



Full wwPDB EM Validation Report ⓘ

Sep 22, 2026 – 10:17 pm BST

PDB ID : 29IY / pdb_000029iy
EMDB ID : EMD-57203
Title : Human monosomes, focus on 60S subunit; control.
Authors : Rabl, J.; Karousis, E.D.
Deposited on : 2026-03-15
Resolution : 2.36 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

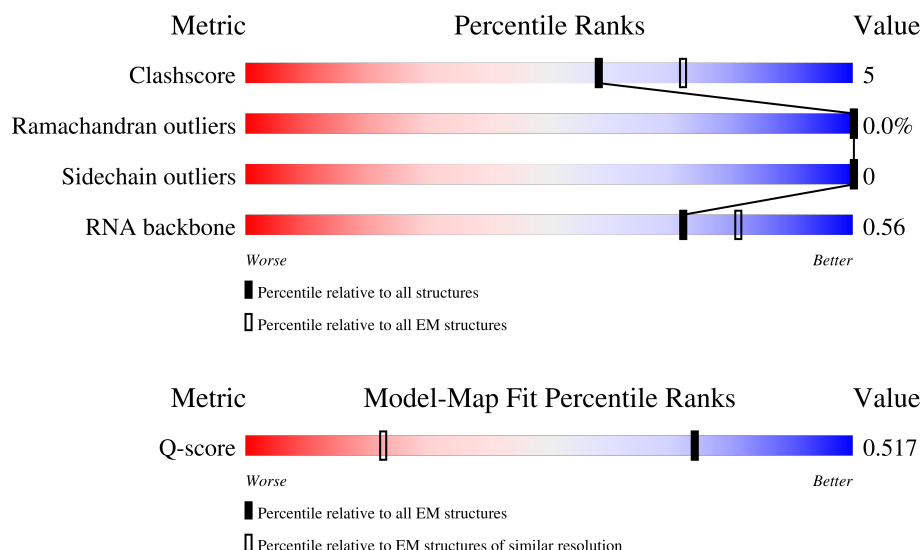
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.36 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	4686 (1.86 - 2.86)

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	AV	159	
2	AW	115	
3	AX	125	

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Mol	Chain	Length	Quality of chain
4	AY	135	
5	AZ	110	
6	Aa	117	
7	Ab	123	
8	Ac	105	
9	Ad	97	
10	Ae	70	
11	Af	51	
12	Ag	128	
13	Ah	106	
14	Ai	92	
15	Aj	137	
16	BA	403	
17	BB	427	
18	BC	297	
19	BD	288	
20	CA	5069	
21	CB	120	
22	CC	157	
23	CD	257	
24	AK	188	
25	AL	196	
26	AM	176	
27	AN	160	
28	AO	128	

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Mol	Chain	Length	Quality of chain
29	AP	140	
30	AQ	157	
31	AR	156	
32	AS	145	
33	AT	136	
34	AU	148	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	PUT	CA	5401	-	-	X	-
38	PUT	CA	5402	-	-	X	-
38	PUT	CA	5403	-	-	X	-
38	PUT	CB	201	-	-	X	-
39	SPD	CA	5410	-	-	X	-

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 203875 atoms, of which 78861 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	AV	100	Total	C	H	N	O	S	0	0
			1687	505	876	177	125	4		

- Molecule 2 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AW	93	Total	C	H	N	O	S	0	0
			1490	462	764	129	129	6		

- Molecule 3 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	AX	109	Total	C	H	N	O	S	0	0
			1848	569	947	173	157	2		

- Molecule 4 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AY	130	Total	C	H	N	O	S	0	0
			2236	676	1166	221	168	5		

- Molecule 5 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	AZ	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	144	3		

- Molecule 6 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	Aa	106	Total	C	H	N	O	S	0	0
			1778	530	933	174	135	6		

- Molecule 7 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Ab	122	Total	C	H	N	O	S	0	0
			2163	641	1148	205	168	1		

- Molecule 8 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Ac	102	Total	C	H	N	O	S	0	0
			1750	521	918	177	129	5		

- Molecule 9 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Ad	86	Total	C	H	N	O	S	0	0
			1441	434	736	155	111	5		

- Molecule 10 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	Ae	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 11 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	Af	50	Total	C	H	N	O	S	0	0
			927	281	483	98	64	1		

- Molecule 12 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Ag	52	Total	C	H	N	O	S	0	0
			896	267	466	90	67	6		

- Molecule 13 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Ah	103	Total	C	H	N	O	S	0	0
			1754	528	912	172	136	6		

- Molecule 14 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Ai	91	Total	C	H	N	O	S	0	0
			1464	445	757	136	119	7		

- Molecule 15 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Aj	125	Total	C	H	N	O	S	0	0
			2071	622	1069	207	168	5		

- Molecule 16 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	BA	396	Total	C	H	N	O	S	0	0
			6537	2037	3339	601	546	14		

- Molecule 17 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	BB	359	Total	C	H	N	O	S	0	0
			5898	1802	3036	572	475	13		

- Molecule 18 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	BC	293	Total	C	H	N	O	S	0	0
			4807	1510	2421	435	427	14		

- Molecule 19 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	BD	216	Total	C	H	N	O	S	0	0
			3625	1119	1888	329	285	4		

- Molecule 20 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	CA	3483	Total	C	H	N	O	P	0	0
			112179	33315	37449	13662	24271	3482		

- Molecule 21 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	CB	119	Total	C	H	N	O	P	0	0
			3823	1132	1285	454	834	118		

- Molecule 22 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	CC	156	Total	C	H	N	O	P	0	0
			4989	1481	1674	585	1094	155		

- Molecule 23 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	CD	246	Total	C	H	N	O	S	0	0
			3867	1183	1979	387	312	6		

- Molecule 24 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AK	187	Total	C	H	N	O	S	0	0
			3142	944	1629	314	250	5		

- Molecule 25 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AL	156	Total	C	H	N	O	S	0	0
			2740	812	1438	279	202	9		

- Molecule 26 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AM	175	Total	C	H	N	O	S	0	0
			2943	925	1490	283	235	10		

- Molecule 27 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	AN	159	Total	C	H	N	O	S	0	0
			2666	823	1368	252	217	6		

- Molecule 28 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	AO	101	Total	C	H	N	O	S	0	0
			1675	529	850	144	150	2		

- Molecule 29 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	AP	131	Total	C	H	N	O	S	0	0
			2018	618	1039	184	172	5		

- Molecule 30 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	AQ	62	Total	C	H	N	O	S	0	0
			1052	332	533	101	83	3		

- Molecule 31 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	AR	119	Total	C	H	N	O	S	0	0
			2029	624	1053	183	168	1		

- Molecule 32 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	AS	134	Total	C	H	N	O	S	0	0
			2320	700	1205	226	186	3		

- Molecule 33 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	AT	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 34 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	AU	147	Total	C	H	N	O	S	0	0
			2373	736	1210	237	187	3		

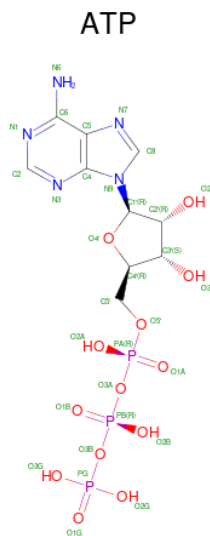
- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	AY	1	Total 1	Mg 1	0
35	AZ	1	Total 1	Mg 1	0
35	Ad	1	Total 1	Mg 1	0
35	BA	1	Total 1	Mg 1	0
35	CA	172	Total 172	Mg 172	0
35	CB	2	Total 2	Mg 2	0
35	CC	3	Total 3	Mg 3	0
35	AP	1	Total 1	Mg 1	0

- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

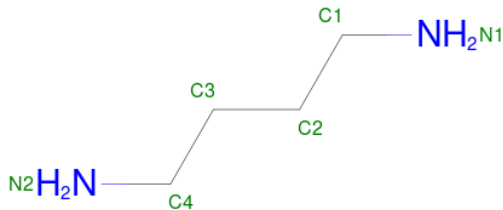
Mol	Chain	Residues	Atoms		AltConf
36	Aa	1	Total 1	Zn 1	0
36	Ad	1	Total 1	Zn 1	0
36	Ag	1	Total 1	Zn 1	0
36	Ah	1	Total 1	Zn 1	0
36	Ai	1	Total 1	Zn 1	0

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						AltConf
37	Ah	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 38 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $\text{C}_4\text{H}_{12}\text{N}_2$).



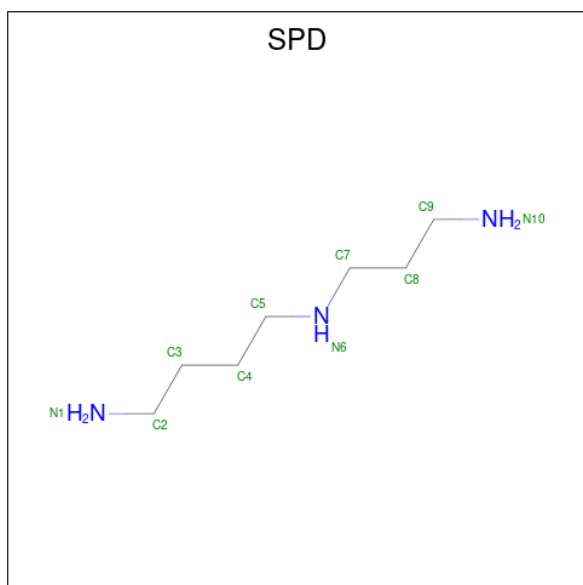
Mol	Chain	Residues	Atoms			AltConf
38	CA	1	Total 6	C 4	N 2	0
38	CA	1	Total 6	C 4	N 2	0
38	CA	1	Total 6	C 4	N 2	0

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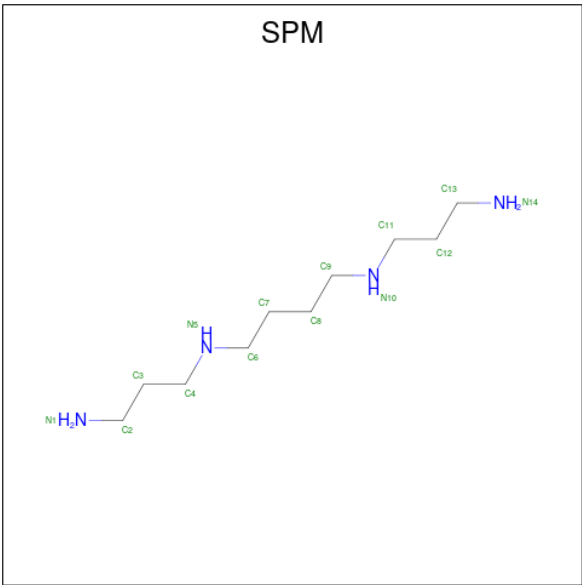
Mol	Chain	Residues	Atoms			AltConf
38	CA	1	Total	C	N	0
			6	4	2	
38	CB	1	Total	C	N	0
			6	4	2	

- Molecule 39 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms				AltConf
39	CA	1	Total	C	H	N	0
			12	7	2	3	
39	CA	1	Total	C	H	N	0
			12	7	2	3	
39	CA	1	Total	C	H	N	0
			12	7	2	3	
39	CA	1	Total	C	H	N	0
			12	7	2	3	
39	CA	1	Total	C	H	N	0
			12	7	2	3	
39	CA	1	Total	C	H	N	0
			12	7	2	3	

- Molecule 40 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
40	CA	1	Total	C	H	N	0
			23	10	9	4	
40	CA	1	Total	C	H	N	0
			23	10	9	4	
40	CA	1	Total	C	H	N	0
			23	10	9	4	
40	CA	1	Total	C	H	N	0
			23	10	9	4	
40	CA	1	Total	C	H	N	0
			23	10	9	4	

- Molecule 41 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
41	CA	41	Total	K	0
			41	41	
41	CD	2	Total	K	0
			2	2	
41	AM	1	Total	K	0
			1	1	
41	AN	1	Total	K	0
			1	1	
41	AP	1	Total	K	0
			1	1	

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	AV	54	Total 54	O 54	0
42	AW	49	Total 49	O 49	0
42	AX	50	Total 50	O 50	0
42	AY	56	Total 56	O 56	0
42	AZ	38	Total 38	O 38	0
42	Aa	31	Total 31	O 31	0
42	Ab	43	Total 43	O 43	0
42	Ac	72	Total 72	O 72	0
42	Ad	42	Total 42	O 42	0
42	Ae	23	Total 23	O 23	0
42	Af	16	Total 16	O 16	0
42	Ag	18	Total 18	O 18	0
42	Ah	64	Total 64	O 64	0
42	Ai	25	Total 25	O 25	0
42	Aj	53	Total 53	O 53	0
42	BA	115	Total 115	O 115	0
42	BB	118	Total 118	O 118	0
42	BC	115	Total 115	O 115	0
42	BD	76	Total 76	O 76	0
42	CA	5815	Total 5815	O 5815	0
42	CB	165	Total 165	O 165	0
42	CC	183	Total 183	O 183	0

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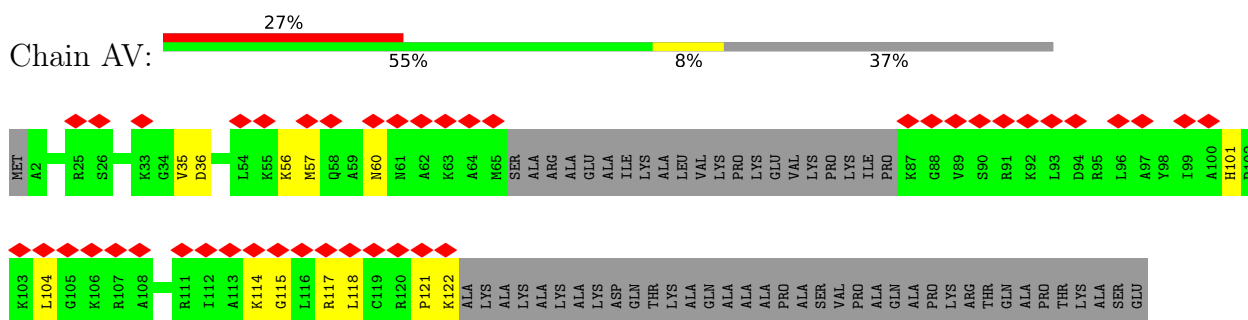
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Mol	Chain	Residues	Atoms		AltConf
42	CD	94	Total 94	O 94	0
42	AK	82	Total 82	O 82	0
42	AL	31	Total 31	O 31	0
42	AM	70	Total 70	O 70	0
42	AN	76	Total 76	O 76	0
42	AO	62	Total 62	O 62	0
42	AP	39	Total 39	O 39	0
42	AQ	25	Total 25	O 25	0
42	AR	41	Total 41	O 41	0
42	AS	43	Total 43	O 43	0
42	AT	67	Total 67	O 67	0
42	AU	60	Total 60	O 60	0

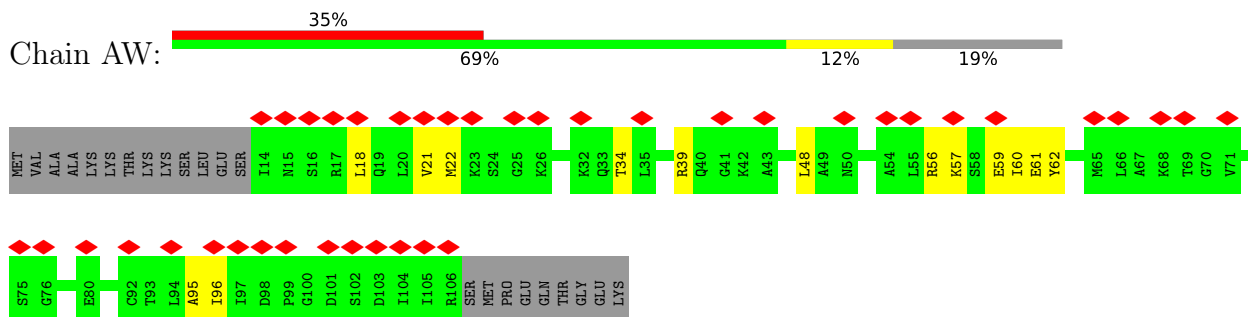
3 Residue-property plots

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

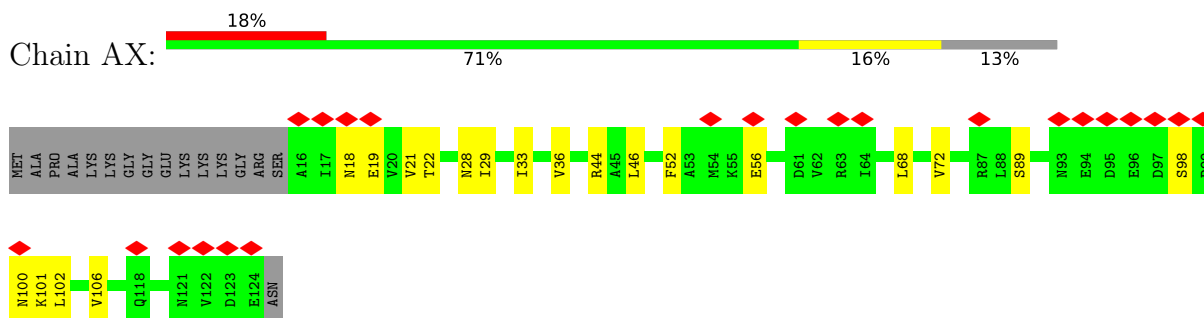
- Molecule 1: 60S ribosomal protein L29



- Molecule 2: 60S ribosomal protein L30



- Molecule 3: 60S ribosomal protein L31

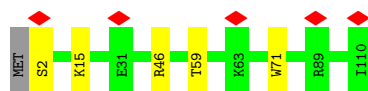


- Molecule 4: 60S ribosomal protein L32

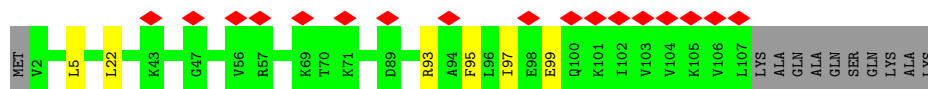




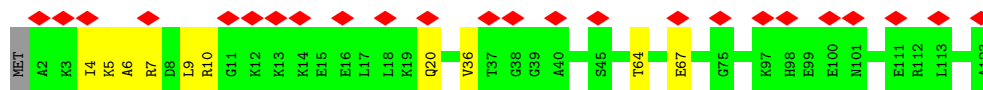
- Molecule 5: Large ribosomal subunit protein eL33



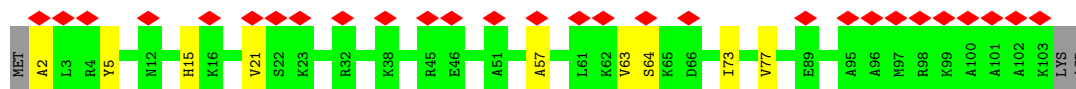
- Molecule 6: 60S ribosomal protein L34



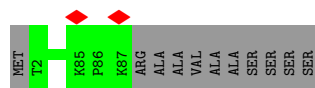
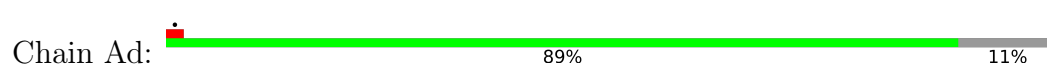
- Molecule 7: 60S ribosomal protein L35



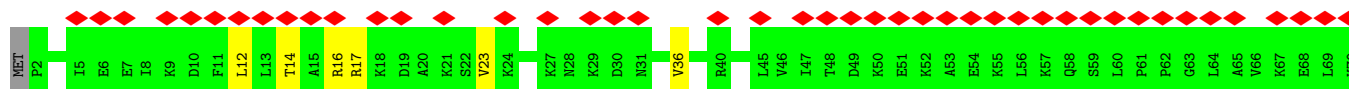
- Molecule 8: 60S ribosomal protein L36



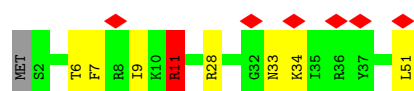
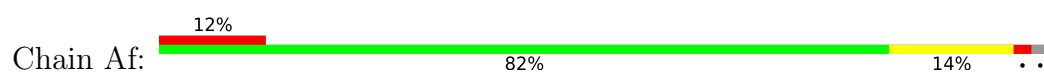
- Molecule 9: Large ribosomal subunit protein eL37



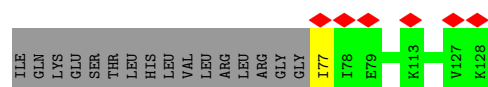
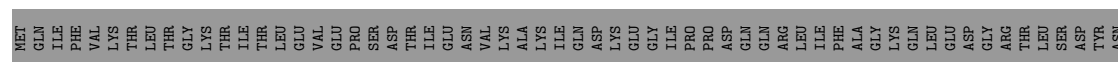
- Molecule 10: 60S ribosomal protein L38



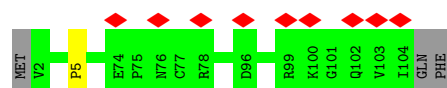
- Molecule 11: 60S ribosomal protein L39



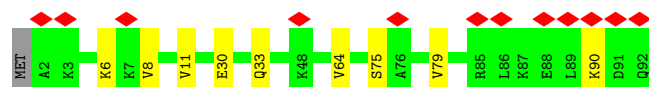
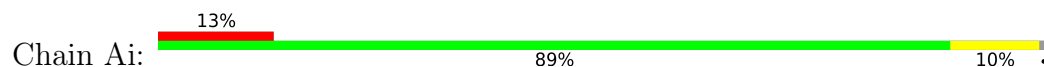
- Molecule 12: Large ribosomal subunit protein eL40



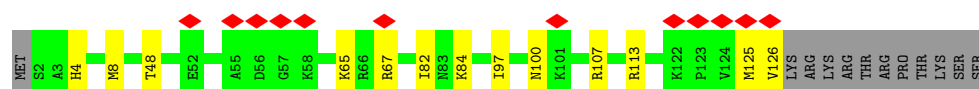
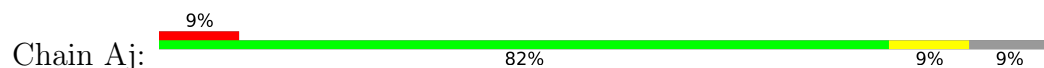
- Molecule 13: 60S ribosomal protein L36a



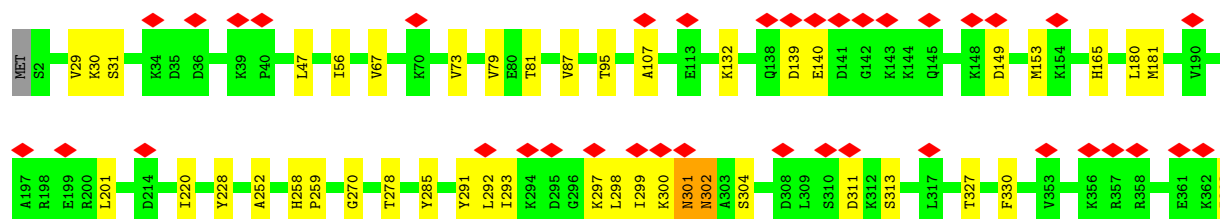
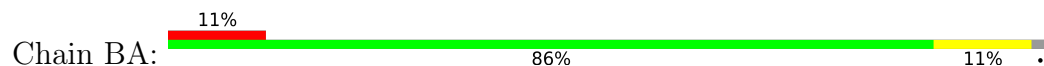
- Molecule 14: 60S ribosomal protein L37a



- Molecule 15: 60S ribosomal protein L28

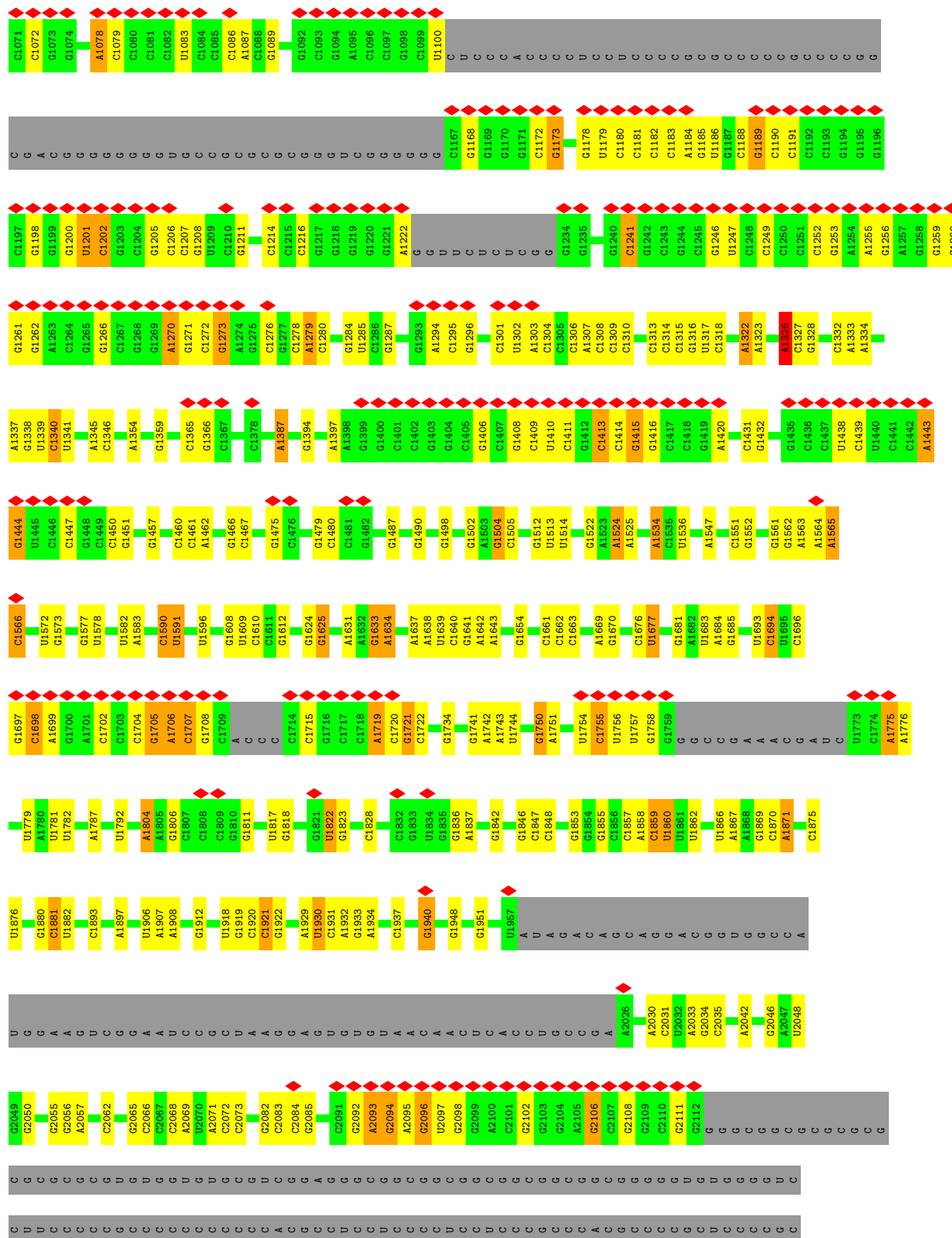


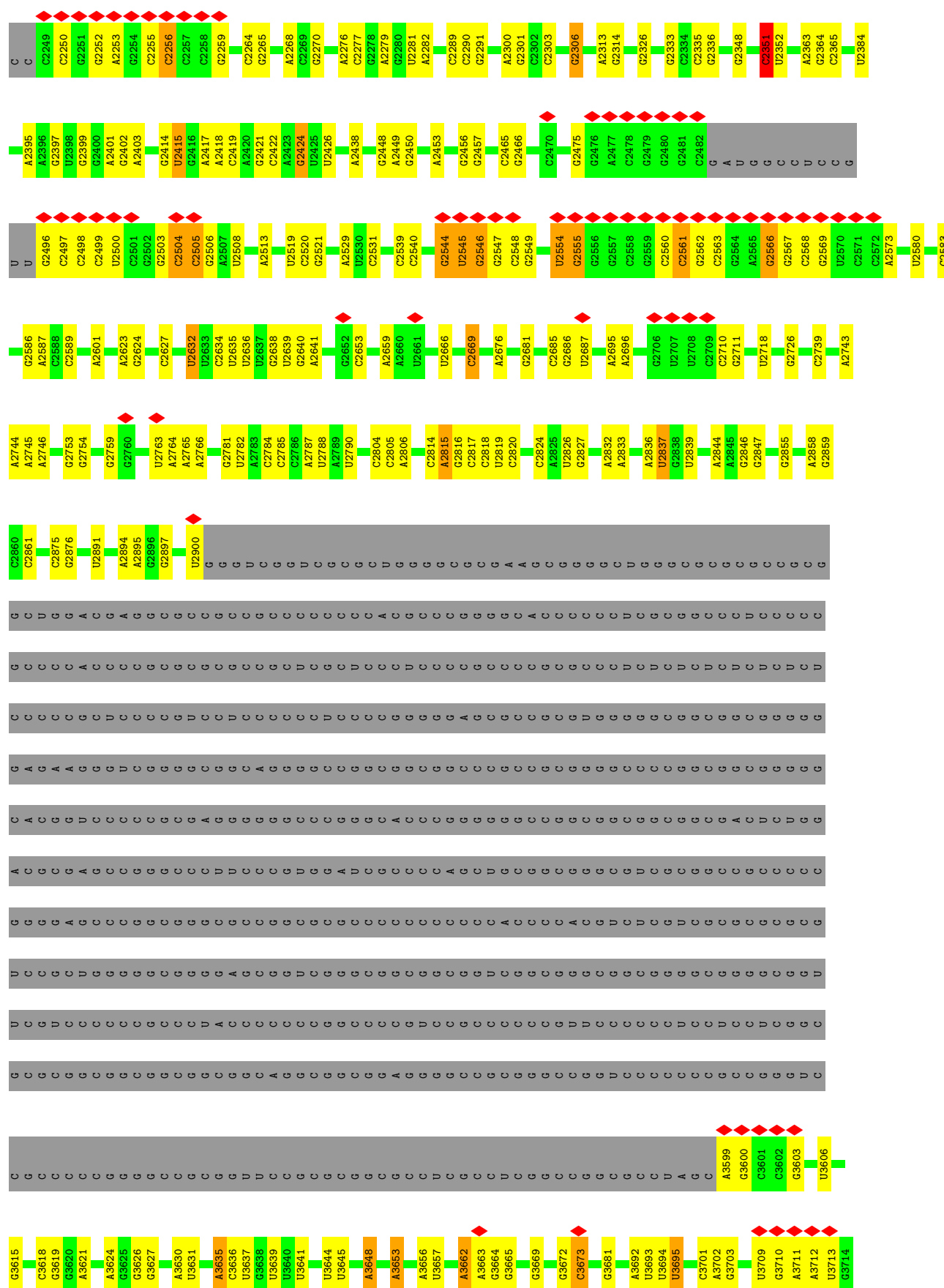
- Molecule 16: Large ribosomal subunit protein uL3



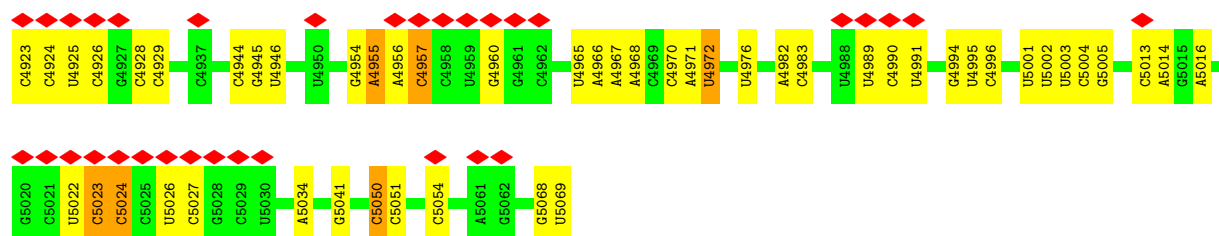
Chain CA:





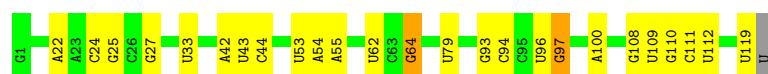






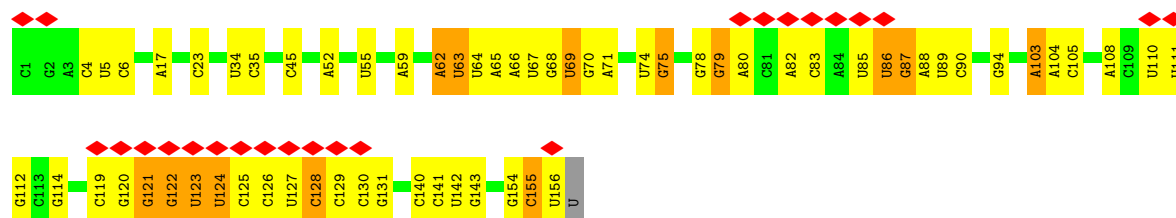
• Molecule 21: 5S rRNA

Chain CB: 78% 19% ..



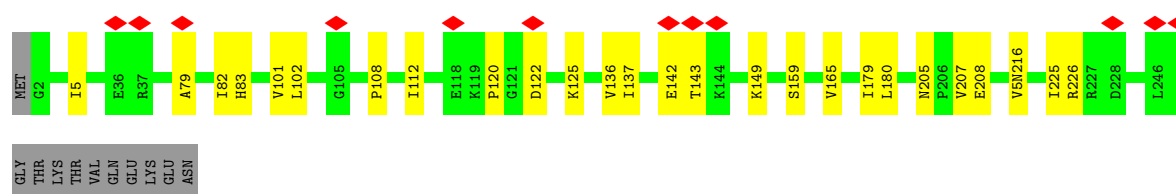
• Molecule 22: 5.8S rRNA

Chain CC: 15% 59% 31% 9% .



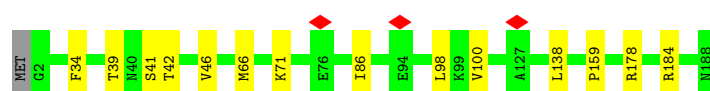
• Molecule 23: Large ribosomal subunit protein uL2

Chain CD: 5% 86% 10% .



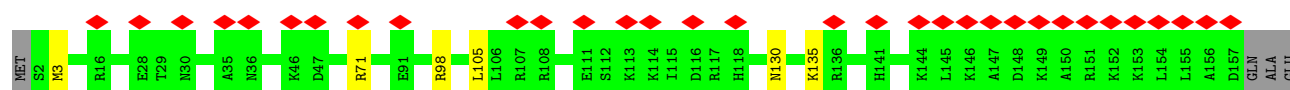
• Molecule 24: 60S ribosomal protein L18

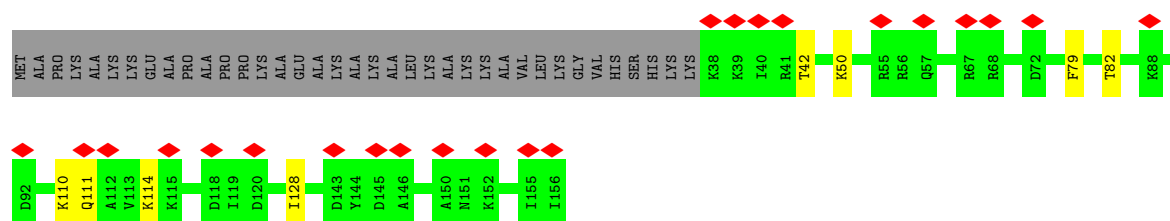
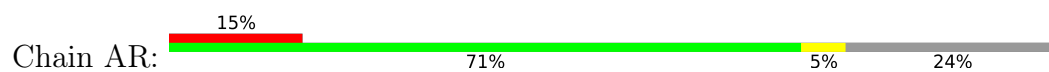
Chain AK: 92% 7% .



