



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 02:58 PM JST

PDB ID : 8INF / pdb_00008inf
EMDB ID : EMD-35597
Title : human nuclear pre-60S ribosomal particle - State F'
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-03-09
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

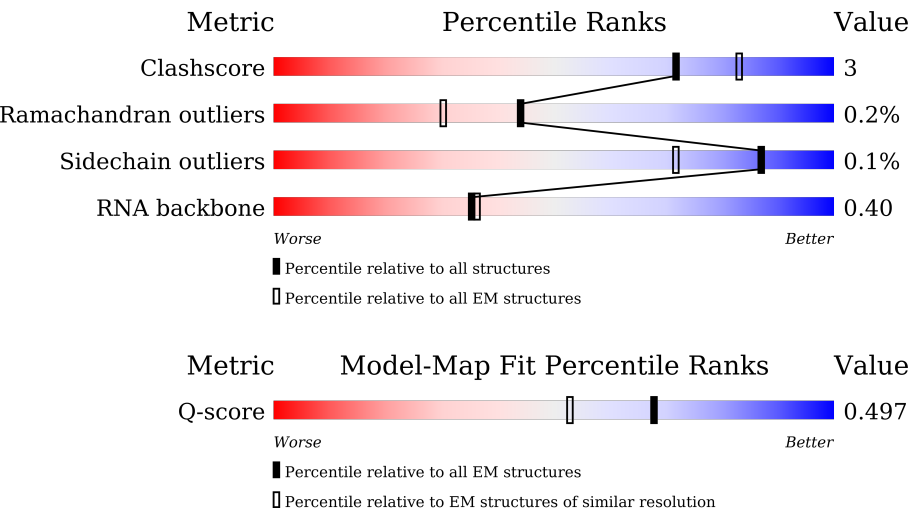
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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.



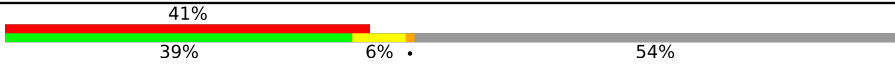
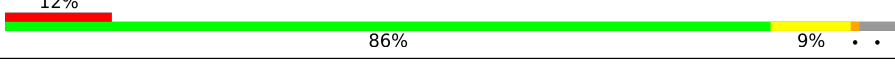
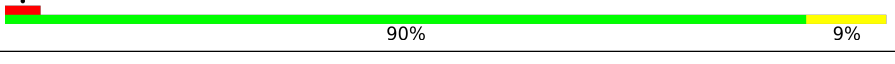
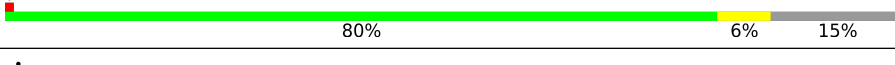
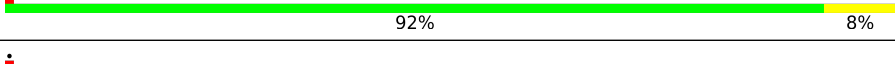
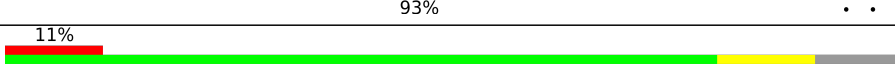
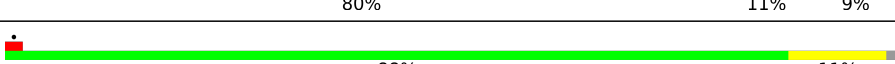
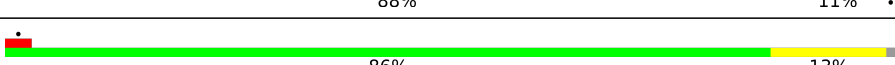
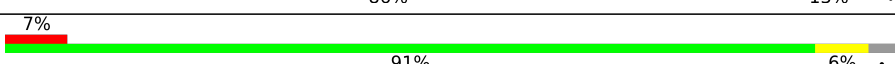
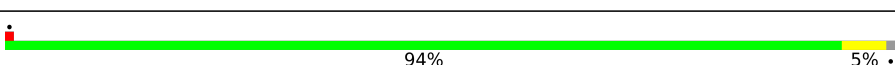
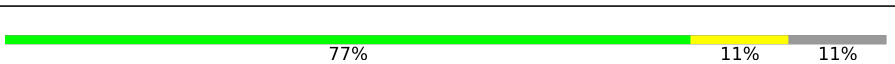
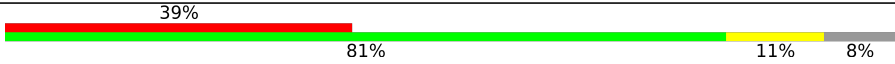
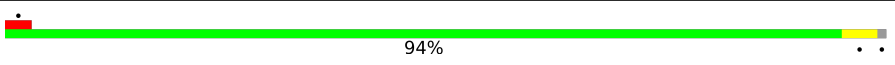
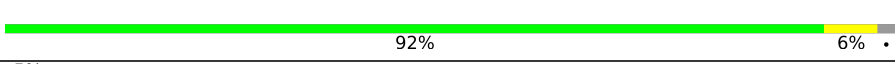
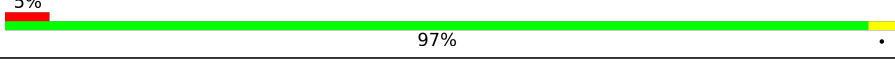
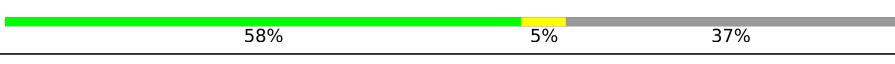
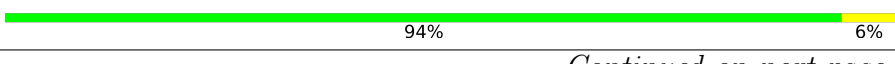
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	u	490	
2	f	687	
3	q	217	

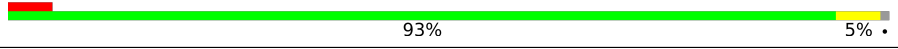
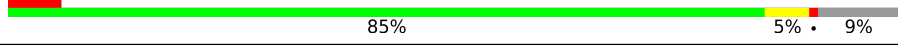
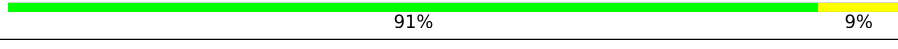
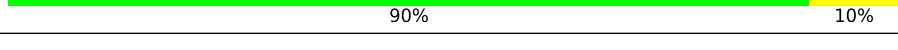
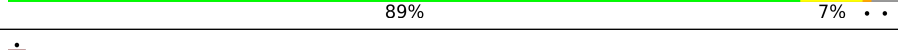
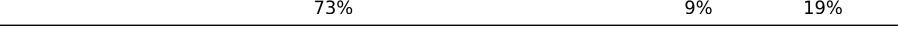
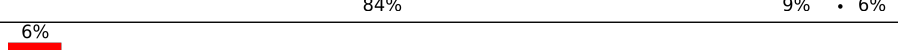
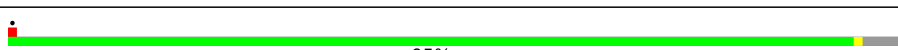
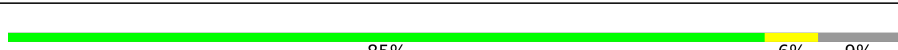
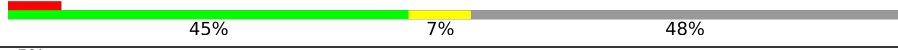
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Mol	Chain	Length	Quality of chain
4	t	293	
5	3	255	
6	2	5054	
7	4	634	
8	5	120	
9	6	245	
10	7	163	
11	9	134	
12	B	403	
13	C	159	
14	D	427	
15	E	115	
16	F	117	
17	G	266	
18	H	123	
19	I	192	
20	K	105	
21	L	148	
22	M	97	
23	N	178	
24	O	70	
25	P	51	
26	Q	211	
27	S	215	
28	U	204	

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Mol	Chain	Length	Quality of chain
29	V	203	
30	W	106	
31	X	92	
32	Y	184	
33	Z	188	
34	a	196	
35	b	176	
36	c	160	
37	d	128	
38	e	140	
39	g	156	
40	h	145	
41	i	136	
42	j	125	
43	k	135	
44	l	137	
45	m	257	
46	n	110	
47	o	288	
48	p	248	
49	r	297	
50	z	129	
51	A	731	
52	R	203	
53	J	239	

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Mol	Chain	Length	Quality of chain
54	T	99	
55	y	165	
56	v	588	
57	8	156	
58	1	123	
59	s	260	
60	w	478	
61	x	120	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 169278 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	u	239	Total	C	N	O	S	0	0
			1924	1232	338	348	6		

- Molecule 2 is a protein called Protein SDA1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	f	554	Total	C	N	O	S	0	0
			4536	2890	810	804	32		

- Molecule 3 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	q	212	Total	C	N	O	S	0	0
			1708	1092	308	300	8		

- Molecule 4 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	t	134	Total	C	N	O	S	0	0
			1135	734	200	197	4		

- Molecule 5 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	229	Total	C	N	O	S	0	0
			1892	1223	356	309	4		

- Molecule 6 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2	3654	Total	C	N	O	P	0	0
			77711	34626	14137	25295	3653		

- Molecule 7 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4	611	Total	C	N	O	S	0	0
			5016	3151	918	920	27		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	5	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 9 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	6	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 10 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	7	139	Total	C	N	O	S	0	0
			1184	754	229	191	10		

- Molecule 11 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	9	97	Total	C	N	O	S	0	0
			787	481	168	134	4		

- Molecule 12 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	402	Total	C	N	O	S	1	0
			3244	2065	609	556	14		

- Molecule 13 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	93	Total	C	N	O	S	0	0
			764	476	167	117	4		

- Molecule 14 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 15 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 16 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	113	Total	C	N	O	S	0	0
			897	560	185	146	6		

- Molecule 17 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 18 is a protein called 60S ribosomal protein L35.

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

- Molecule 19 is a protein called 60S ribosomal protein L9.

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

- Molecule 20 is a protein called 60S ribosomal protein L36.

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

- Molecule 21 is a protein called 60S ribosomal protein L27a.

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

- Molecule 22 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 23 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	164	Total	C	N	O	S	0	0
			1310	830	243	232	5		

- Molecule 24 is a protein called 60S ribosomal protein L38.

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

- Molecule 25 is a protein called 60S ribosomal protein L39.

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

- Molecule 26 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 27 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 28 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 29 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 30 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	96	Total	C	N	O	S	0	0
			785	492	159	128	6		

- Molecule 31 is a protein called 60S ribosomal protein L37a.

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

- Molecule 32 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	167	Total	C	N	O	S	0	0
			1355	848	260	238	9		

- Molecule 33 is a protein called 60S ribosomal protein L18.

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

- Molecule 34 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	148	Total	C	N	O	S	0	0
			1239	772	266	192	9		

- Molecule 35 is a protein called 60S ribosomal protein L18a.

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

- Molecule 36 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	155	Total	C	N	O	S	0	0
			1264	801	248	210	5		

- Molecule 37 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	104	Total	C	N	O	S	0	0
			850	542	149	157	2		

- Molecule 38 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 39 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 40 is a protein called 60S ribosomal protein L26.

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

- Molecule 41 is a protein called 60S ribosomal protein L27.

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

- Molecule 42 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	111	Total	C	N	O	S	0	0
			918	578	178	160	2		

- Molecule 43 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 45 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 46 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 47 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	235	Total	C	N	O	S	0	0
			1897	1217	360	316	4		

- Molecule 48 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 49 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	284	Total	C	N	O	S	0	0
			2312	1463	420	415	14		

- Molecule 50 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 51 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A	333	Total	C	N	O	S	0	0
			2672	1710	457	497	8		

- Molecule 52 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	R	153	Total	C	N	O	S	0	0
			1296	810	248	233	5		

- Molecule 53 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	J	223	Total	C	N	O	S	0	0
			1809	1140	309	349	11		

- Molecule 54 is a protein called Leydig cell tumor 10 kDa protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	T	45	Total	C	N	O	S	0	0
			354	221	75	57	1		

- Molecule 55 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	165	Total	C	N	O	S	0	0
			1250	779	232	234	5		

- Molecule 56 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	v	404	Total	C	N	O	S	0	0
			3317	2140	582	582	13		

- Molecule 57 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	8	154	Total	C	N	O	P	0	0
			3278	1463	580	1081	154		

- Molecule 58 is a protein called Uncharacterized protein C11orf98.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	1	74	Total	C	N	O	0	0
			622	385	142	95		

- Molecule 59 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	s	35	Total	C	N	O	0	0
			316	196	68	52		

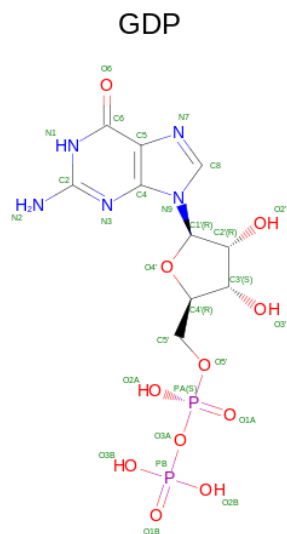
- Molecule 60 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	w	388	Total	C	N	O	S	0	0
			3214	2002	646	564	2		

- Molecule 61 is a RNA chain called Internal Transcribed Spacer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	x	57	Total	C	N	O	P	0	0
			684	285	1	341	57		

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
62	A	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
63	A	1	Total Mg 1 1	0

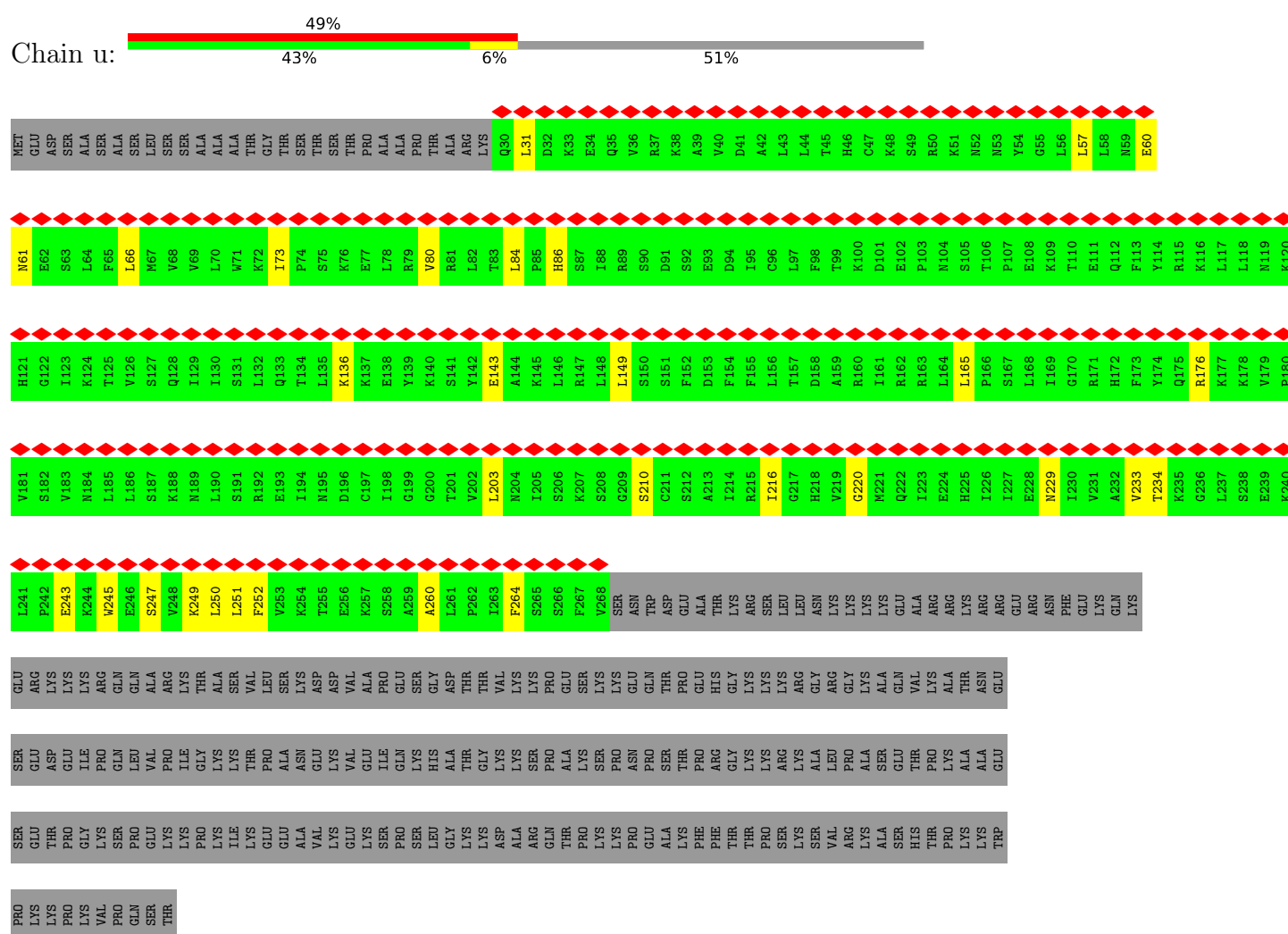
- Molecule 64 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
64	A	1	Total K 1 1	0

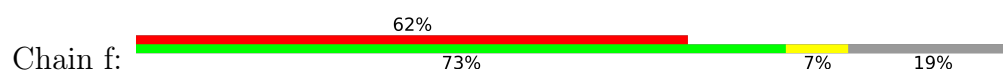
3 Residue-property plots

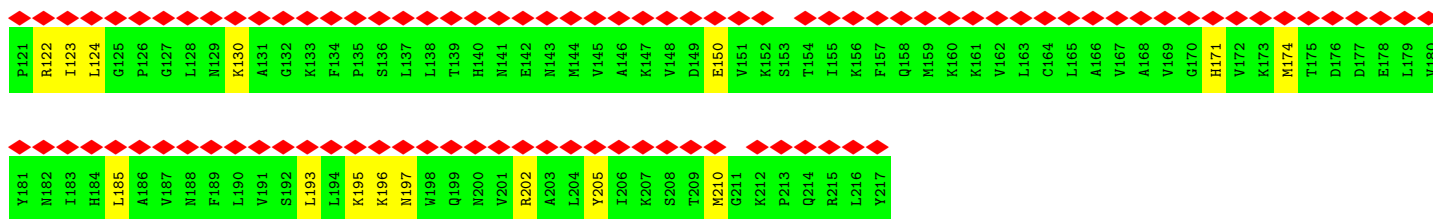
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ribosomal L1 domain-containing protein 1

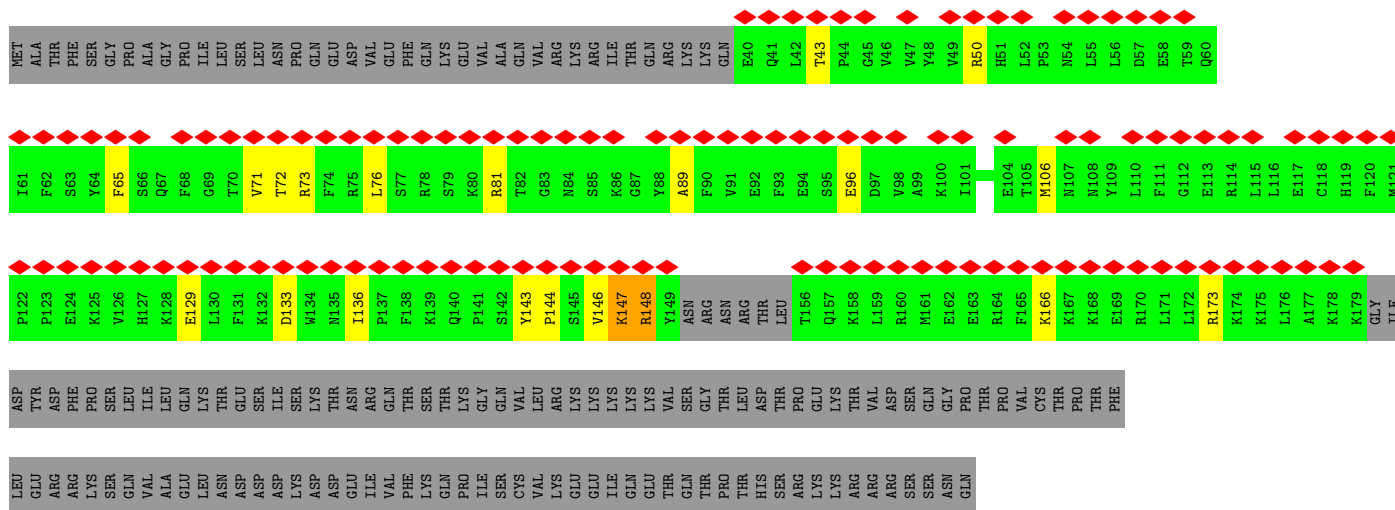
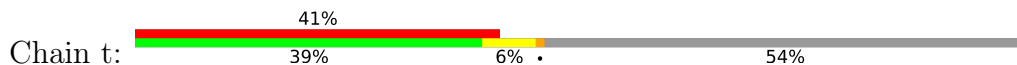


- Molecule 2: Protein SDA1 homolog

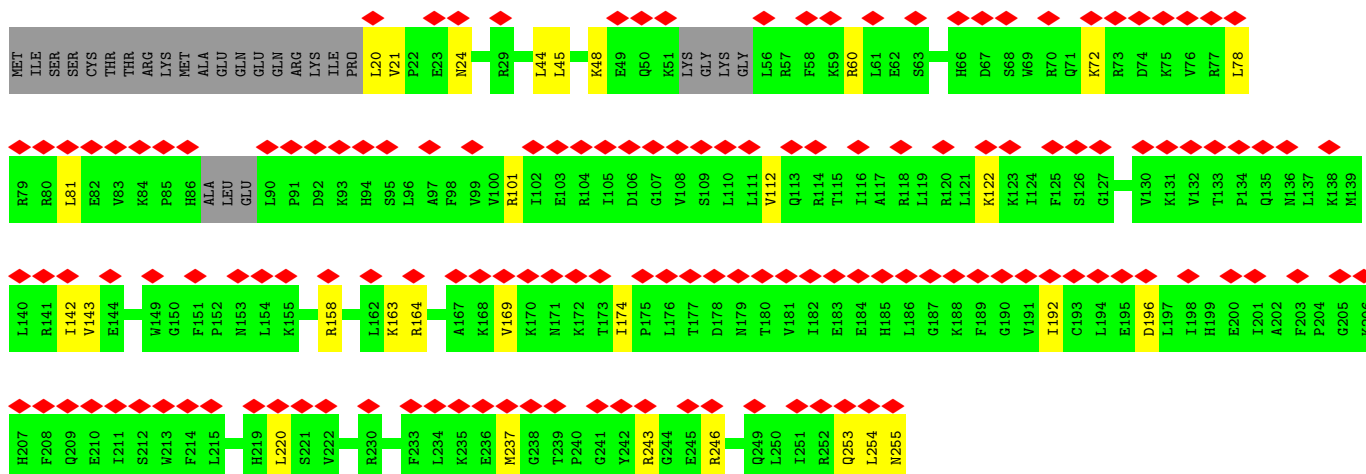
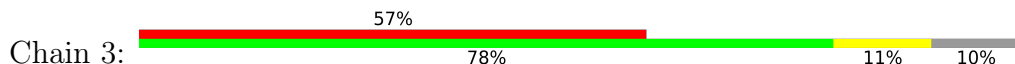




• Molecule 4: MKI67 FHA domain-interacting nucleolar phosphoprotein



• Molecule 5: 60S ribosomal protein L7-like 1

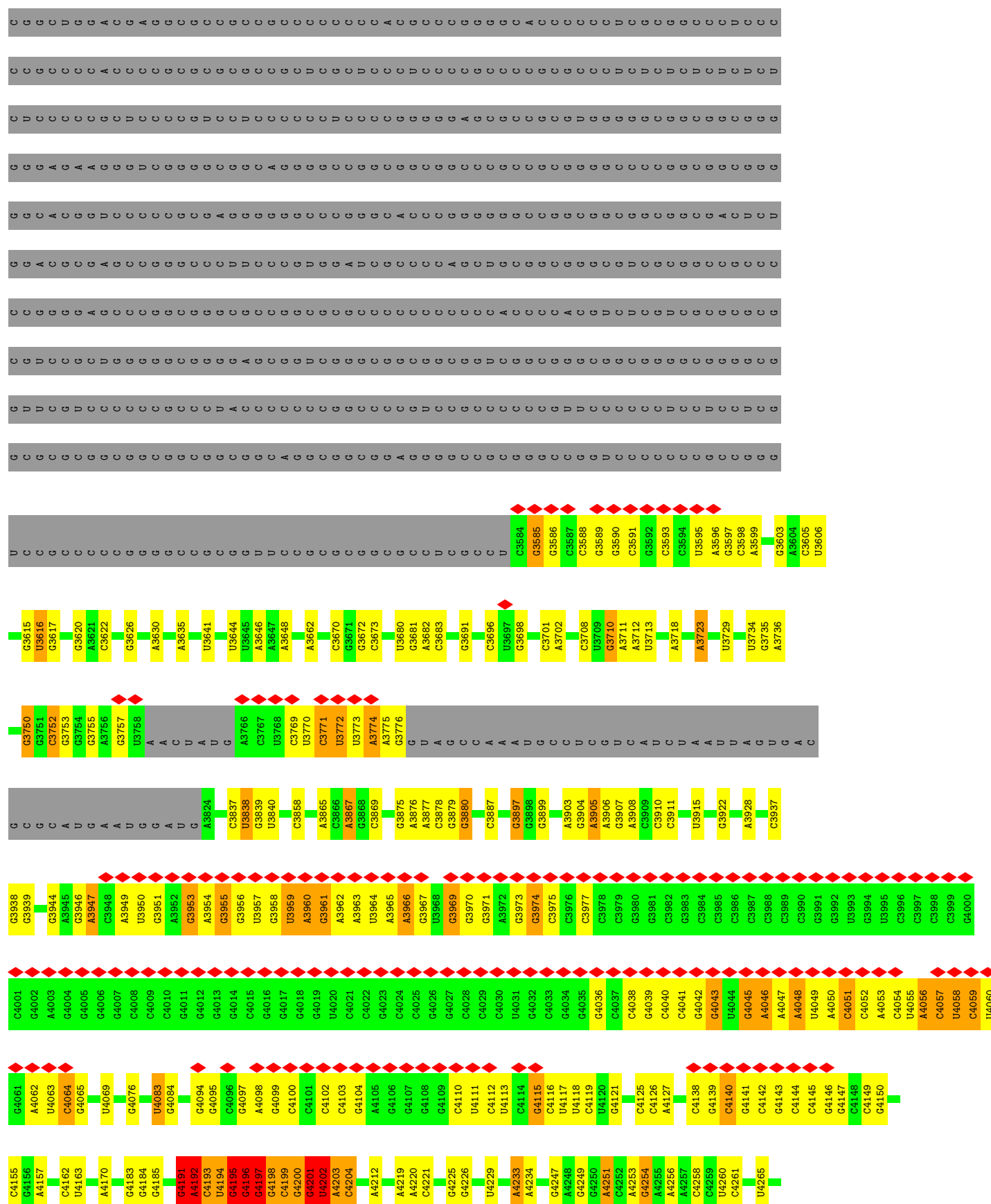


• Molecule 6: 28S rRNA

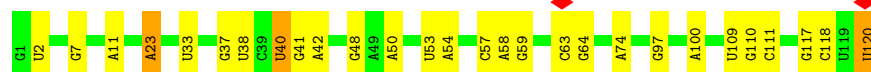








Chain 5:  77% 21%



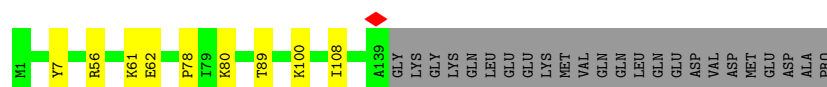
- Molecule 9: Eukaryotic translation initiation factor 6

Chain 6:  90% 9%



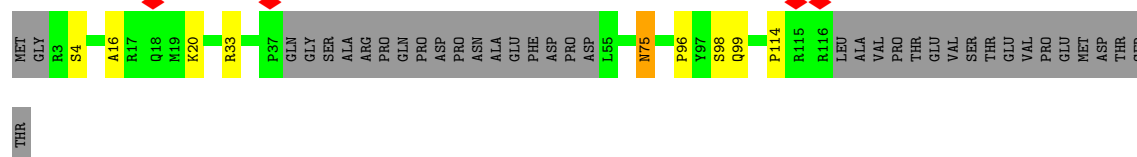
- Molecule 10: Probable ribosome biogenesis protein RLP24

Chain 7:  80% 6% 15%



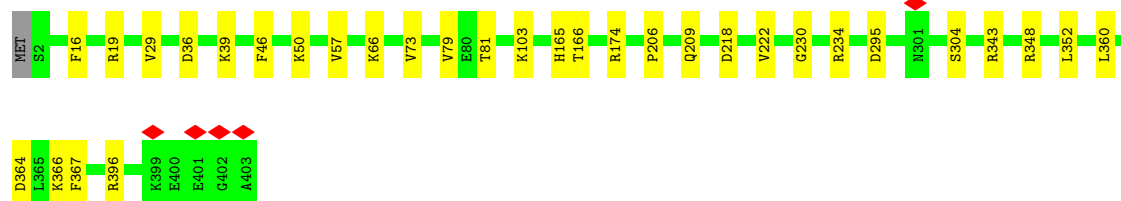
- Molecule 11: Zinc finger protein 593

Chain 9:  66% 6% 28%



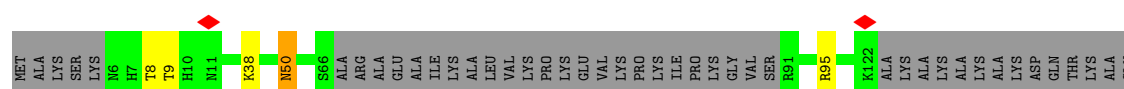
- Molecule 12: 60S ribosomal protein L3

Chain B:  92% 8%

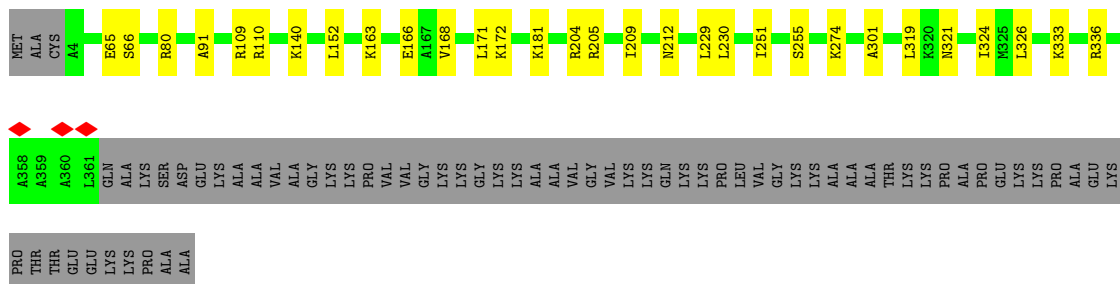
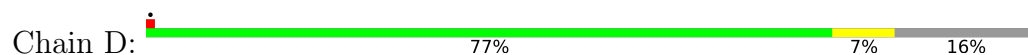


- Molecule 13: 60S ribosomal protein L29

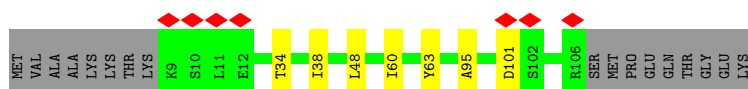
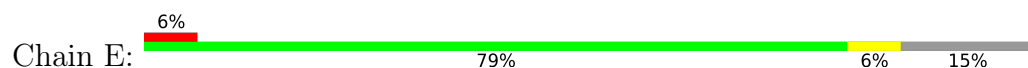
Chain C:  55% 42%



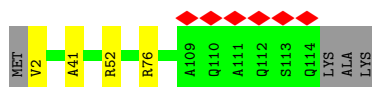
- Molecule 14: 60S ribosomal protein L4



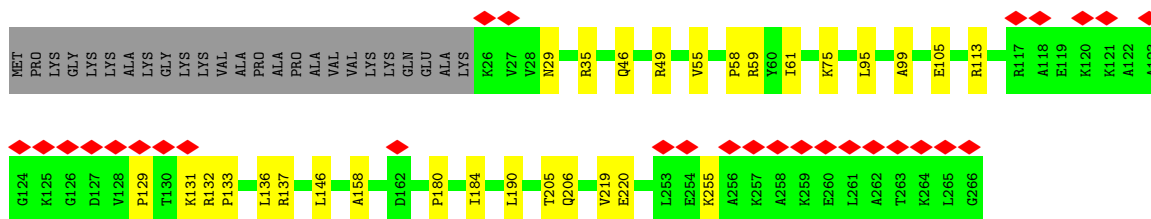
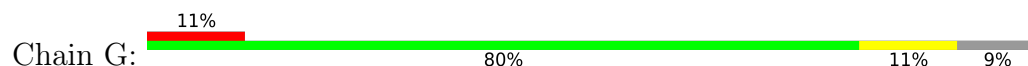
- Molecule 15: 60S ribosomal protein L30



