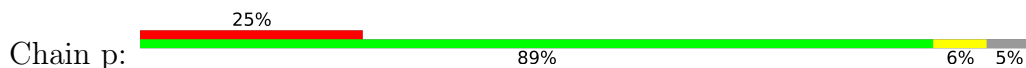
• Molecule 10: 60S ribosomal protein L7a

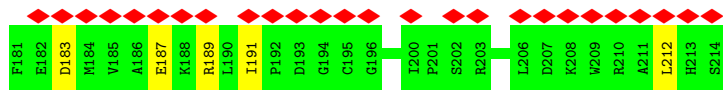


• Molecule 11: 60S ribosomal protein L9

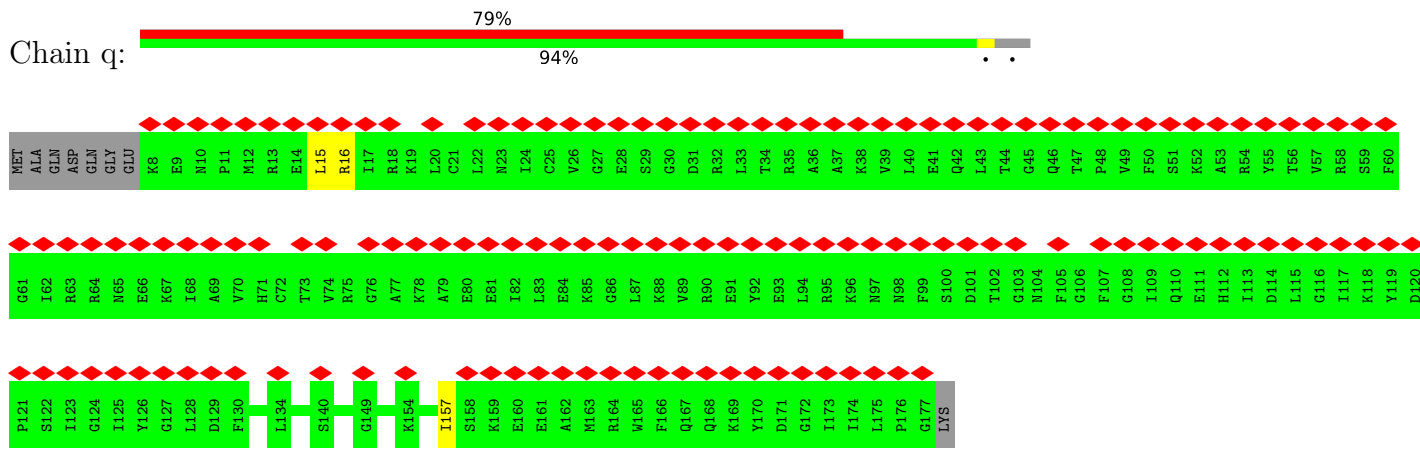


• Molecule 12: 60S ribosomal protein L10

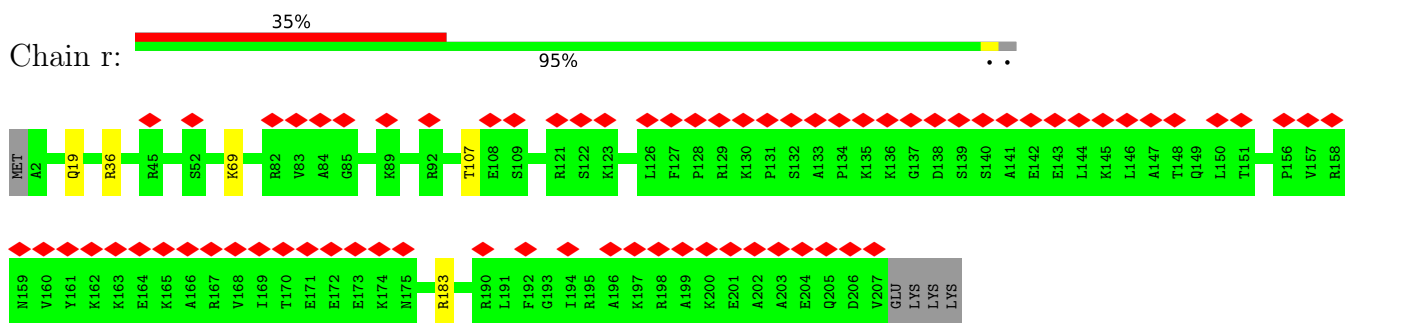




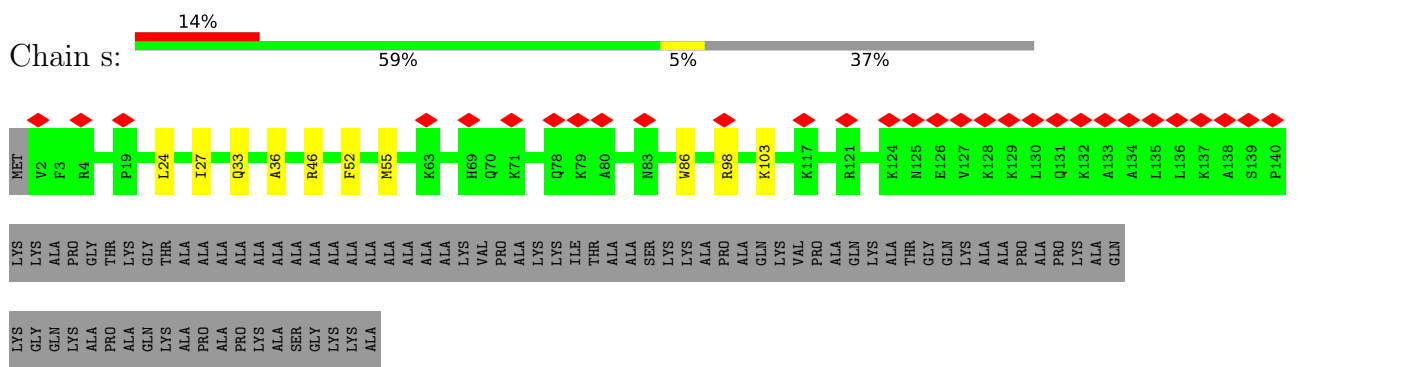
• Molecule 13: 60S ribosomal protein L11



• Molecule 14: 60S ribosomal protein L13



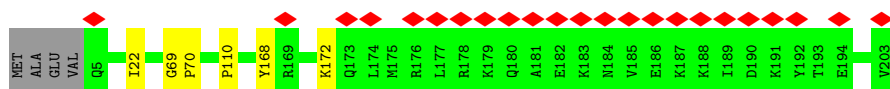
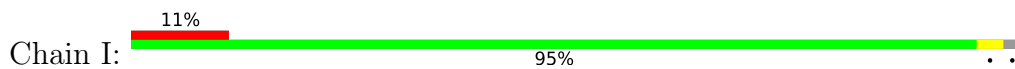
• Molecule 15: 60S ribosomal protein L14



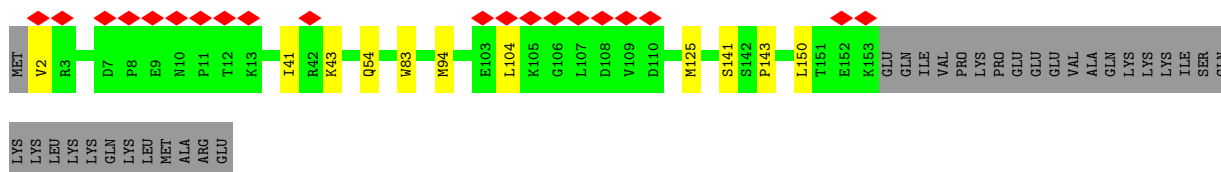
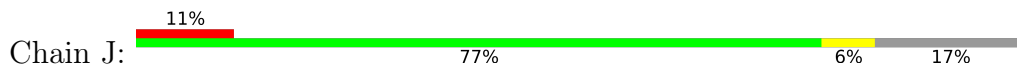
• Molecule 16: 60S ribosomal protein L15



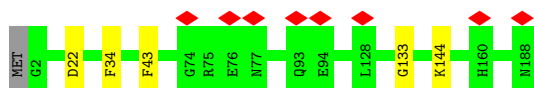
• Molecule 17: 60S ribosomal protein L13a



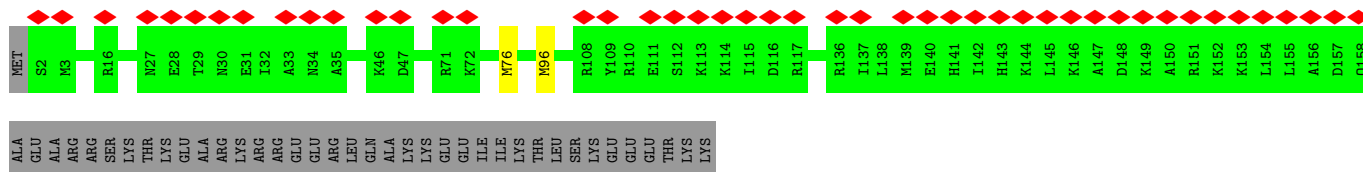
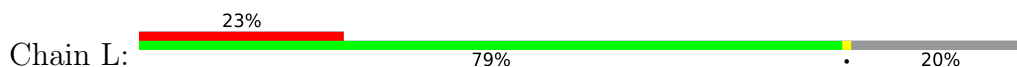
- Molecule 18: 60S ribosomal protein L17



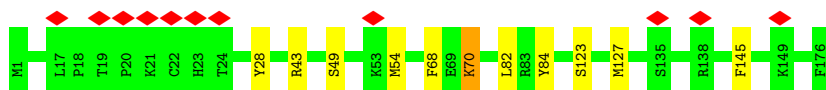
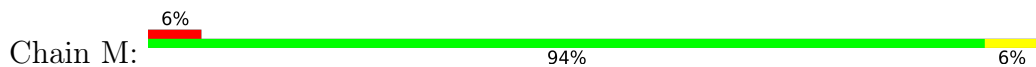
- Molecule 19: 60S ribosomal protein L18



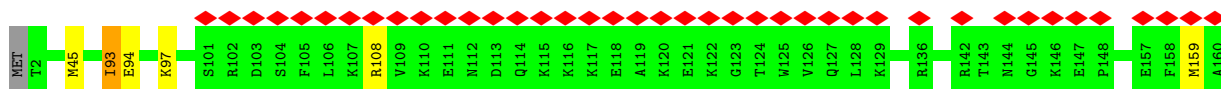
- Molecule 20: 60S ribosomal protein L19



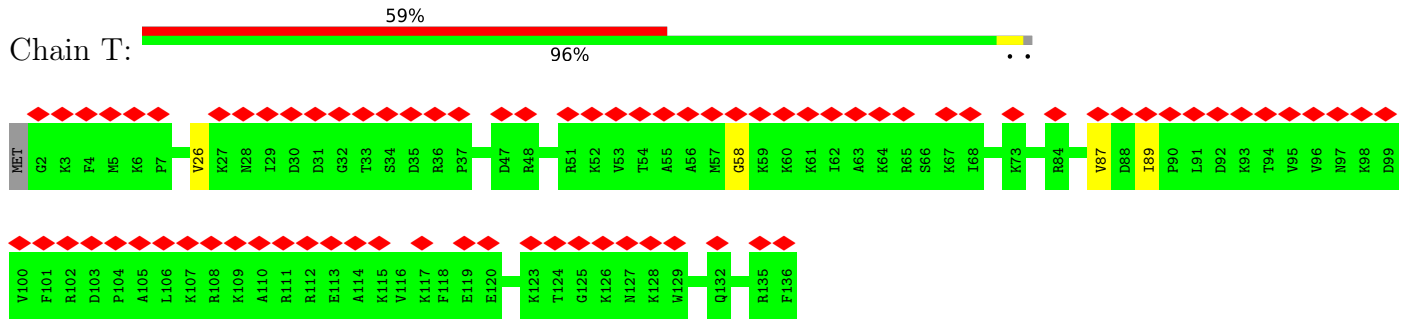
- Molecule 21: 60S ribosomal protein L18a



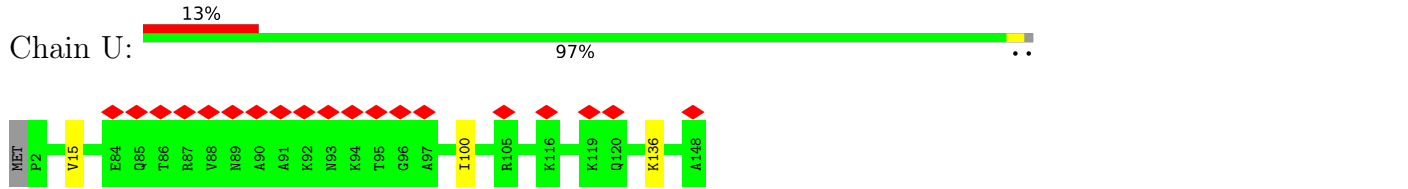
- Molecule 22: 60S ribosomal protein L21



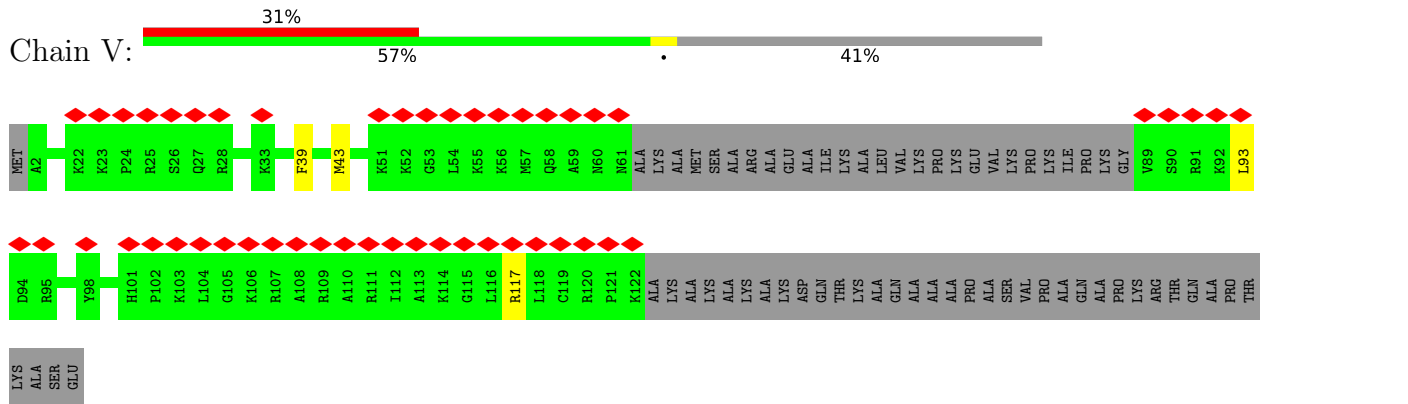
- Molecule 23: 60S ribosomal protein L22



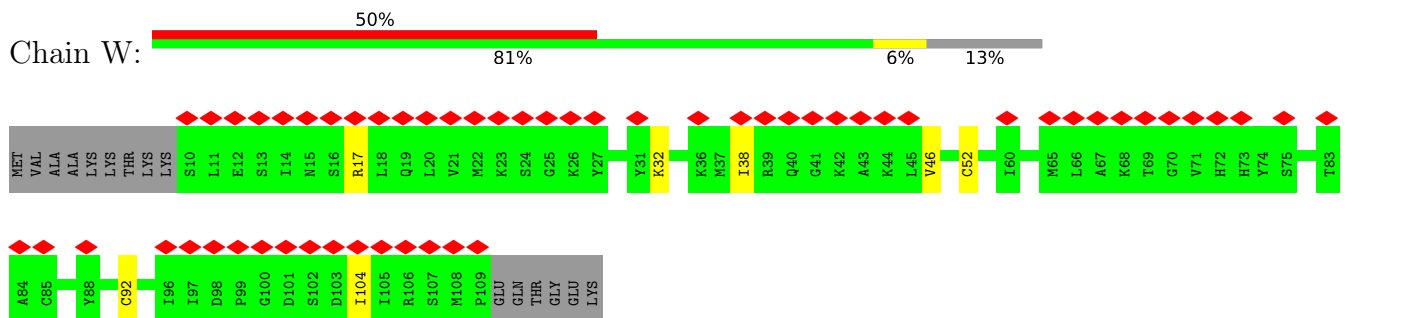
• Molecule 29: 60S ribosomal protein L27a



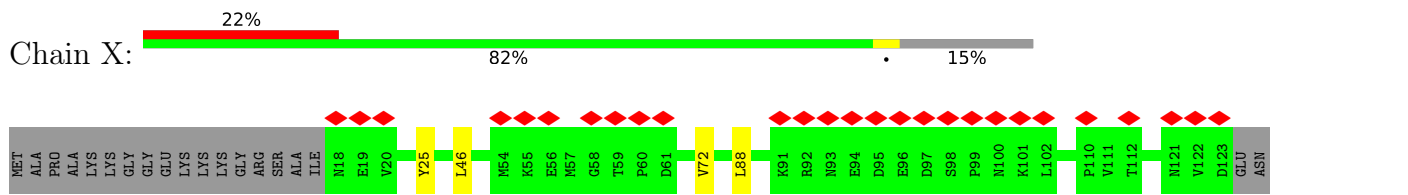
• Molecule 30: 60S ribosomal protein L29



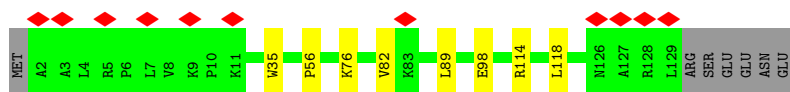
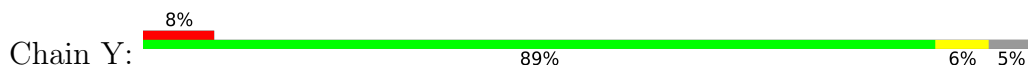
• Molecule 31: 60S ribosomal protein L30



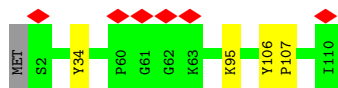
• Molecule 32: 60S ribosomal protein L31



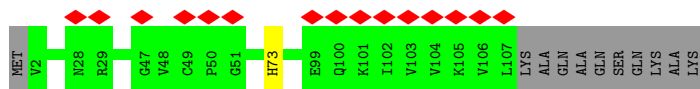
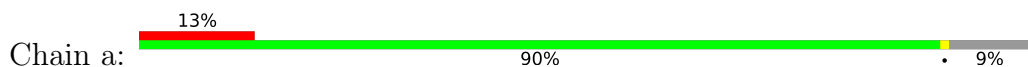
• Molecule 33: 60S ribosomal protein L32



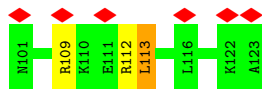
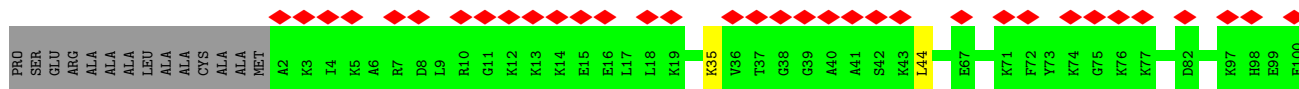
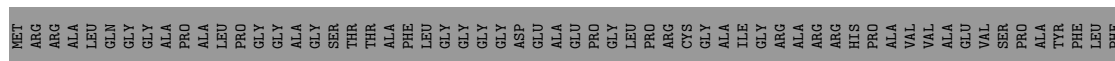
• Molecule 34: 60S ribosomal protein L35a



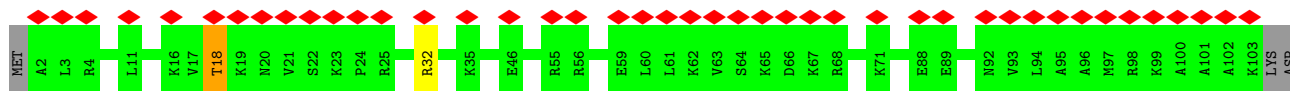
• Molecule 35: 60S ribosomal protein L34



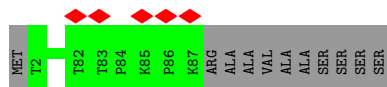
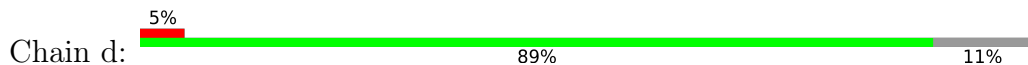
• Molecule 36: Ribosomal protein uL29



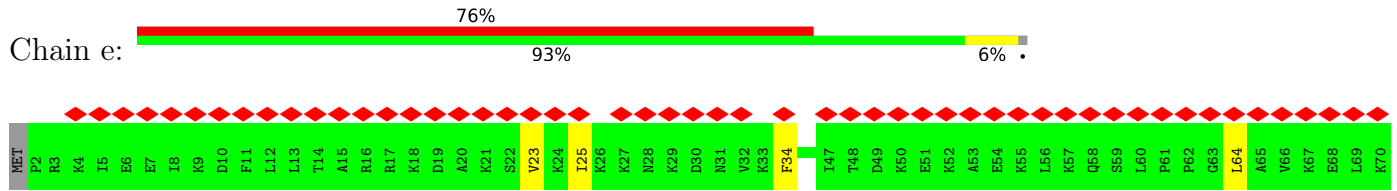
• Molecule 37: 60S ribosomal protein L36



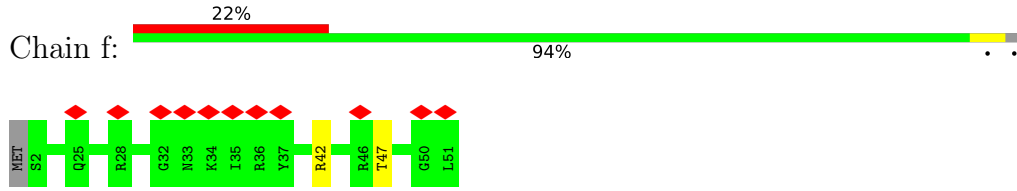
• Molecule 38: 60S ribosomal protein L37



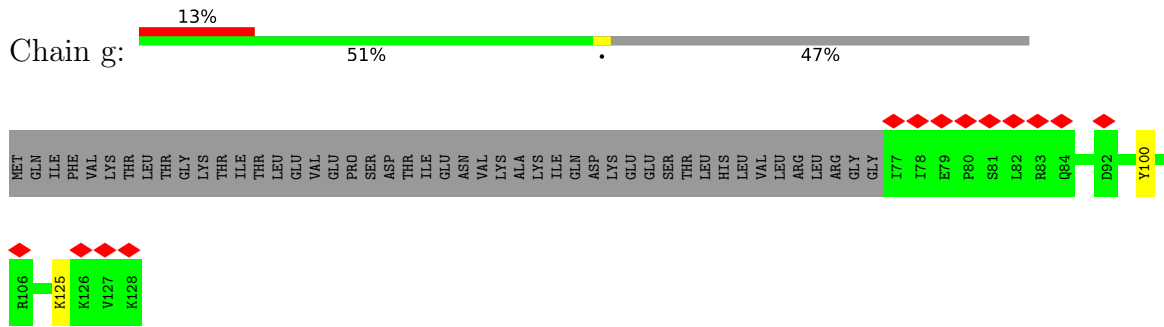
• Molecule 39: 60S ribosomal protein L38



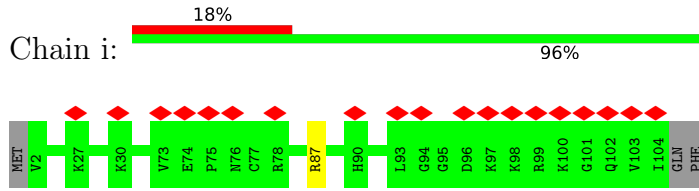
• Molecule 40: 60S ribosomal protein L39



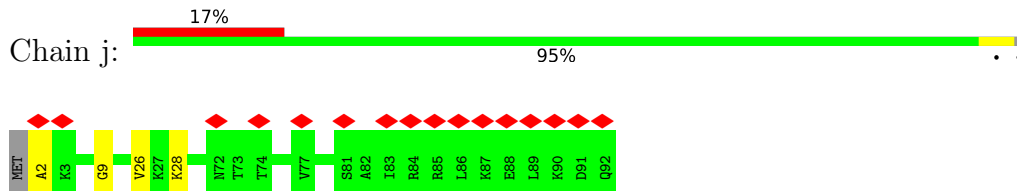
• Molecule 41: Ubiquitin-60S ribosomal protein L40



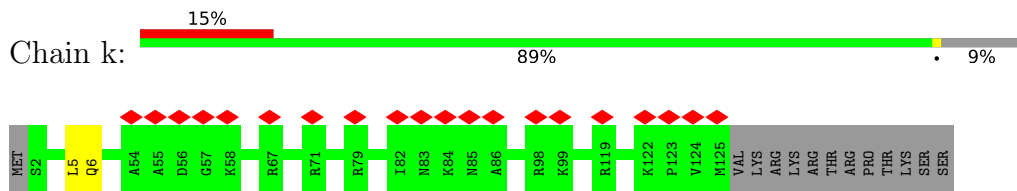
• Molecule 42: 60S ribosomal protein L36a



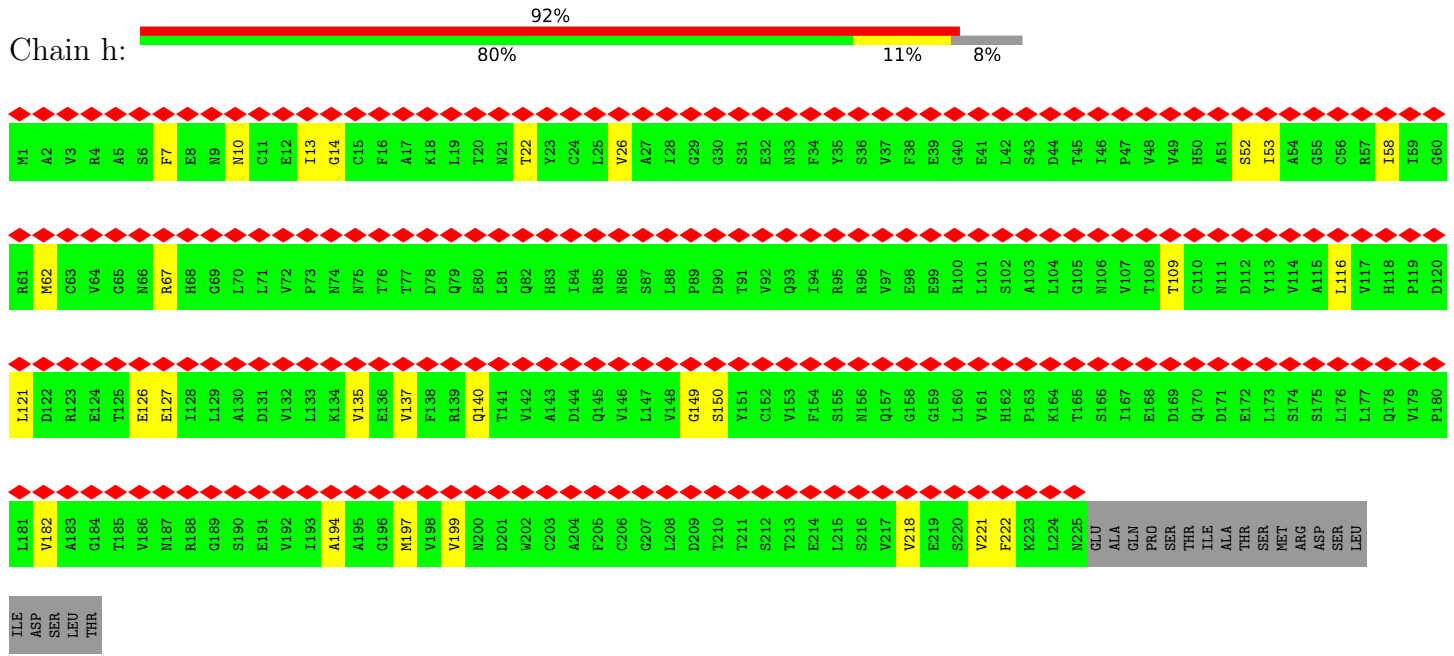
• Molecule 43: 60S ribosomal protein L37a



• Molecule 44: 60S ribosomal protein L28



• Molecule 45: Eukaryotic translation initiation factor 6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1088709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.602	Depositor
Minimum map value	-0.207	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, EPE, PSU, K, HMT, OMG, OMU, A2M, ZN, SPM, 1MA, OMC, UR3, NA, 6MZ, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.68	16/76619 (0.0%)	1.11	197/119498 (0.2%)
2	B	0.66	0/2858	1.08	4/4455 (0.1%)
3	C	0.66	0/3450	1.15	14/5372 (0.3%)
4	D	0.88	0/1925	1.16	0/2581
5	E	0.88	1/3265 (0.0%)	1.20	2/4369 (0.0%)
6	F	0.88	0/2909	1.24	0/3908
7	G	0.90	0/2352	1.31	0/3152
8	H	0.94	1/1791 (0.1%)	1.25	0/2403
9	m	0.83	0/1789	1.20	0/2388
10	n	0.94	0/1840	1.40	2/2476 (0.1%)
11	o	0.89	0/1537	1.19	0/2066
12	p	0.89	0/1692	1.22	1/2258 (0.0%)
13	q	0.94	0/1381	1.38	0/1848
14	r	0.92	0/1695	1.31	0/2270
15	s	0.87	0/1161	1.31	0/1554
16	l	0.86	0/1753	1.19	0/2348
17	I	0.86	0/1666	1.24	1/2228 (0.0%)
18	J	0.87	0/1259	1.20	0/1689
19	K	0.87	0/1537	1.21	1/2052 (0.0%)
20	L	0.90	0/1320	1.36	0/1749
21	M	0.84	0/1501	1.17	1/2013 (0.0%)
22	N	0.88	0/1326	1.22	0/1770
23	O	0.97	0/818	1.33	0/1098
24	P	0.90	0/999	1.18	0/1340
25	Q	0.87	0/532	1.21	0/708
26	R	0.88	0/993	1.23	0/1334
27	S	0.89	0/1132	1.27	0/1504
28	T	0.92	0/1130	1.30	1/1507 (0.1%)
29	U	0.88	0/1191	1.23	0/1591
30	V	0.94	0/786	1.41	0/1038
31	W	0.94	0/783	1.42	0/1052
32	X	0.89	0/883	1.23	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Y	0.88	0/1071	1.18	0/1429
34	Z	0.85	0/901	1.07	0/1206
35	a	0.88	0/855	1.26	0/1140
36	b	0.89	0/1023	1.36	0/1351
37	c	0.91	0/843	1.43	0/1115
38	d	0.86	0/732	1.18	0/968
39	e	0.95	0/575	1.35	0/761
40	f	0.88	0/454	1.17	0/599
41	g	0.91	0/435	1.22	0/575
42	i	0.88	0/855	1.21	0/1128
43	j	0.93	0/718	1.33	0/953
44	k	0.89	0/1007	1.20	0/1351
45	h	1.09	0/1736	1.48	0/2362
All	All	0.77	18/137078 (0.0%)	1.17	224/201747 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
3	C	0	1
All	All	0	17