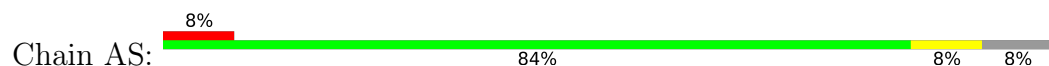
• Molecule 25: 60S ribosomal protein L19

Chain AL: 16% 77% 20%

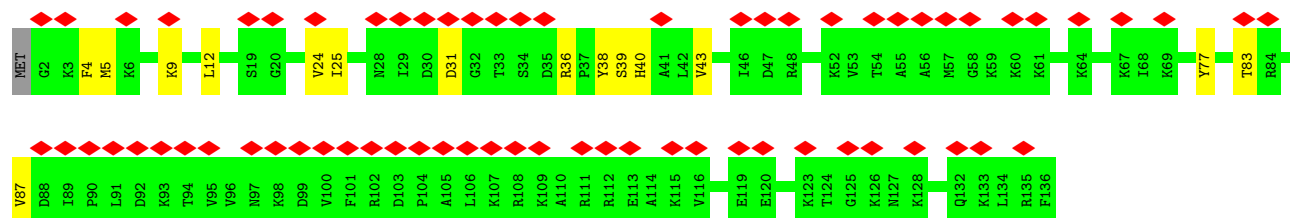
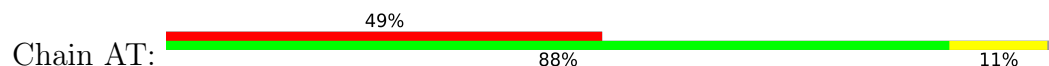




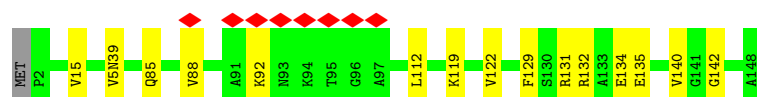
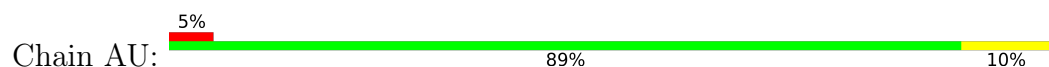
• Molecule 32: 60S ribosomal protein L26



• Molecule 33: 60S ribosomal protein L27



• Molecule 34: Large ribosomal subunit protein uL15



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.797	Depositor
Minimum map value	-0.428	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.648, 0.648, 0.648	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, ATP, 5MC, OMU, PSU, UY1, HIC, SPM, PUT, OMG, ZN, B8T, V5N, SPD, MLZ, OMC, 1MA, UR3, MG, 6MZ, A2M

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	AV	0.25	0/824	0.47	0/1086
2	AW	0.17	0/736	0.38	0/988
3	AX	0.16	0/916	0.36	0/1234
4	AY	0.21	0/1088	0.41	0/1451
5	AZ	0.14	0/895	0.34	0/1198
6	Aa	0.18	0/855	0.39	0/1140
7	Ab	0.18	0/1023	0.45	0/1351
8	Ac	0.17	0/843	0.37	0/1115
9	Ad	0.13	0/720	0.35	0/952
10	Ae	0.25	0/575	0.41	0/761
11	Af	0.29	0/454	0.55	1/599 (0.2%)
12	Ag	0.15	0/425	0.32	0/561
13	Ah	0.16	0/855	0.33	0/1128
14	Ai	0.18	0/717	0.36	0/953
15	Aj	0.20	0/1017	0.38	0/1364
16	BA	0.23	0/3253	0.49	2/4352 (0.0%)
17	BB	0.17	0/2916	0.37	0/3917
18	BC	0.18	0/2432	0.41	0/3256
19	BD	0.17	0/1771	0.38	0/2377
20	CA	0.14	0/80842	0.30	0/126109
21	CB	0.11	0/2836	0.28	0/4421
22	CC	0.13	0/3631	0.29	0/5657
23	CD	0.19	0/1913	0.41	0/2563
24	AK	0.21	0/1537	0.40	0/2052
25	AL	0.22	0/1318	0.42	0/1745
26	AM	0.24	1/1493 (0.1%)	0.41	1/2003 (0.0%)
27	AN	0.22	0/1326	0.42	0/1770
28	AO	0.25	0/839	0.50	0/1126
29	AP	0.21	0/993	0.41	0/1332
30	AQ	0.18	0/532	0.40	0/708
31	AR	0.17	0/993	0.39	0/1334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AS	0.21	0/1132	0.42	0/1504
33	AT	0.21	0/1130	0.39	0/1507
34	AU	0.15	0/1179	0.34	0/1573
All	All	0.16	1/124009 (0.0%)	0.33	4/185187 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	Af	0	1
25	AL	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AM	25	PRO	CA-C	-5.97	1.48	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	BA	301	ASN	N-CA-C	-7.00	99.52	110.36
26	AM	25	PRO	O-C-N	-5.84	118.62	121.31
11	Af	11	ARG	CG-CD-NE	5.50	124.10	112.00
16	BA	302	ASN	N-CA-CB	-5.24	108.20	114.17