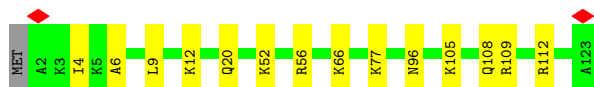
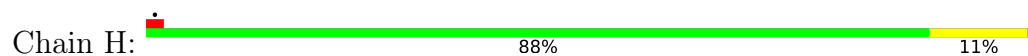
- Molecule 16: 60S ribosomal protein L34



- Molecule 17: 60S ribosomal protein L7a

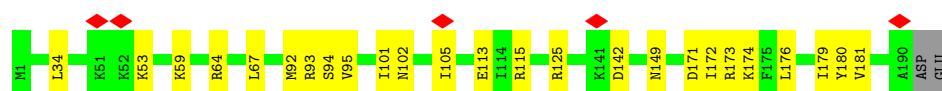


- Molecule 18: 60S ribosomal protein L35

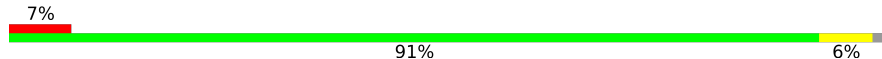


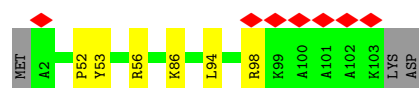
- Molecule 19: 60S ribosomal protein L9

Chain I:  86% 13%

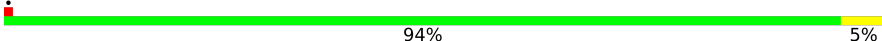


- Molecule 20: 60S ribosomal protein L36

Chain K:  7% 91% 6%



- Molecule 21: 60S ribosomal protein L27a

Chain L:  94% 5%



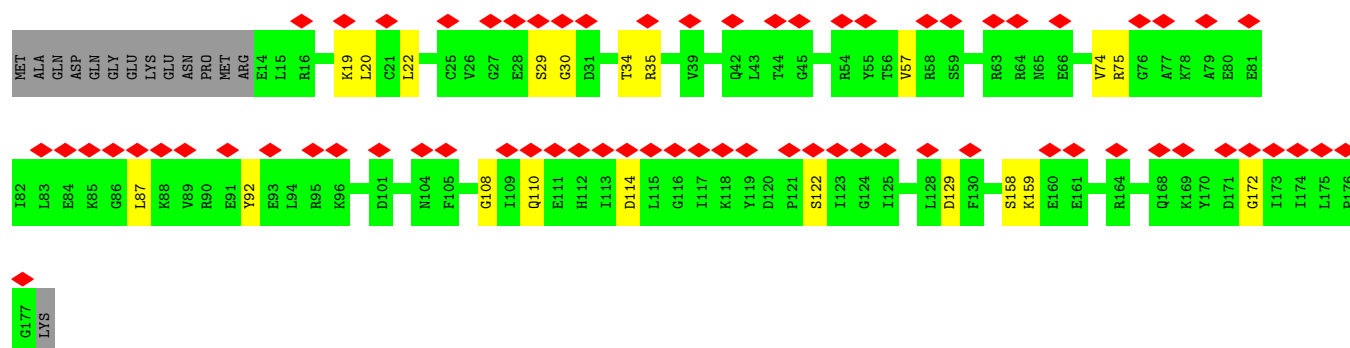
- Molecule 22: 60S ribosomal protein L37

Chain M:  77% 11% 11%

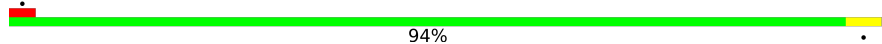


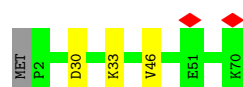
- Molecule 23: 60S ribosomal protein L11

Chain N:  39% 81% 11% 8%



- Molecule 24: 60S ribosomal protein L38

Chain O:  94%

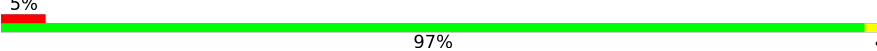


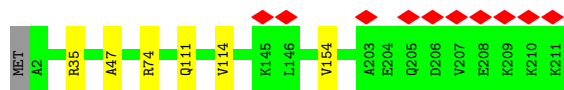
- Molecule 25: 60S ribosomal protein L39

Chain P:  92% 6%



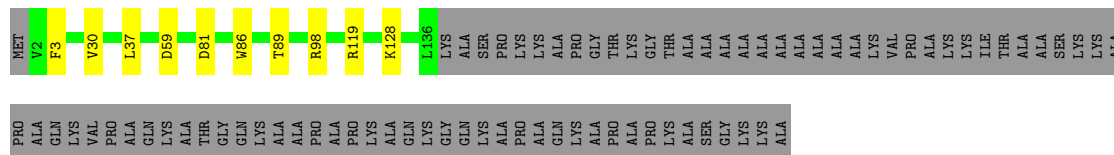
- Molecule 26: 60S ribosomal protein L13

Chain Q:  5% 97%



- Molecule 27: 60S ribosomal protein L14

Chain S:  58% 5% 37%



- Molecule 28: 60S ribosomal protein L15

Chain U:  94% 6%



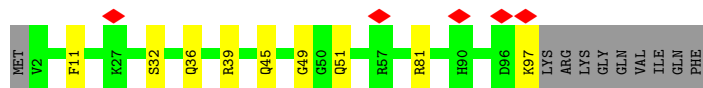
- Molecule 29: 60S ribosomal protein L13a

Chain V:  91% 8%

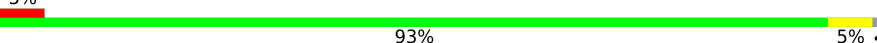


- Molecule 30: 60S ribosomal protein L36a

Chain W:  5% 82% 8% 9%

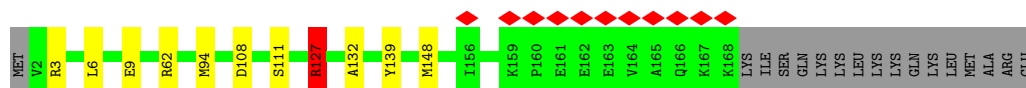
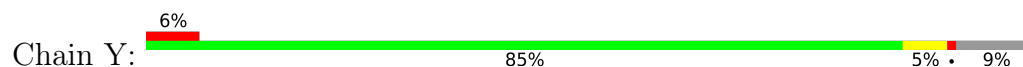


- Molecule 31: 60S ribosomal protein L37a

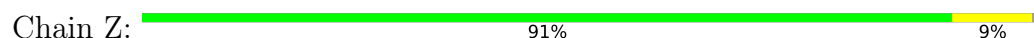
Chain X:  5% 93% 5%



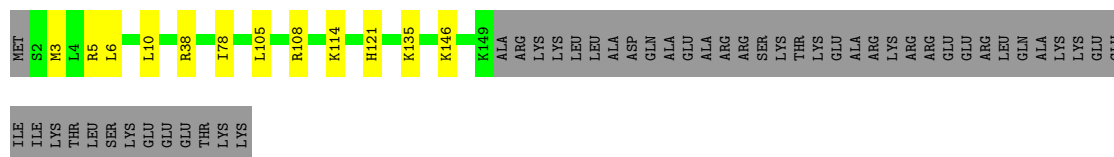
- Molecule 32: 60S ribosomal protein L17



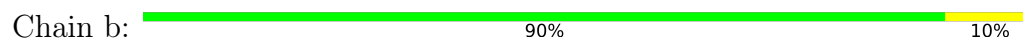
- Molecule 33: 60S ribosomal protein L18



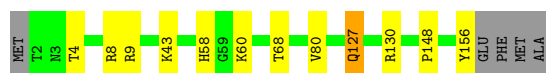
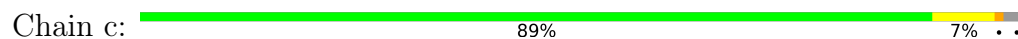
- Molecule 34: 60S ribosomal protein L19



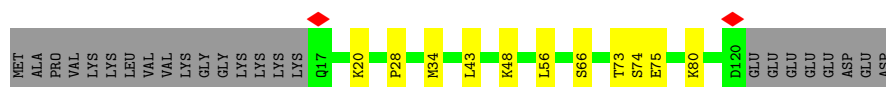
- Molecule 35: 60S ribosomal protein L18a



- Molecule 36: 60S ribosomal protein L21



- Molecule 37: 60S ribosomal protein L22



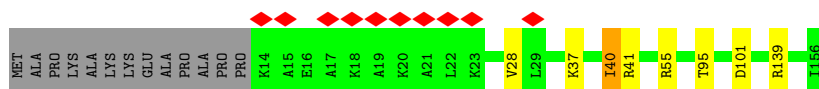
- Molecule 38: 60S ribosomal protein L23

Chain e:  84% 9% • 6%



- Molecule 39: 60S ribosomal protein L23a

Chain g:  6% 87% • • 8%



- Molecule 40: 60S ribosomal protein L26

Chain h:  83% 9% 8%



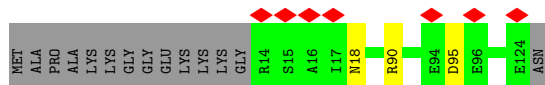
- Molecule 41: 60S ribosomal protein L27

Chain i:  90% 10% •

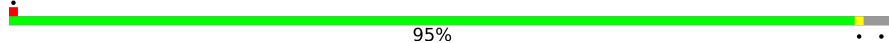


- Molecule 42: 60S ribosomal protein L31

Chain j:  6% 86% • 11%



- Molecule 43: 60S ribosomal protein L32

Chain k:  95% • •

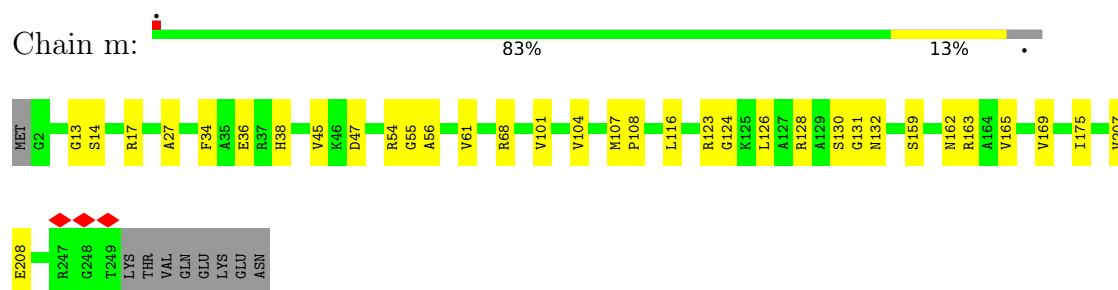


- Molecule 44: 60S ribosomal protein L28

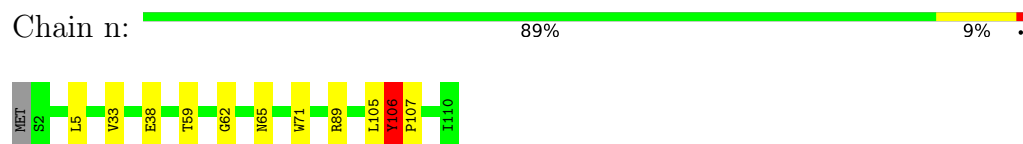
Chain l:  85% 6% 9%



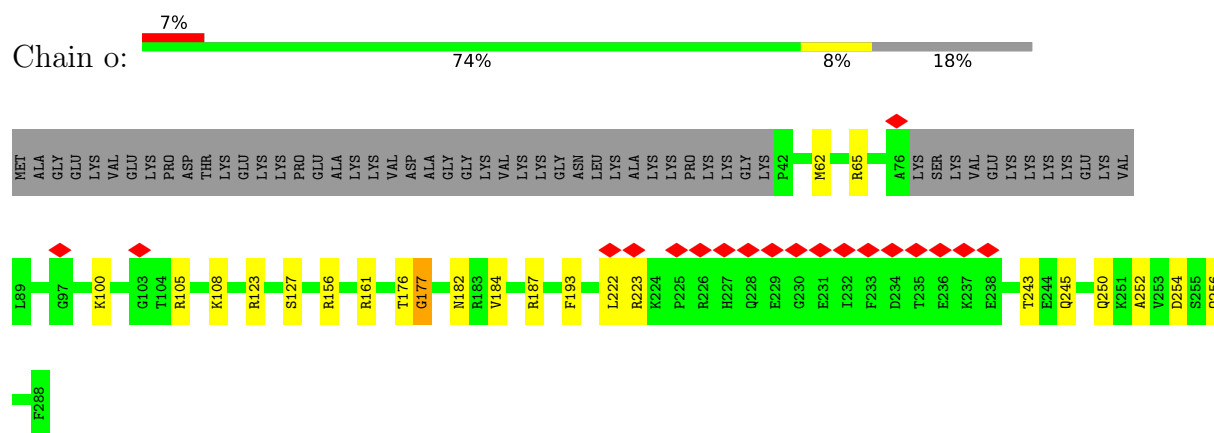
- Molecule 45: 60S ribosomal protein L8



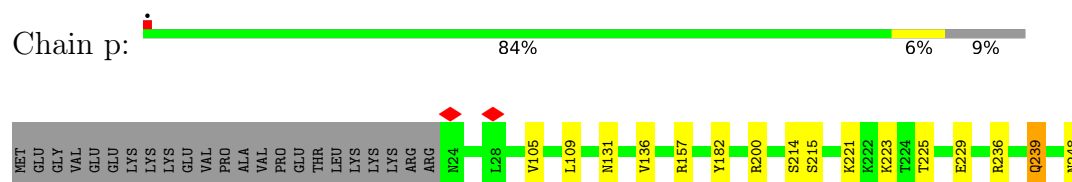
- Molecule 46: 60S ribosomal protein L35a



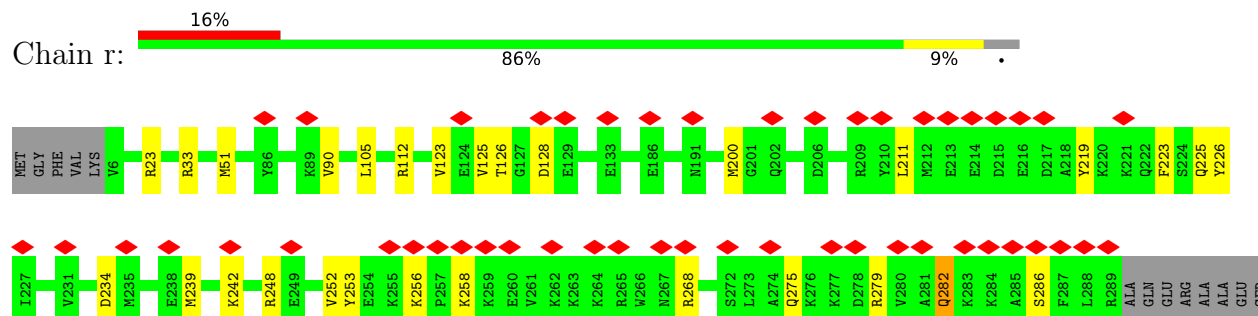
- Molecule 47: 60S ribosomal protein L6



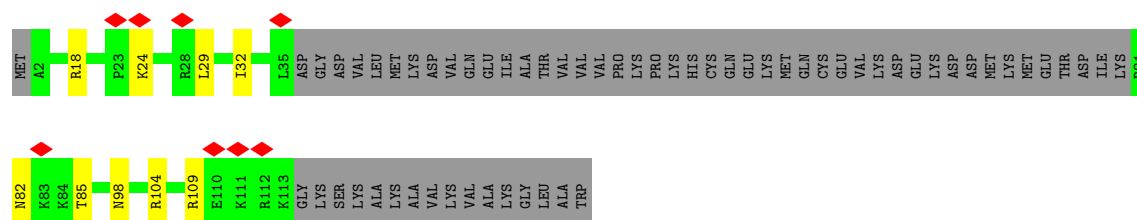
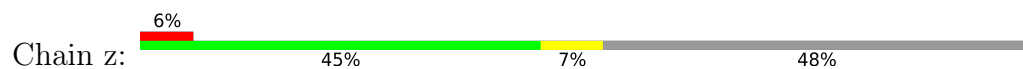
- Molecule 48: 60S ribosomal protein L7



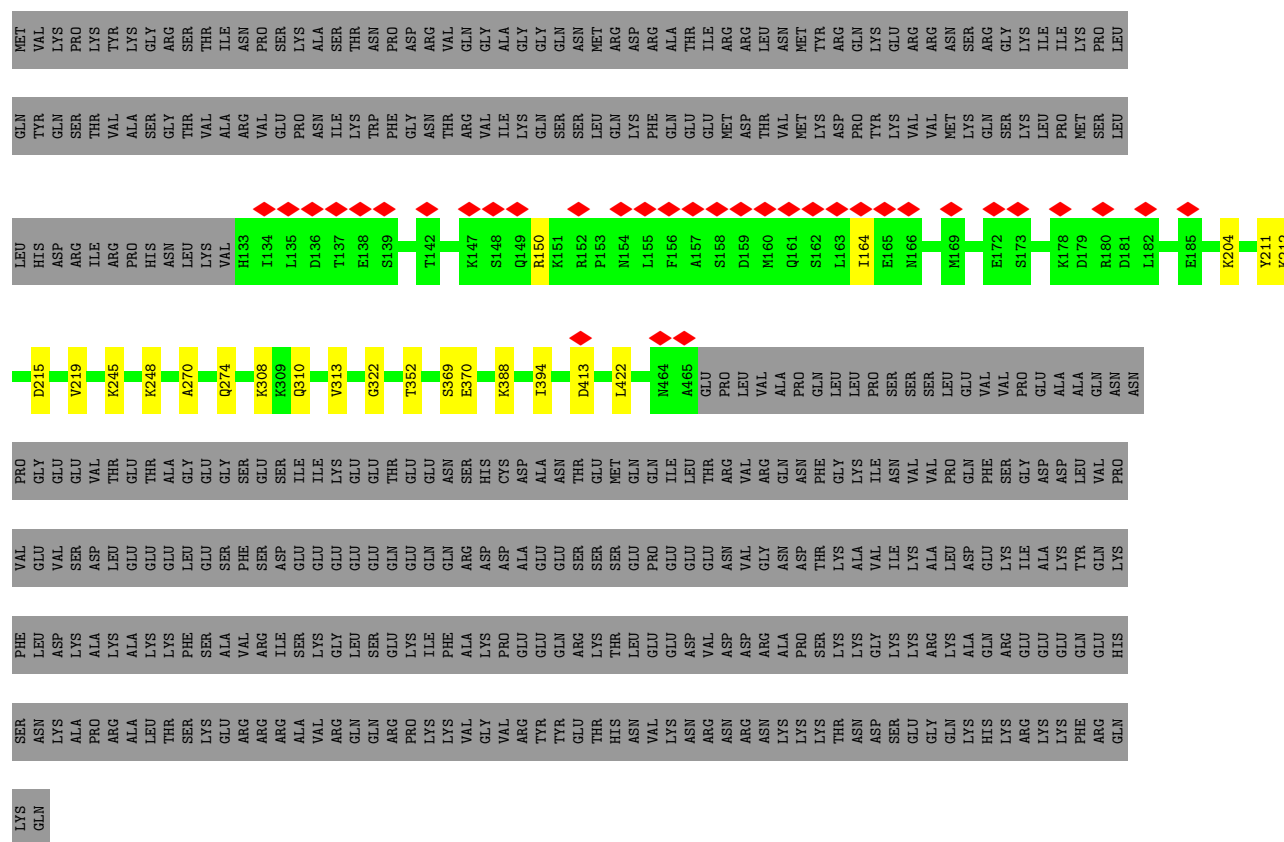
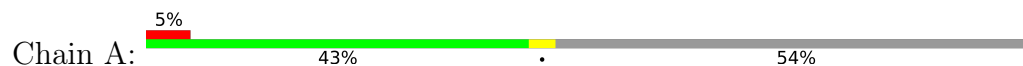
- Molecule 49: 60S ribosomal protein L5



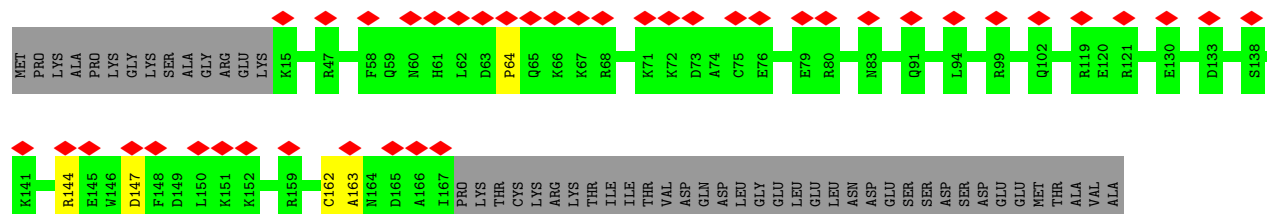
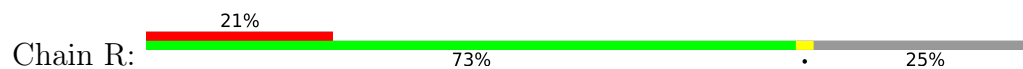
- Molecule 50: Protein LLP homolog



- Molecule 51: G Protein Nucleolar 2



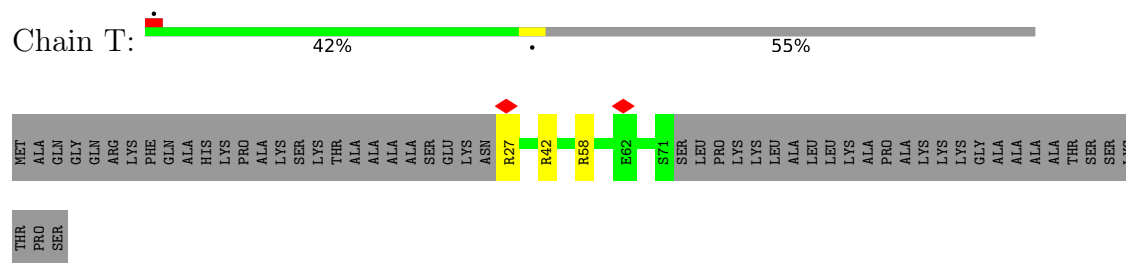
- Molecule 52: Translation machinery-associated protein 16



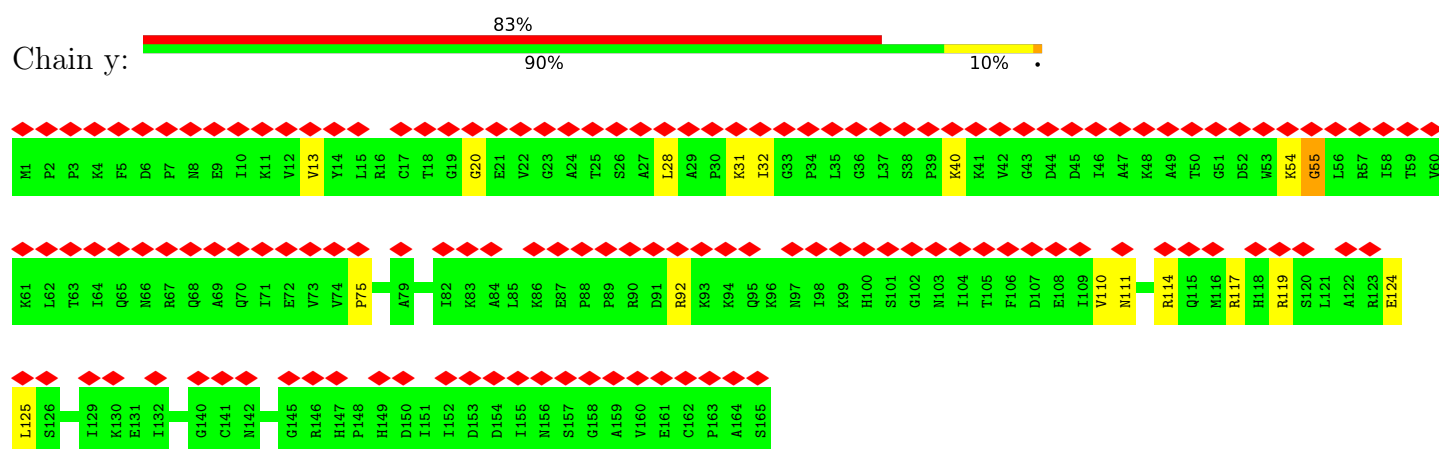
- Molecule 53: mRNA turnover protein 4 homolog



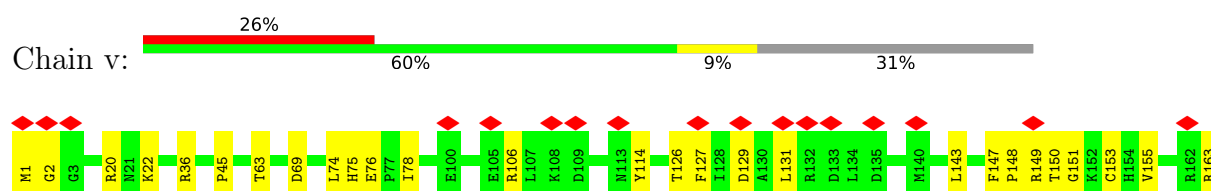
- Molecule 54: Leydig cell tumor 10 kDa protein homolog

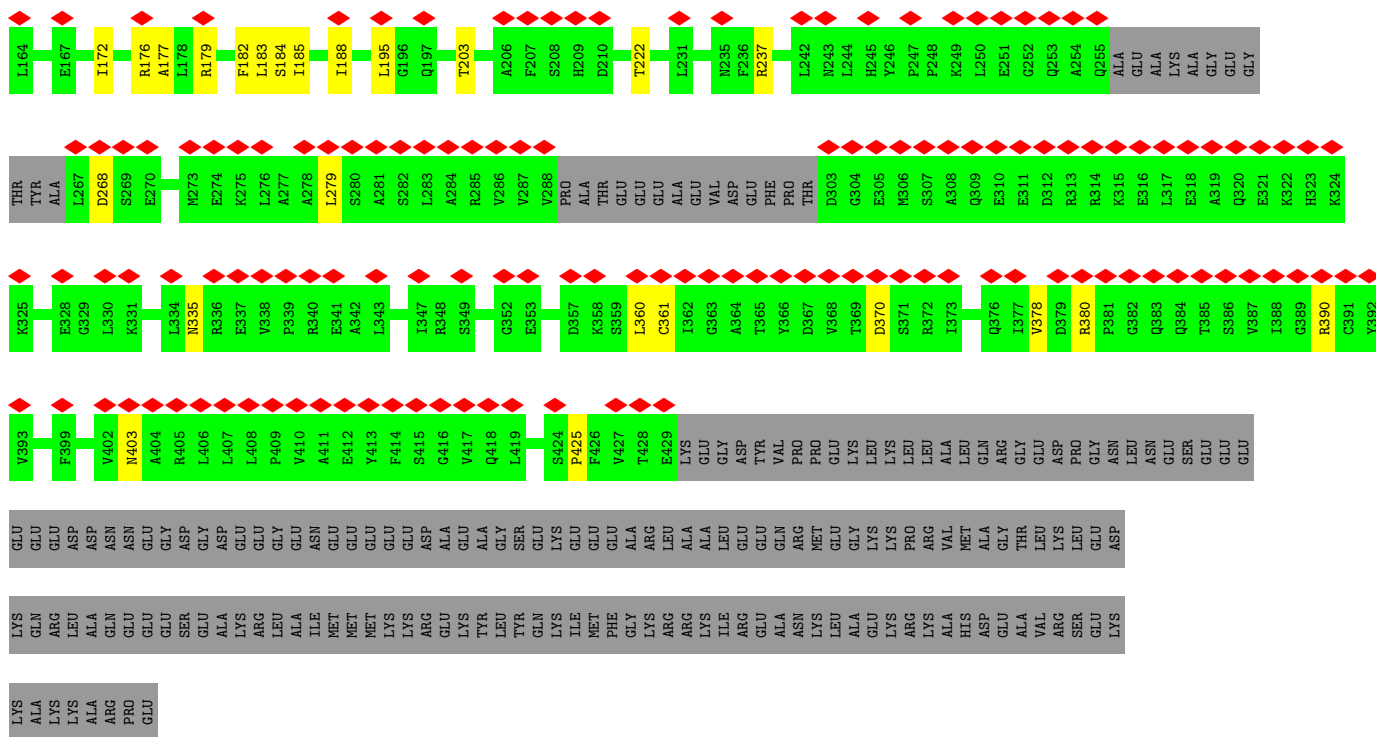


- Molecule 55: 60S ribosomal protein L12

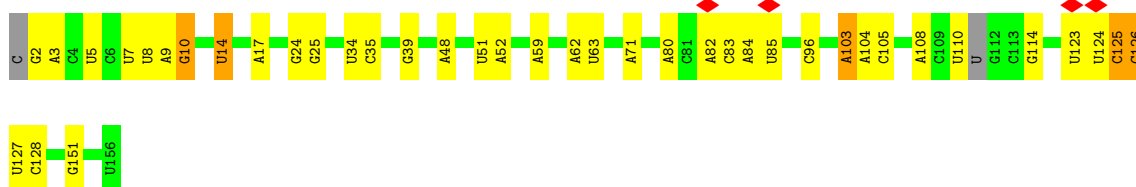


- Molecule 56: Pescadillo homolog

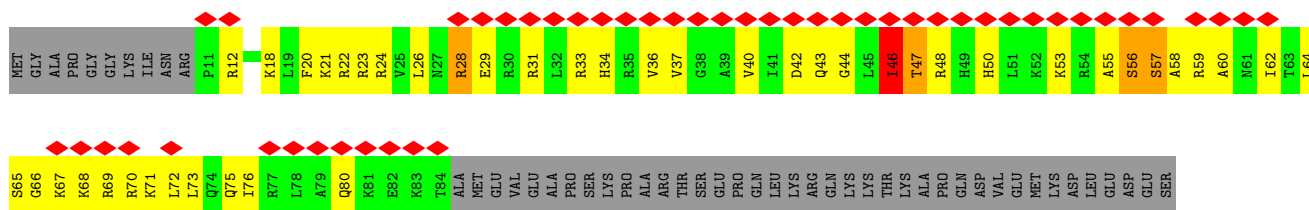
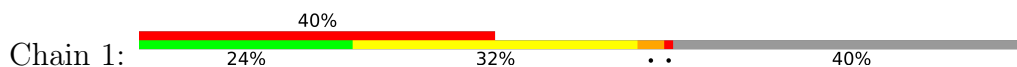