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	245	HIS	CE1-NE2	6.34	1.38	1.32
1	A	3785	A2M	O3'-P	5.93	1.62	1.56
1	A	3718	A2M	O3'-P	5.62	1.61	1.56
1	A	4523	A2M	O3'-P	5.43	1.61	1.56
1	A	2415	OMU	O3'-P	5.42	1.61	1.56
1	A	1534	A2M	O3'-P	5.42	1.61	1.56
1	A	3925	OMU	O3'-P	5.38	1.61	1.56
1	A	2401	A2M	O3'-P	5.37	1.61	1.56
1	A	2787	A2M	O3'-P	5.27	1.61	1.56
1	A	4530	UR3	O3'-P	5.26	1.61	1.56
1	A	3724	A2M	O3'-P	5.23	1.61	1.56
1	A	1326	A2M	O3'-P	5.22	1.61	1.56
1	A	1524	A2M	O3'-P	5.20	1.61	1.56
1	A	4590	A2M	O3'-P	5.16	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3867	A2M	O3'-P	5.15	1.61	1.56
1	A	4306	OMU	O3'-P	5.14	1.61	1.56
8	H	264	ILE	N-CA	5.09	1.50	1.46
1	A	4571	A2M	O3'-P	5.06	1.61	1.56

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2675	G	C2'-C3'-O3'	10.71	125.56	109.50
1	A	232	G	O3'-P-O5'	-10.18	88.73	104.00
1	A	2518	G	O3'-P-O5'	-9.65	89.53	104.00
1	A	1947	U	P-O3'-C3'	-9.03	106.66	120.20
1	A	1653	A	O3'-P-O5'	-8.79	90.81	104.00
1	A	3752	C	C4'-C3'-O3'	-8.46	100.31	113.00
3	C	33	G	C2'-C3'-O3'	-8.22	101.36	113.70
3	C	93	C	C4'-C3'-O3'	-7.94	101.09	113.00
3	C	111	U	P-O3'-C3'	-7.80	108.50	120.20
3	C	93	C	O3'-P-O5'	-7.74	92.39	104.00
1	A	4939	C	O3'-P-O5'	-7.51	92.73	104.00
1	A	1633	G	P-O3'-C3'	7.46	131.40	120.20
3	C	4	C	P-O3'-C3'	-7.41	109.08	120.20
1	A	1935	C	P-O3'-C3'	-7.37	109.15	120.20
1	A	1728	U	O3'-P-O5'	-7.29	93.06	104.00
1	A	4448	G	C4'-C3'-O3'	-7.23	102.16	113.00
1	A	3908	A	C2'-C3'-O3'	7.22	120.33	109.50
2	B	21	G	O3'-P-O5'	-7.14	93.29	104.00
1	A	3614	G	C2'-C3'-O3'	7.06	124.30	113.70
1	A	1419	G	P-O3'-C3'	-6.96	109.77	120.20
1	A	66	A	C4'-C3'-O3'	-6.92	102.62	113.00
3	C	128	C	P-O3'-C3'	6.90	130.55	120.20
1	A	1940	G	P-O3'-C3'	-6.89	109.86	120.20
1	A	2299	G	C2'-C3'-O3'	-6.88	103.38	113.70
1	A	3776	G	C4'-C3'-O3'	6.82	119.64	109.40
1	A	1729	A	C4'-C3'-O3'	-6.82	102.78	113.00
1	A	1424	G	O3'-P-O5'	-6.72	93.92	104.00
1	A	2760	G	C2'-C3'-O3'	6.71	119.57	109.50
1	A	3801	U	C4'-C3'-O3'	-6.70	102.95	113.00
1	A	2089	G	C3'-C2'-C1'	-6.62	94.88	101.50
1	A	208	A	C4'-C3'-O3'	-6.59	103.12	113.00
1	A	4655	A	C4'-C3'-O3'	-6.56	103.16	113.00
1	A	1891	A	C4'-C3'-O3'	-6.49	103.26	113.00
5	E	4	ARG	CB-CA-C	6.48	120.27	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	G	O4'-C1'-N9	6.46	117.89	108.20
1	A	2276	A	O3'-P-O5'	-6.42	94.36	104.00
1	A	3776	G	C4'-C3'-C2'	-6.41	96.19	102.60
1	A	4162	C	P-O3'-C3'	-6.41	110.58	120.20
1	A	4939	C	C2'-C3'-O3'	-6.41	104.08	113.70
1	A	970	G	C1'-O4'-C4'	-6.40	103.50	109.90
1	A	4316	G	C4'-C3'-O3'	-6.40	103.41	113.00
1	A	1590	C	P-O3'-C3'	6.39	129.78	120.20
1	A	1590	C	C2'-C3'-O3'	-6.37	104.14	113.70
3	C	128	C	C4'-C3'-O3'	6.37	118.96	109.40
1	A	4414	A	P-O3'-C3'	-6.36	110.66	120.20
1	A	4718	G	O3'-P-O5'	-6.36	94.46	104.00
1	A	2661	U	O3'-P-O5'	-6.33	94.50	104.00
1	A	3605	C	P-O3'-C3'	-6.31	110.73	120.20
1	A	2349	A	C4'-C3'-O3'	-6.30	103.55	113.00
1	A	4325	A	O3'-P-O5'	-6.30	94.55	104.00
1	A	2061	U	C4'-C3'-O3'	-6.23	103.66	113.00
1	A	1728	U	C4'-C3'-O3'	-6.22	103.67	113.00
1	A	2420	A	C4'-C3'-O3'	-6.19	103.72	113.00
1	A	2844	A	C4'-C3'-O3'	-6.18	103.73	113.00
3	C	61	A	O3'-P-O5'	-6.17	94.75	104.00
1	A	3619	G	C4'-C3'-O3'	-6.17	103.75	113.00
1	A	5068	G	P-O3'-C3'	-6.17	110.95	120.20
10	n	73	ARG	CB-CA-C	-6.15	100.46	110.79
1	A	1669	A	C4'-C3'-O3'	-6.14	103.79	113.00
1	A	2760	G	P-O3'-C3'	6.10	129.35	120.20
1	A	4867	G	P-O3'-C3'	-6.07	111.09	120.20
1	A	3775	A	C4'-C3'-O3'	-6.06	103.90	113.00
1	A	107	G	C4'-C3'-O3'	-6.05	103.93	113.00
1	A	294	G	C4'-C3'-O3'	-6.04	103.95	113.00
1	A	3775	A	O3'-P-O5'	-6.03	94.96	104.00
1	A	439	G	C4'-C3'-O3'	-6.02	103.97	113.00
1	A	4305	G	C1'-O4'-C4'	-6.01	103.69	109.70
1	A	1880	G	C4'-C3'-O3'	-6.01	103.98	113.00
1	A	1590	C	C4'-C3'-O3'	6.00	122.00	113.00
1	A	209	U	C4'-C3'-O3'	-6.00	104.00	113.00
1	A	3937	C	C4'-C3'-O3'	-6.00	104.01	113.00
28	T	58	GLY	CA-C-O	-6.00	118.32	122.22
1	A	914	U	P-O3'-C3'	5.99	129.18	120.20
1	A	1905	U	O3'-P-O5'	5.98	112.97	104.00
1	A	2828	U	C4'-C3'-O3'	-5.97	104.04	113.00
1	A	4913	G	C4'-C3'-O3'	5.97	118.36	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4435	U	C4'-C3'-O3'	-5.97	104.05	113.00
1	A	1730	U	C4'-C3'-O3'	-5.96	104.05	113.00
1	A	4966	A	C4'-C3'-O3'	-5.96	104.05	113.00
1	A	1082	C	C4'-C3'-O3'	5.96	118.33	109.40
1	A	4514	G	O3'-P-O5'	-5.95	95.07	104.00
1	A	1729	A	C5'-C4'-C3'	-5.93	107.10	116.00
1	A	209	U	O5'-C5'-C4'	-5.93	102.60	111.50
1	A	321	U	O3'-P-O5'	-5.89	95.17	104.00
1	A	2442	G	C4'-C3'-C2'	-5.88	96.72	102.60
1	A	3776	G	P-O5'-C5'	-5.87	112.09	120.90
1	A	1457	G	C4'-C3'-O3'	-5.86	104.21	113.00
1	A	4670	C	C4'-C3'-O3'	-5.86	104.22	113.00
1	A	4289	U	C4'-C3'-O3'	-5.85	104.23	113.00
1	A	1425	G	C1'-C2'-O2'	5.84	117.16	108.40
1	A	4267	G	C4'-C3'-O3'	-5.83	104.26	113.00
1	A	3705	G	C4'-C3'-O3'	-5.82	104.27	113.00
1	A	4218	U	C2'-C3'-O3'	-5.82	104.97	113.70
1	A	3704	U	O3'-P-O5'	-5.81	95.29	104.00
1	A	2802	C	C4'-C3'-O3'	-5.80	104.29	113.00
1	A	3837	C	O3'-P-O5'	-5.80	95.30	104.00
1	A	1944	A	C4'-C3'-O3'	-5.79	104.31	113.00
1	A	4075	U	O3'-P-O5'	5.78	112.66	104.00
1	A	4363	A	C4'-C3'-O3'	-5.77	104.34	113.00
1	A	1750	G	P-O3'-C3'	-5.75	111.58	120.20
1	A	3864	C	C2'-C3'-O3'	-5.71	105.13	113.70
1	A	4632	U	C4'-C3'-O3'	-5.71	104.44	113.00
1	A	1276	C	P-O3'-C3'	-5.69	111.66	120.20
1	A	24	G	C4'-C3'-O3'	-5.67	104.50	113.00
1	A	4913	G	P-O3'-C3'	5.67	128.70	120.20
1	A	2518	G	C4'-C3'-O3'	-5.65	104.52	113.00
1	A	384	A	C4'-C3'-O3'	-5.65	104.53	113.00
1	A	407	A	C4'-C3'-O3'	-5.63	104.55	113.00
3	C	135	C	C4'-C3'-O3'	-5.61	104.58	113.00
1	A	1363	C	C4'-C3'-O3'	-5.58	104.62	113.00
1	A	3695	PSU	O3'-P-O5'	-5.58	95.63	104.00
1	A	431	G	O3'-P-O5'	-5.53	95.70	104.00
1	A	1512	G	C4'-C3'-O3'	-5.52	104.71	113.00
1	A	1596	U	C4'-C3'-O3'	-5.52	104.72	113.00
1	A	191	G	C2'-C3'-O3'	-5.52	105.42	113.70
1	A	4211	C	C4'-C3'-O3'	-5.52	104.72	113.00
1	A	1785	C	C4'-C3'-O3'	-5.51	104.73	113.00
1	A	4702	G	C4'-C3'-O3'	-5.50	104.74	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1721	G	C2'-C3'-O3'	-5.50	105.45	113.70
1	A	2042	A	C1'-O4'-C4'	-5.48	104.22	109.70
1	A	1369	C	C4'-C3'-O3'	-5.47	104.79	113.00
3	C	98	C	C4'-C3'-O3'	-5.46	104.80	113.00
3	C	137	A	P-O3'-C3'	-5.46	112.00	120.20
1	A	1546	C	C4'-C3'-O3'	-5.46	104.81	113.00
1	A	4635	A	O3'-P-O5'	-5.46	95.81	104.00
1	A	1944	A	O3'-P-O5'	-5.45	95.82	104.00
1	A	5028	G	C1'-C2'-O2'	-5.45	103.62	111.80
1	A	3669	G	C4'-C3'-O3'	-5.45	104.83	113.00
3	C	24	G	C4'-C3'-O3'	-5.44	104.83	113.00
1	A	4163	U	P-O3'-C3'	-5.44	112.03	120.20
1	A	1906	U	C4'-C3'-C2'	-5.44	97.16	102.60
1	A	2858	A	C2'-C3'-O3'	-5.44	105.55	113.70
1	A	1513	U	C4'-C3'-O3'	-5.43	104.85	113.00
1	A	1424	G	C4'-C3'-O3'	-5.43	104.85	113.00
1	A	3823	G	C4'-C3'-O3'	-5.43	104.86	113.00
1	A	2828	U	O3'-P-O5'	-5.42	95.86	104.00
1	A	1667	G	C4'-C3'-O3'	-5.42	104.87	113.00
1	A	4381	A	C4'-C3'-O3'	-5.42	104.87	113.00
1	A	1546	C	O3'-P-O5'	-5.41	95.89	104.00
1	A	293	G	C2'-C3'-O3'	-5.41	105.59	113.70
1	A	2432	U	O3'-P-O5'	-5.40	95.89	104.00
1	A	2427	G	C4'-C3'-O3'	-5.40	104.91	113.00
1	A	2288	G	C4'-C3'-O3'	-5.39	104.91	113.00
1	A	3818	OMU	OP1-P-O3'	5.39	117.06	105.20
1	A	296	A	O5'-C5'-C4'	-5.39	103.42	111.50
21	M	145	PHE	CA-CB-CG	-5.39	108.41	113.80
1	A	2043	A	C4'-C3'-O3'	-5.39	104.92	113.00
1	A	1722	C	C2'-C3'-O3'	-5.37	105.64	113.70
1	A	4321	U	C4'-C3'-O3'	-5.36	104.95	113.00
1	A	1496	G	C4'-C3'-O3'	-5.36	104.96	113.00
1	A	3878	C	C1'-C2'-O2'	-5.35	103.77	111.80
1	A	4555	U	C1'-C2'-O2'	-5.35	103.77	111.80
3	C	150	C	P-O3'-C3'	-5.35	112.18	120.20
1	A	2280	G	C4'-C3'-O3'	-5.35	104.98	113.00
1	A	71	C	C4'-C3'-O3'	-5.34	104.98	113.00
1	A	219	G	P-O3'-C3'	-5.33	112.20	120.20
10	n	73	ARG	CG-CD-NE	-5.33	100.28	112.00
1	A	2318	G	C1'-C2'-O2'	5.32	116.39	108.40
1	A	2390	G	C4'-C3'-O3'	-5.31	105.03	113.00
1	A	2330	G	C4'-C3'-O3'	-5.31	105.04	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3776	G	O4'-C1'-N9	5.30	116.16	108.20
1	A	3904	G	N9-C1'-C2'	-5.30	106.04	114.00
1	A	2647	A	P-O3'-C3'	-5.30	112.25	120.20
1	A	467	U	P-O3'-C3'	-5.30	112.25	120.20
1	A	1516	G	C4'-C3'-O3'	-5.29	105.06	113.00
1	A	2366	A	O3'-P-O5'	-5.29	96.06	104.00
1	A	4202	U	O3'-P-O5'	-5.29	96.06	104.00
1	A	4326	G	C4'-C3'-O3'	-5.29	105.06	113.00
1	A	5041	G	C2'-C3'-O3'	-5.29	105.76	113.70
1	A	62	A	C4'-C3'-O3'	-5.28	105.08	113.00
1	A	2873	U	C4'-C3'-O3'	-5.26	105.10	113.00
1	A	4475	G	C4'-C3'-O3'	-5.26	105.11	113.00
1	A	1591	U	C4'-C3'-O3'	-5.26	105.12	113.00
1	A	914	U	C2'-C3'-O3'	5.25	117.38	109.50
3	C	5	U	P-O3'-C3'	-5.25	112.32	120.20
2	B	48	G	C4'-C3'-O3'	-5.25	105.13	113.00
1	A	1	C	C4'-C3'-O3'	5.24	117.26	109.40
1	A	1729	A	P-O3'-C3'	-5.24	112.34	120.20
1	A	4892	A	P-O3'-C3'	-5.24	112.35	120.20
1	A	1835	G	P-O3'-C3'	-5.23	112.35	120.20
1	A	4176	C	O3'-P-O5'	-5.23	96.16	104.00
1	A	1453	G	P-O3'-C3'	-5.23	112.36	120.20
1	A	4415	A	C4'-C3'-C2'	-5.21	97.39	102.60
1	A	99	A	C4'-C3'-O3'	-5.21	105.19	113.00
1	A	2734	U	C4'-C3'-O3'	-5.21	105.19	113.00
1	A	2506	G	P-O3'-C3'	-5.20	112.39	120.20
1	A	2724	G	P-O3'-C3'	-5.20	112.39	120.20
1	A	1607	C	C4'-C3'-O3'	-5.19	105.21	113.00
1	A	1548	G	C4'-C3'-O3'	-5.19	105.21	113.00
1	A	917	A	P-O3'-C3'	-5.18	112.44	120.20
19	K	22	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	1833	G	P-O3'-C3'	-5.17	112.45	120.20
1	A	2089	G	N9-C1'-C2'	5.16	121.74	114.00
1	A	232	G	P-O3'-C3'	-5.16	112.46	120.20
5	E	319	GLY	CA-C-O	-5.16	118.67	122.23
1	A	2828	U	P-O3'-C3'	-5.15	112.47	120.20
1	A	4984	C	C4'-C3'-O3'	-5.15	105.28	113.00
1	A	2611	A	P-O3'-C3'	-5.15	112.48	120.20
1	A	1917	A	C4'-C3'-O3'	-5.13	105.30	113.00
1	A	1552	G	O4'-C1'-N9	5.13	115.90	108.20
1	A	1849	U	C4'-C3'-O3'	-5.13	105.30	113.00
1	A	4978	G	C4'-C3'-O3'	-5.12	105.32	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4203	A	C4'-C3'-O3'	-5.11	105.33	113.00
2	B	75	G	C3'-C2'-C1'	-5.11	96.39	101.50
1	A	2444	U	C2'-C3'-O3'	-5.11	106.03	113.70
1	A	2588	C	P-O3'-C3'	-5.09	112.56	120.20
1	A	2267	U	C4'-C3'-O3'	-5.09	105.37	113.00
1	A	4325	A	C4'-C3'-O3'	-5.09	105.37	113.00
1	A	1082	C	P-O3'-C3'	5.08	127.83	120.20
1	A	4974	C	C4'-C3'-O3'	-5.08	105.38	113.00
1	A	2289	C	C4'-C3'-O3'	-5.08	101.78	109.40
1	A	1176	C	P-O3'-C3'	-5.07	112.59	120.20
2	B	2	U	C4'-C3'-O3'	-5.07	105.39	113.00
12	p	189	ARG	N-CA-C	-5.07	106.26	112.90
1	A	1269	G	C4'-C3'-O3'	5.06	116.99	109.40
1	A	1606	U	C4'-C3'-O3'	-5.05	105.42	113.00
1	A	2030	A	P-O3'-C3'	-5.04	112.63	120.20
1	A	339	C	P-O3'-C3'	-5.04	112.64	120.20
1	A	1726	U	C4'-C3'-O3'	-5.03	105.45	113.00
1	A	77	U	C4'-C3'-O3'	-5.02	105.47	113.00
17	I	110	PRO	N-CA-CB	5.01	106.00	103.19
1	A	3704	U	C4'-C3'-O3'	-5.01	105.49	113.00
1	A	1629	G	C2'-C3'-O3'	-5.01	106.19	113.70
1	A	1270	A	C4'-C3'-O3'	-5.00	105.49	113.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1318	C	Sidechain
1	A	1523	A	Sidechain
1	A	1552	G	Sidechain
1	A	1932	A	Sidechain
1	A	2318	G	Sidechain
1	A	2806	A	Sidechain
1	A	292	G	Sidechain
1	A	307	A	Sidechain
1	A	3635	A	Sidechain
1	A	3651	A	Sidechain
1	A	369	G	Sidechain
1	A	3776	G	Sidechain
1	A	3880	G	Sidechain
1	A	417	G	Sidechain
1	A	4583	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	93	G	Sidechain
3	C	16	G	Sidechain

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	A	70928	0	35879	158	0
2	B	2558	0	1295	4	0
3	C	3153	0	1603	15	0
4	D	1887	0	1983	9	0
5	E	3194	0	3336	14	0
6	F	2855	0	3021	14	0
7	G	2308	0	2318	3	0
8	H	1757	0	1910	2	0
9	m	1755	0	1859	3	0
10	n	1809	0	1941	5	0
11	o	1518	0	1600	7	0
12	p	1654	0	1705	6	0
13	q	1358	0	1388	1	0
14	r	1664	0	1773	5	0
15	s	1138	0	1204	7	0
16	l	1708	0	1756	5	0
17	I	1634	0	1779	2	0
18	J	1233	0	1263	9	0
19	K	1513	0	1628	3	0
20	L	1304	0	1433	2	0
21	M	1461	0	1502	8	0
22	N	1298	0	1366	4	0
23	O	804	0	825	1	0
24	P	985	0	1044	4	0
25	Q	519	0	533	1	0
26	R	976	0	1053	3	0
27	S	1115	0	1205	1	0
28	T	1107	0	1182	1	0
29	U	1162	0	1213	2	0
30	V	773	0	828	2	0
31	W	772	0	808	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	X	868	0	913	2	0
33	Y	1053	0	1147	5	0
34	Z	879	0	917	3	0
35	a	845	0	933	1	0
36	b	1015	0	1148	5	0
37	c	832	0	917	2	0
38	d	713	0	746	0	0
39	e	569	0	637	2	0
40	f	444	0	482	2	0
41	g	429	0	465	2	0
42	i	842	0	912	0	0
43	j	708	0	756	4	0
44	k	992	0	1052	2	0
45	h	1712	0	1689	14	0
46	A	214	0	0	0	0
46	B	3	0	0	0	0
46	C	6	0	0	0	0
46	J	1	0	0	0	0
46	L	2	0	0	0	0
46	P	1	0	0	0	0
46	U	1	0	0	0	0
46	d	1	0	0	0	0
47	A	139	0	0	0	0
47	B	1	0	0	0	0
47	D	3	0	0	0	0
47	J	1	0	0	0	0
47	N	1	0	0	0	0
47	V	1	0	0	0	0
47	Y	1	0	0	0	0
47	Z	1	0	0	0	0
47	a	1	0	0	0	0
47	f	1	0	0	0	0
47	i	1	0	0	0	0
47	l	2	0	0	0	0
47	o	1	0	0	0	0
47	p	1	0	0	0	0
48	A	2	0	0	0	0
49	A	39	0	39	1	0
50	A	14	0	26	0	0
51	A	15	0	17	0	0
52	a	1	0	0	0	0
52	d	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	g	1	0	0	0	0
52	i	1	0	0	0	0
52	j	1	0	0	0	0
53	A	8641	0	0	10	0
53	B	261	0	0	0	0
53	C	363	0	0	1	0
53	D	131	0	0	1	0
53	E	177	0	0	0	0
53	F	202	0	0	3	0
53	G	67	0	0	0	0
53	H	49	0	0	0	0
53	I	117	0	0	0	0
53	J	63	0	0	0	0
53	K	139	0	0	0	0
53	L	57	0	0	0	0
53	M	100	0	0	2	0
53	N	87	0	0	1	0
53	O	5	0	0	0	0
53	P	40	0	0	0	0
53	Q	21	0	0	0	0
53	R	35	0	0	0	0
53	S	49	0	0	0	0
53	T	13	0	0	0	0
53	U	92	0	0	0	0
53	V	39	0	0	0	0
53	W	9	0	0	0	0
53	X	37	0	0	0	0
53	Y	112	0	0	0	0
53	Z	72	0	0	2	0
53	a	58	0	0	0	0
53	b	29	0	0	1	0
53	c	32	0	0	0	0
53	d	62	0	0	0	0
53	e	3	0	0	0	0
53	f	19	0	0	1	0
53	g	14	0	0	0	0
53	i	52	0	0	0	0
53	j	40	0	0	1	0
53	k	78	0	0	0	0
53	l	155	0	0	0	0
53	m	131	0	0	0	0
53	n	46	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	o	43	0	0	0	0
53	p	81	0	0	1	0
53	q	13	0	0	0	0
53	r	101	0	0	3	0
53	s	38	0	0	1	0
All	All	142233	0	95029	300	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 1.