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	AL	71	ARG	Sidechain
11	Af	11	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AV	811	876	876	12	0
2	AW	726	764	764	9	0
3	AX	901	947	946	13	0
4	AY	1070	1166	1165	9	0
5	AZ	876	912	912	5	0
6	Aa	845	933	933	6	0
7	Ab	1015	1148	1148	7	0
8	Ac	832	918	917	10	0
9	Ad	705	736	736	0	0
10	Ae	569	637	637	3	0
11	Af	444	483	483	10	0
12	Ag	430	466	466	1	0
13	Ah	842	912	912	1	0
14	Ai	707	757	756	7	0
15	Aj	1002	1069	1068	8	0
16	BA	3198	3339	3339	36	0
17	BB	2862	3036	3036	17	0
18	BC	2386	2421	2421	21	0
19	BD	1737	1888	1888	20	0
20	CA	74730	37449	37836	607	0
21	CB	2538	1285	1286	14	0
22	CC	3315	1674	1685	48	0
23	CD	1888	1979	1976	18	0
24	AK	1513	1629	1628	11	0
25	AL	1302	1438	1438	4	0
26	AM	1453	1490	1490	11	0
27	AN	1298	1368	1366	6	0
28	AO	825	850	850	16	0
29	AP	979	1039	1039	5	0
30	AQ	519	533	533	5	0
31	AR	976	1053	1053	9	0
32	AS	1115	1205	1205	13	0
33	AT	1107	1182	1182	17	0
34	AU	1163	1210	1206	10	0
35	AP	1	0	0	0	0
35	AY	1	0	0	0	0
35	AZ	1	0	0	0	0
35	Ad	1	0	0	0	0
35	BA	1	0	0	0	0
35	CA	172	0	0	0	0
35	CB	2	0	0	0	0
35	CC	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	Aa	1	0	0	0	0
36	Ad	1	0	0	0	0
36	Ag	1	0	0	0	0
36	Ah	1	0	0	0	0
36	Ai	1	0	0	0	0
37	Ah	31	12	12	2	0
38	CA	24	0	48	16	0
38	CB	6	0	12	5	0
39	CA	60	12	113	13	0
40	CA	70	45	130	2	0
41	AM	1	0	0	0	0
41	AN	1	0	0	0	0
41	AP	1	0	0	0	0
41	CA	41	0	0	0	0
41	CD	2	0	0	0	0
42	AK	82	0	0	0	0
42	AL	31	0	0	0	0
42	AM	70	0	0	0	0
42	AN	76	0	0	0	0
42	AO	62	0	0	0	0
42	AP	39	0	0	1	0
42	AQ	25	0	0	0	0
42	AR	41	0	0	0	0
42	AS	43	0	0	0	0
42	AT	67	0	0	0	0
42	AU	60	0	0	0	0
42	AV	54	0	0	0	0
42	AW	49	0	0	0	0
42	AX	50	0	0	0	0
42	AY	56	0	0	0	0
42	AZ	38	0	0	0	0
42	Aa	31	0	0	0	0
42	Ab	43	0	0	0	0
42	Ac	72	0	0	0	0
42	Ad	42	0	0	0	0
42	Ae	23	0	0	0	0
42	Af	16	0	0	0	0
42	Ag	18	0	0	0	0
42	Ah	64	0	0	0	0
42	Ai	25	0	0	0	0
42	Aj	53	0	0	0	0
42	BA	115	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BB	118	0	0	0	0
42	BC	115	0	0	0	0
42	BD	76	0	0	0	0
42	CA	5815	0	0	6	0
42	CB	165	0	0	0	0
42	CC	183	0	0	0	0
42	CD	94	0	0	0	0
All	All	125014	78861	79491	929	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (929) 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)
20:CA:3718:A2M:O4'	20:CA:3718:A2M:C1'	1.63	1.21
2:AW:21:VAL:HG11	2:AW:96:ILE:HD12	1.63	0.81
21:CB:96:U:O4	38:CB:201:PUT:H42	1.81	0.80
20:CA:3717:A:H2'	20:CA:3718:A2M:H8	1.64	0.80
28:AO:44:GLN:HG3	28:AO:63:ILE:HD11	1.67	0.76
20:CA:2050:G:H21	39:CA:5410:SPD:H72	1.51	0.76
20:CA:463:A:H61	20:CA:692:A:H61	1.33	0.75
16:BA:301:ASN:O	16:BA:302:ASN:HB3	1.87	0.74
2:AW:39:ARG:HG2	33:AT:5:MET:HE2	1.69	0.73
29:AP:13:LYS:HD2	29:AP:128:LEU:HD11	1.68	0.73
11:Af:9:ILE:HD12	11:Af:51:LEU:HD21	1.70	0.73
33:AT:5:MET:HE1	33:AT:77:TYR:CE2	2.23	0.73
28:AO:72:VAL:HG12	28:AO:72:VAL:O	1.89	0.72
37:Ah:202:ATP:H8	20:CA:4341:C:H42	1.37	0.71
17:BB:304:ALA:HB1	20:CA:2096:G:H21	1.55	0.70
20:CA:3636:C:H4'	20:CA:3825:A2M:H2	1.72	0.70
20:CA:4744:A:H61	20:CA:4956:A:H62	1.40	0.70
21:CB:97:G:O6	38:CB:201:PUT:H31	1.92	0.69
14:Ai:79:VAL:HG22	23:CD:112:ILE:HD13	1.73	0.69
20:CA:1270:A:H8	20:CA:2106:G:H21	1.42	0.68
20:CA:3917:A:C5	38:CA:5401:PUT:H31	2.29	0.67
24:AK:39:THR:HG22	24:AK:41:SER:H	1.58	0.67
8:Ac:2:ALA:N	8:Ac:5:TYR:HH	1.94	0.66
11:Af:11:ARG:HD3	22:CC:45:C:H4'	1.78	0.66
32:AS:116:LYS:O	32:AS:120:GLU:OE1	2.13	0.66
20:CA:3718:A2M:H2	20:CA:3934:G:O4'	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CA:5410:SPD:H42	39:CA:5410:SPD:H81	1.78	0.65
39:CA:5410:SPD:H42	39:CA:5410:SPD:C8	2.27	0.65
39:CA:5405:SPD:H22	42:CA:6600:HOH:O	1.96	0.65
20:CA:2050:G:C2'	39:CA:5410:SPD:H91	2.30	0.62
16:BA:67:VAL:HG11	29:AP:91:LYS:HD2	1.80	0.62
20:CA:4498:OMU:HM22	20:CA:4499:OMG:C8	2.35	0.62
1:AV:57:MET:HE3	20:CA:1811:G:H21	1.65	0.62
20:CA:455:C:H1'	20:CA:456:C:O2	2.00	0.62
16:BA:301:ASN:O	16:BA:302:ASN:CB	2.48	0.61
31:AR:82:THR:HG22	31:AR:82:THR:O	2.00	0.61
7:Ab:6:ALA:O	7:Ab:10:ARG:HG2	2.01	0.61
8:Ac:57:ALA:CB	8:Ac:73:ILE:HD11	2.31	0.61
16:BA:285:TYR:HD1	16:BA:363:ILE:HG21	1.66	0.61
16:BA:291:TYR:CE2	16:BA:327:THR:HG22	2.36	0.60
19:BD:180:VAL:HG21	19:BD:258:LEU:HD11	1.83	0.60
20:CA:2545:U:H3'	20:CA:2546:G:O4'	2.02	0.60
20:CA:1643:A:N3	38:CA:5403:PUT:H12	2.16	0.60
1:AV:117:ARG:HG3	1:AV:118:LEU:HD22	1.84	0.59
11:Af:34:LYS:HZ1	20:CA:361:C:H4'	1.67	0.59
29:AP:92:ASP:OD1	29:AP:94:VAL:HG22	2.03	0.59
33:AT:4:PHE:O	33:AT:9:LYS:HD2	2.02	0.59
20:CA:4378:A:O2'	20:CA:4379:A:H2'	2.03	0.59
6:Aa:95:PHE:CZ	33:AT:83:THR:HG22	2.37	0.58
22:CC:155:C:H2'	22:CC:156:U:O4'	2.03	0.58
18:BC:228:LYS:O	18:BC:229:ASN:OD1	2.21	0.58
19:BD:104:THR:HG22	19:BD:104:THR:O	2.03	0.58
20:CA:2554:U:O2	20:CA:2764:A:N7	2.37	0.58
20:CA:4393:G:O4'	20:CA:4447:5MC:HM52	2.03	0.58
20:CA:2050:G:O2'	39:CA:5410:SPD:H91	2.02	0.58
20:CA:1577:G:O2'	20:CA:1612:G:H4'	2.04	0.58
20:CA:2414:G:H2'	20:CA:2415:OMU:H6	1.86	0.58
20:CA:2448:G:H2'	20:CA:2449:A:C8	2.39	0.58
20:CA:3917:A:N6	38:CA:5401:PUT:H11	2.19	0.58
20:CA:953:C:N3	20:CA:954:C:C5	2.72	0.58
20:CA:3869:OMC:H6	20:CA:3869:OMC:O5'	1.87	0.58
20:CA:4484:A:C2	20:CA:4485:C:C5	2.91	0.58
20:CA:4563:U:C2	20:CA:4564:A:C8	2.92	0.57
5:AZ:2:SER:N	20:CA:4946:U:HO2'	2.02	0.57
20:CA:1338:G:H4'	20:CA:1339:U:H6	1.69	0.57
23:CD:137:ILE:HD11	23:CD:149:LYS:HB3	1.86	0.57
17:BB:318:PRO:O	17:BB:319:LEU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ab:36:VAL:HG11	31:AR:79:PHE:CD1	2.40	0.57
20:CA:1172:C:H42	20:CA:1188:C:H42	1.53	0.57
27:AN:159:MET:O	27:AN:160:ALA:HB2	2.05	0.57
16:BA:107:ALA:HB2	16:BA:201:LEU:HD22	1.87	0.56
34:AU:131:ARG:O	34:AU:135:GLU:HG3	2.05	0.56
16:BA:149:ASP:O	16:BA:153:MET:HG3	2.05	0.56
17:BB:211:TYR:OH	17:BB:218:ILE:HD11	2.06	0.56
20:CA:4611:A:C8	20:CA:4612:C:C6	2.94	0.56
28:AO:44:GLN:CG	28:AO:63:ILE:HD11	2.35	0.56
16:BA:29:VAL:HG12	16:BA:31:SER:H	1.71	0.56
20:CA:1637:A:OP2	38:CA:5403:PUT:H11	2.04	0.56
20:CA:2050:G:N2	39:CA:5410:SPD:H72	2.19	0.56
20:CA:1326:A2M:H2'	20:CA:1327:C:C6	2.40	0.56
20:CA:4970:C:C2	20:CA:4971:A:C8	2.93	0.56
38:CA:5401:PUT:H21	42:CA:6611:HOH:O	2.05	0.56
28:AO:72:VAL:HG11	28:AO:83:LEU:HD21	1.87	0.56
2:AW:39:ARG:HG2	33:AT:5:MET:CE	2.35	0.55
33:AT:31:ASP:O	33:AT:31:ASP:OD2	2.24	0.55
20:CA:3875:G:OP1	38:CA:5404:PUT:H42	2.06	0.55
2:AW:34:THR:HG23	2:AW:95:ALA:HB2	1.88	0.55
16:BA:378:ARG:HE	30:AQ:32:LEU:HD21	1.70	0.55
33:AT:5:MET:HE1	33:AT:77:TYR:CD2	2.41	0.55
20:CA:2815:A2M:H2'	20:CA:2816:G:C8	2.42	0.55
20:CA:4740:G:H2'	20:CA:4742:G:H5''	1.89	0.55
22:CC:120:G:C6	22:CC:131:G:C6	2.94	0.55
20:CA:1339:U:H2'	20:CA:1340:OMC:C6	2.41	0.55
20:CA:953:C:C2	20:CA:954:C:C6	2.95	0.55
20:CA:1190:C:N3	20:CA:1191:C:C5	2.75	0.55
20:CA:1697:G:H2'	20:CA:1698:C:O4'	2.07	0.55
20:CA:1205:G:H2'	20:CA:1206:C:H6	1.72	0.55
20:CA:1681:G:P	38:CA:5402:PUT:H41	2.47	0.55
20:CA:5004:C:H2'	20:CA:5005:G:O4'	2.07	0.55
3:AX:46:LEU:HD22	3:AX:72:VAL:HG11	1.89	0.54
20:CA:3636:C:C4'	20:CA:3825:A2M:H2	2.38	0.54
20:CA:4860:G:H1'	20:CA:4861:G:H5'	1.88	0.54
20:CA:4257:A:O2'	20:CA:4258:C:C6	2.57	0.54
20:CA:4392:OMG:H2'	20:CA:4447:5MC:HM51	1.89	0.54
20:CA:4653:C:C2	20:CA:4654:C:C5	2.95	0.54
20:CA:2281:U:C2	20:CA:2282:A:C8	2.96	0.54
34:AU:119:LYS:HA	34:AU:140:VAL:HG23	1.90	0.54
24:AK:46:VAL:HG11	24:AK:138:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:711:A:H2'	20:CA:712:C:C6	2.43	0.54
8:Ac:63:VAL:HG12	8:Ac:63:VAL:O	2.08	0.54
20:CA:485:C:H2'	20:CA:485:C:O2	2.07	0.54
20:CA:25:A:C8	20:CA:341:G:C8	2.96	0.54
27:AN:119:ALA:HB1	27:AN:124:THR:O	2.08	0.54
33:AT:5:MET:CE	33:AT:77:TYR:CE2	2.91	0.53
17:BB:276:ASN:OD1	17:BB:276:ASN:O	2.26	0.53
20:CA:2351:OMC:HM22	20:CA:2352:U:H5'	1.89	0.53
20:CA:4314:C:C2	20:CA:4315:A:C8	2.96	0.53
20:CA:4741:C:H4'	20:CA:4742:G:H5'	1.90	0.53
20:CA:954:C:O2'	20:CA:955:G:H5'	2.09	0.53
20:CA:1639:U:O4	38:CA:5403:PUT:H22	2.09	0.53
17:BB:230:LEU:HD21	17:BB:239:LYS:HD2	1.91	0.53
20:CA:3702:A:C2	20:CA:3703:G:C8	2.97	0.53
20:CA:4700:A:C2	20:CA:4701:A:C8	2.97	0.53
20:CA:2424:OMG:HM22	20:CA:2426:U:C6	2.43	0.53
20:CA:2817:C:C2	20:CA:2818:C:C5	2.96	0.53
20:CA:4714:C:C2	20:CA:4715:C:C6	2.96	0.53
20:CA:4258:C:C2	20:CA:4259:C:C5	2.97	0.53
20:CA:4260:U:H2'	20:CA:4261:C:C6	2.43	0.53
3:AX:68:LEU:HD22	3:AX:106:VAL:HG12	1.91	0.53
20:CA:1308:C:H2'	20:CA:1309:C:C6	2.43	0.53
18:BC:62:CYS:HB3	18:BC:105:LEU:HD22	1.91	0.53
20:CA:510:U:O2'	20:CA:511:C:P	2.67	0.53
20:CA:4774:C:HO2'	20:CA:4775:C:H6	1.54	0.53
20:CA:1207:C:C2	20:CA:1208:G:C8	2.96	0.52
20:CA:3664:G:H2'	20:CA:3665:G:H8	1.74	0.52
20:CA:1414:C:C4	20:CA:1415:G:C8	2.97	0.52
30:AQ:1:MET:SD	30:AQ:15:PRO:HB3	2.48	0.52
20:CA:499:G:H21	20:CA:504:G:H1	1.56	0.52
20:CA:4764:A:N7	26:AM:155:PRO:HB2	2.24	0.52
28:AO:28:PRO:HB3	28:AO:33:ILE:HD11	1.90	0.52
20:CA:1450:C:H2'	20:CA:1451:G:O4'	2.10	0.52
28:AO:84:LYS:HB2	28:AO:110:TYR:CZ	2.45	0.52
20:CA:2818:C:C2	20:CA:2819:U:C6	2.98	0.52
20:CA:1306:C:H2'	20:CA:1307:A:H8	1.75	0.52
28:AO:48:LYS:HG2	28:AO:53:ALA:HB2	1.92	0.52
4:AY:84:GLU:O	4:AY:87:VAL:HG22	2.09	0.52
20:CA:911:U:H2'	20:CA:912:G:O4'	2.10	0.52
20:CA:4260:U:H2'	20:CA:4261:C:H6	1.75	0.52
18:BC:191:ASN:O	18:BC:192:ALA:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:1719:A:H2'	20:CA:1720:C:O4'	2.09	0.52
20:CA:1857:C:H2'	20:CA:1858:A:H8	1.74	0.52
24:AK:46:VAL:HG11	24:AK:138:LEU:CD2	2.40	0.52
20:CA:1206:C:C2	20:CA:1207:C:C5	2.97	0.51
20:CA:4440:G:C4	20:CA:4441:A:C8	2.98	0.51
22:CC:70:G:N2	22:CC:87:G:H1'	2.25	0.51
16:BA:297:LYS:HG3	16:BA:299:ILE:HG13	1.92	0.51
20:CA:4921:C:N4	42:CA:5717:HOH:O	2.43	0.51
7:Ab:7:ARG:HH22	22:CC:86:U:H2'	1.75	0.51
20:CA:4610:A:C5	20:CA:4611:A:C2	2.98	0.51
22:CC:121:G:C4	22:CC:122:G:C8	2.98	0.51
20:CA:1447:C:H2'	20:CA:1447:C:O2	2.11	0.51
20:CA:2034:G:H2'	20:CA:2035:C:C6	2.44	0.51
20:CA:4405:G:C4	20:CA:4406:U:C6	2.98	0.51
20:CA:2544:G:H22	22:CC:124:U:H4'	1.75	0.51
22:CC:122:G:H2'	22:CC:123:U:O4'	2.11	0.51
20:CA:952:G:H2'	20:CA:953:C:H6	1.76	0.51
20:CA:4266:G:N3	20:CA:4266:G:H2'	2.25	0.51
20:CA:269:G:H2'	20:CA:270:U:O2	2.11	0.51
20:CA:496:G:H1	20:CA:657:C:H42	1.58	0.51
20:CA:1940:G:H22	20:CA:4434:C:H5''	1.75	0.51
20:CA:2818:C:N3	20:CA:2819:U:C5	2.79	0.51
20:CA:4406:U:C2	20:CA:4407:G:C8	2.99	0.51
32:AS:52:ASP:HB2	32:AS:110:LYS:HD2	1.93	0.51
20:CA:1859:B8T:C4	20:CA:1860:PSU:C2	2.93	0.51
20:CA:120:A:C2	20:CA:152:U:C2	2.98	0.51
20:CA:1633:G:H5'	20:CA:1634:A:OP1	2.10	0.51
20:CA:4536:OMC:HM22	20:CA:4537:C:O4'	2.10	0.51
23:CD:205:ASN:O	23:CD:208:GLU:HG2	2.11	0.51
11:Af:9:ILE:HG23	11:Af:51:LEU:HD11	1.92	0.50
20:CA:50:C:C2	20:CA:51:A:C8	2.99	0.50
20:CA:463:A:H61	20:CA:692:A:N6	2.05	0.50
21:CB:96:U:O4	38:CB:201:PUT:H11	2.11	0.50
21:CB:97:G:O6	38:CB:201:PUT:H12	2.11	0.50
34:AU:85:GLN:HA	34:AU:88:VAL:HG22	1.92	0.50
16:BA:291:TYR:HB3	16:BA:297:LYS:HD2	1.93	0.50
20:CA:672:C:N3	20:CA:673:C:C5	2.79	0.50
16:BA:73:VAL:HG23	30:AQ:1:MET:HE1	1.93	0.50
20:CA:672:C:C2	20:CA:673:C:C5	2.99	0.50
20:CA:1278:C:H2'	20:CA:1279:A:O4'	2.10	0.50
22:CC:89:U:H2'	22:CC:90:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Ae:23:VAL:HG22	10:Ae:36:VAL:HG22	1.93	0.50
16:BA:165:HIS:HB3	16:BA:180:LEU:HD23	1.92	0.50
20:CA:2384:U:O2'	25:AL:3:MET:HE1	2.10	0.50
20:CA:4919:G:C6	20:CA:4920:C:C5	2.99	0.50
21:CB:24:C:H2'	21:CB:25:G:O4'	2.12	0.50
1:AV:117:ARG:HG3	1:AV:118:LEU:N	2.26	0.50
20:CA:2465:C:H2'	20:CA:2466:G:O4'	2.12	0.50
20:CA:3648:A:H1'	20:CA:3785:A2M:N6	2.26	0.50
28:AO:29:VAL:HG21	28:AO:68:SER:HB2	1.93	0.50
4:AY:104:SER:HB2	20:CA:2306:G:OP1	2.11	0.50
18:BC:146:LEU:HD22	18:BC:163:LEU:HD12	1.94	0.50
20:CA:3775:A:H2'	20:CA:3776:G:O4'	2.11	0.50
20:CA:3873:G:H2'	20:CA:3874:G:C8	2.47	0.50
19:BD:47:ASN:HB2	19:BD:62:MET:CE	2.42	0.50
20:CA:2065:G:C5	20:CA:2066:C:C5	3.00	0.50
20:CA:3909:C:C2	20:CA:3910:C:C6	3.00	0.50
22:CC:70:G:H22	22:CC:87:G:H1'	1.77	0.50
3:AX:36:VAL:HG21	3:AX:44:ARG:HG2	1.93	0.50
20:CA:1443:A:N7	20:CA:1444:G:N7	2.60	0.50
20:CA:3635:A:C8	20:CA:3692:A:C8	2.99	0.50
20:CA:4611:A:N7	20:CA:4612:C:C5	2.80	0.50
20:CA:731:G:C6	20:CA:932:A:C4	3.00	0.49
1:AV:118:LEU:O	19:BD:72:LYS:HD2	2.13	0.49
2:AW:57:LYS:O	2:AW:61:GLU:HG3	2.13	0.49
5:AZ:59:THR:HG23	20:CA:4944:C:O2	2.12	0.49
20:CA:286:U:H2'	20:CA:287:U:C6	2.47	0.49
20:CA:1513:U:N3	20:CA:1514:U:C5	2.80	0.49
20:CA:4862:G:H2'	20:CA:4863:G:C8	2.47	0.49
8:Ac:2:ALA:HB3	8:Ac:5:TYR:CE2	2.47	0.49
11:Af:33:ASN:O	11:Af:34:LYS:HB3	2.12	0.49
20:CA:3886:G:P	39:CA:5410:SPD:HN12	2.36	0.49
20:CA:4578:G:H2'	20:CA:4579:PSU:C6	2.47	0.49
20:CA:3692:A:C5	20:CA:3693:U:C5	3.00	0.49
20:CA:3717:A:H2'	20:CA:3718:A2M:C8	2.39	0.49
20:CA:3739:C:C2	20:CA:3740:G:C8	3.00	0.49
2:AW:62:TYR:CE1	6:Aa:99:GLU:OE1	2.65	0.49
18:BC:287:PHE:CE2	18:BC:291:GLN:NE2	2.80	0.49
20:CA:1582:U:C2	20:CA:1583:A:C8	3.00	0.49
20:CA:4535:A:H2'	20:CA:4536:OMC:H6	1.78	0.49
20:CA:1206:C:H2'	20:CA:1207:C:H6	1.77	0.49
20:CA:1332:C:H2'	20:CA:1333:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:2072:C:C2	20:CA:2073:C:C5	3.01	0.49
20:CA:2529:A:H4'	20:CA:2531:C:C5	2.48	0.49
33:AT:87:VAL:O	33:AT:87:VAL:HG13	2.13	0.49
22:CC:83:C:O4'	22:CC:83:C:O2	2.31	0.49
16:BA:47:LEU:HD21	16:BA:181:MET:SD	2.53	0.49
19:BD:92:VAL:HG12	19:BD:93:THR:N	2.27	0.49
20:CA:2402:G:C2	20:CA:2403:A:C8	3.00	0.49
20:CA:2475:G:N1	31:AR:50:LYS:HG3	2.28	0.49
20:CA:3621:A:C8	20:CA:4642:U:H1'	2.48	0.49
16:BA:228:TYR:CE1	16:BA:270:GLY:HA2	2.48	0.49
20:CA:4652:G:H2'	20:CA:4653:C:H6	1.78	0.49
22:CC:108:A:C2	22:CC:112:G:C6	3.01	0.49
23:CD:142:GLU:O	23:CD:143:THR:OG1	2.24	0.49
20:CA:4340:U:C2	20:CA:4341:C:C6	3.01	0.48
22:CC:120:G:C6	22:CC:121:G:N7	2.80	0.48
16:BA:79:VAL:O	16:BA:81:THR:HG23	2.13	0.48
19:BD:114:ARG:HD2	19:BD:114:ARG:O	2.13	0.48
20:CA:734:G:C2	20:CA:735:G:C8	3.01	0.48
20:CA:3868:G:H22	20:CA:3900:G:H1'	1.78	0.48
20:CA:4469:U:C6	20:CA:4708:A:N7	2.80	0.48
20:CA:3774:A:H2'	20:CA:3775:A:N3	2.27	0.48
16:BA:299:ILE:HG23	16:BA:313:SER:HB3	1.96	0.48
20:CA:1206:C:N3	20:CA:1207:C:C5	2.81	0.48
20:CA:4713:G:C5	20:CA:4714:C:C5	3.01	0.48
20:CA:3909:C:O2	20:CA:4396:A:N1	2.47	0.48
24:AK:42:THR:O	24:AK:46:VAL:HG23	2.14	0.48
28:AO:80:LYS:HG2	28:AO:110:TYR:CE2	2.49	0.48
31:AR:111:GLN:HA	31:AR:114:LYS:HZ1	1.77	0.48
20:CA:1590:C:H4'	20:CA:1591:U:OP2	2.13	0.48
20:CA:3641:U:C6	20:CA:3645:U:C4	3.02	0.48
20:CA:4900:C:C5	20:CA:4901:G:C8	3.01	0.48
20:CA:4956:A:O2'	20:CA:4957:C:H6	1.96	0.48
20:CA:4965:U:H4'	20:CA:4966:A:H5'	1.95	0.48
5:AZ:15:LYS:HE3	20:CA:2068:C:OP1	2.13	0.48
19:BD:47:ASN:HB2	19:BD:62:MET:HE1	1.95	0.48
20:CA:511:C:O2'	20:CA:512:U:C6	2.66	0.48
20:CA:683:C:H2'	20:CA:684:G:O4'	2.13	0.48
20:CA:753:C:C5	20:CA:754:U:C5	3.02	0.48
20:CA:1307:A:H2'	20:CA:1308:C:H6	1.78	0.48
20:CA:1307:A:H2'	20:CA:1308:C:C6	2.49	0.48
20:CA:1669:A:H4'	20:CA:1685:G:N2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:3740:G:C5	20:CA:3741:C:C5	3.01	0.48
33:AT:9:LYS:O	33:AT:24:VAL:HA	2.13	0.48
20:CA:418:A:C2	22:CC:17:A:H1'	2.49	0.48
20:CA:1241:C:O4'	20:CA:1241:C:O2	2.32	0.48
20:CA:4489:G:C6	20:CA:4708:A:C5	3.02	0.48
20:CA:4699:U:H4'	20:CA:4700:A:OP1	2.14	0.48
20:CA:4749:C:H2'	20:CA:4750:G:O4'	2.13	0.48
23:CD:101:VAL:HG22	23:CD:165:VAL:HG22	1.96	0.48
24:AK:46:VAL:CG1	24:AK:138:LEU:HD21	2.44	0.48
20:CA:982:U:H2'	20:CA:983:C:C6	2.48	0.48
20:CA:4714:C:C4	20:CA:4715:C:C5	3.02	0.48
22:CC:75:OMG:OP2	32:AS:74:TYR:OH	2.31	0.48
26:AM:30:MET:HE1	26:AM:47:PHE:CB	2.44	0.48
20:CA:415:G:C5	20:CA:416:U:C5	3.02	0.47
20:CA:178:C:H2'	20:CA:178:C:O2	2.14	0.47
20:CA:2817:C:N3	20:CA:2818:C:C5	2.82	0.47
32:AS:120:GLU:O	32:AS:124:LYS:HG2	2.14	0.47
14:AI:30:GLU:HA	14:AI:33:GLN:HG2	1.96	0.47
20:CA:282:C:C2	20:CA:283:G:C8	3.02	0.47
20:CA:1720:C:H3'	20:CA:1721:G:C8	2.49	0.47
20:CA:2417:A:C4	20:CA:2418:A:C8	3.02	0.47
20:CA:2819:U:O2	20:CA:2820:C:C6	2.67	0.47
25:AL:98:ARG:NH2	25:AL:130:ASN:OD1	2.47	0.47
20:CA:456:C:O2	20:CA:456:C:O4'	2.32	0.47
20:CA:1775:A:H3'	20:CA:1776:A:C8	2.49	0.47
20:CA:2264:C:H2'	20:CA:2265:G:O4'	2.14	0.47
20:CA:3909:C:O2	20:CA:3909:C:H2'	2.14	0.47
20:CA:5023:C:H3'	20:CA:5024:C:C5'	2.45	0.47
20:CA:453:G:N3	20:CA:453:G:C2'	2.78	0.47
20:CA:4495:G:C2	20:CA:4496:A:N7	2.82	0.47
6:Aa:5:LEU:HD11	6:Aa:22:LEU:HD22	1.97	0.47
16:BA:302:ASN:OD1	16:BA:330:PHE:HE2	1.98	0.47
20:CA:453:G:N3	20:CA:453:G:H2'	2.29	0.47
20:CA:1189:G:H2'	20:CA:1190:C:H6	1.79	0.47
20:CA:1512:G:H2'	20:CA:1513:U:H6	1.79	0.47
20:CA:2638:G:N2	20:CA:2718:U:H2'	2.29	0.47
20:CA:4956:A:C8	20:CA:4957:C:C5	3.02	0.47
33:AT:39:SER:HB3	33:AT:77:TYR:CD2	2.49	0.47
11:Af:28:ARG:HA	11:Af:33:ASN:ND2	2.29	0.47
19:BD:66:LYS:HB3	19:BD:68:MET:HE3	1.96	0.47
20:CA:259:C:H2'	20:CA:260:C:O2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:750:U:C2	20:CA:751:G:C8	3.03	0.47
20:CA:3783:A:C8	20:CA:3792:OMG:C8	3.03	0.47
20:CA:254:G:H2'	20:CA:255:C:H6	1.78	0.47
20:CA:2844:A:O2'	20:CA:4631:G:H4'	2.15	0.47
20:CA:266:C:HO2'	20:CA:267:G:H8	1.63	0.47
20:CA:1475:G:N2	20:CA:1490:G:C5	2.83	0.47
20:CA:4629:U:C2	20:CA:4630:G:C8	3.03	0.47
22:CC:142:U:H2'	22:CC:143:G:O4'	2.14	0.47
20:CA:1308:C:C2	20:CA:1309:C:C5	3.03	0.46
20:CA:4966:A:H2'	20:CA:4967:A:O4'	2.14	0.46
7:Ab:7:ARG:NH2	22:CC:86:U:H2'	2.31	0.46
16:BA:56:ILE:HD12	16:BA:365:LEU:CD2	2.45	0.46
20:CA:2496:G:H2'	20:CA:2497:C:H6	1.80	0.46
20:CA:3823:G:H2'	20:CA:3824:A:C8	2.50	0.46
20:CA:4537:C:H2'	20:CA:4538:G:C8	2.50	0.46
23:CD:101:VAL:C	23:CD:102:LEU:HD12	2.40	0.46
16:BA:299:ILE:CG2	16:BA:313:SER:HB3	2.45	0.46
16:BA:300:LYS:HG2	16:BA:311:ASP:HA	1.97	0.46
20:CA:1817:U:O2'	20:CA:1818:G:H5'	2.14	0.46
20:CA:3619:G:H22	20:CA:3624:A:H1'	1.80	0.46
20:CA:3648:A:H1'	20:CA:3785:A2M:H61	1.80	0.46
20:CA:3885:G:O5'	39:CA:5410:SPD:H82	2.15	0.46
20:CA:4610:A:C4	20:CA:4611:A:C2	3.04	0.46
34:AU:140:VAL:HG22	34:AU:140:VAL:O	2.16	0.46
1:AV:114:LYS:O	1:AV:117:ARG:HG2	2.16	0.46
11:Af:34:LYS:NZ	20:CA:361:C:H4'	2.30	0.46
20:CA:2567:G:H2'	20:CA:2568:C:H6	1.80	0.46
20:CA:4535:A:C2	20:CA:4536:OMC:C5	3.03	0.46
20:CA:4887:C:H2'	20:CA:4888:U:O4'	2.16	0.46
28:AO:24:ASP:OD1	28:AO:26:THR:HG23	2.16	0.46
20:CA:385:A:H4'	20:CA:386:A:OP1	2.16	0.46
20:CA:2817:C:H2'	20:CA:2818:C:H6	1.79	0.46
20:CA:2897:G:C4	20:CA:3603:G:N2	2.84	0.46
20:CA:3782:5MC:HN41	20:CA:3809:G:H2'	1.80	0.46
20:CA:3896:C:H2'	20:CA:3897:G:C4	2.50	0.46
18:BC:83:LEU:N	18:BC:84:PRO:HD2	2.30	0.46
20:CA:281:U:C2	20:CA:282:C:C6	3.03	0.46
20:CA:1318:C:H42	20:CA:1322:1MA:H8	1.64	0.46
20:CA:1338:G:H4'	20:CA:1339:U:C6	2.50	0.46
20:CA:1870:C:H2'	20:CA:1871:A2M:H8	1.98	0.46
20:CA:1893:C:H1'	20:CA:1937:C:O2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:2816:G:C5	20:CA:2817:C:C5	3.03	0.46
20:CA:4440:G:C5	20:CA:4441:A:N7	2.83	0.46
21:CB:27:G:H21	21:CB:55:A:N6	2.14	0.46
22:CC:121:G:C6	22:CC:122:G:C5	3.04	0.46
28:AO:57:GLY:O	28:AO:60:VAL:HG13	2.16	0.46
16:BA:301:ASN:HA	16:BA:304:SER:OG	2.14	0.46
18:BC:69:ILE:HD12	18:BC:69:ILE:H	1.81	0.46
20:CA:1326:A2M:H2'	20:CA:1327:C:H6	1.81	0.46
20:CA:3825:A2M:HM'3	20:CA:3825:A2M:H1'	1.82	0.46
20:CA:7:C:H2'	20:CA:8:U:C6	2.51	0.46
20:CA:1853:G:H22	38:CA:5402:PUT:H32	1.81	0.46
20:CA:2815:A2M:HM'3	20:CA:2815:A2M:H1'	1.77	0.46
20:CA:3653:A:C2	20:CA:3692:A:O4'	2.68	0.46
20:CA:2505:C:C6	20:CA:2506:G:O6	2.69	0.46
20:CA:2805:C:N4	20:CA:2806:A:N6	2.64	0.46
20:CA:4239:A:H2'	20:CA:4240:G:C8	2.51	0.46
8:Ac:57:ALA:HB2	8:Ac:73:ILE:HD11	1.97	0.45
19:BD:201:ILE:HG13	19:BD:203:ILE:HG23	1.97	0.45
20:CA:1882:U:C4	20:CA:2279:A:C2	3.03	0.45
24:AK:71:LYS:O	24:AK:71:LYS:HG2	2.14	0.45
20:CA:1504:G:H2'	20:CA:1505:C:C6	2.52	0.45
20:CA:1513:U:C2	20:CA:1514:U:C6	3.04	0.45
20:CA:4619:U:H2'	20:CA:4620:OMU:H6	1.97	0.45
20:CA:1387:A:C6	34:AU:112:LEU:HD13	2.52	0.45
20:CA:1853:G:N2	38:CA:5402:PUT:H32	2.31	0.45
20:CA:3744:OMG:HM23	20:CA:3744:OMG:H1'	1.84	0.45
20:CA:4635:A:H3'	20:CA:4636:U:H4'	1.98	0.45
15:Aj:100:ASN:HD21	20:CA:478:G:H21	1.63	0.45
18:BC:65:ALA:HB2	18:BC:74:ILE:HD13	1.98	0.45
20:CA:1565:A:C5	20:CA:1566:C:H1'	2.52	0.45
20:CA:3719:A:C4	20:CA:3720:G:C8	3.05	0.45
20:CA:4638:U:H2'	20:CA:4639:G:N3	2.32	0.45
34:AU:88:VAL:O	34:AU:92:LYS:HG2	2.15	0.45
15:Aj:97:ILE:HD13	15:Aj:107:ARG:HA	1.97	0.45
20:CA:732:A:H2'	20:CA:733:A:O4'	2.17	0.45
20:CA:4758:U:O2	20:CA:4758:U:O4'	2.35	0.45
20:CA:4759:C:H2'	20:CA:4760:G:C8	2.51	0.45
27:AN:118:GLU:O	27:AN:121:GLU:HG2	2.17	0.45
4:AY:65:LYS:O	4:AY:69:MET:HE3	2.16	0.45
16:BA:87:VAL:HG22	16:BA:87:VAL:O	2.16	0.45
20:CA:1206:C:C2	20:CA:1207:C:C6	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:1207:C:N3	20:CA:1208:G:N7	2.65	0.45
20:CA:4347:G:O2'	20:CA:4348:A:H5'	2.16	0.45
20:CA:4537:C:H2'	20:CA:4538:G:H8	1.81	0.45
20:CA:4584:A:H2'	20:CA:4585:U:O4'	2.16	0.45
28:AO:72:VAL:O	28:AO:72:VAL:CG1	2.61	0.45
7:Ab:5:LYS:O	7:Ab:9:LEU:HG	2.17	0.45
8:Ac:15:HIS:HB3	20:CA:72:C:C6	2.51	0.45
13:Ah:5:PRO:HD3	20:CA:4232:U:C2	2.51	0.45
20:CA:1201:U:C2	20:CA:1202:C:C2	3.04	0.45
20:CA:1460:C:H2'	20:CA:1461:C:H6	1.82	0.45
20:CA:2638:G:O2'	20:CA:2639:U:H5'	2.16	0.45
20:CA:4498:OMU:H6	20:CA:4498:OMU:O5'	2.16	0.45
24:AK:178:ARG:HA	24:AK:184:ARG:O	2.16	0.45
18:BC:15:ARG:HD2	20:CA:1743:A:O4'	2.17	0.45
20:CA:23:C:H2'	20:CA:24:G:O4'	2.17	0.45
20:CA:260:C:O2	20:CA:260:C:O4'	2.34	0.45
20:CA:1460:C:C2	20:CA:1461:C:C5	3.05	0.45
20:CA:2566:G:H2'	20:CA:2567:G:C8	2.52	0.45
20:CA:4242:U:H4'	20:CA:4243:C:OP1	2.17	0.45
22:CC:5:U:C2	22:CC:6:C:C5	3.05	0.45
23:CD:207:VAL:HG13	23:CD:208:GLU:HB3	1.99	0.45
16:BA:29:VAL:O	16:BA:30:LYS:HB2	2.17	0.45
17:BB:66:SER:HA	17:BB:77:PRO:HA	1.99	0.45
17:BB:66:SER:O	17:BB:67:TRP:HB2	2.16	0.45
20:CA:255:C:C2	20:CA:256:G:C8	3.05	0.45
20:CA:662:C:N4	20:CA:663:G:O6	2.50	0.45
20:CA:917:A:H2'	20:CA:918:G:O4'	2.17	0.45
20:CA:1089:G:H4'	27:AN:140:PHE:CE2	2.51	0.45
20:CA:1414:C:C4	20:CA:1415:G:N7	2.85	0.45
20:CA:2836:A:H2'	20:CA:2837:OMU:H6	1.99	0.45
20:CA:3672:G:H3'	20:CA:3673:C:H5''	1.98	0.45
20:CA:4232:U:H4'	20:CA:4233:A:O4'	2.17	0.45
20:CA:4956:A:O2'	20:CA:4957:C:C5'	2.64	0.45
22:CC:120:G:C6	22:CC:121:G:C5	3.04	0.45
15:Aj:67:ARG:NE	20:CA:480:C:OP1	2.50	0.45
16:BA:132:LYS:HB2	20:CA:4727:A:OP1	2.17	0.45
18:BC:146:LEU:HD23	20:CA:4323:A:C2	2.52	0.45
20:CA:922:C:H2'	20:CA:923:C:O4'	2.17	0.45
20:CA:4171:C:C2	20:CA:4172:A:C8	3.05	0.45
20:CA:4258:C:N3	20:CA:4259:C:C5	2.84	0.45
22:CC:120:G:C4	22:CC:121:G:C8	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CD:122:ASP:OD1	23:CD:122:ASP:O	2.35	0.45
26:AM:15:ARG:HB3	26:AM:27:LEU:HD23	1.99	0.45
18:BC:124:GLU:O	18:BC:124:GLU:HG2	2.17	0.44
20:CA:1858:A:C2	20:CA:1859:B8T:C5	3.00	0.44
20:CA:2832:A:C4	20:CA:2833:A:C8	3.06	0.44
20:CA:3692:A:C4	20:CA:3693:U:C6	3.05	0.44
20:CA:4652:G:H2'	20:CA:4653:C:C6	2.52	0.44
22:CC:64:U:C2	22:CC:65:A:C8	3.05	0.44
32:AS:51:LYS:O	32:AS:70:VAL:HB	2.18	0.44
33:AT:39:SER:HB3	33:AT:77:TYR:CE2	2.51	0.44
20:CA:285:G:H2'	20:CA:286:U:C6	2.52	0.44
20:CA:952:G:H2'	20:CA:953:C:C6	2.53	0.44
20:CA:2062:C:OP1	26:AM:2:LYS:N	2.50	0.44
20:CA:2520:C:H2'	20:CA:2521:G:H8	1.81	0.44
20:CA:2634:C:C2	20:CA:2635:U:C5	3.04	0.44
20:CA:3896:C:O2	20:CA:4564:A:N1	2.50	0.44
20:CA:4212:A:H4'	20:CA:4213:A:N3	2.32	0.44
20:CA:4261:C:C2	20:CA:4262:C:C5	3.05	0.44
20:CA:4712:C:C2	20:CA:4713:G:C8	3.05	0.44
26:AM:74:ARG:O	26:AM:100:LEU:HD23	2.17	0.44
28:AO:23:LEU:O	28:AO:23:LEU:HD12	2.17	0.44
19:BD:99:ASP:O	19:BD:100:LYS:HB2	2.18	0.44
20:CA:162:A:H2'	20:CA:163:A:N3	2.33	0.44
20:CA:172:C:O2	20:CA:172:C:O4'	2.36	0.44
20:CA:910:G:C6	20:CA:911:U:C4	3.05	0.44
20:CA:1906:U:H2'	20:CA:1907:A:H8	1.81	0.44
20:CA:4254:G:H2'	20:CA:4254:G:N3	2.32	0.44
20:CA:4637:OMG:H2'	20:CA:4638:U:C6	2.52	0.44
20:CA:4922:C:N4	20:CA:4923:C:H41	2.15	0.44
22:CC:78:G:H2'	22:CC:79:G:O4'	2.17	0.44
22:CC:140:C:H2'	22:CC:141:C:H6	1.82	0.44
3:AX:29:ILE:O	3:AX:33:ILE:HG12	2.18	0.44
4:AY:127:ALA:HB2	20:CA:2326:G:H5''	2.00	0.44
18:BC:234:ASP:OD1	18:BC:234:ASP:O	2.35	0.44
20:CA:4:G:H2'	20:CA:5:A:H8	1.81	0.44
20:CA:445:U:H2'	20:CA:446:C:O4'	2.18	0.44
20:CA:1322:1MA:C6	20:CA:1326:A2M:C8	3.00	0.44
20:CA:4355:G:C2	20:CA:4356:G:C8	3.06	0.44
39:CA:5407:SPD:H32	42:CA:9493:HOH:O	2.16	0.44
27:AN:159:MET:O	27:AN:159:MET:HG2	2.18	0.44
18:BC:66:TYR:HE2	18:BC:68:ARG:HE	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:1693:U:H2'	20:CA:1694:C:O4'	2.18	0.44
20:CA:1706:A:O2'	20:CA:1707:C:O4'	2.34	0.44
20:CA:2819:U:O2	20:CA:2819:U:H2'	2.16	0.44
20:CA:4313:A:C6	20:CA:4314:C:C5	3.06	0.44
31:AR:42:THR:HG22	31:AR:42:THR:O	2.17	0.44
32:AS:51:LYS:O	32:AS:70:VAL:O	2.35	0.44
19:BD:151:ILE:HG12	19:BD:161:ARG:HG2	1.99	0.44
20:CA:664:G:H2'	20:CA:665:C:C6	2.53	0.44
20:CA:1317:U:H2'	20:CA:1318:C:C6	2.52	0.44
20:CA:1551:C:C2'	20:CA:1552:G:H5'	2.48	0.44
20:CA:1590:C:H5''	20:CA:1591:U:O5'	2.17	0.44
20:CA:2544:G:C2	20:CA:2545:U:H1'	2.52	0.44
39:CA:5407:SPD:H41	42:CA:6484:HOH:O	2.17	0.44
22:CC:71:A:C2	22:CC:88:A:C1'	3.01	0.44
11:Af:6:THR:OG1	11:Af:9:ILE:HG12	2.18	0.44
18:BC:236:MET:HA	18:BC:239:MET:HG2	1.98	0.44
20:CA:510:U:O2'	20:CA:511:C:OP1	2.36	0.44
20:CA:1804:A:O4'	20:CA:1806:G:C8	2.70	0.44
20:CA:1929:A:H5'	20:CA:1930:U:OP1	2.18	0.44
20:CA:4504:C:H2'	20:CA:4505:C:C6	2.52	0.44
20:CA:4578:G:H2'	20:CA:4579:PSU:H6	1.82	0.44
22:CC:120:G:N1	22:CC:131:G:C6	2.86	0.44
20:CA:282:C:C4	20:CA:283:G:C5	3.05	0.44
20:CA:2635:U:H2'	20:CA:2636:U:C6	2.53	0.44
20:CA:3775:A:O2'	20:CA:3776:G:H5'	2.18	0.44
20:CA:3855:C:H2'	20:CA:3856:A:H8	1.83	0.44
20:CA:4400:G:C6	20:CA:4401:G:N7	2.84	0.44
20:CA:4405:G:C5	20:CA:4406:U:C5	3.06	0.44
20:CA:4901:G:C2	20:CA:4902:C:C5	3.05	0.44
3:AX:98:SER:O	3:AX:101:LYS:HE3	2.18	0.44
4:AY:21:ILE:HG23	4:AY:33:ARG:HE	1.83	0.44
17:BB:168:VAL:O	17:BB:172:LYS:HG3	2.18	0.44
17:BB:317:ASN:OD1	17:BB:318:PRO:O	2.36	0.44
19:BD:244:GLU:O	19:BD:248:ILE:HG12	2.18	0.44
20:CA:1309:C:H2'	20:CA:1310:C:H6	1.83	0.44
20:CA:1662:C:H2'	20:CA:1663:C:C6	2.53	0.44
20:CA:3693:U:N3	20:CA:3694:U:C5	2.85	0.44
20:CA:4647:G:C2	20:CA:4648:A:C8	3.06	0.44
20:CA:4967:A:H2'	20:CA:4968:A:H8	1.83	0.44
19:BD:204:SER:O	19:BD:205:ASN:HB2	2.18	0.43
20:CA:2418:A:C5	20:CA:2419:C:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:4499:OMG:C2	20:CA:4529:G:H1'	2.53	0.43
22:CC:68:G:H2'	22:CC:69:PSU:O4'	2.18	0.43
22:CC:69:PSU:H2'	22:CC:70:G:O4'	2.18	0.43
28:AO:84:LYS:HB2	28:AO:110:TYR:CE2	2.53	0.43
2:AW:18:LEU:O	2:AW:22:MET:HG2	2.17	0.43
17:BB:288:ASP:OD2	17:BB:291:ARG:HB2	2.19	0.43
20:CA:2335:C:H2'	20:CA:2336:G:H8	1.83	0.43
20:CA:2539:C:H2'	20:CA:2540:C:C6	2.53	0.43
20:CA:2744:A:H2'	20:CA:2745:A:C8	2.53	0.43
20:CA:4524:G:H2'	20:CA:4525:C:H6	1.84	0.43
38:CA:5402:PUT:H42	38:CA:5402:PUT:H11	1.84	0.43
29:AP:85:ARG:NH1	42:AP:302:HOH:O	2.50	0.43
3:AX:52:PHE:O	3:AX:56:GLU:HG2	2.18	0.43
4:AY:91:CYS:HA	19:BD:119:GLU:OE2	2.18	0.43
16:BA:79:VAL:O	16:BA:330:PHE:HB2	2.18	0.43
19:BD:153:LEU:HD11	19:BD:195:ILE:HG13	2.00	0.43
20:CA:100:C:C2	20:CA:101:A:C8	3.07	0.43
20:CA:482:G:C2	20:CA:485:C:C4	3.06	0.43
20:CA:733:A:H2'	20:CA:734:G:O4'	2.18	0.43
20:CA:1345:A:H2'	20:CA:1346:C:C6	2.54	0.43
20:CA:3867:A2M:H2'	20:CA:3868:G:C8	2.53	0.43
20:CA:4699:U:H1'	20:CA:4700:A:H5''	2.00	0.43
10:Ae:14:THR:HA	10:Ae:17:ARG:HD3	2.01	0.43
14:Ai:6:LYS:HE2	20:CA:2875:C:O2'	2.19	0.43
16:BA:252:ALA:HB1	20:CA:4524:G:C2	2.53	0.43
18:BC:266:TRP:CH2	21:CB:22:A:H1'	2.53	0.43
20:CA:37:U:H2'	20:CA:38:A:O4'	2.18	0.43
20:CA:284:G:H2'	20:CA:285:G:H8	1.83	0.43
20:CA:484:U:H4'	20:CA:485:C:H5'	2.00	0.43
20:CA:752:G:H2'	20:CA:753:C:O2	2.18	0.43
20:CA:1920:C:H3'	20:CA:1921:C:H5''	2.01	0.43
20:CA:4424:A:N7	20:CA:4475:G:C6	2.87	0.43
26:AM:84:TYR:CE1	26:AM:93:MET:SD	3.11	0.43
33:AT:36:ARG:HG2	33:AT:38:TYR:CZ	2.54	0.43
14:Ai:64:VAL:HG22	23:CD:83:HIS:HB3	2.01	0.43
20:CA:287:U:H2'	20:CA:288:G:C8	2.54	0.43
20:CA:643:C:H3'	20:CA:644:G:C8	2.53	0.43
20:CA:1479:G:C6	20:CA:1487:G:C6	3.07	0.43
20:CA:1669:A:H4'	20:CA:1685:G:H22	1.83	0.43
20:CA:1720:C:H3'	20:CA:1721:G:H8	1.81	0.43
20:CA:2519:U:C2	20:CA:2520:C:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:3718:A2M:O4'	20:CA:3718:A2M:C8	2.66	0.43
20:CA:4306:OMU:OP2	24:AK:159:PRO:HD2	2.18	0.43
20:CA:4410:G:C2	20:CA:4411:G:C8	3.07	0.43
22:CC:128:C:H2'	22:CC:129:C:C6	2.54	0.43
23:CD:179:ILE:O	23:CD:180:LEU:HB2	2.18	0.43
20:CA:222:C:H2'	20:CA:223:G:O4'	2.18	0.43
20:CA:469:C:O2	20:CA:469:C:H2'	2.18	0.43
20:CA:672:C:C2	20:CA:673:C:C6	3.07	0.43
20:CA:1189:G:H2'	20:CA:1190:C:C6	2.54	0.43
20:CA:1413:C:O2	20:CA:1413:C:H2'	2.19	0.43
20:CA:2544:G:H2'	20:CA:2545:U:O4'	2.19	0.43
20:CA:2685:C:H2'	20:CA:2686:G:O4'	2.18	0.43
20:CA:4861:G:H2'	20:CA:4862:G:O4'	2.18	0.43
21:CB:108:G:O2'	21:CB:109:U:H5'	2.17	0.43
22:CC:74:U:C5	32:AS:74:TYR:CE1	3.06	0.43
32:AS:50:ARG:HG2	32:AS:51:LYS:N	2.33	0.43
34:AU:129:PHE:HB2	34:AU:134:GLU:OE2	2.19	0.43
12:Ag:77:ILE:HG13	12:Ag:77:ILE:O	2.19	0.43
14:Ai:90:LYS:HD2	23:CD:108:PRO:HD3	2.00	0.43
15:Aj:82:ILE:HG23	15:Aj:84:LYS:NZ	2.33	0.43
20:CA:270:U:H2'	20:CA:271:C:O2	2.18	0.43
20:CA:325:U:H2'	20:CA:326:C:C6	2.54	0.43
20:CA:1340:OMC:C2	20:CA:1341:U:C5	3.07	0.43
20:CA:3664:G:C2	20:CA:3665:G:N7	2.86	0.43
20:CA:3806:G:C4	20:CA:3807:A:C8	3.06	0.43
20:CA:4238:G:H2'	20:CA:4239:A:H8	1.83	0.43
20:CA:4485:C:C2	20:CA:4486:C:C5	3.07	0.43
22:CC:4:C:H2'	22:CC:5:U:H6	1.83	0.43
22:CC:62:A:H4'	22:CC:63:U:O5'	2.19	0.43
4:AY:90:MET:HE1	15:Aj:113:ARG:HA	2.01	0.43
16:BA:29:VAL:HA	16:BA:220:ILE:HD13	2.00	0.43
17:BB:122:TYR:CD1	17:BB:280:PRO:CG	3.02	0.43
20:CA:1326:A2M:N3	20:CA:1327:C:C5	2.87	0.43
20:CA:1327:C:C2	20:CA:1328:G:N7	2.87	0.43
20:CA:2659:A:C2	20:CA:2676:A:N9	2.87	0.43
20:CA:3702:A:C8	20:CA:3774:A:C1'	3.01	0.43
22:CC:5:U:N3	22:CC:6:C:C5	2.87	0.43
20:CA:131:C:H2'	20:CA:132:G:O4'	2.19	0.43
20:CA:1172:C:O2'	20:CA:1173:G:H8	2.02	0.43
20:CA:1246:G:H2'	20:CA:1247:U:C6	2.53	0.43
20:CA:1466:G:C2	20:CA:1467:C:C6	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:2071:A:C2	20:CA:2072:C:C5	3.06	0.43
22:CC:71:A:H2'	32:AS:50:ARG:NH1	2.33	0.43
22:CC:121:G:C2'	22:CC:122:G:H5'	2.49	0.43
24:AK:98:LEU:HD13	24:AK:100:VAL:HG13	1.99	0.43
30:AQ:55:TYR:O	30:AQ:58:LYS:HG2	2.19	0.43
17:BB:122:TYR:HE1	17:BB:280:PRO:CB	2.31	0.43
18:BC:228:LYS:O	18:BC:229:ASN:CG	2.61	0.43
20:CA:10:A:H2'	20:CA:11:G:C8	2.54	0.43
20:CA:1822:U:C2	20:CA:1823:G:C8	3.06	0.43
20:CA:2071:A:C4	20:CA:2072:C:C5	3.06	0.43
20:CA:2397:G:C8	20:CA:2399:G:C8	3.07	0.43
20:CA:2640:G:H2'	20:CA:2641:A:C8	2.54	0.43
20:CA:4709:U:C2	20:CA:4710:C:C6	3.07	0.43
4:AY:88:LEU:HA	4:AY:91:CYS:SG	2.59	0.42
20:CA:712:C:N3	20:CA:713:C:C5	2.87	0.42
20:CA:2580:U:C6	33:AT:38:TYR:OH	2.71	0.42
20:CA:2846:G:H2'	20:CA:2847:G:H8	1.84	0.42
20:CA:3924:C:H2'	20:CA:3925:OMU:H6	2.01	0.42
20:CA:4474:A:H2'	20:CA:4476:C:O5'	2.19	0.42
20:CA:4498:OMU:HM22	20:CA:4499:OMG:H8	1.81	0.42
20:CA:4535:A:H2'	20:CA:4536:OMC:C6	2.54	0.42
20:CA:4596:C:C4	20:CA:4597:U:C4	3.07	0.42
3:AX:19:GLU:OE1	3:AX:102:LEU:HD11	2.17	0.42
15:Aj:125:MET:O	15:Aj:126:VAL:C	2.62	0.42
16:BA:292:LEU:HD11	16:BA:298:LEU:HD12	2.01	0.42
20:CA:459:C:C2	20:CA:698:G:N2	2.87	0.42
20:CA:493:G:O6	20:CA:660:A:N1	2.52	0.42
20:CA:643:C:H3'	20:CA:644:G:H8	1.83	0.42
20:CA:1314:C:C2	20:CA:1315:C:C5	3.06	0.42
20:CA:2623:A:C2	20:CA:2624:G:C8	3.07	0.42
20:CA:2858:A:H2'	20:CA:2859:G:O4'	2.19	0.42
20:CA:3693:U:C2	20:CA:3694:U:C6	3.07	0.42
23:CD:5:ILE:HG22	23:CD:208:GLU:O	2.19	0.42
17:BB:308:LYS:HG3	20:CA:1702:C:C5'	2.50	0.42
20:CA:424:U:H2'	20:CA:425:U:C6	2.53	0.42
20:CA:671:G:H2'	20:CA:672:C:H6	1.84	0.42
20:CA:965:G:C5	20:CA:2256:C:C5	3.07	0.42
20:CA:2268:A:H4'	20:CA:2270:G:C8	2.55	0.42
20:CA:2438:A:N6	20:CA:2531:C:C4	2.87	0.42
20:CA:2659:A:C2	20:CA:2676:A:C8	3.07	0.42
20:CA:3630:A:C2	20:CA:3631:U:C5	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:4710:C:H2'	20:CA:4711:C:C6	2.54	0.42
20:CA:4736:C:H4'	20:CA:5068:G:C4	2.54	0.42
21:CB:43:U:C2	21:CB:44:C:C6	3.07	0.42
21:CB:62:U:C2	21:CB:64:G:C8	3.07	0.42
3:AX:18:ASN:HB3	3:AX:21:VAL:CG1	2.50	0.42
8:Ac:15:HIS:CB	20:CA:72:C:C6	3.02	0.42
20:CA:153:G:H2'	20:CA:154:G:H8	1.84	0.42
20:CA:179:G:O6	20:CA:259:C:C6	2.72	0.42
20:CA:281:U:O2	20:CA:282:C:C6	2.73	0.42
20:CA:341:G:C6	20:CA:342:G:N7	2.88	0.42
20:CA:1775:A:H2'	20:CA:1776:A:C8	2.53	0.42
20:CA:3717:A:OP2	20:CA:3735:G:N2	2.53	0.42
20:CA:4070:U:O2	20:CA:4070:U:O4'	2.37	0.42
20:CA:4673:PSU:C4	20:CA:4674:C:C5	3.07	0.42
20:CA:4982:A:C5	20:CA:4983:C:C5	3.08	0.42
1:AV:35:VAL:HG12	1:AV:36:ASP:N	2.33	0.42
5:AZ:59:THR:HG21	42:CA:5916:HOH:O	2.19	0.42
16:BA:220:ILE:HG12	16:BA:278:THR:HG23	2.01	0.42
20:CA:964:A:H2'	20:CA:965:G:H4'	2.00	0.42
20:CA:1327:C:H5''	20:CA:4449:A:OP1	2.20	0.42
20:CA:2276:A:H2'	20:CA:2277:C:O4'	2.20	0.42
20:CA:3837:C:H2'	20:CA:3838:U:O4'	2.19	0.42
20:CA:3918:G:N7	38:CA:5401:PUT:H32	2.34	0.42
20:CA:4699:U:C4	20:CA:4702:G:O6	2.73	0.42
20:CA:4956:A:C8	20:CA:4957:C:C6	3.06	0.42
20:CA:5002:U:H2'	20:CA:5003:U:C6	2.54	0.42
25:AL:105:LEU:HD22	25:AL:135:LYS:HG3	2.00	0.42
26:AM:6:THR:O	26:AM:6:THR:HG23	2.20	0.42
34:AU:129:PHE:HB3	34:AU:134:GLU:HG3	2.00	0.42
20:CA:271:C:H2'	20:CA:272:U:O2	2.19	0.42
20:CA:272:U:O2	20:CA:272:U:O4'	2.38	0.42
20:CA:434:A:H2'	20:CA:435:A:O4'	2.20	0.42
20:CA:1572:U:H2'	20:CA:1573:G:C8	2.55	0.42
20:CA:1608:G:O6	40:CA:5415:SPM:H61	2.20	0.42
20:CA:4486:C:H2'	20:CA:4487:A:O4'	2.19	0.42
21:CB:79:U:O4	38:CB:201:PUT:H21	2.19	0.42
22:CC:103:A:OP2	22:CC:104:A:H2'	2.20	0.42
8:Ac:21:VAL:O	8:Ac:21:VAL:HG13	2.19	0.42
14:AI:8:VAL:O	14:AI:11:VAL:HG22	2.20	0.42
20:CA:923:C:H2'	20:CA:924:C:C2	2.54	0.42
20:CA:983:C:H2'	20:CA:984:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:1524:A2M:HM'3	20:CA:3916:G:O2'	2.20	0.42
20:CA:1609:U:H2'	20:CA:1610:C:O4'	2.19	0.42
20:CA:2071:A:N3	20:CA:2072:C:C6	2.88	0.42
20:CA:2666:U:C2	20:CA:2669:C:C5	3.08	0.42
20:CA:3718:A2M:H2'	20:CA:3719:A:H8	1.85	0.42
20:CA:3907:G:N3	20:CA:3909:C:C5	2.87	0.42
20:CA:4261:C:H2'	20:CA:4262:C:H6	1.83	0.42
20:CA:4477:A:C4	20:CA:4478:G:C8	3.08	0.42
20:CA:4637:OMG:HM23	20:CA:4637:OMG:H1'	1.77	0.42
21:CB:111:C:H2'	21:CB:112:U:O4'	2.20	0.42
23:CD:120:PRO:HG3	23:CD:159:SER:HB3	2.02	0.42
16:BA:302:ASN:OD1	16:BA:330:PHE:CE2	2.73	0.42
20:CA:64:A:C4	20:CA:109:G:N7	2.88	0.42
20:CA:751:G:H2'	20:CA:752:G:O4'	2.20	0.42
20:CA:1461:C:C2	20:CA:1462:A:C8	3.08	0.42
20:CA:2065:G:C4	20:CA:2066:C:C6	3.07	0.42
20:CA:4188:U:H2'	20:CA:4189:U:C6	2.55	0.42
20:CA:4928:C:C2	20:CA:4929:C:C5	3.08	0.42
22:CC:119:C:C2	22:CC:120:G:C8	3.08	0.42
10:Ae:12:LEU:O	10:Ae:16:ARG:HG3	2.20	0.42
16:BA:293:ILE:HD11	16:BA:297:LYS:HE3	2.00	0.42
20:CA:1858:A:C6	20:CA:1859:B8T:C41	3.03	0.42
20:CA:2521:G:H5'	20:CA:2640:G:H1'	2.02	0.42
20:CA:3636:C:O2	20:CA:3636:C:H2'	2.20	0.42
20:CA:3711:A:H2'	20:CA:3712:A:O4'	2.20	0.42
20:CA:4415:A:C2	20:CA:4428:A:C4	3.08	0.42
28:AO:94:ASN:HB2	28:AO:96:LEU:HG	2.01	0.42
33:AT:25:ILE:HA	33:AT:43:VAL:HG12	2.02	0.42
1:AV:117:ARG:CZ	20:CA:1273:G:OP2	2.68	0.42
3:AX:100:ASN:O	3:AX:101:LYS:HB2	2.20	0.42
17:BB:293:LEU:HD22	24:AK:34:PHE:CD2	2.55	0.42
19:BD:73:TYR:CE1	20:CA:981:C:C4	3.08	0.42
20:CA:353:A:C4	20:CA:379:G:N7	2.88	0.42
20:CA:1951:G:C6	20:CA:2033:A:C6	3.08	0.42
20:CA:4954:G:H2'	20:CA:4955:A:C8	2.55	0.42
39:CA:5410:SPD:H81	39:CA:5410:SPD:C4	2.48	0.42
24:AK:66:MET:HE1	24:AK:86:ILE:CD1	2.50	0.42
8:Ac:73:ILE:O	8:Ac:77:VAL:HG22	2.20	0.41
17:BB:322:LEU:O	17:BB:326:LEU:HG	2.20	0.41
20:CA:86:U:H2'	20:CA:87:A:C8	2.55	0.41
20:CA:753:C:O2	20:CA:753:C:O4'	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:965:G:H1'	20:CA:2093:A:H61	1.84	0.41
20:CA:1089:G:C6	20:CA:1208:G:C6	3.08	0.41
20:CA:3630:A:C4	20:CA:3631:U:C5	3.09	0.41
20:CA:4355:G:C2	20:CA:4356:G:N7	2.88	0.41
20:CA:4893:A:C4'	20:CA:4894:A:OP1	2.68	0.41
22:CC:122:G:H2'	22:CC:123:U:C1'	2.50	0.41
23:CD:136:VAL:O	23:CD:136:VAL:HG23	2.20	0.41
2:AW:48:LEU:HD21	2:AW:60:ILE:HG21	2.01	0.41
20:CA:288:G:H2'	20:CA:289:C:C6	2.55	0.41
20:CA:1431:C:H2'	20:CA:1432:G:O4'	2.20	0.41
20:CA:1846:G:H2'	20:CA:1847:C:C6	2.55	0.41
20:CA:2753:G:O2'	20:CA:2754:G:H5'	2.20	0.41
20:CA:4173:G:H2'	20:CA:4174:U:C6	2.55	0.41
20:CA:4274:A:H2'	20:CA:4275:G:C8	2.55	0.41
22:CC:141:C:C2	22:CC:142:U:C5	3.08	0.41
32:AS:74:TYR:HD2	32:AS:77:LYS:HB2	1.85	0.41
3:AX:28:ASN:OD1	20:CA:4996:C:OP1	2.39	0.41
8:Ac:63:VAL:O	8:Ac:64:SER:HB2	2.19	0.41
20:CA:379:G:O2'	20:CA:380:U:H5'	2.20	0.41
20:CA:3805:U:H2'	20:CA:3806:G:H8	1.85	0.41
20:CA:4182:G:H4'	23:CD:226:ARG:NH2	2.35	0.41
20:CA:4238:G:H2'	20:CA:4239:A:C8	2.56	0.41
20:CA:4994:G:H2'	20:CA:4995:U:C6	2.55	0.41
2:AW:56:ARG:HA	2:AW:59:GLU:HG2	2.02	0.41
6:Aa:97:ILE:CG2	20:CA:4122:G:O6	2.68	0.41
16:BA:258:HIS:HA	16:BA:259:PRO:C	2.44	0.41
19:BD:267:LEU:O	19:BD:271:LEU:HG	2.21	0.41
20:CA:106:A:H2'	20:CA:107:G:O4'	2.20	0.41
20:CA:112:C:C2	20:CA:113:A:C8	3.09	0.41
20:CA:751:G:C4	20:CA:752:G:C8	3.08	0.41
20:CA:1306:C:H2'	20:CA:1307:A:C8	2.53	0.41
20:CA:1754:U:O2'	20:CA:1755:C:C6	2.70	0.41
20:CA:1880:G:OP2	20:CA:1881:OMC:HM22	2.19	0.41
20:CA:2082:G:O2'	20:CA:2083:C:H5'	2.21	0.41
20:CA:2094:G:H2'	20:CA:2094:G:N3	2.36	0.41
20:CA:2290:C:C2	20:CA:2291:G:C8	3.08	0.41
20:CA:2303:C:O3'	20:CA:2306:G:H5'	2.19	0.41
20:CA:2475:G:C6	31:AR:50:LYS:HG3	2.56	0.41
20:CA:2503:G:O2'	20:CA:2504:C:H2'	2.20	0.41
20:CA:2781:G:O2'	20:CA:2782:U:H5'	2.21	0.41
20:CA:4263:C:H2'	20:CA:4264:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:4341:C:C2	20:CA:4342:C:C6	3.08	0.41
20:CA:4551:U:H2'	20:CA:4552:PSU:C6	2.56	0.41
22:CC:141:C:H2'	22:CC:142:U:C6	2.55	0.41
26:AM:163:HIS:C	26:AM:164:LYS:HD2	2.44	0.41
11:Af:51:LEU:C	11:Af:51:LEU:HD23	2.46	0.41
17:BB:254:GLU:O	17:BB:258:ARG:HG3	2.20	0.41
20:CA:479:G:O2'	20:CA:480:C:H5'	2.20	0.41
20:CA:500:G:H2'	20:CA:505:G:H8	1.86	0.41
20:CA:1684:A:C4	20:CA:1685:G:C8	3.08	0.41
20:CA:1847:C:H2'	20:CA:1848:C:C6	2.56	0.41
20:CA:1866:U:H2'	20:CA:1867:A:O4'	2.20	0.41
20:CA:3630:A:H2'	20:CA:3631:U:H6	1.84	0.41
20:CA:3928:A:H2'	20:CA:3929:G:O4'	2.20	0.41
20:CA:4591:U:H2'	20:CA:4592:C:C6	2.56	0.41
20:CA:4625:C:O2'	20:CA:4626:A:H5'	2.21	0.41
20:CA:4760:G:H2'	20:CA:4761:G:O4'	2.21	0.41
22:CC:120:G:C5	22:CC:121:G:N7	2.88	0.41
31:AR:82:THR:O	31:AR:82:THR:CG2	2.68	0.41
34:AU:131:ARG:NH2	34:AU:132:ARG:NH2	2.69	0.41
3:AX:22:THR:HG23	3:AX:89:SER:OG	2.21	0.41
6:Aa:95:PHE:CD1	33:AT:12:LEU:HD11	2.56	0.41
11:Af:7:PHE:HE1	31:AR:128:ILE:HD13	1.84	0.41
14:Ai:75:SER:O	14:Ai:79:VAL:HG23	2.20	0.41
18:BC:236:MET:O	18:BC:239:MET:HG2	2.20	0.41
20:CA:433:A:H2'	20:CA:434:A:O4'	2.21	0.41
20:CA:1479:G:H2'	20:CA:1480:C:C6	2.54	0.41
20:CA:1750:G:C2	20:CA:1751:A:C8	3.09	0.41
20:CA:2745:A:H2'	20:CA:2746:A:H8	1.86	0.41
20:CA:3694:U:H2'	20:CA:3695:PSU:C6	2.56	0.41
20:CA:3910:C:H1'	20:CA:4396:A:C2	2.55	0.41
20:CA:4484:A:C2	20:CA:4485:C:C6	3.08	0.41
40:CA:5415:SPM:H42	40:CA:5415:SPM:H72	1.74	0.41
22:CC:130:C:H2'	22:CC:131:G:H8	1.84	0.41
1:AV:115:GLY:HA2	20:CA:1241:C:O2	2.20	0.41
20:CA:661:C:H2'	20:CA:662:C:C6	2.55	0.41
20:CA:1681:G:P	38:CA:5402:PUT:H22	2.61	0.41
20:CA:1933:G:H2'	20:CA:1934:A:C8	2.56	0.41
20:CA:2426:U:H5''	25:AL:3:MET:HE3	2.02	0.41
20:CA:3718:A2M:HM'3	20:CA:3718:A2M:H1'	1.85	0.41
20:CA:4728:U:H5'	20:CA:4729:A:OP1	2.20	0.41
20:CA:4967:A:C2	20:CA:4968:A:C5	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CD:79:ALA:O	23:CD:82:ILE:HG12	2.21	0.41
29:AP:112:MET:HE1	29:AP:117:ILE:CG1	2.51	0.41
33:AT:40:HIS:C	33:AT:77:TYR:CE1	2.98	0.41
34:AU:122:VAL:O	34:AU:142:GLY:HA3	2.21	0.41
37:Ah:202:ATP:N1	20:CA:4370:OMG:H2'	2.35	0.41
18:BC:41:LYS:HB2	27:AN:68:THR:O	2.21	0.41
20:CA:332:C:OP2	39:CA:5407:SPD:H91	2.21	0.41
20:CA:511:C:H1'	20:CA:512:U:OP1	2.21	0.41
20:CA:1295:C:H4'	20:CA:1296:G:C8	2.56	0.41
20:CA:2894:A:H2'	20:CA:2895:A:H8	1.86	0.41
20:CA:3681:G:C6	23:CD:125:LYS:HB3	2.56	0.41
20:CA:4687:A:C2	20:CA:4688:C:C6	3.08	0.41
20:CA:4713:G:C4	20:CA:4714:C:C6	3.09	0.41
38:CA:5403:PUT:H11	38:CA:5403:PUT:H42	1.72	0.41
26:AM:74:ARG:C	26:AM:100:LEU:HD23	2.46	0.41
30:AQ:47:ARG:O	30:AQ:55:TYR:HD1	2.04	0.41
32:AS:50:ARG:HB2	32:AS:115:ARG:NH1	2.36	0.41
1:AV:101:HIS:CE1	1:AV:104:LEU:HD13	2.56	0.41
3:AX:33:ILE:HG22	3:AX:44:ARG:HG3	2.02	0.41
6:Aa:93:ARG:HG2	6:Aa:97:ILE:HD12	2.02	0.41
7:Ab:4:ILE:HD12	7:Ab:20:GLN:NE2	2.36	0.41
18:BC:163:LEU:O	18:BC:167:VAL:HG23	2.21	0.41
18:BC:261:VAL:HG11	21:CB:119:U:C2	2.55	0.41
20:CA:35:U:H4'	20:CA:1525:A:C2	2.56	0.41
20:CA:455:C:O2	20:CA:455:C:C2'	2.69	0.41
20:CA:727:C:H2'	20:CA:728:U:C6	2.56	0.41
20:CA:1086:C:H2'	20:CA:1087:A:H8	1.86	0.41
20:CA:1309:C:H2'	20:CA:1310:C:C6	2.56	0.41
20:CA:1479:G:O2'	20:CA:1480:C:H5'	2.21	0.41
20:CA:1875:C:H2'	20:CA:1876:U:C6	2.55	0.41
20:CA:2072:C:N3	20:CA:2073:C:C5	2.89	0.41
20:CA:2456:G:H2'	20:CA:2457:G:H8	1.85	0.41
20:CA:2499:C:C4	20:CA:2500:U:C4	3.08	0.41
20:CA:2544:G:H22	22:CC:124:U:C4'	2.33	0.41
20:CA:2632:PSU:C2	28:AO:85:TYR:CD1	3.09	0.41
20:CA:2764:A:H2'	20:CA:2765:A:H8	1.85	0.41
20:CA:2891:U:O4'	20:CA:5016:A:C2	2.74	0.41
20:CA:4123:C:H2'	20:CA:4124:G:C8	2.55	0.41
20:CA:4125:C:H2'	20:CA:4126:C:C6	2.55	0.41
20:CA:4196:OMG:HM23	20:CA:4196:OMG:H1'	1.92	0.41
20:CA:4222:G:C5	20:CA:4223:C:C5	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:4534:G:O6	20:CA:4553:A:C6	2.74	0.41
20:CA:4876:U:OP2	26:AM:165:PRO:HG3	2.21	0.41
20:CA:4971:A:C6	20:CA:4972:PSU:C2	3.09	0.41
20:CA:5023:C:H3'	20:CA:5024:C:H5''	2.02	0.41
20:CA:5050:C:C2	20:CA:5051:C:C5	3.09	0.41
21:CB:93:G:C5	21:CB:94:C:C5	3.08	0.41
26:AM:95:ARG:HD3	26:AM:97:TYR:OH	2.21	0.41
1:AV:56:LYS:O	1:AV:60:ASN:OD1	2.39	0.41
3:AX:68:LEU:CD2	3:AX:106:VAL:HG12	2.51	0.41
7:Ab:64:THR:O	7:Ab:67:GLU:HG2	2.21	0.41
15:Aj:4:HIS:O	15:Aj:8:MET:HG2	2.21	0.41
16:BA:95:THR:HG22	20:CA:4910:G:H4'	2.03	0.41
16:BA:393:LYS:HA	16:BA:396:ARG:HE	1.86	0.41
19:BD:45:SER:O	19:BD:46:ARG:HB2	2.21	0.41
20:CA:241:G:C5	20:CA:242:U:C5	3.09	0.41
20:CA:1504:G:H2'	20:CA:1505:C:H6	1.85	0.41
20:CA:1670:G:O2'	20:CA:1853:G:H4'	2.21	0.41
20:CA:1696:C:H2'	20:CA:1697:G:O4'	2.21	0.41
20:CA:2030:A:H2'	20:CA:2031:C:O4'	2.21	0.41
20:CA:2497:C:C2	20:CA:2498:C:C6	3.09	0.41
20:CA:2560:C:O2'	20:CA:2561:C:P	2.79	0.41
20:CA:2568:C:C2	20:CA:2569:G:C8	3.09	0.41
5:AZ:46:ARG:HD3	5:AZ:71:TRP:CE3	2.56	0.40
16:BA:139:ASP:OD1	16:BA:140:GLU:N	2.54	0.40
17:BB:41:HIS:CE1	17:BB:45:ARG:HD3	2.56	0.40
18:BC:83:LEU:HB3	18:BC:88:VAL:HB	2.03	0.40
19:BD:190:HIS:HB3	19:BD:193:PHE:HD2	1.86	0.40
20:CA:2555:G:C4	20:CA:2573:A:N1	2.89	0.40
20:CA:3656:A:H2'	20:CA:3657:U:H6	1.86	0.40
20:CA:4259:C:C2	20:CA:4260:U:C5	3.08	0.40
20:CA:4878:C:N3	20:CA:4879:C:C5	2.89	0.40
22:CC:65:A:C4	22:CC:66:A:C8	3.09	0.40
1:AV:57:MET:CE	20:CA:1828:C:H1'	2.52	0.40
20:CA:400:A2M:HM'3	20:CA:400:A2M:H1'	1.89	0.40
20:CA:1202:C:H5''	20:CA:1202:C:O2	2.20	0.40
20:CA:1333:A:H2'	20:CA:1334:A:C8	2.57	0.40
20:CA:1912:G:C6	20:CA:2057:A:C2	3.10	0.40
20:CA:1951:G:C6	20:CA:2033:A:N1	2.90	0.40
20:CA:2765:A:H2'	20:CA:2766:A:C8	2.56	0.40
20:CA:2784:C:C2	20:CA:2785:C:C5	3.10	0.40
20:CA:2846:G:C4	20:CA:2847:G:C8	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CA:3718:A2M:H2'	20:CA:3719:A:C8	2.56	0.40
20:CA:4562:C:C2	20:CA:4563:U:C6	3.10	0.40
20:CA:4656:A:OP1	20:CA:4658:G:H5'	2.21	0.40
20:CA:4878:C:C2	20:CA:4879:C:C6	3.09	0.40
22:CC:154:G:C2'	22:CC:155:C:O5'	2.69	0.40
31:AR:110:LYS:HG2	31:AR:114:LYS:NZ	2.36	0.40
32:AS:74:TYR:HE2	32:AS:77:LYS:HG3	1.86	0.40
20:CA:1202:C:O2	20:CA:1202:C:O4'	2.37	0.40
20:CA:1705:G:H2'	20:CA:1706:A:O4'	2.21	0.40
20:CA:1907:A:H2'	20:CA:1908:A:C8	2.57	0.40
20:CA:3853:U:C2	20:CA:3854:C:C5	3.10	0.40
20:CA:3880:G:O2'	20:CA:3881:G:H5'	2.21	0.40
20:CA:4499:OMG:N3	20:CA:4529:G:H1'	2.37	0.40
20:CA:4694:G:H5''	20:CA:4695:C:H5	1.86	0.40
20:CA:5050:C:O2	20:CA:5050:C:H2'	2.21	0.40
22:CC:67:U:H2'	22:CC:68:G:H8	1.86	0.40
22:CC:140:C:H2'	22:CC:141:C:C6	2.56	0.40
32:AS:47:MET:HE3	32:AS:115:ARG:HE	1.86	0.40
4:AY:108:ARG:CZ	4:AY:128:ARG:HD3	2.51	0.40
15:Aj:48:THR:OG1	15:Aj:65:LYS:HB2	2.21	0.40
20:CA:262:G:H2'	20:CA:263:G:O4'	2.21	0.40
20:CA:416:U:C2'	20:CA:417:G:H5'	2.51	0.40
20:CA:511:C:O2'	20:CA:512:U:H6	2.03	0.40
20:CA:1078:A:C5	20:CA:1079:C:C6	3.09	0.40
20:CA:1582:U:O2	20:CA:1582:U:H2'	2.22	0.40
20:CA:1681:G:OP1	38:CA:5402:PUT:H22	2.21	0.40
20:CA:3599:A:H2'	20:CA:3600:G:C8	2.57	0.40
20:CA:4399:U:C2	20:CA:4400:G:C8	3.10	0.40
20:CA:4714:C:O2	20:CA:4714:C:H2'	2.22	0.40
1:AV:121:PRO:O	1:AV:122:LYS:HB3	2.22	0.40
19:BD:158:ARG:HD2	20:CA:4945:G:N3	2.36	0.40
20:CA:1205:G:H2'	20:CA:1206:C:C6	2.53	0.40
20:CA:1340:OMC:HM23	20:CA:1340:OMC:H1'	1.97	0.40
20:CA:1775:A:H3'	20:CA:1776:A:H8	1.86	0.40
20:CA:3662:A:O4'	20:CA:3664:G:C8	2.75	0.40
20:CA:4189:U:H2'	20:CA:4190:U:C6	2.57	0.40
20:CA:4390:A:H2'	20:CA:4391:G:O4'	2.22	0.40
20:CA:4575:G:N3	20:CA:4576:PSU:C6	2.90	0.40
20:CA:4903:G:H2'	20:CA:4904:G:O4'	2.22	0.40
22:CC:128:C:N3	22:CC:129:C:N4	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AV	96/159 (60%)	93 (97%)	3 (3%)	0	100	100
2	AW	91/115 (79%)	89 (98%)	2 (2%)	0	100	100
3	AX	107/125 (86%)	103 (96%)	4 (4%)	0	100	100
4	AY	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
5	AZ	107/110 (97%)	107 (100%)	0	0	100	100
6	Aa	104/117 (89%)	102 (98%)	2 (2%)	0	100	100
7	Ab	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
8	Ac	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
9	Ad	84/97 (87%)	84 (100%)	0	0	100	100
10	Ae	67/70 (96%)	67 (100%)	0	0	100	100
11	Af	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
12	Ag	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
13	Ah	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
14	Ai	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
15	Aj	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
16	BA	393/403 (98%)	377 (96%)	16 (4%)	0	100	100
17	BB	357/427 (84%)	353 (99%)	4 (1%)	0	100	100
18	BC	291/297 (98%)	282 (97%)	9 (3%)	0	100	100
19	BD	210/288 (73%)	204 (97%)	6 (3%)	0	100	100
23	CD	243/257 (95%)	232 (96%)	11 (4%)	0	100	100
24	AK	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
25	AL	154/196 (79%)	153 (99%)	1 (1%)	0	100	100
26	AM	173/176 (98%)	171 (99%)	2 (1%)	0	100	100
27	AN	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
28	AO	99/128 (77%)	94 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	AP	129/140 (92%)	128 (99%)	1 (1%)	0	100	100
30	AQ	60/157 (38%)	59 (98%)	1 (2%)	0	100	100
31	AR	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
32	AS	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
33	AT	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
34	AU	144/148 (97%)	140 (97%)	3 (2%)	1 (1%)	18	20
All	All	4391/5072 (87%)	4285 (98%)	105 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	AU	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AV	82/126 (65%)	82 (100%)	0	100	100
2	AW	78/97 (80%)	78 (100%)	0	100	100
3	AX	99/110 (90%)	99 (100%)	0	100	100
4	AY	116/121 (96%)	116 (100%)	0	100	100
5	AZ	88/89 (99%)	88 (100%)	0	100	100
6	Aa	92/100 (92%)	92 (100%)	0	100	100
7	Ab	109/110 (99%)	109 (100%)	0	100	100
8	Ac	86/89 (97%)	86 (100%)	0	100	100
9	Ad	73/80 (91%)	73 (100%)	0	100	100
10	Ae	64/65 (98%)	64 (100%)	0	100	100
11	Af	47/48 (98%)	47 (100%)	0	100	100
12	Ag	47/115 (41%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	Ah	91/94 (97%)	91 (100%)	0	100	100
14	Ai	74/75 (99%)	74 (100%)	0	100	100
15	Aj	109/121 (90%)	109 (100%)	0	100	100
16	BA	344/348 (99%)	344 (100%)	0	100	100
17	BB	299/348 (86%)	299 (100%)	0	100	100
18	BC	247/250 (99%)	247 (100%)	0	100	100
19	BD	192/252 (76%)	192 (100%)	0	100	100
23	CD	188/198 (95%)	188 (100%)	0	100	100
24	AK	164/165 (99%)	164 (100%)	0	100	100
25	AL	139/175 (79%)	139 (100%)	0	100	100
26	AM	156/157 (99%)	156 (100%)	0	100	100
27	AN	139/140 (99%)	139 (100%)	0	100	100
28	AO	91/115 (79%)	91 (100%)	0	100	100
29	AP	101/107 (94%)	101 (100%)	0	100	100
30	AQ	54/126 (43%)	54 (100%)	0	100	100
31	AR	107/133 (80%)	107 (100%)	0	100	100
32	AS	124/135 (92%)	124 (100%)	0	100	100
33	AT	117/118 (99%)	117 (100%)	0	100	100
34	AU	119/120 (99%)	119 (100%)	0	100	100
All	All	3836/4327 (89%)	3836 (100%)	0	100	100