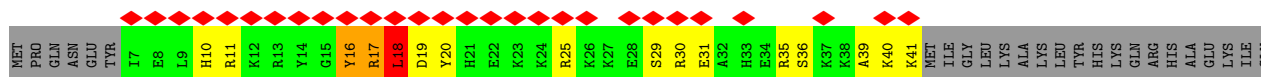
- Molecule 57: 5.8S rRNA



- Molecule 58: Uncharacterized protein C11orf98

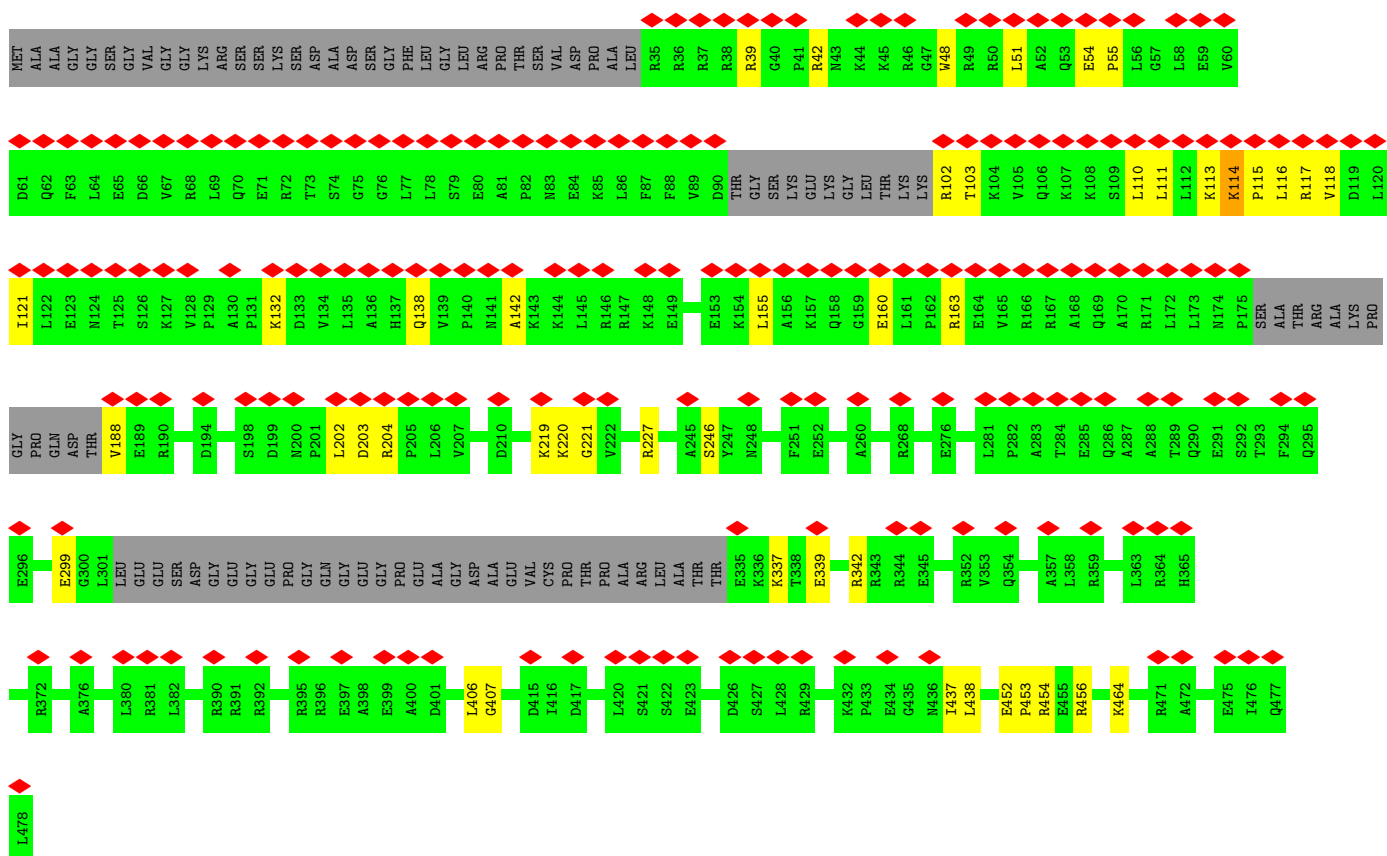
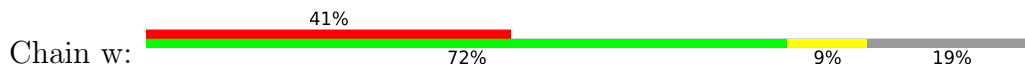


- Molecule 59: Ribosome biogenesis protein NSA2 homolog

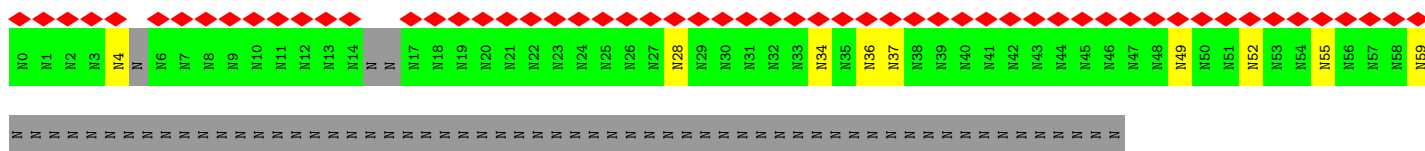
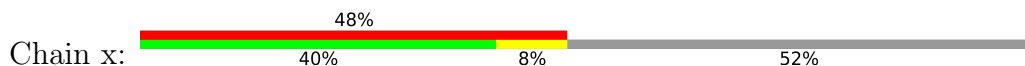


[illegible]

- Molecule 60: Ribosome biogenesis protein NOP53



● Molecule 61: Internal Transcribed Spacer 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45905	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.033	Depositor
Map size ($\text{\AA}$)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.37, 1.37, 1.37	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, P4U, B8H, B8T, 2MG, B9B, B8W, B8K, OMU, 1MA, A2M, E6G, BGH, 7MG, P7G, 6MZ, M7A, OMC, B8Q, B9H, E7G, OMG, 5MU, MHG, UR3, 5MC, MG, GDP, I4U

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	u	0.29	0/1956	0.64	1/2631 (0.0%)
2	f	0.34	2/4614 (0.0%)	0.69	3/6191 (0.0%)
3	q	0.29	0/1736	0.68	1/2328 (0.0%)
4	t	0.29	0/1162	0.74	0/1555
5	3	0.30	0/1928	0.71	0/2584
6	2	0.40	6/84884 (0.0%)	0.55	52/132255 (0.0%)
7	4	0.40	0/5099	0.90	15/6840 (0.2%)
8	5	0.31	0/2858	0.46	0/4455
9	6	0.42	0/1877	0.81	0/2554
10	7	0.41	0/1207	0.81	2/1600 (0.1%)
11	9	0.39	0/802	1.01	6/1069 (0.6%)
12	B	0.43	0/3315	0.80	5/4435 (0.1%)
13	C	0.32	0/777	0.69	0/1026
14	D	0.44	0/2907	0.79	7/3905 (0.2%)
15	E	0.35	0/774	0.74	0/1038
16	F	0.41	0/907	0.75	0/1209
17	G	0.43	0/1971	0.83	4/2651 (0.2%)
18	H	0.40	0/1023	0.65	0/1351
19	I	0.40	0/1537	0.79	1/2066 (0.0%)
20	K	0.35	0/843	0.71	0/1115
21	L	0.39	0/1191	0.70	0/1591
22	M	0.44	0/720	0.74	0/952
23	N	0.31	0/1332	0.78	2/1782 (0.1%)
24	O	0.38	0/575	0.77	0/761
25	P	0.46	0/454	0.68	0/599
26	Q	0.42	0/1732	0.75	1/2315 (0.0%)
27	S	0.42	0/1133	0.73	0/1516
28	U	0.41	0/1746	0.63	0/2338
29	V	0.45	0/1682	0.74	2/2250 (0.1%)
30	W	0.30	0/798	0.67	2/1054 (0.2%)
31	X	0.40	0/718	0.74	1/953 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.43	0/1383	0.80	2/1856 (0.1%)
33	Z	0.42	0/1537	0.69	0/2052
34	a	0.42	0/1255	0.81	3/1662 (0.2%)
35	b	0.41	0/1501	0.62	0/2013
36	c	0.36	0/1291	0.73	1/1725 (0.1%)
37	d	0.41	0/864	0.97	4/1160 (0.3%)
38	e	0.44	0/993	0.79	4/1332 (0.3%)
39	g	0.39	0/1175	0.69	1/1572 (0.1%)
40	h	0.42	0/1132	0.73	0/1504
41	i	0.42	0/1130	0.77	2/1507 (0.1%)
42	j	0.41	0/933	0.74	0/1256
43	k	0.42	0/1082	0.72	0/1443
44	l	0.40	0/1017	0.69	0/1364
45	m	0.43	0/1936	0.82	5/2596 (0.2%)
46	n	0.46	0/895	0.89	7/1198 (0.6%)
47	o	0.38	0/1935	0.80	5/2596 (0.2%)
48	p	0.46	1/1916 (0.1%)	0.77	2/2553 (0.1%)
49	r	0.31	0/2357	0.76	2/3158 (0.1%)
50	z	0.39	0/587	0.80	0/767
51	A	0.33	0/2733	0.62	0/3697
52	R	0.37	0/1317	0.76	0/1757
53	J	0.39	0/1844	0.88	4/2476 (0.2%)
54	T	0.29	0/356	0.75	0/469
55	y	0.30	0/1269	0.74	0/1712
56	v	0.31	0/3395	0.72	1/4578 (0.0%)
57	8	0.46	0/3637	0.59	1/5664 (0.0%)
58	1	0.94	1/626 (0.2%)	1.39	3/825 (0.4%)
59	s	0.30	0/321	0.64	1/418 (0.2%)
60	w	0.26	0/3261	0.64	3/4362 (0.1%)
All	All	0.40	10/177936 (0.0%)	0.65	156/258241 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	f	0	2
6	2	0	2
7	4	0	4
12	B	0	1
26	Q	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	Y	0	1
36	c	0	1
45	m	0	2
46	n	0	1
55	y	0	1
58	1	0	1
60	w	0	1
All	All	0	18

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	668	PHE	CD2-CE2	10.79	1.71	1.38
2	f	668	PHE	CE2-CZ	6.80	1.59	1.38
6	2	4444	C	C1'-N1	6.09	1.57	1.48
48	p	239	GLN	CA-C	-6.03	1.43	1.52
58	1	56	SER	N-CA	-5.74	1.39	1.46
6	2	2488	C	C1'-N1	5.70	1.55	1.47
6	2	4445	U	C1'-N1	5.62	1.55	1.47
6	2	1326	A2M	O3'-P	5.36	1.61	1.56
6	2	2355	G	C2-N2	-5.24	1.24	1.34
6	2	1331	C	N1-C2	5.16	1.50	1.40

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1	56	SER	N-CA-C	-12.29	97.38	111.03
6	2	421	C	C5'-C4'-C3'	11.49	132.44	115.20
6	2	420	A	O3'-P-O5'	10.61	119.92	104.00
6	2	4192	A	P-O3'-C3'	-9.58	105.83	120.20
6	2	4200	G	P-O3'-C3'	-9.37	106.14	120.20
32	Y	127	ARG	CG-CD-NE	9.11	132.03	112.00
6	2	4202	U	P-O3'-C3'	-9.04	106.64	120.20
46	n	62	GLY	CA-C-N	8.94	134.27	120.68
46	n	62	GLY	C-N-CA	8.94	134.27	120.68
6	2	1330	A	N9-C1'-C2'	8.89	125.34	112.00
6	2	1331	C	N3-C2-O2	-8.67	95.89	121.90
7	4	503	THR	CA-C-N	8.09	136.26	121.70
7	4	503	THR	C-N-CA	8.09	136.26	121.70
2	f	668	PHE	CZ-CE2-CD2	-8.03	105.55	120.00
6	2	420	A	OP2-P-O3'	-7.86	84.41	108.00
6	2	4201	G	P-O3'-C3'	-7.65	108.73	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	n	106	TYR	N-CA-C	7.62	126.65	109.81
7	4	406	GLY	CA-C-N	7.57	136.00	121.54
7	4	406	GLY	C-N-CA	7.57	136.00	121.54
6	2	4197	G	P-O3'-C3'	-7.53	108.91	120.20
6	2	4195	G	P-O3'-C3'	-7.51	108.93	120.20
32	Y	132	ALA	N-CA-C	7.44	119.08	110.97
7	4	221	ASP	CA-C-N	7.44	139.71	122.31
7	4	221	ASP	C-N-CA	7.44	139.71	122.31
6	2	4198	G	P-O3'-C3'	-7.43	109.05	120.20
46	n	105	LEU	CA-C-N	7.43	139.93	121.80
46	n	105	LEU	C-N-CA	7.43	139.93	121.80
6	2	4381	A	C2'-C3'-O3'	-7.42	102.57	113.70
10	7	7	TYR	CA-C-N	7.38	135.63	121.54
10	7	7	TYR	C-N-CA	7.38	135.63	121.54
6	2	2328	G	C4-N9-C1'	7.12	147.86	126.50
45	m	124	GLY	N-CA-C	7.12	119.69	111.36
37	d	66	SER	CA-C-N	7.12	135.13	121.54
37	d	66	SER	C-N-CA	7.12	135.13	121.54
48	p	221	LYS	CA-C-N	7.10	135.09	121.54
48	p	221	LYS	C-N-CA	7.10	135.09	121.54
7	4	230	LEU	CA-CB-CG	7.06	141.00	116.30
6	2	4193	C	P-O3'-C3'	-7.05	109.62	120.20
11	9	4	SER	CA-C-N	6.99	134.89	121.54
11	9	4	SER	C-N-CA	6.99	134.89	121.54
41	i	30	ASP	CA-C-N	6.91	133.39	122.61
41	i	30	ASP	C-N-CA	6.91	133.39	122.61
53	J	114	GLU	CA-CB-CG	6.90	127.91	114.10
59	s	16	TYR	N-CA-C	6.90	120.87	109.96
47	o	184	VAL	CB-CA-C	6.89	116.81	110.13
34	a	78	ILE	N-CA-C	-6.82	106.38	111.90
6	2	4196	G	P-O3'-C3'	-6.79	110.01	120.20
60	w	202	LEU	CA-C-N	6.71	134.35	121.54
60	w	202	LEU	C-N-CA	6.71	134.35	121.54
6	2	2327	G	C4'-C3'-O3'	6.64	122.97	113.00
29	V	194	GLU	N-CA-CB	6.58	121.13	110.40
14	D	171	LEU	CA-CB-CG	6.56	139.25	116.30
6	2	1866	UR3	P-O3'-C3'	6.54	127.55	119.70
14	D	230	LEU	N-CA-C	6.51	122.11	114.04
53	J	114	GLU	N-CA-CB	6.49	120.30	110.30
58	1	55	ALA	O-C-N	6.40	128.90	122.12
29	V	110	PRO	N-CA-C	6.37	118.47	110.70
7	4	41	HIS	CA-C-N	6.36	133.69	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	4	41	HIS	C-N-CA	6.36	133.69	121.54
6	2	420	A	P-O3'-C3'	6.35	129.73	120.20
58	1	57	SER	N-CA-C	6.26	118.63	107.80
7	4	391	GLU	CA-C-N	6.25	133.47	121.54
7	4	391	GLU	C-N-CA	6.25	133.47	121.54
47	o	127	SER	CA-C-N	6.25	131.26	122.08
47	o	127	SER	C-N-CA	6.25	131.26	122.08
34	a	38	ARG	CA-C-N	6.18	133.34	121.54
34	a	38	ARG	C-N-CA	6.18	133.34	121.54
36	c	68	THR	OG1-CB-CG2	-6.15	97.00	109.30
6	2	421	C	C1'-C2'-O2'	-6.12	102.62	111.80
14	D	319	LEU	CA-CB-CG	6.07	137.53	116.30
6	2	4194	U	P-O3'-C3'	-6.05	111.12	120.20
12	B	360	LEU	CA-CB-CG	6.05	137.49	116.30
17	G	29	ASN	N-CA-C	-6.03	102.19	109.72
6	2	2470	C	P-O3'-C3'	6.00	129.19	120.20
6	2	420	A	C4'-C3'-O3'	5.96	121.94	113.00
57	8	125	C	P-O3'-C3'	5.95	129.12	120.20
6	2	914	U	P-O3'-C3'	5.94	129.12	120.20
6	2	406	C	C2'-C3'-O3'	5.89	122.53	113.70
6	2	2760	G	P-O3'-C3'	5.86	128.98	120.20
2	f	326	GLY	N-CA-C	5.85	127.05	113.18
6	2	2486	G	P-O3'-C3'	5.84	128.96	120.20
26	Q	47	ALA	N-CA-C	5.82	122.68	109.81
6	2	421	C	N1-C1'-C2'	5.82	122.72	114.00
6	2	3752	C	P-O3'-C3'	5.74	128.81	120.20
6	2	2033	A	P-O3'-C3'	5.69	128.74	120.20
6	2	914	U	C2'-C3'-O3'	5.68	118.03	109.50
6	2	3774	A	P-O3'-C3'	5.67	128.70	120.20
49	r	234	ASP	CA-C-N	5.66	131.43	122.61
49	r	234	ASP	C-N-CA	5.66	131.43	122.61
12	B	304	SER	CA-C-N	5.62	131.38	122.61
12	B	304	SER	C-N-CA	5.62	131.38	122.61
6	2	4199	C	P-O3'-C3'	-5.60	111.80	120.20
7	4	12	VAL	CA-CB-CG1	5.60	119.92	110.40
53	J	238	ASP	CA-C-N	5.60	131.78	121.70
53	J	238	ASP	C-N-CA	5.60	131.78	121.70
17	G	129	PRO	CA-C-N	5.58	130.28	122.08
17	G	129	PRO	C-N-CA	5.58	130.28	122.08
38	e	90	ARG	CA-C-N	5.57	132.18	121.54
38	e	90	ARG	C-N-CA	5.57	132.18	121.54
6	2	420	A	C3'-C2'-O2'	-5.57	102.35	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1331	C	C2-N1-C1'	5.56	135.49	118.80
6	2	1331	C	N1-C2-O2	5.54	135.51	118.90
6	2	1980	U	C2'-C3'-O3'	5.53	117.79	109.50
6	2	4204	C	C2'-C3'-O3'	-5.49	105.47	113.70
17	G	29	ASN	CB-CA-C	5.49	117.26	109.08
6	2	4913	G	P-O3'-C3'	5.47	128.41	120.20
11	9	98	SER	CA-C-N	5.47	131.98	121.54
11	9	98	SER	C-N-CA	5.47	131.98	121.54
6	2	1855	G	P-O3'-C3'	5.45	128.38	120.20
6	2	2356	U	O4'-C1'-N1	5.43	116.65	108.50
14	D	91	ALA	CA-C-N	5.43	131.91	121.54
14	D	91	ALA	C-N-CA	5.43	131.91	121.54
47	o	177	GLY	N-CA-C	-5.43	101.27	112.34
6	2	2327	G	C4-N9-C1'	5.41	142.74	126.50
1	u	165	LEU	CA-CB-CG	5.41	135.24	116.30
23	N	57	VAL	CA-C-N	5.40	131.03	122.61
23	N	57	VAL	C-N-CA	5.40	131.03	122.61
6	2	1980	U	P-O3'-C3'	5.39	128.29	120.20
56	v	279	LEU	CA-CB-CG	5.38	135.15	116.30
6	2	485	C	C2-N1-C1'	5.37	134.90	118.80
6	2	4191	G	C2'-C3'-O3'	5.33	117.50	109.50
37	d	56	LEU	CA-CB-CG	5.33	134.95	116.30
37	d	43	LEU	CA-CB-CG	5.32	134.90	116.30
6	2	1332	C	C2-N1-C1'	5.31	134.74	118.80
6	2	1331	C	N1-C1'-C2'	5.26	119.89	112.00
47	o	62	MET	CB-CG-SD	-5.24	96.99	112.70
6	2	3905	A	P-O3'-C3'	5.23	128.05	120.20
45	m	55	GLY	CA-C-N	5.21	134.52	121.80
45	m	55	GLY	C-N-CA	5.21	134.52	121.80
11	9	114	PRO	CA-C-N	5.21	129.53	122.19
11	9	114	PRO	C-N-CA	5.21	129.53	122.19
60	w	51	LEU	CA-CB-CG	5.20	134.51	116.30
6	2	1332	C	N1-C2-O2	5.19	134.46	118.90
6	2	2014	C	C2'-C3'-O3'	5.18	121.47	113.70
2	f	668	PHE	CB-CG-CD1	-5.17	111.90	120.70
38	e	27	ASN	CA-C-N	5.17	129.71	122.36
38	e	27	ASN	C-N-CA	5.17	129.71	122.36
30	W	32	SER	CA-C-N	5.17	131.42	121.54
30	W	32	SER	C-N-CA	5.17	131.42	121.54
12	B	29	VAL	CA-C-N	5.16	131.40	121.54
12	B	29	VAL	C-N-CA	5.16	131.40	121.54
7	4	430	PRO	CA-C-N	5.16	131.39	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	4	430	PRO	C-N-CA	5.16	131.39	121.54
31	X	88	GLU	N-CA-CB	5.15	117.78	110.16
39	g	40	ILE	CA-CB-CG2	5.14	119.24	110.50
7	4	408	ASP	CA-CB-CG	5.12	117.72	112.60
45	m	13	GLY	CA-C-N	5.10	131.29	121.54
45	m	13	GLY	C-N-CA	5.10	131.29	121.54
46	n	106	TYR	CA-CB-CG	5.09	123.07	113.90
46	n	5	LEU	CA-CB-CG	5.08	134.07	116.30
3	q	197	ASN	CB-CA-C	-5.07	110.33	117.23
6	2	2026	A	O4'-C1'-N9	5.07	116.11	108.50
6	2	2327	G	O3'-P-O5'	5.07	111.61	104.00
14	D	274	LYS	CA-C-N	5.03	131.15	121.54
14	D	274	LYS	C-N-CA	5.03	131.15	121.54
19	I	105	ILE	CA-CB-CG1	5.03	118.95	110.40

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
58	1	44	GLY	Mainchain
6	2	1330	A	Sidechain
6	2	1331	C	Sidechain
7	4	10	THR	Peptide
7	4	294	LYS	Peptide
7	4	365	PRO	Peptide
7	4	503	THR	Peptide
12	B	16	PHE	Peptide
26	Q	154	VAL	Peptide
32	Y	127	ARG	Sidechain
36	c	80	VAL	Peptide
2	f	325	VAL	Peptide
2	f	667	SER	Peptide
45	m	132	ASN	Peptide
45	m	54	ARG	Peptide
46	n	106	TYR	Peptide
60	w	204	ARG	Peptide
55	y	55	GLY	Peptide

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	u	1924	0	2027	24	0
2	f	4536	0	4714	43	0
3	q	1708	0	1815	17	0
4	t	1135	0	1154	26	0
5	3	1892	0	2024	20	0
6	2	77711	0	38933	379	0
7	4	5016	0	5153	37	0
8	5	2558	0	1296	9	0
9	6	1852	0	1828	16	0
10	7	1184	0	1252	6	0
11	9	787	0	796	3	0
12	B	3244	0	3389	18	0
13	C	764	0	822	4	0
14	D	2853	0	3028	17	0
15	E	764	0	804	4	0
16	F	897	0	989	3	0
17	G	1935	0	2087	18	0
18	H	1015	0	1148	10	0
19	I	1518	0	1601	55	0
20	K	832	0	917	5	0
21	L	1162	0	1213	6	0
22	M	705	0	741	7	0
23	N	1310	0	1345	15	0
24	O	569	0	637	2	0
25	P	444	0	483	3	0
26	Q	1701	0	1818	3	0
27	S	1111	0	1174	9	0
28	U	1701	0	1749	10	0
29	V	1650	0	1794	10	0
30	W	785	0	846	5	0
31	X	708	0	760	3	0
32	Y	1355	0	1389	13	0
33	Z	1513	0	1628	10	0
34	a	1239	0	1363	7	0
35	b	1461	0	1502	14	0
36	c	1264	0	1337	8	0
37	d	850	0	868	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	e	979	0	1039	9	0
39	g	1156	0	1268	7	0
40	h	1115	0	1205	11	0
41	i	1107	0	1182	8	0
42	j	918	0	964	2	0
43	k	1064	0	1160	1	0
44	l	1002	0	1068	6	0
45	m	1898	0	1993	18	0
46	n	876	0	912	4	0
47	o	1897	0	2046	14	0
48	p	1878	0	2009	10	0
49	r	2312	0	2339	18	0
50	z	581	0	656	7	0
51	A	2672	0	2695	17	0
52	R	1296	0	1324	3	0
53	J	1809	0	1783	19	0
54	T	354	0	401	3	0
55	y	1250	0	1305	10	0
56	v	3317	0	3368	39	0
57	8	3278	0	1663	34	0
58	1	622	0	700	118	0
59	s	316	0	332	93	0
60	w	3214	0	3361	45	0
61	x	684	0	456	22	0
62	A	28	0	12	1	0
63	A	1	0	0	0	0
64	A	1	0	0	0	0
All	All	169278	0	131665	979	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 3.