All (300) 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)
1:A:1721:G:N2	1:A:1841:C:O2	1.87	1.08
34:Z:95:LYS:NZ	53:Z:301:HOH:O	1.81	1.08
14:r:69:LYS:NZ	53:r:301:HOH:O	1.90	1.03
1:A:1721:G:N2	1:A:1841:C:C2	2.26	1.03
21:M:70:LYS:NZ	53:M:201:HOH:O	1.94	1.01
1:A:5028:G:O2'	1:A:5029:C:O5'	1.91	0.86
1:A:1696:C:H2'	1:A:1697:G:N3	1.93	0.84
15:s:98:ARG:NH2	53:s:301:HOH:O	2.08	0.83
1:A:1695:U:H2'	1:A:1696:C:H1'	1.67	0.77
1:A:5021:C:H2'	1:A:5028:G:H22	1.49	0.76
1:A:3816:A:OP1	1:A:3818:OMU:H5	1.86	0.74
1:A:3638:G:OP2	53:A:5501:HOH:O	2.06	0.73
43:j:28:LYS:HD3	53:j:214:HOH:O	1.88	0.72
1:A:1879:C:OP1	53:A:5502:HOH:O	2.12	0.68
34:Z:34:TYR:O	53:Z:302:HOH:O	2.12	0.68
3:C:122:G:H21	3:C:128:C:H5''	1.59	0.67
1:A:1721:G:C2	1:A:1841:C:N3	2.64	0.66
1:A:4934:A:O2'	1:A:4935:C:O4'	2.13	0.66
1:A:648:G:H2'	1:A:649:A:O4'	1.97	0.65
24:P:62:MET:HE3	24:P:76:VAL:HG12	1.80	0.64
1:A:267:G:H4'	36:b:113:LEU:HD21	1.78	0.64
39:e:25:ILE:HD12	39:e:34:PHE:CD2	2.34	0.62
18:J:125:MET:HE3	18:J:141:SER:OG	2.00	0.61
7:G:62:CYS:HB3	7:G:105:LEU:HD22	1.83	0.61
1:A:3823:G:N2	1:A:3823:G:OP2	2.34	0.60
1:A:1077:C:N3	1:A:1234:G:O6	2.35	0.60
1:A:4538:G:OP1	53:A:5503:HOH:O	2.16	0.60
1:A:2364:OMG:N7	53:A:5528:HOH:O	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:82:THR:HA	26:R:87:MET:HE3	1.83	0.59
6:F:312:ARG:NH2	53:F:502:HOH:O	2.37	0.58
23:O:54:GLY:O	23:O:55:ASN:ND2	2.37	0.57
1:A:4991:U:O2'	1:A:4992:G:O4'	2.21	0.57
1:A:1077:C:O2	1:A:1234:G:O6	2.23	0.57
45:h:197:MET:HE1	45:h:218:VAL:HG22	1.86	0.56
3:C:122:G:H21	3:C:128:C:C5'	2.17	0.56
18:J:54:GLN:HA	18:J:83:TRP:CD1	2.40	0.56
1:A:1077:C:C2	1:A:1234:G:O6	2.58	0.56
1:A:1721:G:C2	1:A:1722:C:N3	2.74	0.56
1:A:4475:G:OP2	1:A:4476:C:O2	2.24	0.55
10:n:63:LEU:HD21	16:l:29:GLN:HG3	1.88	0.55
1:A:2351:OMC:HM23	6:F:95:MET:HG3	1.89	0.55
1:A:1402:C:H1'	1:A:1415:G:C2	2.42	0.55
3:C:71:A:N1	3:C:81:C:O2'	2.38	0.55
40:f:42:ARG:HG3	40:f:47:THR:HG23	1.88	0.55
45:h:182:VAL:HG21	45:h:221:VAL:HG12	1.89	0.55
1:A:3786:U:O2	1:A:3814:U:H4'	2.07	0.54
1:A:2787:A2M:HM'3	1:A:2790:U:OP2	2.07	0.54
24:P:62:MET:HE3	24:P:76:VAL:CG1	2.38	0.54
1:A:2779:C:O2'	3:C:112:G:OP1	2.18	0.54
1:A:1398:A:OP1	29:U:136:LYS:NZ	2.41	0.54
1:A:1064:G:N3	1:A:1064:G:H2'	2.22	0.54
1:A:23:C:H2'	1:A:24:G:O4'	2.09	0.53
1:A:3606:U:H5'	20:L:76:MET:HE1	1.89	0.53
12:p:183:ASP:O	12:p:187:GLU:HG3	2.07	0.53
3:C:78:G:H2'	3:C:79:G:O4'	2.09	0.53
1:A:4266:G:N3	1:A:4266:G:H2'	2.24	0.53
10:n:63:LEU:C	10:n:63:LEU:HD23	2.33	0.52
1:A:960:A:H2'	1:A:970:G:N7	2.24	0.52
1:A:2876:OMG:HM22	1:A:2877:G:O5'	2.10	0.52
31:W:38:ILE:HD11	31:W:46:VAL:HG21	1.92	0.52
1:A:4524:G:N3	5:E:252:ALA:HB1	2.25	0.52
31:W:52:CYS:HA	31:W:92:CYS:SG	2.49	0.52
1:A:4084:G:O6	4:D:68:ARG:HD2	2.10	0.52
1:A:3669:G:O2'	53:A:5504:HOH:O	2.17	0.51
1:A:2638:G:N7	1:A:2697:A:N1	2.57	0.51
4:D:178:PRO:HD2	43:j:26:VAL:HG12	1.91	0.51
1:A:1339:U:H2'	1:A:1340:OMC:C6	2.46	0.51
3:C:128:C:H3'	3:C:129:C:C6	2.46	0.51
18:J:41:ILE:HD12	18:J:150:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:312:ARG:NH1	53:F:503:HOH:O	2.38	0.51
14:r:107:THR:OG1	37:c:18:THR:HG23	2.11	0.51
1:A:1964:A:C4	1:A:1965:G:H1'	2.47	0.50
15:s:24:LEU:HD11	15:s:86:TRP:CG	2.45	0.50
1:A:4452:U:C4	1:A:4531:U:C4	2.99	0.50
26:R:78:LYS:NZ	26:R:133:GLU:OE2	2.42	0.50
33:Y:89:LEU:HD13	33:Y:118:LEU:HD22	1.94	0.50
21:M:82:LEU:C	21:M:82:LEU:HD12	2.37	0.50
1:A:2729:C:H2'	1:A:2730:U:O4'	2.12	0.50
1:A:4260:U:H2'	1:A:4261:C:C6	2.46	0.50
1:A:4860:G:N3	1:A:4860:G:H2'	2.27	0.50
2:B:111:C:H2'	2:B:112:U:O4'	2.12	0.50
1:A:1364:U:OP2	14:r:36:ARG:NH2	2.40	0.50
1:A:1721:G:C2	1:A:1722:C:C2	3.00	0.49
5:E:89:ILE:HG22	5:E:153:MET:HE1	1.94	0.49
39:e:23:VAL:HG23	39:e:64:LEU:HD21	1.94	0.49
1:A:703:G:H2'	1:A:704:C:H4'	1.95	0.49
22:N:93:ILE:HD12	22:N:93:ILE:C	2.38	0.49
34:Z:106:TYR:HA	34:Z:107:PRO:C	2.38	0.49
1:A:1402:C:H2'	1:A:1402:C:O2	2.13	0.49
1:A:3772:U:H5	1:A:3776:G:O6	1.96	0.49
1:A:4524:G:C2	5:E:252:ALA:HB1	2.47	0.49
1:A:2434:G:O2'	1:A:2527:A:N1	2.46	0.49
4:D:175:ILE:HD12	4:D:175:ILE:C	2.37	0.49
26:R:127:LEU:C	26:R:127:LEU:HD12	2.38	0.48
1:A:2351:OMC:HM22	1:A:2352:U:H5'	1.94	0.48
1:A:2673:G:N3	1:A:2673:G:H5'	2.27	0.48
1:A:2476:G:H1'	1:A:2502:G:N2	2.27	0.48
6:F:293:LEU:HD22	19:K:34:PHE:CD2	2.47	0.48
13:q:15:LEU:HD21	13:q:157:ILE:HG12	1.94	0.48
1:A:407:A:O2'	1:A:410:A:OP1	2.16	0.48
1:A:4118:U:H5	53:D:430:HOH:O	1.96	0.48
11:o:128:MET:HA	11:o:128:MET:HE2	1.95	0.48
1:A:4067:U:O2'	1:A:4068:U:C6	2.67	0.48
5:E:122:TRP:CE2	5:E:127:LYS:HE3	2.49	0.48
1:A:4966:A:H2'	1:A:4967:A:O4'	2.14	0.48
5:E:258:HIS:HA	5:E:259:PRO:C	2.39	0.48
12:p:24:ARG:NH1	53:p:402:HOH:O	2.47	0.48
11:o:118:LEU:HD21	11:o:177:ASP:HB2	1.96	0.47
21:M:28:TYR:CD2	21:M:54:MET:HE1	2.49	0.47
49:A:5455:HMT:H28B	53:A:8792:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:o:105:ILE:CG2	11:o:109:GLY:HA2	2.44	0.47
1:A:1940:G:N2	1:A:4434:C:OP1	2.47	0.47
5:E:317:LEU:HD11	5:E:382:MET:HG2	1.95	0.47
7:G:11:ALA:O	7:G:15:ARG:HG2	2.13	0.47
45:h:7:PHE:O	45:h:10:ASN:HB3	2.14	0.47
33:Y:76:LYS:NZ	33:Y:98:GLU:OE1	2.38	0.47
5:E:56:ILE:C	5:E:56:ILE:HD12	2.40	0.47
1:A:1569:U:C5	43:j:2:ALA:HB2	2.50	0.46
2:B:85:G:OP1	9:m:222:LYS:HE2	2.15	0.46
1:A:4291:G:H5'	1:A:4293:PSU:C6	2.50	0.46
1:A:5021:C:H2'	1:A:5028:G:N2	2.24	0.46
5:E:248:LEU:C	5:E:248:LEU:HD12	2.41	0.46
1:A:4476:C:O2	1:A:4476:C:O4'	2.32	0.46
1:A:4926:C:O2	1:A:4926:C:O4'	2.34	0.46
29:U:100:ILE:N	29:U:100:ILE:HD12	2.30	0.46
33:Y:89:LEU:CD1	33:Y:118:LEU:HD22	2.45	0.46
15:s:27:ILE:HD11	15:s:55:MET:HE1	1.97	0.46
17:I:168:TYR:CE2	17:I:172:LYS:HD3	2.50	0.46
1:A:2741:U:H2'	4:D:50:HIS:CD2	2.51	0.46
3:C:155:C:H2'	3:C:156:U:O4'	2.15	0.46
15:s:36:ALA:HB2	15:s:52:PHE:CE1	2.51	0.46
1:A:729:G:H5'	1:A:729:G:N3	2.30	0.46
1:A:4272:G:N7	1:A:4336:A:N1	2.63	0.46
1:A:4419:U:O2	1:A:4419:U:O4'	2.34	0.46
1:A:935:A:O2'	15:s:46:ARG:NH1	2.49	0.46
3:C:76:C:H2'	3:C:77:A:O4'	2.16	0.46
3:C:52:A:OP2	53:C:301:HOH:O	2.21	0.46
5:E:163:ILE:CG2	5:E:180:LEU:HD22	2.45	0.46
1:A:119:G:H3'	1:A:120:A:H5''	1.99	0.45
1:A:906:C:H2'	1:A:906:C:O2	2.16	0.45
1:A:4457:PSU:H1'	5:E:252:ALA:HB3	1.97	0.45
22:N:93:ILE:HD12	22:N:94:GLU:N	2.31	0.45
45:h:22:THR:HG22	45:h:67:ARG:HA	1.99	0.45
1:A:490:C:H2'	1:A:490:C:O2	2.16	0.45
11:o:2:LYS:HD3	15:s:33:GLN:HE22	1.81	0.45
40:f:47:THR:HG22	53:f:210:HOH:O	2.15	0.45
45:h:116:LEU:HD22	45:h:140:GLN:HB3	1.98	0.45
1:A:4456:OMC:HM21	5:E:241:PRO:HD3	1.98	0.45
11:o:92:MET:HE2	11:o:179:ILE:HG22	1.98	0.45
45:h:13:ILE:HD11	45:h:197:MET:HA	1.98	0.45
1:A:309:C:OP2	37:c:32:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2382:A:N1	1:A:2829:U:O2'	2.47	0.45
1:A:2724:G:O2'	1:A:2726:G:OP2	2.33	0.45
1:A:3769:C:O2'	1:A:3770:U:O5'	2.35	0.45
32:X:46:LEU:HD22	32:X:72:VAL:HG11	1.99	0.45
1:A:2416:G:N2	1:A:2427:G:N7	2.60	0.45
1:A:4498:OMU:HM23	1:A:4500:PSU:C6	2.52	0.45
31:W:17:ARG:HD3	31:W:104:ILE:HA	1.99	0.45
1:A:3620:G:N3	1:A:3620:G:H5'	2.32	0.45
1:A:4591:U:H2'	1:A:4592:C:C6	2.52	0.45
11:o:41:ILE:HG22	11:o:43:VAL:HG13	1.99	0.45
1:A:1554:A:H5'	43:j:9:GLY:C	2.42	0.44
1:A:106:A:H2'	1:A:107:G:O4'	2.17	0.44
1:A:1821:G:N3	1:A:1821:G:H2'	2.33	0.44
2:B:24:C:H2'	2:B:25:G:O4'	2.17	0.44
3:C:82:A:N1	27:S:50:ARG:NH2	2.65	0.44
1:A:1721:G:N1	1:A:1841:C:N3	2.66	0.44
1:A:3663:A:N6	1:A:4168:G:O2'	2.50	0.44
1:A:2351:OMC:HM23	6:F:95:MET:CG	2.48	0.44
1:A:3909:C:O2	1:A:4396:A:N1	2.51	0.44
45:h:109:THR:HB	45:h:149:GLY:HA2	2.00	0.44
1:A:4162:C:H5	10:n:73:ARG:HH12	1.65	0.44
6:F:337:ARG:NH1	53:F:501:HOH:O	2.36	0.44
33:Y:82:VAL:HG13	33:Y:114:ARG:HG2	2.00	0.44
1:A:119:G:H3'	1:A:120:A:C5'	2.47	0.44
1:A:4404:U:O2	1:A:4404:U:H2'	2.18	0.44
1:A:2415:OMU:H2'	1:A:2416:G:C8	2.53	0.44
1:A:4393:G:O4'	1:A:4447:5MC:HM53	2.18	0.44
6:F:266:THR:O	6:F:267:TRP:HB2	2.17	0.44
1:A:152:U:O3'	16:l:56:LYS:HE2	2.18	0.44
21:M:68:PHE:O	53:M:201:HOH:O	2.21	0.44
22:N:97:LYS:HG2	53:N:356:HOH:O	2.17	0.44
32:X:25:TYR:CE1	32:X:88:LEU:HD22	2.53	0.44
1:A:1415:G:O2'	1:A:1416:G:O4'	2.21	0.43
1:A:4455:G:OP1	5:E:5:LYS:HE3	2.17	0.43
1:A:4475:G:O6	41:g:125:LYS:NZ	2.51	0.43
5:E:163:ILE:HG22	5:E:180:LEU:HD22	1.99	0.43
21:M:43:ARG:HD2	21:M:43:ARG:HA	1.80	0.43
1:A:368:C:O4'	6:F:83:GLY:HA3	2.17	0.43
1:A:4488:A:H4'	1:A:4489:G:C8	2.54	0.43
45:h:52:SER:C	45:h:53:ILE:HD12	2.44	0.43
1:A:1695:U:O3'	1:A:1696:C:C4'	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4119:C:O2	1:A:4119:C:O4'	2.34	0.43
3:C:91:A:H2'	3:C:92:U:O4'	2.19	0.43
12:p:191:ILE:HD11	12:p:212:LEU:HD21	2.00	0.43
14:r:19:GLN:NE2	53:r:304:HOH:O	2.52	0.43
17:I:69:GLY:HA2	17:I:70:PRO:C	2.44	0.43
45:h:126:GLU:CG	45:h:137:VAL:HG11	2.48	0.43
1:A:266:C:H5'	36:b:112:ARG:HG3	2.01	0.43
1:A:4950:U:O2	1:A:4950:U:O4'	2.36	0.43
6:F:135:ALA:HB3	44:k:6:GLN:NE2	2.34	0.43
12:p:48:LEU:O	12:p:139:ARG:HA	2.18	0.43
1:A:1920:C:H3'	1:A:1921:C:H5''	2.00	0.43
3:C:103:A:C8	3:C:104:A:C8	3.07	0.43
19:K:43:PHE:CD2	19:K:133:GLY:HA3	2.54	0.43
21:M:82:LEU:C	21:M:127:MET:HE2	2.44	0.43
45:h:199:VAL:HG21	45:h:222:PHE:CG	2.54	0.43
45:h:197:MET:HE1	45:h:218:VAL:CG2	2.47	0.43
1:A:168:C:O2	1:A:168:C:O4'	2.37	0.43
1:A:1359:G:H4'	16:l:203:TYR:HB2	2.00	0.43
1:A:1802:A:O2'	22:N:108:ARG:NH2	2.52	0.43
1:A:2607:C:H5''	20:L:96:MET:HE1	2.01	0.42
53:A:8023:HOH:O	9:m:74:MET:HE1	2.19	0.42
18:J:41:ILE:HD12	18:J:150:LEU:HD21	2.01	0.42
18:J:94:MET:HE3	18:J:94:MET:HB2	1.96	0.42
8:H:201:ILE:HG13	8:H:203:ILE:HG23	2.01	0.42
10:n:140:VAL:HG21	10:n:166:LEU:O	2.19	0.42
33:Y:35:TRP:CZ2	33:Y:56:PRO:HD2	2.54	0.42
1:A:1460:C:H5''	19:K:144:LYS:HG3	2.01	0.42
1:A:4992:G:H2'	1:A:4993:G:C8	2.54	0.42
18:J:125:MET:HE2	18:J:143:PRO:HG3	2.00	0.42
1:A:385:A:N3	1:A:387:G:H5''	2.34	0.42
1:A:4507:A:O2'	24:P:41:SER:CB	2.67	0.42
1:A:1721:G:N2	1:A:1722:C:C2	2.87	0.42
1:A:2612:G:N7	53:A:5562:HOH:O	2.37	0.42
1:A:2657:G:O6	31:W:32:LYS:NZ	2.52	0.42
12:p:36:LEU:N	12:p:36:LEU:HD23	2.34	0.42
1:A:2055:G:H3'	1:A:2056:G:H5'	2.02	0.42
1:A:3668:C:H5'	4:D:8:GLN:O	2.19	0.42
1:A:2503:G:O4'	1:A:4084:G:N2	2.52	0.42
4:D:175:ILE:C	4:D:175:ILE:CD1	2.93	0.42
7:G:83:LEU:N	7:G:84:PRO:CD	2.82	0.42
9:m:240:ILE:HD12	9:m:240:ILE:HA	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:C:C5'	36:b:112:ARG:HG3	2.50	0.42
1:A:1927:U:OP1	1:A:1949:U:O2'	2.37	0.42
1:A:1965:G:H2'	1:A:1965:G:N3	2.35	0.42
1:A:106:A:H1'	1:A:336:A:N3	2.34	0.42
1:A:2725:A:N1	53:A:5555:HOH:O	2.36	0.42
2:B:75:G:H5''	21:M:49:SER:O	2.20	0.42
45:h:13:ILE:HD12	45:h:14:GLY:N	2.35	0.42
1:A:21:G:H1'	3:C:103:A:N3	2.35	0.41
1:A:433:A:C2	1:A:3867:A2M:H4'	2.55	0.41
1:A:906:C:O2	1:A:906:C:C2'	2.68	0.41
1:A:2474:G:H1'	1:A:2502:G:N2	2.34	0.41
18:J:104:LEU:C	18:J:104:LEU:HD23	2.45	0.41
1:A:4220:6MZ:O5'	1:A:4220:6MZ:H8	2.21	0.41
10:n:230:TYR:CE2	10:n:234:ARG:HD3	2.55	0.41
1:A:980:U:H2'	1:A:981:C:C6	2.55	0.41
1:A:1964:A:C5	1:A:1965:G:H1'	2.55	0.41
1:A:4438:U:H2'	1:A:4439:U:O4'	2.21	0.41
30:V:93:LEU:HD23	30:V:93:LEU:HA	1.94	0.41
44:k:5:LEU:C	44:k:5:LEU:HD13	2.45	0.41
1:A:1788:A:H2'	12:p:22:PHE:CZ	2.55	0.41
1:A:5028:G:O2'	1:A:5029:C:P	2.78	0.41
4:D:137:ILE:HD11	4:D:149:LYS:HB2	2.02	0.41
11:o:118:LEU:HD13	11:o:118:LEU:HA	1.97	0.41
21:M:84:TYR:HA	21:M:123:SER:O	2.20	0.41
1:A:2658:G:N2	1:A:2676:A:OP2	2.53	0.41
1:A:3767:C:O2'	1:A:3768:U:O4'	2.30	0.41
4:D:101:VAL:C	4:D:102:LEU:HD12	2.46	0.41
18:J:125:MET:HB2	18:J:141:SER:OG	2.20	0.41
1:A:3867:A2M:HM'3	1:A:3880:G:N2	2.36	0.41
1:A:3896:C:O2	1:A:4564:A:N1	2.53	0.41
1:A:4233:A:N3	1:A:4233:A:H2'	2.36	0.41
1:A:4425:G:OP1	41:g:100:TYR:OH	2.35	0.41
16:l:138:PHE:HA	16:l:143:ARG:HD2	2.01	0.41
1:A:3908:A:O2'	1:A:3909:C:H5'	2.20	0.41
1:A:5:A:H2'	1:A:6:C:O4'	2.21	0.41
1:A:27:C:OP1	16:l:193:ARG:CZ	2.69	0.41
1:A:2257:C:O2	1:A:2257:C:O4'	2.38	0.41
1:A:2542:G:O2'	3:C:128:C:H1'	2.21	0.41
1:A:5066:U:OP1	18:J:43:LYS:NZ	2.40	0.41
4:D:42:LYS:HE3	4:D:87:PHE:CG	2.56	0.41
1:A:17:A:N1	3:C:140:C:O2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:G:H3'	1:A:1074:G:H5''	2.03	0.41
1:A:4872:G:O6	15:s:98:ARG:HG3	2.21	0.41
5:E:378:ARG:HD3	25:Q:11:TYR:CD2	2.56	0.41
36:b:109:ARG:NH1	53:b:204:HOH:O	2.54	0.41
45:h:150:SER:HA	45:h:194:ALA:HB3	2.02	0.41
1:A:1380:G:H4'	1:A:1381:U:H6	1.86	0.40
1:A:1601:A:N3	53:A:5567:HOH:O	2.37	0.40
1:A:2297:G:H4'	6:F:242:PRO:HB2	2.03	0.40
45:h:53:ILE:HG22	45:h:62:MET:HE2	2.02	0.40
1:A:2465:C:H2'	1:A:2466:G:O4'	2.21	0.40
1:A:2676:A:OP2	1:A:2676:A:H8	2.05	0.40
6:F:5:ARG:HD2	6:F:24:LEU:O	2.21	0.40
8:H:173:LEU:O	8:H:188:ARG:HA	2.22	0.40
14:r:183:ARG:NH1	53:r:308:HOH:O	2.55	0.40
1:A:233:U:H3'	1:A:234:G:H5''	2.03	0.40
1:A:444:G:O2'	1:A:2313:A:N1	2.49	0.40
6:F:65:GLU:HG2	6:F:80:ARG:HD3	2.02	0.40
24:P:13:LYS:HD3	24:P:128:LEU:HD22	2.03	0.40
28:T:87:VAL:CG1	28:T:89:ILE:HD12	2.52	0.40
36:b:35:LYS:HA	36:b:44:LEU:HD21	2.03	0.40
1:A:2065:G:H2'	1:A:2066:C:O4'	2.21	0.40
30:V:39:PHE:CE2	30:V:43:MET:CE	3.05	0.40
35:a:73:HIS:CD2	35:a:73:HIS:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	244/257 (95%)	240 (98%)	4 (2%)	0	100 100
5	E	394/403 (98%)	389 (99%)	5 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	357/427 (84%)	350 (98%)	7 (2%)	0	100	100
7	G	281/297 (95%)	279 (99%)	2 (1%)	0	100	100
8	H	213/288 (74%)	209 (98%)	4 (2%)	0	100	100
9	m	210/248 (85%)	206 (98%)	4 (2%)	0	100	100
10	n	219/266 (82%)	214 (98%)	5 (2%)	0	100	100
11	o	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
12	p	200/214 (94%)	198 (99%)	2 (1%)	0	100	100
13	q	168/178 (94%)	166 (99%)	2 (1%)	0	100	100
14	r	204/211 (97%)	202 (99%)	2 (1%)	0	100	100
15	s	137/220 (62%)	136 (99%)	1 (1%)	0	100	100
16	l	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
17	I	197/203 (97%)	194 (98%)	3 (2%)	0	100	100
18	J	150/184 (82%)	148 (99%)	2 (1%)	0	100	100
19	K	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
20	L	155/196 (79%)	155 (100%)	0	0	100	100
21	M	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
22	N	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
23	O	97/128 (76%)	93 (96%)	3 (3%)	1 (1%)	12	2
24	P	130/140 (93%)	128 (98%)	2 (2%)	0	100	100
25	Q	60/157 (38%)	59 (98%)	1 (2%)	0	100	100
26	R	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
27	S	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
28	T	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
29	U	145/148 (98%)	140 (97%)	4 (3%)	1 (1%)	18	5
30	V	90/159 (57%)	86 (96%)	4 (4%)	0	100	100
31	W	98/115 (85%)	98 (100%)	0	0	100	100
32	X	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
33	Y	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
34	Z	108/110 (98%)	108 (100%)	0	0	100	100
35	a	104/117 (89%)	102 (98%)	2 (2%)	0	100	100
36	b	120/196 (61%)	119 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	c	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
38	d	85/97 (88%)	84 (99%)	1 (1%)	0	100	100
39	e	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
40	f	48/51 (94%)	48 (100%)	0	0	100	100
41	g	50/99 (50%)	50 (100%)	0	0	100	100
42	i	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
43	j	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
44	k	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
45	h	223/245 (91%)	215 (96%)	7 (3%)	1 (0%)	30	13
All	All	6484/7481 (87%)	6375 (98%)	106 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	O	67	LYS
29	U	15	VAL
45	h	58	ILE

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	
4	D	189/199 (95%)	187 (99%)	2 (1%)	65	47
5	E	345/349 (99%)	344 (100%)	1 (0%)	86	81
6	F	297/348 (85%)	297 (100%)	0	100	100
7	G	237/250 (95%)	236 (100%)	1 (0%)	84	78
8	H	193/252 (77%)	192 (100%)	1 (0%)	81	72
9	m	182/215 (85%)	182 (100%)	0	100	100
10	n	193/223 (86%)	190 (98%)	3 (2%)	55	32
11	o	169/171 (99%)	166 (98%)	3 (2%)	51	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	p	174/181 (96%)	171 (98%)	3 (2%)	53	29
13	q	142/149 (95%)	141 (99%)	1 (1%)	76	62
14	r	172/177 (97%)	172 (100%)	0	100	100
15	s	118/161 (73%)	117 (99%)	1 (1%)	73	59
16	l	172/172 (100%)	172 (100%)	0	100	100
17	I	171/174 (98%)	170 (99%)	1 (1%)	78	67
18	J	133/163 (82%)	132 (99%)	1 (1%)	73	59
19	K	164/165 (99%)	164 (100%)	0	100	100
20	L	138/175 (79%)	138 (100%)	0	100	100
21	M	157/157 (100%)	156 (99%)	1 (1%)	78	67
22	N	139/140 (99%)	136 (98%)	3 (2%)	45	19
23	O	88/115 (76%)	86 (98%)	2 (2%)	44	18
24	P	102/107 (95%)	102 (100%)	0	100	100
25	Q	54/126 (43%)	54 (100%)	0	100	100
26	R	107/133 (80%)	106 (99%)	1 (1%)	70	55
27	S	124/135 (92%)	124 (100%)	0	100	100
28	T	117/118 (99%)	116 (99%)	1 (1%)	70	55
29	U	120/121 (99%)	120 (100%)	0	100	100
30	V	79/126 (63%)	78 (99%)	1 (1%)	61	39
31	W	84/97 (87%)	84 (100%)	0	100	100
32	X	93/110 (84%)	93 (100%)	0	100	100
33	Y	114/121 (94%)	114 (100%)	0	100	100
34	Z	89/89 (100%)	89 (100%)	0	100	100
35	a	92/100 (92%)	92 (100%)	0	100	100
36	b	109/153 (71%)	108 (99%)	1 (1%)	70	55
37	c	86/89 (97%)	85 (99%)	1 (1%)	63	43
38	d	74/80 (92%)	74 (100%)	0	100	100
39	e	64/65 (98%)	64 (100%)	0	100	100
40	f	47/48 (98%)	47 (100%)	0	100	100
41	g	48/91 (53%)	48 (100%)	0	100	100
42	i	91/94 (97%)	90 (99%)	1 (1%)	65	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	j	74/75 (99%)	74 (100%)	0	100	100
44	k	107/121 (88%)	107 (100%)	0	100	100
45	h	195/213 (92%)	191 (98%)	4 (2%)	47	21
All	All	5643/6348 (89%)	5609 (99%)	34 (1%)	76	67

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	175	ILE
4	D	208	GLU
5	E	199	GLU
7	G	220	LYS
8	H	107	VAL
10	n	43	GLN
10	n	87	LEU
10	n	121	LYS
11	o	28	LYS
11	o	112	VAL
11	o	118	LEU
12	p	82	LYS
12	p	142	LEU
12	p	145	LYS
13	q	16	ARG
15	s	103	LYS
17	I	22	ILE
18	J	2	VAL
21	M	70	LYS
22	N	45	MET
22	N	93	ILE
22	N	159	MET
23	O	30	GLU
23	O	55	ASN
26	R	156	ILE
28	T	26	VAL
30	V	117	ARG
36	b	113	LEU
37	c	18	THR
42	i	87	ARG
45	h	26	VAL
45	h	121	LEU
45	h	127	GLU

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Mol	Chain	Res	Type
45	h	135	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	187	GLN
7	G	122	GLN
7	G	291	GLN
8	H	268	GLN
10	n	66	GLN
10	n	90	GLN
11	o	98	HIS
11	o	102	ASN
11	o	188	GLN
12	p	59	GLN
12	p	73	ASN
12	p	130	HIS
13	q	98	ASN
14	r	175	ASN
15	s	33	GLN
15	s	34	ASN
15	s	131	GLN
16	l	29	GLN
17	I	63	ASN
17	I	167	HIS
17	I	184	ASN
18	J	28	ASN
19	K	45	GLN
20	L	27	ASN
22	N	54	HIS
22	N	114	GLN
23	O	95	ASN
24	P	135	ASN
25	Q	59	HIS
26	R	151	ASN
29	U	60	HIS
29	U	120	GLN
30	V	6	ASN
30	V	19	ASN
31	W	15	ASN
32	X	69	ASN
32	X	116	ASN

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Mol	Chain	Res	Type
34	Z	20	ASN
34	Z	21	GLN
34	Z	99	HIS
35	a	100	GLN
36	b	65	GLN
37	c	20	ASN
40	f	33	ASN
41	g	84	GLN
43	j	56	HIS
45	h	157	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3281/5069 (64%)	532 (16%)	71 (2%)
2	B	119/121 (98%)	8 (6%)	0
3	C	147/157 (93%)	21 (14%)	2 (1%)
All	All	3547/5347 (66%)	561 (15%)	73 (2%)

All (561) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	39	A
1	A	42	A
1	A	43	U
1	A	48	G
1	A	59	A
1	A	64	A
1	A	65	A
1	A	73	A
1	A	85	G
1	A	91	G
1	A	98	A
1	A	119	G
1	A	120	A
1	A	129	C
1	A	131	C
1	A	133	C
1	A	134	G
1	A	135	G

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Mol	Chain	Res	Type
1	A	139	G
1	A	141	C
1	A	142	G
1	A	143	C
1	A	144	G
1	A	159	C
1	A	164	G
1	A	165	A
1	A	166	C
1	A	167	C
1	A	168	C
1	A	169	G
1	A	192	G
1	A	200	U
1	A	201	C
1	A	204	U
1	A	216	C
1	A	218	A
1	A	219	G
1	A	233	U
1	A	234	G
1	A	250	C
1	A	253	G
1	A	254	G
1	A	255	C
1	A	269	G
1	A	278	G
1	A	279	A
1	A	297	U
1	A	316	U
1	A	340	C
1	A	387	G
1	A	408	A
1	A	409	G
1	A	410	A
1	A	412	G
1	A	449	C
1	A	450	G
1	A	452	A
1	A	453	G
1	A	454	U
1	A	456	C

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Mol	Chain	Res	Type
1	A	457	G
1	A	461	G
1	A	465	G
1	A	468	U
1	A	472	C
1	A	484	U
1	A	487	G
1	A	489	C
1	A	490	C
1	A	491	G
1	A	505	G
1	A	509	A
1	A	510	U
1	A	512	U
1	A	649	A
1	A	650	C
1	A	653	U
1	A	654	C
1	A	663	G
1	A	666	G
1	A	669	C
1	A	673	C
1	A	686	A
1	A	696	C
1	A	697	G
1	A	703	G
1	A	704	C
1	A	729	G
1	A	730	G
1	A	731	G
1	A	738	C
1	A	739	G
1	A	740	G
1	A	742	G
1	A	746	A
1	A	756	G
1	A	757	G
1	A	907	C
1	A	908	G
1	A	913	U
1	A	914	U
1	A	915	A

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Mol	Chain	Res	Type
1	A	917	A
1	A	918	G
1	A	923	C
1	A	924	C
1	A	926	G
1	A	932	A
1	A	933	G
1	A	934	C
1	A	935	A
1	A	944	A
1	A	945	U
1	A	955	G
1	A	956	A
1	A	959	G
1	A	960	A
1	A	961	G
1	A	971	U
1	A	982	U
1	A	985	C
1	A	988	C
1	A	989	U
1	A	1066	G
1	A	1072	C
1	A	1074	G
1	A	1075	G
1	A	1083	U
1	A	1092	G
1	A	1095	A
1	A	1098	G
1	A	1100	U
1	A	1168	G
1	A	1170	G
1	A	1171	G
1	A	1174	G
1	A	1176	C
1	A	1182	C
1	A	1183	C
1	A	1185	G
1	A	1192	C
1	A	1193	C
1	A	1198	G
1	A	1202	C

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Mol	Chain	Res	Type
1	A	1203	G
1	A	1205	G
1	A	1211	G
1	A	1214	C
1	A	1215	C
1	A	1219	G
1	A	1220	G
1	A	1235	G
1	A	1236	C
1	A	1241	C
1	A	1243	C
1	A	1245	C
1	A	1246	G
1	A	1249	C
1	A	1250	C
1	A	1261	G
1	A	1263	A
1	A	1266	G
1	A	1267	C
1	A	1269	G
1	A	1270	A
1	A	1271	G
1	A	1272	C
1	A	1273	G
1	A	1275	G
1	A	1277	G
1	A	1280	C
1	A	1284	G
1	A	1285	U
1	A	1287	G
1	A	1293	G
1	A	1295	C
1	A	1296	G
1	A	1297	U
1	A	1302	U
1	A	1303	A
1	A	1313	C
1	A	1326	A2M
1	A	1337	A
1	A	1354	A
1	A	1359	G
1	A	1365	C

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Mol	Chain	Res	Type
1	A	1366	G
1	A	1367	C
1	A	1387	A
1	A	1397	A
1	A	1399	G
1	A	1402	C
1	A	1416	G
1	A	1420	A
1	A	1435	G
1	A	1437	C
1	A	1439	C
1	A	1440	U
1	A	1448	G
1	A	1449	C
1	A	1450	C
1	A	1483	C
1	A	1498	G
1	A	1501	C
1	A	1502	G
1	A	1533	A
1	A	1534	A2M
1	A	1547	A
1	A	1564	A
1	A	1566	C
1	A	1578	U
1	A	1591	U
1	A	1596	U
1	A	1613	A
1	A	1614	C
1	A	1624	G
1	A	1625	OMG
1	A	1626	G
1	A	1631	A
1	A	1633	G
1	A	1634	A
1	A	1654	G
1	A	1661	C
1	A	1676	C
1	A	1677	PSU
1	A	1696	C
1	A	1697	G
1	A	1733	G

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Mol	Chain	Res	Type
1	A	1734	G
1	A	1741	G
1	A	1750	G
1	A	1777	C
1	A	1787	A
1	A	1804	A
1	A	1810	G
1	A	1821	G
1	A	1822	U
1	A	1832	C
1	A	1836	G
1	A	1837	A
1	A	1842	G
1	A	1843	A
1	A	1855	G
1	A	1869	G
1	A	1897	A
1	A	1898	C
1	A	1899	G
1	A	1918	U
1	A	1921	C
1	A	1922	G
1	A	1929	A
1	A	1930	U
1	A	1931	C
1	A	1932	A
1	A	1940	G
1	A	1948	G
1	A	1959	U
1	A	1960	A
1	A	1961	G
1	A	1962	A
1	A	2025	A
1	A	2026	A
1	A	2042	A
1	A	2043	A
1	A	2046	G
1	A	2048	U
1	A	2055	G
1	A	2056	G
1	A	2069	A
1	A	2084	C