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

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

Mol	Chain	Res	Type
3	AX	28	ASN
5	AZ	21	GLN
7	Ab	65	GLN
7	Ab	68	ASN
13	Ah	102	GLN
15	Aj	100	ASN
16	BA	11	HIS
16	BA	138	GLN
16	BA	145	GLN

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Mol	Chain	Res	Type
16	BA	203	GLN
17	BB	41	HIS
17	BB	43	ASN
17	BB	89	GLN
17	BB	347	HIS
18	BC	111	ASN
18	BC	250	ASN
18	BC	267	ASN
18	BC	282	GLN
19	BD	211	HIS
23	CD	218	HIS
24	AK	93	GLN
24	AK	162	HIS
26	AM	37	HIS
26	AM	50	GLN
26	AM	122	HIS
26	AM	125	GLN
26	AM	163	HIS
28	AO	41	GLN
31	AR	57	GLN
31	AR	69	ASN
31	AR	111	GLN
32	AS	127	GLN
34	AU	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	CA	3467/5069 (68%)	533 (15%)	12 (0%)
21	CB	118/120 (98%)	8 (6%)	0
22	CC	155/157 (98%)	28 (18%)	0
All	All	3740/5346 (69%)	569 (15%)	12 (0%)

All (569) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	CA	39	A
20	CA	42	A
20	CA	48	G
20	CA	58	G
20	CA	59	A

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Mol	Chain	Res	Type
20	CA	64	A
20	CA	65	A
20	CA	66	A
20	CA	91	G
20	CA	110	C
20	CA	119	G
20	CA	120	A
20	CA	131	C
20	CA	132	G
20	CA	135	G
20	CA	136	C
20	CA	138	G
20	CA	143	C
20	CA	144	G
20	CA	159	C
20	CA	171	U
20	CA	172	C
20	CA	178	C
20	CA	183	C
20	CA	184	U
20	CA	185	C
20	CA	186	G
20	CA	188	G
20	CA	189	G
20	CA	200	U
20	CA	209	U
20	CA	210	C
20	CA	216	C
20	CA	218	A
20	CA	220	C
20	CA	233	U
20	CA	234	G
20	CA	253	G
20	CA	263	G
20	CA	264	C
20	CA	266	C
20	CA	267	G
20	CA	280	G
20	CA	297	U
20	CA	316	U
20	CA	340	C
20	CA	387	G

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Mol	Chain	Res	Type
20	CA	409	G
20	CA	410	A
20	CA	412	G
20	CA	414	C
20	CA	415	G
20	CA	432	U
20	CA	446	C
20	CA	449	C
20	CA	450	G
20	CA	453	G
20	CA	459	C
20	CA	463	A
20	CA	467	U
20	CA	468	U
20	CA	469	C
20	CA	483	G
20	CA	484	U
20	CA	485	C
20	CA	486	C
20	CA	489	C
20	CA	491	G
20	CA	492	U
20	CA	493	G
20	CA	497	G
20	CA	498	C
20	CA	500	G
20	CA	501	C
20	CA	502	C
20	CA	503	C
20	CA	504	G
20	CA	505	G
20	CA	509	A
20	CA	510	U
20	CA	511	C
20	CA	512	U
20	CA	513	U
20	CA	514	U
20	CA	515	C
20	CA	516	C
20	CA	518	G
20	CA	519	C
20	CA	643	C

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Mol	Chain	Res	Type
20	CA	644	G
20	CA	645	G
20	CA	646	G
20	CA	654	C
20	CA	657	C
20	CA	659	G
20	CA	665	C
20	CA	666	G
20	CA	668	C
20	CA	670	G
20	CA	686	A
20	CA	687	U
20	CA	688	U
20	CA	692	A
20	CA	701	G
20	CA	703	G
20	CA	704	C
20	CA	730	G
20	CA	731	G
20	CA	739	G
20	CA	742	G
20	CA	743	G
20	CA	759	G
20	CA	760	G
20	CA	904	C
20	CA	905	C
20	CA	913	U
20	CA	915	A
20	CA	916	C
20	CA	917	A
20	CA	923	C
20	CA	924	C
20	CA	926	G
20	CA	932	A
20	CA	933	G
20	CA	944	A
20	CA	945	U
20	CA	946	C
20	CA	956	A
20	CA	959	G
20	CA	960	A
20	CA	962	C

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Mol	Chain	Res	Type
20	CA	965	G
20	CA	966	A
20	CA	967	C
20	CA	969	C
20	CA	970	G
20	CA	982	U
20	CA	984	C
20	CA	989	U
20	CA	990	C
20	CA	991	C
20	CA	992	C
20	CA	993	G
20	CA	995	C
20	CA	1070	G
20	CA	1072	C
20	CA	1078	A
20	CA	1083	U
20	CA	1100	U
20	CA	1168	G
20	CA	1173	G
20	CA	1178	G
20	CA	1179	U
20	CA	1180	C
20	CA	1181	C
20	CA	1182	C
20	CA	1183	C
20	CA	1184	A
20	CA	1185	G
20	CA	1186	U
20	CA	1189	G
20	CA	1198	G
20	CA	1200	G
20	CA	1201	U
20	CA	1202	C
20	CA	1211	G
20	CA	1214	C
20	CA	1216	C
20	CA	1222	A
20	CA	1241	C
20	CA	1249	C
20	CA	1252	C
20	CA	1253	G

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Mol	Chain	Res	Type
20	CA	1255	A
20	CA	1256	G
20	CA	1259	G
20	CA	1260	G
20	CA	1261	G
20	CA	1262	G
20	CA	1266	G
20	CA	1270	A
20	CA	1271	G
20	CA	1272	C
20	CA	1273	G
20	CA	1276	C
20	CA	1279	A
20	CA	1280	C
20	CA	1284	G
20	CA	1285	U
20	CA	1287	G
20	CA	1294	A
20	CA	1301	C
20	CA	1302	U
20	CA	1303	A
20	CA	1304	C
20	CA	1313	C
20	CA	1326	A2M
20	CA	1337	A
20	CA	1354	A
20	CA	1359	G
20	CA	1365	C
20	CA	1366	G
20	CA	1387	A
20	CA	1394	G
20	CA	1397	A
20	CA	1406	G
20	CA	1408	G
20	CA	1409	C
20	CA	1410	U
20	CA	1411	C
20	CA	1413	C
20	CA	1415	G
20	CA	1416	G
20	CA	1420	A
20	CA	1438	U

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Mol	Chain	Res	Type
20	CA	1439	C
20	CA	1443	A
20	CA	1444	G
20	CA	1457	G
20	CA	1498	G
20	CA	1502	G
20	CA	1504	G
20	CA	1534	A2M
20	CA	1547	A
20	CA	1561	G
20	CA	1562	G
20	CA	1563	A
20	CA	1564	A
20	CA	1565	A
20	CA	1566	C
20	CA	1578	U
20	CA	1591	U
20	CA	1596	U
20	CA	1624	G
20	CA	1625	OMG
20	CA	1631	A
20	CA	1633	G
20	CA	1634	A
20	CA	1638	A
20	CA	1640	C
20	CA	1641	G
20	CA	1642	A
20	CA	1654	G
20	CA	1661	C
20	CA	1676	C
20	CA	1677	PSU
20	CA	1694	C
20	CA	1698	C
20	CA	1699	A
20	CA	1704	C
20	CA	1705	G
20	CA	1706	A
20	CA	1707	C
20	CA	1708	G
20	CA	1715	C
20	CA	1719	A
20	CA	1721	G

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Mol	Chain	Res	Type
20	CA	1722	C
20	CA	1734	G
20	CA	1741	G
20	CA	1742	A
20	CA	1750	G
20	CA	1755	C
20	CA	1756	U
20	CA	1757	U
20	CA	1758	G
20	CA	1775	A
20	CA	1787	A
20	CA	1804	A
20	CA	1822	U
20	CA	1836	G
20	CA	1837	A
20	CA	1842	G
20	CA	1855	G
20	CA	1869	G
20	CA	1897	A
20	CA	1918	U
20	CA	1919	G
20	CA	1921	C
20	CA	1922	G
20	CA	1930	U
20	CA	1931	C
20	CA	1932	A
20	CA	1940	G
20	CA	1948	G
20	CA	2042	A
20	CA	2046	G
20	CA	2048	U
20	CA	2055	G
20	CA	2056	G
20	CA	2069	A
20	CA	2084	C
20	CA	2085	G
20	CA	2092	G
20	CA	2093	A
20	CA	2094	G
20	CA	2095	A
20	CA	2096	G
20	CA	2097	U

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Mol	Chain	Res	Type
20	CA	2098	G
20	CA	2102	G
20	CA	2106	G
20	CA	2108	G
20	CA	2111	G
20	CA	2250	C
20	CA	2252	G
20	CA	2253	A
20	CA	2255	C
20	CA	2256	C
20	CA	2259	G
20	CA	2289	C
20	CA	2300	A
20	CA	2301	G
20	CA	2306	G
20	CA	2313	A
20	CA	2314	G
20	CA	2333	G
20	CA	2348	G
20	CA	2351	OMC
20	CA	2395	A
20	CA	2421	G
20	CA	2450	G
20	CA	2453	A
20	CA	2504	C
20	CA	2505	C
20	CA	2513	A
20	CA	2544	G
20	CA	2545	U
20	CA	2546	G
20	CA	2547	G
20	CA	2548	C
20	CA	2549	G
20	CA	2554	U
20	CA	2555	G
20	CA	2561	C
20	CA	2562	G
20	CA	2563	C
20	CA	2566	G
20	CA	2583	C
20	CA	2586	G
20	CA	2587	A

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Mol	Chain	Res	Type
20	CA	2589	C
20	CA	2601	A
20	CA	2627	C
20	CA	2653	C
20	CA	2669	C
20	CA	2681	G
20	CA	2687	U
20	CA	2695	A
20	CA	2696	A
20	CA	2710	C
20	CA	2711	G
20	CA	2726	G
20	CA	2739	C
20	CA	2743	A
20	CA	2759	G
20	CA	2763	U
20	CA	2788	U
20	CA	2790	U
20	CA	2814	C
20	CA	2826	U
20	CA	2827	G
20	CA	2855	G
20	CA	2900	U
20	CA	3606	U
20	CA	3615	G
20	CA	3618	C
20	CA	3626	G
20	CA	3635	A
20	CA	3644	U
20	CA	3648	A
20	CA	3653	A
20	CA	3662	A
20	CA	3663	A
20	CA	3673	C
20	CA	3709	U
20	CA	3710	G
20	CA	3713	U
20	CA	3748	A
20	CA	3753	G
20	CA	3773	U
20	CA	3774	A
20	CA	3777	G

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Mol	Chain	Res	Type
20	CA	3783	A
20	CA	3784	A
20	CA	3785	A2M
20	CA	3792	OMG
20	CA	3809	G
20	CA	3811	G
20	CA	3812	C
20	CA	3814	U
20	CA	3817	A
20	CA	3819	G
20	CA	3823	G
20	CA	3838	U
20	CA	3840	U
20	CA	3867	A2M
20	CA	3877	A
20	CA	3878	C
20	CA	3879	G
20	CA	3897	G
20	CA	3901	A
20	CA	3906	A
20	CA	3907	G
20	CA	3908	A
20	CA	3915	U
20	CA	4076	G
20	CA	4077	A
20	CA	4084	G
20	CA	4119	C
20	CA	4122	G
20	CA	4141	G
20	CA	4143	G
20	CA	4144	C
20	CA	4145	C
20	CA	4146	G
20	CA	4149	C
20	CA	4152	G
20	CA	4162	C
20	CA	4163	U
20	CA	4170	A
20	CA	4183	G
20	CA	4184	G
20	CA	4191	G
20	CA	4203	A

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Mol	Chain	Res	Type
20	CA	4225	G
20	CA	4229	U
20	CA	4233	A
20	CA	4254	G
20	CA	4256	A
20	CA	4266	G
20	CA	4268	A
20	CA	4273	A
20	CA	4281	A
20	CA	4291	G
20	CA	4305	G
20	CA	4329	G
20	CA	4330	G
20	CA	4332	C
20	CA	4339	A
20	CA	4349	C
20	CA	4373	G
20	CA	4376	A
20	CA	4377	G
20	CA	4378	A
20	CA	4380	A
20	CA	4387	C
20	CA	4391	G
20	CA	4394	A
20	CA	4421	C
20	CA	4422	A
20	CA	4448	G
20	CA	4455	G
20	CA	4464	A
20	CA	4466	C
20	CA	4512	U
20	CA	4513	A
20	CA	4519	C
20	CA	4524	G
20	CA	4548	A
20	CA	4549	G
20	CA	4560	C
20	CA	4567	G
20	CA	4572	U
20	CA	4573	G
20	CA	4584	A
20	CA	4590	A

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Mol	Chain	Res	Type
20	CA	4606	G
20	CA	4608	G
20	CA	4610	A
20	CA	4627	U
20	CA	4636	U
20	CA	4637	OMG
20	CA	4670	C
20	CA	4672	A
20	CA	4694	G
20	CA	4700	A
20	CA	4708	A
20	CA	4709	U
20	CA	4719	G
20	CA	4720	C
20	CA	4731	G
20	CA	4732	G
20	CA	4734	A
20	CA	4735	G
20	CA	4740	G
20	CA	4741	C
20	CA	4742	G
20	CA	4754	G
20	CA	4757	C
20	CA	4759	C
20	CA	4761	G
20	CA	4765	G
20	CA	4771	C
20	CA	4774	C
20	CA	4775	C
20	CA	4861	G
20	CA	4870	G
20	CA	4871	C
20	CA	4875	G
20	CA	4882	U
20	CA	4883	C
20	CA	4889	G
20	CA	4894	A
20	CA	4895	C
20	CA	4896	G
20	CA	4900	C
20	CA	4910	G
20	CA	4912	G

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Mol	Chain	Res	Type
20	CA	4914	C
20	CA	4919	G
20	CA	4924	C
20	CA	4925	U
20	CA	4926	C
20	CA	4955	A
20	CA	4957	C
20	CA	4960	G
20	CA	4976	U
20	CA	4989	U
20	CA	4990	C
20	CA	4991	U
20	CA	5013	C
20	CA	5014	A
20	CA	5022	U
20	CA	5023	C
20	CA	5024	C
20	CA	5026	U
20	CA	5027	C
20	CA	5034	A
20	CA	5041	G
20	CA	5050	C
20	CA	5054	C
20	CA	5069	U
21	CB	33	U
21	CB	42	A
21	CB	53	U
21	CB	54	A
21	CB	64	G
21	CB	97	G
21	CB	100	A
21	CB	110	G
22	CC	23	C
22	CC	34	U
22	CC	35	C
22	CC	52	A
22	CC	59	A
22	CC	62	A
22	CC	63	U
22	CC	79	G
22	CC	80	A
22	CC	82	A

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Mol	Chain	Res	Type
22	CC	85	U
22	CC	86	U
22	CC	87	G
22	CC	94	G
22	CC	103	A
22	CC	105	C
22	CC	110	U
22	CC	111	U
22	CC	114	G
22	CC	121	G
22	CC	122	G
22	CC	123	U
22	CC	124	U
22	CC	125	C
22	CC	126	C
22	CC	127	U
22	CC	128	C
22	CC	155	C

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	CA	510	U
20	CA	511	C
20	CA	1201	U
20	CA	1252	C
20	CA	1590	C
20	CA	1633	G
20	CA	1677	PSU
20	CA	2252	G
20	CA	2562	G
20	CA	4142	C
20	CA	4699	U
20	CA	4893	A

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

122 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
20	A2M	CA	1524	20	22,25,26	3.39	8 (36%)	31,36,39	2.77	13 (41%)
20	PSU	CA	4293	20	18,21,22	1.27	3 (16%)	22,30,33	1.52	3 (13%)
20	A2M	CA	400	20	22,25,26	3.35	9 (40%)	31,36,39	2.83	12 (38%)
20	OMC	CA	4456	20	19,22,23	3.13	8 (42%)	26,31,34	0.71	0
20	OMU	CA	4498	20,35	19,22,23	0.79	1 (5%)	26,31,34	1.25	4 (15%)
20	PSU	CA	1779	20	18,21,22	1.27	3 (16%)	22,30,33	1.47	3 (13%)
20	PSU	CA	4972	20	18,21,22	1.30	2 (11%)	22,30,33	1.48	3 (13%)
20	PSU	CA	3920	20,35	18,21,22	1.29	3 (16%)	22,30,33	1.36	3 (13%)
16	HIC	BA	245	16	10,11,12	0.48	0	8,14,16	0.51	0
20	OMG	CA	4392	20	23,26,27	2.50	6 (26%)	33,38,41	1.88	10 (30%)
20	PSU	CA	4576	20	18,21,22	1.31	3 (16%)	22,30,33	1.32	3 (13%)
20	PSU	CA	1792	20	18,21,22	1.27	3 (16%)	22,30,33	1.50	3 (13%)
20	OMG	CA	2364	20,35	23,26,27	2.51	6 (26%)	33,38,41	1.85	10 (30%)
20	OMU	CA	4620	20	19,22,23	0.73	1 (5%)	26,31,34	1.23	2 (7%)
20	PSU	CA	4493	20,41	18,21,22	1.28	3 (16%)	22,30,33	1.53	4 (18%)
20	1MA	CA	1322	20,35	21,25,26	2.89	5 (23%)	31,37,40	2.13	8 (25%)
20	PSU	CA	2508	20	18,21,22	1.27	3 (16%)	22,30,33	1.52	3 (13%)
20	PSU	CA	4532	20	18,21,22	1.28	3 (16%)	22,30,33	1.53	3 (13%)
20	PSU	CA	4471	20	18,21,22	1.29	3 (16%)	22,30,33	1.50	3 (13%)
20	PSU	CA	3844	20	18,21,22	1.32	3 (16%)	22,30,33	1.41	3 (13%)
20	A2M	CA	3830	20	22,25,26	3.38	9 (40%)	31,36,39	2.71	12 (38%)
20	OMC	CA	2422	20,35	19,22,23	3.21	8 (42%)	26,31,34	0.77	0
20	OMU	CA	2415	20	19,22,23	0.77	1 (5%)	26,31,34	1.21	3 (11%)
20	OMU	CA	2837	20	19,22,23	0.82	1 (5%)	26,31,34	1.27	3 (11%)
20	PSU	CA	4579	20	18,21,22	1.27	3 (16%)	22,30,33	1.36	3 (13%)
20	OMG	CA	4499	20	23,26,27	2.54	6 (26%)	33,38,41	1.92	8 (24%)
20	OMC	CA	3841	20	19,22,23	3.11	8 (42%)	26,31,34	0.57	0
20	A2M	CA	2401	20	22,25,26	3.32	9 (40%)	31,36,39	2.73	13 (41%)
20	PSU	CA	3822	20	18,21,22	1.32	2 (11%)	22,30,33	1.17	2 (9%)
20	OMU	CA	4227	20	19,22,23	0.83	2 (10%)	26,31,34	1.31	4 (15%)
20	PSU	CA	4420	20	18,21,22	1.32	2 (11%)	22,30,33	1.20	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PSU	CA	4521	20,35	18,21,22	1.29	3 (16%)	22,30,33	1.55	5 (22%)
20	OMG	CA	1625	20	23,26,27	2.54	6 (26%)	33,38,41	1.85	8 (24%)
20	OMG	CA	4228	20	23,26,27	2.49	8 (34%)	33,38,41	1.96	11 (33%)
20	PSU	CA	3695	20	18,21,22	1.27	2 (11%)	22,30,33	1.29	3 (13%)
20	UR3	CA	4530	20	19,22,23	3.08	8 (42%)	26,32,35	1.46	3 (11%)
20	PSU	CA	3639	20	18,21,22	1.28	3 (16%)	22,30,33	1.39	3 (13%)
22	PSU	CC	55	22	18,21,22	1.29	3 (16%)	22,30,33	1.54	3 (13%)
20	PSU	CA	4312	20	18,21,22	1.32	3 (16%)	22,30,33	1.57	3 (13%)
20	OMC	CA	3887	20	19,22,23	3.11	8 (42%)	26,31,34	0.83	1 (3%)
20	OMU	CA	3925	20	19,22,23	0.89	2 (10%)	26,31,34	1.24	3 (11%)
20	OMG	CA	4196	20	23,26,27	2.53	6 (26%)	33,38,41	1.85	7 (21%)
20	A2M	CA	1534	20,35	22,25,26	3.52	9 (40%)	31,36,39	2.68	10 (32%)
20	PSU	CA	1860	20	18,21,22	1.22	1 (5%)	22,30,33	1.66	4 (18%)
20	A2M	CA	2787	20	22,25,26	3.42	9 (40%)	31,36,39	2.43	9 (29%)
20	PSU	CA	4299	20	18,21,22	1.27	3 (16%)	22,30,33	1.50	3 (13%)
20	OMC	CA	2804	20	19,22,23	3.11	8 (42%)	26,31,34	0.67	0
20	PSU	CA	1683	20,41	18,21,22	1.24	3 (16%)	22,30,33	1.54	4 (18%)
20	PSU	CA	4353	20	18,21,22	1.27	3 (16%)	22,30,33	1.57	3 (13%)
20	OMU	CA	4306	20	19,22,23	0.79	1 (5%)	26,31,34	1.33	4 (15%)
23	V5N	CD	216	23	9,11,12	1.51	1 (11%)	9,14,16	1.86	3 (33%)
20	PSU	CA	1862	20	18,21,22	1.25	3 (16%)	22,30,33	1.56	3 (13%)
20	PSU	CA	4403	20	18,21,22	1.27	3 (16%)	22,30,33	1.51	3 (13%)
20	OMG	CA	1522	20	23,26,27	2.52	6 (26%)	33,38,41	1.91	10 (30%)
34	V5N	AU	39	34	9,11,12	1.45	2 (22%)	9,14,16	2.02	3 (33%)
20	PSU	CA	4442	20	18,21,22	1.26	2 (11%)	22,30,33	1.21	2 (9%)
20	6MZ	CA	4220	20	22,25,26	3.77	9 (40%)	30,36,39	2.55	11 (36%)
20	UY1	CA	3818	20,41	19,22,23	4.30	5 (26%)	22,31,34	2.07	6 (27%)
22	PSU	CC	69	22	18,21,22	1.28	2 (11%)	22,30,33	1.22	2 (9%)
20	A2M	CA	3785	20	22,25,26	3.40	9 (40%)	31,36,39	2.78	12 (38%)
20	PSU	CA	1781	20	18,21,22	1.29	3 (16%)	22,30,33	1.48	4 (18%)
20	A2M	CA	1326	20	22,25,26	3.39	9 (40%)	31,36,39	2.75	14 (45%)
20	OMG	CA	4370	20	23,26,27	2.53	7 (30%)	33,38,41	1.92	10 (30%)
20	A2M	CA	3867	20	22,25,26	3.38	9 (40%)	31,36,39	2.78	15 (48%)
20	OMG	CA	3744	20	23,26,27	2.50	7 (30%)	33,38,41	1.85	9 (27%)
20	5MC	CA	3782	20,35	18,22,23	3.56	7 (38%)	26,32,35	1.03	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PSU	CA	3884	20	18,21,22	1.22	3 (16%)	22,30,33	1.53	3 (13%)
20	A2M	CA	398	20	22,25,26	3.32	9 (40%)	31,36,39	2.87	13 (41%)
20	PSU	CA	4689	20	18,21,22	1.20	1 (5%)	22,30,33	1.46	3 (13%)
20	A2M	CA	1871	20,35	22,25,26	3.40	9 (40%)	31,36,39	2.75	11 (35%)
20	PSU	CA	4500	20	18,21,22	1.32	3 (16%)	22,30,33	1.43	3 (13%)
12	MLZ	Ag	98	12	8,9,10	0.78	0	4,9,11	0.77	0
20	PSU	CA	5001	20	18,21,22	1.32	3 (16%)	22,30,33	1.36	3 (13%)
20	OMC	CA	3869	20	19,22,23	3.12	8 (42%)	26,31,34	0.72	0
20	PSU	CA	3851	20	18,21,22	1.33	2 (11%)	22,30,33	1.45	3 (13%)
20	OMG	CA	4618	20	23,26,27	2.50	7 (30%)	33,38,41	1.89	10 (30%)
20	OMG	CA	4623	20	23,26,27	2.53	6 (26%)	33,38,41	1.86	9 (27%)
20	A2M	CA	2363	20,35	22,25,26	3.28	9 (40%)	31,36,39	2.75	12 (38%)
20	PSU	CA	1744	20	18,21,22	1.28	3 (16%)	22,30,33	1.56	3 (13%)
20	OMG	CA	4494	20	23,26,27	2.54	6 (26%)	33,38,41	1.85	9 (27%)
20	OMC	CA	3701	20,41	19,22,23	3.09	8 (42%)	26,31,34	0.70	0
20	B8T	CA	1859	20	19,22,23	1.00	1 (5%)	26,31,34	0.86	1 (3%)
20	PSU	CA	1536	20	18,21,22	1.24	3 (16%)	22,30,33	1.55	3 (13%)
20	OMC	CA	2861	20	19,22,23	3.14	8 (42%)	26,31,34	0.64	0
20	OMG	CA	2876	20	23,26,27	2.54	6 (26%)	33,38,41	1.95	10 (30%)
20	OMC	CA	2351	20,35	19,22,23	3.09	8 (42%)	26,31,34	0.87	1 (3%)
20	A2M	CA	3825	20	22,25,26	3.38	9 (40%)	31,36,39	2.80	12 (38%)
20	PSU	CA	4431	20	18,21,22	1.26	3 (16%)	22,30,33	1.52	3 (13%)
20	OMC	CA	1881	20,35	19,22,23	3.14	8 (42%)	26,31,34	0.79	0
20	OMC	CA	1340	20	19,22,23	3.11	8 (42%)	26,31,34	0.66	0
20	PSU	CA	2839	20	18,21,22	1.28	3 (16%)	22,30,33	1.45	3 (13%)
20	A2M	CA	3718	20	22,25,26	3.36	9 (40%)	31,36,39	2.79	12 (38%)
20	PSU	CA	4457	20	18,21,22	1.23	1 (5%)	22,30,33	1.32	3 (13%)
20	OMC	CA	4536	20	19,22,23	3.13	8 (42%)	26,31,34	0.70	0
20	OMC	CA	2824	20	19,22,23	3.15	8 (42%)	26,31,34	0.69	0
20	PSU	CA	3637	20,41	18,21,22	1.16	1 (5%)	22,30,33	1.56	5 (22%)
20	PSU	CA	1677	20	18,21,22	1.43	4 (22%)	22,30,33	1.54	3 (13%)
20	OMG	CA	2424	20	23,26,27	2.53	7 (30%)	33,38,41	1.86	10 (30%)
20	PSU	CA	1782	20	18,21,22	1.26	3 (16%)	22,30,33	1.60	4 (18%)
20	A2M	CA	4523	20,35	22,25,26	3.32	9 (40%)	31,36,39	2.94	13 (41%)
20	5MC	CA	4447	20,41	18,22,23	3.55	7 (38%)	26,32,35	1.16	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	A2M	CA	2815	20	22,25,26	3.40	9 (40%)	31,36,39	2.74	15 (48%)
20	PSU	CA	4552	20	18,21,22	1.26	3 (16%)	22,30,33	1.52	3 (13%)
20	PSU	CA	3715	20	18,21,22	1.45	4 (22%)	22,30,33	1.36	3 (13%)
20	OMG	CA	3669	20	23,26,27	2.54	7 (30%)	33,38,41	1.92	10 (30%)
20	PSU	CA	4628	20	18,21,22	1.29	3 (16%)	22,30,33	1.44	3 (13%)
22	OMG	CC	75	22	23,26,27	2.53	7 (30%)	33,38,41	1.88	9 (27%)
20	PSU	CA	4423	20	18,21,22	1.32	3 (16%)	22,30,33	1.56	3 (13%)
20	PSU	CA	4361	20	18,21,22	1.26	3 (16%)	22,30,33	1.57	3 (13%)
20	A2M	CA	4571	20	22,25,26	3.29	9 (40%)	31,36,39	2.94	17 (54%)
20	OMC	CA	2365	20	19,22,23	3.13	8 (42%)	26,31,34	0.70	0
20	OMG	CA	3792	20	23,26,27	2.53	7 (30%)	33,38,41	1.87	9 (27%)
20	OMC	CA	3808	20	19,22,23	3.14	8 (42%)	26,31,34	0.78	0
20	OMG	CA	3899	20,35	23,26,27	2.52	7 (30%)	33,38,41	1.85	10 (30%)
20	A2M	CA	1323	20	22,25,26	3.40	8 (36%)	31,36,39	2.74	12 (38%)
20	PSU	CA	2632	20	18,21,22	1.33	3 (16%)	22,30,33	1.35	3 (13%)
20	PSU	CA	224	20	18,21,22	1.33	3 (16%)	22,30,33	1.48	4 (18%)
20	PSU	CA	4673	20,35	18,21,22	1.26	2 (11%)	22,30,33	1.42	3 (13%)
20	OMG	CA	3627	20	23,26,27	2.52	6 (26%)	33,38,41	1.88	10 (30%)
20	PSU	CA	4296	20	18,21,22	1.31	3 (16%)	22,30,33	1.47	3 (13%)
20	OMG	CA	4637	20	23,26,27	2.51	6 (26%)	33,38,41	1.83	9 (27%)
20	OMG	CA	1316	20	23,26,27	2.50	6 (26%)	33,38,41	1.84	9 (27%)