All (979) 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)
6:2:4083:5MU:C5	6:2:4083:5MU:C4	1.78	1.61
6:2:1860:B8H:C5	6:2:1860:B8H:C4	1.81	1.54
6:2:4296:B8H:C5	6:2:4296:B8H:C4	1.81	1.54
4:t:173:ARG:NH1	61:x:34:N:H5'	1.27	1.50
57:8:3:A:N6	58:1:20:PHE:HE1	1.15	1.40
4:t:50:ARG:NH2	61:x:55:N:OP2	1.63	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8:2:G:OP1	58:1:31:ARG:HD3	1.19	1.26
57:8:3:A:N6	58:1:20:PHE:CE1	1.93	1.25
4:t:173:ARG:HH12	61:x:34:N:C5'	1.48	1.24
4:t:166:LYS:HE2	61:x:36:N:OP1	1.35	1.23
6:2:1948:G:OP1	59:s:36:SER:OG	1.60	1.17
6:2:1332:C:N4	6:2:2354:G:O6	1.81	1.14
6:2:4697:U:H5'	59:s:29:SER:CB	1.78	1.11
4:t:81:ARG:NH2	61:x:28:N:OP2	1.82	1.10
57:8:2:G:OP1	58:1:31:ARG:CD	2.02	1.08
32:Y:6:LEU:HA	58:1:60:ALA:HA	1.32	1.07
1:u:60:GLU:HG3	60:w:103:THR:HG22	1.38	1.04
56:v:163:ARG:NH2	60:w:188:VAL:O	1.91	1.03
19:I:180:TYR:CD1	59:s:18:LEU:HD12	1.93	1.03
6:2:430:G:OP1	58:1:18:LYS:HD3	1.59	1.01
4:t:50:ARG:HH12	61:x:55:N:H1'	1.22	1.01
4:t:166:LYS:CE	61:x:36:N:OP1	2.09	1.00
19:I:93:ARG:NH2	59:s:18:LEU:HD13	1.74	1.00
6:2:1323:A:H61	6:2:3875:G:H21	1.01	1.00
6:2:406:C:O2	58:1:67:LYS:HE3	1.60	0.99
2:f:651:PHE:HD2	6:2:4199:C:C6	1.80	0.99
6:2:4697:U:H5'	59:s:29:SER:OG	1.62	0.98
6:2:4573:G:H5''	58:1:22:ARG:NH1	1.78	0.96
59:s:17:ARG:HB3	59:s:20:TYR:HB2	1.47	0.96
58:1:46:ILE:HG13	58:1:50:HIS:CE1	2.01	0.95
6:2:407:A:H4'	58:1:67:LYS:H	1.31	0.95
19:I:180:TYR:HD1	59:s:18:LEU:HD12	1.29	0.95
6:2:1948:G:OP1	59:s:36:SER:CB	2.16	0.94
6:2:1323:A:N6	6:2:3875:G:H21	1.65	0.93
60:w:117:ARG:HG2	61:x:52:N:OP2	1.69	0.93
2:f:651:PHE:HD2	6:2:4199:C:C5	1.86	0.92
6:2:4745:G:H1	6:2:4955:A:H61	1.12	0.92
6:2:407:A:H4'	58:1:67:LYS:N	1.85	0.91
57:8:2:G:O6	58:1:23:ARG:NH1	1.98	0.90
1:u:176:ARG:CZ	61:x:49:N:OP2	2.20	0.89
6:2:407:A:O4'	58:1:67:LYS:HB2	1.71	0.89
19:I:95:VAL:CG1	59:s:18:LEU:HD11	2.04	0.88
6:2:2306:G:O6	58:1:71:LYS:HE2	1.75	0.86
6:2:4697:U:O3'	59:s:30:ARG:HG3	1.75	0.86
6:2:4697:U:C5'	59:s:29:SER:CB	2.54	0.86
19:I:93:ARG:CZ	59:s:18:LEU:HD13	2.05	0.85
6:2:4697:U:C5'	59:s:29:SER:HB3	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8:10:G:H1'	58:1:56:SER:HB2	1.57	0.84
6:2:4697:U:H5'	59:s:29:SER:HB3	1.58	0.84
6:2:4415:A:N6	6:2:4427:G:H22	1.76	0.84
2:f:685:ARG:NE	6:2:4192:A:O4'	2.10	0.83
1:u:60:GLU:CG	60:w:103:THR:HG22	2.07	0.83
6:2:407:A:C4'	58:1:67:LYS:HB2	2.09	0.83
6:2:4573:G:H5''	58:1:22:ARG:HH12	1.43	0.82
19:I:93:ARG:HH21	59:s:18:LEU:HD13	1.41	0.82
6:2:4697:U:C5'	59:s:29:SER:OG	2.27	0.82
6:2:1443:A:N6	6:2:2104:G:C6	2.49	0.81
6:2:2306:G:O6	58:1:71:LYS:CE	2.20	0.81
28:U:165:THR:O	28:U:169:ARG:HB2	1.81	0.81
6:2:1323:A:H61	6:2:3875:G:N2	1.78	0.80
57:8:9:A:N3	58:1:56:SER:HA	1.96	0.80
6:2:4697:U:C4'	59:s:29:SER:OG	2.30	0.79
19:I:95:VAL:CG2	59:s:18:LEU:HD11	2.13	0.79
2:f:651:PHE:CD2	6:2:4199:C:C5	2.71	0.79
57:8:10:G:H1'	58:1:56:SER:CB	2.13	0.78
57:8:2:G:P	58:1:31:ARG:HD3	2.23	0.78
57:8:3:A:N6	58:1:20:PHE:CD1	2.51	0.78
6:2:3951:G:H1	6:2:4060:U:H3	1.29	0.77
6:2:263:G:OP1	60:w:163:ARG:NH2	2.18	0.77
6:2:4698:C:C5	59:s:30:ARG:NH1	2.53	0.77
59:s:17:ARG:CB	59:s:20:TYR:HB2	2.13	0.77
6:2:4415:A:H61	6:2:4427:G:H22	1.32	0.77
4:t:166:LYS:HE2	61:x:36:N:P	2.24	0.77
4:t:173:ARG:NH1	61:x:34:N:C5'	2.20	0.77
58:1:28:ARG:HA	58:1:31:ARG:HH21	1.49	0.77
6:2:4720:C:O2	58:1:12:ARG:NH1	2.18	0.77
32:Y:9:GLU:HG3	58:1:37:VAL:O	1.86	0.76
6:2:4291:G:H4'	6:2:4292:A:H5''	1.68	0.76
6:2:4698:C:H41	59:s:30:ARG:NH1	1.81	0.76
6:2:2329:U:P	58:1:68:LYS:HG3	2.25	0.76
6:2:4745:G:H1	6:2:4955:A:N6	1.84	0.76
59:s:18:LEU:C	59:s:20:TYR:H	1.93	0.76
6:2:4155:C:OP2	60:w:464:LYS:NZ	2.16	0.75
6:2:4056:A:H2'	6:2:4057:C:H5''	1.68	0.75
2:f:651:PHE:CD2	6:2:4199:C:C6	2.70	0.73
2:f:681:LYS:HE2	6:2:4192:A:OP2	1.88	0.73
6:2:4415:A:O5'	6:2:4415:A:H8	1.71	0.73
6:2:4698:C:N4	59:s:30:ARG:NH1	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:1948:G:H5'	59:s:40:LYS:HE3	1.70	0.72
58:1:46:ILE:HG21	58:1:50:HIS:ND1	2.05	0.71
6:2:1948:G:H5'	59:s:40:LYS:CE	2.21	0.71
32:Y:9:GLU:HG3	58:1:37:VAL:C	2.16	0.71
19:I:95:VAL:HG13	59:s:18:LEU:HD11	1.73	0.70
58:1:31:ARG:HA	58:1:34:HIS:CE1	2.26	0.70
6:2:4720:C:O2'	58:1:12:ARG:NH2	2.24	0.70
6:2:4697:U:OP1	59:s:25:ARG:NH2	2.21	0.70
6:2:163:A:H5''	60:w:142:ALA:H	1.55	0.70
57:8:3:A:C6	58:1:20:PHE:HE1	2.03	0.70
4:t:148:ARG:HD3	61:x:37:N:H4'	1.72	0.69
4:t:129:GLU:CG	61:x:59:N:H1'2	2.22	0.69
57:8:10:G:O2'	58:1:53:LYS:HD2	1.91	0.69
6:2:4721:G:OP2	58:1:12:ARG:NH2	2.25	0.69
19:I:93:ARG:NE	59:s:18:LEU:HD13	2.07	0.69
19:I:93:ARG:HH21	59:s:18:LEU:CD1	2.06	0.68
2:f:685:ARG:NE	6:2:4192:A:C1'	2.57	0.68
6:2:4698:C:C6	59:s:30:ARG:HD3	2.28	0.68
1:u:176:ARG:NH1	61:x:49:N:OP2	2.26	0.67
6:2:4414:A:H2	6:2:4427:G:C2	2.13	0.67
6:2:273:U:O2	60:w:138:GLN:NE2	2.28	0.67
6:2:3944:G:H1	6:2:4069:U:H3	1.43	0.66
19:I:93:ARG:NH2	59:s:18:LEU:HB3	2.10	0.66
6:2:3955:G:H4'	6:2:4057:C:H2'	1.78	0.66
6:2:4698:C:H41	59:s:30:ARG:HH12	1.41	0.66
57:8:9:A:N3	58:1:56:SER:CA	2.58	0.66
6:2:406:C:O2	58:1:67:LYS:CE	2.42	0.66
6:2:4413:C:H2'	6:2:4414:A:C8	2.31	0.65
46:n:33:VAL:HG23	46:n:38:GLU:HG3	1.79	0.65
19:I:176:LEU:HD22	59:s:17:ARG:HA	1.77	0.65
4:t:129:GLU:HG3	61:x:59:N:H1'2	1.79	0.65
19:I:176:LEU:HD22	59:s:17:ARG:CA	2.26	0.65
6:2:1100:U:C2	6:2:1195:G:O6	2.50	0.65
19:I:93:ARG:HH21	59:s:18:LEU:HD22	1.62	0.64
19:I:180:TYR:CD1	59:s:18:LEU:CD1	2.78	0.64
19:I:93:ARG:NH2	59:s:18:LEU:CD1	2.55	0.64
6:2:4413:C:H2'	6:2:4414:A:H8	1.60	0.64
56:v:63:THR:HG22	60:w:407:GLY:HA2	1.78	0.64
32:Y:9:GLU:CG	58:1:37:VAL:O	2.46	0.63
6:2:4573:G:C5'	58:1:22:ARG:NH1	2.57	0.63
58:1:53:LYS:HE2	58:1:62:ILE:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:1098:G:H1	6:2:1197:C:H42	1.45	0.63
6:2:1971:C:H2'	6:2:1972:G:H8	1.63	0.62
6:2:2486:G:H2'	6:2:2488:C:H41	1.64	0.62
6:2:1948:G:H5'	59:s:40:LYS:NZ	2.14	0.62
6:2:2329:U:OP1	58:1:68:LYS:CB	2.48	0.62
60:w:110:LEU:HA	60:w:113:LYS:HD2	1.80	0.62
6:2:1969:G:H3'	6:2:1970:A:H8	1.65	0.62
6:2:4200:G:HO2'	6:2:4201:G:H8	1.46	0.62
19:I:172:ILE:HD11	59:s:17:ARG:NH2	2.15	0.62
60:w:111:LEU:HD23	60:w:114:LYS:HG2	1.80	0.62
6:2:515:C:H42	6:2:647:G:H1	1.47	0.62
40:h:50:ARG:NH2	57:8:83:C:N3	2.48	0.62
50:z:82:ASN:HB3	50:z:85:THR:HG22	1.82	0.62
19:I:174:LYS:NZ	59:s:10:HIS:CD2	2.68	0.61
20:K:94:LEU:O	20:K:98:ARG:HB2	2.00	0.61
6:2:498:C:H42	6:2:657:C:H42	1.47	0.61
19:I:95:VAL:HG21	59:s:18:LEU:CG	2.30	0.61
11:9:75:ASN:N	11:9:75:ASN:HD22	1.97	0.61
19:I:95:VAL:CG2	59:s:18:LEU:CD1	2.78	0.61
1:u:243:GLU:HB3	1:u:247:SER:HB3	1.82	0.61
6:2:4202:U:H2'	6:2:4203:A:C8	2.35	0.61
19:I:95:VAL:HG22	59:s:18:LEU:HD11	1.82	0.61
19:I:174:LYS:HZ1	59:s:10:HIS:CD2	2.17	0.61
57:8:9:A:H2	58:1:56:SER:C	2.09	0.61
20:K:56:ARG:HD3	60:w:48:TRP:NE1	2.16	0.60
59:s:18:LEU:C	59:s:20:TYR:N	2.58	0.60
12:B:352:LEU:HD13	50:z:18:ARG:HH21	1.66	0.60
6:2:2902:G:N7	6:2:2903:G:N2	2.50	0.60
38:e:90:ARG:HH12	38:e:123:LYS:HB3	1.66	0.60
3:q:122:ARG:HG3	3:q:123:ILE:HG13	1.84	0.60
19:I:95:VAL:HG21	59:s:18:LEU:HG	1.83	0.60
58:1:46:ILE:HG12	58:1:64:LEU:HD11	1.83	0.60
59:s:17:ARG:HD3	59:s:18:LEU:H	1.65	0.60
19:I:93:ARG:NH2	59:s:18:LEU:CB	2.65	0.59
29:V:34:VAL:HG12	29:V:103:LYS:HB2	1.84	0.59
6:2:2327:G:O2'	58:1:48:ARG:CZ	2.51	0.59
2:f:682:LYS:HE2	6:2:4221:C:H42	1.68	0.59
5:3:44:LEU:HD12	60:w:456:ARG:HH12	1.66	0.59
6:2:4573:G:H5''	58:1:22:ARG:CZ	2.32	0.59
6:2:2562:G:N2	6:2:2565:A:OP2	2.36	0.59
6:2:4195:G:H5''	6:2:4195:G:H8	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:6:39:GLU:O	9:6:43:SER:HB2	2.02	0.59
57:8:9:A:C2	58:1:56:SER:C	2.81	0.59
57:8:10:G:C1'	58:1:56:SER:HB2	2.30	0.59
6:2:2489:C:H42	56:v:155:VAL:HG23	1.68	0.59
4:t:173:ARG:HH12	61:x:34:N:H5'	0.77	0.59
2:f:655:ARG:NH2	6:2:4197:G:C6	2.71	0.58
53:J:40:LEU:HB3	53:J:208:TRP:HB3	1.84	0.58
6:2:3961:G:N2	6:2:4048:A:C2	2.71	0.58
56:v:45:PRO:HG2	60:w:406:LEU:HD12	1.85	0.58
19:I:176:LEU:HB2	59:s:17:ARG:HE	1.69	0.58
32:Y:94:MET:HG2	32:Y:148:MET:HE2	1.84	0.58
53:J:74:MET:HB3	53:J:79:ARG:HD2	1.84	0.58
6:2:1971:C:H2'	6:2:1972:G:C8	2.39	0.58
6:2:4573:G:C5'	58:1:22:ARG:HH12	2.14	0.58
58:1:31:ARG:HA	58:1:34:HIS:NE2	2.19	0.58
32:Y:9:GLU:OE2	58:1:37:VAL:O	2.21	0.58
56:v:147:PHE:HZ	60:w:438:LEU:HD11	1.69	0.58
6:2:4698:C:C4	59:s:30:ARG:NH1	2.71	0.58
4:t:129:GLU:HG2	61:x:59:N:H1'2	1.85	0.58
6:2:3937:C:H1'	28:U:125:SER:HB2	1.86	0.58
6:2:5025:C:O2	6:2:5028:G:N2	2.37	0.58
6:2:3960:A:N7	6:2:4043:G:O6	2.37	0.57
60:w:155:LEU:HB3	60:w:160:GLU:HB2	1.84	0.57
8:5:74:A:N3	35:b:53:LYS:NZ	2.52	0.57
58:1:40:VAL:HB	58:1:43:GLN:HB2	1.86	0.57
6:2:1443:A:N6	6:2:2104:G:N1	2.52	0.57
51:A:322:GLY:HA2	62:A:801:GDP:O2A	2.03	0.57
20:K:56:ARG:HD3	60:w:48:TRP:HE1	1.70	0.57
6:2:4740:G:H1'	6:2:4742:G:H5''	1.85	0.57
6:2:3955:G:OP2	6:2:3955:G:H8	1.87	0.57
6:2:1865:G:H21	6:2:1868:A:H62	1.53	0.57
7:4:196:GLN:HG3	7:4:198:TYR:H	1.70	0.57
6:2:407:A:H4'	58:1:67:LYS:HB2	1.83	0.56
19:I:95:VAL:HG22	59:s:18:LEU:CD1	2.35	0.56
57:8:126:C:O2'	57:8:128:C:N4	2.38	0.56
6:2:4698:C:H5	59:s:30:ARG:NH1	2.03	0.56
7:4:405:MET:HE2	7:4:409:TYR:HA	1.85	0.56
57:8:9:A:C2	58:1:56:SER:O	2.58	0.56
6:2:2431:A:OP1	25:P:41:ARG:NH1	2.37	0.56
19:I:174:LYS:HZ2	59:s:10:HIS:HB2	1.70	0.56
47:o:222:LEU:HD12	47:o:223:ARG:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:2329:U:OP2	58:1:68:LYS:HG3	2.05	0.56
6:2:4698:C:H5	59:s:30:ARG:CZ	2.18	0.56
45:m:207:VAL:HG13	45:m:208:GLU:HG3	1.88	0.56
6:2:4198:G:N2	51:A:310:GLN:O	2.39	0.56
57:8:10:G:H1'	58:1:56:SER:OG	2.04	0.56
19:I:113:GLU:HG2	19:I:125:ARG:HG2	1.88	0.56
7:4:230:LEU:O	7:4:233:ARG:NH1	2.39	0.56
58:1:76:ILE:HG22	58:1:80:GLN:CD	2.31	0.56
6:2:1969:G:H3'	6:2:1970:A:C8	2.41	0.56
6:2:3959:U:O2'	6:2:3961:G:N7	2.38	0.56
12:B:206:PRO:HG2	12:B:209:GLN:HG3	1.87	0.56
49:r:123:VAL:HA	49:r:248:ARG:HH12	1.71	0.56
6:2:1333:A:HO2'	57:8:17:A:HO2'	1.54	0.55
33:Z:81:VAL:HG12	33:Z:101:CYS:HB3	1.87	0.55
57:8:9:A:N3	58:1:56:SER:HB2	2.21	0.55
40:h:8:THR:HB	40:h:10:ASP:H	1.70	0.55
6:2:469:C:N3	47:o:105:ARG:NH2	2.55	0.55
19:I:93:ARG:HH21	59:s:18:LEU:CG	2.19	0.55
1:u:66:LEU:HB2	1:u:216:ILE:HD11	1.87	0.55
9:6:126:GLU:OE2	9:6:139:ARG:NH1	2.39	0.55
52:R:64:PRO:HA	52:R:144:ARG:HH22	1.72	0.55
6:2:4618:G:H5''	38:e:15:ARG:HB2	1.88	0.55
6:2:4720:C:O2'	58:1:12:ARG:NH1	2.39	0.55
12:B:66:LYS:NZ	38:e:12:ALA:O	2.39	0.55
19:I:95:VAL:HG11	59:s:18:LEU:HD11	1.85	0.55
6:2:4539:U:H5''	51:A:352:THR:HG23	1.89	0.55
30:W:11:PHE:O	30:W:81:ARG:NH2	2.39	0.55
6:2:3951:G:N2	6:2:4060:U:O2	2.40	0.55
40:h:50:ARG:HH12	57:8:83:C:H42	1.53	0.55
59:s:17:ARG:HD3	59:s:18:LEU:N	2.21	0.55
3:q:171:HIS:H	3:q:174:MET:HE1	1.72	0.55
6:2:3953:G:C2	6:2:3954:A:H1'	2.42	0.55
6:2:4196:G:H8	6:2:4196:G:OP2	1.89	0.55
31:X:38:THR:HA	31:X:45:THR:HA	1.89	0.55
6:2:4195:G:H3'	6:2:4196:G:C8	2.42	0.55
6:2:961:G:N2	6:2:964:A:N6	2.55	0.54
6:2:3960:A:C5	6:2:4043:G:O6	2.61	0.54
2:f:4:ARG:HD3	6:2:3682:A:H3'	1.89	0.54
58:1:36:VAL:HB	58:1:59:ARG:HH22	1.72	0.54
6:2:4698:C:C5	59:s:30:ARG:CD	2.91	0.54
17:G:137[A]:ARG:HD2	17:G:146:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:3910:C:H2'	6:2:3911:C:C6	2.43	0.54
58:1:57:SER:HB3	58:1:60:ALA:HB3	1.90	0.54
58:1:58:ALA:C	58:1:60:ALA:H	2.15	0.54
1:u:143:GLU:OE2	60:w:118:VAL:HG23	2.07	0.54
41:i:54:THR:H	41:i:57:MET:HE3	1.72	0.54
6:2:3949:A:H62	6:2:4064:C:H42	1.55	0.54
1:u:252:PHE:HB3	1:u:260:ALA:HB1	1.90	0.54
8:5:40:U:O2	23:N:75:ARG:NH1	2.40	0.54
60:w:452:GLU:OE2	60:w:454:ARG:NH2	2.41	0.54
60:w:337:LYS:HD2	60:w:342:ARG:HE	1.73	0.54
5:3:163:LYS:HB3	56:v:148:PRO:HB3	1.90	0.53
6:2:2092:G:O2'	6:2:2262:G:N2	2.41	0.53
35:b:77:ASN:ND2	35:b:137:CYS:SG	2.81	0.53
58:1:24:ARG:HG2	58:1:31:ARG:HH22	1.74	0.53
6:2:406:C:H1'	58:1:70:ARG:NH2	2.23	0.53
35:b:29:ARG:HG3	36:c:148:PRO:HB2	1.90	0.53
35:b:88:SER:HB3	54:T:42:ARG:HH12	1.73	0.53
6:2:2329:U:OP1	58:1:68:LYS:HG3	2.08	0.53
19:I:93:ARG:HH21	59:s:18:LEU:CD2	2.22	0.53
50:z:85:THR:OG1	50:z:109:ARG:NH2	2.42	0.53
6:2:4195:G:H5''	6:2:4195:G:C8	2.43	0.53
6:2:3957:U:OP1	6:2:4046:A:N6	2.42	0.53
6:2:219:G:O6	14:D:181:LYS:NZ	2.42	0.53
12:B:57:VAL:HG12	12:B:73:VAL:HG22	1.89	0.53
2:f:465:GLN:NE2	2:f:469:GLU:O	2.41	0.53
19:I:92:MET:HG2	19:I:181:VAL:HA	1.90	0.53
23:N:158:SER:OG	23:N:159:LYS:N	2.42	0.53
58:1:68:LYS:O	58:1:72:LEU:HG	2.08	0.53
5:3:45:LEU:HA	5:3:48:LYS:HE2	1.91	0.53
7:4:428:LYS:NZ	12:B:364:ASP:OD2	2.42	0.53
25:P:21:ARG:NH2	57:8:51:U:OP2	2.42	0.53
35:b:15:ARG:HB3	35:b:27:LEU:HD23	1.91	0.53
6:2:2037:C:O2'	59:s:40:LYS:O	2.20	0.53
6:2:4985:U:O2	12:B:174:ARG:NH1	2.42	0.53
2:f:283:ASN:O	3:q:44:GLN:NE2	2.41	0.52
5:3:196:ASP:OD2	56:v:380:ARG:NH2	2.43	0.52
19:I:34:LEU:HD11	19:I:149:ASN:HB3	1.92	0.52
45:m:36:GLU:OE1	45:m:163:ARG:NH1	2.42	0.52
2:f:640:SER:HB3	2:f:645:LYS:HE3	1.91	0.52
6:2:407:A:C4'	58:1:67:LYS:N	2.65	0.52
6:2:2562:G:O2'	6:2:2565:A:N6	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:5040:U:OP2	12:B:396:ARG:NH2	2.42	0.52
9:6:129:LEU:O	9:6:133:LEU:HB2	2.09	0.52
6:2:3910:C:H2'	6:2:3911:C:H6	1.74	0.52
19:I:171:ASP:OD1	19:I:173:ARG:NH1	2.42	0.52
40:h:34:LEU:HD23	40:h:38:LEU:HB3	1.92	0.52
5:3:60:ARG:NH2	39:g:28:VAL:O	2.41	0.52
6:2:4341:C:N4	6:2:4371:MHG:O6	2.43	0.52
59:s:31:GLU:OE2	59:s:35:ARG:NH2	2.42	0.52
4:t:81:ARG:NH2	61:x:28:N:P	2.82	0.52
6:2:4547:C:O2'	6:2:4548:A:H5'	2.10	0.52
6:2:4606:G:H21	7:4:4:TYR:HE1	1.57	0.52
19:I:180:TYR:CD1	59:s:18:LEU:CB	2.92	0.52
40:h:8:THR:HG21	40:h:13:LYS:HD2	1.90	0.52
45:m:116:LEU:HB3	45:m:126:LEU:HB2	1.90	0.52
53:J:128:GLY:H	53:J:182:LEU:HB2	1.75	0.52
1:u:143:GLU:CD	60:w:118:VAL:HG23	2.35	0.52
2:f:385:LYS:HE3	23:N:34:THR:HA	1.92	0.52
3:q:27:LYS:HB2	6:2:3974:G:H5'	1.92	0.52
12:B:222:VAL:O	12:B:343:ARG:NH1	2.42	0.52
42:j:18:ASN:O	42:j:90:ARG:NH2	2.42	0.52
58:1:68:LYS:HE3	58:1:71:LYS:HB2	1.90	0.52
6:2:2501:C:OP1	45:m:68:ARG:NH1	2.43	0.52
33:Z:67:ILE:HD11	33:Z:95:VAL:HG23	1.90	0.52
58:1:68:LYS:HD2	58:1:71:LYS:HG3	1.91	0.52
7:4:292:ASP:OD1	7:4:292:ASP:N	2.43	0.52
21:L:56:VAL:O	33:Z:172:ARG:NH1	2.43	0.52
58:1:46:ILE:CD1	58:1:47:THR:H	2.23	0.52
6:2:63:G:OP2	28:U:169:ARG:NH2	2.39	0.52
47:o:250:GLN:NE2	47:o:254:ASP:OD2	2.43	0.52
2:f:109:ASN:HB3	6:2:3711:A:H4'	1.93	0.51
3:q:31:THR:OG1	3:q:60:ARG:NH1	2.43	0.51
6:2:1992:U:H5'	6:2:1993:C:H5'	1.91	0.51
6:2:3928:A:OP1	28:U:90:ASN:ND2	2.43	0.51
17:G:180:PRO:HG3	17:G:219:VAL:HG13	1.91	0.51
32:Y:6:LEU:HD21	58:1:59:ARG:HG2	1.92	0.51
47:o:243:THR:HG22	47:o:245:GLN:H	1.74	0.51
55:y:55:GLY:HA2	55:y:92:ARG:HH12	1.75	0.51
2:f:294:GLN:HB3	2:f:330:LEU:HD22	1.91	0.51
3:q:35:GLN:HB2	3:q:205:TYR:HB2	1.91	0.51
34:a:108:ARG:NH1	60:w:339:GLU:OE1	2.42	0.51
53:J:19:GLY:HA2	53:J:22:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:1100:U:O2	6:2:1195:G:C6	2.63	0.51
6:2:4083:5MU:OP1	45:m:123:ARG:NH2	2.44	0.51
6:2:4139:G:H21	6:2:4140:C:H41	1.58	0.51
7:4:226:LEU:O	7:4:233:ARG:NH2	2.44	0.51
6:2:1332:C:N4	6:2:2354:G:C6	2.59	0.51
6:2:1646:A:OP2	14:D:80:ARG:NH1	2.43	0.51
6:2:2329:U:OP1	58:1:68:LYS:HB2	2.10	0.51
6:2:2557:G:H1	6:2:2570:U:H3	1.59	0.51
6:2:3946:G:N3	6:2:3947:A:N6	2.57	0.51
6:2:3969:G:O2'	6:2:4054:C:N4	2.43	0.51
6:2:4199:C:H4'	6:2:4200:G:H5'	1.91	0.51
6:2:4200:G:O2'	6:2:4201:G:H8	1.94	0.51
14:D:301:ALA:HB1	33:Z:132:LYS:HD3	1.93	0.51
36:c:127:GLN:HA	36:c:127:GLN:HE21	1.76	0.51
56:v:184:SER:OG	56:v:185:ILE:N	2.43	0.51
4:t:106:MET:HE1	39:g:28:VAL:HG21	1.93	0.51
6:2:4197:G:H22	51:A:215:ASP:CG	2.18	0.51
6:2:4434:C:H2'	6:2:4435:U:O4'	2.11	0.51
7:4:359:ARG:HD2	9:6:163:PRO:HB3	1.92	0.51
35:b:1:MET:HE3	35:b:35:PRO:HD3	1.91	0.51
41:i:21:ARG:NH1	41:i:47:ASP:O	2.44	0.51
9:6:155:SER:OG	9:6:156:ASN:N	2.43	0.51
18:H:12:LYS:NZ	18:H:20:GLN:OE1	2.44	0.51
6:2:1100:U:O2	6:2:1195:G:O6	2.29	0.51
6:2:2343:G:OP2	14:D:109:ARG:NH2	2.43	0.51
6:2:2469:C:H5	6:2:2471:G:H1	1.58	0.51
6:2:2664:G:OP2	34:a:121:HIS:ND1	2.42	0.51
6:2:3969:G:O6	6:2:4051:C:N4	2.43	0.51
58:1:72:LEU:O	58:1:76:ILE:HG13	2.11	0.51
1:u:80:VAL:HB	1:u:203:LEU:HB3	1.92	0.51
6:2:136:C:H5''	18:H:96:ASN:HD22	1.74	0.51
6:2:194:C:O2	40:h:121:ARG:NH1	2.44	0.51
6:2:4261:C:OP1	23:N:19:LYS:NZ	2.43	0.51
2:f:685:ARG:NE	6:2:4192:A:H1'	2.26	0.51
6:2:4572:U:OP1	58:1:23:ARG:NH2	2.44	0.51
6:2:4720:C:C2'	58:1:12:ARG:HH22	2.24	0.51
19:I:180:TYR:CE1	59:s:18:LEU:HB2	2.46	0.51
6:2:729:2MG:N2	35:b:66:GLN:O	2.40	0.50
6:2:4415:A:O5'	6:2:4415:A:C8	2.60	0.50
19:I:102:ASN:HB3	19:I:115:ARG:HB3	1.92	0.50
2:f:193:TRP:HB3	2:f:198:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:3616:U:OP2	6:2:3617:G:N2	2.44	0.50
6:2:4415:A:H61	6:2:4427:G:N2	2.05	0.50
6:2:2262:G:OP2	44:l:98:ARG:NH2	2.43	0.50
6:2:4939:C:OP1	47:o:187:ARG:NH1	2.45	0.50
49:r:90:VAL:HG21	49:r:225:GLN:HB3	1.93	0.50
14:D:152:LEU:HD23	14:D:251:ILE:HG12	1.93	0.50
27:S:59:ASP:OD1	27:S:59:ASP:N	2.44	0.50
58:1:69:ARG:O	58:1:73:LEU:HG	2.11	0.50
1:u:249:LYS:HG2	1:u:250:LEU:HG	1.94	0.50
5:3:253:GLN:O	56:v:149:ARG:NH1	2.44	0.50
6:2:4280:A:OP2	49:r:23:ARG:NH2	2.45	0.50
9:6:119:PRO:O	9:6:139:ARG:NH2	2.45	0.50
52:R:147:ASP:OD1	52:R:147:ASP:N	2.45	0.50
6:2:1443:A:C6	6:2:2104:G:N1	2.79	0.50
6:2:2391:G:OP2	7:4:504:GLN:NE2	2.45	0.50
6:2:136:C:N4	18:H:77:LYS:O	2.45	0.50
6:2:1703:C:H42	6:2:2096:G:H22	1.59	0.50
6:2:4434:C:OP2	7:4:143:ARG:NH2	2.45	0.50
14:D:204:ARG:NH1	14:D:205:ARG:O	2.44	0.50
19:I:94:SER:HB2	19:I:101:ILE:HD11	1.94	0.50
6:2:4693:C:OP1	19:I:64:ARG:NH1	2.44	0.50
7:4:347:LYS:NZ	9:6:242:ASP:OD1	2.44	0.50
2:f:163:ASN:OD1	2:f:197:LYS:NZ	2.44	0.50
2:f:167:THR:HA	2:f:170:ARG:HG2	1.94	0.50
6:2:387:G:O2'	6:2:412:G:N1	2.43	0.50
6:2:1468:C:OP1	21:L:132:ARG:NH2	2.44	0.50
6:2:3967:G:H4'	6:2:4047:A:H61	1.77	0.50
6:2:4434:C:H2'	6:2:4435:U:C6	2.46	0.50
6:2:5022:U:O2'	6:2:5025:C:N4	2.45	0.50
42:j:95:ASP:OD1	42:j:95:ASP:N	2.45	0.50
51:A:394:ILE:HG13	51:A:422:LEU:HD11	1.94	0.50
6:2:2263:A:OP1	44:l:107:ARG:NH2	2.45	0.49
6:2:4043:G:OP1	6:2:4045:G:N2	2.45	0.49
7:4:258:SER:OG	7:4:259:GLU:N	2.42	0.49
45:m:14:SER:H	45:m:17:ARG:HG3	1.76	0.49
58:1:57:SER:CB	58:1:60:ALA:HB3	2.42	0.49
1:u:61:ASN:HB3	1:u:220:GLY:H	1.77	0.49
6:2:2583:C:OP2	16:F:76:ARG:NH1	2.44	0.49
6:2:2601:A:N6	6:2:2744:A:OP2	2.45	0.49
12:B:218:ASP:OD2	12:B:348:ARG:NH1	2.44	0.49
27:S:3:PHE:H	35:b:175:PHE:HZ	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8:10:G:C2	58:1:57:SER:OG	2.58	0.49
6:2:172:C:O2	18:H:112:ARG:NH2	2.45	0.49
6:2:1173:G:OP1	6:2:1189:G:N2	2.43	0.49
6:2:1256:G:OP2	6:2:1257:A:N6	2.45	0.49
12:B:57:VAL:HG22	12:B:367:PHE:HB3	1.95	0.49
37:d:20:LYS:HG2	37:d:73:THR:HG22	1.94	0.49
55:y:117:ARG:HH22	55:y:124:GLU:HA	1.77	0.49
6:2:2773:OMG:HM22	6:2:2774:C:H5'	1.95	0.49
6:2:4896:G:OP1	27:S:128:LYS:NZ	2.46	0.49
56:v:188:ILE:HB	56:v:203:THR:HB	1.95	0.49
2:f:158:ASN:OD1	2:f:193:TRP:NE1	2.45	0.49
5:3:164:ARG:HH21	5:3:255:ASN:HA	1.77	0.49
6:2:407:A:C5'	58:1:67:LYS:N	2.75	0.49
6:2:2544:G:H8	6:2:2546:G:H5'	1.77	0.49
6:2:2613:C:H4'	16:F:2:VAL:HG23	1.93	0.49
6:2:4191:G:H1'	6:2:4192:A:C5'	2.43	0.49
7:4:293:VAL:HG23	7:4:294:LYS:HG3	1.93	0.49
23:N:92:TYR:HB3	23:N:172:GLY:HA2	1.93	0.49
38:e:83:ARG:NH1	38:e:120:PRO:O	2.44	0.49
51:A:270:ALA:O	51:A:274:GLN:NE2	2.45	0.49
55:y:13:VAL:HG21	55:y:31:LYS:HD3	1.95	0.49
6:2:4697:U:O4'	59:s:29:SER:OG	2.29	0.49
33:Z:39:THR:HG22	33:Z:41:SER:H	1.77	0.49
45:m:159:SER:O	45:m:162:ASN:ND2	2.45	0.49
53:J:137:LEU:HD12	53:J:173:TYR:HB3	1.95	0.49
58:1:71:LYS:O	58:1:75:GLN:HG3	2.12	0.49
56:v:36:ARG:NH2	56:v:114:TYR:OH	2.46	0.49
2:f:429:MET:HE2	2:f:433:ARG:HH21	1.77	0.49
3:q:54:ARG:HE	3:q:150:GLU:HA	1.78	0.49
6:2:1552:G:O2'	6:2:1574:B9B:N2	2.45	0.49
6:2:3620:G:OP1	6:2:3622:C:N4	2.45	0.49
56:v:184:SER:HA	60:w:246:SER:HA	1.94	0.49
2:f:647:LYS:HB3	6:2:4199:C:O2	2.12	0.49
55:y:117:ARG:HH21	55:y:125:LEU:HG	1.78	0.49
6:2:1508:A:OP1	14:D:110:ARG:NH2	2.43	0.49
6:2:3955:G:H4'	6:2:4057:C:C2'	2.43	0.49
6:2:4251:A:H1'	23:N:110:GLN:HG3	1.94	0.49
23:N:20:LEU:HD13	23:N:22:LEU:HD21	1.95	0.49
51:A:245:LYS:HG2	51:A:248:LYS:HE3	1.94	0.49
56:v:172:ILE:HG13	56:v:177:ALA:HB3	1.95	0.49
58:1:56:SER:HG	58:1:57:SER:H	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:1854:G:H1	6:2:1880:G:H21	1.59	0.48
6:2:3681:G:OP2	45:m:128:ARG:NH1	2.46	0.48
6:2:3954:A:C2	6:2:4057:C:H5	2.31	0.48
44:l:19:LYS:HG2	44:l:24:THR:HG22	1.94	0.48
4:t:133:ASP:HB3	4:t:136:ILE:HB	1.95	0.48
6:2:2898:G:OP2	34:a:135:LYS:NZ	2.42	0.48
7:4:442:ILE:HD13	10:7:89:THR:HG21	1.95	0.48
45:m:45:VAL:HG12	45:m:61:VAL:HG22	1.94	0.48
6:2:4408:G:OP1	54:T:58:ARG:NH2	2.46	0.48
6:2:4726:G:OP2	50:z:98:ASN:ND2	2.45	0.48
31:X:90:LYS:HE3	45:m:108:PRO:HD3	1.94	0.48
4:t:129:GLU:HG2	61:x:59:N:C1'	2.43	0.48
6:2:263:G:OP1	60:w:163:ARG:CZ	2.61	0.48
6:2:2621:A:OP1	37:d:80:LYS:NZ	2.45	0.48
6:2:3585:G:H2'	6:2:3586:G:H8	1.77	0.48
7:4:475:GLU:HG2	7:4:476:GLU:HG3	1.95	0.48
15:E:101:ASP:N	15:E:101:ASP:OD1	2.45	0.48
23:N:114:ASP:N	23:N:114:ASP:OD1	2.46	0.48
6:2:430:G:OP1	58:1:18:LYS:CD	2.48	0.48
6:2:4415:A:C6	6:2:4416:G:C5	3.01	0.48
14:D:140:LYS:O	14:D:204:ARG:NH2	2.46	0.48
6:2:423:G:OP1	32:Y:62:ARG:NH1	2.46	0.48
7:4:73:ASP:OD1	7:4:73:ASP:N	2.47	0.48
9:6:150:SER:HA	9:6:194:ALA:HB3	1.96	0.48
48:p:214:SER:OG	48:p:215:SER:N	2.47	0.48
55:y:75:PRO:O	55:y:119:ARG:NH1	2.44	0.48
6:2:4872:2MG:O6	27:S:98:ARG:NH1	2.46	0.48
40:h:34:LEU:HD11	40:h:47:MET:HG2	1.95	0.48
5:3:78:LEU:HD23	5:3:81:LEU:HD13	1.96	0.48
6:2:116:G:O5'	60:w:132:LYS:NZ	2.47	0.48
6:2:406:C:H1'	58:1:70:ARG:HH21	1.78	0.48
8:5:23:A:N3	8:5:118:C:O2'	2.43	0.48
60:w:219:LYS:HE3	60:w:221:GLY:HA3	1.96	0.48
6:2:407:A:H4'	58:1:67:LYS:CB	2.44	0.48
6:2:505:G:H1	6:2:653:U:H3	1.61	0.48
6:2:4097:G:H2'	6:2:4098:A:H8	1.79	0.48
7:4:580:LEU:HB3	7:4:585:MET:HG3	1.95	0.48
28:U:46:ASP:OD1	28:U:46:ASP:N	2.46	0.48
51:A:413:ASP:OD1	51:A:413:ASP:N	2.46	0.48
6:2:1948:G:C5'	59:s:40:LYS:NZ	2.76	0.48
6:2:2364:OMG:N2	6:2:3858:C:O2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:364:ILE:HG22	7:4:366:THR:H	1.78	0.48
18:H:105:LYS:HA	18:H:108:GLN:HG2	1.96	0.48
54:T:27:ARG:O	59:s:39:ALA:HA	2.13	0.48
55:y:111:ASN:HA	55:y:114:ARG:HD2	1.96	0.48
6:2:375:G:OP2	22:M:52:LYS:NZ	2.43	0.47
6:2:382:G:N1	6:2:385:A:OP2	2.46	0.47
6:2:1931:C:N4	6:2:2040:A:O2'	2.46	0.47
6:2:4698:C:C5	59:s:30:ARG:CZ	2.95	0.47
11:9:33:ARG:HG3	11:9:96:PRO:HD3	1.96	0.47
1:u:86:HIS:HB2	1:u:229:ASN:HD21	1.78	0.47
4:t:166:LYS:CD	61:x:36:N:OP1	2.61	0.47
6:2:4910:G:N2	29:V:106:ASP:O	2.47	0.47
27:S:81:ASP:OD1	27:S:81:ASP:N	2.47	0.47
41:i:50:PRO:HD3	41:i:68:ILE:HG12	1.95	0.47
1:u:143:GLU:OE1	60:w:118:VAL:HB	2.14	0.47
7:4:458:GLU:HA	7:4:461:THR:HG22	1.95	0.47
8:5:120:U:O2	49:r:258:LYS:NZ	2.44	0.47
17:G:55:VAL:HG21	39:g:41:ARG:HD2	1.97	0.47
49:r:112:ARG:HH22	49:r:252:VAL:HG22	1.79	0.47
51:A:219:VAL:HB	51:A:313:VAL:HG22	1.96	0.47
6:2:2579:G:N2	6:2:2582:A:OP2	2.41	0.47
56:v:20:ARG:NH1	60:w:454:ARG:HH22	2.12	0.47
29:V:121:PRO:HA	29:V:124:LEU:HD12	1.96	0.47
43:k:84:GLU:OE1	44:l:20:ARG:NH1	2.43	0.47
1:u:149:LEU:HD21	1:u:176:ARG:HG3	1.97	0.47
7:4:170:THR:HG22	7:4:218:GLN:HB2	1.96	0.47
9:6:62:MET:HE2	38:e:139:ILE:HD11	1.97	0.47