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Mol	Chain	Res	Type
1	A	2089	G
1	A	2090	U
1	A	2257	C
1	A	2258	C
1	A	2259	G
1	A	2260	C
1	A	2300	A
1	A	2301	G
1	A	2313	A
1	A	2314	G
1	A	2332	A
1	A	2348	G
1	A	2351	OMC
1	A	2360	A
1	A	2389	A
1	A	2395	A
1	A	2397	G
1	A	2417	A
1	A	2421	G
1	A	2425	U
1	A	2447	U
1	A	2470	C
1	A	2471	G
1	A	2474	G
1	A	2475	G
1	A	2476	G
1	A	2503	G
1	A	2504	C
1	A	2513	A
1	A	2519	U
1	A	2548	C
1	A	2554	U
1	A	2556	G
1	A	2559	G
1	A	2560	C
1	A	2569	G
1	A	2577	C
1	A	2587	A
1	A	2588	C
1	A	2589	C
1	A	2601	A
1	A	2611	A

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Mol	Chain	Res	Type
1	A	2627	C
1	A	2653	C
1	A	2662	G
1	A	2669	C
1	A	2675	G
1	A	2676	A
1	A	2687	U
1	A	2694	G
1	A	2695	A
1	A	2696	A
1	A	2703	G
1	A	2705	G
1	A	2706	G
1	A	2707	U
1	A	2708	U
1	A	2710	C
1	A	2711	G
1	A	2712	G
1	A	2726	G
1	A	2743	A
1	A	2760	G
1	A	2761	U
1	A	2762	G
1	A	2763	U
1	A	2788	U
1	A	2790	U
1	A	2794	C
1	A	2795	A
1	A	2814	C
1	A	2826	U
1	A	2827	G
1	A	2855	G
1	A	2899	C
1	A	3600	G
1	A	3601	C
1	A	3604	A
1	A	3605	C
1	A	3615	G
1	A	3618	C
1	A	3626	G
1	A	3635	A
1	A	3644	U

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Mol	Chain	Res	Type
1	A	3662	A
1	A	3673	C
1	A	3674	G
1	A	3709	U
1	A	3710	G
1	A	3713	U
1	A	3714	G
1	A	3735	G
1	A	3736	A
1	A	3755	G
1	A	3756	A
1	A	3757	G
1	A	3768	U
1	A	3769	C
1	A	3770	U
1	A	3771	C
1	A	3776	G
1	A	3777	G
1	A	3783	A
1	A	3784	A
1	A	3785	A2M
1	A	3811	G
1	A	3814	U
1	A	3817	A
1	A	3819	G
1	A	3838	U
1	A	3839	G
1	A	3840	U
1	A	3876	A
1	A	3877	A
1	A	3878	C
1	A	3879	G
1	A	3897	G
1	A	3901	A
1	A	3905	A
1	A	3906	A
1	A	3907	G
1	A	3908	A
1	A	3915	U
1	A	3939	G
1	A	3942	A
1	A	3944	G

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Mol	Chain	Res	Type
1	A	3945	A
1	A	4068	U
1	A	4070	U
1	A	4073	A
1	A	4076	G
1	A	4077	A
1	A	4092	G
1	A	4093	G
1	A	4116	C
1	A	4119	C
1	A	4122	G
1	A	4127	A
1	A	4131	G
1	A	4135	G
1	A	4149	C
1	A	4150	G
1	A	4152	G
1	A	4160	C
1	A	4162	C
1	A	4163	U
1	A	4170	A
1	A	4177	C
1	A	4183	G
1	A	4184	G
1	A	4191	G
1	A	4203	A
1	A	4214	A
1	A	4229	U
1	A	4233	A
1	A	4251	A
1	A	4254	G
1	A	4257	A
1	A	4258	C
1	A	4266	G
1	A	4268	A
1	A	4281	A
1	A	4291	G
1	A	4306	OMU
1	A	4330	G
1	A	4339	A
1	A	4373	G
1	A	4376	A

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Mol	Chain	Res	Type
1	A	4377	G
1	A	4378	A
1	A	4387	C
1	A	4394	A
1	A	4422	A
1	A	4448	G
1	A	4449	A
1	A	4450	U
1	A	4464	A
1	A	4512	U
1	A	4513	A
1	A	4519	C
1	A	4524	G
1	A	4548	A
1	A	4549	G
1	A	4567	G
1	A	4573	G
1	A	4575	G
1	A	4590	A2M
1	A	4635	A
1	A	4636	U
1	A	4637	OMG
1	A	4656	A
1	A	4670	C
1	A	4672	A
1	A	4700	A
1	A	4708	A
1	A	4709	U
1	A	4720	C
1	A	4730	C
1	A	4731	G
1	A	4733	C
1	A	4734	A
1	A	4740	G
1	A	4741	C
1	A	4742	G
1	A	4745	G
1	A	4747	C
1	A	4754	G
1	A	4757	C
1	A	4759	C
1	A	4765	G

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Mol	Chain	Res	Type
1	A	4771	C
1	A	4772	C
1	A	4773	C
1	A	4861	G
1	A	4863	G
1	A	4870	G
1	A	4871	C
1	A	4882	U
1	A	4883	C
1	A	4888	U
1	A	4889	G
1	A	4895	C
1	A	4896	G
1	A	4897	G
1	A	4900	C
1	A	4901	G
1	A	4909	A
1	A	4910	A
1	A	4912	G
1	A	4913	G
1	A	4914	C
1	A	4916	G
1	A	4926	C
1	A	4935	C
1	A	4937	C
1	A	4938	A
1	A	4940	C
1	A	4951	G
1	A	4955	A
1	A	4960	G
1	A	4966	A
1	A	4976	U
1	A	4988	U
1	A	4993	G
1	A	4994	G
1	A	5007	A
1	A	5013	C
1	A	5014	A
1	A	5017	G
1	A	5021	C
1	A	5029	C
1	A	5030	U

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Mol	Chain	Res	Type
1	A	5031	G
1	A	5034	A
1	A	5041	G
1	A	5050	C
1	A	5053	U
1	A	5054	C
1	A	5061	A
1	A	5062	G
1	A	5069	U
2	B	22	A
2	B	25	G
2	B	33	U
2	B	42	A
2	B	53	U
2	B	54	A
2	B	64	G
2	B	110	G
3	C	34	U
3	C	35	C
3	C	51	U
3	C	52	A
3	C	59	A
3	C	62	A
3	C	63	U
3	C	79	G
3	C	82	A
3	C	86	U
3	C	87	G
3	C	94	G
3	C	104	A
3	C	105	C
3	C	110	U
3	C	114	G
3	C	120	G
3	C	121	G
3	C	122	G
3	C	129	C
3	C	156	U

All (73) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	A	1	C
1	A	42	A
1	A	58	G
1	A	64	A
1	A	73	A
1	A	92	C
1	A	167	C
1	A	200	U
1	A	233	U
1	A	278	G
1	A	408	A
1	A	483	G
1	A	648	G
1	A	729	G
1	A	906	C
1	A	914	U
1	A	933	G
1	A	955	G
1	A	1082	C
1	A	1175	A
1	A	1269	G
1	A	1324	A
1	A	1380	G
1	A	1448	G
1	A	1501	C
1	A	1590	C
1	A	1613	A
1	A	1625	OMG
1	A	1633	G
1	A	1677	PSU
1	A	1733	G
1	A	1776	A
1	A	1804	A
1	A	1898	C
1	A	1929	A
1	A	2042	A
1	A	2055	G
1	A	2088	A
1	A	2257	C
1	A	2313	A
1	A	2529	A

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Mol	Chain	Res	Type
1	A	2587	A
1	A	2588	C
1	A	2675	G
1	A	2760	G
1	A	2790	U
1	A	2794	C
1	A	2798	A
1	A	2827	G
1	A	3614	G
1	A	3673	C
1	A	3735	G
1	A	3776	G
1	A	3876	A
1	A	3878	C
1	A	4076	G
1	A	4115	G
1	A	4116	C
1	A	4233	A
1	A	4266	G
1	A	4449	A
1	A	4464	A
1	A	4635	A
1	A	4699	U
1	A	4750	G
1	A	4870	G
1	A	4909	A
1	A	4913	G
1	A	4993	G
1	A	5005	G
1	A	5061	A
3	C	51	U
3	C	128	C

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

117 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	PSU	A	5001	47,1	18,21,22	1.46	3 (16%)	22,30,33	2.37	4 (18%)
1	PSU	A	4403	47,1	18,21,22	1.64	2 (11%)	22,30,33	2.18	5 (22%)
1	OMG	A	4196	46,1	23,26,27	1.25	4 (17%)	33,38,41	2.08	11 (33%)
3	OMG	C	75	3	23,26,27	1.13	4 (17%)	33,38,41	1.90	8 (24%)
1	OMC	A	3841	1	19,22,23	0.75	0	26,31,34	1.13	2 (7%)
1	PSU	A	1536	1	18,21,22	1.44	2 (11%)	22,30,33	2.31	4 (18%)
1	PSU	A	1782	1	18,21,22	1.60	3 (16%)	22,30,33	2.06	5 (22%)
1	OMU	A	2837	1	19,22,23	1.31	2 (10%)	26,31,34	2.02	7 (26%)
1	PSU	A	4457	1	18,21,22	1.37	3 (16%)	22,30,33	2.31	5 (22%)
1	PSU	A	1582	47,1	18,21,22	1.85	5 (27%)	22,30,33	2.12	5 (22%)
1	PSU	A	3920	46,1	18,21,22	1.28	1 (5%)	22,30,33	2.05	5 (22%)
1	PSU	A	1781	1	18,21,22	1.43	2 (11%)	22,30,33	2.13	5 (22%)
1	PSU	A	4552	1	18,21,22	1.53	3 (16%)	22,30,33	2.25	6 (27%)
1	OMC	A	2804	1	19,22,23	0.86	1 (5%)	26,31,34	0.99	1 (3%)
1	PSU	A	4299	1	18,21,22	1.40	4 (22%)	22,30,33	2.36	5 (22%)
1	OMC	A	2861	1	19,22,23	0.93	2 (10%)	26,31,34	0.86	0
1	A2M	A	2815	47,1	22,25,26	1.34	4 (18%)	31,36,39	1.95	9 (29%)
1	PSU	A	5010	1	18,21,22	1.28	2 (11%)	22,30,33	1.94	5 (22%)
1	OMC	A	3808	1	19,22,23	0.80	1 (5%)	26,31,34	0.97	1 (3%)
1	PSU	A	1792	47,1	18,21,22	1.44	3 (16%)	22,30,33	2.29	7 (31%)
1	A2M	A	4590	1	22,25,26	1.25	4 (18%)	31,36,39	2.06	11 (35%)
1	OMG	A	1522	1	23,26,27	1.16	4 (17%)	33,38,41	1.85	6 (18%)
1	PSU	A	4673	47,1	18,21,22	1.15	3 (16%)	22,30,33	1.81	3 (13%)
1	A2M	A	400	1	22,25,26	1.41	4 (18%)	31,36,39	1.94	9 (29%)
1	OMG	A	4618	47,1	23,26,27	1.12	2 (8%)	33,38,41	1.85	9 (27%)
1	PSU	A	3884	47,1	18,21,22	1.23	3 (16%)	22,30,33	2.05	4 (18%)
1	PSU	A	4361	47,1	18,21,22	1.77	4 (22%)	22,30,33	2.12	5 (22%)
1	OMC	A	2351	46,1	19,22,23	0.77	0	26,31,34	1.45	2 (7%)
1	OMG	A	2876	1	23,26,27	1.29	4 (17%)	33,38,41	2.09	8 (24%)
1	A2M	A	1524	1	22,25,26	1.39	5 (22%)	31,36,39	1.96	9 (29%)
1	OMG	A	3899	1	23,26,27	1.20	4 (17%)	33,38,41	2.06	9 (27%)
1	PSU	A	4442	1	18,21,22	1.44	2 (11%)	22,30,33	2.18	6 (27%)
3	PSU	C	55	3	18,21,22	1.23	3 (16%)	22,30,33	1.93	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	A	3724	1	22,25,26	1.40	5 (22%)	31,36,39	2.03	9 (29%)
1	PSU	A	3715	1	18,21,22	1.29	2 (11%)	22,30,33	2.05	4 (18%)
1	OMG	A	3792	1	23,26,27	1.09	2 (8%)	33,38,41	1.79	6 (18%)
1	PSU	A	3853	46,1	18,21,22	1.28	3 (16%)	22,30,33	2.33	5 (22%)
1	PSU	A	1677	47,1	18,21,22	1.66	3 (16%)	22,30,33	2.41	6 (27%)
1	PSU	A	4296	1	18,21,22	1.41	3 (16%)	22,30,33	2.07	5 (22%)
1	A2M	A	4523	46,1	22,25,26	1.27	3 (13%)	31,36,39	2.35	11 (35%)
1	PSU	A	4579	1	18,21,22	1.45	3 (16%)	22,30,33	2.09	4 (18%)
1	A2M	A	3718	1	22,25,26	1.48	3 (13%)	31,36,39	2.04	9 (29%)
1	A2M	A	3830	1	22,25,26	1.32	4 (18%)	31,36,39	1.92	8 (25%)
1	PSU	A	4521	47,46,1	18,21,22	1.49	3 (16%)	22,30,33	2.40	7 (31%)
3	PSU	C	69	3	18,21,22	1.53	3 (16%)	22,30,33	2.20	5 (22%)
1	OMG	A	4370	1	23,26,27	1.14	4 (17%)	33,38,41	1.87	7 (21%)
1	PSU	A	3639	1	18,21,22	1.39	2 (11%)	22,30,33	2.14	3 (13%)
1	OMC	A	2824	1	19,22,23	0.89	0	26,31,34	0.97	1 (3%)
1	A2M	A	1326	1	22,25,26	1.33	3 (13%)	31,36,39	2.01	10 (32%)
1	PSU	A	1860	1	18,21,22	1.37	3 (16%)	22,30,33	2.15	6 (27%)
1	OMG	A	4228	1	23,26,27	1.15	2 (8%)	33,38,41	2.04	13 (39%)
1	5MC	A	4447	47,1	18,22,23	1.00	1 (5%)	26,32,35	1.51	5 (19%)
1	OMG	A	4494	1	23,26,27	1.26	4 (17%)	33,38,41	1.88	7 (21%)
1	PSU	A	4493	47,1	18,21,22	1.31	2 (11%)	22,30,33	2.34	6 (27%)
1	PSU	A	4500	1	18,21,22	1.44	4 (22%)	22,30,33	2.21	5 (22%)
1	OMU	A	4620	1	19,22,23	1.15	2 (10%)	26,31,34	2.18	6 (23%)
1	OMU	A	3818	47,1	19,22,23	1.35	3 (15%)	26,31,34	1.98	6 (23%)
1	A2M	A	3867	1	22,25,26	1.19	3 (13%)	31,36,39	1.94	8 (25%)
1	PSU	A	4576	47,1	18,21,22	1.35	3 (16%)	22,30,33	2.18	5 (22%)
1	6MZ	A	4220	1	22,25,26	1.43	4 (18%)	30,36,39	2.12	9 (30%)
1	OMC	A	2422	46,1	19,22,23	1.12	2 (10%)	26,31,34	0.84	1 (3%)
1	PSU	A	3844	1	18,21,22	1.39	3 (16%)	22,30,33	2.32	5 (22%)
1	A2M	A	3785	1	22,25,26	1.28	3 (13%)	31,36,39	2.53	14 (45%)
1	PSU	A	1683	47,1	18,21,22	1.39	3 (16%)	22,30,33	2.34	6 (27%)
1	OMG	A	1316	47,1	23,26,27	1.21	4 (17%)	33,38,41	1.79	6 (18%)
1	A2M	A	398	1	22,25,26	1.55	4 (18%)	31,36,39	2.17	9 (29%)
1	OMC	A	2365	46,1	19,22,23	1.01	1 (5%)	26,31,34	1.06	2 (7%)
1	OMC	A	1340	1	19,22,23	0.92	1 (5%)	26,31,34	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	3729	1	18,21,22	1.45	4 (22%)	22,30,33	1.95	4 (18%)
1	PSU	A	4420	1	18,21,22	1.35	2 (11%)	22,30,33	1.99	5 (22%)
1	PSU	A	4293	1	18,21,22	1.47	3 (16%)	22,30,33	2.08	6 (27%)
1	A2M	A	2363	46,1	22,25,26	1.27	3 (13%)	31,36,39	2.11	10 (32%)
1	UR3	A	4530	1	19,22,23	0.92	1 (5%)	26,32,35	1.64	4 (15%)
1	PSU	A	4972	47,1	18,21,22	1.31	2 (11%)	22,30,33	2.42	6 (27%)
1	OMU	A	4498	47,1	19,22,23	1.27	3 (15%)	26,31,34	2.31	7 (26%)
1	PSU	A	2632	1	18,21,22	1.46	3 (16%)	22,30,33	2.12	5 (22%)
1	PSU	A	4689	1	18,21,22	1.26	3 (16%)	22,30,33	2.19	4 (18%)
1	PSU	A	4628	1	18,21,22	1.40	4 (22%)	22,30,33	2.35	5 (22%)
1	OMC	A	4456	1	19,22,23	0.85	0	26,31,34	0.85	1 (3%)
1	OMG	A	1625	47,1	23,26,27	1.25	2 (8%)	33,38,41	1.81	7 (21%)
1	OMG	A	2424	1	23,26,27	1.38	4 (17%)	33,38,41	1.77	6 (18%)
1	OMC	A	3701	47,1	19,22,23	0.93	0	26,31,34	1.45	4 (15%)
1	OMU	A	2415	1	19,22,23	1.33	2 (10%)	26,31,34	1.85	8 (30%)
1	OMG	A	4623	1	23,26,27	1.15	3 (13%)	33,38,41	1.83	7 (21%)
1	PSU	A	4532	47,1	18,21,22	1.50	3 (16%)	22,30,33	2.33	6 (27%)
1	PSU	A	2839	1	18,21,22	1.41	3 (16%)	22,30,33	1.95	7 (31%)
1	PSU	A	3637	47,1	18,21,22	1.31	3 (16%)	22,30,33	2.29	4 (18%)
1	OMG	A	3744	1	23,26,27	1.06	2 (8%)	33,38,41	1.69	5 (15%)
1	1MA	A	1322	46,1	21,25,26	1.13	2 (9%)	31,37,40	1.61	5 (16%)
1	OMG	A	2364	1	23,26,27	1.20	3 (13%)	33,38,41	1.69	7 (21%)
1	PSU	A	1862	1	18,21,22	1.49	3 (16%)	22,30,33	2.51	4 (18%)
1	OMU	A	4227	1	19,22,23	1.24	3 (15%)	26,31,34	1.84	5 (19%)
1	PSU	A	3851	1	18,21,22	1.31	3 (16%)	22,30,33	2.35	6 (27%)
1	OMG	A	3627	1	23,26,27	1.29	4 (17%)	33,38,41	1.92	9 (27%)
1	PSU	A	4312	1	18,21,22	1.44	2 (11%)	22,30,33	2.16	4 (18%)
1	5MC	A	3782	46,1	18,22,23	1.11	1 (5%)	26,32,35	1.29	4 (15%)
1	A2M	A	2787	46,1	22,25,26	1.28	3 (13%)	31,36,39	2.52	15 (48%)
1	OMC	A	4536	46,1	19,22,23	0.85	0	26,31,34	0.89	1 (3%)
1	PSU	A	4423	1	18,21,22	1.29	3 (16%)	22,30,33	1.88	3 (13%)
1	PSU	A	3695	47,1	18,21,22	1.34	2 (11%)	22,30,33	2.08	6 (27%)
1	A2M	A	3825	1	22,25,26	1.12	3 (13%)	31,36,39	1.93	11 (35%)
1	OMG	A	4637	47,1	23,26,27	1.15	3 (13%)	33,38,41	1.94	8 (24%)
1	OMC	A	3869	1	19,22,23	0.84	1 (5%)	26,31,34	1.21	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	2508	1	18,21,22	1.32	3 (16%)	22,30,33	1.99	6 (27%)
1	OMU	A	4306	1	19,22,23	1.28	3 (15%)	26,31,34	1.78	6 (23%)
1	PSU	A	4471	47,1	18,21,22	1.53	3 (16%)	22,30,33	1.92	4 (18%)
1	PSU	A	4431	47,1	18,21,22	1.44	3 (16%)	22,30,33	2.41	7 (31%)
1	OMU	A	3925	1	19,22,23	1.16	2 (10%)	26,31,34	1.92	5 (19%)
1	OMG	A	4499	1	23,26,27	1.30	4 (17%)	33,38,41	2.08	7 (21%)
1	PSU	A	1744	47,1	18,21,22	1.38	2 (11%)	22,30,33	2.10	4 (18%)
1	OMC	A	3887	1	19,22,23	0.85	1 (5%)	26,31,34	1.24	2 (7%)
1	A2M	A	4571	1	22,25,26	1.48	4 (18%)	31,36,39	2.01	9 (29%)
1	A2M	A	1871	46,1	22,25,26	1.09	2 (9%)	31,36,39	1.80	7 (22%)
1	PSU	A	4353	47,1	18,21,22	1.53	3 (16%)	22,30,33	2.37	5 (22%)
1	A2M	A	1534	46,1	22,25,26	1.63	4 (18%)	31,36,39	1.99	11 (35%)
1	A2M	A	2401	46,1	22,25,26	1.23	3 (13%)	31,36,39	2.14	11 (35%)
1	OMG	A	4392	1	23,26,27	1.10	3 (13%)	33,38,41	1.89	8 (24%)

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	PSU	A	5001	47,1	-	0/7/25/26	0/2/2/2
1	PSU	A	4403	47,1	-	0/7/25/26	0/2/2/2
1	OMG	A	4196	46,1	-	0/9/27/28	0/3/3/3
3	OMG	C	75	3	-	0/9/27/28	0/3/3/3
1	OMC	A	3841	1	-	0/9/27/28	0/2/2/2
1	PSU	A	1536	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1782	1	-	0/7/25/26	0/2/2/2
1	OMU	A	2837	1	-	0/9/27/28	0/2/2/2
1	PSU	A	4457	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1582	47,1	-	0/7/25/26	0/2/2/2
1	PSU	A	3920	46,1	-	0/7/25/26	0/2/2/2
1	PSU	A	1781	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4552	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2804	1	-	0/9/27/28	0/2/2/2
1	PSU	A	4299	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2861	1	-	0/9/27/28	0/2/2/2
1	A2M	A	2815	47,1	-	0/9/27/28	0/3/3/3
1	PSU	A	5010	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	A	3808	1	-	0/9/27/28	0/2/2/2
1	PSU	A	1792	47,1	-	0/7/25/26	0/2/2/2
1	A2M	A	4590	1	-	1/9/27/28	0/3/3/3
1	OMG	A	1522	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4673	47,1	-	0/7/25/26	0/2/2/2
1	A2M	A	400	1	-	0/9/27/28	0/3/3/3
1	OMG	A	4618	47,1	-	0/9/27/28	0/3/3/3
1	PSU	A	3884	47,1	-	0/7/25/26	0/2/2/2
1	PSU	A	4361	47,1	-	0/7/25/26	0/2/2/2
1	OMC	A	2351	46,1	-	1/9/27/28	0/2/2/2
1	OMG	A	2876	1	-	0/9/27/28	0/3/3/3
1	A2M	A	1524	1	-	0/9/27/28	0/3/3/3
1	OMG	A	3899	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4442	1	-	0/7/25/26	0/2/2/2
3	PSU	C	55	3	-	0/7/25/26	0/2/2/2
1	A2M	A	3724	1	-	0/9/27/28	0/3/3/3
1	PSU	A	3715	1	-	0/7/25/26	0/2/2/2
1	OMG	A	3792	1	-	0/9/27/28	0/3/3/3
1	PSU	A	3853	46,1	-	0/7/25/26	0/2/2/2
1	PSU	A	1677	47,1	-	1/7/25/26	0/2/2/2
1	PSU	A	4296	1	-	0/7/25/26	0/2/2/2
1	A2M	A	4523	46,1	-	0/9/27/28	0/3/3/3
1	PSU	A	4579	1	-	0/7/25/26	0/2/2/2
1	A2M	A	3718	1	-	0/9/27/28	0/3/3/3
1	A2M	A	3830	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4521	47,46,1	-	0/7/25/26	0/2/2/2
3	PSU	C	69	3	-	0/7/25/26	0/2/2/2
1	OMG	A	4370	1	-	0/9/27/28	0/3/3/3
1	PSU	A	3639	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2824	1	-	0/9/27/28	0/2/2/2
1	A2M	A	1326	1	-	1/9/27/28	0/3/3/3
1	PSU	A	1860	1	-	0/7/25/26	0/2/2/2
1	OMG	A	4228	1	-	0/9/27/28	0/3/3/3
1	5MC	A	4447	47,1	-	4/7/25/26	0/2/2/2
1	OMG	A	4494	1	-	1/9/27/28	0/3/3/3
1	PSU	A	4493	47,1	-	0/7/25/26	0/2/2/2
1	PSU	A	4500	1	-	1/7/25/26	0/2/2/2
1	OMU	A	4620	1	-	0/9/27/28	0/2/2/2
1	OMU	A	3818	47,1	-	1/9/27/28	0/2/2/2
1	A2M	A	3867	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4576	47,1	-	0/7/25/26	0/2/2/2
1	6MZ	A	4220	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	A	2422	46,1	-	2/9/27/28	0/2/2/2
1	PSU	A	3844	1	-	1/7/25/26	0/2/2/2
1	A2M	A	3785	1	-	2/9/27/28	0/3/3/3
1	PSU	A	1683	47,1	-	0/7/25/26	0/2/2/2
1	OMG	A	1316	47,1	-	0/9/27/28	0/3/3/3
1	A2M	A	398	1	-	0/9/27/28	0/3/3/3
1	OMC	A	2365	46,1	-	0/9/27/28	0/2/2/2
1	OMC	A	1340	1	-	0/9/27/28	0/2/2/2
1	PSU	A	3729	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4420	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4293	1	-	0/7/25/26	0/2/2/2
1	A2M	A	2363	46,1	-	1/9/27/28	0/3/3/3
1	UR3	A	4530	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4972	47,1	-	0/7/25/26	0/2/2/2
1	OMU	A	4498	47,1	-	0/9/27/28	0/2/2/2
1	PSU	A	2632	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4689	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4628	1	-	0/7/25/26	0/2/2/2
1	OMC	A	4456	1	-	0/9/27/28	0/2/2/2
1	OMG	A	1625	47,1	-	0/9/27/28	0/3/3/3
1	OMG	A	2424	1	-	0/9/27/28	0/3/3/3
1	OMC	A	3701	47,1	-	4/9/27/28	0/2/2/2
1	OMU	A	2415	1	-	1/9/27/28	0/2/2/2
1	OMG	A	4623	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4532	47,1	-	0/7/25/26	0/2/2/2
1	PSU	A	2839	1	-	0/7/25/26	0/2/2/2
1	PSU	A	3637	47,1	-	0/7/25/26	0/2/2/2
1	OMG	A	3744	1	-	0/9/27/28	0/3/3/3
1	1MA	A	1322	46,1	-	0/7/25/26	0/3/3/3
1	OMG	A	2364	1	-	2/9/27/28	0/3/3/3
1	PSU	A	1862	1	-	0/7/25/26	0/2/2/2
1	OMU	A	4227	1	-	0/9/27/28	0/2/2/2
1	PSU	A	3851	1	-	0/7/25/26	0/2/2/2
1	OMG	A	3627	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4312	1	-	0/7/25/26	0/2/2/2
1	5MC	A	3782	46,1	-	0/7/25/26	0/2/2/2
1	A2M	A	2787	46,1	-	3/9/27/28	0/3/3/3
1	OMC	A	4536	46,1	-	0/9/27/28	0/2/2/2
1	PSU	A	4423	1	-	0/7/25/26	0/2/2/2
1	PSU	A	3695	47,1	-	0/7/25/26	0/2/2/2
1	A2M	A	3825	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A	4637	47,1	-	0/9/27/28	0/3/3/3
1	OMC	A	3869	1	-	0/9/27/28	0/2/2/2
1	PSU	A	2508	1	-	0/7/25/26	0/2/2/2
1	OMU	A	4306	1	-	0/9/27/28	0/2/2/2
1	PSU	A	4471	47,1	-	0/7/25/26	0/2/2/2
1	PSU	A	4431	47,1	-	0/7/25/26	0/2/2/2
1	OMU	A	3925	1	-	0/9/27/28	0/2/2/2
1	OMG	A	4499	1	-	0/9/27/28	0/3/3/3
1	PSU	A	1744	47,1	-	0/7/25/26	0/2/2/2
1	OMC	A	3887	1	-	0/9/27/28	0/2/2/2
1	A2M	A	4571	1	-	0/9/27/28	0/3/3/3
1	A2M	A	1871	46,1	-	0/9/27/28	0/3/3/3
1	PSU	A	4353	47,1	-	0/7/25/26	0/2/2/2
1	A2M	A	1534	46,1	-	2/9/27/28	0/3/3/3
1	A2M	A	2401	46,1	-	1/9/27/28	0/3/3/3
1	OMG	A	4392	1	-	0/9/27/28	0/3/3/3