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
20	A2M	CA	1524	20	-	1/9/27/28	0/3/3/3
20	PSU	CA	4293	20	-	0/7/25/26	0/2/2/2
20	A2M	CA	400	20	-	1/9/27/28	0/3/3/3
20	OMC	CA	4456	20	-	0/9/27/28	0/2/2/2
20	OMU	CA	4498	20,35	-	1/9/27/28	0/2/2/2
20	PSU	CA	1779	20	-	0/7/25/26	0/2/2/2
20	PSU	CA	4972	20	-	0/7/25/26	0/2/2/2
20	PSU	CA	3920	20,35	-	0/7/25/26	0/2/2/2
16	HIC	BA	245	16	-	1/5/6/8	0/1/1/1
20	OMG	CA	4392	20	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PSU	CA	4576	20	-	0/7/25/26	0/2/2/2
20	PSU	CA	1792	20	-	0/7/25/26	0/2/2/2
20	OMG	CA	2364	20,35	-	0/9/27/28	0/3/3/3
20	OMU	CA	4620	20	-	0/9/27/28	0/2/2/2
20	PSU	CA	4493	20,41	-	0/7/25/26	0/2/2/2
20	1MA	CA	1322	20,35	-	1/7/25/26	0/3/3/3
20	PSU	CA	2508	20	-	0/7/25/26	0/2/2/2
20	PSU	CA	4532	20	-	0/7/25/26	0/2/2/2
20	PSU	CA	4471	20	-	0/7/25/26	0/2/2/2
20	PSU	CA	3844	20	-	1/7/25/26	0/2/2/2
20	A2M	CA	3830	20	-	1/9/27/28	0/3/3/3
20	OMC	CA	2422	20,35	-	2/9/27/28	0/2/2/2
20	OMU	CA	2415	20	-	0/9/27/28	0/2/2/2
20	OMU	CA	2837	20	-	0/9/27/28	0/2/2/2
20	PSU	CA	4579	20	-	0/7/25/26	0/2/2/2
20	OMG	CA	4499	20	-	0/9/27/28	0/3/3/3
20	OMC	CA	3841	20	-	0/9/27/28	0/2/2/2
20	A2M	CA	2401	20	-	2/9/27/28	0/3/3/3
20	PSU	CA	3822	20	-	0/7/25/26	0/2/2/2
20	OMU	CA	4227	20	-	0/9/27/28	0/2/2/2
20	PSU	CA	4420	20	-	3/7/25/26	0/2/2/2
20	PSU	CA	4521	20,35	-	1/7/25/26	0/2/2/2
20	OMG	CA	1625	20	-	0/9/27/28	0/3/3/3
20	OMG	CA	4228	20	-	0/9/27/28	0/3/3/3
20	PSU	CA	3695	20	-	0/7/25/26	0/2/2/2
20	UR3	CA	4530	20	-	2/7/25/26	0/2/2/2
20	PSU	CA	3639	20	-	0/7/25/26	0/2/2/2
22	PSU	CC	55	22	-	0/7/25/26	0/2/2/2
20	PSU	CA	4312	20	-	0/7/25/26	0/2/2/2
20	OMC	CA	3887	20	-	0/9/27/28	0/2/2/2
20	OMU	CA	3925	20	-	0/9/27/28	0/2/2/2
20	OMG	CA	4196	20	-	0/9/27/28	0/3/3/3
20	A2M	CA	1534	20,35	-	2/9/27/28	0/3/3/3
20	PSU	CA	1860	20	-	0/7/25/26	0/2/2/2
20	A2M	CA	2787	20	-	3/9/27/28	0/3/3/3
20	PSU	CA	4299	20	-	0/7/25/26	0/2/2/2
20	OMC	CA	2804	20	-	0/9/27/28	0/2/2/2
20	PSU	CA	1683	20,41	-	0/7/25/26	0/2/2/2
20	PSU	CA	4353	20	-	0/7/25/26	0/2/2/2
20	OMU	CA	4306	20	-	0/9/27/28	0/2/2/2
23	V5N	CD	216	23	-	1/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PSU	CA	1862	20	-	0/7/25/26	0/2/2/2
20	PSU	CA	4403	20	-	0/7/25/26	0/2/2/2
20	OMG	CA	1522	20	-	0/9/27/28	0/3/3/3
34	V5N	AU	39	34	-	2/9/10/12	0/1/1/1
20	PSU	CA	4442	20	-	0/7/25/26	0/2/2/2
20	6MZ	CA	4220	20	-	0/9/27/28	0/3/3/3
20	UY1	CA	3818	20,41	-	2/9/27/28	0/2/2/2
22	PSU	CC	69	22	-	0/7/25/26	0/2/2/2
20	A2M	CA	3785	20	-	2/9/27/28	0/3/3/3
20	PSU	CA	1781	20	-	1/7/25/26	0/2/2/2
20	A2M	CA	1326	20	-	1/9/27/28	0/3/3/3
20	OMG	CA	4370	20	-	1/9/27/28	0/3/3/3
20	A2M	CA	3867	20	-	3/9/27/28	0/3/3/3
20	OMG	CA	3744	20	-	1/9/27/28	0/3/3/3
20	5MC	CA	3782	20,35	-	0/7/25/26	0/2/2/2
20	PSU	CA	3884	20	-	0/7/25/26	0/2/2/2
20	A2M	CA	398	20	-	2/9/27/28	0/3/3/3
20	PSU	CA	4689	20	-	0/7/25/26	0/2/2/2
20	A2M	CA	1871	20,35	-	0/9/27/28	0/3/3/3
20	PSU	CA	4500	20	-	3/7/25/26	0/2/2/2
12	MLZ	Ag	98	12	-	1/7/8/10	-
20	PSU	CA	5001	20	-	0/7/25/26	0/2/2/2
20	OMC	CA	3869	20	-	0/9/27/28	0/2/2/2
20	PSU	CA	3851	20	-	1/7/25/26	0/2/2/2
20	OMG	CA	4618	20	-	0/9/27/28	0/3/3/3
20	OMG	CA	4623	20	-	0/9/27/28	0/3/3/3
20	A2M	CA	2363	20,35	-	1/9/27/28	0/3/3/3
20	PSU	CA	1744	20	-	0/7/25/26	0/2/2/2
20	OMG	CA	4494	20	-	1/9/27/28	0/3/3/3
20	OMC	CA	3701	20,41	-	4/9/27/28	0/2/2/2
20	B8T	CA	1859	20	-	1/7/27/28	0/2/2/2
20	PSU	CA	1536	20	-	0/7/25/26	0/2/2/2
20	OMC	CA	2861	20	-	0/9/27/28	0/2/2/2
20	OMG	CA	2876	20	-	1/9/27/28	0/3/3/3
20	OMC	CA	2351	20,35	-	4/9/27/28	0/2/2/2
20	A2M	CA	3825	20	-	1/9/27/28	0/3/3/3
20	PSU	CA	4431	20	-	0/7/25/26	0/2/2/2
20	OMC	CA	1881	20,35	-	0/9/27/28	0/2/2/2
20	OMC	CA	1340	20	-	0/9/27/28	0/2/2/2
20	PSU	CA	2839	20	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	A2M	CA	3718	20	-	1/9/27/28	0/3/3/3
20	PSU	CA	4457	20	-	0/7/25/26	0/2/2/2
20	OMC	CA	4536	20	-	0/9/27/28	0/2/2/2
20	OMC	CA	2824	20	-	0/9/27/28	0/2/2/2
20	PSU	CA	3637	20,41	-	0/7/25/26	0/2/2/2
20	PSU	CA	1677	20	-	0/7/25/26	0/2/2/2
20	OMG	CA	2424	20	-	0/9/27/28	0/3/3/3
20	PSU	CA	1782	20	-	0/7/25/26	0/2/2/2
20	A2M	CA	4523	20,35	-	1/9/27/28	0/3/3/3
20	5MC	CA	4447	20,41	-	4/7/25/26	0/2/2/2
20	A2M	CA	2815	20	-	1/9/27/28	0/3/3/3
20	PSU	CA	4552	20	-	0/7/25/26	0/2/2/2
20	PSU	CA	3715	20	-	0/7/25/26	0/2/2/2
20	OMG	CA	3669	20	-	2/9/27/28	0/3/3/3
20	PSU	CA	4628	20	-	0/7/25/26	0/2/2/2
22	OMG	CC	75	22	-	0/9/27/28	0/3/3/3
20	PSU	CA	4423	20	-	0/7/25/26	0/2/2/2
20	PSU	CA	4361	20	-	0/7/25/26	0/2/2/2
20	A2M	CA	4571	20	-	2/9/27/28	0/3/3/3
20	OMC	CA	2365	20	-	0/9/27/28	0/2/2/2
20	OMG	CA	3792	20	-	2/9/27/28	0/3/3/3
20	OMC	CA	3808	20	-	0/9/27/28	0/2/2/2
20	OMG	CA	3899	20,35	-	0/9/27/28	0/3/3/3
20	A2M	CA	1323	20	-	1/9/27/28	0/3/3/3
20	PSU	CA	2632	20	-	0/7/25/26	0/2/2/2
20	PSU	CA	224	20	-	2/7/25/26	0/2/2/2
20	PSU	CA	4673	20,35	-	0/7/25/26	0/2/2/2
20	OMG	CA	3627	20	-	0/9/27/28	0/3/3/3
20	PSU	CA	4296	20	-	0/7/25/26	0/2/2/2
20	OMG	CA	4637	20	-	1/9/27/28	0/3/3/3
20	OMG	CA	1316	20	-	0/9/27/28	0/3/3/3

All (606) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	3818	UY1	C6-C5	12.13	1.49	1.35
20	CA	4220	6MZ	C6-N6	11.81	1.47	1.34
20	CA	3818	UY1	C2-N1	9.82	1.50	1.36
20	CA	4447	5MC	C6-C5	9.25	1.49	1.34
20	CA	3782	5MC	C6-C5	9.21	1.49	1.34
20	CA	3718	A2M	O4'-C1'	9.06	1.63	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	3830	A2M	O4'-C1'	8.95	1.63	1.42
20	CA	2815	A2M	O4'-C1'	8.94	1.63	1.42
20	CA	1524	A2M	O4'-C1'	8.94	1.63	1.42
20	CA	1871	A2M	O4'-C1'	8.86	1.63	1.42
20	CA	3825	A2M	O4'-C1'	8.86	1.63	1.42
20	CA	1534	A2M	O4'-C1'	8.85	1.63	1.42
20	CA	1323	A2M	O4'-C1'	8.82	1.62	1.42
20	CA	1326	A2M	O4'-C1'	8.80	1.62	1.42
20	CA	400	A2M	O4'-C1'	8.77	1.62	1.42
20	CA	398	A2M	O4'-C1'	8.74	1.62	1.42
20	CA	1322	1MA	C2-N3	8.74	1.46	1.30
20	CA	3867	A2M	O4'-C1'	8.72	1.62	1.42
20	CA	2401	A2M	O4'-C1'	8.64	1.62	1.42
20	CA	4523	A2M	O4'-C1'	8.64	1.62	1.42
20	CA	2363	A2M	O4'-C1'	8.56	1.62	1.42
20	CA	2787	A2M	O4'-C1'	8.53	1.62	1.42
20	CA	4571	A2M	O4'-C1'	8.53	1.62	1.42
20	CA	2787	A2M	C2'-C1'	-8.46	1.31	1.53
20	CA	3785	A2M	C2'-C1'	-8.44	1.31	1.53
20	CA	3785	A2M	O4'-C1'	8.43	1.62	1.42
20	CA	1534	A2M	C2'-C1'	-8.30	1.31	1.53
20	CA	1871	A2M	C2'-C1'	-8.29	1.31	1.53
20	CA	1524	A2M	C2'-C1'	-8.23	1.31	1.53
20	CA	1326	A2M	C2'-C1'	-8.11	1.32	1.53
20	CA	3867	A2M	C2'-C1'	-8.09	1.32	1.53
20	CA	4220	6MZ	O4'-C1'	8.06	1.61	1.42
20	CA	2815	A2M	C2'-C1'	-8.04	1.32	1.53
20	CA	4523	A2M	C2'-C1'	-8.00	1.32	1.53
20	CA	3818	UY1	C2-N3	8.00	1.51	1.37
20	CA	1323	A2M	C2'-C1'	-7.99	1.32	1.53
20	CA	3825	A2M	C2'-C1'	-7.99	1.32	1.53
20	CA	3830	A2M	C2'-C1'	-7.92	1.32	1.53
20	CA	400	A2M	C2'-C1'	-7.87	1.32	1.53
20	CA	398	A2M	C2'-C1'	-7.83	1.32	1.53
20	CA	2401	A2M	C2'-C1'	-7.78	1.33	1.53
20	CA	2363	A2M	C2'-C1'	-7.75	1.33	1.53
20	CA	3718	A2M	C2'-C1'	-7.70	1.33	1.53
20	CA	4530	UR3	C2-N1	7.53	1.49	1.38
20	CA	4571	A2M	C2'-C1'	-7.43	1.33	1.53
20	CA	1625	OMG	C4-N3	7.29	1.51	1.34
20	CA	3792	OMG	C4-N3	7.23	1.51	1.34
20	CA	2876	OMG	C4-N3	7.22	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	4494	OMG	C4-N3	7.21	1.51	1.34
20	CA	4196	OMG	C4-N3	7.18	1.51	1.34
20	CA	1522	OMG	C4-N3	7.17	1.51	1.34
20	CA	4392	OMG	C4-N3	7.16	1.51	1.34
20	CA	3669	OMG	C4-N3	7.15	1.51	1.34
20	CA	2424	OMG	C4-N3	7.15	1.51	1.34
20	CA	3627	OMG	C4-N3	7.14	1.51	1.34
20	CA	3899	OMG	C4-N3	7.14	1.51	1.34
20	CA	4623	OMG	C4-N3	7.13	1.51	1.34
20	CA	2364	OMG	C4-N3	7.12	1.51	1.34
22	CC	75	OMG	C4-N3	7.12	1.51	1.34
20	CA	4637	OMG	C4-N3	7.11	1.51	1.34
20	CA	4370	OMG	C4-N3	7.11	1.51	1.34
20	CA	4499	OMG	C4-N3	7.08	1.51	1.34
20	CA	3744	OMG	C4-N3	7.08	1.51	1.34
20	CA	1534	A2M	O4'-C4'	-7.08	1.29	1.45
20	CA	1316	OMG	C4-N3	7.06	1.51	1.34
20	CA	4228	OMG	C4-N3	6.99	1.50	1.34
20	CA	4618	OMG	C4-N3	6.96	1.50	1.34
20	CA	1322	1MA	C4-N3	6.74	1.49	1.35
20	CA	4530	UR3	C6-C5	6.69	1.50	1.35
20	CA	1323	A2M	O4'-C4'	-6.64	1.30	1.45
20	CA	1326	A2M	O4'-C4'	-6.60	1.30	1.45
20	CA	3867	A2M	O4'-C4'	-6.58	1.30	1.45
20	CA	2422	OMC	C2-N3	6.55	1.49	1.36
20	CA	3785	A2M	O4'-C4'	-6.50	1.30	1.45
20	CA	2815	A2M	O4'-C4'	-6.48	1.30	1.45
20	CA	4571	A2M	O4'-C4'	-6.47	1.30	1.45
20	CA	2401	A2M	O4'-C4'	-6.45	1.30	1.45
20	CA	1881	OMC	C6-C5	6.45	1.50	1.35
20	CA	2787	A2M	O4'-C4'	-6.41	1.30	1.45
20	CA	3782	5MC	C4-N3	6.40	1.45	1.34
20	CA	4536	OMC	C2-N3	6.36	1.49	1.36
20	CA	3841	OMC	C6-C5	6.35	1.49	1.35
20	CA	2422	OMC	C6-C5	6.31	1.49	1.35
20	CA	1340	OMC	C6-C5	6.31	1.49	1.35
20	CA	1340	OMC	C2-N3	6.30	1.49	1.36
20	CA	3701	OMC	C6-C5	6.30	1.49	1.35
20	CA	2824	OMC	C2-N3	6.30	1.49	1.36
20	CA	2861	OMC	C6-C5	6.30	1.49	1.35
20	CA	4456	OMC	C2-N3	6.29	1.49	1.36
20	CA	2824	OMC	C6-C5	6.28	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	3869	OMC	C2-N3	6.28	1.49	1.36
20	CA	2365	OMC	C6-C5	6.27	1.49	1.35
20	CA	3808	OMC	C6-C5	6.26	1.49	1.35
20	CA	2804	OMC	C6-C5	6.26	1.49	1.35
20	CA	3808	OMC	C2-N3	6.26	1.49	1.36
20	CA	2861	OMC	C2-N3	6.26	1.49	1.36
20	CA	2365	OMC	C2-N3	6.25	1.49	1.36
20	CA	400	A2M	O4'-C4'	-6.24	1.31	1.45
20	CA	2351	OMC	C6-C5	6.22	1.49	1.35
20	CA	4456	OMC	C6-C5	6.22	1.49	1.35
20	CA	3869	OMC	C6-C5	6.21	1.49	1.35
20	CA	2363	A2M	O4'-C4'	-6.21	1.31	1.45
20	CA	4536	OMC	C6-C5	6.21	1.49	1.35
20	CA	3887	OMC	C6-C5	6.20	1.49	1.35
20	CA	2804	OMC	C2-N3	6.20	1.48	1.36
20	CA	4220	6MZ	O4'-C4'	-6.18	1.31	1.45
20	CA	3887	OMC	C2-N3	6.18	1.48	1.36
20	CA	4447	5MC	C4-N3	6.17	1.44	1.34
20	CA	3841	OMC	C2-N3	6.15	1.48	1.36
20	CA	3825	A2M	O4'-C4'	-6.14	1.31	1.45
20	CA	3830	A2M	O4'-C4'	-6.10	1.31	1.45
20	CA	1881	OMC	C2-N3	6.09	1.48	1.36
20	CA	3701	OMC	C2-N3	6.08	1.48	1.36
20	CA	2351	OMC	C2-N3	6.08	1.48	1.36
20	CA	3782	5MC	C2-N3	6.05	1.48	1.36
20	CA	1871	A2M	O4'-C4'	-6.04	1.31	1.45
20	CA	1524	A2M	O4'-C4'	-6.04	1.31	1.45
20	CA	3718	A2M	O4'-C4'	-6.02	1.31	1.45
20	CA	398	A2M	O4'-C4'	-5.94	1.31	1.45
20	CA	4447	5MC	C2-N3	5.92	1.48	1.36
20	CA	4523	A2M	O4'-C4'	-5.81	1.32	1.45
20	CA	4499	OMG	C2-N3	5.71	1.47	1.33
20	CA	4530	UR3	C2-N3	5.71	1.50	1.39
20	CA	4494	OMG	C2-N3	5.70	1.46	1.33
20	CA	1625	OMG	C2-N3	5.68	1.46	1.33
20	CA	4196	OMG	C2-N3	5.68	1.46	1.33
20	CA	2422	OMC	C4-N3	5.66	1.45	1.34
20	CA	2876	OMG	C2-N3	5.63	1.46	1.33
20	CA	1881	OMC	C2-N1	5.62	1.52	1.40
20	CA	4370	OMG	C2-N3	5.62	1.46	1.33
20	CA	3669	OMG	C2-N3	5.62	1.46	1.33
20	CA	2824	OMC	C2-N1	5.62	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	3808	OMC	C2-N1	5.60	1.52	1.40
20	CA	2422	OMC	C2-N1	5.59	1.52	1.40
20	CA	2424	OMG	C2-N3	5.56	1.46	1.33
20	CA	1522	OMG	C2-N3	5.55	1.46	1.33
20	CA	4536	OMC	C2-N1	5.54	1.52	1.40
20	CA	3627	OMG	C2-N3	5.53	1.46	1.33
20	CA	2364	OMG	C2-N3	5.53	1.46	1.33
20	CA	4637	OMG	C2-N3	5.53	1.46	1.33
20	CA	3792	OMG	C2-N3	5.52	1.46	1.33
20	CA	4623	OMG	C2-N3	5.52	1.46	1.33
20	CA	2351	OMC	C2-N1	5.52	1.52	1.40
20	CA	2365	OMC	C2-N1	5.52	1.52	1.40
20	CA	4456	OMC	C2-N1	5.52	1.52	1.40
20	CA	3899	OMG	C2-N3	5.51	1.46	1.33
22	CC	75	OMG	C2-N3	5.51	1.46	1.33
20	CA	3887	OMC	C2-N1	5.50	1.51	1.40
20	CA	4392	OMG	C2-N3	5.48	1.46	1.33
20	CA	3869	OMC	C2-N1	5.46	1.51	1.40
20	CA	3744	OMG	C2-N3	5.45	1.46	1.33
20	CA	2861	OMC	C2-N1	5.44	1.51	1.40
20	CA	1316	OMG	C2-N3	5.44	1.46	1.33
20	CA	2861	OMC	C4-N3	5.44	1.45	1.34
20	CA	2824	OMC	C4-N3	5.41	1.45	1.34
20	CA	3869	OMC	C4-N3	5.41	1.45	1.34
20	CA	3808	OMC	C4-N3	5.39	1.45	1.34
20	CA	4536	OMC	C4-N3	5.39	1.45	1.34
20	CA	2804	OMC	C2-N1	5.39	1.51	1.40
20	CA	4456	OMC	C4-N3	5.38	1.45	1.34
20	CA	2365	OMC	C4-N3	5.38	1.45	1.34
20	CA	3701	OMC	C2-N1	5.38	1.51	1.40
20	CA	4618	OMG	C2-N3	5.35	1.46	1.33
20	CA	3701	OMC	C4-N3	5.34	1.45	1.34
20	CA	3841	OMC	C4-N3	5.33	1.45	1.34
20	CA	3887	OMC	C4-N3	5.32	1.45	1.34
20	CA	1881	OMC	C4-N3	5.30	1.45	1.34
20	CA	2804	OMC	C4-N3	5.29	1.45	1.34
20	CA	1340	OMC	C4-N3	5.29	1.45	1.34
20	CA	2351	OMC	C4-N3	5.26	1.45	1.34
20	CA	3841	OMC	C2-N1	5.25	1.51	1.40
20	CA	4228	OMG	C2-N3	5.24	1.45	1.33
20	CA	1340	OMC	C2-N1	5.23	1.51	1.40
20	CA	2422	OMC	C4-N4	5.11	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	1340	OMC	C4-N4	5.05	1.45	1.33
20	CA	2861	OMC	C4-N4	5.04	1.45	1.33
20	CA	2804	OMC	C4-N4	5.03	1.45	1.33
20	CA	2824	OMC	C4-N4	5.03	1.45	1.33
20	CA	3841	OMC	C4-N4	5.02	1.45	1.33
20	CA	3869	OMC	C4-N4	5.01	1.45	1.33
20	CA	4456	OMC	C4-N4	5.00	1.45	1.33
20	CA	2365	OMC	C4-N4	4.98	1.45	1.33
20	CA	4536	OMC	C4-N4	4.98	1.45	1.33
20	CA	3808	OMC	C4-N4	4.96	1.45	1.33
20	CA	3887	OMC	C4-N4	4.93	1.45	1.33
20	CA	1881	OMC	C4-N4	4.91	1.45	1.33
20	CA	2351	OMC	C4-N4	4.88	1.45	1.33
20	CA	4220	6MZ	C2'-C1'	-4.87	1.37	1.53
20	CA	3701	OMC	C4-N4	4.87	1.45	1.33
20	CA	4571	A2M	C6-N6	4.82	1.46	1.34
20	CA	2787	A2M	C6-N6	4.81	1.46	1.34
20	CA	1322	1MA	C2-N1	4.79	1.44	1.35
20	CA	1524	A2M	C6-N6	4.74	1.46	1.34
20	CA	1534	A2M	C6-N6	4.69	1.45	1.34
20	CA	400	A2M	C6-N6	4.61	1.45	1.34
20	CA	3818	UY1	C6-N1	4.61	1.43	1.36
20	CA	2401	A2M	C6-N6	4.60	1.45	1.34
20	CA	2363	A2M	C6-N6	4.57	1.45	1.34
20	CA	3718	A2M	C6-N6	4.56	1.45	1.34
20	CA	398	A2M	C6-N6	4.56	1.45	1.34
20	CA	3867	A2M	C6-N6	4.56	1.45	1.34
20	CA	2815	A2M	C6-N6	4.55	1.45	1.34
20	CA	1871	A2M	C6-N6	4.54	1.45	1.34
20	CA	3830	A2M	C6-N6	4.52	1.45	1.34
20	CA	4523	A2M	C6-N6	4.52	1.45	1.34
20	CA	1323	A2M	C6-N6	4.48	1.45	1.34
20	CA	1326	A2M	C6-N6	4.48	1.45	1.34
20	CA	4447	5MC	C6-N1	4.47	1.45	1.38
20	CA	3825	A2M	C6-N6	4.46	1.45	1.34
20	CA	3782	5MC	C6-N1	4.46	1.45	1.38
20	CA	3785	A2M	C6-N6	4.37	1.45	1.34
20	CA	4447	5MC	C4-N4	4.36	1.45	1.34
20	CA	4447	5MC	C2-N1	4.31	1.49	1.40
20	CA	3782	5MC	C4-N4	4.29	1.45	1.34
20	CA	4499	OMG	C2-N2	4.26	1.44	1.34
20	CA	3669	OMG	C2-N2	4.20	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	3782	5MC	C2-N1	4.18	1.49	1.40
20	CA	2424	OMG	C2-N2	4.18	1.44	1.34
20	CA	4623	OMG	C2-N2	4.17	1.44	1.34
20	CA	4196	OMG	C2-N2	4.16	1.44	1.34
20	CA	1625	OMG	C2-N2	4.16	1.44	1.34
20	CA	2876	OMG	C2-N2	4.15	1.44	1.34
22	CC	75	OMG	C2-N2	4.15	1.44	1.34
20	CA	4370	OMG	C2-N2	4.15	1.44	1.34
20	CA	2364	OMG	C2-N2	4.14	1.44	1.34
20	CA	1316	OMG	C2-N2	4.14	1.44	1.34
20	CA	4618	OMG	C2-N2	4.13	1.44	1.34
20	CA	3744	OMG	C2-N2	4.13	1.44	1.34
20	CA	3792	OMG	C2-N2	4.13	1.44	1.34
20	CA	3899	OMG	C2-N2	4.13	1.44	1.34
20	CA	4494	OMG	C2-N2	4.13	1.44	1.34
20	CA	3627	OMG	C2-N2	4.12	1.44	1.34
20	CA	1522	OMG	C2-N2	4.12	1.44	1.34
20	CA	4637	OMG	C2-N2	4.10	1.43	1.34
20	CA	4228	OMG	C2-N2	4.08	1.43	1.34
20	CA	4392	OMG	C2-N2	4.07	1.43	1.34
20	CA	4530	UR3	C6-N1	3.98	1.47	1.38
20	CA	1322	1MA	C5-C6	3.92	1.54	1.43
20	CA	1677	PSU	C2-N1	3.77	1.41	1.36
20	CA	3715	PSU	C2-N1	3.72	1.41	1.36
20	CA	4499	OMG	C5-N7	-3.71	1.31	1.39
20	CA	3851	PSU	C2-N1	3.71	1.41	1.36
20	CA	4196	OMG	C5-N7	-3.67	1.32	1.39
20	CA	4494	OMG	C5-N7	-3.65	1.32	1.39
20	CA	4500	PSU	C2-N1	3.64	1.41	1.36
20	CA	1625	OMG	C5-N7	-3.63	1.32	1.39
20	CA	3669	OMG	C2-N1	3.63	1.46	1.37
20	CA	3792	OMG	C5-N7	-3.62	1.32	1.39
20	CA	2876	OMG	C5-N7	-3.61	1.32	1.39
20	CA	4228	OMG	C2-N1	3.61	1.46	1.37
20	CA	4370	OMG	C2-N1	3.60	1.46	1.37
20	CA	4618	OMG	C2-N1	3.59	1.46	1.37
20	CA	2424	OMG	C2-N1	3.58	1.46	1.37
20	CA	1316	OMG	C5-N7	-3.58	1.32	1.39
22	CC	75	OMG	C2-N1	3.57	1.46	1.37
20	CA	4623	OMG	C2-N1	3.57	1.46	1.37
20	CA	3744	OMG	C2-N1	3.56	1.46	1.37
20	CA	3627	OMG	C5-N7	-3.56	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	4370	OMG	C5-N7	-3.56	1.32	1.39
20	CA	1522	OMG	C2-N1	3.55	1.46	1.37
20	CA	3627	OMG	C2-N1	3.55	1.46	1.37
20	CA	4637	OMG	C5-N7	-3.55	1.32	1.39
20	CA	2424	OMG	C5-N7	-3.54	1.32	1.39
20	CA	3899	OMG	C2-N1	3.53	1.46	1.37
20	CA	4623	OMG	C5-N7	-3.53	1.32	1.39
20	CA	4618	OMG	C5-N7	-3.53	1.32	1.39
20	CA	1323	A2M	O2'-C2'	3.53	1.51	1.42
20	CA	4571	A2M	O2'-C2'	3.52	1.51	1.42
20	CA	2364	OMG	C5-N7	-3.52	1.32	1.39
22	CC	55	PSU	C2-N1	3.52	1.41	1.36
20	CA	4494	OMG	C2-N1	3.51	1.46	1.37
20	CA	4312	PSU	C2-N1	3.51	1.41	1.36
20	CA	3899	OMG	C5-N7	-3.51	1.32	1.39
20	CA	1316	OMG	C2-N1	3.50	1.46	1.37
22	CC	75	OMG	C5-N7	-3.50	1.32	1.39
20	CA	4196	OMG	C2-N1	3.50	1.46	1.37
20	CA	3792	OMG	C2-N1	3.50	1.46	1.37
20	CA	4637	OMG	C2-N1	3.49	1.46	1.37
20	CA	4972	PSU	C2-N1	3.49	1.41	1.36
20	CA	1522	OMG	C5-N7	-3.49	1.32	1.39
20	CA	3744	OMG	C5-N7	-3.48	1.32	1.39
20	CA	4499	OMG	C2-N1	3.47	1.46	1.37
20	CA	2364	OMG	C2-N1	3.47	1.46	1.37
20	CA	4392	OMG	C2-N1	3.47	1.46	1.37
20	CA	3818	UY1	C4-N3	3.47	1.45	1.38
20	CA	3669	OMG	C5-N7	-3.46	1.32	1.39
20	CA	2876	OMG	C2-N1	3.46	1.46	1.37
20	CA	4392	OMG	C5-N7	-3.45	1.32	1.39
20	CA	1625	OMG	C2-N1	3.45	1.46	1.37
20	CA	4353	PSU	C2-N1	3.44	1.41	1.36
20	CA	3867	A2M	O2'-C2'	3.43	1.51	1.42
20	CA	1792	PSU	C2-N1	3.43	1.41	1.36
20	CA	4296	PSU	C2-N1	3.42	1.41	1.36
20	CA	3844	PSU	C2-N1	3.42	1.41	1.36
20	CA	4423	PSU	C2-N1	3.40	1.41	1.36
20	CA	4420	PSU	C2-N1	3.39	1.41	1.36
20	CA	4521	PSU	C2-N1	3.39	1.41	1.36
20	CA	4471	PSU	C2-N1	3.38	1.41	1.36
20	CA	3822	PSU	C2-N1	3.37	1.41	1.36
20	CA	2632	PSU	C2-N1	3.37	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	4493	PSU	C2-N1	3.37	1.41	1.36
20	CA	398	A2M	O2'-C2'	3.36	1.51	1.42
20	CA	2508	PSU	C2-N1	3.36	1.41	1.36
20	CA	4293	PSU	C2-N1	3.36	1.41	1.36
20	CA	4228	OMG	C5-N7	-3.36	1.32	1.39
20	CA	4299	PSU	C2-N1	3.35	1.41	1.36
20	CA	2839	PSU	C2-N1	3.35	1.41	1.36
20	CA	224	PSU	C2-N1	3.34	1.41	1.36
20	CA	3637	PSU	C2-N1	3.34	1.41	1.36
20	CA	1744	PSU	C2-N1	3.34	1.41	1.36
20	CA	4361	PSU	C2-N1	3.34	1.41	1.36
20	CA	4532	PSU	C2-N1	3.34	1.41	1.36
20	CA	4576	PSU	C2-N1	3.32	1.41	1.36
20	CA	4431	PSU	C2-N1	3.32	1.41	1.36
20	CA	1862	PSU	C2-N1	3.32	1.41	1.36
22	CC	69	PSU	C2-N1	3.31	1.41	1.36
20	CA	4673	PSU	C2-N1	3.30	1.41	1.36
20	CA	4403	PSU	C2-N1	3.29	1.41	1.36
20	CA	1781	PSU	C2-N1	3.28	1.41	1.36
20	CA	3825	A2M	O2'-C2'	3.28	1.51	1.42
20	CA	3920	PSU	C2-N1	3.27	1.41	1.36
20	CA	4623	OMG	C5-C6	3.27	1.56	1.44
20	CA	4392	OMG	C5-C6	3.26	1.56	1.44
20	CA	1536	PSU	C2-N1	3.26	1.41	1.36
20	CA	3669	OMG	C5-C6	3.25	1.56	1.44
20	CA	3899	OMG	C5-C6	3.25	1.56	1.44
20	CA	4618	OMG	C5-C6	3.25	1.56	1.44
20	CA	4552	PSU	C2-N1	3.24	1.41	1.36
20	CA	1782	PSU	C2-N1	3.24	1.41	1.36
20	CA	4628	PSU	C2-N1	3.24	1.41	1.36
20	CA	1860	PSU	C2-N1	3.23	1.41	1.36
20	CA	400	A2M	O2'-C2'	3.23	1.50	1.42
20	CA	3830	A2M	O2'-C2'	3.23	1.50	1.42
20	CA	2876	OMG	C5-C6	3.23	1.56	1.44
20	CA	2424	OMG	C5-C6	3.23	1.56	1.44
20	CA	3627	OMG	C5-C6	3.22	1.56	1.44
22	CC	75	OMG	C5-C6	3.22	1.56	1.44
20	CA	2364	OMG	C5-C6	3.22	1.56	1.44
20	CA	3792	OMG	C5-C6	3.21	1.56	1.44
20	CA	3639	PSU	C2-N1	3.21	1.41	1.36
20	CA	1534	A2M	O3'-C3'	-3.21	1.35	1.43
20	CA	4228	OMG	C5-C6	3.21	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	4196	OMG	C5-C6	3.21	1.56	1.44
20	CA	1534	A2M	O2'-C2'	3.21	1.50	1.42
20	CA	3744	OMG	C5-C6	3.21	1.56	1.44
20	CA	3718	A2M	O2'-C2'	3.21	1.50	1.42
20	CA	4494	OMG	C5-C6	3.20	1.56	1.44
20	CA	4442	PSU	C2-N1	3.19	1.41	1.36
20	CA	3695	PSU	C2-N1	3.19	1.41	1.36
20	CA	4499	OMG	C5-C6	3.19	1.56	1.44
20	CA	4370	OMG	C5-C6	3.19	1.56	1.44
20	CA	4457	PSU	C2-N1	3.19	1.41	1.36
20	CA	4637	OMG	C5-C6	3.18	1.56	1.44
20	CA	1522	OMG	C5-C6	3.18	1.56	1.44
20	CA	2815	A2M	O2'-C2'	3.18	1.50	1.42
20	CA	4523	A2M	O2'-C2'	3.17	1.50	1.42
20	CA	1683	PSU	C2-N1	3.17	1.41	1.36
20	CA	5001	PSU	C2-N1	3.16	1.41	1.36
20	CA	1779	PSU	C2-N1	3.14	1.41	1.36
20	CA	4689	PSU	C2-N1	3.14	1.41	1.36
20	CA	1881	OMC	C5-C4	3.14	1.50	1.42
20	CA	4579	PSU	C2-N1	3.14	1.41	1.36
20	CA	1524	A2M	O2'-C2'	3.14	1.50	1.42
20	CA	1625	OMG	C5-C6	3.13	1.56	1.44
20	CA	1316	OMG	C5-C6	3.13	1.56	1.44
20	CA	4530	UR3	C4-N3	3.12	1.47	1.40
20	CA	3884	PSU	C2-N1	3.11	1.40	1.36
20	CA	2787	A2M	C5-N7	-3.09	1.33	1.39
20	CA	3841	OMC	C5-C4	3.07	1.50	1.42
20	CA	2861	OMC	C5-C4	3.07	1.49	1.42
20	CA	3785	A2M	O2'-C2'	3.07	1.50	1.42
20	CA	3701	OMC	C5-C4	3.06	1.49	1.42
20	CA	1326	A2M	O2'-C2'	3.04	1.50	1.42
20	CA	3785	A2M	C5-N7	-3.03	1.33	1.39
20	CA	2365	OMC	C5-C4	2.97	1.49	1.42
20	CA	2824	OMC	C5-C4	2.97	1.49	1.42
20	CA	4456	OMC	C5-C4	2.96	1.49	1.42
20	CA	2401	A2M	O2'-C2'	2.96	1.50	1.42
20	CA	2422	OMC	C5-C4	2.96	1.49	1.42
20	CA	2804	OMC	C5-C4	2.96	1.49	1.42
20	CA	3785	A2M	O3'-C3'	-2.95	1.36	1.43
20	CA	4536	OMC	C5-C4	2.95	1.49	1.42
20	CA	2363	A2M	O2'-C2'	2.95	1.50	1.42
20	CA	1871	A2M	O2'-C2'	2.94	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	1524	A2M	C5-N7	-2.94	1.33	1.39
20	CA	1871	A2M	O3'-C3'	-2.93	1.36	1.43
20	CA	3887	OMC	C5-C4	2.93	1.49	1.42
20	CA	3808	OMC	C5-C4	2.93	1.49	1.42
20	CA	2787	A2M	O3'-C3'	-2.92	1.36	1.43
20	CA	3869	OMC	C5-C4	2.91	1.49	1.42
20	CA	1326	A2M	C5-C4	-2.90	1.33	1.39
20	CA	2351	OMC	C5-C4	2.89	1.49	1.42
20	CA	3825	A2M	O3'-C3'	-2.89	1.36	1.43
20	CA	1340	OMC	C5-C4	2.88	1.49	1.42
20	CA	2861	OMC	C6-N1	2.86	1.44	1.38
20	CA	1323	A2M	C5-C4	-2.85	1.33	1.39
20	CA	4523	A2M	O3'-C3'	-2.84	1.36	1.43
20	CA	2815	A2M	C5-C4	-2.84	1.33	1.39
20	CA	3701	OMC	C6-N1	2.83	1.44	1.38
20	CA	2351	OMC	C6-N1	2.83	1.44	1.38
20	CA	2365	OMC	C6-N1	2.82	1.44	1.38
20	CA	3841	OMC	C6-N1	2.82	1.44	1.38
20	CA	1322	1MA	C5-N7	-2.81	1.33	1.39
20	CA	2824	OMC	C6-N1	2.81	1.44	1.38
20	CA	1881	OMC	C6-N1	2.80	1.44	1.38
20	CA	2804	OMC	C6-N1	2.80	1.44	1.38
20	CA	3808	OMC	C6-N1	2.79	1.44	1.38
20	CA	3830	A2M	O3'-C3'	-2.79	1.36	1.43
20	CA	1534	A2M	C5-C4	-2.79	1.33	1.39
20	CA	3869	OMC	C6-N1	2.79	1.44	1.38
20	CA	3887	OMC	C6-N1	2.78	1.44	1.38
20	CA	1326	A2M	O3'-C3'	-2.78	1.36	1.43
23	CD	216	V5N	CE1-ND1	2.76	1.39	1.35
20	CA	4456	OMC	C6-N1	2.76	1.44	1.38
20	CA	2401	A2M	O3'-C3'	-2.75	1.36	1.43
20	CA	2422	OMC	C6-N1	2.73	1.44	1.38
20	CA	1340	OMC	C6-N1	2.73	1.44	1.38
20	CA	3830	A2M	C5-C4	-2.72	1.33	1.39
20	CA	4536	OMC	C6-N1	2.71	1.44	1.38
20	CA	2815	A2M	O3'-C3'	-2.71	1.36	1.43
20	CA	398	A2M	C5-C4	-2.70	1.34	1.39
20	CA	400	A2M	O3'-C3'	-2.69	1.36	1.43
20	CA	3825	A2M	C5-C4	-2.69	1.34	1.39
20	CA	4530	UR3	O4-C4	-2.69	1.17	1.23
20	CA	3718	A2M	C5-N7	-2.69	1.33	1.39
20	CA	1871	A2M	C5-C4	-2.68	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	3867	A2M	C5-C4	-2.68	1.34	1.39
20	CA	4220	6MZ	O3'-C3'	-2.68	1.36	1.43
20	CA	400	A2M	C5-C4	-2.67	1.34	1.39
20	CA	2787	A2M	O2'-C2'	2.67	1.49	1.42
20	CA	4447	5MC	O2-C2	-2.67	1.18	1.23
20	CA	3782	5MC	O2-C2	-2.66	1.18	1.23
20	CA	3718	A2M	O3'-C3'	-2.66	1.36	1.43
20	CA	3715	PSU	C4-N3	2.66	1.43	1.38
20	CA	1323	A2M	O3'-C3'	-2.66	1.36	1.43
20	CA	4523	A2M	C5-C4	-2.65	1.34	1.39
20	CA	4571	A2M	C5-C4	-2.64	1.34	1.39
20	CA	4530	UR3	O2-C2	-2.64	1.17	1.22
20	CA	3825	A2M	C5-N7	-2.62	1.34	1.39
20	CA	3925	OMU	C2-N1	2.60	1.42	1.38
20	CA	2787	A2M	C8-N9	-2.60	1.32	1.37
20	CA	2401	A2M	C5-N7	-2.59	1.34	1.39
34	AU	39	V5N	CE1-ND1	2.58	1.39	1.35
20	CA	2363	A2M	O3'-C3'	-2.57	1.36	1.43
20	CA	2363	A2M	C5-C4	-2.55	1.34	1.39
20	CA	4523	A2M	C8-N9	-2.55	1.32	1.37
20	CA	3718	A2M	C5-C4	-2.54	1.34	1.39
20	CA	5001	PSU	C4-N3	2.54	1.43	1.38
20	CA	3718	A2M	C8-N9	-2.53	1.33	1.37
20	CA	3841	OMC	O2-C2	-2.53	1.19	1.23
20	CA	1326	A2M	C5-N7	-2.53	1.34	1.39
20	CA	3822	PSU	C4-N3	2.52	1.43	1.38
20	CA	1871	A2M	C5-N7	-2.50	1.34	1.39
20	CA	4523	A2M	C5-N7	-2.50	1.34	1.39
20	CA	1534	A2M	C5-N7	-2.50	1.34	1.39
20	CA	4220	6MZ	C5-C4	-2.49	1.34	1.39
20	CA	398	A2M	O3'-C3'	-2.49	1.37	1.43
20	CA	3825	A2M	C8-N9	-2.48	1.33	1.37
20	CA	3867	A2M	C5-N7	-2.47	1.34	1.39
20	CA	2351	OMC	O2-C2	-2.47	1.19	1.23
20	CA	1534	A2M	C8-N9	-2.47	1.33	1.37
20	CA	2363	A2M	C5-N7	-2.46	1.34	1.39
20	CA	3887	OMC	O2-C2	-2.45	1.19	1.23
20	CA	3867	A2M	O3'-C3'	-2.45	1.37	1.43
20	CA	398	A2M	C5-N7	-2.44	1.34	1.39
20	CA	224	PSU	C4-N3	2.44	1.43	1.38
20	CA	2401	A2M	C5-C4	-2.43	1.34	1.39
20	CA	4420	PSU	C4-N3	2.43	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	400	A2M	C5-N7	-2.42	1.34	1.39
20	CA	1871	A2M	C8-N9	-2.42	1.33	1.37
20	CA	2422	OMC	O2-C2	-2.41	1.19	1.23
20	CA	2804	OMC	O2-C2	-2.41	1.19	1.23
20	CA	3830	A2M	C5-N7	-2.41	1.34	1.39
20	CA	1677	PSU	O4'-C1'	-2.41	1.40	1.43
20	CA	1340	OMC	O2-C2	-2.41	1.19	1.23
20	CA	4571	A2M	O3'-C3'	-2.40	1.37	1.43
20	CA	3785	A2M	C5-C4	-2.39	1.34	1.39
20	CA	2365	OMC	O2-C2	-2.39	1.19	1.23
20	CA	4456	OMC	O2-C2	-2.39	1.19	1.23
20	CA	1524	A2M	C5-C4	-2.38	1.34	1.39
20	CA	3808	OMC	O2-C2	-2.37	1.19	1.23
20	CA	1881	OMC	O2-C2	-2.36	1.19	1.23
20	CA	3869	OMC	O2-C2	-2.35	1.19	1.23
20	CA	3830	A2M	C8-N9	-2.35	1.33	1.37
20	CA	1323	A2M	C5-N7	-2.35	1.34	1.39
20	CA	4576	PSU	C4-N3	2.35	1.43	1.38
20	CA	1524	A2M	O3'-C3'	-2.34	1.37	1.43
20	CA	4500	PSU	C4-N3	2.34	1.43	1.38
20	CA	1859	B8T	C4-N4	2.34	1.40	1.35
20	CA	3701	OMC	O2-C2	-2.34	1.19	1.23
20	CA	3785	A2M	C8-N9	-2.34	1.33	1.37
20	CA	4579	PSU	C4-N3	2.34	1.43	1.38
20	CA	3695	PSU	C4-N3	2.33	1.43	1.38
20	CA	4296	PSU	C4-N3	2.33	1.43	1.38
20	CA	2861	OMC	O2-C2	-2.33	1.19	1.23
20	CA	4552	PSU	C4-N3	2.32	1.43	1.38
20	CA	4536	OMC	O2-C2	-2.32	1.19	1.23
20	CA	4628	PSU	C4-N3	2.32	1.43	1.38
20	CA	400	A2M	C8-N9	-2.32	1.33	1.37
20	CA	2632	PSU	C4-N3	2.32	1.43	1.38
20	CA	1779	PSU	C4-N3	2.31	1.43	1.38
20	CA	3715	PSU	C6-N1	2.31	1.40	1.36
20	CA	4423	PSU	C2-N3	2.30	1.41	1.37
20	CA	1677	PSU	C4-N3	2.29	1.43	1.38
20	CA	4220	6MZ	C8-N9	-2.29	1.33	1.37
20	CA	4972	PSU	C4-N3	2.29	1.43	1.38
20	CA	398	A2M	C8-N9	-2.29	1.33	1.37
20	CA	3920	PSU	C4-N3	2.28	1.43	1.38
20	CA	4579	PSU	C2-N3	2.28	1.41	1.37
20	CA	2824	OMC	O2-C2	-2.28	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	224	PSU	C2-N3	2.28	1.41	1.37
20	CA	1779	PSU	C2-N3	2.28	1.41	1.37
20	CA	4571	A2M	C5-N7	-2.28	1.34	1.39
20	CA	1744	PSU	C2-N3	2.26	1.41	1.37
20	CA	4220	6MZ	O2'-C2'	2.26	1.48	1.43
20	CA	2837	OMU	C4-N3	2.26	1.42	1.38
20	CA	3715	PSU	C2-N3	2.25	1.41	1.37
20	CA	2787	A2M	C5-C4	-2.25	1.34	1.39
20	CA	4423	PSU	C4-N3	2.25	1.43	1.38
20	CA	4442	PSU	C4-N3	2.25	1.43	1.38
20	CA	2815	A2M	C5-N7	-2.24	1.34	1.39
20	CA	4403	PSU	C4-N3	2.24	1.43	1.38
20	CA	4618	OMG	C6-N1	2.23	1.43	1.38
20	CA	1781	PSU	C4-N3	2.22	1.43	1.38
20	CA	4431	PSU	C4-N3	2.22	1.43	1.38
20	CA	4471	PSU	C4-N3	2.22	1.43	1.38
20	CA	1782	PSU	C2-N3	2.22	1.41	1.37
20	CA	5001	PSU	C2-N3	2.22	1.41	1.37
20	CA	4493	PSU	C2-N3	2.22	1.41	1.37
20	CA	1862	PSU	C2-N3	2.22	1.41	1.37
20	CA	1782	PSU	C4-N3	2.21	1.42	1.38
20	CA	4628	PSU	C2-N3	2.21	1.41	1.37
20	CA	4673	PSU	C4-N3	2.21	1.42	1.38
20	CA	4228	OMG	C4-N9	-2.20	1.32	1.38
20	CA	1683	PSU	C4-N3	2.20	1.42	1.38
20	CA	3639	PSU	C4-N3	2.20	1.42	1.38
20	CA	3851	PSU	C4-N3	2.19	1.42	1.38
20	CA	1792	PSU	C4-N3	2.19	1.42	1.38
20	CA	2839	PSU	C4-N3	2.19	1.42	1.38
20	CA	1683	PSU	C2-N3	2.19	1.41	1.37
20	CA	3844	PSU	C4-N3	2.19	1.42	1.38
20	CA	4220	6MZ	C5-N7	-2.18	1.34	1.39
20	CA	4228	OMG	C6-N1	2.18	1.42	1.38
20	CA	4312	PSU	C2-N3	2.18	1.41	1.37
20	CA	4361	PSU	C4-N3	2.17	1.42	1.38
20	CA	1781	PSU	C2-N3	2.17	1.41	1.37
20	CA	4296	PSU	C2-N3	2.17	1.41	1.37
20	CA	1326	A2M	C8-N9	-2.17	1.33	1.37
20	CA	4493	PSU	C4-N3	2.17	1.42	1.38
20	CA	2415	OMU	C4-N3	2.17	1.42	1.38
20	CA	3669	OMG	C6-N1	2.16	1.42	1.38
20	CA	4293	PSU	C4-N3	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	4498	OMU	C2-N1	2.16	1.41	1.38
20	CA	2815	A2M	C8-N9	-2.16	1.33	1.37
20	CA	4312	PSU	C4-N3	2.16	1.42	1.38
20	CA	4532	PSU	C2-N3	2.15	1.41	1.37
20	CA	1744	PSU	C4-N3	2.15	1.42	1.38
20	CA	2424	OMG	C6-N1	2.15	1.42	1.38
20	CA	2632	PSU	C2-N3	2.15	1.41	1.37
20	CA	4227	OMU	C4-N3	2.15	1.42	1.38
20	CA	4403	PSU	C2-N3	2.15	1.41	1.37
20	CA	4530	UR3	C5-C4	2.15	1.49	1.43
20	CA	4571	A2M	C8-N9	-2.14	1.33	1.37
20	CA	4361	PSU	C2-N3	2.14	1.41	1.37
20	CA	4552	PSU	C2-N3	2.14	1.41	1.37
20	CA	2839	PSU	C2-N3	2.14	1.41	1.37
20	CA	3920	PSU	C2-N3	2.14	1.41	1.37
20	CA	4227	OMU	C2-N1	2.14	1.41	1.38
20	CA	3925	OMU	C4-N3	2.14	1.42	1.38
20	CA	4306	OMU	C4-N3	2.13	1.42	1.38
20	CA	3639	PSU	C2-N3	2.13	1.41	1.37
22	CC	69	PSU	C4-N3	2.13	1.42	1.38
20	CA	4353	PSU	C2-N3	2.13	1.41	1.37
20	CA	4431	PSU	C2-N3	2.13	1.41	1.37
20	CA	4299	PSU	C2-N3	2.12	1.41	1.37
20	CA	4353	PSU	C4-N3	2.12	1.42	1.38
20	CA	3884	PSU	C2-N3	2.12	1.41	1.37
22	CC	55	PSU	C4-N3	2.12	1.42	1.38
20	CA	1862	PSU	C4-N3	2.11	1.42	1.38
20	CA	4532	PSU	C4-N3	2.11	1.42	1.38
20	CA	1536	PSU	C2-N3	2.10	1.41	1.37
20	CA	4521	PSU	C4-N3	2.10	1.42	1.38
20	CA	4293	PSU	C2-N3	2.10	1.41	1.37
20	CA	3844	PSU	C2-N3	2.10	1.41	1.37
20	CA	2508	PSU	C2-N3	2.10	1.41	1.37
20	CA	4500	PSU	C6-N1	2.09	1.39	1.36
20	CA	1792	PSU	C2-N3	2.09	1.41	1.37
20	CA	4521	PSU	C2-N3	2.09	1.41	1.37
20	CA	3792	OMG	C6-N1	2.08	1.42	1.38
20	CA	4576	PSU	C2-N3	2.08	1.41	1.37
22	CC	75	OMG	C6-N1	2.08	1.42	1.38
20	CA	4471	PSU	C2-N3	2.08	1.41	1.37
20	CA	2401	A2M	C8-N9	-2.07	1.33	1.37
20	CA	2363	A2M	C8-N9	-2.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CA	1536	PSU	C4-N3	2.06	1.42	1.38
22	CC	55	PSU	C2-N3	2.05	1.41	1.37
34	AU	39	V5N	CG-ND1	2.05	1.39	1.37
20	CA	3884	PSU	C4-N3	2.05	1.42	1.38
20	CA	1677	PSU	C6-N1	2.05	1.39	1.36
20	CA	4370	OMG	C6-N1	2.05	1.42	1.38
20	CA	3867	A2M	C8-N9	-2.04	1.33	1.37
20	CA	4299	PSU	C4-N3	2.04	1.42	1.38
20	CA	4620	OMU	C4-N3	2.04	1.42	1.38
20	CA	3899	OMG	C6-N1	2.02	1.42	1.38
20	CA	2508	PSU	C4-N3	2.02	1.42	1.38
20	CA	3744	OMG	C6-N1	2.01	1.42	1.38