51:A:369:SER:OG	51:A:370:GLU:N	2.46	0.47
4:t:65:PHE:HD2	4:t:71:VAL:HG22	1.80	0.47
6:2:407:A:C1'	58:1:67:LYS:HB2	2.45	0.47
6:2:947:C:OP1	14:D:336:ARG:NH1	2.47	0.47
6:2:1179:U:H2'	49:r:286:SER:HA	1.96	0.47
6:2:3907:G:H2'	6:2:3908:A:H8	1.78	0.47
6:2:3960:A:N7	6:2:4043:G:C6	2.83	0.47
15:E:48:LEU:HD21	15:E:60:ILE:HG21	1.95	0.47
45:m:47:ASP:OD2	45:m:47:ASP:N	2.48	0.47
48:p:105:VAL:HG13	48:p:136:VAL:HG12	1.96	0.47
4:t:146:VAL:O	4:t:148:ARG:N	2.47	0.47
6:2:337:U:OP1	26:Q:35:ARG:NH2	2.45	0.47
6:2:3771:C:O2'	6:2:3772:U:O2	2.30	0.47
6:2:4893:A:OP1	29:V:188:LYS:NZ	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:107:ASP:N	7:4:107:ASP:OD1	2.44	0.47
9:6:123:ARG:NH1	9:6:127:GLU:OE2	2.44	0.47
15:E:34:THR:HG23	15:E:95:ALA:HB2	1.97	0.47
34:a:6:LEU:O	34:a:10:LEU:HB2	2.15	0.47
45:m:101:VAL:HG22	45:m:165:VAL:HG22	1.96	0.47
47:o:161:ARG:O	47:o:182:ASN:ND2	2.47	0.47
56:v:176:ARG:O	56:v:179:ARG:NH2	2.48	0.47
5:3:243:ARG:HB3	5:3:246:ARG:HB2	1.96	0.47
6:2:4435:U:H3'	6:2:4436:U:O2	2.15	0.47
7:4:85:ILE:O	51:A:150:ARG:NH1	2.47	0.47
14:D:66:SER:O	14:D:66:SER:OG	2.33	0.47
34:a:114:LYS:O	34:a:146:LYS:NZ	2.42	0.47
40:h:26:ARG:NH1	40:h:75:ARG:O	2.47	0.47
49:r:239:MET:HA	49:r:242:LYS:HD3	1.95	0.47
58:1:46:ILE:HD12	58:1:47:THR:H	1.80	0.47
6:2:4233:A:OP2	30:W:97:LYS:NZ	2.43	0.47
59:s:18:LEU:O	59:s:20:TYR:N	2.48	0.47
6:2:1998:A:H62	53:J:67:PHE:HE2	1.62	0.46
6:2:2631:U:OP1	37:d:48:LYS:NZ	2.46	0.46
6:2:4940:C:OP1	47:o:156:ARG:NH1	2.47	0.46
33:Z:157:GLY:O	33:Z:188:ASN:ND2	2.47	0.46
44:l:7:TRP:O	44:l:11:ARG:HB2	2.14	0.46
6:2:4203:A:H4'	6:2:4203:A:OP1	2.15	0.46
27:S:30:VAL:HG21	35:b:150:ILE:HD13	1.97	0.46
6:2:2572:C:O2'	41:i:112:ARG:NH2	2.48	0.46
6:2:4720:C:O2'	58:1:12:ARG:CZ	2.63	0.46
17:G:137[B]:ARG:HD3	17:G:146:LEU:HD11	1.97	0.46
17:G:220:GLU:OE2	60:w:121:ILE:HG23	2.14	0.46
47:o:252:ALA:O	47:o:256:GLN:NE2	2.45	0.46
53:J:188:ARG:HG3	53:J:192:LEU:HD23	1.97	0.46
57:8:9:A:H2	58:1:56:SER:O	1.97	0.46
6:2:1255:A:H5'	6:2:1257:A:H61	1.79	0.46
7:4:42:ARG:HA	7:4:45:HIS:HB3	1.97	0.46
46:n:71:TRP:HB2	46:n:89:ARG:HE	1.81	0.46
2:f:560:ARG:NH2	3:q:195:LYS:O	2.49	0.46
3:q:120:ILE:HG23	3:q:124:LEU:HB2	1.97	0.46
7:4:264:GLY:O	7:4:268:GLN:NE2	2.48	0.46
22:M:20:ARG:NH1	22:M:39:TYR:OH	2.48	0.46
52:R:162:CYS:SG	52:R:163:ALA:N	2.89	0.46
56:v:403:ASN:HD22	56:v:425:PRO:HG3	1.81	0.46
6:2:407:A:C4'	58:1:67:LYS:CB	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:4304:A:OP2	6:2:4305:G:N2	2.45	0.46
14:D:168:VAL:O	14:D:172:LYS:HB2	2.15	0.46
21:L:85:GLN:HA	21:L:88:VAL:HG12	1.98	0.46
58:1:65:SER:O	58:1:66:GLY:C	2.59	0.46
2:f:623:ASP:N	2:f:623:ASP:OD1	2.49	0.46
6:2:1:C:O5'	39:g:37:LYS:NZ	2.49	0.46
6:2:517:C:N4	6:2:646:G:O5'	2.48	0.46
6:2:1865:G:N2	6:2:1868:A:H62	2.13	0.46
6:2:4620:OMU:OP1	38:e:51:ARG:NH1	2.49	0.46
6:2:4698:C:N4	59:s:30:ARG:HH11	2.14	0.46
29:V:47:PHE:HZ	29:V:144:GLU:HG3	1.80	0.46
30:W:45:GLN:NE2	30:W:51:GLN:OE1	2.49	0.46
41:i:5:MET:O	41:i:28:ASN:ND2	2.47	0.46
49:r:279:ARG:HA	49:r:282:GLN:HG3	1.98	0.46
55:y:28:LEU:O	55:y:32:ILE:N	2.44	0.46
5:3:220:LEU:HB3	5:3:254:LEU:HB3	1.97	0.46
6:2:961:G:N2	6:2:964:A:C6	2.84	0.46
6:2:4043:G:N2	6:2:4045:G:N3	2.64	0.46
6:2:4607:A:O2'	6:2:4608:G:O4'	2.33	0.46
7:4:258:SER:HB2	7:4:294:LYS:HD3	1.97	0.46
19:I:95:VAL:HG21	59:s:18:LEU:CD1	2.45	0.46
45:m:56:ALA:HB2	45:m:130:SER:HB3	1.98	0.46
45:m:131:GLY:H	45:m:169:VAL:HG13	1.81	0.46
2:f:656:TYR:HB3	51:A:212:LYS:HE2	1.97	0.46
6:2:28:C:OP2	28:U:193:ARG:NH2	2.48	0.46
6:2:1816:C:O3'	13:C:38:LYS:NZ	2.46	0.46
6:2:2778:G:OP2	56:v:2:GLY:N	2.49	0.46
7:4:311:GLN:HB3	7:4:317:VAL:HG23	1.98	0.46
12:B:46:PHE:HE2	12:B:81:THR:HB	1.81	0.46
19:I:172:ILE:HD11	59:s:17:ARG:CZ	2.46	0.46
27:S:86:TRP:O	27:S:89:THR:OG1	2.34	0.46
2:f:293:PRO:HD2	3:q:130:LYS:HZ3	1.81	0.46
6:2:4306:OMU:HM23	6:2:4306:OMU:H1'	1.78	0.46
6:2:4698:C:P	59:s:30:ARG:HG3	2.56	0.46
8:5:2:U:H3	8:5:117:G:H1	1.62	0.46
10:7:62:GLU:HG2	10:7:108:ILE:HD11	1.97	0.46
19:I:95:VAL:HG21	59:s:18:LEU:HD11	1.96	0.46
6:2:4698:C:C5	59:s:30:ARG:HD3	2.50	0.45
8:5:59:G:H21	49:r:268:ARG:HD3	1.80	0.45
19:I:92:MET:HE2	19:I:179:ILE:HG22	1.97	0.45
6:2:1646:A:O2'	22:M:49:TRP:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:2327:G:O2'	58:1:48:ARG:NE	2.49	0.45
6:2:4200:G:O2'	6:2:4201:G:O5'	2.34	0.45
7:4:90:ASP:O	7:4:94:LEU:HB2	2.16	0.45
16:F:41:ALA:O	16:F:52:ARG:NH1	2.45	0.45
53:J:20:LEU:HA	53:J:23:LYS:HD2	1.98	0.45
3:q:55:LEU:HD13	3:q:185:LEU:HD23	1.98	0.45
6:2:407:A:H5'	58:1:67:LYS:HA	1.98	0.45
6:2:3961:G:C2	6:2:4048:A:N1	2.84	0.45
6:2:4623:OMG:OP1	12:B:19:ARG:NH2	2.48	0.45
23:N:129:ASP:N	23:N:129:ASP:OD1	2.48	0.45
39:g:55:ARG:HH12	56:v:74:LEU:HD13	1.82	0.45
53:J:53:LEU:HB3	53:J:57:ARG:HH21	1.81	0.45
1:u:245:TRP:HH2	1:u:251:LEU:HD11	1.81	0.45
6:2:4301:U:OP2	6:2:4303:C:N4	2.49	0.45
19:I:172:ILE:HD11	59:s:17:ARG:HH22	1.80	0.45
56:v:182:PHE:HB2	56:v:425:PRO:HD2	1.99	0.45
1:u:31:LEU:HD22	1:u:234:THR:HG21	1.99	0.45
2:f:655:ARG:NH2	6:2:4197:G:C5	2.84	0.45
6:2:4637:OMG:HM23	6:2:4637:OMG:H1'	1.79	0.45
6:2:4293:U:C6	6:2:4294:C:H5	2.34	0.45
14:D:212:ASN:HD22	14:D:255:SER:HB3	1.82	0.45
17:G:35:ARG:HH22	41:i:52:LYS:HG3	1.81	0.45
2:f:668:PHE:HZ	6:2:1866:UR3:H4'	1.46	0.45
5:3:169:VAL:HB	5:3:174:ILE:HD12	1.99	0.45
6:2:1070:G:OP2	47:o:65:ARG:NH2	2.50	0.45
6:2:3907:G:H2'	6:2:3908:A:C8	2.51	0.45
6:2:4094:G:N1	6:2:4115:G:OP1	2.49	0.45
6:2:4253:A:N3	6:2:4254:G:N2	2.65	0.45
32:Y:3:ARG:HH22	58:1:62:ILE:HG23	1.81	0.45
56:v:76:GLU:HB3	56:v:78:ILE:HG22	1.99	0.45
56:v:150:THR:HG23	56:v:153:CYS:H	1.81	0.45
6:2:1480:C:O2'	6:2:1482:G:OP2	2.34	0.45
6:2:1727:U:OP1	48:p:131:ASN:ND2	2.50	0.45
6:2:1945:G:N2	59:s:39:ALA:O	2.47	0.45
6:2:1963:C:N4	53:J:234:ASP:OD1	2.50	0.45
58:1:29:GLU:H	58:1:29:GLU:CD	2.25	0.45
58:1:68:LYS:CE	58:1:71:LYS:HB2	2.47	0.45
6:2:153:G:OP2	28:U:54:LYS:NZ	2.46	0.45
12:B:36:ASP:HB3	12:B:39:LYS:HD2	1.98	0.45
14:D:321:ASN:HB3	14:D:324:ILE:HB	1.99	0.45
33:Z:95:VAL:HG13	33:Z:116:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:p:157:ARG:HE	48:p:248:ASN:HB2	1.82	0.45
58:1:28:ARG:HA	58:1:31:ARG:NH2	2.25	0.45
1:u:73:ILE:HG12	1:u:210:SER:HB3	1.99	0.45
1:u:136:LYS:NZ	61:x:4:N:H2'	2.32	0.45
6:2:1398:A:N1	6:2:1419:G:O2'	2.47	0.45
6:2:1969:G:H4'	53:J:49:ARG:HH12	1.82	0.45
6:2:1994:C:H2'	6:2:1995:G:H8	1.82	0.45
6:2:3953:G:H2'	6:2:3954:A:C8	2.52	0.45
17:G:205:THR:OG1	17:G:206:GLN:N	2.50	0.45
56:v:143:LEU:HD22	60:w:437:ILE:HG22	1.99	0.45
2:f:676:ARG:HH12	6:2:1871:A2M:H5''	1.69	0.44
6:2:145:G:OP1	56:v:106:ARG:NH1	2.50	0.44
6:2:3589:G:N2	6:2:3590:G:O6	2.49	0.44
12:B:57:VAL:HG23	12:B:366:LYS:HB3	1.98	0.44
12:B:230:GLY:O	12:B:234:ARG:HB2	2.17	0.44
23:N:20:LEU:HD12	23:N:74:VAL:HB	1.98	0.44
29:V:51:LYS:HE3	29:V:144:GLU:HB3	1.98	0.44
32:Y:108:ASP:OD1	32:Y:111:SER:OG	2.33	0.44
58:1:22:ARG:O	58:1:26:LEU:HG	2.17	0.44
6:2:1872:G:O2'	6:2:4219:A:N3	2.44	0.44
6:2:2007:G:H21	6:2:2012:A:H62	1.65	0.44
6:2:4198:G:C6	51:A:308:LYS:HD3	2.52	0.44
6:2:4251:A:H5''	23:N:108:GLY:HA3	1.99	0.44
6:2:4913:G:O6	50:z:104:ARG:NH1	2.50	0.44
7:4:302:ASP:N	7:4:302:ASP:OD1	2.48	0.44
13:C:8:THR:OG1	13:C:9:THR:N	2.48	0.44
2:f:98:MET:HE1	2:f:136:THR:HG21	1.99	0.44
2:f:364:LEU:O	2:f:467:TYR:OH	2.35	0.44
4:t:43:THR:OG1	4:t:96:GLU:OE1	2.35	0.44
6:2:4191:G:O2'	6:2:4192:A:P	2.74	0.44
6:2:4419:U:OP1	6:2:4421:C:N4	2.50	0.44
23:N:29:SER:OG	23:N:30:GLY:N	2.49	0.44
6:2:1969:G:OP1	53:J:49:ARG:NH2	2.40	0.44
6:2:3953:G:H2'	6:2:3954:A:H8	1.83	0.44
19:I:93:ARG:HE	59:s:18:LEU:HD13	1.77	0.44
49:r:125:VAL:HG21	49:r:200:MET:HE2	2.00	0.44
5:3:101:ARG:NH1	5:3:122:LYS:O	2.50	0.44
6:2:2329:U:OP1	58:1:68:LYS:CG	2.66	0.44
40:h:67:ILE:HD13	40:h:107:THR:HG21	1.99	0.44
55:y:110:VAL:HG12	55:y:114:ARG:HE	1.81	0.44
60:w:114:LYS:HZ3	60:w:114:LYS:HG3	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:39:LYS:HE3	3:q:202:ARG:HA	1.99	0.44
10:7:100:LYS:HE2	10:7:100:LYS:HB3	1.75	0.44
1:u:143:GLU:OE1	60:w:116:LEU:HB3	2.17	0.44
2:f:618:MET:HA	2:f:621:LYS:HB2	1.98	0.44
6:2:2484:A:OP1	60:w:454:ARG:NH1	2.51	0.44
17:G:46:GLN:OE1	17:G:49:ARG:NH2	2.51	0.44
17:G:58:PRO:HG2	17:G:61:ILE:HD12	1.98	0.44
24:O:30:ASP:OD2	24:O:30:ASP:N	2.49	0.44
53:J:77:LEU:HD11	53:J:89:LEU:HD22	1.99	0.44
58:1:58:ALA:C	58:1:60:ALA:N	2.75	0.44
6:2:684:G:H5'	47:o:100:LYS:HD3	1.99	0.44
7:4:178:ASN:ND2	7:4:197:PRO:O	2.51	0.44
14:D:326:LEU:HD21	14:D:333:LYS:HB2	2.00	0.44
50:z:29:LEU:HD23	50:z:32:ILE:HD11	2.00	0.44
57:8:9:A:N3	58:1:56:SER:CB	2.81	0.44
58:1:40:VAL:HG12	58:1:42:ASP:H	1.82	0.44
5:3:78:LEU:HD21	5:3:142:ILE:HG23	2.00	0.44
6:2:3702:A:H62	6:2:3750:G:H21	1.66	0.44
6:2:4333:C:O2	36:c:8:ARG:NH1	2.51	0.44
19:I:94:SER:OG	19:I:142:ASP:OD1	2.31	0.44
53:J:87:ASP:OD1	53:J:87:ASP:N	2.49	0.44
58:1:53:LYS:CE	58:1:62:ILE:HG13	2.46	0.44
6:2:4448:G:OP1	51:A:204:LYS:NZ	2.42	0.43
11:9:16:ALA:O	11:9:20:LYS:HB2	2.17	0.43
25:P:21:ARG:O	25:P:38:ASN:ND2	2.43	0.43
33:Z:69:LYS:HA	33:Z:69:LYS:HD3	1.84	0.43
36:c:43:LYS:O	36:c:58:HIS:ND1	2.38	0.43
6:2:62:A:N3	6:2:77:U:O2'	2.47	0.43
9:6:109:THR:HB	9:6:149:GLY:HA2	2.00	0.43
19:I:180:TYR:OH	59:s:17:ARG:CZ	2.66	0.43
22:M:21:ARG:NH2	57:8:103:A:OP1	2.45	0.43
26:Q:111:GLN:HA	26:Q:114:VAL:HG12	2.00	0.43
28:U:98:LEU:HA	28:U:101:VAL:HG12	1.99	0.43
2:f:609:ASP:OD1	2:f:609:ASP:N	2.51	0.43
5:3:158:ARG:NH2	56:v:360:LEU:O	2.51	0.43
6:2:1207:C:H2'	6:2:1208:G:H8	1.83	0.43
6:2:3708:C:O2'	6:2:3710:G:OP1	2.36	0.43
6:2:3755:G:H1	6:2:3770:U:H3	1.65	0.43
14:D:65:GLU:OE1	14:D:80:ARG:NH2	2.51	0.43
14:D:163:LYS:HB2	14:D:166:GLU:HG3	2.00	0.43
18:H:66:LYS:HD2	57:8:96:C:H5''	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:M:27:TYR:HA	22:M:34:CYS:HA	2.00	0.43
53:J:124:TYR:HE1	53:J:194:GLY:HA2	1.84	0.43
56:v:183:LEU:HD13	56:v:188:ILE:HD13	1.99	0.43
18:H:6:ALA:HA	18:H:9:LEU:HB2	1.99	0.43
6:2:5047:C:O2'	6:2:5050:C:OP2	2.34	0.43
7:4:303:ASP:HA	7:4:306:ILE:HG12	2.00	0.43
35:b:92:ASN:HD21	36:c:156:TYR:HB3	1.84	0.43
58:1:24:ARG:O	58:1:28:ARG:N	2.51	0.43
6:2:75:G:H3'	26:Q:74:ARG:HD2	2.00	0.43
6:2:407:A:H4'	58:1:67:LYS:CA	2.47	0.43
6:2:500:G:OP2	6:2:503:C:O2'	2.35	0.43
6:2:1735:U:H2'	6:2:1736:A:H8	1.83	0.43
6:2:3641:U:OP2	6:2:3646:A:N6	2.51	0.43
6:2:4195:G:C2	6:2:4200:G:C5	3.06	0.43
7:4:62:LEU:HD22	7:4:99:ILE:HG23	2.00	0.43
7:4:384:ARG:HD2	7:4:386:LYS:HD2	2.00	0.43
23:N:108:GLY:HA2	23:N:129:ASP:HA	2.00	0.43
46:n:106:TYR:HB2	47:o:193:PHE:HD2	1.83	0.43
1:u:136:LYS:HZ3	61:x:4:N:H2'	1.83	0.43
6:2:958:G:O2'	47:o:123:ARG:O	2.37	0.43
6:2:1305:C:H4'	57:8:7:U:C2	2.54	0.43
6:2:4736:C:H2'	6:2:4737:G:H8	1.83	0.43
55:y:20:GLY:HA3	55:y:54:LYS:HD3	2.00	0.43
56:v:335:ASN:HD22	56:v:378:VAL:HG13	1.83	0.43
2:f:314:LYS:HA	2:f:317:LEU:HB2	2.00	0.43
6:2:2394:G:O2'	6:2:2819:U:O4	2.34	0.43
6:2:3757:G:O6	6:2:3769:C:N4	2.52	0.43
6:2:4353:U:H5''	6:2:4354:U:H5'	2.00	0.43
32:Y:9:GLU:CD	58:1:37:VAL:O	2.62	0.43
33:Z:79:THR:HB	33:Z:136:THR:HG22	2.01	0.43
49:r:223:PHE:HB3	49:r:226:TYR:HB2	2.01	0.43
57:8:10:G:O3'	58:1:53:LYS:NZ	2.49	0.43
6:2:4761:G:OP2	29:V:37:ARG:NH2	2.51	0.43
21:L:38:LEU:O	21:L:42:ARG:NH1	2.51	0.43
32:Y:6:LEU:CD2	58:1:59:ARG:HG2	2.49	0.43
34:a:3:MET:SD	34:a:5:ARG:NH1	2.92	0.43
56:v:75:HIS:HB2	60:w:220:LYS:HE2	2.01	0.43
58:1:24:ARG:HG3	58:1:31:ARG:HH12	1.84	0.43
6:2:760:G:H22	6:2:903:C:H2'	1.84	0.43
17:G:99:ALA:HB1	17:G:136:LEU:HD11	2.01	0.43
6:2:2478:C:H5	56:v:22:LYS:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:4448:G:H22	6:2:4502:C:H5	1.67	0.42
7:4:161:LEU:HD12	7:4:162:PRO:HD2	2.01	0.42
9:6:107:VAL:HG22	9:6:118:HIS:HB2	2.00	0.42
37:d:28:PRO:HB2	37:d:34:MET:HG2	2.01	0.42
58:1:72:LEU:HA	58:1:75:GLN:CD	2.44	0.42
59:s:18:LEU:N	59:s:18:LEU:HD23	2.34	0.42
4:t:143:TYR:O	4:t:147:LYS:HG3	2.18	0.42
5:3:112:VAL:HG13	5:3:143:VAL:HG12	2.00	0.42
6:2:2262:G:OP1	44:l:94:ARG:NH1	2.51	0.42
6:2:2362:U:H2'	6:2:2363:A2M:H8	2.01	0.42
6:2:3955:G:N3	6:2:3966:A:N7	2.67	0.42
6:2:4447:C:H5'	51:A:211:TYR:HE2	1.85	0.42
53:J:41:PHE:HB3	53:J:103:LEU:HB3	2.01	0.42
53:J:86:LYS:H	53:J:89:LEU:HD12	1.84	0.42
58:1:46:ILE:CG2	58:1:50:HIS:ND1	2.80	0.42
2:f:210:VAL:HB	2:f:213:ILE:HG12	2.01	0.42
6:2:430:G:OP2	58:1:21:LYS:HB2	2.20	0.42
6:2:4697:U:C4'	59:s:29:SER:CB	2.95	0.42
33:Z:159:PRO:HA	33:Z:160:HIS:HA	1.87	0.42
57:8:14:OMU:HM22	57:8:14:OMU:H1'	1.79	0.42
60:w:114:LYS:HA	60:w:115:PRO:HD2	1.85	0.42
2:f:153:LYS:O	6:2:4058:U:H4'	2.19	0.42
2:f:155:ASN:H	6:2:4058:U:H4'	1.83	0.42
6:2:2364:OMG:HM23	6:2:2364:OMG:H1'	1.79	0.42
6:2:2483:G:O2'	6:2:2485:U:OP2	2.36	0.42
6:2:4140:C:N3	6:2:4145:C:O2'	2.52	0.42
15:E:38:ILE:HG21	15:E:63:TYR:HB3	2.02	0.42
37:d:74:SER:OG	37:d:75:GLU:N	2.51	0.42
57:8:9:A:C2	58:1:56:SER:CA	3.02	0.42
17:G:95:LEU:HD23	17:G:184:ILE:HD12	2.01	0.42
46:n:59:THR:OG1	46:n:65:ASN:OD1	2.38	0.42
58:1:56:SER:OG	58:1:57:SER:N	2.53	0.42
2:f:92:LEU:O	2:f:97:ARG:NH2	2.52	0.42
17:G:255:LYS:HE3	17:G:255:LYS:HB2	1.79	0.42
18:H:52:LYS:HA	18:H:52:LYS:HD3	1.85	0.42
19:I:53:LYS:HA	19:I:53:LYS:HD2	1.83	0.42
27:S:119:ARG:NH1	29:V:193:THR:OG1	2.52	0.42
6:2:4698:C:OP1	59:s:30:ARG:NE	2.53	0.42
13:C:50:ASN:HD22	13:C:50:ASN:HA	1.65	0.42
28:U:85:VAL:HA	30:W:49:GLY:HA2	2.01	0.42
60:w:54:GLU:HA	60:w:55:PRO:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:399:LYS:HB2	2:f:435:LEU:HD12	2.02	0.42
5:3:20:LEU:HB3	5:3:21:VAL:H	1.74	0.42
5:3:237:MET:HE1	5:3:254:LEU:HD21	2.01	0.42
6:2:1950:U:O2'	35:b:116:ARG:NH1	2.53	0.42
19:I:174:LYS:HZ2	59:s:10:HIS:CG	2.38	0.42
19:I:180:TYR:CD1	59:s:18:LEU:HB2	2.55	0.42
41:i:84:ARG:NH1	60:w:299:GLU:O	2.48	0.42
48:p:225:THR:OG1	48:p:229:GLU:OE2	2.37	0.42
56:v:131:LEU:HD11	56:v:195:LEU:HD12	2.02	0.42
58:1:68:LYS:HD2	58:1:68:LYS:HA	1.90	0.42
59:s:11:ARG:HH11	59:s:16:TYR:HD2	1.66	0.42
60:w:113:LYS:O	60:w:114:LYS:C	2.62	0.42
3:q:103:LEU:HB3	3:q:110:PHE:HZ	1.85	0.42
6:2:267:G:OP1	18:H:109:ARG:NH2	2.45	0.42
6:2:2471:G:OP1	17:G:59:ARG:NH2	2.48	0.42
6:2:3961:G:N2	6:2:4048:A:N1	2.67	0.42
9:6:39:GLU:O	9:6:43:SER:CB	2.67	0.42
48:p:109:LEU:HG	48:p:136:VAL:HG11	2.01	0.42
48:p:236:ARG:HB2	48:p:239:GLN:HB2	2.02	0.42
3:q:51:GLY:HA3	3:q:193:LEU:HD11	2.02	0.42
6:2:4697:U:H5''	59:s:29:SER:HB3	1.99	0.42
7:4:206:PHE:HB2	7:4:221:ASP:HB3	2.01	0.42
22:M:17:THR:OG1	22:M:18:LEU:N	2.50	0.42
59:s:41:LYS:HA	59:s:41:LYS:HD2	1.85	0.42
4:t:76:LEU:HD12	4:t:89:ALA:HB2	2.01	0.41
6:2:4040:C:H5'	6:2:4045:G:H1	1.85	0.41
7:4:585:MET:HE2	7:4:585:MET:HB3	1.98	0.41
19:I:59:LYS:HG2	19:I:67:LEU:HD23	2.02	0.41
19:I:174:LYS:HZ1	59:s:10:HIS:HD2	1.63	0.41
22:M:67:LEU:HD23	22:M:67:LEU:HA	1.95	0.41
39:g:101:ASP:OD1	39:g:101:ASP:N	2.48	0.41
1:u:84:LEU:HD21	1:u:233:VAL:HG23	2.01	0.41
6:2:1683:U:OP1	21:L:44:ASN:ND2	2.50	0.41
6:2:2016:C:H5''	6:2:2016:C:H6	1.85	0.41
6:2:2488:C:H5'	56:v:151:GLY:HA3	2.02	0.41
6:2:2529:A:O2'	6:2:2531:C:OP2	2.37	0.41
8:5:117:G:OP1	49:r:253:TYR:OH	2.37	0.41
9:6:85:ARG:O	10:7:80:LYS:NZ	2.46	0.41
18:H:4:ILE:O	18:H:56:ARG:NH1	2.46	0.41
28:U:73:ARG:HG2	28:U:75:VAL:HG13	2.02	0.41
34:a:105:LEU:HD22	34:a:135:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:c:60:LYS:HA	36:c:60:LYS:HD3	1.93	0.41
45:m:34:PHE:O	45:m:38:HIS:HB2	2.20	0.41
59:s:11:ARG:HD3	59:s:16:TYR:CE2	2.56	0.41
5:3:158:ARG:NH2	56:v:361:CYS:SG	2.94	0.41
6:2:1187:G:H8	49:r:275:GLN:HG3	1.85	0.41
6:2:1802:A:N3	36:c:130:ARG:NH2	2.68	0.41
6:2:2439:G:O5'	56:v:1:MET:N	2.50	0.41
6:2:4394:A:H3'	6:2:4395:U:H2'	2.02	0.41
19:I:174:LYS:HZ2	59:s:10:HIS:CB	2.33	0.41
21:L:88:VAL:O	21:L:92:LYS:HB2	2.19	0.41
23:N:35:ARG:HH11	23:N:122:SER:HB2	1.84	0.41
36:c:4:THR:O	36:c:9:ARG:NH1	2.43	0.41
57:8:10:G:H21	58:1:60:ALA:CB	2.33	0.41
59:s:16:TYR:O	59:s:17:ARG:C	2.61	0.41
60:w:452:GLU:HA	60:w:453:PRO:HD3	1.91	0.41
6:2:2754:B9B:OP2	41:i:133:LYS:NZ	2.41	0.41
6:2:4414:A:C2	6:2:4427:G:C2	3.02	0.41
12:B:50:LYS:HA	12:B:79:VAL:HG12	2.02	0.41
17:G:75:LYS:HE3	17:G:75:LYS:HB2	1.96	0.41
38:e:90:ARG:NH1	38:e:124:GLU:OE1	2.51	0.41
50:z:98:ASN:OD1	50:z:98:ASN:N	2.52	0.41
1:u:57:LEU:H	60:w:102:ARG:N	2.19	0.41
2:f:3:ASN:HB3	45:m:175:ILE:HD11	2.02	0.41
5:3:192:ILE:HB	56:v:380:ARG:HH12	1.85	0.41
6:2:961:G:N2	6:2:964:A:H61	2.19	0.41
6:2:1896:A:OP1	48:p:223:LYS:NZ	2.53	0.41
20:K:53:TYR:OH	20:K:86:LYS:NZ	2.53	0.41
23:N:87:LEU:HD23	23:N:87:LEU:HA	1.93	0.41
38:e:82:ILE:HD12	38:e:121:VAL:HG12	2.02	0.41
39:g:95:THR:HG22	39:g:139:ARG:HG3	2.03	0.41
47:o:176:THR:OG1	47:o:177:GLY:O	2.37	0.41
49:r:51:MET:HE1	49:r:105:LEU:HD23	2.03	0.41
59:s:11:ARG:HD3	59:s:16:TYR:HE2	1.85	0.41
6:2:1265:G:OP1	13:C:95:ARG:NH1	2.46	0.41
6:2:2859:G:N2	6:2:3837:C:O2	2.48	0.41
7:4:278:LEU:HA	51:A:164:ILE:HD11	2.02	0.41
8:5:7:G:OP1	49:r:33:ARG:NH1	2.53	0.41
24:O:33:LYS:HG2	24:O:46:VAL:HG22	2.03	0.41
40:h:10:ASP:HB3	40:h:13:LYS:HB2	2.03	0.41
48:p:182:TYR:HB3	48:p:200:ARG:HG3	2.02	0.41
49:r:256:LYS:HE2	49:r:256:LYS:HB3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:251:LEU:HD12	1:u:264:PHE:HB3	2.03	0.41
3:q:70:ASP:HA	3:q:87:ILE:HD11	2.02	0.41
6:2:1717:C:OP2	48:p:200:ARG:NH2	2.54	0.41
35:b:77:ASN:HB3	35:b:98:ARG:HG2	2.02	0.41
58:1:69:ARG:HG2	58:1:73:LEU:HD11	2.02	0.41
2:f:560:ARG:HH22	3:q:196:LYS:HA	1.85	0.41
2:f:681:LYS:CE	6:2:4192:A:OP2	2.65	0.41
3:q:26:ARG:HH12	3:q:210:MET:HB3	1.86	0.41
6:2:407:A:O2'	6:2:410:A:OP1	2.36	0.41
6:2:4721:G:P	58:1:12:ARG:NH2	2.93	0.41
29:V:61:ARG:HG2	29:V:66:PRO:HB3	2.02	0.41
45:m:104:VAL:HA	45:m:107:MET:HE3	2.03	0.41
47:o:108:LYS:HB3	47:o:108:LYS:HE2	1.88	0.41
60:w:39:ARG:HG2	60:w:42:ARG:HH22	1.86	0.41
6:2:425:U:O2	58:1:57:SER:OG	2.38	0.41
6:2:2705:G:H1	6:2:2710:C:H5	1.68	0.41
6:2:4193:C:H2'	6:2:4194:U:C6	2.55	0.41
6:2:4418:G:N2	6:2:4422:A:O3'	2.44	0.41
9:6:85:ARG:HD3	10:7:78:PRO:HG2	2.01	0.41
12:B:165:HIS:ND1	12:B:166:THR:O	2.49	0.41
35:b:30:MET:HE2	35:b:30:MET:HB3	1.92	0.41
35:b:113:MET:HG3	35:b:119:ALA:HB3	2.02	0.41
45:m:27:ALA:O	45:m:128:ARG:NH2	2.54	0.41
56:v:268:ASP:N	56:v:268:ASP:OD1	2.54	0.41
58:1:46:ILE:HG23	58:1:47:THR:N	2.36	0.41
4:t:143:TYR:HA	4:t:144:PRO:HD3	1.89	0.41
6:2:426:A:C2	58:1:56:SER:O	2.74	0.41
6:2:703:G:H2'	6:2:704:C:H4'	2.03	0.41
12:B:103:LYS:HB2	12:B:103:LYS:HE3	1.85	0.41
17:G:158:ALA:HB2	17:G:190:LEU:HD12	2.03	0.41
51:A:388:LYS:HA	51:A:388:LYS:HD2	1.95	0.41
4:t:72:THR:HG22	4:t:73:ARG:HG3	2.03	0.40
6:2:1554:A:OP1	31:X:5:THR:OG1	2.38	0.40
6:2:4058:U:H3'	6:2:4059:C:H4'	2.03	0.40
6:2:4202:U:H5''	6:2:4202:U:H6	1.86	0.40
6:2:4872:2MG:HM21	29:V:202:LEU:H	1.86	0.40
17:G:105:GLU:OE2	17:G:113:ARG:NH2	2.52	0.40
20:K:52:PRO:HB3	60:w:48:TRP:HB2	2.02	0.40
30:W:36:GLN:HB3	30:W:39:ARG:HH21	1.86	0.40
49:r:211:LEU:HG	49:r:219:TYR:HB2	2.02	0.40
56:v:36:ARG:HG2	56:v:222:THR:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:72:LYS:HB3	5:3:72:LYS:HE3	1.90	0.40
6:2:1366:G:O2'	6:2:1367:C:O2	2.34	0.40
6:2:4448:G:H1	6:2:4502:C:H41	1.68	0.40
7:4:264:GLY:HA3	55:y:40:LYS:HE3	2.02	0.40
9:6:20:THR:OG1	9:6:21:ASN:N	2.45	0.40
17:G:131:LYS:HB2	17:G:131:LYS:HE2	1.87	0.40
56:v:370:ASP:O	56:v:390:ARG:NH2	2.50	0.40
60:w:110:LEU:HD23	60:w:113:LYS:HD2	2.03	0.40
6:2:1969:G:O3'	53:J:49:ARG:NH1	2.55	0.40
6:2:2906:G:N2	6:2:3586:G:O6	2.54	0.40
6:2:4573:G:OP1	58:1:22:ARG:NH1	2.54	0.40
19:I:180:TYR:OH	59:s:17:ARG:NE	2.54	0.40
49:r:126:THR:HG22	49:r:128:ASP:H	1.85	0.40
60:w:111:LEU:HA	60:w:114:LYS:HB2	2.03	0.40
6:2:2848:G:O2'	6:2:3838:U:O4	2.37	0.40
19:I:176:LEU:HD22	59:s:17:ARG:N	2.36	0.40
27:S:37:LEU:HD12	27:S:37:LEU:HA	1.94	0.40
32:Y:127:ARG:HD2	32:Y:139:TYR:HD2	1.86	0.40
53:J:42:ILE:HD12	53:J:206:TYR:HB2	2.04	0.40
56:v:127:PHE:O	56:v:237:ARG:NH1	2.55	0.40
6:2:404:U:O3'	40:h:87:ARG:NH2	2.55	0.40
6:2:753:C:H41	6:2:910:G:H1	1.68	0.40
6:2:1437:C:H1'	6:2:2098:G:H8	1.87	0.40
8:5:57:C:H2'	8:5:58:A:H8	1.85	0.40
10:7:56:ARG:HE	10:7:61:LYS:HG3	1.86	0.40
14:D:209:ILE:HB	14:D:229:LEU:HD13	2.02	0.40
17:G:132:ARG:HA	17:G:133:PRO:HD3	1.83	0.40
38:e:69:LYS:HD3	38:e:69:LYS:HA	1.84	0.40
56:v:69:ASP:HB3	60:w:227:ARG:HH22	1.86	0.40
56:v:126:THR:OG1	56:v:129:ASP:OD1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	237/490 (48%)	228 (96%)	9 (4%)	0	100	100
2	f	546/687 (80%)	520 (95%)	24 (4%)	2 (0%)	30	65
3	q	210/217 (97%)	202 (96%)	8 (4%)	0	100	100
4	t	130/293 (44%)	122 (94%)	6 (5%)	2 (2%)	8	35
5	3	223/255 (88%)	209 (94%)	13 (6%)	1 (0%)	30	65
7	4	607/634 (96%)	559 (92%)	44 (7%)	4 (1%)	18	53
9	6	242/245 (99%)	230 (95%)	12 (5%)	0	100	100
10	7	137/163 (84%)	132 (96%)	5 (4%)	0	100	100
11	9	93/134 (69%)	82 (88%)	10 (11%)	1 (1%)	11	43
12	B	401/403 (100%)	376 (94%)	24 (6%)	1 (0%)	43	76
13	C	89/159 (56%)	86 (97%)	3 (3%)	0	100	100
14	D	356/427 (83%)	331 (93%)	25 (7%)	0	100	100
15	E	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
16	F	111/117 (95%)	108 (97%)	3 (3%)	0	100	100
17	G	240/266 (90%)	226 (94%)	14 (6%)	0	100	100
18	H	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
19	I	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
20	K	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
21	L	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
22	M	84/97 (87%)	77 (92%)	6 (7%)	1 (1%)	10	40
23	N	162/178 (91%)	142 (88%)	20 (12%)	0	100	100
24	O	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
25	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
26	Q	208/211 (99%)	190 (91%)	18 (9%)	0	100	100
27	S	133/215 (62%)	126 (95%)	7 (5%)	0	100	100
28	U	201/204 (98%)	188 (94%)	13 (6%)	0	100	100
29	V	199/203 (98%)	191 (96%)	8 (4%)	0	100	100
30	W	94/106 (89%)	89 (95%)	5 (5%)	0	100	100
31	X	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
32	Y	165/184 (90%)	155 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Z	185/188 (98%)	174 (94%)	11 (6%)	0	100	100
34	a	146/196 (74%)	141 (97%)	5 (3%)	0	100	100
35	b	174/176 (99%)	164 (94%)	10 (6%)	0	100	100
36	c	153/160 (96%)	147 (96%)	6 (4%)	0	100	100
37	d	102/128 (80%)	95 (93%)	7 (7%)	0	100	100
38	e	129/140 (92%)	114 (88%)	15 (12%)	0	100	100
39	g	141/156 (90%)	135 (96%)	5 (4%)	1 (1%)	18	53
40	h	132/145 (91%)	126 (96%)	6 (4%)	0	100	100
41	i	133/136 (98%)	122 (92%)	11 (8%)	0	100	100
42	j	109/125 (87%)	104 (95%)	5 (5%)	0	100	100
43	k	127/135 (94%)	116 (91%)	11 (9%)	0	100	100
44	l	123/137 (90%)	112 (91%)	11 (9%)	0	100	100
45	m	246/257 (96%)	222 (90%)	24 (10%)	0	100	100
46	n	107/110 (97%)	101 (94%)	4 (4%)	2 (2%)	6	30
47	o	231/288 (80%)	217 (94%)	14 (6%)	0	100	100
48	p	224/248 (90%)	209 (93%)	15 (7%)	0	100	100
49	r	282/297 (95%)	270 (96%)	12 (4%)	0	100	100
50	z	63/129 (49%)	60 (95%)	2 (3%)	1 (2%)	7	34
51	A	331/731 (45%)	320 (97%)	11 (3%)	0	100	100
52	R	151/203 (74%)	138 (91%)	13 (9%)	0	100	100
53	J	221/239 (92%)	207 (94%)	14 (6%)	0	100	100
54	T	43/99 (43%)	42 (98%)	1 (2%)	0	100	100
55	y	163/165 (99%)	161 (99%)	2 (1%)	0	100	100
56	v	398/588 (68%)	385 (97%)	13 (3%)	0	100	100
58	l	72/123 (58%)	62 (86%)	7 (10%)	3 (4%)	2	13
59	s	33/260 (13%)	30 (91%)	1 (3%)	2 (6%)	1	7
60	w	380/478 (80%)	355 (93%)	24 (6%)	1 (0%)	36	70
All	All	10320/12821 (80%)	9703 (94%)	595 (6%)	22 (0%)	44	76