All (317) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4403	PSU	C6-C5	4.87	1.41	1.35
1	A	4361	PSU	C6-C5	4.66	1.40	1.35
1	A	398	A2M	C5-C4	4.53	1.47	1.39
1	A	3718	A2M	C5-C4	4.35	1.47	1.39
1	A	1534	A2M	C5-C4	4.30	1.47	1.39
1	A	1782	PSU	C6-C5	4.21	1.40	1.35
1	A	4532	PSU	C6-C5	4.19	1.40	1.35
1	A	2632	PSU	C6-C5	4.15	1.40	1.35
1	A	4420	PSU	C6-C5	4.09	1.40	1.35
1	A	1781	PSU	C6-C5	4.05	1.40	1.35
1	A	400	A2M	C5-C4	4.01	1.46	1.39
1	A	3724	A2M	C5-C4	3.89	1.46	1.39
1	A	2787	A2M	C5-C4	3.84	1.46	1.39
3	C	69	PSU	C6-C5	3.83	1.39	1.35
1	A	4972	PSU	C6-C5	3.78	1.39	1.35
1	A	4571	A2M	C5-C4	3.77	1.46	1.39
1	A	4293	PSU	C6-C5	3.76	1.39	1.35
1	A	3637	PSU	C6-C5	3.75	1.39	1.35
1	A	2815	A2M	C5-C4	3.74	1.46	1.39
1	A	2401	A2M	C5-C4	3.74	1.46	1.39
1	A	1582	PSU	C4-N3	-3.72	1.31	1.38
1	A	4471	PSU	C6-C5	3.65	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4361	PSU	C2-N1	-3.60	1.31	1.36
1	A	1582	PSU	C6-C5	3.60	1.39	1.35
1	A	4220	6MZ	C5-C4	3.59	1.45	1.39
1	A	4521	PSU	C4-N3	-3.57	1.32	1.38
1	A	1862	PSU	C6-C5	3.56	1.39	1.35
1	A	1536	PSU	C6-C5	3.54	1.39	1.35
1	A	4431	PSU	C4-N3	-3.53	1.32	1.38
1	A	4552	PSU	C4-N3	-3.52	1.32	1.38
1	A	1524	A2M	C5-C4	3.50	1.45	1.39
1	A	3639	PSU	C6-C5	3.48	1.39	1.35
1	A	1534	A2M	C5-N7	-3.47	1.32	1.39
1	A	4403	PSU	C2-N1	-3.45	1.32	1.36
1	A	5001	PSU	C6-C5	3.44	1.39	1.35
1	A	1683	PSU	C6-C5	3.40	1.39	1.35
1	A	3729	PSU	C6-C5	3.39	1.39	1.35
1	A	4296	PSU	C6-C5	3.37	1.39	1.35
1	A	4312	PSU	C4-N3	-3.37	1.32	1.38
1	A	4361	PSU	C4-N3	-3.37	1.32	1.38
1	A	4590	A2M	C5-C4	3.36	1.45	1.39
1	A	3844	PSU	C4-N3	-3.35	1.32	1.38
1	A	3627	OMG	C6-N1	-3.35	1.32	1.38
1	A	3785	A2M	C5-C4	3.35	1.45	1.39
1	A	1862	PSU	C4-N3	-3.34	1.32	1.38
1	A	4353	PSU	C2-N1	-3.32	1.32	1.36
1	A	4493	PSU	C6-C5	3.32	1.39	1.35
1	A	1536	PSU	C4-N3	-3.32	1.32	1.38
1	A	2508	PSU	C4-N3	-3.31	1.32	1.38
1	A	3695	PSU	C6-C5	3.30	1.39	1.35
1	A	1534	A2M	C4-N9	-3.28	1.30	1.37
1	A	4306	OMU	C4-N3	-3.27	1.32	1.38
1	A	4628	PSU	C6-C5	3.27	1.39	1.35
1	A	4523	A2M	C5-C4	3.27	1.45	1.39
1	A	2837	OMU	C4-N3	-3.27	1.32	1.38
1	A	4442	PSU	C6-C5	3.23	1.39	1.35
1	A	1782	PSU	C4-N3	-3.22	1.32	1.38
1	A	4494	OMG	C6-N1	-3.21	1.32	1.38
1	A	1860	PSU	C2-N3	-3.21	1.32	1.37
1	A	3853	PSU	C6-C5	3.20	1.39	1.35
1	A	4552	PSU	C6-C5	3.17	1.39	1.35
1	A	4457	PSU	C6-C5	3.16	1.39	1.35
1	A	1326	A2M	C5-C4	3.16	1.44	1.39
1	A	4500	PSU	C6-C5	3.16	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1677	PSU	C2-N1	-3.16	1.32	1.36
1	A	3715	PSU	C6-C5	3.14	1.39	1.35
1	A	1677	PSU	C4-N3	-3.14	1.33	1.38
1	A	1316	OMG	C5-C4	3.14	1.47	1.38
1	A	4576	PSU	C6-C5	3.11	1.38	1.35
1	A	2363	A2M	C5-C4	3.11	1.44	1.39
1	A	1625	OMG	C6-N1	-3.11	1.33	1.38
1	A	1792	PSU	C4-N3	-3.09	1.33	1.38
1	A	2839	PSU	C4-N3	-3.08	1.33	1.38
1	A	4579	PSU	C6-C5	3.08	1.38	1.35
1	A	1582	PSU	C2-N1	-3.07	1.32	1.36
1	A	4312	PSU	C2-N3	-3.06	1.32	1.37
1	A	3718	A2M	C5-N7	-3.04	1.33	1.39
1	A	1582	PSU	O5'-C5'	-3.04	1.37	1.44
1	A	4442	PSU	C4-N3	-3.03	1.33	1.38
3	C	75	OMG	C5-C4	3.03	1.47	1.38
1	A	2876	OMG	C6-N1	-3.03	1.33	1.38
1	A	4299	PSU	C4-N3	-3.03	1.33	1.38
1	A	4392	OMG	C5-C4	3.00	1.47	1.38
1	A	4689	PSU	C6-C5	3.00	1.38	1.35
1	A	3830	A2M	C5-C4	2.99	1.44	1.39
1	A	3851	PSU	C6-C5	2.99	1.38	1.35
1	A	3729	PSU	C4-N3	-2.97	1.33	1.38
1	A	2415	OMU	C2-N3	-2.97	1.32	1.38
1	A	1625	OMG	C5-C4	2.94	1.46	1.38
1	A	5010	PSU	C6-C5	2.94	1.38	1.35
1	A	1744	PSU	C4-N3	-2.93	1.33	1.38
3	C	69	PSU	C4-N3	-2.93	1.33	1.38
1	A	1792	PSU	C6-C5	2.93	1.38	1.35
1	A	4471	PSU	C4-N3	-2.92	1.33	1.38
1	A	398	A2M	C5-N7	-2.91	1.33	1.39
1	A	4228	OMG	C6-N1	-2.90	1.33	1.38
1	A	1683	PSU	C4-N3	-2.90	1.33	1.38
1	A	2422	OMC	O5'-C5'	-2.89	1.37	1.44
1	A	3920	PSU	C6-C5	2.89	1.38	1.35
1	A	4571	A2M	C5-N7	-2.88	1.33	1.39
1	A	2364	OMG	C6-N1	-2.87	1.33	1.38
1	A	4196	OMG	C5-C4	2.86	1.46	1.38
1	A	4576	PSU	C4-N3	-2.85	1.33	1.38
1	A	2363	A2M	C5-N7	-2.84	1.33	1.39
1	A	4579	PSU	C4-N3	-2.83	1.33	1.38
1	A	1322	1MA	C6-N6	2.82	1.34	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1582	PSU	C2-N3	-2.81	1.32	1.37
1	A	1326	A2M	C5-N7	-2.81	1.33	1.39
1	A	3899	OMG	C4-N9	-2.81	1.30	1.38
1	A	3925	OMU	C4-N3	-2.80	1.33	1.38
1	A	3851	PSU	C2-N3	-2.80	1.32	1.37
1	A	1782	PSU	C2-N1	-2.80	1.32	1.36
1	A	4499	OMG	C5-N7	-2.79	1.33	1.39
1	A	2508	PSU	C6-C5	2.79	1.38	1.35
1	A	2839	PSU	C2-N3	-2.78	1.32	1.37
1	A	2839	PSU	C6-C5	2.78	1.38	1.35
1	A	4423	PSU	C4-N3	-2.78	1.33	1.38
1	A	3718	A2M	C4-N9	-2.78	1.31	1.37
1	A	3782	5MC	C6-C5	2.77	1.39	1.34
1	A	4353	PSU	C4-N3	-2.77	1.33	1.38
1	A	4532	PSU	C4-N3	-2.74	1.33	1.38
1	A	4220	6MZ	C8-N7	2.74	1.36	1.31
1	A	2424	OMG	C5-C4	2.74	1.46	1.38
1	A	4620	OMU	C4-N3	-2.73	1.33	1.38
1	A	1781	PSU	C4-N3	-2.73	1.33	1.38
1	A	4299	PSU	C6-C5	2.73	1.38	1.35
1	A	1860	PSU	C4-N3	-2.73	1.33	1.38
1	A	2424	OMG	C6-N1	-2.73	1.33	1.38
1	A	4571	A2M	C4-N9	-2.72	1.31	1.37
1	A	4493	PSU	C4-N3	-2.72	1.33	1.38
1	A	4353	PSU	C6-C5	2.72	1.38	1.35
1	A	4296	PSU	C4-N3	-2.71	1.33	1.38
1	A	5001	PSU	C4-N3	-2.71	1.33	1.38
1	A	3715	PSU	C4-N3	-2.71	1.33	1.38
1	A	3884	PSU	C4-N3	-2.70	1.33	1.38
1	A	4673	PSU	C6-C5	2.70	1.38	1.35
1	A	4220	6MZ	C4-N9	-2.70	1.31	1.37
1	A	2876	OMG	C5-N7	-2.70	1.33	1.39
1	A	4498	OMU	C4-N3	-2.69	1.33	1.38
3	C	55	PSU	C4-N3	-2.68	1.33	1.38
1	A	2876	OMG	C5-C4	2.68	1.46	1.38
1	A	1522	OMG	C5-C4	2.68	1.46	1.38
1	A	2422	OMC	C6-C5	2.68	1.41	1.35
1	A	4227	OMU	C4-N3	-2.68	1.33	1.38
1	A	3825	A2M	C5-C4	2.67	1.44	1.39
1	A	4499	OMG	C5-C4	2.67	1.46	1.38
1	A	2364	OMG	O5'-C5'	-2.67	1.38	1.44
1	A	3867	A2M	C8-N7	2.66	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2632	PSU	C4-N3	-2.65	1.33	1.38
1	A	1524	A2M	C8-N7	2.64	1.36	1.31
1	A	3818	OMU	C4-N3	-2.63	1.33	1.38
1	A	3695	PSU	C4-N3	-2.63	1.34	1.38
1	A	3844	PSU	C2-N1	-2.63	1.33	1.36
1	A	4499	OMG	C6-N1	-2.62	1.34	1.38
3	C	55	PSU	C2-N3	-2.62	1.33	1.37
1	A	3884	PSU	C6-C5	2.61	1.38	1.35
1	A	2424	OMG	C4-N9	-2.61	1.31	1.38
1	A	1871	A2M	C5-C4	2.61	1.43	1.39
1	A	3899	OMG	C5-C4	2.60	1.46	1.38
1	A	2415	OMU	C4-N3	-2.60	1.33	1.38
1	A	4628	PSU	C2-N3	-2.60	1.33	1.37
1	A	2424	OMG	C5-N7	-2.59	1.34	1.39
1	A	3844	PSU	C6-C5	2.59	1.38	1.35
1	A	4293	PSU	C2-N3	-2.59	1.33	1.37
1	A	4521	PSU	C2-N3	-2.58	1.33	1.37
1	A	1860	PSU	C6-C5	2.58	1.38	1.35
1	A	4228	OMG	C5-C4	2.58	1.45	1.38
1	A	398	A2M	C8-N7	2.57	1.36	1.31
1	A	2837	OMU	C2-N3	-2.56	1.33	1.38
1	A	1744	PSU	C6-C5	2.56	1.38	1.35
1	A	3925	OMU	C2-N3	-2.55	1.33	1.38
1	A	4689	PSU	C2-N3	-2.55	1.33	1.37
1	A	4392	OMG	C6-N1	-2.55	1.34	1.38
1	A	2632	PSU	C2-N1	-2.54	1.33	1.36
1	A	4293	PSU	C4-N3	-2.54	1.34	1.38
1	A	3792	OMG	C5-C4	2.54	1.45	1.38
1	A	4423	PSU	C6-C5	2.53	1.38	1.35
1	A	4494	OMG	C5-C4	2.53	1.45	1.38
1	A	4620	OMU	C2-N3	-2.53	1.33	1.38
1	A	3785	A2M	C5-N7	-2.53	1.34	1.39
1	A	4306	OMU	C6-C5	2.53	1.40	1.35
1	A	3818	OMU	C5-C4	-2.53	1.38	1.43
1	A	4196	OMG	C5-N7	-2.52	1.34	1.39
1	A	3818	OMU	C2-N1	2.51	1.42	1.38
1	A	3830	A2M	C5-N7	-2.49	1.34	1.39
1	A	4590	A2M	C4-N9	-2.49	1.32	1.37
1	A	3627	OMG	C4-N9	-2.49	1.31	1.38
1	A	2364	OMG	C4-N9	-2.46	1.31	1.38
1	A	4457	PSU	C4-N3	-2.46	1.34	1.38
1	A	4521	PSU	C6-C5	2.46	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4571	A2M	C5-C6	2.45	1.47	1.41
1	A	4370	OMG	C6-N1	-2.45	1.34	1.38
1	A	4498	OMU	C2-N3	-2.45	1.33	1.38
1	A	3825	A2M	C5-N7	-2.44	1.34	1.39
1	A	4637	OMG	C6-N1	-2.44	1.34	1.38
1	A	4196	OMG	C6-N1	-2.44	1.34	1.38
1	A	4637	OMG	C5-C4	2.43	1.45	1.38
1	A	4623	OMG	C6-N1	-2.43	1.34	1.38
1	A	4447	5MC	C6-C5	2.43	1.38	1.34
1	A	4590	A2M	C5-N7	-2.43	1.34	1.39
1	A	2876	OMG	C4-N9	-2.43	1.31	1.38
1	A	4972	PSU	C4-N3	-2.42	1.34	1.38
1	A	4532	PSU	C2-N3	-2.42	1.33	1.37
1	A	3627	OMG	C5-C4	2.42	1.45	1.38
1	A	4299	PSU	C2-N3	-2.41	1.33	1.37
1	A	3792	OMG	C4-N9	-2.41	1.31	1.38
1	A	2363	A2M	C4-N9	-2.41	1.32	1.37
1	A	3639	PSU	C4-N3	-2.40	1.34	1.38
1	A	1524	A2M	C4-N9	-2.40	1.32	1.37
1	A	3808	OMC	C6-C5	2.40	1.40	1.35
1	A	3724	A2M	C5-C6	2.39	1.47	1.41
1	A	4579	PSU	C2-N1	-2.38	1.33	1.36
1	A	400	A2M	C5-C6	2.37	1.47	1.41
1	A	3851	PSU	C4-N3	-2.37	1.34	1.38
1	A	5010	PSU	C4-N3	-2.37	1.34	1.38
1	A	4499	OMG	C4-N9	-2.36	1.31	1.38
1	A	3744	OMG	C5-C4	2.36	1.45	1.38
1	A	3867	A2M	C4-N9	-2.36	1.32	1.37
1	A	1524	A2M	C5-N7	-2.36	1.34	1.39
1	A	2365	OMC	C6-C5	2.35	1.40	1.35
1	A	2861	OMC	C6-C5	2.35	1.40	1.35
1	A	4296	PSU	C2-N3	-2.35	1.33	1.37
1	A	2815	A2M	C5-N7	-2.34	1.34	1.39
1	A	4431	PSU	C2-N3	-2.33	1.33	1.37
1	A	4370	OMG	C5-N7	-2.32	1.34	1.39
1	A	4370	OMG	C4-N9	-2.32	1.32	1.38
1	A	3724	A2M	C5-N7	-2.31	1.34	1.39
1	A	1316	OMG	C4-N9	-2.31	1.32	1.38
1	A	4523	A2M	C4-N9	-2.31	1.32	1.37
1	A	3887	OMC	C6-C5	2.30	1.40	1.35
1	A	4196	OMG	C4-N9	-2.30	1.32	1.38
1	A	4431	PSU	C6-C5	2.30	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1871	A2M	C4-N9	-2.29	1.32	1.37
1	A	4689	PSU	C4-N3	-2.28	1.34	1.38
1	A	4220	6MZ	C5-N7	-2.28	1.34	1.39
1	A	398	A2M	C5-C6	2.28	1.47	1.41
1	A	4523	A2M	C5-N7	-2.27	1.34	1.39
1	A	4500	PSU	C2'-C1'	-2.27	1.50	1.53
3	C	69	PSU	C2-N3	-2.27	1.33	1.37
1	A	1677	PSU	C2'-C1'	-2.27	1.50	1.53
1	A	4552	PSU	C2-N3	-2.27	1.33	1.37
1	A	4500	PSU	C4-N3	-2.26	1.34	1.38
1	A	4370	OMG	C5-C4	2.26	1.45	1.38
1	A	4471	PSU	C2-N1	-2.26	1.33	1.36
1	A	1316	OMG	C6-N1	-2.26	1.34	1.38
1	A	4498	OMU	C5-C4	-2.26	1.38	1.43
1	A	5001	PSU	C2-N1	-2.24	1.33	1.36
1	A	2815	A2M	C8-N7	2.24	1.35	1.31
1	A	4306	OMU	C2-N3	-2.23	1.34	1.38
1	A	1683	PSU	C2-N3	-2.23	1.33	1.37
1	A	400	A2M	C5-N7	-2.23	1.34	1.39
1	A	4494	OMG	C5-N7	-2.23	1.34	1.39
1	A	4423	PSU	C2-N3	-2.22	1.33	1.37
1	A	1522	OMG	C5-N7	-2.22	1.34	1.39
1	A	3724	A2M	C4-N9	-2.21	1.32	1.37
1	A	3853	PSU	C2'-C1'	-2.21	1.50	1.53
1	A	2804	OMC	C6-C5	2.21	1.40	1.35
1	A	3869	OMC	C6-C5	2.21	1.40	1.35
1	A	3884	PSU	C2-N3	-2.21	1.33	1.37
1	A	3637	PSU	C4-N3	-2.19	1.34	1.38
1	A	4673	PSU	C4-N3	-2.19	1.34	1.38
1	A	4530	UR3	C6-C5	2.19	1.40	1.35
3	C	75	OMG	C6-N1	-2.17	1.34	1.38
1	A	400	A2M	C4-N9	-2.17	1.32	1.37
1	A	3744	OMG	C5-N7	-2.17	1.34	1.39
1	A	4420	PSU	C4-N3	-2.17	1.34	1.38
3	C	75	OMG	C5-N7	-2.16	1.34	1.39
1	A	4392	OMG	C4-N9	-2.16	1.32	1.38
1	A	4500	PSU	O4'-C4'	-2.16	1.40	1.45
1	A	4494	OMG	C4-N9	-2.16	1.32	1.38
1	A	3637	PSU	C2-N1	-2.16	1.33	1.36
1	A	1340	OMC	C6-C5	2.16	1.40	1.35
1	A	2508	PSU	C2-N3	-2.16	1.33	1.37
1	A	1326	A2M	C4-N9	-2.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	55	PSU	C6-C5	2.15	1.37	1.35
1	A	4623	OMG	C4-N9	-2.14	1.32	1.38
1	A	4623	OMG	C5-N7	-2.14	1.34	1.39
1	A	4227	OMU	C2-N3	-2.14	1.34	1.38
1	A	3867	A2M	C5-C4	2.14	1.43	1.39
1	A	2401	A2M	C4-N9	-2.13	1.32	1.37
1	A	4590	A2M	C8-N7	2.12	1.35	1.31
1	A	3724	A2M	C8-N7	2.12	1.35	1.31
1	A	3729	PSU	O5'-C5'	-2.12	1.39	1.44
1	A	4673	PSU	C2-N3	-2.11	1.33	1.37
1	A	3729	PSU	C2-N3	-2.11	1.33	1.37
1	A	4618	OMG	C5-C4	2.11	1.44	1.38
1	A	4457	PSU	C4-C5	2.10	1.50	1.44
1	A	4628	PSU	C4-N3	-2.09	1.35	1.38
1	A	1534	A2M	C5-C6	2.09	1.46	1.41
1	A	3830	A2M	C4-N9	-2.09	1.33	1.37
1	A	4299	PSU	C2-N1	-2.09	1.33	1.36
1	A	2787	A2M	C5-N7	-2.09	1.35	1.39
1	A	2861	OMC	C5-C4	-2.09	1.38	1.42
3	C	75	OMG	C4-N9	-2.09	1.32	1.38
1	A	4618	OMG	C5-N7	-2.07	1.35	1.39
1	A	3830	A2M	C8-N7	2.07	1.35	1.31
1	A	4227	OMU	C6-C5	2.06	1.39	1.35
1	A	3825	A2M	C4-N9	-2.06	1.33	1.37
1	A	4637	OMG	C4-N9	-2.06	1.32	1.38
1	A	2787	A2M	C4-N9	-2.06	1.33	1.37
1	A	3785	A2M	C4-N9	-2.05	1.33	1.37
1	A	3627	OMG	C5-N7	-2.05	1.35	1.39
1	A	1862	PSU	C2-N1	-2.04	1.34	1.36
1	A	4628	PSU	C2-N1	-2.04	1.34	1.36
1	A	2815	A2M	C4-N9	-2.04	1.33	1.37
1	A	1322	1MA	C5-C4	2.04	1.44	1.38
1	A	1792	PSU	O5'-C5'	-2.03	1.39	1.44
1	A	1524	A2M	C5-C6	2.03	1.46	1.41
1	A	1522	OMG	C6-N1	-2.03	1.35	1.38
1	A	3899	OMG	C6-N1	-2.03	1.35	1.38
1	A	1522	OMG	C4-N9	-2.02	1.32	1.38
1	A	1316	OMG	C5-N7	-2.02	1.35	1.39
1	A	2401	A2M	C5-N7	-2.02	1.35	1.39
1	A	4576	PSU	C2-N3	-2.01	1.34	1.37
1	A	4361	PSU	C6-N1	-2.01	1.32	1.36
1	A	3899	OMG	C5-N7	-2.00	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3853	PSU	C2-N3	-2.00	1.34	1.37