All (644) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	3785	A2M	N6-C6-N1	-6.74	103.59	118.35
20	CA	3867	A2M	C5-C4-N3	-6.45	118.33	126.75
20	CA	3785	A2M	C5-C4-N3	-6.45	118.34	126.75
20	CA	1524	A2M	N6-C6-N1	-6.42	104.28	118.35
20	CA	4571	A2M	C5-C4-N3	-6.42	118.37	126.75
20	CA	3718	A2M	C5-C4-N3	-6.35	118.47	126.75
20	CA	4571	A2M	N6-C6-N1	-6.34	104.46	118.35
20	CA	1534	A2M	C5-C4-N3	-6.31	118.52	126.75
20	CA	1326	A2M	C5-C4-N3	-6.29	118.55	126.75
20	CA	1534	A2M	N6-C6-N1	-6.28	104.60	118.35
20	CA	2401	A2M	C5-C4-N3	-6.23	118.62	126.75
20	CA	4523	A2M	C5-C4-N3	-6.18	118.69	126.75
20	CA	2363	A2M	C5-C4-N3	-6.17	118.70	126.75
20	CA	2363	A2M	N6-C6-N1	-6.17	104.83	118.35
20	CA	4523	A2M	C2'-C1'-N9	-6.05	103.34	113.53
20	CA	1871	A2M	N6-C6-N1	-6.05	105.10	118.35
20	CA	2363	A2M	C5-C6-N6	6.04	136.58	123.43
20	CA	398	A2M	N6-C6-N1	-6.04	105.12	118.35
20	CA	3825	A2M	C5-C4-N3	-6.04	118.88	126.75
20	CA	2815	A2M	N6-C6-N1	-6.04	105.13	118.35
20	CA	1323	A2M	C5-C4-N3	-6.03	118.88	126.75
20	CA	400	A2M	N6-C6-N1	-6.03	105.15	118.35
20	CA	2815	A2M	C5-C4-N3	-5.97	118.95	126.75
20	CA	3718	A2M	N6-C6-N1	-5.97	105.28	118.35
20	CA	4523	A2M	N6-C6-N1	-5.96	105.30	118.35
20	CA	1871	A2M	C5-C6-N6	5.94	136.36	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	400	A2M	C5-C4-N3	-5.94	119.00	126.75
20	CA	3830	A2M	N6-C6-N1	-5.92	105.38	118.35
20	CA	398	A2M	C5-C4-N3	-5.91	119.04	126.75
20	CA	1323	A2M	N6-C6-N1	-5.91	105.41	118.35
20	CA	2787	A2M	N6-C6-N1	-5.91	105.41	118.35
20	CA	400	A2M	C5-C6-N6	5.90	136.27	123.43
20	CA	4220	6MZ	C5-C4-N3	-5.90	119.06	126.75
20	CA	1524	A2M	C5-C6-N6	5.90	136.26	123.43
20	CA	4571	A2M	C5-C6-N6	5.86	136.18	123.43
20	CA	2815	A2M	C5-C6-N6	5.84	136.15	123.43
20	CA	398	A2M	C5-C6-N6	5.84	136.13	123.43
20	CA	1326	A2M	N6-C6-N1	-5.80	105.65	118.35
20	CA	3825	A2M	N6-C6-N1	-5.78	105.70	118.35
20	CA	3830	A2M	C5-C6-N6	5.77	135.99	123.43
20	CA	3718	A2M	C5-C6-N6	5.77	135.98	123.43
20	CA	2876	OMG	C5-C4-N3	-5.77	119.11	128.46
20	CA	2401	A2M	C5-C6-N6	5.77	135.98	123.43
20	CA	2401	A2M	N6-C6-N1	-5.74	105.79	118.35
20	CA	4499	OMG	C5-C4-N3	-5.72	119.18	128.46
20	CA	1323	A2M	C5-C6-N6	5.72	135.87	123.43
20	CA	3825	A2M	C5-C6-N6	5.71	135.85	123.43
20	CA	4196	OMG	C5-C4-N3	-5.66	119.28	128.46
20	CA	4523	A2M	C5-C6-N6	5.63	135.68	123.43
20	CA	3867	A2M	N6-C6-N1	-5.62	106.04	118.35
20	CA	1625	OMG	C5-C4-N3	-5.61	119.36	128.46
20	CA	4220	6MZ	C4-C5-C6	5.60	121.15	116.81
20	CA	1326	A2M	C5-C6-N6	5.56	135.53	123.43
20	CA	1871	A2M	C5-C4-N3	-5.56	119.49	126.75
20	CA	4494	OMG	C5-C4-N3	-5.55	119.46	128.46
20	CA	1524	A2M	C5-C4-N3	-5.49	119.59	126.75
20	CA	3830	A2M	C5-C4-N3	-5.45	119.63	126.75
20	CA	3867	A2M	C5-C6-N6	5.45	135.29	123.43
20	CA	2787	A2M	C5-C6-N6	5.42	135.22	123.43
20	CA	1534	A2M	C5-C6-N6	5.41	135.19	123.43
20	CA	3792	OMG	C5-C4-N3	-5.41	119.69	128.46
20	CA	3785	A2M	C5-C6-N6	5.36	135.09	123.43
20	CA	2364	OMG	C5-C4-N3	-5.34	119.79	128.46
20	CA	2424	OMG	C5-C4-N3	-5.32	119.83	128.46
20	CA	4370	OMG	C5-C4-N3	-5.31	119.85	128.46
20	CA	3669	OMG	C5-C4-N3	-5.30	119.86	128.46
20	CA	4637	OMG	C5-C4-N3	-5.29	119.88	128.46
20	CA	2787	A2M	C5-C4-N3	-5.27	119.87	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	3627	OMG	C5-C4-N3	-5.24	119.95	128.46
20	CA	4623	OMG	C5-C4-N3	-5.19	120.04	128.46
22	CC	75	OMG	C5-C4-N3	-5.16	120.09	128.46
20	CA	4392	OMG	C5-C4-N3	-5.13	120.13	128.46
20	CA	1322	1MA	C1'-N9-C4	-5.13	111.27	126.50
20	CA	398	A2M	C2'-C1'-N9	-5.13	104.90	113.53
20	CA	1522	OMG	C5-C4-N3	-5.12	120.15	128.46
20	CA	1860	PSU	C6-C5-C4	5.12	121.78	118.20
20	CA	1524	A2M	N3-C2-N1	-5.11	120.61	128.60
20	CA	3785	A2M	N3-C2-N1	-5.04	120.72	128.60
20	CA	3830	A2M	N3-C2-N1	-5.03	120.74	128.60
20	CA	3744	OMG	C5-C4-N3	-5.02	120.31	128.46
20	CA	4220	6MZ	N1-C2-N3	-5.01	120.77	128.60
20	CA	3818	UY1	C4-N3-C2	-4.98	119.16	126.34
20	CA	1316	OMG	C5-C4-N3	-4.97	120.40	128.46
20	CA	3899	OMG	C5-C4-N3	-4.96	120.41	128.46
20	CA	2787	A2M	N3-C2-N1	-4.95	120.86	128.60
20	CA	4618	OMG	C5-C4-N3	-4.95	120.44	128.46
20	CA	1871	A2M	N3-C2-N1	-4.90	120.94	128.60
20	CA	1322	1MA	N1-C2-N3	-4.88	120.20	126.00
20	CA	2815	A2M	N3-C2-N1	-4.84	121.03	128.60
20	CA	4530	UR3	C4-N3-C2	-4.78	120.06	124.56
20	CA	398	A2M	N3-C2-N1	-4.78	121.12	128.60
20	CA	1782	PSU	C6-C5-C4	4.74	121.51	118.20
20	CA	3818	UY1	N1-C2-N3	4.73	120.49	115.13
20	CA	1534	A2M	N3-C2-N1	-4.72	121.22	128.60
20	CA	1322	1MA	C5-C4-N3	-4.71	120.24	127.26
20	CA	2401	A2M	N3-C2-N1	-4.68	121.29	128.60
20	CA	1326	A2M	N3-C2-N1	-4.65	121.34	128.60
20	CA	1323	A2M	N3-C2-N1	-4.64	121.34	128.60
20	CA	1524	A2M	N9-C8-N7	-4.64	107.57	113.91
20	CA	400	A2M	N3-C2-N1	-4.63	121.36	128.60
20	CA	4523	A2M	N3-C2-N1	-4.63	121.37	128.60
20	CA	2876	OMG	C2-N3-C4	4.62	120.53	112.30
20	CA	4361	PSU	C6-C5-C4	4.61	121.42	118.20
20	CA	4423	PSU	C6-C5-C4	4.61	121.42	118.20
20	CA	4312	PSU	C6-C5-C4	4.59	121.41	118.20
20	CA	1744	PSU	C6-C5-C4	4.59	121.41	118.20
20	CA	4353	PSU	C6-C5-C4	4.59	121.40	118.20
20	CA	3884	PSU	C6-C5-C4	4.58	121.40	118.20
20	CA	2363	A2M	N3-C2-N1	-4.57	121.45	128.60
20	CA	1871	A2M	C2'-C1'-N9	-4.55	105.88	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	3867	A2M	N3-C4-N9	4.54	134.56	127.08
20	CA	4293	PSU	C6-C5-C4	4.50	121.34	118.20
20	CA	1536	PSU	C6-C5-C4	4.49	121.34	118.20
20	CA	1862	PSU	C6-C5-C4	4.48	121.33	118.20
20	CA	4499	OMG	C2-N3-C4	4.44	120.21	112.30
20	CA	4220	6MZ	N9-C8-N7	-4.44	107.84	113.91
22	CC	55	PSU	C6-C5-C4	4.43	121.30	118.20
20	CA	4523	A2M	N3-C4-N9	4.42	134.37	127.08
20	CA	4571	A2M	N3-C2-N1	-4.42	121.69	128.60
20	CA	1322	1MA	C1'-N9-C8	4.42	139.27	126.70
20	CA	3792	OMG	C2-N3-C4	4.42	120.17	112.30
20	CA	4493	PSU	C6-C5-C4	4.40	121.28	118.20
20	CA	4532	PSU	C6-C5-C4	4.40	121.27	118.20
20	CA	4618	OMG	C2-N3-C4	4.39	120.13	112.30
20	CA	2508	PSU	C6-C5-C4	4.37	121.26	118.20
20	CA	4196	OMG	C2-N3-C4	4.37	120.08	112.30
20	CA	4228	OMG	C5-C4-N3	-4.35	121.40	128.46
20	CA	1683	PSU	C6-C5-C4	4.33	121.23	118.20
20	CA	4552	PSU	C6-C5-C4	4.33	121.22	118.20
20	CA	3637	PSU	C6-C5-C4	4.32	121.22	118.20
20	CA	4228	OMG	C1'-N9-C4	-4.32	113.67	126.50
20	CA	2401	A2M	N3-C4-N9	4.32	134.20	127.08
20	CA	3718	A2M	N3-C2-N1	-4.30	121.87	128.60
20	CA	4392	OMG	C2-N3-C4	4.30	119.96	112.30
22	CC	75	OMG	C2-N3-C4	4.30	119.96	112.30
20	CA	4494	OMG	C2-N3-C4	4.29	119.95	112.30
20	CA	4431	PSU	C6-C5-C4	4.29	121.20	118.20
20	CA	4523	A2M	N9-C8-N7	-4.29	108.05	113.91
20	CA	1625	OMG	C2-N3-C4	4.29	119.94	112.30
20	CA	3830	A2M	N9-C8-N7	-4.28	108.06	113.91
20	CA	4299	PSU	C6-C5-C4	4.28	121.19	118.20
20	CA	1522	OMG	C2-N3-C4	4.27	119.91	112.30
20	CA	3825	A2M	N3-C4-N9	4.27	134.12	127.08
20	CA	3627	OMG	C2-N3-C4	4.27	119.90	112.30
20	CA	2364	OMG	C2-N3-C4	4.26	119.89	112.30
20	CA	2424	OMG	C2-N3-C4	4.26	119.89	112.30
20	CA	4623	OMG	C2-N3-C4	4.24	119.85	112.30
20	CA	4370	OMG	C2-N3-C4	4.24	119.85	112.30
20	CA	3669	OMG	C2-N3-C4	4.24	119.85	112.30
20	CA	3718	A2M	C2'-C1'-N9	-4.22	106.42	113.53
20	CA	3744	OMG	C2-N3-C4	4.22	119.82	112.30
20	CA	4571	A2M	N3-C4-N9	4.20	134.01	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	3899	OMG	C2-N3-C4	4.19	119.77	112.30
20	CA	4521	PSU	C6-C5-C4	4.19	121.13	118.20
20	CA	3830	A2M	C2'-C1'-N9	-4.18	106.50	113.53
20	CA	400	A2M	C2'-C1'-N9	-4.17	106.51	113.53
20	CA	224	PSU	C6-C5-C4	4.17	121.11	118.20
20	CA	4637	OMG	C2-N3-C4	4.17	119.72	112.30
20	CA	4471	PSU	C6-C5-C4	4.16	121.11	118.20
20	CA	3867	A2M	N3-C2-N1	-4.16	122.10	128.60
20	CA	1677	PSU	C6-C5-C4	4.15	121.10	118.20
20	CA	1316	OMG	C2-N3-C4	4.15	119.70	112.30
20	CA	2839	PSU	C6-C5-C4	4.15	121.10	118.20
20	CA	3825	A2M	N9-C8-N7	-4.14	108.25	113.91
20	CA	3718	A2M	N3-C4-N9	4.13	133.89	127.08
20	CA	1779	PSU	C6-C5-C4	4.12	121.08	118.20
20	CA	400	A2M	N9-C8-N7	-4.12	108.28	113.91
20	CA	3867	A2M	C6-C5-C4	4.11	122.72	117.18
20	CA	4403	PSU	C6-C5-C4	4.11	121.07	118.20
20	CA	398	A2M	N9-C8-N7	-4.10	108.30	113.91
20	CA	400	A2M	N3-C4-N9	4.10	133.84	127.08
20	CA	1326	A2M	N3-C4-N9	4.08	133.81	127.08
20	CA	4220	6MZ	N3-C4-N9	4.07	133.78	127.08
20	CA	4228	OMG	C2-N3-C4	4.06	119.53	112.30
20	CA	1871	A2M	N9-C8-N7	-4.02	108.42	113.91
20	CA	3785	A2M	N3-C4-N9	4.01	133.69	127.08
20	CA	1792	PSU	C6-C5-C4	4.00	120.99	118.20
20	CA	1781	PSU	C6-C5-C4	3.99	120.99	118.20
20	CA	4296	PSU	C6-C5-C4	3.99	120.99	118.20
20	CA	3818	UY1	C6-C5-C4	3.98	120.98	118.20
20	CA	3825	A2M	C2'-C1'-N9	-3.98	106.84	113.53
20	CA	3825	A2M	N3-C2-N1	-3.97	122.39	128.60
20	CA	398	A2M	N3-C4-N9	3.97	133.62	127.08
20	CA	2363	A2M	N3-C4-N9	3.95	133.59	127.08
20	CA	3785	A2M	C2-N3-C4	3.93	121.04	111.75
20	CA	4972	PSU	C6-C5-C4	3.93	120.95	118.20
20	CA	4228	OMG	C1'-N9-C8	3.93	137.88	126.70
20	CA	1323	A2M	N3-C4-N9	3.91	133.53	127.08
20	CA	4628	PSU	C6-C5-C4	3.89	120.92	118.20
20	CA	1534	A2M	N3-C4-N9	3.89	133.49	127.08
20	CA	4500	PSU	C6-C5-C4	3.88	120.91	118.20
20	CA	1322	1MA	C2-N3-C4	3.88	120.03	112.41
20	CA	1323	A2M	N9-C8-N7	-3.87	108.62	113.91
20	CA	3825	A2M	C6-C5-C4	3.85	122.36	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	3867	A2M	N9-C8-N7	-3.85	108.64	113.91
20	CA	3844	PSU	C6-C5-C4	3.83	120.88	118.20
20	CA	3718	A2M	C6-C5-C4	3.83	122.33	117.18
20	CA	4571	A2M	N9-C8-N7	-3.81	108.70	113.91
20	CA	4689	PSU	C6-C5-C4	3.81	120.86	118.20
20	CA	2363	A2M	N9-C8-N7	-3.78	108.74	113.91
20	CA	3785	A2M	N9-C8-N7	-3.77	108.75	113.91
20	CA	1326	A2M	N9-C8-N7	-3.77	108.76	113.91
20	CA	2401	A2M	C6-C5-C4	3.76	122.24	117.18
20	CA	4673	PSU	C6-C5-C4	3.76	120.83	118.20
20	CA	3782	5MC	C5-C6-N1	-3.75	119.48	123.34
20	CA	1326	A2M	C6-C5-C4	3.73	122.20	117.18
20	CA	1625	OMG	N9-C4-N3	3.72	133.41	125.94
20	CA	1534	A2M	N9-C8-N7	-3.71	108.84	113.91
20	CA	2815	A2M	N9-C8-N7	-3.70	108.85	113.91
20	CA	1524	A2M	C5-N7-C8	3.70	108.77	103.51
34	AU	39	V5N	O2-CB-CG	-3.69	104.07	110.73
20	CA	1871	A2M	N3-C4-N9	3.68	133.15	127.08
20	CA	4196	OMG	N9-C4-N3	3.67	133.30	125.94
20	CA	4499	OMG	N9-C4-N3	3.67	133.30	125.94
20	CA	2815	A2M	N3-C4-N9	3.65	133.10	127.08
20	CA	3851	PSU	C6-C5-C4	3.65	120.75	118.20
20	CA	2401	A2M	N9-C8-N7	-3.65	108.92	113.91
20	CA	2787	A2M	N3-C4-N9	3.63	133.07	127.08
20	CA	4494	OMG	N9-C4-N3	3.62	133.20	125.94
20	CA	1534	A2M	C2-N3-C4	3.60	120.25	111.75
20	CA	4447	5MC	C5-C6-N1	-3.59	119.64	123.34
20	CA	2876	OMG	N9-C4-N3	3.59	133.15	125.94
20	CA	3830	A2M	N3-C4-N9	3.58	132.98	127.08
20	CA	4552	PSU	C4-N3-C2	-3.58	121.19	126.34
20	CA	2363	A2M	C6-C5-C4	3.54	121.94	117.18
20	CA	1323	A2M	C6-C5-C4	3.54	121.94	117.18
20	CA	4571	A2M	C6-C5-C4	3.53	121.93	117.18
20	CA	224	PSU	C4-N3-C2	-3.53	121.26	126.34
20	CA	4306	OMU	C4-N3-C2	-3.52	121.94	126.58
20	CA	3639	PSU	C6-C5-C4	3.51	120.65	118.20
20	CA	3715	PSU	C6-C5-C4	3.51	120.65	118.20
20	CA	4972	PSU	C4-N3-C2	-3.51	121.29	126.34
20	CA	2837	OMU	C4-N3-C2	-3.50	121.97	126.58
20	CA	400	A2M	C6-C5-C4	3.49	121.88	117.18
20	CA	4403	PSU	C4-N3-C2	-3.49	121.31	126.34
20	CA	1782	PSU	C4-N3-C2	-3.49	121.32	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AU	39	V5N	O2-CB-CA	3.48	114.63	107.28
20	CA	3925	OMU	C4-N3-C2	-3.48	121.99	126.58
20	CA	4227	OMU	C4-N3-C2	-3.48	121.99	126.58
20	CA	4431	PSU	C4-N3-C2	-3.46	121.35	126.34
20	CA	1524	A2M	C2-N3-C4	3.46	119.93	111.75
20	CA	2415	OMU	C4-N3-C2	-3.44	122.04	126.58
20	CA	3792	OMG	N9-C4-N3	3.43	132.83	125.94
20	CA	1862	PSU	C4-N3-C2	-3.43	121.39	126.34
20	CA	1860	PSU	C4-N3-C2	-3.43	121.39	126.34
20	CA	4521	PSU	C4-N3-C2	-3.43	121.40	126.34
20	CA	4571	A2M	C5-N7-C8	3.43	108.38	103.51
20	CA	4523	A2M	C6-C5-C4	3.43	121.79	117.18
20	CA	4579	PSU	C6-C5-C4	3.42	120.59	118.20
20	CA	4220	6MZ	C2-N3-C4	3.42	119.82	111.75
20	CA	2787	A2M	N9-C8-N7	-3.41	109.24	113.91
20	CA	2815	A2M	C6-C5-C4	3.41	121.77	117.18
20	CA	3637	PSU	C4-N3-C2	-3.41	121.43	126.34
20	CA	3851	PSU	C4-N3-C2	-3.40	121.43	126.34
20	CA	4423	PSU	C4-N3-C2	-3.40	121.44	126.34
20	CA	4571	A2M	O2'-C2'-C1'	3.40	115.70	109.08
20	CA	1792	PSU	C4-N3-C2	-3.39	121.45	126.34
20	CA	4353	PSU	C4-N3-C2	-3.39	121.45	126.34
20	CA	4370	OMG	N9-C4-N3	3.39	132.75	125.94
20	CA	1744	PSU	C4-N3-C2	-3.39	121.45	126.34
20	CA	1781	PSU	C4-N3-C2	-3.39	121.46	126.34
20	CA	1683	PSU	C4-N3-C2	-3.38	121.47	126.34
20	CA	4361	PSU	C4-N3-C2	-3.38	121.47	126.34
20	CA	4493	PSU	C4-N3-C2	-3.38	121.47	126.34
20	CA	4571	A2M	C2-N3-C4	3.38	119.73	111.75
20	CA	4532	PSU	C4-N3-C2	-3.38	121.47	126.34
20	CA	3695	PSU	C4-N3-C2	-3.36	121.49	126.34
20	CA	1322	1MA	N9-C8-N7	-3.36	107.06	113.39
20	CA	1534	A2M	C5-N7-C8	3.36	108.28	103.51
20	CA	2815	A2M	C2-N3-C4	3.35	119.67	111.75
20	CA	1536	PSU	C4-N3-C2	-3.34	121.52	126.34
20	CA	4312	PSU	C4-N3-C2	-3.34	121.52	126.34
20	CA	4296	PSU	C4-N3-C2	-3.34	121.53	126.34
20	CA	2363	A2M	C2-N3-C4	3.34	119.63	111.75
20	CA	1326	A2M	C2-N3-C4	3.33	119.61	111.75
23	CD	216	V5N	O2-CB-CG	-3.32	104.73	110.73
20	CA	4498	OMU	C4-N3-C2	-3.32	122.20	126.58
20	CA	2364	OMG	N9-C4-N3	3.32	132.61	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	4628	PSU	C4-N3-C2	-3.32	121.56	126.34
20	CA	4523	A2M	C2-N3-C4	3.31	119.58	111.75
20	CA	3715	PSU	C4-N3-C2	-3.31	121.57	126.34
20	CA	398	A2M	C6-C5-C4	3.31	121.63	117.18
20	CA	3669	OMG	N9-C4-N3	3.31	132.58	125.94
20	CA	3785	A2M	C5-N7-C8	3.31	108.20	103.51
20	CA	5001	PSU	C4-N3-C2	-3.30	121.58	126.34
20	CA	4457	PSU	C4-N3-C2	-3.30	121.58	126.34
22	CC	55	PSU	C4-N3-C2	-3.30	121.58	126.34
20	CA	2508	PSU	C4-N3-C2	-3.30	121.59	126.34
20	CA	2424	OMG	N9-C4-N3	3.28	132.53	125.94
20	CA	3884	PSU	C4-N3-C2	-3.28	121.61	126.34
20	CA	1323	A2M	C2-N3-C4	3.28	119.50	111.75
20	CA	4299	PSU	C4-N3-C2	-3.28	121.62	126.34
20	CA	1779	PSU	C4-N3-C2	-3.28	121.62	126.34
20	CA	4293	PSU	C4-N3-C2	-3.28	121.62	126.34
20	CA	4471	PSU	C4-N3-C2	-3.27	121.62	126.34
20	CA	4523	A2M	C5-N7-C8	3.27	108.15	103.51
20	CA	398	A2M	C2-N3-C4	3.26	119.46	111.75
20	CA	3627	OMG	N9-C4-N3	3.26	132.49	125.94
20	CA	3920	PSU	C6-C5-C4	3.25	120.47	118.20
20	CA	4576	PSU	C4-N3-C2	-3.25	121.66	126.34
20	CA	2401	A2M	C2-N3-C4	3.25	119.42	111.75
20	CA	4673	PSU	C4-N3-C2	-3.25	121.66	126.34
23	CD	216	V5N	O2-CB-CA	3.24	114.11	107.28
20	CA	1522	OMG	N9-C4-N3	3.22	132.41	125.94
20	CA	2632	PSU	C6-C5-C4	3.22	120.45	118.20
20	CA	4442	PSU	C4-N3-C2	-3.22	121.70	126.34
20	CA	4620	OMU	C4-N3-C2	-3.21	122.35	126.58
20	CA	3920	PSU	C4-N3-C2	-3.21	121.72	126.34
20	CA	4637	OMG	N9-C4-N3	3.21	132.38	125.94
20	CA	3718	A2M	C2-N3-C4	3.20	119.32	111.75
20	CA	1524	A2M	N3-C4-N9	3.20	132.36	127.08
20	CA	3830	A2M	C2-N3-C4	3.20	119.31	111.75
20	CA	3844	PSU	C4-N3-C2	-3.20	121.73	126.34
20	CA	4220	6MZ	C5-N7-C8	3.20	108.05	103.51
22	CC	69	PSU	C4-N3-C2	-3.19	121.74	126.34
20	CA	4530	UR3	C1'-N1-C2	3.19	122.37	116.99
20	CA	1524	A2M	C2'-C1'-N9	-3.18	108.17	113.53
20	CA	2787	A2M	C2-N3-C4	3.18	119.27	111.75
20	CA	1871	A2M	C2-N3-C4	3.18	119.26	111.75
20	CA	2632	PSU	C4-N3-C2	-3.17	121.77	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	4579	PSU	C4-N3-C2	-3.17	121.77	126.34
20	CA	400	A2M	C2-N3-C4	3.16	119.22	111.75
20	CA	400	A2M	C5-N7-C8	3.15	107.98	103.51
20	CA	3639	PSU	C4-N3-C2	-3.15	121.80	126.34
20	CA	4623	OMG	N9-C4-N3	3.14	132.25	125.94
20	CA	1316	OMG	N9-C4-N3	3.14	132.24	125.94
20	CA	1677	PSU	C4-N3-C2	-3.13	121.83	126.34
20	CA	3899	OMG	C1'-N9-C4	-3.13	117.21	126.50
20	CA	3867	A2M	C2-N3-C4	3.12	119.13	111.75
20	CA	2839	PSU	C4-N3-C2	-3.12	121.84	126.34
34	AU	39	V5N	O-C-CA	-3.12	116.61	124.78
20	CA	2363	A2M	C5-N7-C8	3.11	107.93	103.51
20	CA	4392	OMG	N9-C4-N3	3.11	132.19	125.94
20	CA	398	A2M	C5-N7-C8	3.11	107.93	103.51
20	CA	4618	OMG	C1'-N9-C4	-3.09	117.31	126.50
20	CA	3744	OMG	N9-C4-N3	3.09	132.15	125.94
20	CA	5001	PSU	C6-C5-C4	3.09	120.36	118.20
20	CA	3825	A2M	C5-N7-C8	3.08	107.89	103.51
20	CA	1522	OMG	C1'-N9-C4	-3.08	117.35	126.50
20	CA	3818	UY1	C6-N1-C2	-3.08	119.53	122.68
20	CA	4228	OMG	N9-C8-N7	-3.07	107.60	113.39
20	CA	3822	PSU	C4-N3-C2	-3.07	121.92	126.34
20	CA	1871	A2M	C6-C5-C4	3.06	121.30	117.18
20	CA	3830	A2M	C5-N7-C8	3.06	107.85	103.51
20	CA	2787	A2M	C5-N7-C8	3.04	107.83	103.51
20	CA	4500	PSU	C4-N3-C2	-3.02	121.98	126.34
20	CA	1326	A2M	C5-N7-C8	3.02	107.80	103.51
22	CC	75	OMG	C1'-N9-C4	-3.01	117.55	126.50
20	CA	3867	A2M	C5-N7-C8	3.01	107.78	103.51
20	CA	4499	OMG	C2-N1-C6	-3.01	119.62	125.10
20	CA	1534	A2M	C6-C5-C4	3.00	121.22	117.18
22	CC	75	OMG	N9-C4-N3	3.00	131.97	125.94
20	CA	1524	A2M	C3'-C2'-C1'	3.00	108.53	102.89
20	CA	4392	OMG	C1'-N9-C4	-3.00	117.59	126.50
20	CA	4576	PSU	C6-C5-C4	3.00	120.30	118.20
20	CA	4689	PSU	C4-N3-C2	-3.00	122.02	126.34
20	CA	3718	A2M	N9-C8-N7	-2.99	109.82	113.91
20	CA	3899	OMG	N9-C4-N3	2.99	131.94	125.94
20	CA	4370	OMG	C1'-N9-C4	-2.98	117.65	126.50
20	CA	4420	PSU	C4-N3-C2	-2.97	122.06	126.34
20	CA	1871	A2M	C5-N7-C8	2.95	107.70	103.51
20	CA	2876	OMG	C2-N1-C6	-2.95	119.73	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	3830	A2M	C6-C5-C4	2.94	121.14	117.18
20	CA	3744	OMG	C1'-N9-C4	-2.93	117.79	126.50
20	CA	4571	A2M	O4'-C1'-N9	-2.93	102.28	108.06
20	CA	2401	A2M	C5-N7-C8	2.93	107.67	103.51
20	CA	1316	OMG	C1'-N9-C4	-2.93	117.81	126.50
20	CA	4220	6MZ	C2'-C1'-N9	-2.92	105.91	113.30
20	CA	3825	A2M	C2-N3-C4	2.92	118.64	111.75
20	CA	4618	OMG	C1'-N9-C8	2.92	135.00	126.70
20	CA	1323	A2M	C5-N7-C8	2.91	107.64	103.51
20	CA	4623	OMG	C1'-N9-C4	-2.89	117.91	126.50
20	CA	3867	A2M	C1'-N9-C8	-2.89	120.61	127.14
20	CA	4220	6MZ	C4-N9-C8	2.88	108.85	105.73
20	CA	4196	OMG	C2-N1-C6	-2.88	119.85	125.10
22	CC	75	OMG	C1'-N9-C8	2.87	134.86	126.70
20	CA	2401	A2M	C1'-N9-C8	-2.87	120.66	127.14
20	CA	4618	OMG	N9-C4-N3	2.86	131.68	125.94
20	CA	1326	A2M	C1'-N9-C8	-2.85	120.69	127.14
20	CA	3627	OMG	C1'-N9-C4	-2.85	118.03	126.50
23	CD	216	V5N	O-C-CA	-2.84	117.32	124.78
20	CA	3899	OMG	C1'-N9-C8	2.84	134.79	126.70
20	CA	4370	OMG	C2-N1-C6	-2.82	119.96	125.10
20	CA	1326	A2M	O4'-C1'-N9	-2.80	102.54	108.06
20	CA	3818	UY1	O2-C2-N1	-2.80	119.71	122.79
20	CA	2364	OMG	C2-N1-C6	-2.79	120.00	125.10
20	CA	3669	OMG	C2-N1-C6	-2.78	120.03	125.10
20	CA	2815	A2M	C5-N7-C8	2.77	107.44	103.51
20	CA	2424	OMG	C2-N1-C6	-2.77	120.05	125.10
20	CA	3792	OMG	C2-N1-C6	-2.76	120.06	125.10
20	CA	3825	A2M	C1'-N9-C8	-2.76	120.90	127.14
20	CA	1522	OMG	C1'-N9-C8	2.74	134.51	126.70
20	CA	4523	A2M	C4-N9-C8	2.74	108.70	105.73
20	CA	4457	PSU	C6-C5-C4	2.74	120.11	118.20
22	CC	69	PSU	O4-C4-N3	-2.74	114.86	120.12
20	CA	4392	OMG	C1'-N9-C8	2.74	134.49	126.70
20	CA	1522	OMG	N9-C8-N7	-2.73	108.24	113.39
20	CA	1625	OMG	C2-N1-C6	-2.73	120.12	125.10
20	CA	4392	OMG	C2-N1-C6	-2.72	120.14	125.10
20	CA	3899	OMG	N9-C8-N7	-2.69	108.32	113.39
22	CC	75	OMG	C2-N1-C6	-2.69	120.19	125.10
20	CA	4370	OMG	C1'-N9-C8	2.69	134.36	126.70
20	CA	4494	OMG	C2-N1-C6	-2.69	120.20	125.10
20	CA	4623	OMG	C1'-N9-C8	2.69	134.35	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	2415	OMU	C6-C5-C4	2.68	123.18	119.52
20	CA	2424	OMG	C1'-N9-C4	-2.68	118.53	126.50
20	CA	4306	OMU	C6-C5-C4	2.68	123.18	119.52
20	CA	4420	PSU	O4-C4-N3	-2.68	114.99	120.12
20	CA	3822	PSU	O4-C4-N3	-2.67	114.99	120.12
20	CA	2363	A2M	C1'-N9-C8	-2.67	121.11	127.14
20	CA	4442	PSU	O4-C4-N3	-2.67	115.01	120.12
20	CA	4618	OMG	C2-N1-C6	-2.66	120.25	125.10
20	CA	3669	OMG	C1'-N9-C4	-2.66	118.60	126.50
20	CA	4392	OMG	N9-C8-N7	-2.65	108.39	113.39
20	CA	3627	OMG	C2-N1-C6	-2.65	120.27	125.10
20	CA	3744	OMG	N9-C8-N7	-2.65	108.40	113.39
20	CA	3627	OMG	N9-C8-N7	-2.65	108.41	113.39
20	CA	4637	OMG	C1'-N9-C4	-2.64	118.65	126.50
20	CA	4370	OMG	N9-C8-N7	-2.64	108.42	113.39
20	CA	3830	A2M	C4-N9-C8	2.64	108.59	105.73
20	CA	3695	PSU	C6-C5-C4	2.64	120.04	118.20
20	CA	3744	OMG	C1'-N9-C8	2.63	134.20	126.70
20	CA	3785	A2M	O4'-C1'-N9	2.63	113.25	108.06
20	CA	2364	OMG	N9-C8-N7	-2.63	108.43	113.39
20	CA	3925	OMU	C6-C5-C4	2.63	123.11	119.52
20	CA	1859	B8T	C4-N3-C2	-2.63	116.54	120.12
20	CA	2837	OMU	C6-C5-C4	2.63	123.11	119.52
20	CA	4227	OMU	C6-C5-C4	2.63	123.10	119.52
20	CA	4623	OMG	C2-N1-C6	-2.62	120.32	125.10
20	CA	1316	OMG	C1'-N9-C8	2.62	134.15	126.70
20	CA	3851	PSU	O4-C4-N3	-2.61	115.11	120.12
20	CA	5001	PSU	O4-C4-N3	-2.61	115.12	120.12
20	CA	4571	A2M	C5'-C4'-C3'	-2.60	105.42	115.18
20	CA	3744	OMG	C2-N1-C6	-2.60	120.35	125.10
20	CA	3669	OMG	CM2-O2'-C2'	2.59	121.32	114.52
20	CA	3627	OMG	C1'-N9-C8	2.59	134.07	126.70
20	CA	4637	OMG	C2-N1-C6	-2.59	120.38	125.10
20	CA	4457	PSU	O4-C4-N3	-2.58	115.16	120.12
20	CA	2876	OMG	C5-C6-N1	2.58	119.75	113.19
20	CA	3825	A2M	C4-N9-C8	2.58	108.52	105.73
20	CA	2424	OMG	N9-C8-N7	-2.57	108.54	113.39
20	CA	1316	OMG	N9-C8-N7	-2.57	108.54	113.39
20	CA	3718	A2M	C5-N7-C8	2.57	107.16	103.51
20	CA	4618	OMG	N9-C8-N7	-2.56	108.57	113.39
20	CA	4623	OMG	N9-C8-N7	-2.56	108.57	113.39
20	CA	4370	OMG	O6-C6-C5	-2.56	119.81	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	3669	OMG	N9-C8-N7	-2.56	108.57	113.39
20	CA	3867	A2M	O4'-C1'-N9	-2.56	103.02	108.06
20	CA	4576	PSU	O4-C4-N3	-2.56	115.22	120.12
20	CA	4571	A2M	CM'-O2'-C2'	2.55	121.22	114.52
20	CA	2364	OMG	C1'-N9-C4	-2.55	118.92	126.50
20	CA	4499	OMG	C5-C6-N1	2.55	119.66	113.19
22	CC	75	OMG	N9-C8-N7	-2.55	108.60	113.39
20	CA	3920	PSU	O4-C4-N3	-2.54	115.24	120.12
20	CA	2632	PSU	O4-C4-N3	-2.53	115.26	120.12
20	CA	1522	OMG	C2-N1-C6	-2.53	120.48	125.10
20	CA	4673	PSU	O4-C4-N3	-2.53	115.27	120.12
20	CA	4500	PSU	O4-C4-N3	-2.52	115.28	120.12
20	CA	4618	OMG	O6-C6-C5	-2.52	119.92	126.60
20	CA	4637	OMG	N9-C8-N7	-2.52	108.65	113.39
20	CA	1677	PSU	O4-C4-N3	-2.52	115.29	120.12
20	CA	4392	OMG	C5-C6-N1	2.51	119.57	113.19
20	CA	4498	OMU	C6-C5-C4	2.51	122.94	119.52
20	CA	1792	PSU	O4-C4-N3	-2.51	115.31	120.12
20	CA	1322	1MA	N9-C4-N3	2.51	132.78	126.94
20	CA	3695	PSU	O4-C4-N3	-2.50	115.32	120.12
20	CA	3899	OMG	C2-N1-C6	-2.49	120.55	125.10
20	CA	3639	PSU	O4-C4-N3	-2.49	115.34	120.12
20	CA	2876	OMG	N9-C8-N7	-2.49	108.70	113.39
20	CA	2876	OMG	C1'-N9-C4	-2.49	119.11	126.50
20	CA	3792	OMG	N9-C8-N7	-2.49	108.70	113.39
20	CA	4499	OMG	O6-C6-C5	-2.48	120.01	126.60
20	CA	4196	OMG	C5-C6-N1	2.48	119.50	113.19
20	CA	4296	PSU	O4-C4-N3	-2.48	115.36	120.12
20	CA	1316	OMG	C2-N1-C6	-2.48	120.59	125.10
20	CA	3792	OMG	C5-C6-N1	2.47	119.47	113.19
20	CA	3792	OMG	O6-C6-C5	-2.47	120.04	126.60
20	CA	4521	PSU	O4-C4-N3	-2.47	115.38	120.12
20	CA	3637	PSU	O4-C4-N3	-2.47	115.38	120.12
20	CA	4579	PSU	O4-C4-N3	-2.47	115.38	120.12
20	CA	4196	OMG	O6-C6-C5	-2.47	120.05	126.60
20	CA	4689	PSU	O4-C4-N3	-2.46	115.39	120.12
20	CA	224	PSU	O4-C4-N3	-2.46	115.39	120.12
20	CA	1781	PSU	O4-C4-N3	-2.46	115.40	120.12
20	CA	1323	A2M	C3'-C2'-C1'	2.46	107.51	102.89
20	CA	4471	PSU	O4-C4-N3	-2.46	115.41	120.12
20	CA	3844	PSU	O4-C4-N3	-2.46	115.41	120.12
20	CA	1534	A2M	C4-C5-N7	-2.46	107.63	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	2424	OMG	C1'-N9-C8	2.45	133.68	126.70
20	CA	1625	OMG	O6-C6-C5	-2.45	120.11	126.60
20	CA	4620	OMU	C6-C5-C4	2.45	122.86	119.52
20	CA	4532	PSU	O4-C4-N3	-2.44	115.43	120.12
20	CA	1536	PSU	O4-C4-N3	-2.44	115.43	120.12
20	CA	2876	OMG	O6-C6-C5	-2.44	120.13	126.60
20	CA	4228	OMG	C2-N1-C6	-2.44	120.66	125.10
20	CA	4637	OMG	C1'-N9-C8	2.43	133.63	126.70
20	CA	2364	OMG	C5-C6-N1	2.43	119.37	113.19
22	CC	55	PSU	O4-C4-N3	-2.43	115.45	120.12
22	CC	75	OMG	C5-C6-N1	2.43	119.36	113.19
20	CA	1683	PSU	O4-C4-N3	-2.43	115.46	120.12
20	CA	400	A2M	C1'-N9-C8	-2.43	121.66	127.14
20	CA	3669	OMG	C1'-N9-C8	2.42	133.60	126.70
20	CA	400	A2M	C4-N9-C8	2.42	108.36	105.73
20	CA	1862	PSU	O4-C4-N3	-2.42	115.47	120.12
20	CA	4299	PSU	O4-C4-N3	-2.42	115.47	120.12
20	CA	4618	OMG	C5-C6-N1	2.42	119.34	113.19
20	CA	4530	UR3	C6-N1-C2	-2.42	119.62	121.79
20	CA	4370	OMG	C5-C6-N1	2.42	119.33	113.19
20	CA	4353	PSU	O4-C4-N3	-2.42	115.48	120.12
20	CA	1779	PSU	O4-C4-N3	-2.42	115.48	120.12
20	CA	1316	OMG	O6-C6-C5	-2.41	120.21	126.60
20	CA	3792	OMG	C1'-N9-C4	-2.41	119.35	126.50
20	CA	4494	OMG	N9-C8-N7	-2.40	108.86	113.39
20	CA	4972	PSU	O4-C4-N3	-2.40	115.51	120.12
20	CA	1522	OMG	O6-C6-C5	-2.40	120.23	126.60
20	CA	4312	PSU	O4-C4-N3	-2.40	115.51	120.12
20	CA	1625	OMG	C5-C6-N1	2.40	119.28	113.19
20	CA	4293	PSU	O4-C4-N3	-2.40	115.52	120.12
20	CA	2839	PSU	O4-C4-N3	-2.40	115.53	120.12
20	CA	4628	PSU	O4-C4-N3	-2.39	115.53	120.12
20	CA	4494	OMG	O6-C6-C5	-2.39	120.25	126.60
20	CA	3744	OMG	C5-C6-N1	2.39	119.27	113.19
20	CA	1871	A2M	C4-N9-C8	2.39	108.32	105.73
20	CA	4523	A2M	C1'-N9-C8	-2.39	121.75	127.14
20	CA	1522	OMG	C5-C6-N1	2.39	119.25	113.19
20	CA	4220	6MZ	C1'-N9-C8	-2.39	121.75	127.14
20	CA	2508	PSU	O4-C4-N3	-2.38	115.55	120.12
20	CA	4403	PSU	O4-C4-N3	-2.38	115.55	120.12
20	CA	4361	PSU	O4-C4-N3	-2.38	115.55	120.12
22	CC	75	OMG	O6-C6-C5	-2.38	120.28	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	3627	OMG	C5-C6-N1	2.38	119.23	113.19
20	CA	3669	OMG	C5-C6-N1	2.38	119.23	113.19
20	CA	2364	OMG	O6-C6-C5	-2.37	120.30	126.60
20	CA	2401	A2M	O4'-C1'-N9	-2.37	103.39	108.06
20	CA	2424	OMG	C5-C6-N1	2.37	119.21	113.19
20	CA	2876	OMG	C1'-N9-C8	2.37	133.44	126.70
20	CA	2787	A2M	C6-C5-C4	2.37	120.37	117.18
20	CA	1625	OMG	N9-C8-N7	-2.37	108.93	113.39
20	CA	4494	OMG	C5-C6-N1	2.37	119.20	113.19
20	CA	4499	OMG	N9-C8-N7	-2.36	108.94	113.39
20	CA	4423	PSU	O4-C4-N3	-2.36	115.59	120.12
20	CA	4228	OMG	C5-C6-N1	2.36	119.18	113.19
20	CA	3899	OMG	C5-C6-N1	2.36	119.18	113.19
20	CA	4493	PSU	O4-C4-N3	-2.36	115.60	120.12
20	CA	3627	OMG	O6-C6-C5	-2.35	120.35	126.60
20	CA	3744	OMG	O6-C6-C5	-2.35	120.36	126.60
20	CA	4228	OMG	O6-C6-C5	-2.35	120.36	126.60
20	CA	3718	A2M	C1'-N9-C8	-2.35	121.83	127.14
20	CA	4623	OMG	C5-C6-N1	2.35	119.15	113.19
20	CA	3669	OMG	O6-C6-C5	-2.34	120.38	126.60
20	CA	1744	PSU	O4-C4-N3	-2.34	115.62	120.12
20	CA	2424	OMG	O6-C6-C5	-2.34	120.39	126.60
20	CA	3785	A2M	C4-C5-N7	-2.33	107.78	110.62
20	CA	1524	A2M	O4'-C1'-N9	2.33	112.65	108.06
20	CA	398	A2M	C4-N9-C8	2.32	108.24	105.73
20	CA	1316	OMG	C5-C6-N1	2.32	119.08	113.19
20	CA	4431	PSU	O4-C4-N3	-2.31	115.68	120.12
20	CA	1782	PSU	O4-C4-N3	-2.31	115.69	120.12
20	CA	3884	PSU	O4-C4-N3	-2.31	115.70	120.12
20	CA	4392	OMG	O6-C6-C5	-2.30	120.49	126.60
20	CA	4228	OMG	N9-C4-N3	2.30	130.56	125.94
20	CA	1323	A2M	C1'-N9-C8	-2.30	121.94	127.14
20	CA	4637	OMG	C5-C6-N1	2.30	119.03	113.19
20	CA	4571	A2M	C2'-C3'-C4'	2.30	106.98	101.99
20	CA	4196	OMG	N9-C8-N7	-2.29	109.08	113.39
20	CA	4571	A2M	C4-C5-N7	-2.29	107.83	110.62
20	CA	4623	OMG	O6-C6-C5	-2.29	120.53	126.60
20	CA	2351	OMC	C1'-N1-C2	2.29	123.52	118.42
20	CA	2364	OMG	C1'-N9-C8	2.28	133.20	126.70
20	CA	1322	1MA	C8-N7-C5	2.28	108.37	104.24
20	CA	2815	A2M	C3'-C2'-C1'	2.28	107.17	102.89
20	CA	4637	OMG	O6-C6-C5	-2.28	120.56	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	1524	A2M	C4-C5-N7	-2.28	107.85	110.62
20	CA	3715	PSU	O4-C4-N3	-2.28	115.75	120.12
20	CA	2363	A2M	O4'-C1'-N9	-2.27	103.59	108.06
20	CA	2815	A2M	C2'-C1'-N9	-2.27	109.71	113.53
20	CA	3899	OMG	O6-C6-C5	-2.25	120.63	126.60
20	CA	1860	PSU	O4-C4-N3	-2.25	115.81	120.12
20	CA	1326	A2M	C3'-C2'-C1'	2.23	107.07	102.89
20	CA	4447	5MC	CM5-C5-C6	-2.21	119.90	122.85
20	CA	4552	PSU	O4-C4-N3	-2.20	115.90	120.12
20	CA	4571	A2M	C1'-N9-C8	-2.20	122.18	127.14
20	CA	4498	OMU	O4-C4-N3	-2.19	116.09	119.31
20	CA	3792	OMG	C1'-N9-C8	2.19	132.93	126.70
20	CA	4494	OMG	C1'-N9-C4	-2.19	120.00	126.50
20	CA	4571	A2M	C3'-C2'-C1'	2.19	107.00	102.89
20	CA	1326	A2M	C4-N9-C1'	2.17	131.77	126.59
20	CA	3867	A2M	CM'-O2'-C2'	2.16	120.20	114.52
20	CA	1860	PSU	N1-C2-N3	2.16	117.58	115.13
20	CA	2837	OMU	N3-C2-N1	2.15	117.75	114.89
20	CA	4228	OMG	C8-N7-C5	2.14	108.12	104.24
20	CA	4227	OMU	N3-C2-N1	2.14	117.73	114.89
20	CA	1524	A2M	C6-C5-C4	2.13	120.04	117.18
20	CA	4618	OMG	N2-C2-N1	2.13	121.24	116.71
20	CA	3637	PSU	O4'-C1'-C2'	2.12	108.13	105.14
20	CA	3785	A2M	O2'-C2'-C1'	2.12	113.20	109.08
20	CA	2401	A2M	C2'-C1'-N9	-2.11	109.97	113.53
20	CA	2363	A2M	C4-C5-N7	-2.11	108.05	110.62
20	CA	3818	UY1	O4'-C1'-C2'	2.11	108.40	104.48
20	CA	4227	OMU	O4-C4-N3	-2.11	116.21	119.31
20	CA	2401	A2M	C4-N9-C1'	2.11	131.61	126.59
20	CA	4498	OMU	N3-C2-N1	2.10	117.68	114.89
20	CA	4521	PSU	N1-C2-N3	2.10	117.51	115.13
20	CA	4306	OMU	N3-C2-N1	2.09	117.67	114.89
20	CA	398	A2M	C1'-N9-C8	-2.09	122.41	127.14
20	CA	1326	A2M	C2'-C1'-N9	-2.09	110.01	113.53
20	CA	3867	A2M	C3'-C2'-C1'	2.09	106.82	102.89
20	CA	2815	A2M	C5'-C4'-C3'	-2.09	107.36	115.18
20	CA	3785	A2M	C6-C5-C4	2.09	119.99	117.18
20	CA	4228	OMG	N2-C2-N1	2.08	121.15	116.71
20	CA	3718	A2M	C3'-C2'-C1'	2.08	106.80	102.89
20	CA	4499	OMG	C1'-N9-C4	-2.08	120.32	126.50
20	CA	3627	OMG	C8-N7-C5	2.08	108.00	104.24
20	CA	4220	6MZ	C4-C5-N7	-2.07	108.09	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	3887	OMC	C1'-N1-C2	2.07	123.05	118.42
20	CA	1683	PSU	N1-C2-N3	2.06	117.47	115.13
20	CA	4521	PSU	O4'-C1'-C2'	2.06	108.04	105.14
20	CA	3830	A2M	C4-C5-N7	-2.05	108.12	110.62
20	CA	3782	5MC	CM5-C5-C6	-2.05	120.11	122.85
20	CA	2815	A2M	C1'-N9-C8	-2.05	122.51	127.14
20	CA	4306	OMU	O4-C4-N3	-2.05	116.30	119.31
20	CA	1522	OMG	C8-N7-C5	2.05	107.94	104.24
20	CA	398	A2M	O2'-C2'-C1'	2.05	113.07	109.08
20	CA	3867	A2M	C4-N9-C1'	2.04	131.47	126.59
20	CA	1782	PSU	N1-C2-N3	2.04	117.44	115.13
20	CA	2876	OMG	C8-N7-C5	2.04	107.94	104.24
20	CA	2364	OMG	C8-N7-C5	2.04	107.93	104.24
20	CA	3899	OMG	C8-N7-C5	2.04	107.93	104.24
20	CA	2415	OMU	N3-C2-N1	2.04	117.59	114.89
20	CA	1323	A2M	C2'-C1'-N9	-2.04	110.10	113.53
20	CA	224	PSU	N1-C2-N3	2.03	117.43	115.13
20	CA	3637	PSU	N1-C2-N3	2.03	117.43	115.13
20	CA	2424	OMG	C8-N7-C5	2.03	107.91	104.24
20	CA	2815	A2M	C4-C5-N7	-2.02	108.15	110.62
20	CA	4523	A2M	C4-C5-N7	-2.02	108.16	110.62
20	CA	2815	A2M	O2'-C2'-C1'	2.02	113.02	109.08
20	CA	3925	OMU	N3-C2-N1	2.02	117.57	114.89
20	CA	4370	OMG	C8-N7-C5	2.02	107.89	104.24
20	CA	1781	PSU	N1-C2-N3	2.01	117.41	115.13
20	CA	4392	OMG	C8-N7-C5	2.01	107.87	104.24
20	CA	4493	PSU	N1-C2-N3	2.01	117.40	115.13
20	CA	4494	OMG	C1'-N9-C8	2.01	132.41	126.70
20	CA	3867	A2M	C4-N9-C8	2.00	107.90	105.73
20	CA	1625	OMG	C1'-N9-C4	-2.00	120.56	126.50