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	f	326	GLY

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Mol	Chain	Res	Type
4	t	147	LYS
5	3	24	ASN
46	n	106	TYR
60	w	203	ASP
4	t	148	ARG
7	4	88	ASP
7	4	427	ASP
11	9	99	GLN
12	B	295	ASP
50	z	24	LYS
58	1	28	ARG
58	1	46	ILE
58	1	47	THR
59	s	18	LEU
59	s	19	ASP
39	g	40	ILE
7	4	230	LEU
7	4	366	THR
2	f	325	VAL
46	n	107	PRO
22	M	85	LYS

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	u	222/437 (51%)	222 (100%)	0	100	100
2	f	509/629 (81%)	509 (100%)	0	100	100
3	q	191/196 (97%)	191 (100%)	0	100	100
4	t	125/274 (46%)	125 (100%)	0	100	100
5	3	206/228 (90%)	206 (100%)	0	100	100
7	4	554/574 (96%)	554 (100%)	0	100	100
9	6	212/213 (100%)	212 (100%)	0	100	100
10	7	128/149 (86%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	9	81/114 (71%)	80 (99%)	1 (1%)	63	82
12	B	349/349 (100%)	349 (100%)	0	100	100
13	C	78/126 (62%)	77 (99%)	1 (1%)	61	81
14	D	298/348 (86%)	298 (100%)	0	100	100
15	E	83/97 (86%)	83 (100%)	0	100	100
16	F	97/100 (97%)	97 (100%)	0	100	100
17	G	204/223 (92%)	204 (100%)	0	100	100
18	H	109/110 (99%)	109 (100%)	0	100	100
19	I	169/171 (99%)	169 (100%)	0	100	100
20	K	86/89 (97%)	86 (100%)	0	100	100
21	L	120/121 (99%)	120 (100%)	0	100	100
22	M	73/80 (91%)	73 (100%)	0	100	100
23	N	137/149 (92%)	137 (100%)	0	100	100
24	O	64/65 (98%)	64 (100%)	0	100	100
25	P	47/48 (98%)	47 (100%)	0	100	100
26	Q	176/177 (99%)	176 (100%)	0	100	100
27	S	115/161 (71%)	115 (100%)	0	100	100
28	U	171/172 (99%)	171 (100%)	0	100	100
29	V	173/174 (99%)	173 (100%)	0	100	100
30	W	85/94 (90%)	85 (100%)	0	100	100
31	X	74/75 (99%)	74 (100%)	0	100	100
32	Y	147/163 (90%)	147 (100%)	0	100	100
33	Z	164/165 (99%)	164 (100%)	0	100	100
34	a	133/175 (76%)	133 (100%)	0	100	100
35	b	157/157 (100%)	157 (100%)	0	100	100
36	c	136/140 (97%)	135 (99%)	1 (1%)	76	86
37	d	94/115 (82%)	94 (100%)	0	100	100
38	e	101/107 (94%)	101 (100%)	0	100	100
39	g	124/133 (93%)	124 (100%)	0	100	100
40	h	124/135 (92%)	124 (100%)	0	100	100
41	i	117/118 (99%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	j	101/110 (92%)	101 (100%)	0	100	100
43	k	115/121 (95%)	115 (100%)	0	100	100
44	l	109/121 (90%)	109 (100%)	0	100	100
45	m	190/199 (96%)	190 (100%)	0	100	100
46	n	88/89 (99%)	88 (100%)	0	100	100
47	o	208/252 (82%)	208 (100%)	0	100	100
48	p	195/215 (91%)	195 (100%)	0	100	100
49	r	240/250 (96%)	239 (100%)	1 (0%)	84	90
50	z	61/115 (53%)	61 (100%)	0	100	100
51	A	296/654 (45%)	296 (100%)	0	100	100
52	R	141/184 (77%)	141 (100%)	0	100	100
53	J	199/214 (93%)	199 (100%)	0	100	100
54	T	38/76 (50%)	38 (100%)	0	100	100
55	y	137/137 (100%)	137 (100%)	0	100	100
56	v	359/509 (70%)	359 (100%)	0	100	100
58	l	66/107 (62%)	64 (97%)	2 (3%)	36	69
59	s	32/228 (14%)	30 (94%)	2 (6%)	16	48
60	w	338/402 (84%)	337 (100%)	1 (0%)	86	91
All	All	9146/11134 (82%)	9137 (100%)	9 (0%)	87	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	9	75	ASN
13	C	50	ASN
36	c	127	GLN
49	r	282	GLN
58	l	33	ARG
58	l	46	ILE
59	s	17	ARG
59	s	18	LEU
60	w	114	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	u	46	HIS
1	u	229	ASN
2	f	34	GLN
2	f	152	HIS
2	f	288	HIS
2	f	340	GLN
2	f	635	ASN
3	q	19	HIS
3	q	21	ASN
3	q	44	GLN
3	q	214	GLN
7	4	98	GLN
7	4	482	GLN
9	6	86	ASN
9	6	140	GLN
9	6	178	GLN
9	6	228	GLN
10	7	17	HIS
10	7	119	GLN
10	7	130	ASN
11	9	79	HIS
11	9	85	HIS
12	B	121	ASN
13	C	19	ASN
14	D	317	ASN
14	D	347	HIS
16	F	14	ASN
18	H	96	ASN
18	H	108	GLN
19	I	39	ASN
19	I	156	ASN
19	I	169	ASN
20	K	12	ASN
21	L	19	HIS
21	L	60	HIS
21	L	66	ASN
23	N	46	GLN
25	P	25	GLN
25	P	33	ASN
26	Q	15	HIS
26	Q	159	ASN
26	Q	175	ASN
26	Q	205	GLN

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Mol	Chain	Res	Type
27	S	44	GLN
27	S	66	HIS
28	U	90	ASN
28	U	109	HIS
28	U	149	GLN
29	V	50	ASN
29	V	63	ASN
29	V	180	GLN
30	W	19	GLN
32	Y	34	GLN
32	Y	166	GLN
33	Z	7	HIS
33	Z	21	GLN
33	Z	77	ASN
35	b	77	ASN
35	b	92	ASN
36	c	112	ASN
36	c	127	GLN
36	c	131	GLN
38	e	50	ASN
38	e	84	GLN
40	h	20	ASN
41	i	78	ASN
42	j	18	ASN
42	j	34	HIS
42	j	79	ASN
43	k	23	HIS
43	k	57	ASN
43	k	63	ASN
44	l	85	ASN
45	m	187	HIS
47	o	227	HIS
47	o	279	ASN
48	p	24	ASN
48	p	248	ASN
49	r	111	ASN
49	r	222	GLN
49	r	225	GLN
49	r	267	ASN
49	r	282	GLN
51	A	176	GLN
52	R	65	GLN

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Mol	Chain	Res	Type
55	y	70	GLN
56	v	253	GLN
58	1	74	GLN
59	s	10	HIS
60	w	43	ASN
60	w	124	ASN
60	w	255	GLN
60	w	286	GLN
60	w	341	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
57	8	152/156 (97%)	30 (19%)	2 (1%)
6	2	3580/5054 (70%)	904 (25%)	32 (0%)
61	x	0/120	-	-
8	5	119/120 (99%)	20 (16%)	0
All	All	3851/5450 (70%)	954 (24%)	34 (0%)

All (954) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	2	6	C
6	2	21	G
6	2	25	A
6	2	39	A
6	2	42	A
6	2	48	G
6	2	56	A
6	2	59	A
6	2	64	A
6	2	65	A
6	2	69	A
6	2	72	C
6	2	73	A
6	2	91	G
6	2	98	A
6	2	108	A
6	2	109	G
6	2	110	C
6	2	119	G

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Mol	Chain	Res	Type
6	2	120	A
6	2	122	U
6	2	133	C
6	2	134	G
6	2	135	G
6	2	136	C
6	2	137	G
6	2	141	C
6	2	144	G
6	2	145	G
6	2	146	G
6	2	151	G
6	2	152	U
6	2	159	C
6	2	164	G
6	2	165	A
6	2	172	C
6	2	178	C
6	2	181	C
6	2	182	G
6	2	183	C
6	2	184	U
6	2	185	C
6	2	187	U
6	2	188	G
6	2	189	G
6	2	197	A
6	2	200	U
6	2	209	U
6	2	210	C
6	2	218	A
6	2	219	G
6	2	220	C
6	2	234	G
6	2	254	G
6	2	255	C
6	2	256	G
6	2	259	C
6	2	261	G
6	2	262	G
6	2	264	C
6	2	265	C

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Mol	Chain	Res	Type
6	2	266	C
6	2	267	G
6	2	279	A
6	2	280	G
6	2	281	U
6	2	297	U
6	2	306	A
6	2	315	G
6	2	316	U
6	2	326	C
6	2	340	C
6	2	363	A
6	2	385	A
6	2	387	G
6	2	398	A2M
6	2	407	A
6	2	408	A
6	2	409	G
6	2	410	A
6	2	411	G
6	2	412	G
6	2	413	G
6	2	422	C
6	2	423	G
6	2	426	A
6	2	427	A
6	2	428	G
6	2	433	A
6	2	449	C
6	2	450	G
6	2	452	A
6	2	453	G
6	2	454	U
6	2	464	G
6	2	465	G
6	2	467	U
6	2	468	U
6	2	483	G
6	2	484	U
6	2	485	C
6	2	486	C
6	2	489	C

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Mol	Chain	Res	Type
6	2	493	G
6	2	494	U
6	2	496	G
6	2	497	G
6	2	499	G
6	2	500	G
6	2	502	C
6	2	503	C
6	2	504	G
6	2	505	G
6	2	509	A
6	2	510	U
6	2	513	U
6	2	514	U
6	2	515	C
6	2	517	C
6	2	518	G
6	2	519	C
6	2	653	U
6	2	654	C
6	2	656	C
6	2	657	C
6	2	666	G
6	2	667	A
6	2	669	C
6	2	673	C
6	2	686	A
6	2	688	U
6	2	692	A
6	2	696	C
6	2	697	G
6	2	703	G
6	2	704	C
6	2	731	G
6	2	738	C
6	2	739	G
6	2	740	G
6	2	742	G
6	2	759	G
6	2	904	C
6	2	905	C
6	2	910	G

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Mol	Chain	Res	Type
6	2	913	U
6	2	914	U
6	2	915	A
6	2	916	C
6	2	917	A
6	2	918	G
6	2	923	C
6	2	924	C
6	2	925	C
6	2	926	G
6	2	932	A
6	2	933	G
6	2	936	C
6	2	937	U
6	2	941	C
6	2	943	A
6	2	944	A
6	2	945	U
6	2	959	G
6	2	960	A
6	2	961	G
6	2	962	C
6	2	963	G
6	2	964	A
6	2	965	G
6	2	966	A
6	2	967	C
6	2	969	C
6	2	970	G
6	2	972	C
6	2	982	U
6	2	988	C
6	2	990	C
6	2	991	C
6	2	992	C
6	2	993	G
6	2	994	G
6	2	995	C
6	2	996	G
6	2	1048	G
6	2	1049	C
6	2	1051	G

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Mol	Chain	Res	Type
6	2	1066	G
6	2	1070	G
6	2	1072	C
6	2	1081	C
6	2	1082	C
6	2	1083	U
6	2	1095	A
6	2	1100	U
6	2	1168	G
6	2	1172	C
6	2	1173	G
6	2	1176	C
6	2	1178	G
6	2	1179	U
6	2	1180	C
6	2	1181	C
6	2	1182	C
6	2	1183	C
6	2	1184	A
6	2	1186	U
6	2	1187	G
6	2	1194	G
6	2	1198	G
6	2	1199	G
6	2	1200	G
6	2	1201	U
6	2	1202	C
6	2	1203	G
6	2	1211	G
6	2	1215	C
6	2	1216	C
6	2	1220	G
6	2	1222	A
6	2	1235	G
6	2	1241	C
6	2	1245	C
6	2	1253	G
6	2	1254	A
6	2	1255	A
6	2	1257	A
6	2	1260	G
6	2	1265	G

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Mol	Chain	Res	Type
6	2	1266	G
6	2	1269	G
6	2	1270	A
6	2	1271	G
6	2	1272	C
6	2	1275	G
6	2	1280	C
6	2	1283	G
6	2	1284	G
6	2	1287	G
6	2	1294	A
6	2	1295	C
6	2	1296	G
6	2	1301	C
6	2	1302	U
6	2	1303	A
6	2	1304	C
6	2	1314	C
6	2	1320	U
6	2	1323	A
6	2	1324	A
6	2	1326	A2M
6	2	1330	A
6	2	1331	C
6	2	1337	A
6	2	1354	A
6	2	1358	G
6	2	1359	G
6	2	1362	G
6	2	1365	C
6	2	1366	G
6	2	1370	G
6	2	1371	A
6	2	1377	G
6	2	1378	C
6	2	1379	C
6	2	1387	A
6	2	1394	G
6	2	1397	A
6	2	1398	A
6	2	1402	C
6	2	1404	G

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Mol	Chain	Res	Type
6	2	1405	C
6	2	1407	C
6	2	1409	C
6	2	1410	U
6	2	1414	C
6	2	1417	C
6	2	1419	G
6	2	1420	A
6	2	1425	G
6	2	1434	G
6	2	1439	C
6	2	1442	C
6	2	1443	A
6	2	1444	G
6	2	1447	C
6	2	1482	G
6	2	1483	C
6	2	1497	A
6	2	1498	G
6	2	1502	G
6	2	1503	A
6	2	1518	A
6	2	1525	A
6	2	1534	A2M
6	2	1547	A
6	2	1554	A
6	2	1566	C
6	2	1575	A
6	2	1578	U
6	2	1592	G
6	2	1612	G
6	2	1613	A
6	2	1618	G
6	2	1624	G
6	2	1625	OMG
6	2	1631	A
6	2	1633	G
6	2	1634	A
6	2	1637	A
6	2	1642	A
6	2	1650	A
6	2	1654	G

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Mol	Chain	Res	Type
6	2	1661	C
6	2	1676	C
6	2	1677	U
6	2	1678	C
6	2	1685	G
6	2	1691	G
6	2	1697	G
6	2	1699	A
6	2	1700	G
6	2	1701	A
6	2	1703	C
6	2	1704	C
6	2	1705	G
6	2	1707	C
6	2	1709	C
6	2	1716	G
6	2	1718	C
6	2	1719	A
6	2	1724	G
6	2	1726	U
6	2	1734	G
6	2	1790	U
6	2	1797	E7G
6	2	1803	G
6	2	1804	A
6	2	1806	G
6	2	1821	G
6	2	1822	U
6	2	1836	G
6	2	1837	A
6	2	1842	G
6	2	1843	A
6	2	1853	G
6	2	1854	G
6	2	1855	G
6	2	1856	C
6	2	1866	UR3
6	2	1867	A
6	2	1868	A
6	2	1869	G
6	2	1870	C
6	2	1881	C

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Mol	Chain	Res	Type
6	2	1883	OMG
6	2	1888	A
6	2	1891	A
6	2	1897	A
6	2	1900	C
6	2	1916	G
6	2	1918	U
6	2	1919	G
6	2	1920	C
6	2	1922	G
6	2	1925	G
6	2	1931	C
6	2	1932	A
6	2	1938	C
6	2	1941	A
6	2	1948	G
6	2	1949	U
6	2	1951	G
6	2	1958	A
6	2	1959	U
6	2	1961	G
6	2	1962	A
6	2	1963	C
6	2	1968	G
6	2	1969	G
6	2	1970	A
6	2	1971	C
6	2	1979	A
6	2	1980	U
6	2	1981	G
6	2	1983	A
6	2	1984	A
6	2	1985	G
6	2	1990	A
6	2	2001	G
6	2	2002	A
6	2	2003	G
6	2	2004	U
6	2	2008	U
6	2	2010	A
6	2	2011	C
6	2	2016	C

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Mol	Chain	Res	Type
6	2	2018	C
6	2	2021	G
6	2	2024	G
6	2	2025	A
6	2	2026	A
6	2	2033	A
6	2	2034	G
6	2	2043	A
6	2	2044	U
6	2	2046	G
6	2	2048	U
6	2	2055	G
6	2	2056	G
6	2	2069	A
6	2	2071	A
6	2	2084	C
6	2	2085	G
6	2	2090	U
6	2	2092	G
6	2	2093	A
6	2	2095	A
6	2	2097	U
6	2	2098	G
6	2	2100	A
6	2	2101	C
6	2	2102	G
6	2	2104	G
6	2	2105	A
6	2	2106	G
6	2	2108	G
6	2	2111	G
6	2	2112	G
6	2	2113	C
6	2	2250	C
6	2	2252	G
6	2	2253	A
6	2	2255	C
6	2	2256	C
6	2	2258	C
6	2	2259	G
6	2	2260	C
6	2	2268	A

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Mol	Chain	Res	Type
6	2	2277	C
6	2	2289	C
6	2	2300	A
6	2	2301	G
6	2	2306	G
6	2	2313	A
6	2	2327	G
6	2	2328	G
6	2	2331	G
6	2	2333	G
6	2	2348	G
6	2	2350	U
6	2	2351	C
6	2	2354	G
6	2	2356	U
6	2	2364	OMG
6	2	2395	A
6	2	2416	G
6	2	2417	A
6	2	2418	A
6	2	2422	OMC
6	2	2424	OMG
6	2	2425	U
6	2	2437	C
6	2	2439	G
6	2	2441	C
6	2	2445	C
6	2	2447	U
6	2	2450	G
6	2	2453	A
6	2	2470	C
6	2	2471	G
6	2	2475	G
6	2	2476	G
6	2	2477	A
6	2	2478	C
6	2	2484	A
6	2	2485	U
6	2	2486	G
6	2	2487	G
6	2	2488	C
6	2	2489	C

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Mol	Chain	Res	Type
6	2	2490	U
6	2	2497	C
6	2	2501	C
6	2	2511	A
6	2	2512	A
6	2	2513	A
6	2	2519	U
6	2	2520	C
6	2	2529	A
6	2	2543	A
6	2	2544	G
6	2	2545	U
6	2	2546	G
6	2	2548	C
6	2	2554	U
6	2	2559	G
6	2	2566	G
6	2	2583	C
6	2	2586	G
6	2	2587	A
6	2	2589	C
6	2	2593	C
6	2	2601	A
6	2	2602	G
6	2	2611	A
6	2	2618	G
6	2	2627	C
6	2	2638	G
6	2	2652	G
6	2	2653	C
6	2	2661	U
6	2	2662	G
6	2	2669	C
6	2	2670	C
6	2	2674	A
6	2	2675	G
6	2	2687	U
6	2	2694	G
6	2	2695	A
6	2	2696	A
6	2	2697	A
6	2	2707	U

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Mol	Chain	Res	Type
6	2	2708	U
6	2	2711	G
6	2	2719	C
6	2	2724	G
6	2	2726	G
6	2	2739	C
6	2	2742	G
6	2	2743	A
6	2	2756	G
6	2	2761	U
6	2	2763	U
6	2	2764	A
6	2	2765	A
6	2	2769	U
6	2	2770	C
6	2	2786	B9H
6	2	2787	A
6	2	2788	U
6	2	2790	U
6	2	2799	G
6	2	2814	C
6	2	2815	A
6	2	2826	U
6	2	2827	G
6	2	2842	G
6	2	2846	G
6	2	2849	A
6	2	2850	A
6	2	2855	G
6	2	2875	C
6	2	2877	G
6	2	2879	A
6	2	2897	G
6	2	2900	U
6	2	2901	G
6	2	2902	G
6	2	2903	G
6	2	2904	U
6	2	2905	C
6	2	2906	G
6	2	2907	G
6	2	2908	U

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Mol	Chain	Res	Type
6	2	3585	G
6	2	3588	C
6	2	3591	C
6	2	3593	C
6	2	3595	U
6	2	3596	A
6	2	3597	G
6	2	3598	C
6	2	3599	A
6	2	3603	G
6	2	3605	C
6	2	3606	U
6	2	3615	G
6	2	3616	U
6	2	3626	G
6	2	3630	A
6	2	3635	A
6	2	3644	U
6	2	3648	A
6	2	3662	A
6	2	3670	C
6	2	3672	G
6	2	3673	C
6	2	3680	U
6	2	3683	C
6	2	3691	G
6	2	3696	C
6	2	3698	G
6	2	3710	G
6	2	3712	A
6	2	3713	U
6	2	3723	A2M
6	2	3729	U
6	2	3734	U
6	2	3735	G
6	2	3736	A
6	2	3750	G
6	2	3753	G
6	2	3771	C
6	2	3772	U
6	2	3774	A
6	2	3775	A

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Mol	Chain	Res	Type
6	2	3776	G
6	2	3838	U
6	2	3839	G
6	2	3840	U
6	2	3865	A
6	2	3867	A2M
6	2	3876	A
6	2	3877	A
6	2	3878	C
6	2	3879	G
6	2	3880	P7G
6	2	3897	B8K
6	2	3903	A
6	2	3904	G
6	2	3905	A
6	2	3906	A
6	2	3915	U
6	2	3922	G
6	2	3938	G
6	2	3939	G
6	2	3947	A
6	2	3950	U
6	2	3953	G
6	2	3955	G
6	2	3956	G
6	2	3958	G
6	2	3959	U
6	2	3960	A
6	2	3961	G
6	2	3962	A
6	2	3963	A
6	2	3964	U
6	2	3965	A
6	2	3966	A
6	2	3969	G
6	2	3970	G
6	2	3971	G
6	2	3973	G
6	2	3974	G
6	2	3975	C
6	2	3977	C
6	2	4036	G

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Mol	Chain	Res	Type
6	2	4038	C
6	2	4039	G
6	2	4041	C
6	2	4042	G
6	2	4043	G
6	2	4045	G
6	2	4046	A
6	2	4048	A
6	2	4049	U
6	2	4050	A
6	2	4051	C
6	2	4052	C
6	2	4053	A
6	2	4055	U
6	2	4056	A
6	2	4057	C
6	2	4058	U
6	2	4059	C
6	2	4062	A
6	2	4063	U
6	2	4064	C
6	2	4065	G
6	2	4076	G
6	2	4084	G
6	2	4095	G
6	2	4099	G
6	2	4100	C
6	2	4102	C
6	2	4103	C
6	2	4104	G
6	2	4110	C
6	2	4111	U
6	2	4112	C
6	2	4113	U
6	2	4115	G
6	2	4116	C
6	2	4117	U
6	2	4118	U
6	2	4119	C
6	2	4121	G
6	2	4125	C
6	2	4127	A

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Mol	Chain	Res	Type
6	2	4138	C
6	2	4140	C
6	2	4141	G
6	2	4142	C
6	2	4143	G
6	2	4144	C
6	2	4146	G
6	2	4147	G
6	2	4149	C
6	2	4150	G
6	2	4157	A
6	2	4162	C
6	2	4163	U
6	2	4170	A
6	2	4183	G
6	2	4184	G
6	2	4191	G
6	2	4192	A
6	2	4195	G
6	2	4196	G
6	2	4197	G
6	2	4201	G
6	2	4202	U
6	2	4203	A
6	2	4204	C
6	2	4212	A
6	2	4225	G
6	2	4226	G
6	2	4229	U
6	2	4233	A
6	2	4234	A
6	2	4247	G
6	2	4249	G
6	2	4251	A
6	2	4254	G
6	2	4256	A
6	2	4258	C
6	2	4260	U
6	2	4265	U
6	2	4268	A
6	2	4271	A
6	2	4273	A