All (700) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4353	PSU	N1-C2-N3	7.77	123.94	115.13
1	A	1862	PSU	N1-C2-N3	7.45	123.57	115.13
1	A	5001	PSU	N1-C2-N3	7.41	123.53	115.13
1	A	4628	PSU	N1-C2-N3	7.17	123.26	115.13
1	A	4521	PSU	N1-C2-N3	7.15	123.23	115.13
1	A	3637	PSU	N1-C2-N3	7.14	123.22	115.13
1	A	1536	PSU	N1-C2-N3	6.92	122.97	115.13
1	A	1683	PSU	N1-C2-N3	6.83	122.87	115.13
1	A	4500	PSU	N1-C2-N3	6.80	122.83	115.13
1	A	3851	PSU	N1-C2-N3	6.73	122.75	115.13
3	C	69	PSU	N1-C2-N3	6.65	122.66	115.13
1	A	4442	PSU	N1-C2-N3	6.63	122.64	115.13
1	A	1677	PSU	N1-C2-N3	6.60	122.61	115.13
1	A	4972	PSU	N1-C2-N3	6.59	122.60	115.13
1	A	3844	PSU	N1-C2-N3	6.52	122.51	115.13
1	A	4403	PSU	N1-C2-N3	6.50	122.49	115.13
1	A	4312	PSU	N1-C2-N3	6.39	122.36	115.13
1	A	4689	PSU	N1-C2-N3	6.37	122.34	115.13
1	A	2787	A2M	C5-C4-N3	-6.33	118.49	126.75
1	A	1782	PSU	N1-C2-N3	6.29	122.26	115.13
1	A	3884	PSU	N1-C2-N3	6.27	122.23	115.13
1	A	3715	PSU	N1-C2-N3	6.26	122.22	115.13
1	A	4361	PSU	N1-C2-N3	6.25	122.21	115.13
1	A	3853	PSU	N1-C2-N3	6.24	122.20	115.13
1	A	4299	PSU	N1-C2-N3	6.23	122.19	115.13
1	A	4457	PSU	N1-C2-N3	6.22	122.18	115.13
1	A	4293	PSU	N1-C2-N3	6.18	122.13	115.13
1	A	2876	OMG	C5-C4-N3	-6.16	118.47	128.46
1	A	4431	PSU	N1-C2-N3	6.12	122.07	115.13
1	A	1744	PSU	N1-C2-N3	6.12	122.06	115.13
1	A	4296	PSU	N1-C2-N3	6.11	122.05	115.13
1	A	1582	PSU	N1-C2-N3	6.11	122.05	115.13
1	A	398	A2M	C5-C4-N3	-6.10	118.79	126.75
1	A	4493	PSU	N1-C2-N3	6.05	121.99	115.13
1	A	4471	PSU	N1-C2-N3	6.04	121.98	115.13
1	A	3639	PSU	C6-C5-C4	-6.03	113.98	118.20
1	A	4530	UR3	C4-N3-C2	-6.01	118.90	124.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4423	PSU	N1-C2-N3	6.00	121.93	115.13
1	A	4620	OMU	N3-C2-N1	5.99	122.85	114.89
1	A	4576	PSU	N1-C2-N3	5.97	121.89	115.13
1	A	1860	PSU	N1-C2-N3	5.90	121.82	115.13
1	A	1862	PSU	C4-N3-C2	-5.88	117.87	126.34
1	A	1792	PSU	N1-C2-N3	5.85	121.75	115.13
1	A	3729	PSU	N1-C2-N3	5.83	121.73	115.13
1	A	3785	A2M	O4'-C1'-N9	5.80	119.49	108.06
1	A	1781	PSU	N1-C2-N3	5.79	121.69	115.13
1	A	3695	PSU	N1-C2-N3	5.77	121.67	115.13
1	A	4532	PSU	N1-C2-N3	5.76	121.66	115.13
1	A	4579	PSU	N1-C2-N3	5.74	121.63	115.13
1	A	4196	OMG	C5-C4-N3	-5.69	119.22	128.46
1	A	4498	OMU	N3-C2-N1	5.65	122.39	114.89
1	A	2508	PSU	N1-C2-N3	5.63	121.51	115.13
1	A	4499	OMG	C5-C4-N3	-5.63	119.33	128.46
1	A	2632	PSU	N1-C2-N3	5.60	121.48	115.13
1	A	4494	OMG	C5-C4-N3	-5.58	119.41	128.46
3	C	55	PSU	N1-C2-N3	5.56	121.43	115.13
1	A	4420	PSU	N1-C2-N3	5.54	121.41	115.13
1	A	2424	OMG	C5-C4-N3	-5.53	119.50	128.46
1	A	1677	PSU	O2'-C2'-C1'	-5.51	98.09	111.23
1	A	4552	PSU	N1-C2-N3	5.48	121.34	115.13
1	A	4552	PSU	C6-C5-C4	-5.45	114.39	118.20
1	A	4637	OMG	C5-C4-N3	-5.44	119.64	128.46
1	A	3724	A2M	C5-C4-N3	-5.44	119.66	126.75
1	A	3920	PSU	N1-C2-N3	5.42	121.28	115.13
1	A	5010	PSU	N1-C2-N3	5.39	121.24	115.13
1	A	4620	OMU	C4-N3-C2	-5.38	119.48	126.58
1	A	4673	PSU	N1-C2-N3	5.31	121.15	115.13
1	A	4196	OMG	C2-N3-C4	5.30	121.74	112.30
1	A	4353	PSU	C4-N3-C2	-5.29	118.72	126.34
1	A	3718	A2M	C5-C4-N3	-5.26	119.88	126.75
1	A	4370	OMG	C5-C4-N3	-5.26	119.93	128.46
1	A	3830	A2M	C5-C4-N3	-5.19	119.98	126.75
1	A	2815	A2M	C5-C4-N3	-5.18	119.99	126.75
1	A	5001	PSU	C4-N3-C2	-5.17	118.89	126.34
1	A	2351	OMC	O2'-C2'-C1'	-5.16	99.01	109.08
1	A	3639	PSU	N1-C2-N3	5.16	120.98	115.13
1	A	3899	OMG	C2-N3-C4	5.16	121.49	112.30
1	A	2839	PSU	N1-C2-N3	5.13	120.94	115.13
1	A	3818	OMU	C4-N3-C2	-5.12	119.82	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4972	PSU	C4-N3-C2	-5.10	118.99	126.34
1	A	2632	PSU	C6-C5-C4	-5.08	114.65	118.20
1	A	4499	OMG	C2-N3-C4	5.07	121.33	112.30
1	A	3792	OMG	C5-C4-N3	-5.05	120.27	128.46
1	A	4689	PSU	O2-C2-N1	-5.05	117.23	122.79
3	C	75	OMG	C5-C4-N3	-5.04	120.29	128.46
1	A	4306	OMU	N3-C2-N1	5.00	121.53	114.89
1	A	4431	PSU	C4-N3-C2	-4.99	119.15	126.34
1	A	4227	OMU	C4-N3-C2	-4.96	120.03	126.58
1	A	1536	PSU	O2-C2-N1	-4.96	117.33	122.79
1	A	4299	PSU	C6-C5-C4	-4.96	114.73	118.20
1	A	3825	A2M	C5-C4-N3	-4.96	120.28	126.75
1	A	4637	OMG	C2-N3-C4	4.92	121.07	112.30
1	A	3853	PSU	C4-N3-C2	-4.91	119.26	126.34
1	A	1792	PSU	C6-C5-C4	-4.91	114.77	118.20
1	A	4590	A2M	N3-C2-N1	-4.91	120.93	128.60
1	A	4571	A2M	C5-C4-N3	-4.90	120.36	126.75
1	A	4498	OMU	C4-N3-C2	-4.90	120.12	126.58
1	A	4523	A2M	C5-C4-N3	-4.89	120.37	126.75
1	A	3785	A2M	N3-C4-N9	4.89	135.13	127.08
1	A	3853	PSU	C6-C5-C4	-4.88	114.78	118.20
1	A	2787	A2M	N3-C4-N9	4.87	135.11	127.08
1	A	2876	OMG	C2-N3-C4	4.87	120.98	112.30
1	A	3785	A2M	C5-C4-N3	-4.86	120.40	126.75
1	A	400	A2M	C5-C4-N3	-4.86	120.41	126.75
1	A	4370	OMG	C2-N3-C4	4.85	120.94	112.30
1	A	4293	PSU	C4-N3-C2	-4.85	119.35	126.34
1	A	2837	OMU	N3-C2-N1	4.82	121.29	114.89
1	A	4457	PSU	C4-N3-C2	-4.82	119.40	126.34
1	A	4523	A2M	C4-N9-C8	4.78	110.91	105.73
1	A	2876	OMG	N9-C4-N3	4.78	135.53	125.94
1	A	4392	OMG	C5-C4-N3	-4.77	120.73	128.46
1	A	1326	A2M	N3-C2-N1	-4.76	121.16	128.60
1	A	3844	PSU	C4-N3-C2	-4.75	119.49	126.34
1	A	1792	PSU	C4-N3-C2	-4.74	119.51	126.34
1	A	4493	PSU	C6-C5-C4	-4.74	114.89	118.20
1	A	4312	PSU	O2-C2-N1	-4.73	117.58	122.79
1	A	4523	A2M	N3-C4-N9	4.73	134.87	127.08
1	A	4623	OMG	C5-C4-N3	-4.73	120.79	128.46
1	A	1860	PSU	O2-C2-N1	-4.71	117.61	122.79
1	A	4228	OMG	C5-C4-N3	-4.70	120.84	128.46
1	A	3899	OMG	C5-C4-N3	-4.69	120.85	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4493	PSU	C4-N3-C2	-4.69	119.59	126.34
1	A	1683	PSU	C4-N3-C2	-4.68	119.60	126.34
1	A	4403	PSU	C4-N3-C2	-4.67	119.61	126.34
3	C	75	OMG	C2-N3-C4	4.66	120.61	112.30
1	A	4220	6MZ	C5-C4-N3	-4.65	120.68	126.75
1	A	4500	PSU	O2-C2-N1	-4.65	117.67	122.79
1	A	2401	A2M	C5-C4-N3	-4.63	120.71	126.75
1	A	1744	PSU	O2-C2-N1	-4.62	117.71	122.79
1	A	1625	OMG	C5-C4-N3	-4.61	120.98	128.46
1	A	398	A2M	N3-C4-N9	4.60	134.66	127.08
1	A	1522	OMG	C2'-C1'-N9	-4.59	105.32	114.22
1	A	3627	OMG	C5-C4-N3	-4.54	121.10	128.46
1	A	3925	OMU	N3-C2-N1	4.54	120.91	114.89
1	A	4457	PSU	C6-C5-C4	-4.52	115.03	118.20
1	A	4532	PSU	C6-C5-C4	-4.51	115.05	118.20
1	A	3884	PSU	C4-N3-C2	-4.50	119.86	126.34
1	A	1522	OMG	C5-C4-N3	-4.48	121.19	128.46
1	A	4361	PSU	C4-N3-C2	-4.47	119.90	126.34
1	A	3724	A2M	N3-C4-N9	4.47	134.44	127.08
1	A	3851	PSU	O2-C2-N1	-4.47	117.87	122.79
1	A	1781	PSU	C4-N3-C2	-4.46	119.91	126.34
1	A	4576	PSU	O2-C2-N1	-4.46	117.88	122.79
1	A	4196	OMG	N9-C4-N3	4.45	134.88	125.94
1	A	2415	OMU	C4-N3-C2	-4.44	120.72	126.58
1	A	4628	PSU	C4-N3-C2	-4.44	119.94	126.34
1	A	4228	OMG	C2-N3-C4	4.43	120.19	112.30
1	A	3715	PSU	C4-N3-C2	-4.42	119.97	126.34
1	A	3785	A2M	C4-N9-C8	4.42	110.52	105.73
1	A	4521	PSU	C4-N3-C2	-4.42	119.97	126.34
1	A	4628	PSU	O2-C2-N1	-4.42	117.93	122.79
1	A	4523	A2M	N3-C2-N1	-4.41	121.70	128.60
1	A	4689	PSU	C4-N3-C2	-4.41	119.99	126.34
1	A	4392	OMG	C2-N3-C4	4.40	120.14	112.30
1	A	1316	OMG	C5-C4-N3	-4.40	121.33	128.46
1	A	3744	OMG	C5-C4-N3	-4.40	121.33	128.46
1	A	3920	PSU	O2-C2-N1	-4.39	117.96	122.79
1	A	4637	OMG	N9-C4-N3	4.38	134.74	125.94
1	A	4442	PSU	C4-N3-C2	-4.38	120.03	126.34
1	A	2837	OMU	C4-N3-C2	-4.38	120.81	126.58
1	A	4227	OMU	N3-C2-N1	4.37	120.69	114.89
1	A	4498	OMU	O4-C4-C5	-4.36	117.49	125.16
1	A	3718	A2M	N3-C4-N9	4.35	134.25	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4220	6MZ	N3-C4-N9	4.34	134.23	127.08
3	C	69	PSU	C4-N3-C2	-4.32	120.11	126.34
1	A	4579	PSU	C6-C5-C4	-4.32	115.18	118.20
1	A	4431	PSU	O2-C2-N1	-4.31	118.05	122.79
1	A	4499	OMG	N9-C4-N3	4.29	134.55	125.94
1	A	2815	A2M	N3-C4-N9	4.29	134.15	127.08
1	A	3867	A2M	C5-C4-N3	-4.29	121.16	126.75
1	A	4494	OMG	C2-N3-C4	4.28	119.92	112.30
1	A	4590	A2M	C5-C4-N3	-4.26	121.19	126.75
1	A	1524	A2M	C5-C4-N3	-4.25	121.20	126.75
1	A	4299	PSU	C4-N3-C2	-4.25	120.22	126.34
1	A	3818	OMU	N3-C2-N1	4.25	120.53	114.89
1	A	2363	A2M	C5-C4-N3	-4.25	121.21	126.75
1	A	2401	A2M	N3-C2-N1	-4.24	121.97	128.60
1	A	3818	OMU	C5-C4-N3	4.23	121.17	114.84
1	A	4618	OMG	C2-N3-C4	4.23	119.84	112.30
1	A	3792	OMG	C2-N3-C4	4.23	119.84	112.30
1	A	4673	PSU	C4-N3-C2	-4.23	120.25	126.34
1	A	3925	OMU	O2-C2-N1	-4.22	117.18	122.79
1	A	5001	PSU	O2-C2-N1	-4.22	118.15	122.79
1	A	4498	OMU	O2-C2-N1	-4.21	117.18	122.79
1	A	4576	PSU	C4-N3-C2	-4.21	120.28	126.34
1	A	1326	A2M	C5-C4-N3	-4.20	121.27	126.75
1	A	4618	OMG	C5-C4-N3	-4.20	121.65	128.46
1	A	4431	PSU	C6-C5-C4	-4.19	115.27	118.20
1	A	4227	OMU	C5-C4-N3	4.19	121.11	114.84
1	A	1326	A2M	C2-N1-C6	4.19	125.96	118.77
1	A	4392	OMG	C6-C5-N7	4.19	138.03	130.25
1	A	2632	PSU	C4-N3-C2	-4.18	120.31	126.34
1	A	2363	A2M	N3-C4-N9	4.18	133.97	127.08
1	A	3637	PSU	O2-C2-N1	-4.18	118.19	122.79
1	A	1536	PSU	C4-N3-C2	-4.17	120.34	126.34
1	A	1871	A2M	N3-C2-N1	-4.16	122.09	128.60
1	A	1744	PSU	C4-N3-C2	-4.16	120.34	126.34
1	A	4471	PSU	C4-N3-C2	-4.16	120.34	126.34
1	A	2424	OMG	N9-C4-N3	4.16	134.29	125.94
1	A	1862	PSU	O2-C2-N1	-4.16	118.21	122.79
1	A	2415	OMU	N3-C2-N1	4.15	120.40	114.89
1	A	2364	OMG	C5-C4-N3	-4.14	121.74	128.46
1	A	3899	OMG	N9-C4-N3	4.14	134.24	125.94
1	A	1677	PSU	O2-C2-N1	-4.13	118.25	122.79
1	A	3695	PSU	C4-N3-C2	-4.13	120.39	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4571	A2M	N3-C4-N9	4.12	133.88	127.08
1	A	4552	PSU	C4-N3-C2	-4.11	120.42	126.34
1	A	1782	PSU	C4-N3-C2	-4.09	120.44	126.34
1	A	400	A2M	N3-C2-N1	-4.09	122.20	128.60
1	A	3851	PSU	C4-N3-C2	-4.09	120.45	126.34
1	A	1582	PSU	C4-N3-C2	-4.09	120.45	126.34
1	A	2363	A2M	N3-C2-N1	-4.09	122.21	128.60
3	C	75	OMG	N9-C4-N3	4.08	134.13	125.94
1	A	4618	OMG	C6-C5-N7	4.08	137.83	130.25
1	A	4620	OMU	C5-C4-N3	4.07	120.94	114.84
1	A	4220	6MZ	N1-C2-N3	-4.07	122.23	128.60
1	A	4579	PSU	O2-C2-N1	-4.07	118.31	122.79
1	A	1522	OMG	C2-N3-C4	4.05	119.52	112.30
1	A	3627	OMG	C2'-C1'-N9	-4.05	106.36	114.22
1	A	4423	PSU	C4-N3-C2	-4.04	120.51	126.34
1	A	3639	PSU	C4-N3-C2	-4.03	120.53	126.34
1	A	1534	A2M	C5-C4-N3	-4.03	121.49	126.75
1	A	3744	OMG	C2-N3-C4	4.02	119.47	112.30
1	A	4228	OMG	C6-C5-N7	4.01	137.71	130.25
1	A	2787	A2M	C4-C5-N7	-4.01	105.73	110.62
1	A	1871	A2M	C2-N1-C6	4.01	125.64	118.77
1	A	3867	A2M	N3-C2-N1	-4.00	122.35	128.60
1	A	4220	6MZ	C9-N6-C6	-4.00	119.43	122.87
1	A	4494	OMG	N9-C4-N3	3.99	133.96	125.94
1	A	2401	A2M	N3-C4-N9	3.99	133.66	127.08
1	A	3818	OMU	C2'-C1'-N1	-3.99	106.48	114.22
1	A	3724	A2M	N3-C2-N1	-3.98	122.37	128.60
1	A	4220	6MZ	C4-N9-C8	3.98	110.04	105.73
1	A	2363	A2M	O2'-C2'-C1'	-3.97	101.33	109.08
1	A	4972	PSU	O2-C2-N1	-3.97	118.42	122.79
1	A	4532	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A	4623	OMG	C2'-C1'-N9	-3.96	106.53	114.22
1	A	5010	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A	1534	A2M	N3-C2-N1	-3.96	122.42	128.60
1	A	4370	OMG	N9-C4-N3	3.95	133.87	125.94
1	A	1316	OMG	C2-N3-C4	3.94	119.32	112.30
1	A	1625	OMG	N9-C4-N3	3.94	133.85	125.94
3	C	55	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A	3792	OMG	N9-C4-N3	3.93	133.84	125.94
1	A	1322	1MA	C2-N3-C4	3.92	120.12	112.41
1	A	1860	PSU	C6-C5-C4	-3.92	115.46	118.20
1	A	1316	OMG	N9-C4-N3	3.92	133.81	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4523	A2M	N9-C8-N7	-3.91	108.56	113.91
1	A	4196	OMG	C6-C5-N7	3.91	137.51	130.25
1	A	2837	OMU	C5-C4-N3	3.90	120.67	114.84
1	A	4623	OMG	C2-N3-C4	3.89	119.23	112.30
1	A	4457	PSU	O2-C2-N1	-3.88	118.52	122.79
1	A	3637	PSU	C6-N1-C2	-3.88	118.71	122.68
1	A	3925	OMU	C4-N3-C2	-3.88	121.46	126.58
1	A	400	A2M	N3-C4-N9	3.88	133.47	127.08
1	A	4312	PSU	C4-N3-C2	-3.87	120.76	126.34
1	A	1322	1MA	C5-C4-N3	-3.87	121.48	127.26
1	A	4576	PSU	C6-C5-C4	-3.87	115.49	118.20
1	A	3627	OMG	C6-C5-N7	3.84	137.39	130.25
1	A	3627	OMG	C2-N3-C4	3.84	119.14	112.30
1	A	4296	PSU	O2-C2-N1	-3.84	118.57	122.79
1	A	4579	PSU	C4-N3-C2	-3.83	120.81	126.34
1	A	4361	PSU	O2-C2-N1	-3.83	118.57	122.79
1	A	3744	OMG	N9-C4-N3	3.82	133.60	125.94
1	A	3887	OMC	C2'-C1'-N1	-3.81	106.83	114.22
1	A	4296	PSU	C4-N3-C2	-3.80	120.87	126.34
1	A	2787	A2M	C5-N7-C8	3.79	108.89	103.51
1	A	3920	PSU	C4-N3-C2	-3.78	120.89	126.34
1	A	4500	PSU	C4-N3-C2	-3.78	120.89	126.34
1	A	3867	A2M	C4-N9-C8	3.78	109.83	105.73
1	A	1683	PSU	O2-C2-N1	-3.77	118.64	122.79
1	A	3830	A2M	C2'-C1'-N9	-3.76	107.20	113.53
1	A	3724	A2M	C2-N3-C4	3.75	120.62	111.75
1	A	3825	A2M	N3-C4-N9	3.75	133.25	127.08
1	A	3867	A2M	N3-C4-N9	3.74	133.25	127.08
1	A	2839	PSU	O2-C2-N1	-3.74	118.67	122.79
1	A	2508	PSU	C4-N3-C2	-3.73	120.96	126.34
1	A	4420	PSU	C3'-C2'-C1'	3.73	105.98	101.64
1	A	2787	A2M	C2-N3-C4	3.73	120.56	111.75
1	A	4420	PSU	C4-N3-C2	-3.72	120.97	126.34
1	A	1625	OMG	C2-N3-C4	3.72	118.93	112.30
1	A	3718	A2M	C2'-C1'-N9	-3.71	107.29	113.53
1	A	398	A2M	N3-C2-N1	-3.71	122.81	128.60
1	A	3729	PSU	C4-N3-C2	-3.70	121.01	126.34
1	A	3899	OMG	C6-C5-N7	3.67	137.08	130.25
1	A	4521	PSU	C6-C5-C4	-3.67	115.63	118.20
1	A	2424	OMG	C2-N3-C4	3.66	118.81	112.30
1	A	4523	A2M	C2-N3-C4	3.65	120.39	111.75
1	A	2815	A2M	N3-C2-N1	-3.64	122.90	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3729	PSU	O2-C2-N1	-3.64	118.78	122.79
1	A	2363	A2M	C4-N9-C8	3.63	109.67	105.73
1	A	3853	PSU	O2-C2-N1	-3.62	118.81	122.79
1	A	1524	A2M	N3-C4-N9	3.61	133.03	127.08
1	A	3851	PSU	C6-C5-C4	-3.61	115.67	118.20
1	A	398	A2M	C2-N3-C4	3.60	120.27	111.75
1	A	3920	PSU	C6-C5-C4	-3.60	115.68	118.20
1	A	4590	A2M	C2-N3-C4	3.58	120.20	111.75
1	A	2401	A2M	C4-N9-C8	3.57	109.60	105.73
1	A	4220	6MZ	C2-N3-C4	3.57	120.18	111.75
1	A	4228	OMG	N9-C4-N3	3.56	133.09	125.94
1	A	4972	PSU	C6-C5-C4	-3.55	115.71	118.20
1	A	3925	OMU	C5-C4-N3	3.55	120.14	114.84
1	A	398	A2M	C4-C5-N7	-3.54	106.31	110.62
1	A	1781	PSU	C6-C5-C4	-3.53	115.73	118.20
1	A	3718	A2M	N3-C2-N1	-3.53	123.08	128.60
1	A	2787	A2M	N3-C2-N1	-3.53	123.09	128.60
1	A	2415	OMU	C5-C4-N3	3.53	120.11	114.84
1	A	4392	OMG	N9-C4-N3	3.51	132.99	125.94
1	A	4499	OMG	C6-C5-N7	3.51	136.78	130.25
1	A	4571	A2M	C2-N3-C4	3.51	120.04	111.75
1	A	4521	PSU	O2-C2-N1	-3.51	118.93	122.79
1	A	1522	OMG	N9-C4-N3	3.50	132.97	125.94
1	A	5010	PSU	O2-C2-N1	-3.50	118.94	122.79
1	A	4299	PSU	O2-C2-N1	-3.49	118.94	122.79
1	A	3844	PSU	C6-C5-C4	-3.49	115.76	118.20
1	A	1524	A2M	N3-C2-N1	-3.49	123.14	128.60
1	A	4590	A2M	C2-N1-C6	3.49	124.75	118.77
1	A	3718	A2M	C2-N3-C4	3.49	119.98	111.75
1	A	4571	A2M	N3-C2-N1	-3.48	123.15	128.60
1	A	2401	A2M	C2-N1-C6	3.48	124.74	118.77
1	A	3844	PSU	O2-C2-N1	-3.47	118.97	122.79
1	A	1582	PSU	C6-C5-C4	-3.47	115.77	118.20
1	A	3637	PSU	C4-N3-C2	-3.46	121.35	126.34
1	A	2837	OMU	O2-C2-N1	-3.46	118.19	122.79
1	A	1326	A2M	N3-C4-N9	3.45	132.77	127.08
1	A	4306	OMU	C4-N3-C2	-3.44	122.04	126.58
1	A	3701	OMC	O3'-C3'-C4'	-3.42	101.15	111.05
1	A	4623	OMG	N9-C4-N3	3.41	132.78	125.94
1	A	3785	A2M	N9-C8-N7	-3.40	109.26	113.91
1	A	400	A2M	C2-N3-C4	3.40	119.77	111.75
1	A	4423	PSU	O2-C2-N1	-3.37	119.08	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4620	OMU	O2-C2-N1	-3.37	118.31	122.79
1	A	2839	PSU	C4-N3-C2	-3.36	121.49	126.34
1	A	2815	A2M	C2-N3-C4	3.36	119.70	111.75
1	A	1534	A2M	N3-C4-N9	3.35	132.60	127.08
1	A	2364	OMG	C2-N3-C4	3.35	118.27	112.30
1	A	3627	OMG	N9-C4-N3	3.34	132.66	125.94
1	A	1677	PSU	C4-N3-C2	-3.34	121.53	126.34
1	A	3830	A2M	N3-C2-N1	-3.34	123.39	128.60
1	A	1860	PSU	C4-N3-C2	-3.33	121.54	126.34
1	A	4532	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A	4447	5MC	C5-C4-N3	-3.32	118.09	121.67
1	A	400	A2M	C2-N1-C6	3.31	124.45	118.77
1	A	398	A2M	C5-N7-C8	3.30	108.20	103.51
1	A	3715	PSU	O2-C2-N1	-3.29	119.16	122.79
1	A	2363	A2M	C2-N1-C6	3.29	124.42	118.77
1	A	2787	A2M	O4'-C1'-C2'	-3.29	100.80	106.57
1	A	1625	OMG	O6-C6-C5	-3.29	117.88	126.60
1	A	3830	A2M	C2-N1-C6	3.28	124.40	118.77
3	C	75	OMG	C6-C5-N7	3.28	136.35	130.25
1	A	4498	OMU	C5-C4-N3	3.27	119.74	114.84
1	A	3830	A2M	N3-C4-N9	3.27	132.47	127.08
1	A	4447	5MC	C5-C6-N1	-3.25	119.99	123.34
1	A	3785	A2M	C5-N7-C8	3.25	108.13	103.51
1	A	1524	A2M	C4-N9-C8	3.25	109.25	105.73
1	A	1781	PSU	O2-C2-N1	-3.25	119.21	122.79
1	A	1871	A2M	C5-C4-N3	-3.25	122.52	126.75
1	A	4420	PSU	O2-C2-N1	-3.24	119.23	122.79
1	A	4637	OMG	C6-C5-N7	3.24	136.26	130.25
1	A	4590	A2M	N3-C4-N9	3.23	132.41	127.08
1	A	4618	OMG	N9-C4-N3	3.23	132.43	125.94
1	A	2415	OMU	O4-C4-C5	-3.23	119.48	125.16
1	A	4228	OMG	O3'-C3'-C2'	-3.22	102.01	111.17
1	A	2401	A2M	C4-C5-N7	-3.21	106.71	110.62
1	A	1524	A2M	C2-N3-C4	3.21	119.33	111.75
1	A	1782	PSU	C6-C5-C4	-3.20	115.96	118.20
1	A	2364	OMG	C6-C5-N7	3.19	136.19	130.25
3	C	69	PSU	O2-C2-N1	-3.19	119.28	122.79
1	A	4523	A2M	C5-N7-C8	3.19	108.04	103.51
3	C	55	PSU	C6-C5-C4	-3.18	115.97	118.20
1	A	3867	A2M	C2-N3-C4	3.18	119.26	111.75
3	C	55	PSU	O2-C2-N1	-3.14	119.33	122.79
1	A	4442	PSU	O2-C2-N1	-3.14	119.34	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3785	A2M	C2'-C1'-N9	-3.14	108.25	113.53
1	A	4306	OMU	O2-C2-N1	-3.14	118.62	122.79
1	A	1534	A2M	C2-N3-C4	3.13	119.14	111.75
1	A	1683	PSU	C6-C5-C4	-3.12	116.02	118.20
1	A	1316	OMG	C6-C5-N7	3.12	136.05	130.25
1	A	4552	PSU	O2-C2-N1	-3.12	119.36	122.79
1	A	2815	A2M	C4-N9-C8	3.12	109.11	105.73
1	A	2401	A2M	C2-N3-C4	3.10	119.07	111.75
1	A	4353	PSU	O2-C2-N1	-3.09	119.39	122.79
1	A	3701	OMC	O2-C2-N3	-3.08	117.31	122.33
1	A	3825	A2M	N3-C2-N1	-3.08	123.78	128.60
1	A	4361	PSU	C6-C5-C4	-3.07	116.05	118.20
1	A	3818	OMU	O4-C4-C5	-3.06	119.78	125.16
1	A	4370	OMG	C6-C5-N7	3.06	135.93	130.25
1	A	4493	PSU	O2-C2-N1	-3.06	119.43	122.79
1	A	4523	A2M	C2'-C1'-N9	-3.05	108.39	113.53
1	A	4431	PSU	O4-C4-C5	-3.04	116.09	124.05
1	A	4403	PSU	C6-C5-C4	-3.04	116.07	118.20
1	A	3925	OMU	O4-C4-C5	-3.03	119.83	125.16
1	A	1534	A2M	C4-N9-C8	3.03	109.01	105.73
1	A	3744	OMG	C6-C5-N7	3.02	135.87	130.25
1	A	2787	A2M	C4-N9-C8	3.02	109.00	105.73
1	A	1322	1MA	N9-C4-N3	3.01	133.95	126.94
1	A	4306	OMU	C5-C4-N3	3.01	119.34	114.84
1	A	4571	A2M	C4-N9-C8	3.01	108.98	105.73
1	A	3899	OMG	O6-C6-C5	-3.00	118.63	126.60
1	A	1871	A2M	C2'-C1'-N9	-3.00	108.48	113.53
1	A	1524	A2M	N6-C6-N1	3.00	124.92	118.35
1	A	4447	5MC	O2-C2-N3	-2.97	117.50	122.33
1	A	3782	5MC	CM5-C5-C6	-2.97	118.89	122.85
1	A	3884	PSU	O2-C2-N1	-2.96	119.53	122.79
1	A	2364	OMG	N9-C4-N3	2.96	131.89	125.94
1	A	4499	OMG	O6-C6-C5	-2.95	118.76	126.60
1	A	4532	PSU	C2'-C3'-C4'	-2.95	96.90	102.64
1	A	3785	A2M	O4'-C4'-C3'	2.95	110.95	105.11
1	A	2401	A2M	C5-N7-C8	2.94	107.69	103.51
1	A	2363	A2M	C2-N3-C4	2.94	118.69	111.75
1	A	2837	OMU	O4-C4-C5	-2.93	120.00	125.16
1	A	1582	PSU	O2-C2-N3	-2.93	116.30	121.82
1	A	2837	OMU	C2'-C1'-N1	-2.92	108.55	114.22
1	A	3785	A2M	O4'-C4'-C5'	-2.92	99.77	109.37
1	A	1522	OMG	C6-C5-N7	2.92	135.67	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4532	PSU	O4'-C1'-C2'	-2.91	101.04	105.14
1	A	1322	1MA	N1-C2-N3	-2.91	122.54	126.00
1	A	4590	A2M	C4-N9-C8	2.91	108.88	105.73
1	A	4471	PSU	C6-C5-C4	-2.90	116.17	118.20
1	A	3782	5MC	C5-C6-N1	-2.89	120.36	123.34
1	A	2876	OMG	C6-C5-N7	2.89	135.62	130.25
1	A	2787	A2M	N9-C8-N7	-2.89	109.97	113.91
1	A	4530	UR3	C6-N1-C2	-2.89	119.20	121.79
1	A	1326	A2M	C2-N3-C4	2.89	118.57	111.75
1	A	1536	PSU	C6-N1-C2	-2.88	119.74	122.68
1	A	4392	OMG	C4-C5-N7	-2.88	106.16	110.72
1	A	3792	OMG	C6-C5-N7	2.85	135.55	130.25
1	A	3825	A2M	C5-N7-C8	2.85	107.56	103.51
1	A	3808	OMC	O2-C2-N3	-2.83	117.73	122.33
1	A	4494	OMG	C6-C5-N7	2.82	135.49	130.25
1	A	4228	OMG	O6-C6-C5	-2.82	119.12	126.60
1	A	4312	PSU	C6-C5-C4	-2.82	116.23	118.20
1	A	4220	6MZ	N9-C8-N7	-2.81	110.07	113.91
1	A	3724	A2M	C4-N9-C8	2.81	108.77	105.73
1	A	3899	OMG	C2'-C1'-N9	-2.81	108.77	114.22
1	A	3695	PSU	O2-C2-N1	-2.78	119.72	122.79
1	A	4590	A2M	N9-C8-N7	-2.78	110.11	113.91
1	A	4623	OMG	C6-C5-N7	2.78	135.41	130.25
1	A	2508	PSU	O2-C2-N1	-2.78	119.73	122.79
1	A	400	A2M	C4-C5-N7	-2.77	107.24	110.62
1	A	4420	PSU	C6-C5-C4	-2.77	116.26	118.20
1	A	1871	A2M	C4-N9-C8	2.77	108.73	105.73
1	A	3830	A2M	C4-C5-N7	-2.77	107.25	110.62
1	A	1625	OMG	C6-C5-N7	2.77	135.40	130.25
1	A	3867	A2M	N9-C8-N7	-2.77	110.13	113.91
1	A	398	A2M	C2-N1-C6	2.77	123.51	118.77
1	A	2365	OMC	C2'-C1'-N1	-2.76	108.86	114.22
1	A	4196	OMG	C5-C6-N1	2.76	120.20	113.19
1	A	3785	A2M	N3-C2-N1	-2.76	124.29	128.60
1	A	2364	OMG	O6-C6-C5	-2.76	119.29	126.60
1	A	4353	PSU	O2-C2-N3	-2.75	116.63	121.82
3	C	69	PSU	O2'-C2'-C1'	-2.74	104.69	111.23
1	A	4552	PSU	O4-C4-C5	-2.74	116.88	124.05
1	A	3825	A2M	C4-C5-N7	-2.74	107.28	110.62
1	A	3825	A2M	C2-N3-C4	2.74	118.22	111.75
1	A	1534	A2M	C4-C5-N7	-2.73	107.29	110.62
1	A	1677	PSU	C6-N1-C2	-2.73	119.89	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1326	A2M	C5-N7-C8	2.73	107.39	103.51
3	C	75	OMG	O6-C6-C5	-2.73	119.36	126.60
1	A	1871	A2M	C2-N3-C4	2.73	118.20	111.75
1	A	3830	A2M	C2-N3-C4	2.73	118.19	111.75
1	A	2815	A2M	N9-C8-N7	-2.73	110.19	113.91
1	A	1316	OMG	C2'-C1'-N9	-2.72	108.94	114.22
1	A	4370	OMG	C2'-C1'-N9	-2.72	108.94	114.22
1	A	4972	PSU	O4-C4-C5	-2.72	116.93	124.05
1	A	4620	OMU	O4-C4-C5	-2.72	120.38	125.16
1	A	4552	PSU	C2'-C3'-C4'	-2.72	97.37	102.64
1	A	1871	A2M	N3-C4-N9	2.71	131.55	127.08
1	A	1524	A2M	C5-C6-N6	-2.71	117.54	123.43
1	A	2815	A2M	C5-N7-C8	2.70	107.35	103.51
1	A	4972	PSU	C3'-C2'-C1'	2.70	104.78	101.64
1	A	1782	PSU	O2-C2-N1	-2.69	119.82	122.79
1	A	4590	A2M	C6-C5-N7	2.69	137.04	132.02
1	A	3695	PSU	C6-C5-C4	-2.69	116.32	118.20
1	A	2508	PSU	C6-C5-C4	-2.69	116.32	118.20
1	A	1326	A2M	C4-N9-C8	2.69	108.64	105.73
1	A	3744	OMG	O6-C6-C5	-2.69	119.48	126.60
1	A	4296	PSU	C2'-C3'-C4'	-2.68	97.44	102.64
1	A	4590	A2M	C4-C5-N7	-2.68	107.36	110.62
1	A	4523	A2M	C2-N1-C6	2.67	123.35	118.77
1	A	4293	PSU	C6-C5-C4	-2.67	116.33	118.20
1	A	2876	OMG	O6-C6-C5	-2.67	119.53	126.60
1	A	3785	A2M	C2-N3-C4	2.66	118.03	111.75
1	A	4299	PSU	C2'-C3'-C4'	-2.65	97.49	102.64
1	A	1582	PSU	C5'-C4'-C3'	-2.65	105.25	115.18
1	A	2839	PSU	C6-C5-C4	-2.64	116.35	118.20
1	A	3718	A2M	C4-N9-C8	2.64	108.59	105.73
1	A	3825	A2M	C2-N1-C6	2.64	123.30	118.77
1	A	4590	A2M	C5-N7-C8	2.64	107.26	103.51
1	A	1534	A2M	C2-N1-C6	2.64	123.29	118.77
1	A	1326	A2M	C4-C5-N7	-2.63	107.41	110.62
1	A	1534	A2M	C5-N7-C8	2.63	107.25	103.51
1	A	4196	OMG	O6-C6-C5	-2.63	119.63	126.60
1	A	1792	PSU	C3'-C2'-C1'	2.63	104.70	101.64
1	A	3715	PSU	C3'-C2'-C1'	2.62	104.69	101.64
1	A	4227	OMU	O4-C4-C5	-2.61	120.56	125.16
1	A	4499	OMG	C5-C6-N1	2.59	119.77	113.19
1	A	3825	A2M	N6-C6-N1	2.59	124.02	118.35
1	A	3782	5MC	O2-C2-N3	-2.59	118.12	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2401	A2M	N9-C8-N7	-2.59	110.38	113.91
1	A	4306	OMU	C6-N1-C2	-2.59	117.69	120.99
1	A	4521	PSU	C6-N1-C2	-2.58	120.05	122.68
1	A	4296	PSU	C6-C5-C4	-2.58	116.40	118.20
1	A	2815	A2M	C4-C5-N7	-2.57	107.49	110.62
1	A	3825	A2M	C2'-C1'-N9	-2.57	109.21	113.53
1	A	1316	OMG	O6-C6-C5	-2.57	119.79	126.60
1	A	5010	PSU	C6-C5-C4	-2.56	116.41	118.20
1	A	2787	A2M	C2-N1-C6	2.56	123.16	118.77
1	A	4494	OMG	C2'-C1'-N9	-2.56	109.25	114.22
1	A	4392	OMG	O6-C6-C5	-2.55	119.83	126.60
1	A	3724	A2M	C4-C5-N7	-2.54	107.52	110.62
1	A	2424	OMG	O6-C6-C5	-2.54	119.86	126.60
1	A	1744	PSU	C6-C5-C4	-2.53	116.43	118.20
1	A	3851	PSU	C6-N1-C2	-2.52	120.10	122.68
1	A	3869	OMC	C4-N3-C2	2.51	124.31	120.25
1	A	3825	A2M	N9-C8-N7	-2.51	110.49	113.91
1	A	3718	A2M	C4-C5-N7	-2.51	107.57	110.62
1	A	2363	A2M	C4-N9-C1'	-2.50	120.64	126.59
1	A	4293	PSU	O2-C2-N1	-2.49	120.05	122.79
1	A	3627	OMG	O6-C6-C5	-2.49	119.99	126.60
1	A	4571	A2M	C4-C5-N7	-2.49	107.59	110.62
1	A	4228	OMG	C4-C5-N7	-2.49	106.79	110.72
1	A	4403	PSU	O2-C2-N1	-2.48	120.06	122.79
1	A	4498	OMU	C6-N1-C2	-2.48	117.82	120.99
1	A	4623	OMG	O6-C6-C5	-2.48	120.03	126.60
1	A	4620	OMU	C6-N1-C2	-2.47	117.83	120.99
1	A	4500	PSU	C6-N1-C2	-2.47	120.16	122.68
1	A	4618	OMG	C2'-C3'-C4'	-2.47	96.63	101.99
1	A	2415	OMU	O2-C2-N1	-2.47	119.51	122.79
1	A	1326	A2M	N9-C8-N7	-2.46	110.55	113.91
1	A	3899	OMG	C6-C5-C4	-2.46	115.00	118.77
1	A	3785	A2M	C4-C5-N7	-2.45	107.64	110.62
1	A	4618	OMG	O6-C6-C5	-2.44	120.11	126.60
1	A	3627	OMG	C5-C6-N1	2.43	119.37	113.19
1	A	4196	OMG	C4-C5-N7	-2.43	106.88	110.72
1	A	2424	OMG	C2'-C1'-N9	2.43	118.94	114.22
1	A	4628	PSU	C6-C5-C4	-2.42	116.51	118.20
1	A	4457	PSU	O4-C4-C5	-2.42	117.73	124.05
1	A	400	A2M	C4-N9-C8	2.41	108.34	105.73
1	A	3869	OMC	C5-C4-N3	-2.41	117.22	121.33
1	A	3887	OMC	O2-C2-N3	-2.41	118.41	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4442	PSU	C3'-C2'-C1'	2.41	104.44	101.64
1	A	3867	A2M	C5-C6-N6	-2.40	118.21	123.43
1	A	1860	PSU	C6-N1-C2	-2.40	120.23	122.68
1	A	398	A2M	N9-C8-N7	-2.39	110.64	113.91
1	A	1524	A2M	N9-C8-N7	-2.39	110.64	113.91
1	A	4536	OMC	C2'-C1'-N1	-2.39	109.59	114.22
1	A	2363	A2M	N9-C8-N7	-2.39	110.65	113.91
1	A	4370	OMG	O6-C6-C5	-2.39	120.27	126.60
1	A	4523	A2M	C4-C5-N7	-2.38	107.72	110.62
1	A	398	A2M	C4-N9-C8	2.38	108.31	105.73
1	A	3695	PSU	O4-C4-C5	-2.38	117.83	124.05
1	A	4571	A2M	O3'-C3'-C4'	-2.37	104.18	111.05
1	A	4471	PSU	O2-C2-N3	-2.37	117.34	121.82
1	A	2876	OMG	C4-C5-N7	-2.37	106.97	110.72
1	A	3701	OMC	O4'-C1'-C2'	-2.36	102.43	106.57
1	A	4618	OMG	C6-C5-C4	-2.36	115.15	118.77
1	A	4618	OMG	C4-C5-N7	-2.35	107.00	110.72
1	A	3627	OMG	C4-C5-N7	-2.35	107.00	110.72
1	A	4498	OMU	O4-C4-N3	2.35	122.76	119.31
1	A	4196	OMG	C8-N7-C5	2.35	108.49	104.24
1	A	2837	OMU	C6-N1-C2	-2.35	117.99	120.99
1	A	3724	A2M	C2-N1-C6	2.35	122.79	118.77
1	A	4403	PSU	O2-C2-N3	-2.34	117.40	121.82
1	A	1326	A2M	N6-C6-N1	2.34	123.47	118.35
1	A	2363	A2M	N6-C6-N1	2.34	123.47	118.35
1	A	4590	A2M	C2'-C1'-N9	-2.34	109.59	113.53
1	A	1792	PSU	O2-C2-N1	-2.34	120.22	122.79
1	A	2401	A2M	C6-C5-N7	2.33	136.37	132.02
1	A	1862	PSU	C5-C6-N1	-2.33	118.62	122.11
1	A	400	A2M	C5-N7-C8	2.32	106.81	103.51
1	A	3899	OMG	C5-C6-N1	2.31	119.07	113.19
1	A	5001	PSU	C6-N1-C2	-2.31	120.32	122.68
1	A	2815	A2M	C2-N1-C6	2.31	122.73	118.77
1	A	2365	OMC	C4-N3-C2	2.31	123.98	120.25
1	A	4637	OMG	O6-C6-C5	-2.31	120.47	126.60
1	A	2401	A2M	O2'-C2'-C1'	-2.31	104.58	109.08
1	A	3782	5MC	C5-C4-N3	-2.30	119.19	121.67
1	A	2424	OMG	C2-N1-C6	-2.30	120.91	125.10
1	A	4228	OMG	N9-C8-N7	-2.29	109.08	113.39
1	A	3825	A2M	C4-N9-C8	2.29	108.21	105.73
3	C	69	PSU	C6-C5-C4	-2.29	116.60	118.20
1	A	1683	PSU	C6-N1-C2	-2.28	120.35	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4571	A2M	C5-N7-C8	2.28	106.75	103.51
1	A	2839	PSU	O2'-C2'-C1'	-2.28	105.79	111.23
1	A	4637	OMG	C4-C5-N7	-2.28	107.12	110.72
1	A	2804	OMC	C5-C4-N3	-2.27	117.46	121.33
1	A	1534	A2M	N9-C8-N7	-2.27	110.81	113.91
1	A	3830	A2M	O2'-C2'-C1'	2.27	113.50	109.08
1	A	3853	PSU	O4-C4-C5	-2.27	118.12	124.05
1	A	4196	OMG	N9-C8-N7	-2.26	109.13	113.39
1	A	2632	PSU	O2-C2-N1	-2.26	120.31	122.79
1	A	3899	OMG	C8-N9-C4	2.25	110.33	106.05
1	A	3724	A2M	C2'-C1'-N9	-2.25	109.74	113.53
1	A	2508	PSU	C3'-C2'-C1'	2.24	104.25	101.64
1	A	2787	A2M	C4'-O4'-C1'	2.23	114.40	109.47
1	A	3841	OMC	C5-C4-N3	-2.23	117.53	121.33
1	A	3869	OMC	N4-C4-N3	2.23	121.87	117.97
1	A	3718	A2M	C5-N7-C8	2.22	106.67	103.51
1	A	4447	5MC	O2'-C2'-C1'	-2.22	102.60	110.02
1	A	4499	OMG	C4-C5-N7	-2.21	107.22	110.72
1	A	1534	A2M	C6-C5-N7	2.21	136.14	132.02
1	A	1322	1MA	C8-N9-C4	2.21	110.25	106.05
1	A	4361	PSU	C2'-C3'-C4'	-2.21	98.35	102.64
1	A	1524	A2M	C2-N1-C6	2.20	122.54	118.77
1	A	4530	UR3	O2-C2-N1	-2.20	117.57	122.72
1	A	4628	PSU	C3'-C2'-C1'	2.20	104.19	101.64
1	A	4571	A2M	N9-C8-N7	-2.20	110.91	113.91
1	A	1683	PSU	O4-C4-C5	-2.19	118.31	124.05
1	A	4220	6MZ	C6-C5-N7	2.19	134.76	132.39
1	A	4637	OMG	C5-C6-N1	2.19	118.74	113.19
1	A	3818	OMU	O2-C2-N3	-2.19	117.43	121.50
1	A	4689	PSU	O4-C4-C5	-2.18	118.35	124.05
1	A	4494	OMG	C4-C5-N7	-2.17	107.28	110.72
1	A	2787	A2M	C5'-C4'-C3'	-2.17	107.04	115.18
1	A	3867	A2M	N6-C6-N1	2.17	123.10	118.35
1	A	4523	A2M	N6-C6-N1	2.16	123.09	118.35
1	A	4521	PSU	O2-C2-N3	-2.16	117.74	121.82
1	A	1625	OMG	N2-C2-N3	-2.16	115.53	119.73
1	A	4228	OMG	C6-C5-C4	-2.16	115.46	118.77
1	A	1860	PSU	O4-C4-C5	-2.15	118.41	124.05
1	A	2364	OMG	C1'-N9-C4	-2.15	120.11	126.50
1	A	4442	PSU	C6-C5-C4	-2.15	116.69	118.20
1	A	4228	OMG	C8-N7-C5	2.15	108.12	104.24
1	A	4392	OMG	C5-C6-N1	2.14	118.63	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3724	A2M	C5-N7-C8	2.14	106.55	103.51
1	A	4220	6MZ	C2-N1-C6	2.14	122.43	115.25
1	A	4493	PSU	O4-C4-C5	-2.14	118.46	124.05
1	A	3785	A2M	C4-N9-C1'	-2.14	121.50	126.59
1	A	3884	PSU	O4-C4-C5	-2.13	118.47	124.05
1	A	4673	PSU	O4-C4-C5	-2.13	118.47	124.05
1	A	2632	PSU	C3'-C2'-C1'	2.13	104.12	101.64
1	A	4306	OMU	O4-C4-C5	-2.13	121.42	125.16
1	A	2415	OMU	CM2-O2'-C2'	2.13	120.11	114.52
1	A	4227	OMU	O2-C2-N1	-2.13	119.96	122.79
1	A	3792	OMG	C4-C5-N7	-2.13	107.36	110.72
1	A	2508	PSU	O4-C4-C5	-2.13	118.49	124.05
1	A	1522	OMG	O6-C6-C5	-2.13	120.96	126.60
1	A	4623	OMG	C5-C6-N1	2.12	118.59	113.19
1	A	4293	PSU	O2-C2-N3	-2.12	117.81	121.82
1	A	2876	OMG	C5-C6-N1	2.12	118.58	113.19
1	A	4228	OMG	C5-C6-N1	2.12	118.57	113.19
1	A	1625	OMG	C5-C6-N1	2.12	118.56	113.19
1	A	4530	UR3	C3U-N3-C2	2.12	121.02	117.31
1	A	3785	A2M	O2'-C2'-C1'	2.11	113.20	109.08
1	A	2351	OMC	CM2-O2'-C2'	2.11	120.07	114.52
1	A	4494	OMG	O6-C6-C5	-2.11	120.99	126.60
1	A	2839	PSU	C6-N1-C2	-2.11	120.52	122.68
1	A	2824	OMC	O3'-C3'-C4'	-2.11	104.95	111.05
1	A	1781	PSU	O4-C4-C5	-2.11	118.53	124.05
1	A	2364	OMG	C5-C6-N1	2.11	118.54	113.19
1	A	4431	PSU	C2'-C3'-C4'	-2.10	98.55	102.64
1	A	3701	OMC	C1'-N1-C6	2.10	125.42	120.84
1	A	1534	A2M	O4'-C1'-C2'	-2.10	102.88	106.57
1	A	2422	OMC	O2-C2-N3	-2.10	118.92	122.33
1	A	3718	A2M	N6-C6-N1	2.08	122.92	118.35
1	A	4493	PSU	C5-C4-N3	2.08	121.29	116.58
1	A	4293	PSU	C5-C6-N1	-2.08	118.98	122.11
1	A	4447	5MC	N1-C2-N3	2.08	122.59	118.81
1	A	2787	A2M	C3'-C2'-C1'	2.07	106.79	102.89
1	A	3851	PSU	O4-C4-C5	-2.07	118.62	124.05
3	C	75	OMG	C3'-C2'-C1'	-2.07	98.99	102.89
1	A	4521	PSU	C3'-C2'-C1'	2.07	104.05	101.64
1	A	4456	OMC	C1'-N1-C6	2.07	125.36	120.84
1	A	2839	PSU	O4-C4-C5	-2.07	118.63	124.05
1	A	2787	A2M	N6-C6-N1	2.07	122.89	118.35
1	A	1782	PSU	O2-C2-N3	-2.07	117.92	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4196	OMG	C2-N1-C6	-2.07	121.33	125.10
1	A	1792	PSU	C2'-C3'-C4'	-2.07	98.63	102.64
1	A	3729	PSU	C6-C5-C4	-2.06	116.76	118.20
1	A	3695	PSU	O2'-C2'-C1'	-2.06	106.32	111.23
1	A	400	A2M	C6-C5-N7	2.06	135.86	132.02
1	A	4228	OMG	C8-N9-C4	2.06	109.97	106.05
1	A	1677	PSU	O3'-C3'-C4'	-2.06	105.10	111.05
1	A	3627	OMG	C6-C5-C4	-2.06	115.61	118.77
1	A	4353	PSU	C5-C6-N1	-2.06	119.02	122.11
1	A	4196	OMG	C6-C5-C4	-2.06	115.61	118.77
1	A	3844	PSU	O4-C4-C5	-2.05	118.68	124.05
1	A	4431	PSU	C5-C4-N3	2.05	121.22	116.58
3	C	55	PSU	O4-C4-C5	-2.05	118.69	124.05
3	C	75	OMG	C4-C5-N7	-2.05	107.48	110.72
1	A	4228	OMG	C1'-N9-C4	-2.04	120.43	126.50
1	A	4500	PSU	O4'-C1'-C2'	2.04	108.03	105.14
1	A	2415	OMU	C2'-C1'-N1	-2.04	110.26	114.22
1	A	2876	OMG	C2-N1-C6	-2.04	121.38	125.10
1	A	5010	PSU	O2'-C2'-C1'	-2.04	106.37	111.23
1	A	3920	PSU	O4-C4-C5	-2.04	118.72	124.05
1	A	4618	OMG	C5-C6-N1	2.03	118.35	113.19
1	A	4576	PSU	O4-C4-C5	-2.03	118.74	124.05
1	A	2415	OMU	O4'-C1'-N1	2.03	113.00	108.36
1	A	1792	PSU	O2-C2-N3	-2.02	118.00	121.82
1	A	2787	A2M	O4'-C4'-C5'	2.02	116.03	109.37
1	A	3869	OMC	C6-N1-C2	-2.02	116.98	120.49
1	A	4442	PSU	O2-C2-N3	-2.02	118.01	121.82
3	C	75	OMG	C5-C6-N1	2.02	118.32	113.19
1	A	3841	OMC	C6-N1-C2	-2.01	117.01	120.49
1	A	3792	OMG	C8-N9-C4	2.01	109.87	106.05
1	A	4637	OMG	C8-N9-C4	2.00	109.86	106.05
1	A	4392	OMG	C6-C5-C4	-2.00	115.69	118.77
1	A	4370	OMG	C4-C5-N7	-2.00	107.55	110.72