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	BA	245	HIC	O-C-CA-CB
20	CA	224	PSU	C2'-C1'-C5-C4
20	CA	398	A2M	C1'-C2'-O2'-CM'
20	CA	400	A2M	C1'-C2'-O2'-CM'
20	CA	1323	A2M	C1'-C2'-O2'-CM'
20	CA	2815	A2M	C1'-C2'-O2'-CM'
20	CA	3669	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
20	CA	3701	OMC	C2'-C1'-N1-C2
20	CA	3701	OMC	C2'-C1'-N1-C6
20	CA	3718	A2M	C1'-C2'-O2'-CM'
20	CA	3785	A2M	C3'-C4'-C5'-O5'
20	CA	3792	OMG	O4'-C4'-C5'-O5'
20	CA	3825	A2M	C1'-C2'-O2'-CM'
20	CA	3830	A2M	C1'-C2'-O2'-CM'
20	CA	3867	A2M	C1'-C2'-O2'-CM'
20	CA	4420	PSU	C2'-C1'-C5-C4
20	CA	4420	PSU	O4'-C1'-C5-C4
20	CA	4420	PSU	O4'-C1'-C5-C6
20	CA	4500	PSU	O4'-C1'-C5-C4
20	CA	4500	PSU	O4'-C1'-C5-C6
20	CA	4523	A2M	C1'-C2'-O2'-CM'
20	CA	4530	UR3	O4'-C1'-N1-C6
20	CA	4530	UR3	O4'-C1'-N1-C2
20	CA	4571	A2M	C1'-C2'-O2'-CM'
20	CA	4637	OMG	C1'-C2'-O2'-CM2
20	CA	3785	A2M	O4'-C4'-C5'-O5'
20	CA	3792	OMG	C3'-C4'-C5'-O5'
20	CA	3867	A2M	C3'-C4'-C5'-O5'
20	CA	2401	A2M	C3'-C4'-C5'-O5'
20	CA	3669	OMG	C3'-C2'-O2'-CM2
20	CA	2401	A2M	O4'-C4'-C5'-O5'
20	CA	2422	OMC	O4'-C4'-C5'-O5'
20	CA	3867	A2M	O4'-C4'-C5'-O5'
20	CA	2787	A2M	C2'-C1'-N9-C8
20	CA	3818	UY1	C4'-C5'-O5'-P
20	CA	2422	OMC	C3'-C4'-C5'-O5'
12	Ag	98	MLZ	CD-CE-NZ-CM
20	CA	4447	5MC	C2'-C1'-N1-C6
20	CA	1534	A2M	C4'-C5'-O5'-P
20	CA	2787	A2M	C2'-C1'-N9-C4
20	CA	2876	OMG	C3'-C2'-O2'-CM2
20	CA	4370	OMG	C3'-C2'-O2'-CM2
20	CA	4498	OMU	C3'-C2'-O2'-CM2
20	CA	1326	A2M	C4'-C5'-O5'-P
20	CA	4500	PSU	C4'-C5'-O5'-P
20	CA	1781	PSU	C3'-C4'-C5'-O5'
20	CA	3701	OMC	O4'-C1'-N1-C6
20	CA	4447	5MC	O4'-C1'-N1-C6
20	CA	3844	PSU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
34	AU	39	V5N	O2-CB-CG-CD2
20	CA	3701	OMC	O4'-C1'-N1-C2
34	AU	39	V5N	O2-CB-CG-ND1
20	CA	4447	5MC	O4'-C1'-N1-C2
20	CA	4521	PSU	O4'-C1'-C5-C4
20	CA	2351	OMC	C3'-C2'-O2'-CM2
20	CA	4494	OMG	C3'-C2'-O2'-CM2
20	CA	4571	A2M	C3'-C2'-O2'-CM'
20	CA	2351	OMC	C2'-C1'-N1-C2
20	CA	2351	OMC	C2'-C1'-N1-C6
20	CA	1524	A2M	O4'-C1'-N9-C8
20	CA	398	A2M	O4'-C4'-C5'-O5'
20	CA	2787	A2M	O4'-C1'-N9-C8
20	CA	3744	OMG	C1'-C2'-O2'-CM2
20	CA	224	PSU	O4'-C1'-C5-C6
20	CA	3818	UY1	O4'-C1'-C5-C6
20	CA	4447	5MC	C2'-C1'-N1-C2
20	CA	1534	A2M	O4'-C4'-C5'-O5'
20	CA	2351	OMC	O4'-C4'-C5'-O5'
20	CA	3851	PSU	C3'-C4'-C5'-O5'
20	CA	1322	1MA	C2'-C1'-N9-C8
20	CA	1859	B8T	C2'-C1'-N1-C2
20	CA	2363	A2M	C3'-C2'-O2'-CM'
23	CD	216	V5N	O-C-CA-CB

There are no ring outliers.

42 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	CA	1524	A2M	1	0
20	CA	400	A2M	1	0
20	CA	4498	OMU	3	0
20	CA	4972	PSU	1	0
20	CA	4392	OMG	1	0
20	CA	4576	PSU	1	0
20	CA	4620	OMU	1	0
20	CA	1322	1MA	2	0
20	CA	2415	OMU	1	0
20	CA	2837	OMU	1	0
20	CA	4579	PSU	2	0
20	CA	4499	OMG	4	0
20	CA	3695	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	CA	3925	OMU	1	0
20	CA	4196	OMG	1	0
20	CA	1860	PSU	1	0
20	CA	4306	OMU	1	0
22	CC	69	PSU	2	0
20	CA	3785	A2M	2	0
20	CA	1326	A2M	4	0
20	CA	4370	OMG	1	0
20	CA	3867	A2M	1	0
20	CA	3744	OMG	1	0
20	CA	3782	5MC	1	0
20	CA	1871	A2M	1	0
20	CA	3869	OMC	1	0
20	CA	1859	B8T	3	0
20	CA	2351	OMC	1	0
20	CA	3825	A2M	3	0
20	CA	1881	OMC	1	0
20	CA	1340	OMC	3	0
20	CA	3718	A2M	8	0
20	CA	4536	OMC	4	0
20	CA	2424	OMG	1	0
20	CA	4447	5MC	2	0
20	CA	2815	A2M	2	0
20	CA	4552	PSU	1	0
22	CC	75	OMG	1	0
20	CA	3792	OMG	1	0
20	CA	2632	PSU	1	0
20	CA	4673	PSU	1	0
20	CA	4637	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 250 ligands modelled in this entry, 233 are monoatomic - leaving 17 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
38	PUT	CA	5403	-	5,5,5	0.26	0	4,4,4	0.45	0
37	ATP	Ah	202	-	29,33,33	0.24	0	44,52,52	0.82	2 (4%)
40	SPM	CA	5411	-	13,13,13	0.56	0	12,12,12	0.89	0
40	SPM	CA	5414	-	13,13,13	0.37	0	12,12,12	1.05	0
40	SPM	CA	5413	-	13,13,13	0.48	0	12,12,12	1.01	0
38	PUT	CA	5401	-	5,5,5	0.17	0	4,4,4	0.38	0
40	SPM	CA	5412	-	13,13,13	0.47	0	12,12,12	0.95	0
40	SPM	CA	5415	-	13,13,13	0.51	0	12,12,12	0.94	0
38	PUT	CA	5404	-	5,5,5	0.28	0	4,4,4	0.30	0
39	SPD	CA	5406	-	9,9,9	0.57	0	8,8,8	1.43	1 (12%)
39	SPD	CA	5410	-	9,9,9	0.41	0	8,8,8	1.35	1 (12%)
39	SPD	CA	5408	-	9,9,9	0.43	0	8,8,8	1.39	1 (12%)
38	PUT	CA	5402	-	5,5,5	0.32	0	4,4,4	0.28	0
38	PUT	CB	201	-	5,5,5	0.24	0	4,4,4	0.32	0
39	SPD	CA	5409	-	9,9,9	0.59	0	8,8,8	1.35	1 (12%)
39	SPD	CA	5405	35	9,9,9	0.47	0	8,8,8	1.41	1 (12%)
39	SPD	CA	5407	-	9,9,9	0.66	0	8,8,8	1.37	1 (12%)

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
38	PUT	CA	5403	-	-	1/3/3/3	-
37	ATP	Ah	202	-	-	3/22/38/38	0/3/3/3
40	SPM	CA	5411	-	-	1/11/11/11	-
40	SPM	CA	5414	-	-	4/11/11/11	-
40	SPM	CA	5413	-	-	2/11/11/11	-
38	PUT	CA	5401	-	-	1/3/3/3	-
40	SPM	CA	5412	-	-	2/11/11/11	-
40	SPM	CA	5415	-	-	8/11/11/11	-
38	PUT	CA	5404	-	-	0/3/3/3	-
39	SPD	CA	5406	-	-	3/7/7/7	-
39	SPD	CA	5410	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	SPD	CA	5408	-	-	6/7/7/7	-
38	PUT	CA	5402	-	-	1/3/3/3	-
38	PUT	CB	201	-	-	1/3/3/3	-
39	SPD	CA	5409	-	-	3/7/7/7	-
39	SPD	CA	5405	35	-	4/7/7/7	-
39	SPD	CA	5407	-	-	3/7/7/7	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	CA	5406	SPD	C4-C5-N6	3.39	121.29	112.14
39	CA	5408	SPD	C4-C5-N6	3.30	121.04	112.14
39	CA	5405	SPD	C4-C5-N6	3.24	120.89	112.14
39	CA	5407	SPD	C4-C5-N6	3.12	120.55	112.14
39	CA	5410	SPD	C4-C5-N6	3.12	120.55	112.14
39	CA	5409	SPD	C4-C5-N6	3.09	120.47	112.14
37	Ah	202	ATP	PB-O3B-PG	2.42	141.13	132.83
37	Ah	202	ATP	O3'-C3'-C4'	-2.05	105.11	111.05

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	CA	5405	SPD	C8-C7-N6-C5
39	CA	5407	SPD	C8-C7-N6-C5
39	CA	5408	SPD	C4-C5-N6-C7
39	CA	5410	SPD	C4-C5-N6-C7
39	CA	5408	SPD	N6-C7-C8-C9
38	CA	5403	PUT	C1-C2-C3-C4
40	CA	5415	SPM	N10-C11-C12-C13
39	CA	5408	SPD	C3-C4-C5-N6
39	CA	5410	SPD	C3-C4-C5-N6
40	CA	5413	SPM	C2-C3-C4-N5
39	CA	5409	SPD	C3-C4-C5-N6
39	CA	5410	SPD	N6-C7-C8-C9
40	CA	5415	SPM	C2-C3-C4-N5
40	CA	5415	SPM	C12-C11-N10-C9
39	CA	5407	SPD	C3-C4-C5-N6
37	Ah	202	ATP	O4'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
39	CA	5406	SPD	N6-C7-C8-C9
37	Ah	202	ATP	O4'-C1'-N9-C8
39	CA	5408	SPD	C8-C7-N6-C5
39	CA	5405	SPD	N6-C7-C8-C9
40	CA	5411	SPM	C7-C8-C9-N10
37	Ah	202	ATP	O4'-C4'-C5'-O5'
39	CA	5408	SPD	C2-C3-C4-C5
39	CA	5407	SPD	N6-C7-C8-C9
39	CA	5405	SPD	C7-C8-C9-N10
39	CA	5410	SPD	C7-C8-C9-N10
40	CA	5415	SPM	N1-C2-C3-C4
38	CA	5402	PUT	C1-C2-C3-C4
39	CA	5409	SPD	C2-C3-C4-C5
40	CA	5413	SPM	C7-C6-N5-C4
38	CB	201	PUT	C1-C2-C3-C4
40	CA	5414	SPM	C12-C11-N10-C9
40	CA	5414	SPM	N5-C6-C7-C8
40	CA	5414	SPM	C11-C12-C13-N14
40	CA	5415	SPM	C11-C12-C13-N14
39	CA	5409	SPD	N1-C2-C3-C4
40	CA	5412	SPM	N5-C6-C7-C8
40	CA	5414	SPM	C6-C7-C8-C9
40	CA	5415	SPM	C8-C9-N10-C11
39	CA	5405	SPD	C4-C5-N6-C7
38	CA	5401	PUT	C1-C2-C3-C4
39	CA	5406	SPD	C8-C7-N6-C5
39	CA	5410	SPD	C8-C7-N6-C5
40	CA	5415	SPM	C3-C4-N5-C6
40	CA	5415	SPM	C7-C6-N5-C4
39	CA	5406	SPD	C7-C8-C9-N10
39	CA	5408	SPD	C7-C8-C9-N10
40	CA	5412	SPM	C8-C9-N10-C11

There are no ring outliers.

10 monomers are involved in 38 short contacts:

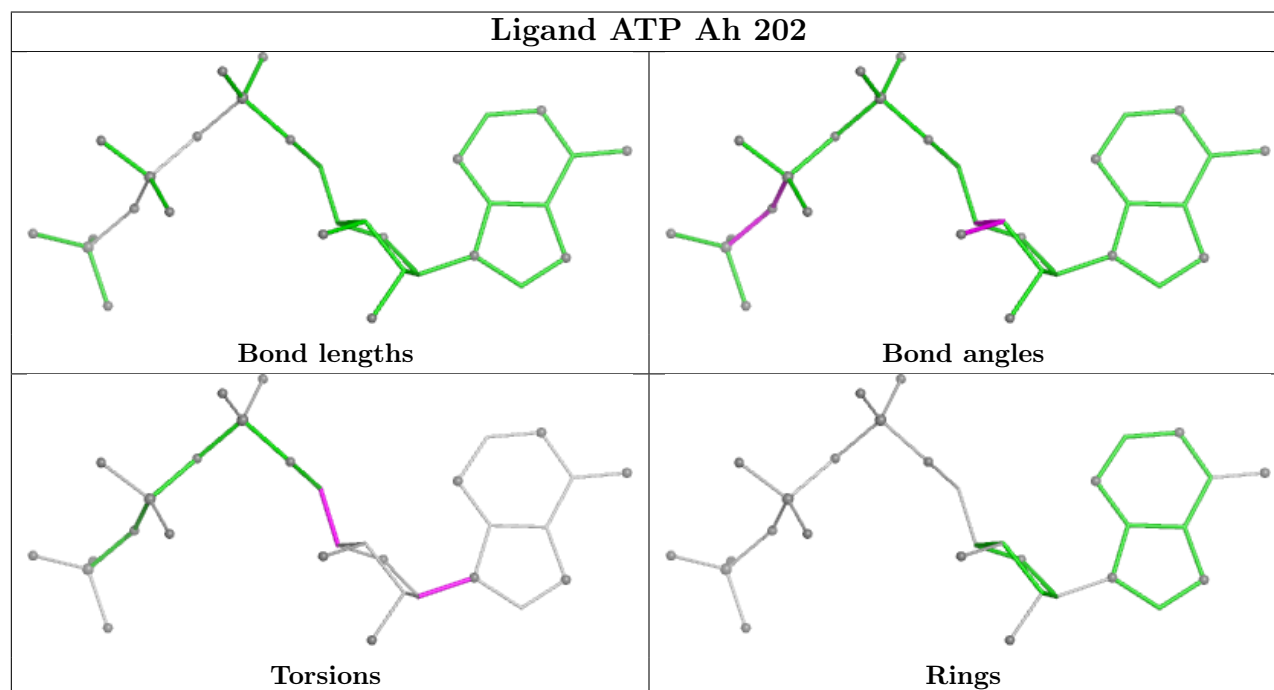
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	CA	5403	PUT	4	0
37	Ah	202	ATP	2	0
38	CA	5401	PUT	4	0
40	CA	5415	SPM	2	0
38	CA	5404	PUT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	CA	5410	SPD	9	0
38	CA	5402	PUT	6	0
38	CB	201	PUT	5	0
39	CA	5405	SPD	1	0
39	CA	5407	SPD	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

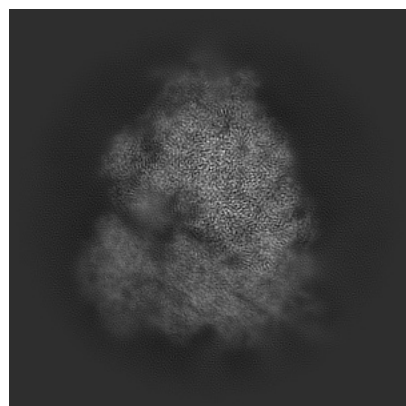
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57203. These allow visual inspection of the internal detail of the map and identification of artifacts.