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Mol	Chain	Res	Type
6	2	4279	A
6	2	4281	A
6	2	4291	G
6	2	4292	A
6	2	4293	U
6	2	4294	C
6	2	4295	U
6	2	4296	B8H
6	2	4304	A
6	2	4305	G
6	2	4314	C
6	2	4329	G
6	2	4330	G
6	2	4332	C
6	2	4339	A
6	2	4349	C
6	2	4354	U
6	2	4364	G
6	2	4373	G
6	2	4377	G
6	2	4378	A
6	2	4379	A
6	2	4380	A
6	2	4381	A
6	2	4382	G
6	2	4387	C
6	2	4395	U
6	2	4396	A
6	2	4415	A
6	2	4418	G
6	2	4422	A
6	2	4424	A
6	2	4427	G
6	2	4428	A
6	2	4430	G
6	2	4437	U
6	2	4440	G
6	2	4446	U
6	2	4447	C
6	2	4448	G
6	2	4451	G
6	2	4452	U

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Mol	Chain	Res	Type
6	2	4453	C
6	2	4464	A
6	2	4466	C
6	2	4475	G
6	2	4476	C
6	2	4484	A
6	2	4488	A
6	2	4498	U
6	2	4508	C
6	2	4510	A
6	2	4512	U
6	2	4513	A
6	2	4518	A
6	2	4519	C
6	2	4523	A2M
6	2	4524	G
6	2	4529	B8W
6	2	4531	U
6	2	4545	G
6	2	4547	C
6	2	4548	A
6	2	4549	G
6	2	4554	G
6	2	4555	U
6	2	4556	U
6	2	4557	U
6	2	4558	U
6	2	4560	C
6	2	4567	G
6	2	4570	G
6	2	4584	A
6	2	4589	A
6	2	4590	A
6	2	4597	UR3
6	2	4600	G
6	2	4601	U
6	2	4606	G
6	2	4607	A
6	2	4608	G
6	2	4627	U
6	2	4636	U
6	2	4637	OMG

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Mol	Chain	Res	Type
6	2	4656	A
6	2	4670	C
6	2	4672	A
6	2	4678	G
6	2	4693	C
6	2	4694	G
6	2	4695	C
6	2	4702	G
6	2	4708	A
6	2	4709	U
6	2	4719	G
6	2	4720	C
6	2	4721	G
6	2	4730	C
6	2	4731	G
6	2	4732	G
6	2	4733	C
6	2	4734	A
6	2	4735	G
6	2	4740	G
6	2	4741	C
6	2	4742	G
6	2	4745	G
6	2	4754	G
6	2	4757	C
6	2	4759	C
6	2	4761	G
6	2	4764	A
6	2	4765	G
6	2	4771	C
6	2	4775	C
6	2	4776	G
6	2	4862	G
6	2	4870	OMG
6	2	4871	C
6	2	4873	G
6	2	4875	G
6	2	4877	G
6	2	4882	U
6	2	4883	C
6	2	4895	C
6	2	4896	G

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Mol	Chain	Res	Type
6	2	4899	G
6	2	4900	C
6	2	4901	G
6	2	4907	G
6	2	4910	G
6	2	4912	G
6	2	4914	C
6	2	4915	G
6	2	4927	G
6	2	4928	C
6	2	4931	G
6	2	4935	C
6	2	4937	C
6	2	4938	A
6	2	4940	C
6	2	4941	G
6	2	4943	A
6	2	4944	C
6	2	4949	G
6	2	4958	C
6	2	4960	G
6	2	4961	G
6	2	4976	U
6	2	4989	U
6	2	4990	C
6	2	4991	U
6	2	5014	A
6	2	5017	G
6	2	5022	U
6	2	5023	C
6	2	5026	U
6	2	5027	C
6	2	5028	G
6	2	5030	U
6	2	5031	G
6	2	5034	A
6	2	5040	U
6	2	5041	G
6	2	5050	C
6	2	5053	U
6	2	5054	C
6	2	5055	G

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Mol	Chain	Res	Type
6	2	5058	A
6	2	5062	G
6	2	5069	U
8	5	11	A
8	5	23	A
8	5	33	U
8	5	37	G
8	5	38	U
8	5	40	U
8	5	41	G
8	5	42	A
8	5	48	G
8	5	50	A
8	5	53	U
8	5	54	A
8	5	63	C
8	5	64	G
8	5	97	G
8	5	100	A
8	5	109	U
8	5	110	G
8	5	111	C
8	5	120	U
57	8	5	U
57	8	8	U
57	8	10	G
57	8	24	G
57	8	25	G
57	8	34	U
57	8	35	C
57	8	39	G
57	8	48	A
57	8	52	A
57	8	59	A
57	8	62	A
57	8	63	U
57	8	71	A
57	8	80	A
57	8	82	A
57	8	84	A
57	8	85	U
57	8	103	A

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Mol	Chain	Res	Type
57	8	104	A
57	8	105	C
57	8	108	A
57	8	110	U
57	8	114	G
57	8	123	U
57	8	124	U
57	8	125	C
57	8	126	C
57	8	127	U
57	8	151	G

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	2	406	C
6	2	408	A
6	2	421	C
6	2	422	C
6	2	914	U
6	2	1322	1MA
6	2	1625	OMG
6	2	1676	C
6	2	1855	G
6	2	1980	U
6	2	2014	C
6	2	2033	A
6	2	2348	G
6	2	2470	C
6	2	2486	G
6	2	2487	G
6	2	2496	G
6	2	2760	G
6	2	3596	A
6	2	3752	C
6	2	3773	U
6	2	3774	A
6	2	3905	A
6	2	4126	C
6	2	4191	G
6	2	4195	G
6	2	4202	U

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Mol	Chain	Res	Type
6	2	4204	C
6	2	4445	U
6	2	4547	C
6	2	4555	U
6	2	4913	G
57	8	124	U
57	8	125	C

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

76 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$
6	OMG	2	4370	6	23,26,27	2.58	9 (39%)	33,38,41	2.73	15 (45%)
6	B9B	2	1574	6	25,28,29	1.80	6 (24%)	35,40,43	5.27	10 (28%)
6	A2M	2	1524	6	22,25,26	3.26	10 (45%)	31,36,39	2.96	11 (35%)
6	B8T	2	4671	6	19,22,23	3.36	8 (42%)	26,31,34	0.96	1 (3%)
6	A2M	2	398	6	22,25,26	3.24	10 (45%)	31,36,39	2.93	10 (32%)
6	OMU	2	4306	6	19,22,23	2.87	8 (42%)	26,31,34	1.74	5 (19%)
6	B8Q	2	1456	6	17,22,23	2.79	5 (29%)	22,32,35	2.45	6 (27%)
6	A2M	2	2401	6	22,25,26	3.29	10 (45%)	31,36,39	3.04	11 (35%)
6	OMC	2	2861	6	19,22,23	2.91	8 (42%)	26,31,34	1.02	2 (7%)
6	OMG	2	1522	6	23,26,27	2.59	9 (39%)	33,38,41	2.74	13 (39%)
6	A2M	2	1534	6	22,25,26	3.22	11 (50%)	31,36,39	3.20	13 (41%)
6	A2M	2	4523	6	22,25,26	3.18	10 (45%)	31,36,39	3.03	10 (32%)
6	UR3	2	4530	6	19,22,23	2.77	6 (31%)	26,32,35	1.36	2 (7%)
6	UR3	2	4597	6	19,22,23	2.69	6 (31%)	26,32,35	2.26	7 (26%)
6	6MZ	2	4220	6	22,25,26	2.56	4 (18%)	30,36,39	3.39	10 (33%)
6	A2M	2	3718	6	22,25,26	3.26	10 (45%)	31,36,39	2.66	10 (32%)
6	OMC	2	3887	6	19,22,23	2.91	8 (42%)	26,31,34	0.94	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OMC	2	4536	6	19,22,23	2.83	7 (36%)	26,31,34	1.08	2 (7%)
57	OMU	8	14	6,57	19,22,23	2.74	7 (36%)	26,31,34	2.00	5 (19%)
6	P4U	2	1348	6	21,24,25	3.37	8 (38%)	27,33,36	1.17	2 (7%)
6	2MG	2	729	6	23,26,27	2.82	8 (34%)	32,38,41	2.36	8 (25%)
6	A2M	2	4571	6	22,25,26	3.21	11 (50%)	31,36,39	2.95	10 (32%)
6	OMG	2	4870	6	23,26,27	2.64	9 (39%)	33,38,41	2.92	10 (30%)
6	OMC	2	3869	6	19,22,23	2.87	7 (36%)	26,31,34	1.83	6 (23%)
6	OMC	2	2365	6	19,22,23	2.74	7 (36%)	26,31,34	0.90	0
6	B8H	2	4296	6	20,22,23	6.64	6 (30%)	21,32,35	2.46	5 (23%)
6	OMG	2	1625	6	23,26,27	2.59	9 (39%)	33,38,41	2.71	9 (27%)
6	MHG	2	4371	6	29,32,33	3.93	11 (37%)	34,46,49	2.36	12 (35%)
6	OMG	2	2424	6	23,26,27	2.64	9 (39%)	33,38,41	2.74	9 (27%)
6	OMG	2	4494	6	23,26,27	2.61	8 (34%)	33,38,41	2.76	10 (30%)
6	OMG	2	1883	6	23,26,27	2.59	9 (39%)	33,38,41	2.63	12 (36%)
6	E7G	2	1797	6	24,27,28	3.87	11 (45%)	30,40,43	2.28	9 (30%)
6	A2M	2	3867	6	22,25,26	3.18	10 (45%)	31,36,39	2.95	12 (38%)
6	B8H	2	1860	6	20,22,23	6.60	6 (30%)	21,32,35	2.41	5 (23%)
6	UR3	2	1866	6	19,22,23	3.04	7 (36%)	26,32,35	2.16	6 (23%)
6	7MG	2	4550	6	22,26,27	3.38	10 (45%)	29,39,42	1.83	8 (27%)
6	5MU	2	4083	6	19,22,23	7.17	8 (42%)	28,32,35	3.49	10 (35%)
6	E6G	2	4355	6	24,27,28	2.02	5 (20%)	34,39,42	2.80	12 (35%)
6	A2M	2	1326	6	22,25,26	3.18	10 (45%)	31,36,39	2.90	12 (38%)
6	A2M	2	2363	6	22,25,26	3.27	11 (50%)	31,36,39	3.00	11 (35%)
6	7MG	2	2522	6	22,26,27	3.25	10 (45%)	29,39,42	1.90	9 (31%)
6	P7G	2	1909	6	24,28,29	3.67	11 (45%)	27,41,44	1.98	5 (18%)
6	B8W	2	2380	6	23,26,27	2.62	5 (21%)	33,38,41	2.60	15 (45%)
6	P7G	2	3880	6	24,28,29	3.78	11 (45%)	27,41,44	1.53	3 (11%)
6	I4U	2	1659	6	21,24,25	3.31	9 (42%)	27,34,37	1.11	1 (3%)
6	7MG	2	1605	6	22,26,27	3.49	10 (45%)	29,39,42	2.03	9 (31%)
6	OMG	2	2364	6	23,26,27	2.55	9 (39%)	33,38,41	2.70	13 (39%)
6	B9B	2	237	6	25,28,29	1.84	6 (24%)	35,40,43	5.05	12 (34%)
6	B9B	2	2754	6	25,28,29	1.77	7 (28%)	35,40,43	5.06	11 (31%)
6	B8K	2	3897	6	24,28,29	3.11	11 (45%)	30,42,45	2.56	11 (36%)
6	OMC	2	3701	6	19,22,23	2.80	8 (42%)	26,31,34	0.88	0
6	BGH	2	3899	6	25,29,30	4.35	16 (64%)	31,43,46	2.79	13 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	B8W	2	4472	6	23,26,27	2.75	6 (26%)	33,38,41	2.86	12 (36%)
6	B8T	2	4483	6	19,22,23	3.59	8 (42%)	26,31,34	1.42	4 (15%)
6	A2M	2	1871	6	22,25,26	3.21	10 (45%)	31,36,39	2.91	11 (35%)
6	1MA	2	1322	6	21,25,26	3.04	4 (19%)	31,37,40	1.86	6 (19%)
6	B8W	2	4529	6	23,26,27	2.86	5 (21%)	33,38,41	2.74	12 (36%)
6	OMU	2	4620	6	19,22,23	2.74	7 (36%)	26,31,34	1.80	4 (15%)
6	B9H	2	2786	6	20,25,26	3.18	4 (20%)	22,35,38	3.26	7 (31%)
6	M7A	2	4564	6	20,25,26	1.84	3 (15%)	28,37,40	3.95	7 (25%)
6	OMG	2	373	6	23,26,27	2.59	9 (39%)	33,38,41	2.72	16 (48%)
6	2MG	2	1517	6	23,26,27	2.94	8 (34%)	32,38,41	2.74	8 (25%)
6	OMC	2	2422	6	19,22,23	2.87	7 (36%)	26,31,34	1.38	4 (15%)
6	2MG	2	978	6	23,26,27	2.92	9 (39%)	32,38,41	2.26	10 (31%)
6	B8W	2	4185	6	23,26,27	2.79	5 (21%)	33,38,41	2.47	13 (39%)
6	OMG	2	1316	6	23,26,27	2.66	9 (39%)	33,38,41	2.74	11 (33%)
6	OMC	2	2804	6	19,22,23	2.75	7 (36%)	26,31,34	1.21	3 (11%)
6	OMG	2	2773	6	23,26,27	2.62	8 (34%)	33,38,41	2.71	11 (33%)
6	2MG	2	4872	6	23,26,27	2.76	8 (34%)	32,38,41	2.39	8 (25%)
6	OMG	2	2050	6	23,26,27	2.60	9 (39%)	33,38,41	2.65	10 (30%)
6	OMG	2	4623	6	23,26,27	2.55	9 (39%)	33,38,41	2.70	13 (39%)
6	OMG	2	4637	6	23,26,27	2.56	9 (39%)	33,38,41	2.76	12 (36%)
6	B8K	2	4690	6	24,28,29	3.08	12 (50%)	30,42,45	2.78	12 (40%)
6	A2M	2	3723	6	22,25,26	3.15	10 (45%)	31,36,39	2.79	10 (32%)
6	5MC	2	4335	6	18,22,23	3.46	7 (38%)	26,32,35	1.14	2 (7%)
6	E7G	2	2297	6	24,27,28	3.59	11 (45%)	30,40,43	2.15	9 (30%)

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
6	OMG	2	4370	6	-	0/9/27/28	0/3/3/3
6	B9B	2	1574	6	-	2/11/29/30	0/3/3/3
6	A2M	2	1524	6	-	2/9/27/28	0/3/3/3
6	B8T	2	4671	6	-	0/7/27/28	0/2/2/2
6	A2M	2	398	6	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMU	2	4306	6	-	1/9/27/28	0/2/2/2
6	B8Q	2	1456	6	-	0/7/42/43	0/2/2/2
6	A2M	2	2401	6	-	1/9/27/28	0/3/3/3
6	OMC	2	2861	6	-	0/9/27/28	0/2/2/2
6	OMG	2	1522	6	-	0/9/27/28	0/3/3/3
6	A2M	2	1534	6	-	1/9/27/28	0/3/3/3
6	A2M	2	4523	6	-	3/9/27/28	0/3/3/3
6	UR3	2	4530	6	-	0/7/25/26	0/2/2/2
6	UR3	2	4597	6	-	0/7/25/26	0/2/2/2
6	6MZ	2	4220	6	-	1/9/27/28	0/3/3/3
6	A2M	2	3718	6	-	1/9/27/28	0/3/3/3
6	OMC	2	3887	6	-	1/9/27/28	0/2/2/2
6	OMC	2	4536	6	-	0/9/27/28	0/2/2/2
57	OMU	8	14	6,57	-	1/9/27/28	0/2/2/2
6	P4U	2	1348	6	-	1/10/29/30	0/2/2/2
6	2MG	2	729	6	-	1/9/27/28	0/3/3/3
6	A2M	2	4571	6	-	0/9/27/28	0/3/3/3
6	OMG	2	4870	6	-	3/9/27/28	0/3/3/3
6	OMC	2	3869	6	-	4/9/27/28	0/2/2/2
6	OMC	2	2365	6	-	0/9/27/28	0/2/2/2
6	B8H	2	4296	6	-	3/7/25/26	0/2/2/2
6	OMG	2	1625	6	-	2/9/27/28	0/3/3/3
6	MHG	2	4371	6	-	7/16/46/47	0/3/3/3
6	OMG	2	2424	6	-	2/9/27/28	0/3/3/3
6	OMG	2	4494	6	-	0/9/27/28	0/3/3/3
6	OMG	2	1883	6	-	2/9/27/28	0/3/3/3
6	E7G	2	1797	6	-	3/9/39/40	0/3/3/3
6	A2M	2	3867	6	-	3/9/27/28	0/3/3/3
6	B8H	2	1860	6	-	0/7/25/26	0/2/2/2
6	UR3	2	1866	6	-	2/7/25/26	0/2/2/2
6	7MG	2	4550	6	-	0/7/37/38	0/3/3/3
6	5MU	2	4083	6	-	0/7/25/26	0/2/2/2
6	E6G	2	4355	6	-	2/10/28/29	0/3/3/3
6	A2M	2	1326	6	-	1/9/27/28	0/3/3/3
6	A2M	2	2363	6	-	0/9/27/28	0/3/3/3
6	7MG	2	2522	6	-	0/7/37/38	0/3/3/3
6	P7G	2	1909	6	-	3/10/40/41	0/3/3/3
6	B8W	2	2380	6	-	2/9/27/28	0/3/3/3
6	P7G	2	3880	6	-	3/10/40/41	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	I4U	2	1659	6	-	2/9/29/30	0/2/2/2
6	7MG	2	1605	6	-	2/7/37/38	0/3/3/3
6	OMG	2	2364	6	-	2/9/27/28	0/3/3/3
6	B9B	2	237	6	-	4/11/29/30	0/3/3/3
6	B9B	2	2754	6	-	2/11/29/30	0/3/3/3
6	B8K	2	3897	6	-	3/11/41/42	0/3/3/3
6	OMC	2	3701	6	-	4/9/27/28	0/2/2/2
6	BGH	2	3899	6	-	1/13/43/44	0/3/3/3
6	B8W	2	4472	6	-	0/9/27/28	0/3/3/3
6	B8T	2	4483	6	-	0/7/27/28	0/2/2/2
6	A2M	2	1871	6	-	0/9/27/28	0/3/3/3
6	1MA	2	1322	6	-	0/7/25/26	0/3/3/3
6	B8W	2	4529	6	-	2/9/27/28	0/3/3/3
6	OMU	2	4620	6	-	0/9/27/28	0/2/2/2
6	B9H	2	2786	6	-	2/12/47/48	0/2/2/2
6	M7A	2	4564	6	-	0/7/37/38	0/3/3/3
6	OMG	2	373	6	-	1/9/27/28	0/3/3/3
6	2MG	2	1517	6	-	0/9/27/28	0/3/3/3
6	OMC	2	2422	6	-	1/9/27/28	0/2/2/2
6	2MG	2	978	6	-	0/9/27/28	0/3/3/3
6	B8W	2	4185	6	-	2/9/27/28	0/3/3/3
6	OMG	2	1316	6	-	0/9/27/28	0/3/3/3
6	OMC	2	2804	6	-	0/9/27/28	0/2/2/2
6	OMG	2	2773	6	-	0/9/27/28	0/3/3/3
6	2MG	2	4872	6	-	2/9/27/28	0/3/3/3
6	OMG	2	2050	6	-	0/9/27/28	0/3/3/3
6	OMG	2	4623	6	-	0/9/27/28	0/3/3/3
6	OMG	2	4637	6	-	3/9/27/28	0/3/3/3
6	B8K	2	4690	6	-	0/11/41/42	0/3/3/3
6	A2M	2	3723	6	-	2/9/27/28	0/3/3/3
6	5MC	2	4335	6	-	1/7/25/26	0/2/2/2
6	E7G	2	2297	6	-	2/9/39/40	0/3/3/3