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2415	OMU	C1'-C2'-O2'-CM2
1	A	3701	OMC	C2'-C1'-N1-C2
1	A	3701	OMC	C2'-C1'-N1-C6
1	A	4590	A2M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	A	3785	A2M	O4'-C4'-C5'-O5'
1	A	2787	A2M	C2'-C1'-N9-C4
1	A	3785	A2M	C3'-C4'-C5'-O5'
1	A	2787	A2M	C2'-C1'-N9-C8
1	A	2422	OMC	O4'-C4'-C5'-O5'
1	A	2422	OMC	C3'-C4'-C5'-O5'
1	A	2363	A2M	C3'-C2'-O2'-CM'
1	A	2401	A2M	C3'-C2'-O2'-CM'
1	A	4494	OMG	C3'-C2'-O2'-CM2
1	A	1326	A2M	C4'-C5'-O5'-P
1	A	3818	OMU	C4'-C5'-O5'-P
1	A	1534	A2M	C4'-C5'-O5'-P
1	A	4500	PSU	C4'-C5'-O5'-P
1	A	3701	OMC	O4'-C1'-N1-C6
1	A	4447	5MC	O4'-C1'-N1-C6
1	A	4447	5MC	C2'-C1'-N1-C6
1	A	2364	OMG	O4'-C4'-C5'-O5'
1	A	3701	OMC	O4'-C1'-N1-C2
1	A	4447	5MC	O4'-C1'-N1-C2
1	A	1677	PSU	O4'-C1'-C5-C4
1	A	2787	A2M	O4'-C1'-N9-C8
1	A	4447	5MC	C2'-C1'-N1-C2
1	A	1534	A2M	O4'-C4'-C5'-O5'
1	A	2364	OMG	C3'-C4'-C5'-O5'
1	A	2351	OMC	O4'-C4'-C5'-O5'
1	A	3844	PSU	C4'-C5'-O5'-P

There are no ring outliers.

15 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4457	PSU	1	0
1	A	2351	OMC	3	0
1	A	2876	OMG	1	0
1	A	4447	5MC	1	0
1	A	4500	PSU	1	0
1	A	3818	OMU	1	0
1	A	3867	A2M	2	0
1	A	4220	6MZ	1	0
1	A	1340	OMC	1	0
1	A	4293	PSU	1	0
1	A	4498	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4456	OMC	1	0
1	A	2415	OMU	1	0
1	A	2364	OMG	1	0
1	A	2787	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 394 ligands modelled in this entry, 391 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
49	HMT	A	5455	-	40,43,43	0.62	0	41,66,66	0.67	0
50	SPM	A	5456	-	13,13,13	0.22	0	12,12,12	0.24	0
51	EPE	A	5457	-	15,15,15	0.91	1 (6%)	18,20,20	1.89	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	HMT	A	5455	-	-	0/27/74/74	0/5/5/5
50	SPM	A	5456	-	-	3/11/11/11	-
51	EPE	A	5457	-	-	1/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A	5457	EPE	O2S-S	3.20	1.54	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	A	5457	EPE	O2S-S-C10	-7.35	98.06	106.92
51	A	5457	EPE	O3S-S-O1S	2.76	118.01	111.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	A	5456	SPM	C2-C3-C4-N5
50	A	5456	SPM	C6-C7-C8-C9
51	A	5457	EPE	C9-C10-S-O3S
50	A	5456	SPM	C7-C6-N5-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	A	5455	HMT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

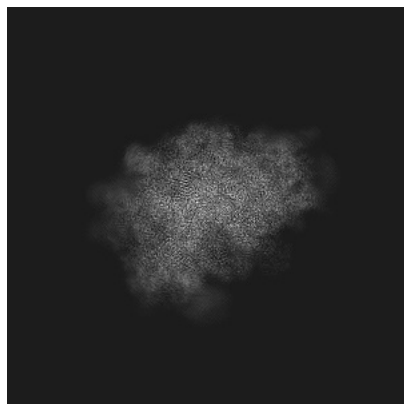
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15113. These allow visual inspection of the internal detail of the map and identification of artifacts.

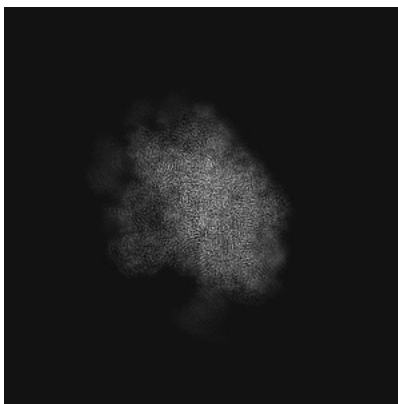
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

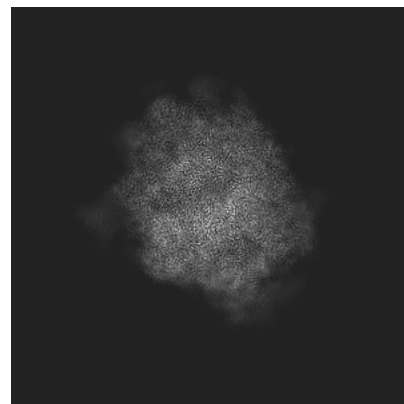
6.1.1 Primary map



X

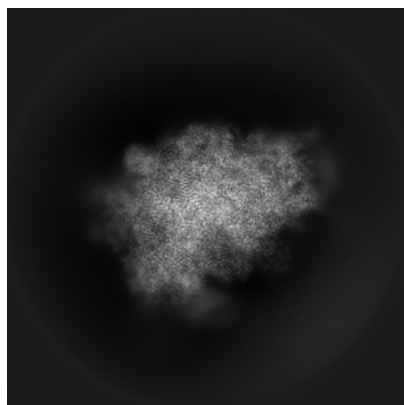


Y

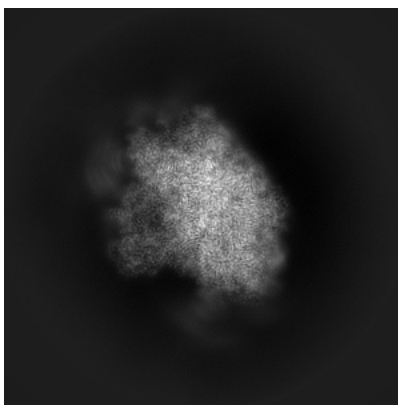


Z

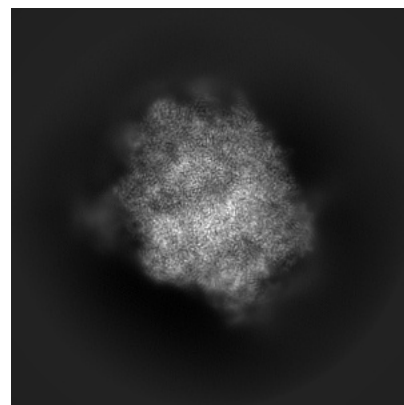
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

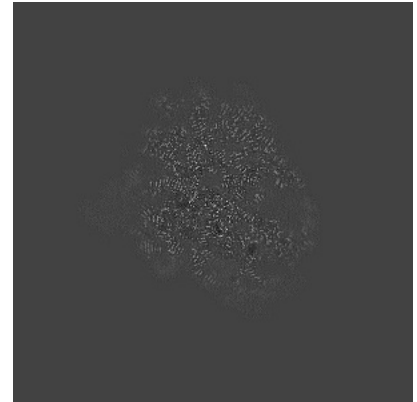
6.2.1 Primary map



X Index: 256

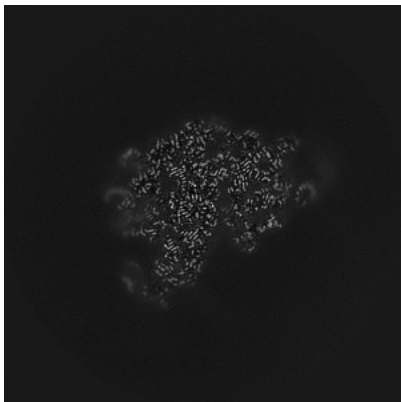


Y Index: 256

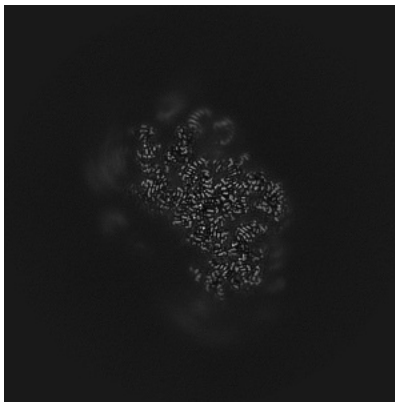


Z Index: 256

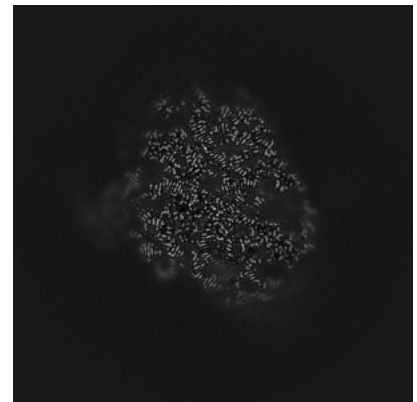
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

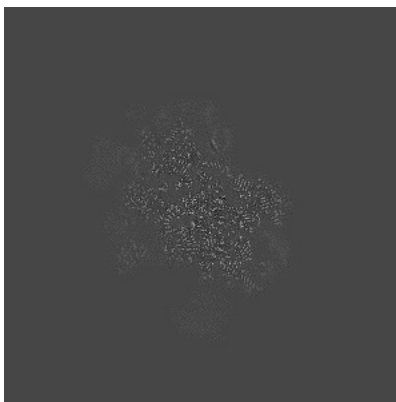
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

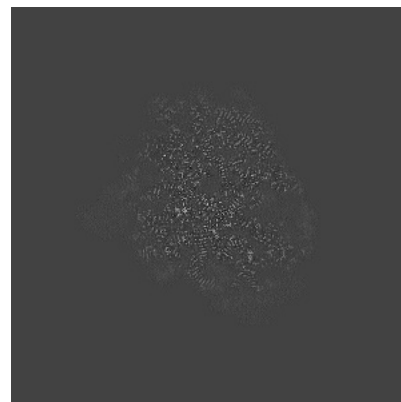
6.3.1 Primary map



X Index: 253

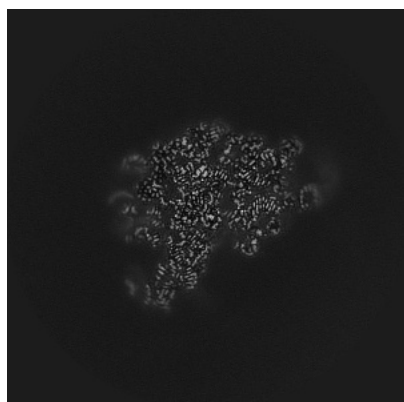


Y Index: 239

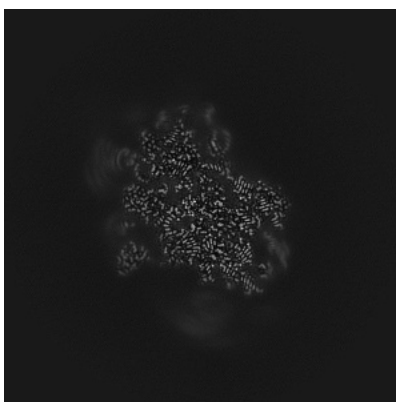


Z Index: 258

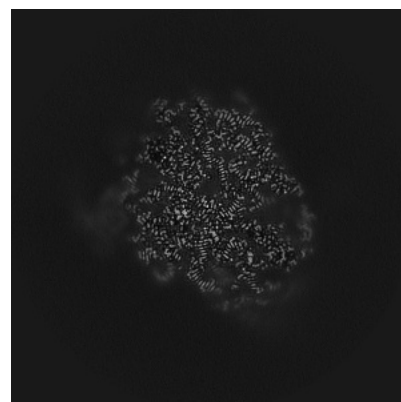
6.3.2 Raw map



X Index: 253



Y Index: 239

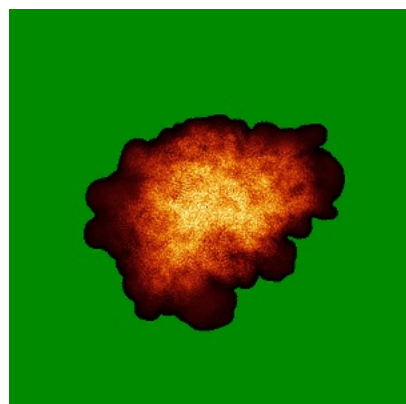


Z Index: 258

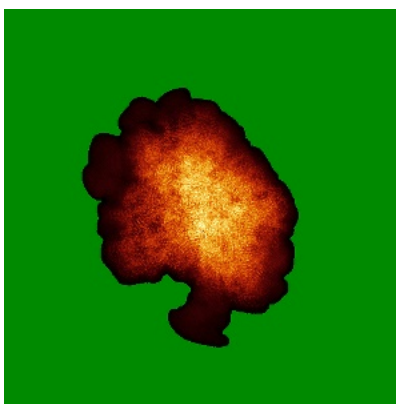
The images above show the largest variance slices of the map in three orthogonal directions.