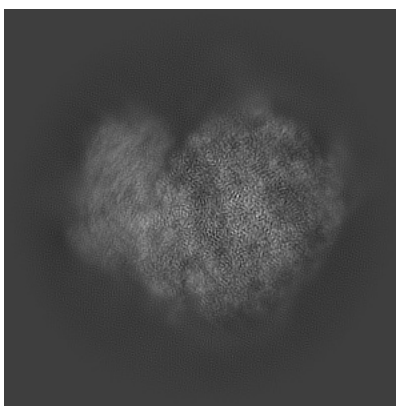
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

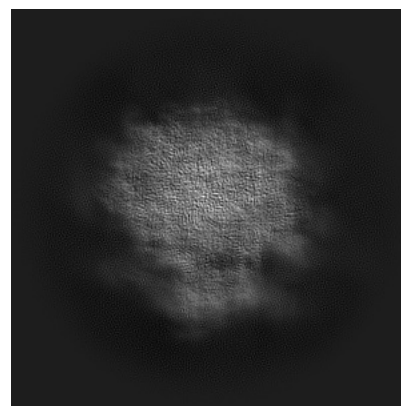
6.1.1 Primary map



X

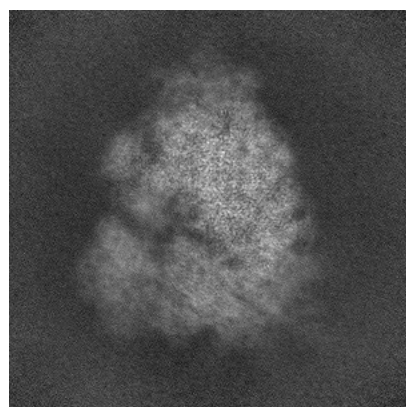


Y

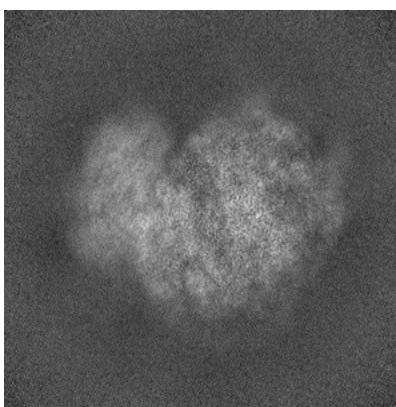


Z

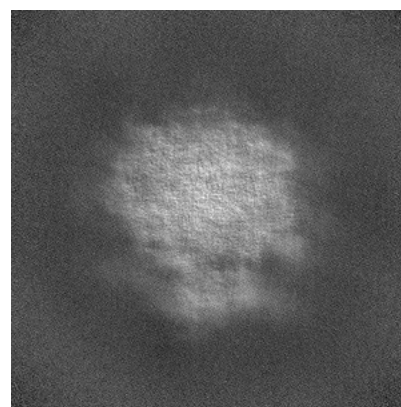
6.1.2 Raw map



X



Y

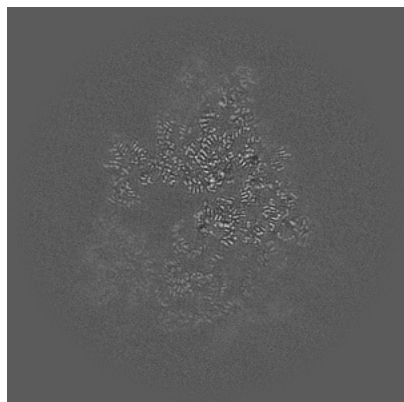


Z

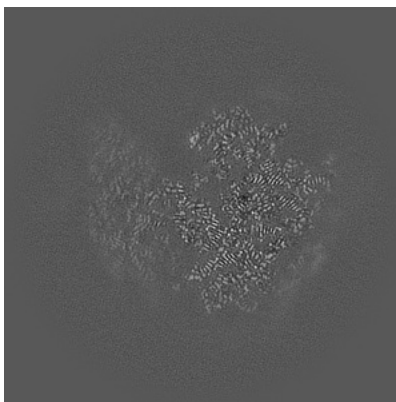
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

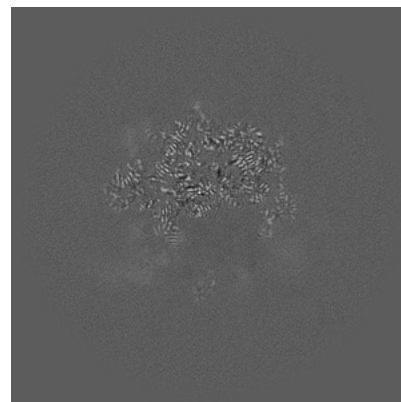
6.2.1 Primary map



X Index: 320

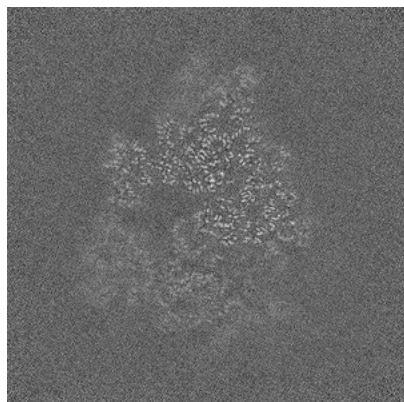


Y Index: 320

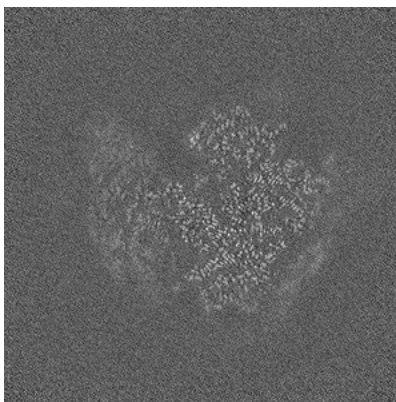


Z Index: 320

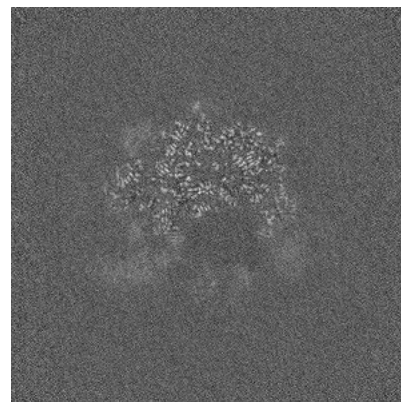
6.2.2 Raw map



X Index: 320



Y Index: 320

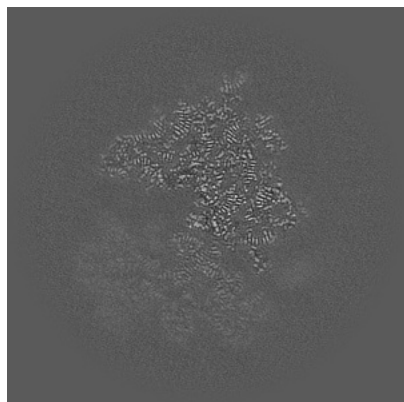


Z Index: 320

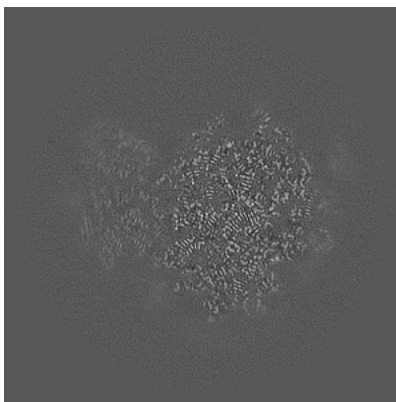
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

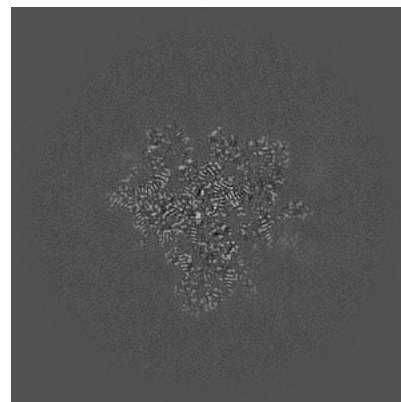
6.3.1 Primary map



X Index: 286

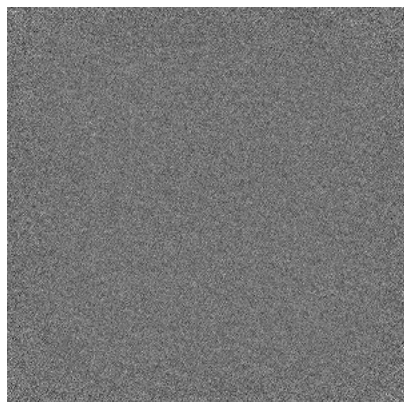


Y Index: 339

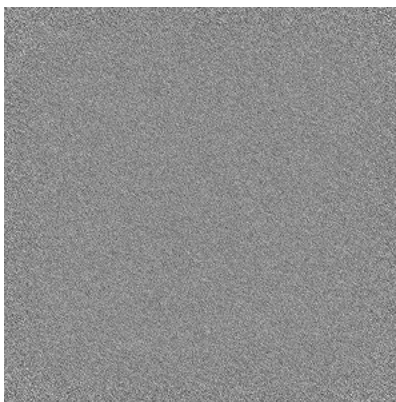


Z Index: 386

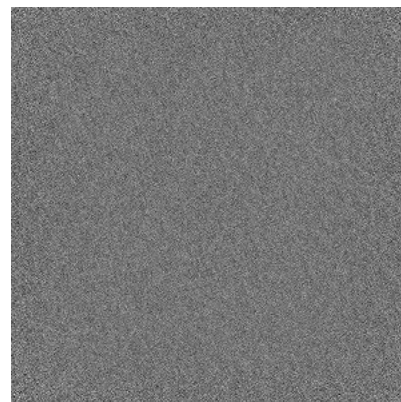
6.3.2 Raw map



X Index: 0



Y Index: 0

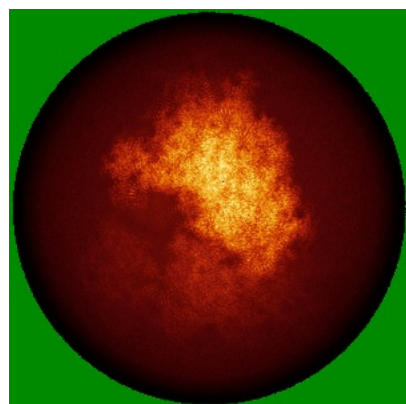


Z Index: 0

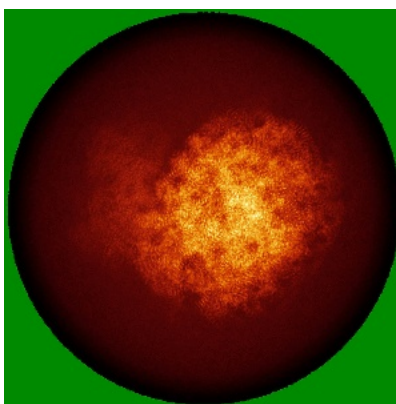
The images above show the largest variance slices of the map in three orthogonal directions.

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

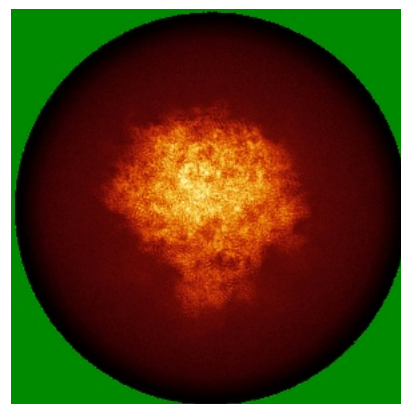
6.4.1 Primary map



X

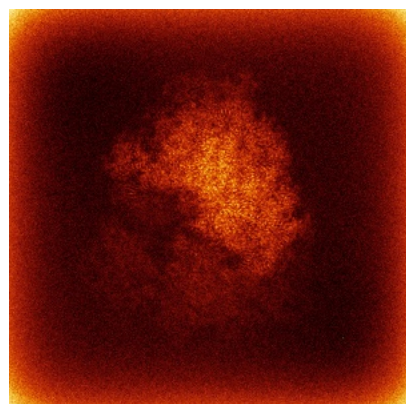


Y

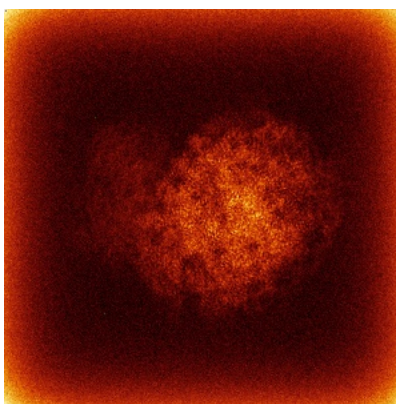


Z

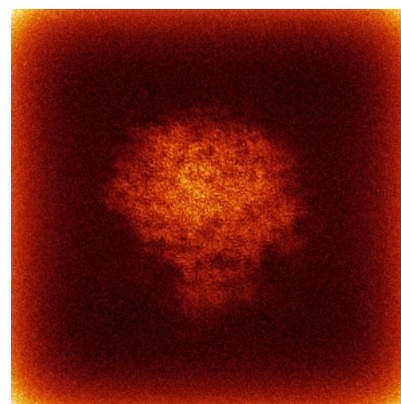
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



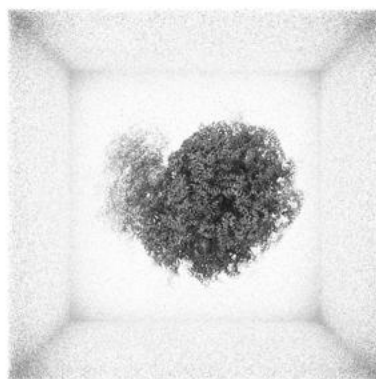
Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

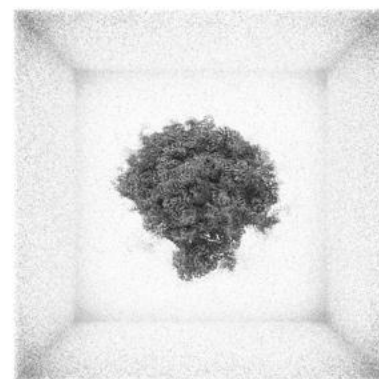
6.5.2 Raw map



X



Y



Z

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

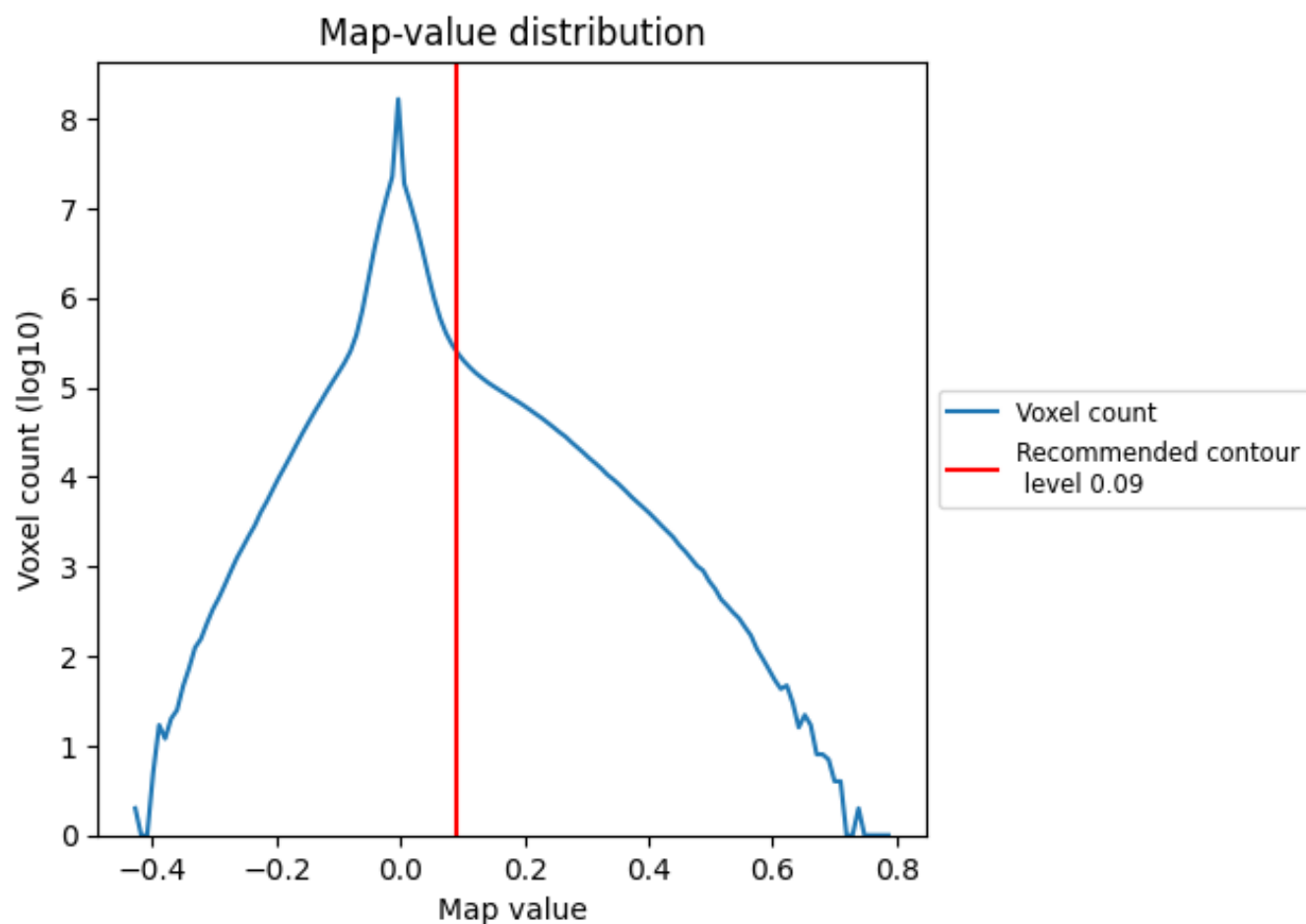
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

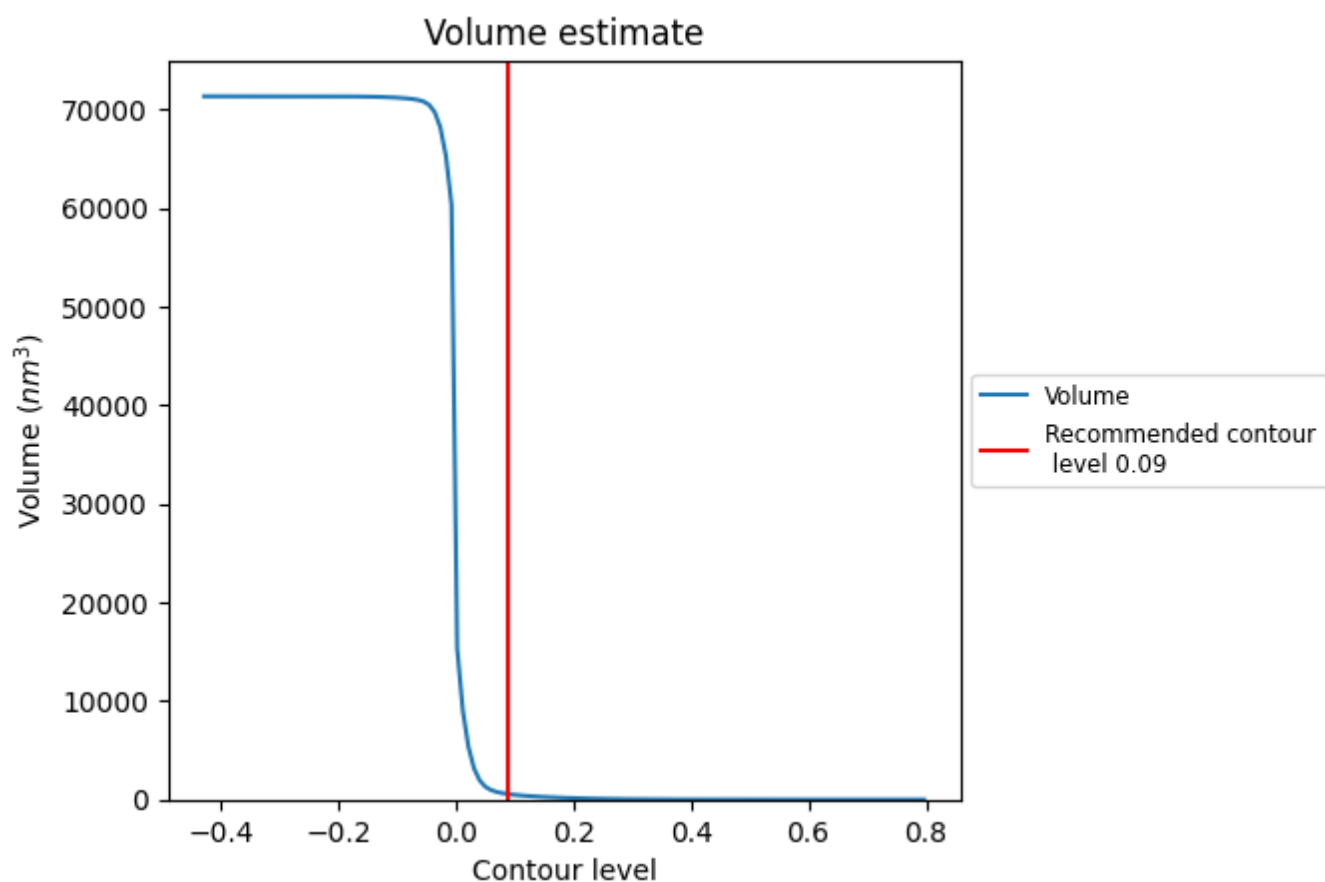
This section contains the results of statistical analysis of the map.

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.

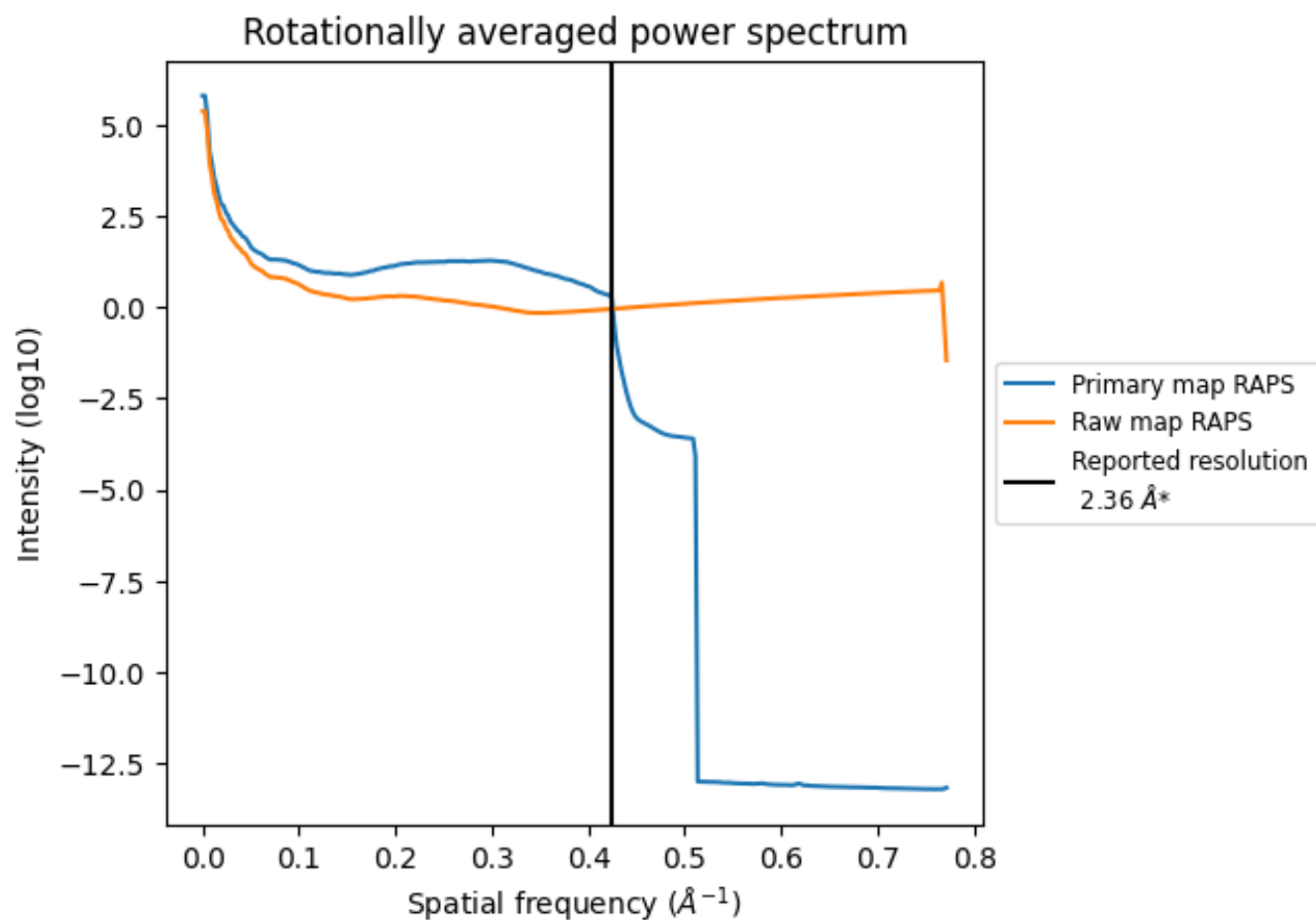
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 553 nm³; this corresponds to an approximate mass of 499 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

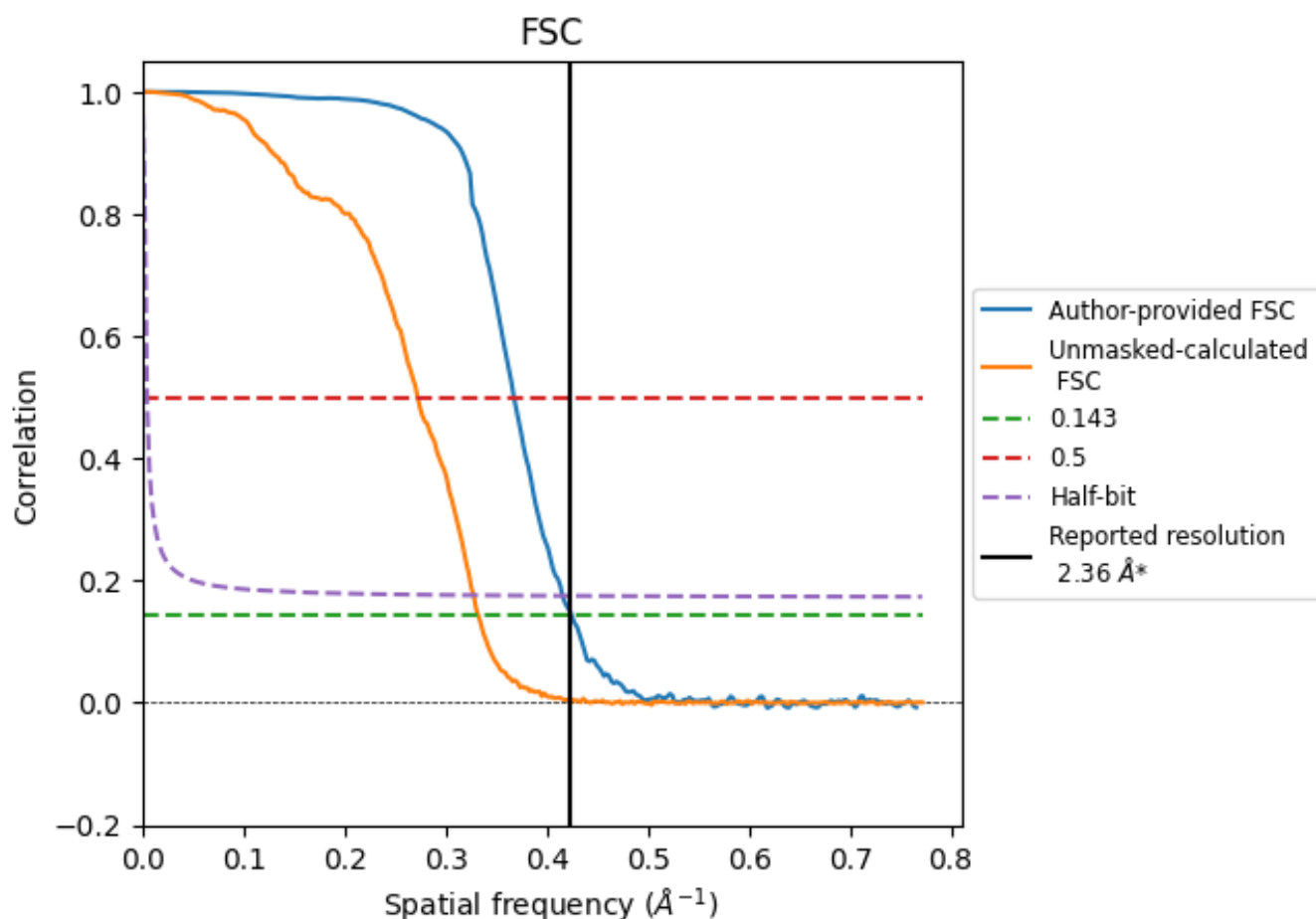


*Reported resolution corresponds to spatial frequency of 0.424 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.424 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

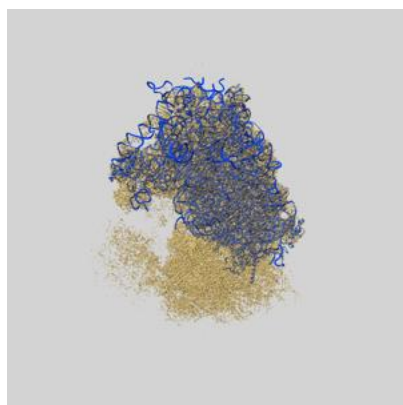
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.36	-	-
Author-provided FSC curve	2.36	2.72	2.41
Unmasked-calculated*	3.01	3.67	3.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.01 differs from the reported value 2.36 by more than 10 %

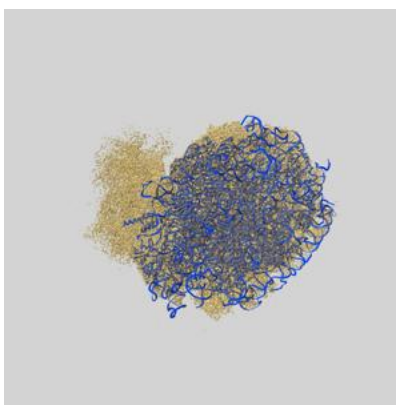
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57203 and PDB model 29IY. Per-residue inclusion information can be found in section 3 on page 16.

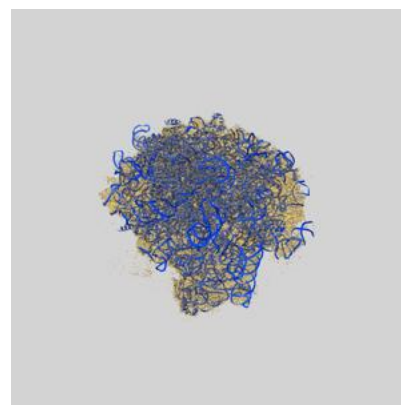
9.1 Map-model overlay [i](#)



X



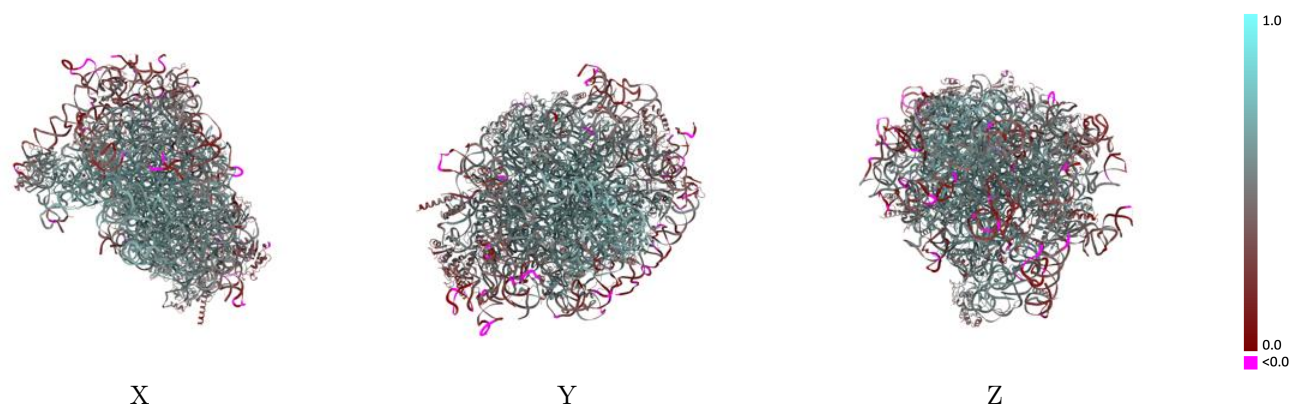
Y



Z

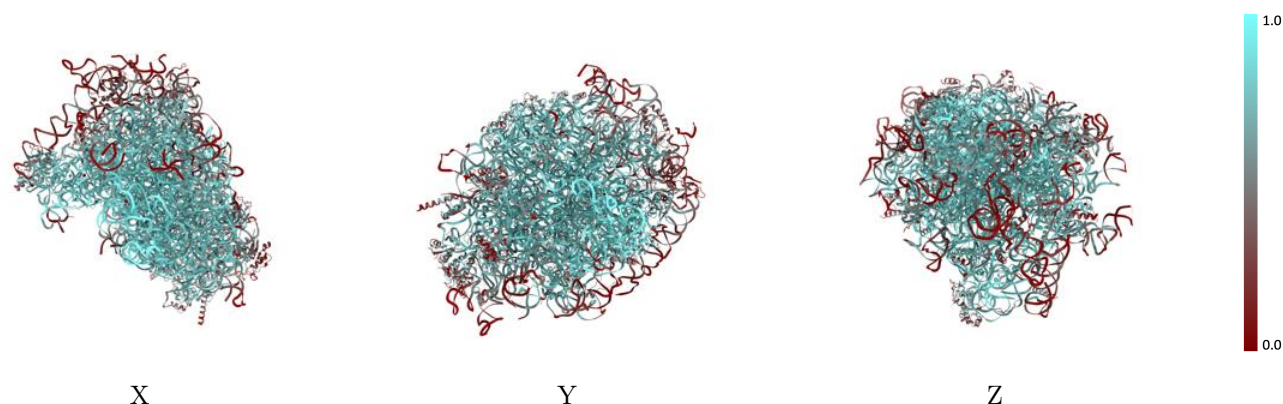
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



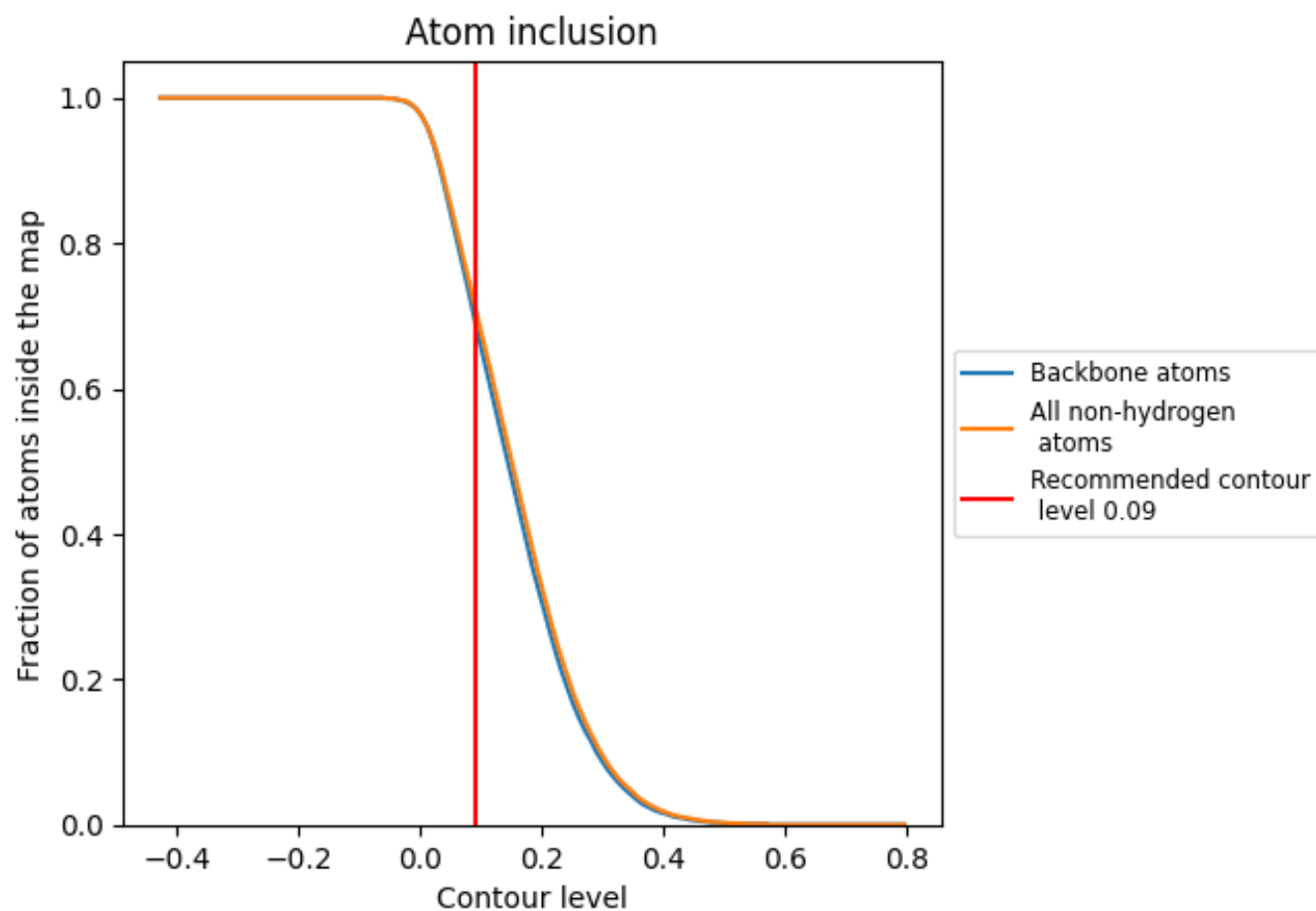
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 71% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.5170
AK	 0.8320	 0.5980
AL	 0.6290	 0.4650
AM	 0.7430	 0.5350
AN	 0.6910	 0.5360
AO	 0.2730	 0.3040
AP	 0.7470	 0.5590
AQ	 0.6540	 0.4930
AR	 0.6220	 0.4870
AS	 0.7490	 0.5700
AT	 0.4080	 0.3080
AU	 0.8100	 0.5910
AV	 0.5310	 0.4730
AW	 0.4640	 0.3490
AX	 0.6140	 0.4730
AY	 0.8270	 0.6090
AZ	 0.8170	 0.5670
Aa	 0.6400	 0.4660
Ab	 0.6220	 0.5120
Ac	 0.5500	 0.4420
Ad	 0.8860	 0.6290
Ae	 0.3250	 0.2840
Af	 0.7470	 0.5780
Ag	 0.7120	 0.5100
Ah	 0.7880	 0.5950
Ai	 0.6830	 0.5190
Aj	 0.7560	 0.5690
BA	 0.7080	 0.5160
BB	 0.7910	 0.5870
BC	 0.5710	 0.4620
BD	 0.5020	 0.4170
CA	 0.7150	 0.5180
CB	 0.8350	 0.5740
CC	 0.7350	 0.5230
CD	 0.7990	 0.5660