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

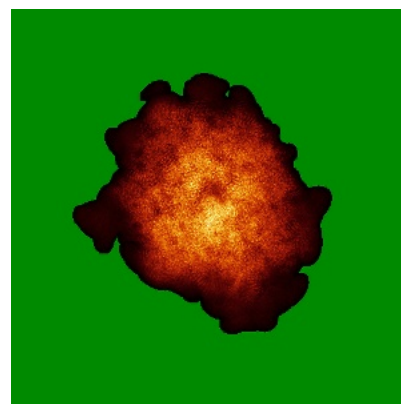
6.4.1 Primary map



X

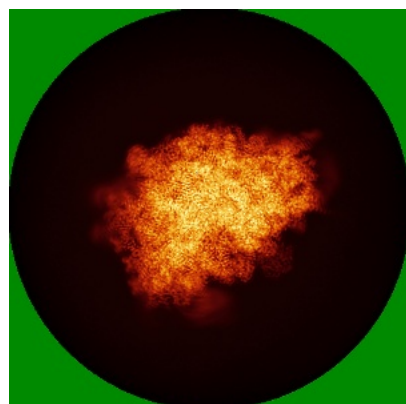


Y

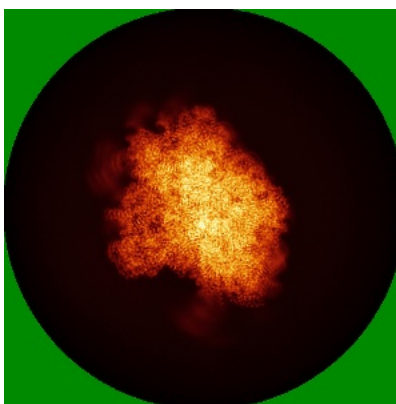


Z

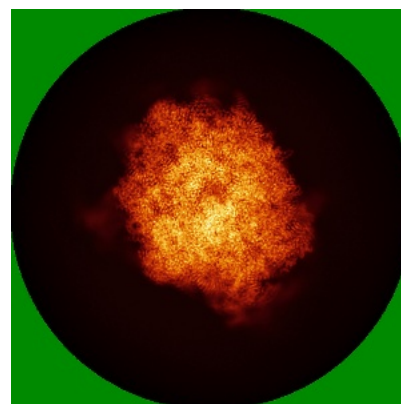
6.4.2 Raw map



X



Y

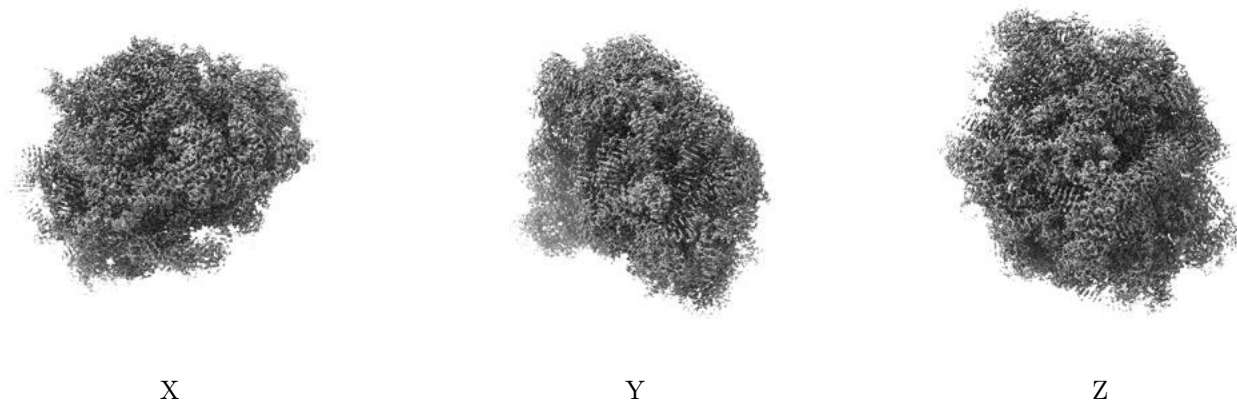


Z

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

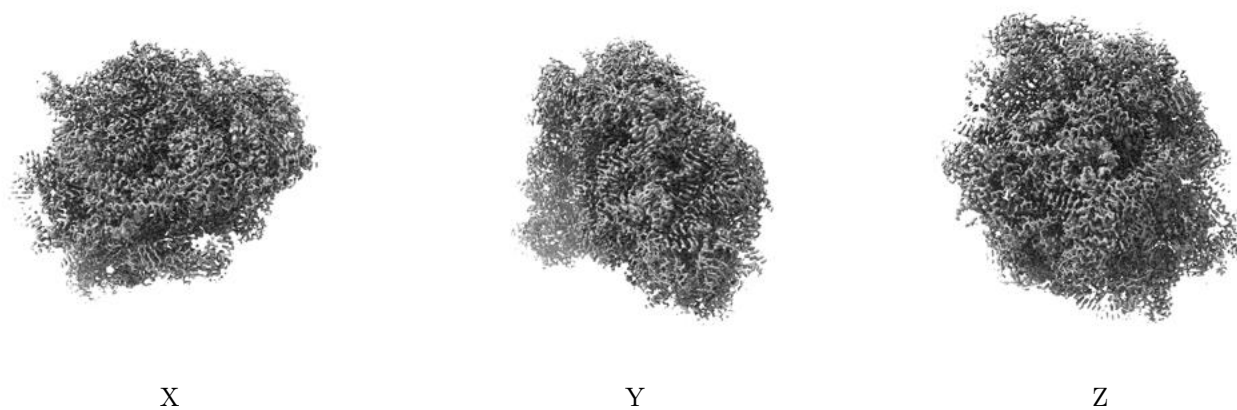
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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

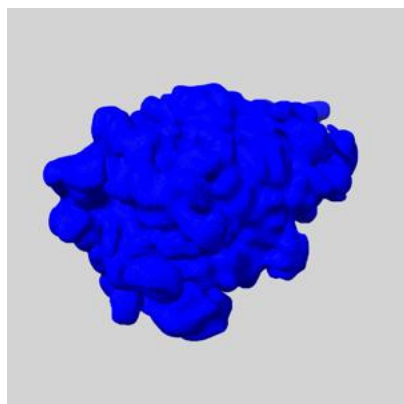
6.6 Mask visualisation [i](#)

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

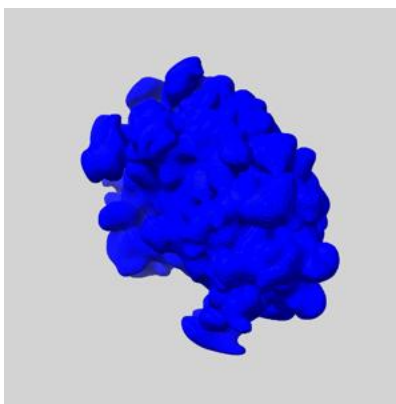
A mask typically either:

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

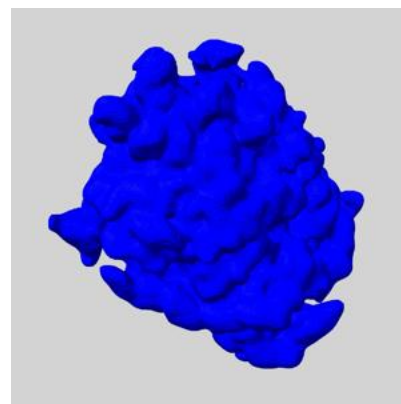
6.6.1 emd_15113_msk_1.map [i](#)



X



Y

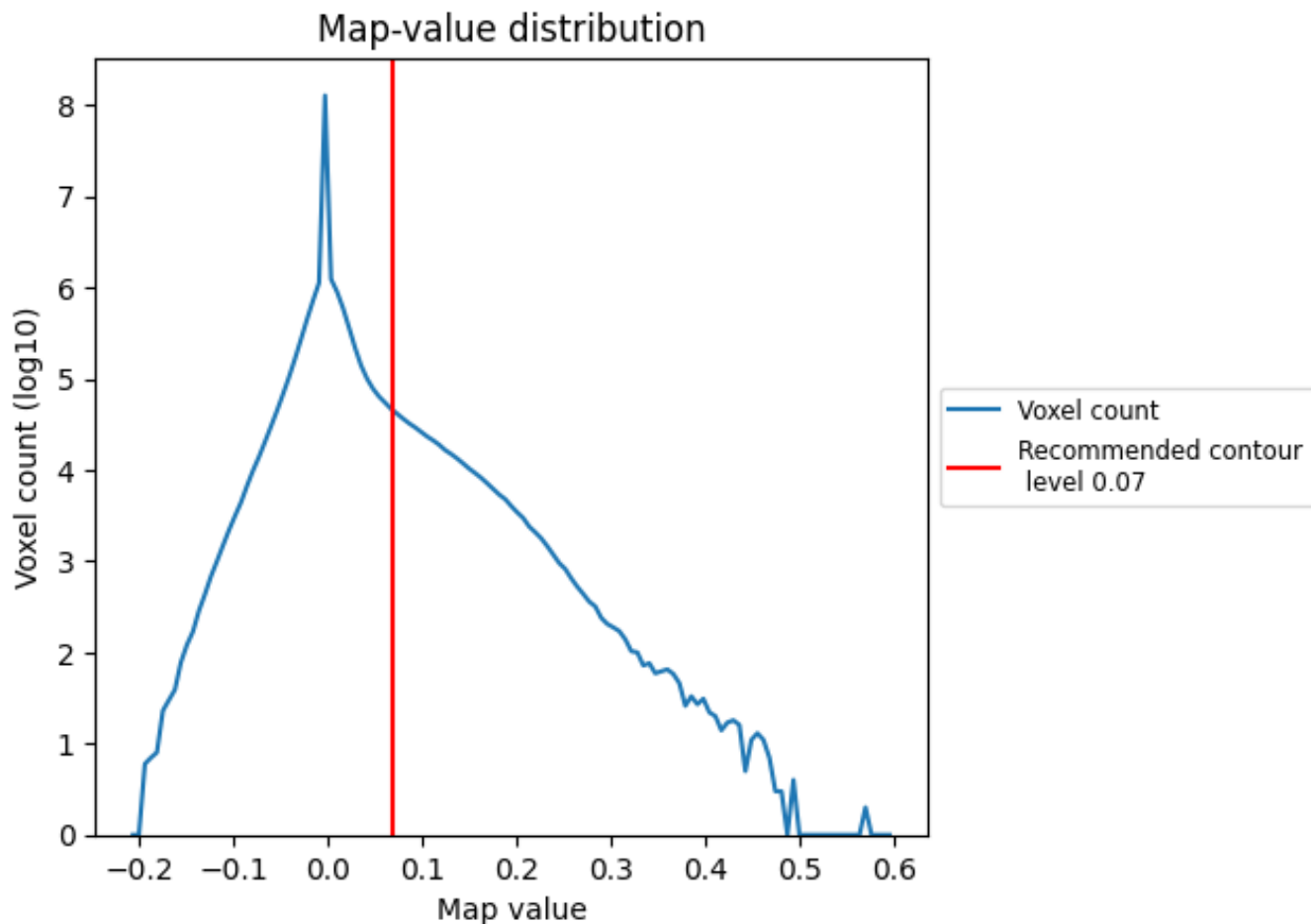


Z

7 Map analysis [i](#)

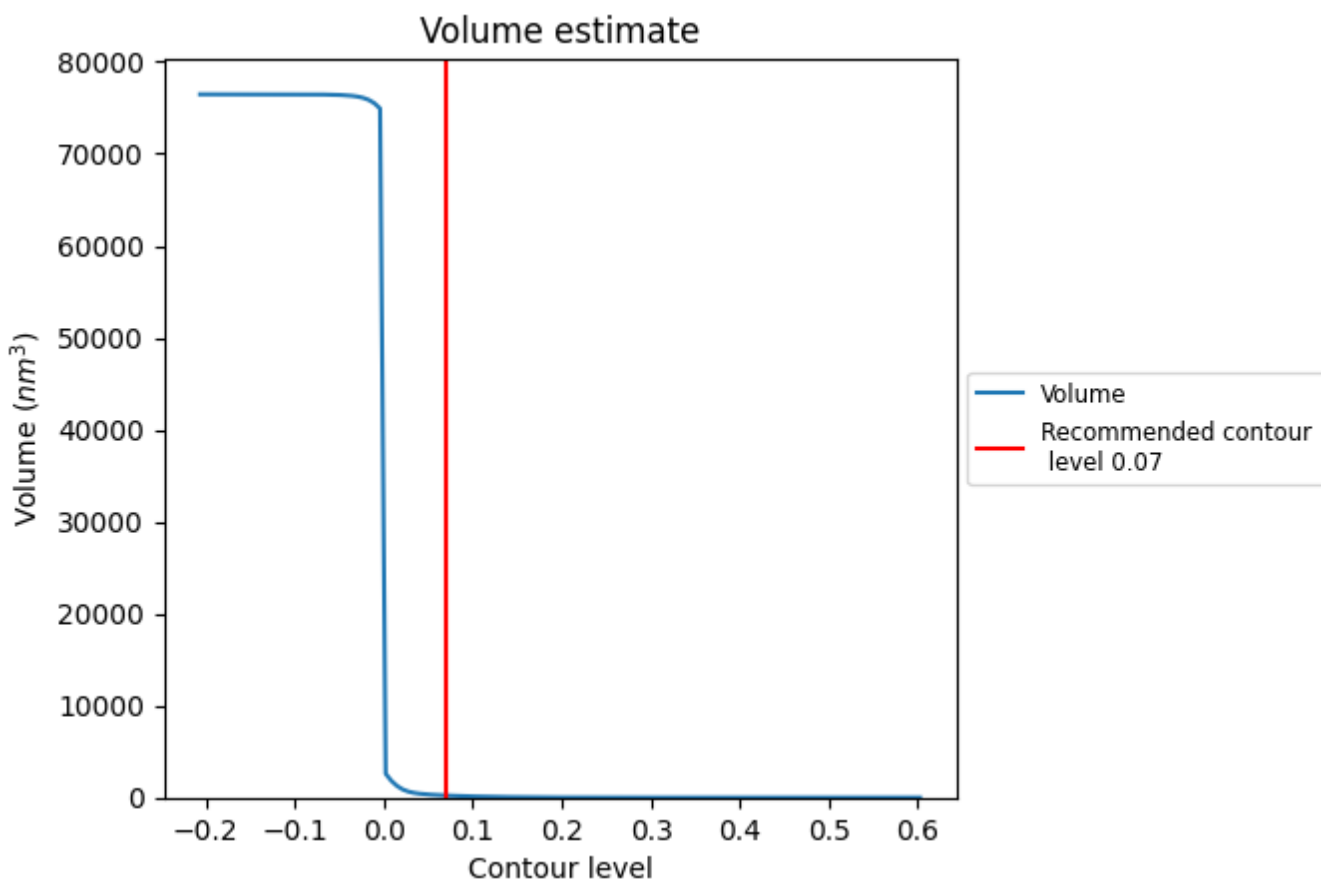
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

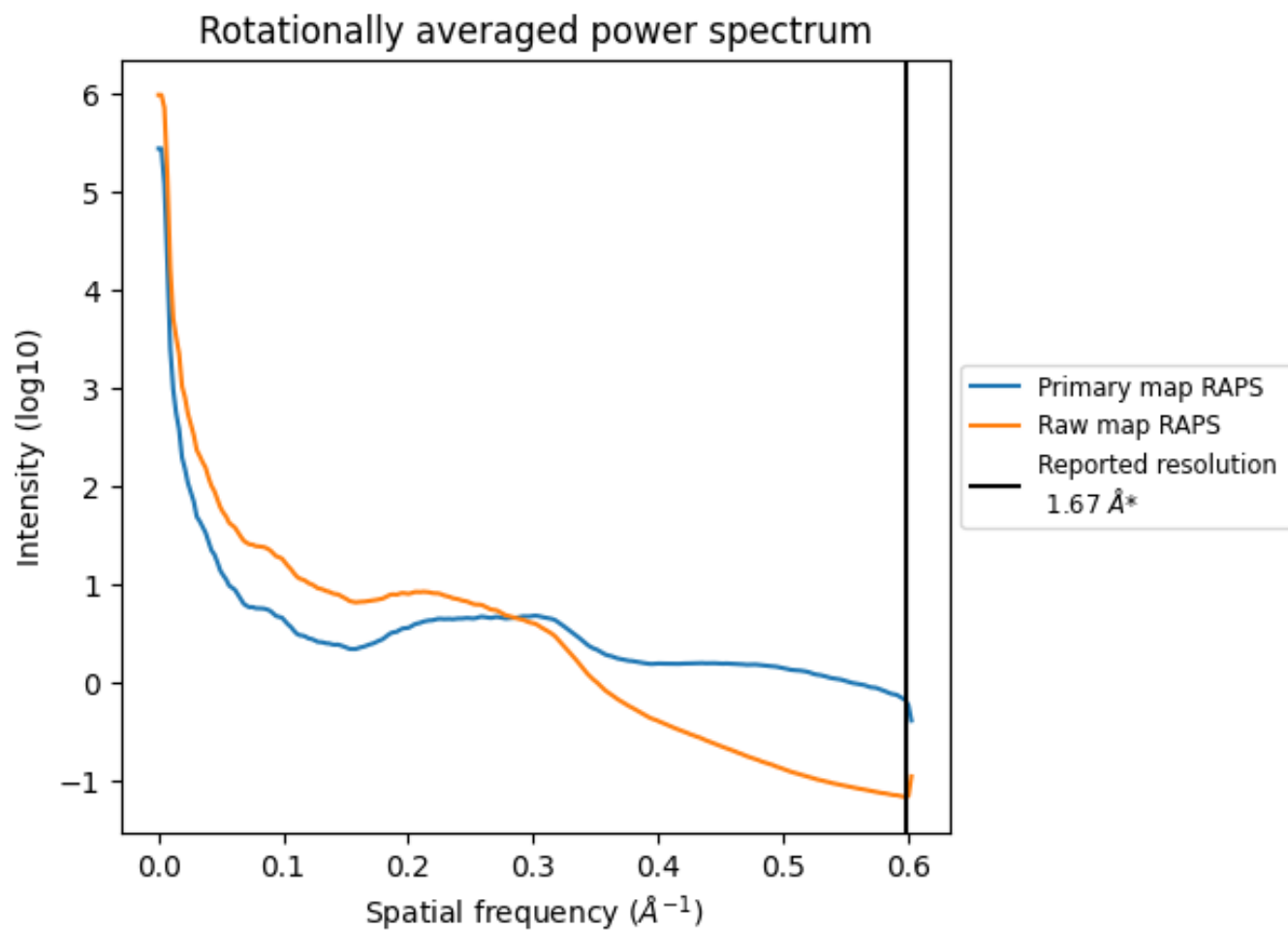
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222 nm³; this corresponds to an approximate mass of 200 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

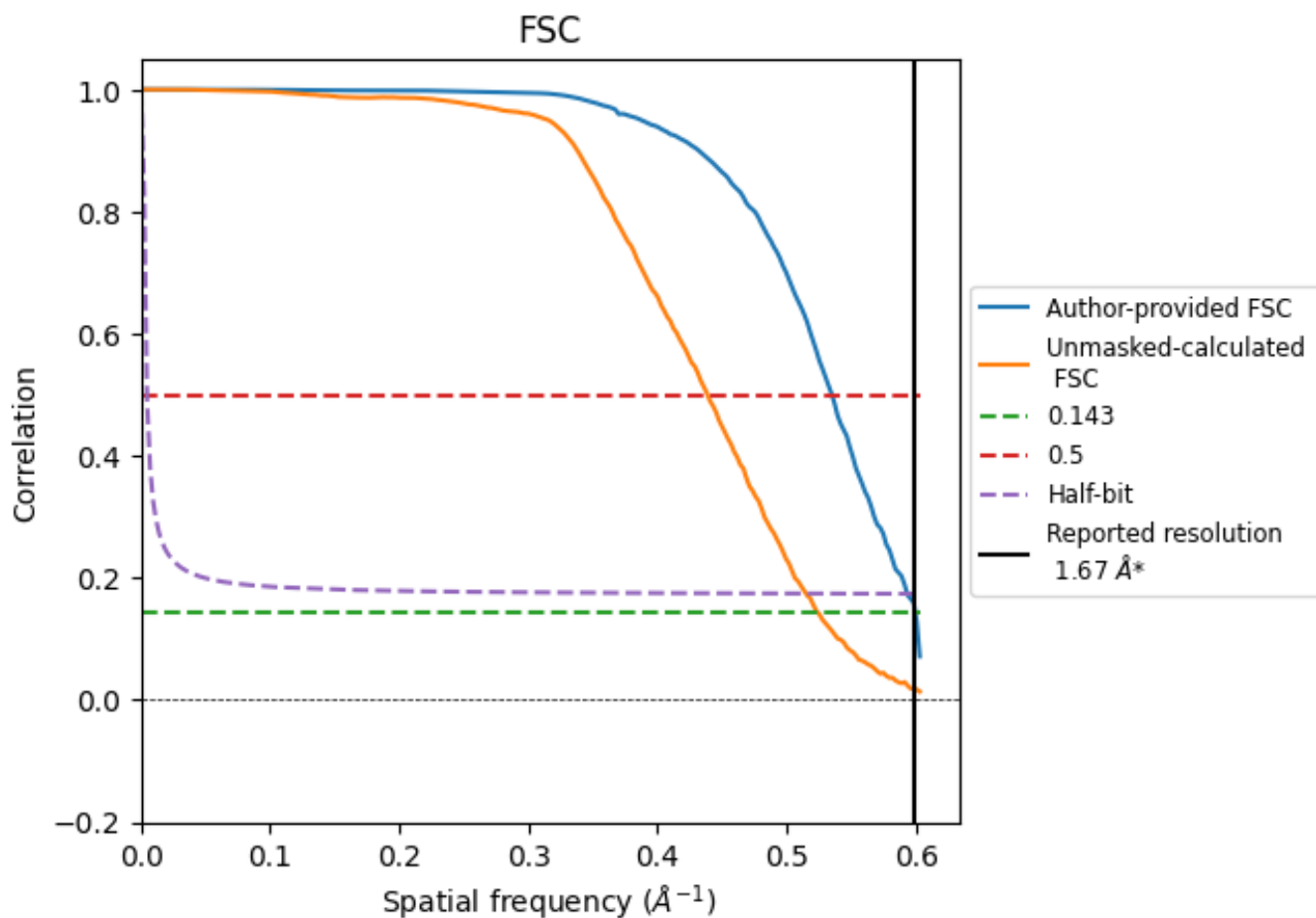


*Reported resolution corresponds to spatial frequency of 0.599 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.599 Å⁻¹

8.2 Resolution estimates [i](#)

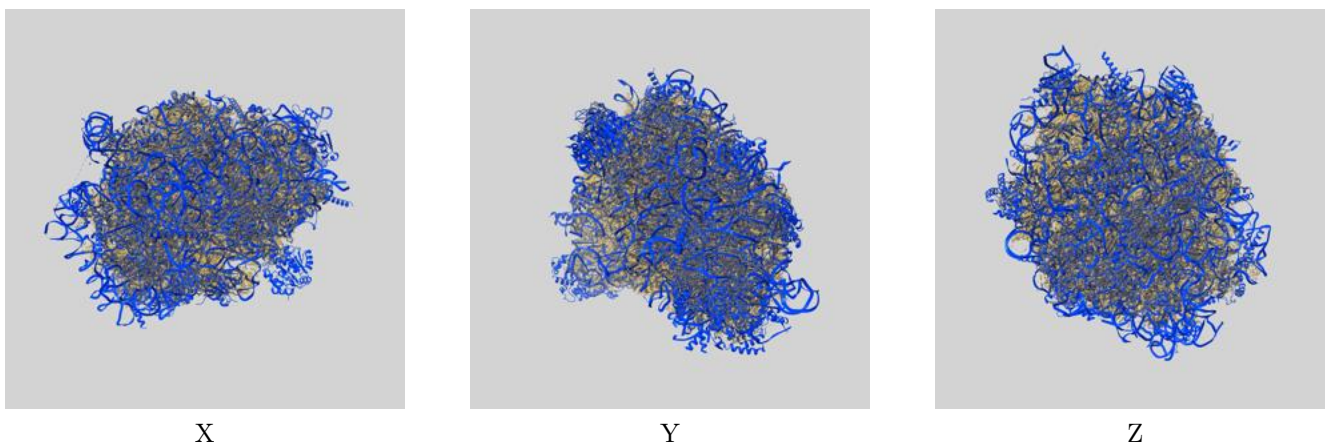
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.67	-	-
Author-provided FSC curve	1.67	1.87	1.69
Unmasked-calculated*	1.91	2.28	1.94

*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 1.91 differs from the reported value 1.67 by more than 10 %

9 Map-model fit [i](#)

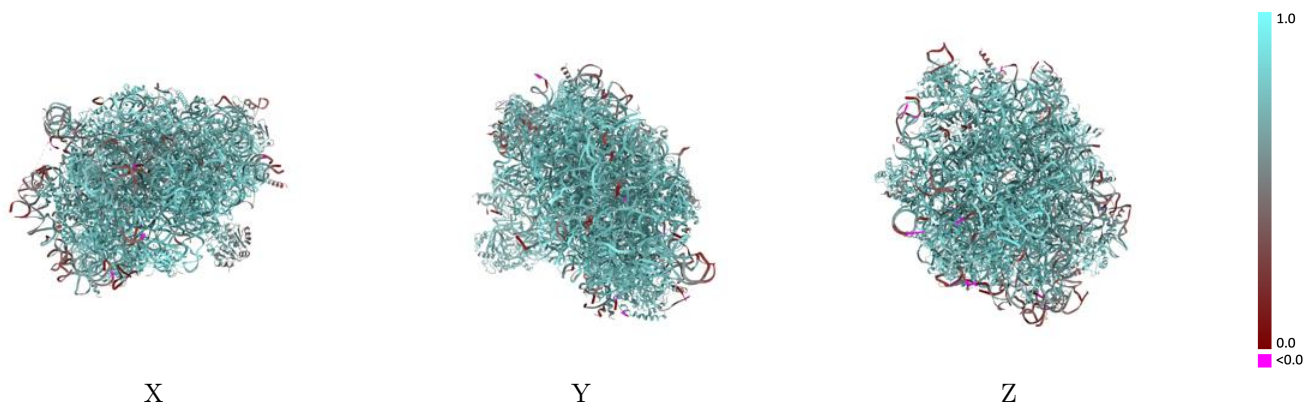
This section contains information regarding the fit between EMDB map EMD-15113 and PDB model 8A3D. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



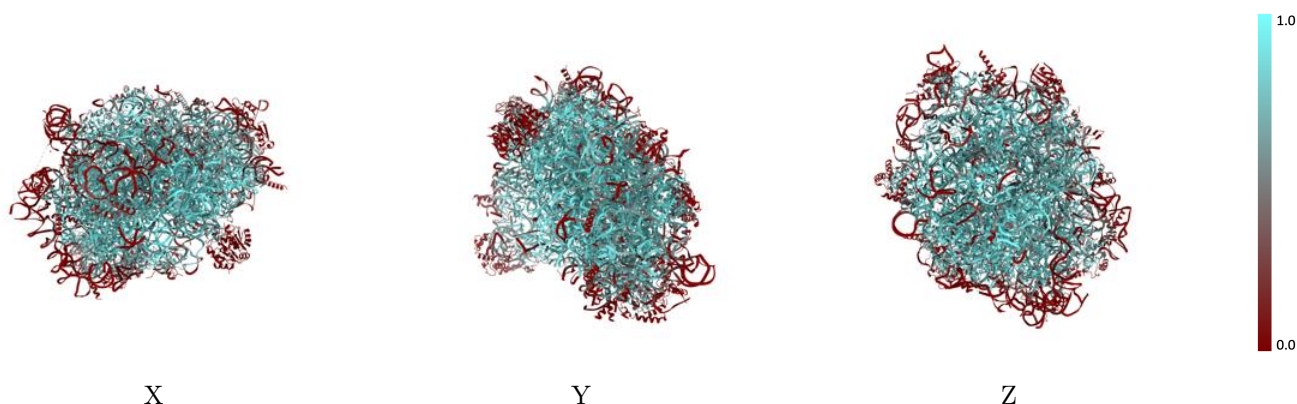
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



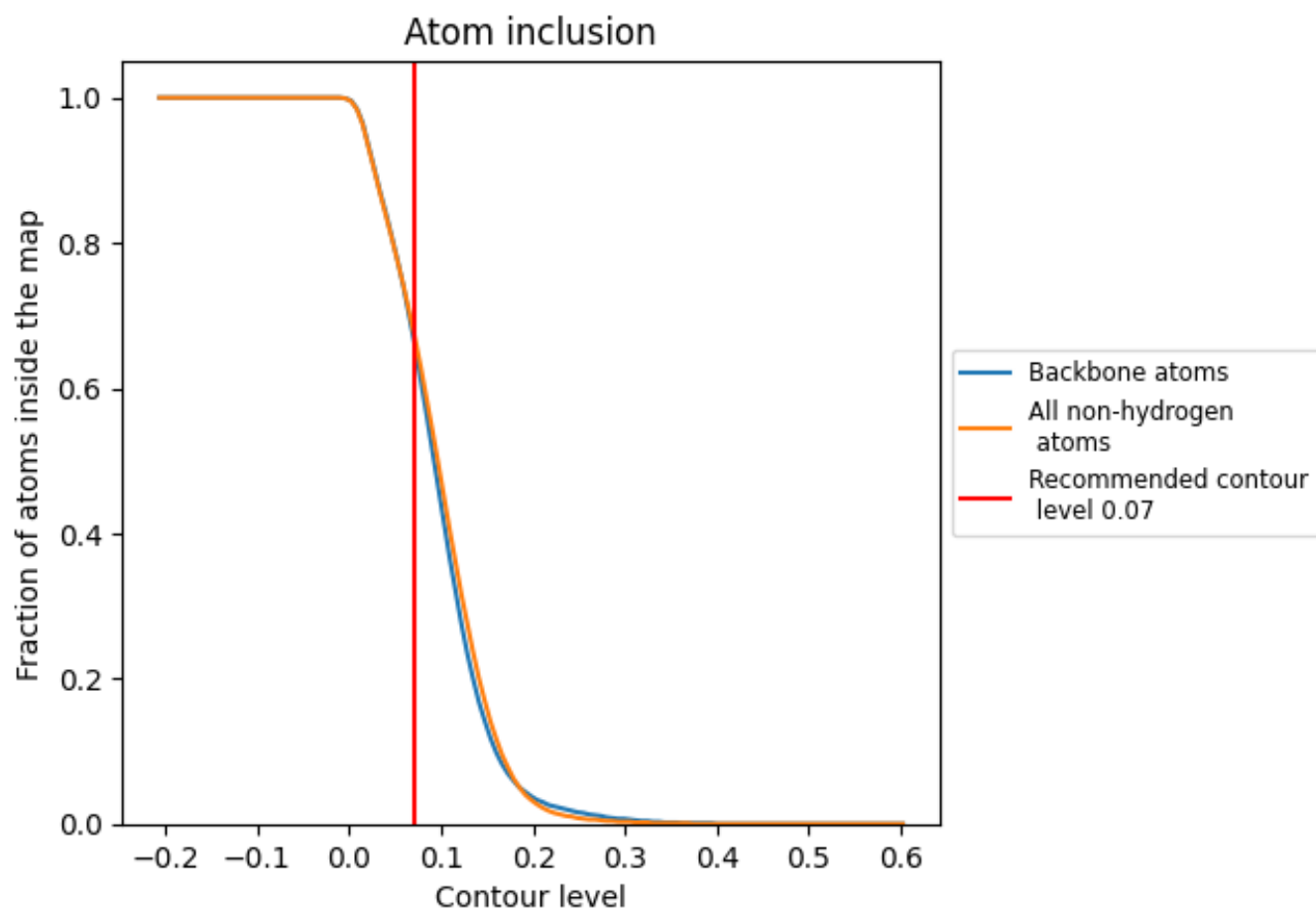
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 68% 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	0.6780	0.7690
A	0.7080	0.7530
B	0.7760	0.8070
C	0.7530	0.7850
D	0.8600	0.8430
E	0.7290	0.8170
F	0.8100	0.8270
G	0.4810	0.7720
H	0.4480	0.7450
I	0.7900	0.8260
J	0.7950	0.8340
K	0.8480	0.8450
L	0.6360	0.7650
M	0.8230	0.8330
N	0.6770	0.7700
O	0.0760	0.6310
P	0.7260	0.8190
Q	0.6560	0.8060
R	0.5980	0.7930
S	0.6800	0.8010
T	0.3670	0.7540
U	0.8020	0.8270
V	0.4420	0.7200
W	0.3790	0.7370
X	0.6270	0.7870
Y	0.8380	0.8400
Z	0.8640	0.8480
a	0.7510	0.8200
b	0.5590	0.7800
c	0.4710	0.7460
d	0.8550	0.8470
e	0.2350	0.6880
f	0.7030	0.8080
g	0.6680	0.7950
h	0.0000	0.5730



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Chain	Atom inclusion	Q-score
i	 0.6770	 0.8140
j	 0.6980	 0.7920
k	 0.7690	 0.8200
l	 0.9170	 0.8500
m	 0.8760	 0.8480
n	 0.4020	 0.7310
o	 0.5350	 0.7840
p	 0.6680	 0.8120
q	 0.1650	 0.6920
r	 0.6020	 0.7690
s	 0.6620	 0.7840