All (629) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	4083	5MU	C4-C5	20.27	1.78	1.44
6	2	4296	B8H	C6-C5	-16.82	1.11	1.34
6	2	1860	B8H	C6-C5	-16.42	1.11	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	4296	B8H	C4-N3	-16.02	1.09	1.38
6	2	1860	B8H	C4-N3	-15.78	1.09	1.38
6	2	4083	5MU	C6-N1	15.61	1.64	1.38
6	2	1860	B8H	C4-C5	13.17	1.81	1.44
6	2	4296	B8H	C4-C5	12.97	1.81	1.44
6	2	1860	B8H	C6-N1	12.13	1.66	1.36
6	2	4296	B8H	C6-N1	12.01	1.66	1.36
6	2	4083	5MU	C6-C5	-11.92	1.15	1.34
6	2	4083	5MU	C4-N3	-11.41	1.17	1.38
6	2	4220	6MZ	C6-N6	10.72	1.45	1.34
6	2	2786	B9H	C2-N3	10.19	1.50	1.37
6	2	4371	MHG	C8-N9	10.09	1.51	1.46
6	2	1348	P4U	C4-N3	9.99	1.44	1.31
6	2	1322	1MA	C2-N3	9.90	1.49	1.30
6	2	1659	I4U	C4-N3	9.77	1.44	1.31
6	2	1524	A2M	C3'-C4'	-9.11	1.29	1.53
6	2	1797	E7G	C5-N7	9.10	1.45	1.35
6	2	2297	E7G	C5-N7	9.05	1.45	1.35
6	2	4371	MHG	C5-N7	9.04	1.45	1.35
6	2	1534	A2M	C3'-C4'	-8.98	1.30	1.53
6	2	398	A2M	C3'-C4'	-8.98	1.30	1.53
6	2	3899	BGH	C2'-C1'	-8.98	1.30	1.53
6	2	2401	A2M	C3'-C4'	-8.96	1.30	1.53
6	2	2363	A2M	C3'-C4'	-8.93	1.30	1.53
6	2	3867	A2M	C3'-C4'	-8.91	1.30	1.53
6	2	1797	E7G	C8-N9	8.87	1.50	1.46
6	2	4571	A2M	C3'-C4'	-8.86	1.30	1.53
6	2	3880	P7G	C5-N7	8.83	1.45	1.35
6	2	1909	P7G	C5-N7	8.82	1.45	1.35
6	2	3718	A2M	C3'-C4'	-8.82	1.30	1.53
6	2	1871	A2M	C3'-C4'	-8.80	1.30	1.53
6	2	4185	B8W	O6-C6	8.80	1.49	1.35
6	2	3723	A2M	C3'-C4'	-8.72	1.30	1.53
6	2	3899	BGH	O4'-C1'	8.66	1.62	1.42
6	2	4523	A2M	C3'-C4'	-8.64	1.30	1.53
6	2	4529	B8W	O6-C6	8.61	1.48	1.35
6	2	4335	5MC	C6-C5	8.59	1.48	1.34
6	2	4472	B8W	O6-C6	8.45	1.48	1.35
6	2	1605	7MG	C5-N7	8.30	1.45	1.35
6	2	4690	B8K	C8-N9	8.26	1.50	1.46
6	2	1326	A2M	C3'-C4'	-8.25	1.31	1.53
6	2	4550	7MG	C5-N7	8.21	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	2522	7MG	C5-N7	8.21	1.45	1.35
6	2	4371	MHG	C2-N3	8.02	1.47	1.31
6	2	3897	B8K	C8-N9	8.00	1.50	1.46
6	2	1456	B8Q	C6-C5	7.96	1.51	1.33
6	2	4529	B8W	C2-N2	7.96	1.49	1.33
6	2	2380	B8W	O6-C6	7.91	1.47	1.35
6	2	1909	P7G	C8-N9	7.85	1.50	1.46
6	2	3899	BGH	O4'-C4'	-7.85	1.27	1.45
6	2	4472	B8W	C2-N2	7.84	1.49	1.33
6	2	3899	BGH	C8-N9	7.82	1.50	1.46
6	2	398	A2M	O4'-C4'	7.73	1.62	1.45
6	2	2401	A2M	O4'-C4'	7.69	1.62	1.45
6	2	1326	A2M	O4'-C4'	7.68	1.62	1.45
6	2	4550	7MG	C8-N9	7.66	1.50	1.46
6	2	978	2MG	C2-N3	7.65	1.46	1.31
6	2	1871	A2M	O4'-C4'	7.62	1.62	1.45
6	2	4185	B8W	C2-N2	7.62	1.49	1.33
6	2	4872	2MG	C2-N3	7.61	1.46	1.31
6	2	3880	P7G	C8-N9	7.58	1.50	1.46
6	2	2363	A2M	O4'-C4'	7.49	1.61	1.45
6	2	4483	B8T	C2-N3	7.44	1.51	1.36
6	2	4523	A2M	O4'-C4'	7.41	1.61	1.45
6	2	1517	2MG	C2-N3	7.39	1.46	1.31
6	2	1866	UR3	C2-N1	7.37	1.49	1.38
6	2	3718	A2M	O4'-C4'	7.35	1.61	1.45
6	2	1605	7MG	C8-N9	7.34	1.50	1.46
6	2	3723	A2M	O4'-C4'	7.31	1.61	1.45
6	2	2380	B8W	C2-N2	7.23	1.48	1.33
6	2	729	2MG	C2-N3	7.22	1.45	1.31
6	2	1322	1MA	C4-N3	7.13	1.50	1.35
6	2	4571	A2M	O4'-C4'	7.10	1.60	1.45
6	2	1524	A2M	O4'-C4'	7.07	1.60	1.45
6	2	4483	B8T	C4-N3	7.06	1.45	1.32
6	2	2522	7MG	C8-N9	7.05	1.49	1.46
6	2	1534	A2M	O4'-C4'	7.05	1.60	1.45
6	2	3867	A2M	O4'-C4'	7.02	1.60	1.45
6	2	1866	UR3	C6-C5	6.94	1.51	1.35
6	2	2297	E7G	C8-N9	6.93	1.49	1.46
6	2	1517	2MG	C4-N3	6.93	1.50	1.34
6	2	4671	B8T	C2-N3	6.87	1.50	1.36
6	2	1517	2MG	C2-N2	6.77	1.48	1.33
6	2	4671	B8T	C6-C5	6.66	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	4371	MHG	C8-N7	6.60	1.52	1.45
6	2	978	2MG	C2-N2	6.60	1.48	1.33
6	2	4620	OMU	C2-N1	6.55	1.49	1.38
6	2	4597	UR3	C6-C5	6.54	1.50	1.35
6	2	4530	UR3	C2-N1	6.51	1.47	1.38
6	2	4306	OMU	C2-N1	6.51	1.48	1.38
6	2	729	2MG	C4-N3	6.49	1.49	1.34
6	2	978	2MG	C4-N3	6.47	1.49	1.34
6	2	4335	5MC	C4-N3	6.44	1.45	1.34
6	2	4530	UR3	C6-C5	6.41	1.50	1.35
6	2	2786	B9H	C2-N1	6.41	1.47	1.38
6	2	4671	B8T	C4-N3	6.39	1.43	1.32
6	2	4306	OMU	C2-N3	6.36	1.49	1.38
6	2	4483	B8T	C6-C5	6.34	1.49	1.35
57	8	14	OMU	C2-N1	6.29	1.48	1.38
6	2	3897	B8K	C2-N3	6.29	1.48	1.33
6	2	4690	B8K	C2-N3	6.27	1.48	1.33
6	2	2786	B9H	C6-C5	6.24	1.47	1.33
6	2	2861	OMC	C2-N3	6.23	1.49	1.36
6	2	4483	B8T	C4-N4	6.22	1.48	1.35
6	2	4335	5MC	C2-N3	6.21	1.48	1.36
6	2	729	2MG	C2-N2	6.19	1.47	1.33
6	2	3880	P7G	C4-N9	6.18	1.44	1.35
6	2	1866	UR3	C2-N3	6.18	1.51	1.39
6	2	3887	OMC	C2-N3	6.13	1.48	1.36
6	2	1909	P7G	C4-N3	6.10	1.48	1.37
57	8	14	OMU	C2-N3	6.05	1.48	1.38
6	2	4536	OMC	C2-N3	6.04	1.48	1.36
6	2	4597	UR3	C2-N3	6.01	1.50	1.39
6	2	3869	OMC	C2-N3	6.01	1.48	1.36
6	2	3880	P7G	C4-N3	6.01	1.48	1.37
6	2	1909	P7G	C4-N9	5.98	1.44	1.35
6	2	4870	OMG	C4-N3	5.96	1.48	1.34
6	2	1316	OMG	C2-N2	5.94	1.48	1.34
6	2	1659	I4U	C6-C5	5.94	1.48	1.35
6	2	4355	E6G	C2-N2	5.93	1.45	1.33
6	2	4872	2MG	C2-N2	5.93	1.46	1.33
6	2	2424	OMG	C2-N3	5.91	1.47	1.33
6	2	4870	OMG	C2-N3	5.91	1.47	1.33
6	2	1456	B8Q	C2-N3	5.91	1.45	1.35
6	2	4494	OMG	C4-N3	5.89	1.48	1.34
6	2	4371	MHG	C2-N1	5.89	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	1316	OMG	C2-N3	5.88	1.47	1.33
6	2	2422	OMC	C6-C5	5.88	1.48	1.35
6	2	1797	E7G	C4-N9	5.88	1.44	1.37
6	2	4620	OMU	C2-N3	5.88	1.48	1.38
6	2	2422	OMC	C2-N3	5.86	1.48	1.36
6	2	4671	B8T	C4-N4	5.85	1.47	1.35
6	2	2773	OMG	C2-N2	5.84	1.48	1.34
6	2	4494	OMG	C2-N3	5.83	1.47	1.33
6	2	3887	OMC	C6-C5	5.83	1.48	1.35
6	2	3701	OMC	C2-N3	5.82	1.48	1.36
6	2	2773	OMG	C4-N3	5.81	1.48	1.34
6	2	2773	OMG	C2-N3	5.81	1.47	1.33
6	2	2424	OMG	C2-N2	5.80	1.48	1.34
6	2	1348	P4U	C2-N3	5.79	1.48	1.36
6	2	1659	I4U	C2-N3	5.79	1.48	1.36
6	2	373	OMG	C2-N2	5.79	1.47	1.34
6	2	1797	E7G	C8-N7	5.77	1.51	1.45
6	2	2365	OMC	C2-N3	5.77	1.48	1.36
6	2	4370	OMG	C2-N2	5.77	1.47	1.34
6	2	2424	OMG	C4-N3	5.77	1.48	1.34
6	2	4870	OMG	C2-N2	5.76	1.47	1.34
6	2	1625	OMG	C2-N2	5.75	1.47	1.34
6	2	4536	OMC	C6-C5	5.74	1.48	1.35
6	2	2050	OMG	C4-N3	5.73	1.47	1.34
6	2	1316	OMG	C4-N3	5.72	1.47	1.34
6	2	1625	OMG	C4-N3	5.72	1.47	1.34
6	2	2050	OMG	C2-N3	5.72	1.47	1.33
6	2	1522	OMG	C2-N2	5.71	1.47	1.34
6	2	3880	P7G	C2-N2	5.70	1.47	1.34
6	2	3701	OMC	C6-C5	5.69	1.48	1.35
6	2	2861	OMC	C6-C5	5.68	1.48	1.35
6	2	1883	OMG	C4-N3	5.68	1.47	1.34
6	2	2050	OMG	C2-N2	5.66	1.47	1.34
6	2	4530	UR3	C2-N3	5.66	1.50	1.39
6	2	2804	OMC	C2-N3	5.65	1.47	1.36
6	2	4494	OMG	C2-N2	5.64	1.47	1.34
6	2	1883	OMG	C2-N2	5.64	1.47	1.34
6	2	2364	OMG	C2-N2	5.63	1.47	1.34
6	2	4370	OMG	C4-N3	5.63	1.47	1.34
6	2	373	OMG	C4-N3	5.62	1.47	1.34
6	2	1522	OMG	C4-N3	5.61	1.47	1.34
6	2	4623	OMG	C2-N2	5.60	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	4371	MHG	C2-N2	5.59	1.45	1.33
6	2	1625	OMG	C2-N3	5.58	1.46	1.33
6	2	1348	P4U	C6-C5	5.57	1.48	1.35
6	2	1883	OMG	C2-N3	5.57	1.46	1.33
6	2	3880	P7G	C8-N7	5.57	1.51	1.45
6	2	2297	E7G	C8-N7	5.57	1.51	1.45
6	2	1797	E7G	C4-N3	5.54	1.47	1.34
6	2	2365	OMC	C6-C5	5.54	1.47	1.35
6	2	4370	OMG	C2-N3	5.54	1.46	1.33
6	2	2364	OMG	C4-N3	5.53	1.47	1.34
6	2	1909	P7G	C2-N2	5.52	1.47	1.34
6	2	4637	OMG	C4-N3	5.51	1.47	1.34
6	2	373	OMG	C2-N3	5.50	1.46	1.33
6	2	4355	E6G	O6-C6	5.49	1.43	1.35
6	2	4637	OMG	C2-N2	5.44	1.47	1.34
6	2	4371	MHG	C4-N3	5.43	1.47	1.34
6	2	3869	OMC	C6-C5	5.43	1.47	1.35
6	2	1797	E7G	C2-N3	5.43	1.46	1.33
6	2	2804	OMC	C6-C5	5.42	1.47	1.35
6	2	4623	OMG	C2-N3	5.42	1.46	1.33
6	2	4597	UR3	C2-N1	5.42	1.46	1.38
6	2	2297	E7G	C4-N3	5.41	1.47	1.34
6	2	4623	OMG	C4-N3	5.40	1.47	1.34
6	2	4306	OMU	C6-C5	5.40	1.47	1.35
6	2	2297	E7G	C2-N3	5.38	1.46	1.33
6	2	237	B9B	C2-N2	5.36	1.44	1.33
6	2	2364	OMG	C2-N3	5.35	1.46	1.33
6	2	1605	7MG	C2-N3	5.33	1.46	1.33
6	2	4637	OMG	C2-N3	5.32	1.46	1.33
6	2	4872	2MG	C4-N3	5.31	1.46	1.34
6	2	2754	B9B	C2-N2	5.29	1.44	1.33
6	2	1522	OMG	C2-N3	5.28	1.45	1.33
6	2	3869	OMC	C2-N1	5.28	1.51	1.40
6	2	1605	7MG	C4-N3	5.28	1.46	1.34
6	2	1574	B9B	C2-N2	5.27	1.44	1.33
6	2	4620	OMU	C6-C5	5.25	1.47	1.35
6	2	4483	B8T	C2-N1	5.21	1.51	1.40
6	2	4550	7MG	C2-N3	5.17	1.45	1.33
6	2	1524	A2M	O4'-C1'	-5.15	1.29	1.42
6	2	3897	B8K	C4-N9	5.06	1.43	1.37
6	2	4550	7MG	C4-N3	5.06	1.46	1.34
6	2	3718	A2M	O4'-C1'	-5.02	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	3899	BGH	C4-N3	5.00	1.46	1.34
57	8	14	OMU	C6-C5	4.99	1.46	1.35
6	2	3899	BGH	C2-N3	4.98	1.45	1.33
6	2	1797	E7G	C2-N2	4.98	1.46	1.34
6	2	2297	E7G	C2-N2	4.96	1.46	1.34
6	2	1534	A2M	O4'-C1'	-4.96	1.30	1.42
6	2	4564	M7A	C4-N9	4.96	1.47	1.38
6	2	4571	A2M	O4'-C1'	-4.91	1.30	1.42
6	2	4371	MHG	C4-N9	4.88	1.43	1.37
6	2	4523	A2M	O4'-C1'	-4.88	1.30	1.42
6	2	2363	A2M	O4'-C1'	-4.87	1.30	1.42
6	2	3880	P7G	C2-N1	4.86	1.44	1.33
6	2	2522	7MG	C2-N3	4.84	1.44	1.33
6	2	2401	A2M	O4'-C1'	-4.82	1.30	1.42
6	2	2522	7MG	C4-N3	4.81	1.45	1.34
6	2	3899	BGH	C4-N9	4.80	1.43	1.37
6	2	3867	A2M	O4'-C1'	-4.77	1.30	1.42
6	2	3887	OMC	C4-N3	4.77	1.44	1.34
6	2	2422	OMC	C2-N1	4.76	1.50	1.40
6	2	4536	OMC	C4-N4	4.76	1.45	1.33
6	2	2297	E7G	C4-N9	4.74	1.43	1.37
6	2	1326	A2M	O4'-C1'	-4.73	1.30	1.42
6	2	2422	OMC	C4-N4	4.73	1.45	1.33
6	2	2804	OMC	C4-N4	4.72	1.45	1.33
6	2	2861	OMC	C2-N1	4.71	1.50	1.40
6	2	3701	OMC	C4-N3	4.67	1.43	1.34
6	2	2861	OMC	C4-N4	4.65	1.44	1.33
6	2	1605	7MG	C4-N9	4.65	1.43	1.37
6	2	3723	A2M	O4'-C1'	-4.63	1.31	1.42
6	2	3887	OMC	C4-N4	4.62	1.44	1.33
6	2	1605	7MG	C2-N2	4.61	1.45	1.34
6	2	1871	A2M	O4'-C1'	-4.61	1.31	1.42
6	2	3869	OMC	C4-N4	4.60	1.44	1.33
6	2	2861	OMC	C4-N3	4.59	1.43	1.34
6	2	398	A2M	O4'-C1'	-4.59	1.31	1.42
6	2	4550	7MG	C2-N2	4.55	1.45	1.34
6	2	3701	OMC	C4-N4	4.54	1.44	1.33
6	2	1326	A2M	C6-N6	4.53	1.45	1.34
6	2	1909	P7G	C2-N1	4.52	1.44	1.33
6	2	2365	OMC	C4-N4	4.49	1.44	1.33
6	2	1348	P4U	O4-C4	4.48	1.40	1.35
6	2	1322	1MA	C5-C6	4.48	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	4637	OMG	C5-N7	-4.45	1.30	1.39
6	2	2365	OMC	C4-N3	4.45	1.43	1.34
6	2	1456	B8Q	C2-N1	4.44	1.44	1.38
6	2	1871	A2M	C6-N6	4.44	1.45	1.34
6	2	3867	A2M	C6-N6	4.43	1.45	1.34
6	2	2804	OMC	C2-N1	4.42	1.49	1.40
6	2	4335	5MC	C4-N4	4.42	1.45	1.34
6	2	3899	BGH	C2-N2	4.40	1.44	1.34
6	2	3887	OMC	C2-N1	4.39	1.49	1.40
6	2	1625	OMG	C5-N7	-4.39	1.30	1.39
6	2	2401	A2M	C6-N6	4.39	1.45	1.34
6	2	3723	A2M	C6-N6	4.38	1.45	1.34
6	2	2422	OMC	C4-N3	4.36	1.43	1.34
6	2	1524	A2M	C6-N6	4.35	1.45	1.34
6	2	4690	B8K	C4-N9	4.35	1.42	1.37
6	2	4523	A2M	C6-N6	4.34	1.45	1.34
6	2	4536	OMC	C2-N1	4.33	1.49	1.40
6	2	4536	OMC	C4-N3	4.29	1.43	1.34
6	2	1860	B8H	C2-N3	4.27	1.45	1.38
6	2	4571	A2M	C6-N6	4.24	1.44	1.34
6	2	3718	A2M	C6-N6	4.24	1.44	1.34
6	2	398	A2M	C6-N6	4.23	1.44	1.34
6	2	4083	5MU	C2-N3	4.23	1.45	1.38
6	2	2424	OMG	C5-N7	-4.20	1.30	1.39
6	2	2522	7MG	C2-N2	4.18	1.44	1.34
6	2	2804	OMC	C4-N3	4.17	1.42	1.34
6	2	4564	M7A	C6-N6	4.17	1.44	1.34
6	2	2050	OMG	C5-N7	-4.17	1.31	1.39
6	2	3899	BGH	C5-N7	4.17	1.46	1.39
6	2	3897	B8K	C4-N3	4.16	1.44	1.34
6	2	2363	A2M	C6-N6	4.16	1.44	1.34
6	2	4494	OMG	C5-N7	-4.15	1.31	1.39
6	2	4335	5MC	C6-N1	4.14	1.45	1.38
6	2	1522	OMG	C5-N7	-4.14	1.31	1.39
6	2	1316	OMG	C5-N7	-4.14	1.31	1.39
6	2	3869	OMC	C4-N3	4.10	1.42	1.34
6	2	3701	OMC	C2-N1	4.06	1.48	1.40
6	2	1348	P4U	C2-N1	4.05	1.48	1.40
6	2	1534	A2M	C6-N6	4.03	1.44	1.34
6	2	4690	B8K	C4-N3	4.02	1.43	1.34
6	2	4296	B8H	C2-N3	3.98	1.45	1.38
6	2	1883	OMG	C5-N7	-3.97	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	3897	B8K	C5-C6	3.94	1.53	1.43
6	2	4335	5MC	C2-N1	3.94	1.48	1.40
6	2	2364	OMG	C5-N7	-3.93	1.31	1.39
6	2	1322	1MA	C2-N1	3.91	1.43	1.35
6	2	4623	OMG	C5-N7	-3.90	1.31	1.39
6	2	4690	B8K	C5-N7	3.90	1.46	1.39
6	2	1659	I4U	C5-C4	3.89	1.48	1.43
6	2	4671	B8T	C2-N1	3.83	1.48	1.40
6	2	1909	P7G	O6-C6	-3.82	1.17	1.23
6	2	978	2MG	C2-N1	3.82	1.42	1.36
6	2	4870	OMG	C5-N7	-3.82	1.31	1.39
6	2	4306	OMU	C4-N3	3.80	1.45	1.38
6	2	2773	OMG	C5-N7	-3.80	1.31	1.39
6	2	4529	B8W	C5-N7	-3.79	1.31	1.39
6	2	3897	B8K	C5-N7	3.77	1.46	1.39
6	2	3899	BGH	C5-C6	3.75	1.53	1.43
6	2	2365	OMC	C2-N1	3.73	1.48	1.40
6	2	1659	I4U	C2-N1	3.69	1.48	1.40
6	2	4370	OMG	C5-N7	-3.69	1.31	1.39
6	2	729	2MG	C2-N1	3.68	1.42	1.36
6	2	4371	MHG	C5-C6	3.68	1.53	1.43
6	2	1517	2MG	C2-N1	3.66	1.42	1.36
6	2	1574	B9B	C5-C4	-3.64	1.32	1.39
6	2	373	OMG	C5-N7	-3.61	1.32	1.39
6	2	3899	BGH	C71-N7	3.61	1.47	1.39
6	2	4872	2MG	C2-N1	3.61	1.42	1.36
6	2	2380	B8W	C5-N7	-3.61	1.32	1.39
6	2	4550	7MG	C4-N9	3.60	1.41	1.37
6	2	1797	E7G	C5-C6	3.59	1.52	1.43
6	2	4185	B8W	C5-C4	-3.56	1.32	1.39
6	2	4690	B8K	C5-C6	3.55	1.52	1.43
6	2	1316	OMG	O6-C6	-3.53	1.16	1.23
57	8	14	OMU	C4-N3	3.52	1.44	1.38
6	2	2050	OMG	O6-C6	-3.51	1.16	1.23
6	2	4690	B8K	C71-N7	3.51	1.47	1.39
6	2	4671	B8T	C5-C4	3.50	1.48	1.40
6	2	1517	2MG	C5-N7	-3.49	1.32	1.39
6	2	2297	E7G	C5-C6	3.47	1.52	1.43
6	2	4637	OMG	O6-C6	-3.47	1.17	1.23
6	2	2364	OMG	O6-C6	-3.47	1.17	1.23
6	2	1605	7MG	C5-C6	3.47	1.52	1.43
6	2	237	B9B	C5-C4	-3.47	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	1883	OMG	O6-C6	-3.46	1.17	1.23
6	2	1348	P4U	C5-C4	3.45	1.47	1.43
6	2	1909	P7G	C2-N3	3.44	1.46	1.37
6	2	4623	OMG	O6-C6	-3.44	1.17	1.23
6	2	1625	OMG	O6-C6	-3.43	1.17	1.23
6	2	4564	M7A	C5-N7	3.42	1.47	1.39
6	2	1522	OMG	O6-C6	-3.42	1.17	1.23
6	2	4870	OMG	O6-C6	-3.42	1.17	1.23
6	2	1605	7MG	C2-N1	3.41	1.46	1.37
6	2	3897	B8K	C71-N7	3.40	1.47	1.39
6	2	2754	B9B	C5-C4	-3.40	1.32	1.39
6	2	4355	E6G	C5-C4	-3.39	1.32	1.39
6	2	1909	P7G	C8-N7	3.37	1.49	1.45
6	2	4483	B8T	C6-N1	3.35	1.46	1.38
6	2	3887	OMC	C6-N1	3.35	1.46	1.38
6	2	3880	P7G	O6-C6	-3.34	1.18	1.23
6	2	729	2MG	C5-N7	-3.34	1.32	1.39
6	2	2522	7MG	C4-N9	3.34	1.41	1.37
6	2	4472	B8W	C5-C4	-3.33	1.32	1.39
6	2	2773	OMG	O6-C6	-3.33	1.17	1.23
6	2	4529	B8W	C8-N9	-3.32	1.31	1.37
6	2	373	OMG	O6-C6	-3.32	1.17	1.23
6	2	4530	UR3	C6-N1	3.32	1.46	1.38
6	2	2424	OMG	O6-C6	-3.31	1.17	1.23
6	2	4483	B8T	C5-C4	3.31	1.47	1.40
6	2	3899	BGH	O2'-C2'	3.31	1.51	1.42
6	2	4872	2MG	C5-N7	-3.30	1.32	1.39
6	2	3897	B8K	C2-N2	3.29	1.42	1.34
6	2	3880	P7G	C2-N3	3.29	1.45	1.37
6	2	2380	B8W	C5-C4	-3.28	1.32	1.39
6	2	4620	OMU	C4-N3	3.28	1.44	1.38
6	2	4690	B8K	C2-N2	3.26	1.42	1.34
6	2	2754	B9B	O6-C6	3.26	1.40	1.35
57	8	14	OMU	O4-C4	-3.25	1.18	1.24
6	2	1326	A2M	O3'-C3'	3.24	1.50	1.43
6	2	2401	A2M	C5-C4	-3.23	1.33	1.39
6	2	4550	7MG	C5-C6	3.23	1.51	1.43
6	2	3897	B8K	C6-N1	3.23	1.44	1.38
6	2	4083	5MU	O4-C4	-3.22	1.17	1.23
6	2	4370	OMG	O6-C6	-3.21	1.17	1.23
6	2	4472	B8W	C5-N7	-3.21	1.33	1.39
6	2	2363	A2M	C5-C4	-3.20	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	4185	B8W	C5-N7	-3.20	1.33	1.39
6	2	4371	MHG	C6-N1	3.19	1.44	1.38
6	2	2522	7MG	C2-N1	3.19	1.45	1.37
6	2	2363	A2M	C8-N9	-3.19	1.31	1.37
6	2	978	2MG	C5-N7	-3.18	1.32	1.39
6	2	237	B9B	C5-N7	-3.18	1.33	1.39
6	2	1348	P4U	O2-C2	-3.18	1.17	1.23
6	2	4671	B8T	O2-C2	-3.17	1.17	1.23
6	2	1797	E7G	C2-N1	3.17	1.45	1.37
6	2	2365	OMC	C6-N1	3.16	1.45	1.38
6	2	4494	OMG	O6-C6	-3.14	1.17	1.23
6	2	2297	E7G	C2-N1	3.14	1.45	1.37
6	2	4571	A2M	C5-C4	-3.14	1.33	1.39
6	2	1534	A2M	C5-C4	-3.14	1.33	1.39
6	2	398	A2M	C5-C4	-3.12	1.33	1.39
6	2	3880	P7G	C6-N1	3.12	1.43	1.38
6	2	4370	OMG	C6-N1	3.12	1.44	1.38
6	2	4083	5MU	O2-C2	-3.11	1.17	1.23
6	2	2804	OMC	O2-C2	-3.11	1.17	1.23
6	2	4083	5MU	C2-N1	3.11	1.43	1.38
6	2	4306	OMU	O4-C4	-3.10	1.18	1.24
6	2	1605	7MG	C6-N1	3.09	1.44	1.38
6	2	4620	OMU	O4-C4	-3.09	1.18	1.24
6	2	1871	A2M	C5-C4	-3.09	1.33	1.39
6	2	1866	UR3	C6-N1	3.09	1.45	1.38
6	2	2422	OMC	O2-C2	-3.08	1.18	1.23
6	2	2861	OMC	C6-N1	3.08	1.45	1.38
6	2	1659	I4U	C6-N1	3.07	1.45	1.38
6	2	4494	OMG	C6-N1	3.06	1.44	1.38
6	2	3899	BGH	O6-C6	-3.06	1.17	1.23
6	2	2522	7MG	C5-C6	3.06	1.51	1.43
6	2	1574	B9B	C5-N7	-3.06	1.33	1.39
6	2	3869	OMC	C6-N1	3.06	1.45	1.38
6	2	4529	B8W	C5-C4	-3.05	1.33	1.39
6	2	2365	OMC	O2-C2	-3.04	1.18	1.23
6	2	1574	B9B	O6-C6	3.03	1.39	1.35
6	2	1348	P4U	C6-N1	3.03	1.45	1.38
6	2	1797	E7G	C6-N1	3.01	1.44	1.38
6	2	237	B9B	O6-C6	3.01	1.39	1.35
6	2	4690	B8K	C6-N1	3.01	1.44	1.38
6	2	1659	I4U	O2-C2	-2.99	1.18	1.23
6	2	3701	OMC	O2-C2	-2.99	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	1524	A2M	O2'-C2'	-2.99	1.35	1.42
6	2	3897	B8K	C2-N1	2.99	1.45	1.37
6	2	1524	A2M	C5-C4	-2.99	1.33	1.39
6	2	3869	OMC	O2-C2	-2.99	1.18	1.23
6	2	3718	A2M	C5-C4	-2.98	1.33	1.39
6	2	3718	A2M	C5-N7	-2.98	1.33	1.39
6	2	3880	P7G	C5-C4	2.97	1.43	1.37
6	2	373	OMG	C6-N1	2.96	1.44	1.38
6	2	3899	BGH	C6-N1	2.96	1.44	1.38
6	2	2522	7MG	O6-C6	-2.94	1.18	1.23
6	2	3899	BGH	O3'-C3'	-2.93	1.36	1.43
6	2	2754	B9B	C5-N7	-2.93	1.33	1.39
6	2	4523	A2M	C5-C4	-2.93	1.33	1.39
6	2	1534	A2M	O2'-C2'	-2.93	1.35	1.42
6	2	4550	7MG	C2-N1	2.93	1.44	1.37
6	2	1909	P7G	C5-C4	2.93	1.43	1.37
6	2	4536	OMC	O2-C2	-2.93	1.18	1.23
6	2	2401	A2M	O2'-C2'	-2.92	1.35	1.42
6	2	4872	2MG	C4-N9	-2.92	1.30	1.38
6	2	4536	OMC	C6-N1	2.92	1.45	1.38
6	2	4597	UR3	C6-N1	2.91	1.45	1.38
6	2	237	B9B	C5-C6	-2.91	1.36	1.41
6	2	2380	B8W	C8-N9	-2.90	1.32	1.37
6	2	4483	B8T	O2-C2	-2.90	1.18	1.23
6	2	1326	A2M	C8-N9	-2.90	1.32	1.37
6	2	2424	OMG	C6-N1	2.89	1.44	1.38
6	2	3867	A2M	O2'-C2'	-2.88	1.35	1.42
6	2	2401	A2M	O3'-C3'	2.87	1.49	1.43
6	2	2422	OMC	C6-N1	2.87	1.44	1.38
6	2	1659	I4U	O4-C41	-2.86	1.40	1.47
6	2	1883	OMG	C6-N1	2.86	1.44	1.38
6	2	3899	BGH	C2-N1	2.86	1.44	1.37
6	2	3718	A2M	C8-N9	-2.86	1.32	1.37
6	2	3723	A2M	C5-C4	-2.85	1.33	1.39
6	2	2861	OMC	O2-C2	-2.85	1.18	1.23
6	2	4550	7MG	O6-C6	-2.85	1.18	1.23
6	2	4671	B8T	C6-N1	2.84	1.44	1.38
6	2	2804	OMC	C6-N1	2.83	1.44	1.38
6	2	1522	OMG	C6-N1	2.82	1.44	1.38
6	2	2364	OMG	C6-N1	2.81	1.44	1.38
6	2	2363	A2M	O2'-C2'	-2.81	1.35	1.42
6	2	4185	B8W	C8-N9	-2.81	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	1909	P7G	C6-N1	2.81	1.43	1.38
6	2	4623	OMG	C6-N1	2.81	1.44	1.38
6	2	2297	E7G	O6-C6	-2.80	1.18	1.23
6	2	4220	6MZ	C5-C4	-2.80	1.33	1.39
6	2	2363	A2M	C5-N7	-2.79	1.33	1.39
6	2	3867	A2M	C5-C4	-2.79	1.33	1.39
6	2	2401	A2M	C8-N9	-2.79	1.32	1.37
6	2	3718	A2M	C4-N9	-2.78	1.31	1.37
6	2	2773	OMG	C6-N1	2.78	1.44	1.38
6	2	4690	B8K	C2-N1	2.77	1.44	1.37
6	2	4523	A2M	O2'-C2'	-2.77	1.35	1.42
6	2	3718	A2M	O3'-C3'	2.77	1.49	1.43
6	2	1534	A2M	O3'-C3'	2.76	1.49	1.43
6	2	2363	A2M	O3'-C3'	2.76	1.49	1.43
6	2	4571	A2M	O2'-C2'	-2.76	1.35	1.42
6	2	4571	A2M	C8-N9	-2.76	1.32	1.37
6	2	2297	E7G	C6-N1	2.75	1.43	1.38
6	2	398	A2M	O2'-C2'	-2.74	1.35	1.42
6	2	1605	7MG	O6-C6	-2.74	1.18	1.23
6	2	4550	7MG	C6-N1	2.74	1.43	1.38
6	2	3701	OMC	C6-N1	2.74	1.44	1.38
6	2	2401	A2M	C5-N7	-2.73	1.33	1.39
6	2	237	B9B	C8-N9	-2.73	1.32	1.37
6	2	1524	A2M	O3'-C3'	2.73	1.49	1.43
6	2	3723	A2M	O3'-C3'	2.72	1.49	1.43
6	2	3887	OMC	O2-C2	-2.71	1.18	1.23
6	2	4335	5MC	O2-C2	-2.70	1.18	1.23
6	2	3718	A2M	O2'-C2'	-2.70	1.35	1.42
6	2	1534	A2M	C8-N9	-2.69	1.32	1.37
6	2	1326	A2M	O2'-C2'	-2.69	1.35	1.42
6	2	398	A2M	C5-N7	-2.69	1.33	1.39
6	2	4523	A2M	C8-N9	-2.68	1.32	1.37
57	8	14	OMU	O2-C2	-2.68	1.18	1.23
6	2	4220	6MZ	C5-N7	-2.68	1.34	1.39
6	2	4870	OMG	C6-N1	2.68	1.43	1.38
6	2	1524	A2M	C5-N7	-2.68	1.34	1.39
6	2	4523	A2M	O3'-C3'	2.67	1.49	1.43
6	2	398	A2M	C8-N9	-2.67	1.32	1.37
6	2	3867	A2M	O3'-C3'	2.67	1.49	1.43
6	2	1625	OMG	C6-N1	2.66	1.43	1.38
6	2	1871	A2M	O2'-C2'	-2.65	1.35	1.42
6	2	1524	A2M	C8-N9	-2.65	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	4306	OMU	O2-C2	-2.65	1.18	1.23
6	2	978	2MG	C5-C6	2.64	1.54	1.44
6	2	4620	OMU	O2-C2	-2.64	1.18	1.23
6	2	1326	A2M	C5-N7	-2.63	1.34	1.39
6	2	4370	OMG	C5-C6	2.62	1.54	1.44
6	2	398	A2M	O3'-C3'	2.62	1.49	1.43
6	2	4371	MHG	O6-C6	-2.62	1.18	1.23
6	2	1574	B9B	C8-N9	-2.62	1.32	1.37
6	2	4872	2MG	C5-C6	2.61	1.54	1.44
6	2	2522	7MG	C6-N1	2.61	1.43	1.38
6	2	3867	A2M	C5-N7	-2.60	1.34	1.39
6	2	1797	E7G	O6-C6	-2.60	1.18	1.23
6	2	1326	A2M	C5-C4	-2.59	1.34	1.39
6	2	4571	A2M	O3'-C3'	2.59	1.49	1.43
6	2	4690	B8K	O6-C6	-2.59	1.18	1.23
6	2	4637	OMG	C6-N1	2.58	1.43	1.38
6	2	4571	A2M	C5-N7	-2.57	1.34	1.39
6	2	4306	OMU	C6-N1	2.57	1.44	1.38
6	2	1316	OMG	C6-N1	2.57	1.43	1.38
6	2	3723	A2M	O2'-C2'	-2.56	1.36	1.42
6	2	1534	A2M	C5-N7	-2.56	1.34	1.39
6	2	1871	A2M	O3'-C3'	2.56	1.49	1.43
6	2	3897	B8K	C5-C4	2.55	1.46	1.38
6	2	2050	OMG	C6-N1	2.55	1.43	1.38
6	2	4571	A2M	C4-N9	-2.54	1.32	1.37
6	2	1659	I4U	O4-C4	2.54	1.40	1.35
6	2	3723	A2M	C5-N7	-2.51	1.34	1.39
6	2	1574	B9B	C5-C6	-2.50	1.36	1.41
6	2	4623	OMG	C5-C6	2.50	1.53	1.44
6	2	4370	OMG	C2-N1	2.49	1.43	1.37
6	2	1883	OMG	C4-N9	-2.47	1.31	1.38
6	2	729	2MG	C5-C6	2.47	1.53	1.44
6	2	1522	OMG	C4-N9	-2.46	1.31	1.38
6	2	4870	OMG	C5-C6	2.46	1.53	1.44
6	2	4690	B8K	C5-C4	2.46	1.46	1.38
6	2	2773	OMG	C5-C6	2.46	1.53	1.44
6	2	373	OMG	C5-C6	2.43	1.53	1.44
6	2	4597	UR3	O2-C2	-2.43	1.18	1.22
6	2	2364	OMG	C5-C6	2.42	1.53	1.44
6	2	3867	A2M	C8-N9	-2.41	1.33	1.37
6	2	1522	OMG	C5-C6	2.41	1.53	1.44
6	2	1316	OMG	C5-C6	2.41	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	1517	2MG	C5-C6	2.41	1.53	1.44
6	2	1871	A2M	C5-N7	-2.40	1.34	1.39
6	2	2786	B9H	C6-N1	2.39	1.43	1.38
6	2	4523	A2M	C5-N7	-2.38	1.34	1.39
6	2	373	OMG	C4-N9	-2.37	1.31	1.38
6	2	2754	B9B	C5-C6	-2.36	1.37	1.41
6	2	4296	B8H	O4-C4	-2.36	1.19	1.23
6	2	1866	UR3	C4-N3	2.35	1.46	1.40
6	2	4637	OMG	C5-C6	2.35	1.53	1.44
6	2	1871	A2M	C8-N9	-2.35	1.33	1.37
6	2	4623	OMG	C4-N9	-2.34	1.32	1.38
6	2	729	2MG	O6-C6	-2.34	1.19	1.23
6	2	1517	2MG	O6-C6	-2.33	1.19	1.23
6	2	2050	OMG	C4-N9	-2.33	1.32	1.38
6	2	2424	OMG	C2-N1	2.33	1.43	1.37
6	2	2754	B9B	C8-N9	-2.33	1.33	1.37
6	2	4872	2MG	O6-C6	-2.32	1.19	1.23
6	2	2364	OMG	C4-N9	-2.32	1.32	1.38
6	2	978	2MG	C6-N1	2.31	1.43	1.38
6	2	4637	OMG	C4-N9	-2.30	1.32	1.38
6	2	1456	B8Q	C6-N1	2.28	1.43	1.38
6	2	4472	B8W	C8-N9	-2.28	1.33	1.37
6	2	4494	OMG	C5-C6	2.27	1.52	1.44
6	2	4355	E6G	C8-N9	-2.26	1.33	1.37
6	2	2773	OMG	C2-N1	2.26	1.43	1.37
6	2	4355	E6G	C5-N7	-2.26	1.34	1.39
6	2	1860	B8H	O4-C4	-2.25	1.19	1.23
6	2	3723	A2M	C8-N9	-2.24	1.33	1.37
6	2	1524	A2M	C4-N9	-2.24	1.32	1.37
6	2	4494	OMG	C2-N1	2.22	1.43	1.37
6	2	4530	UR3	C4-N3	2.22	1.45	1.40
6	2	1456	B8Q	O2-C2	-2.21	1.18	1.22
6	2	978	2MG	C4-N9	-2.21	1.32	1.38
6	2	3701	OMC	C5-C4	2.21	1.48	1.42
57	8	14	OMU	C6-N1	2.21	1.43	1.38
6	2	1517	2MG	C6-N1	2.20	1.42	1.38
6	2	1866	UR3	C5-C4	2.20	1.49	1.43
6	2	4597	UR3	C5-C4	2.20	1.49	1.43
6	2	4623	OMG	C2-N1	2.19	1.43	1.37
6	2	398	A2M	C4-N9	-2.19	1.32	1.37
6	2	1883	OMG	C2-N1	2.18	1.43	1.37
6	2	4571	A2M	O5'-C5'	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	1871	A2M	C4-N9	-2.18	1.32	1.37
6	2	1534	A2M	C4-N9	-2.17	1.32	1.37
6	2	2754	B9B	C4-N9	-2.17	1.32	1.37
6	2	4620	OMU	C6-N1	2.17	1.43	1.38
6	2	1316	OMG	C2-N1	2.16	1.43	1.37
6	2	1534	A2M	O5'-C5'	-2.15	1.39	1.44
6	2	4220	6MZ	C8-N9	-2.15	1.33	1.37
6	2	1625	OMG	C5-C6	2.15	1.52	1.44
6	2	1883	OMG	C5-C6	2.14	1.52	1.44
6	2	373	OMG	C2-N1	2.14	1.43	1.37
6	2	2424	OMG	C4-N9	-2.13	1.32	1.38
6	2	4870	OMG	C4-N9	-2.13	1.32	1.38
6	2	3887	OMC	C5-C4	2.11	1.47	1.42
6	2	4530	UR3	O2-C2	-2.11	1.18	1.22
6	2	4523	A2M	C4-N9	-2.11	1.33	1.37
6	2	2050	OMG	C2-N1	2.11	1.42	1.37
6	2	2364	OMG	C2-N1	2.11	1.42	1.37
6	2	729	2MG	C4-N9	-2.11	1.32	1.38
6	2	2050	OMG	C5-C6	2.10	1.52	1.44
6	2	4870	OMG	C2-N1	2.10	1.42	1.37
6	2	2363	A2M	O5'-C5'	-2.10	1.39	1.44
6	2	4306	OMU	C5-C4	2.08	1.48	1.43
6	2	1522	OMG	C2-N1	2.08	1.42	1.37
6	2	1316	OMG	C4-N9	-2.08	1.32	1.38
6	2	2401	A2M	C4-N9	-2.07	1.33	1.37
6	2	1326	A2M	C4-N9	-2.07	1.33	1.37
6	2	4370	OMG	C4-N9	-2.07	1.32	1.38
6	2	978	2MG	O6-C6	-2.06	1.19	1.23
6	2	1625	OMG	C2-N1	2.06	1.42	1.37
6	2	3867	A2M	C4-N9	-2.05	1.33	1.37
6	2	2861	OMC	C5-C4	2.05	1.47	1.42
6	2	4637	OMG	C2-N1	2.05	1.42	1.37
6	2	2424	OMG	C5-C6	2.05	1.52	1.44
6	2	3723	A2M	C4-N9	-2.04	1.33	1.37
6	2	1625	OMG	C4-N9	-2.04	1.32	1.38
6	2	1866	UR3	O2-C2	-2.04	1.18	1.22
6	2	4472	B8W	C4-N3	2.03	1.36	1.34
6	2	2363	A2M	C4-N9	-2.00	1.33	1.37

All (639) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1574	B9B	O6-C6-C5	21.62	143.95	116.57
6	2	2754	B9B	O6-C6-C5	20.90	143.03	116.57
6	2	237	B9B	O6-C6-C5	20.02	141.92	116.57
6	2	1574	B9B	O6-C6-N1	-18.80	93.81	120.00
6	2	2754	B9B	O6-C6-N1	-17.81	95.20	120.00
6	2	237	B9B	O6-C6-N1	-17.29	95.92	120.00
6	2	4564	M7A	C5-C6-N6	14.20	147.99	123.74
6	2	4564	M7A	N6-C6-N1	-11.57	93.00	118.35
6	2	4083	5MU	C5-C4-N3	10.33	124.13	115.31
6	2	4597	UR3	C4-N3-C2	-9.38	115.73	124.56
6	2	4220	6MZ	C4-N9-C1'	-9.34	104.33	126.59
6	2	4870	OMG	C1'-N9-C8	-9.23	100.42	126.70
6	2	4220	6MZ	C1'-N9-C8	9.21	147.93	127.14
6	2	2786	B9H	C31-N3-C2	9.09	128.56	117.21
6	2	4870	OMG	C1'-N9-C4	8.90	152.93	126.50
6	2	1517	2MG	C2-N3-C4	8.74	122.88	112.04
6	2	2424	OMG	C1'-N9-C4	8.72	152.40	126.50
6	2	4494	OMG	C1'-N9-C4	8.63	152.13	126.50
6	2	1625	OMG	C1'-N9-C4	8.60	152.06	126.50
6	2	2424	OMG	C1'-N9-C8	-8.57	102.31	126.70
6	2	2773	OMG	C1'-N9-C4	8.31	151.17	126.50
6	2	1522	OMG	C1'-N9-C4	8.27	151.06	126.50
6	2	1522	OMG	C1'-N9-C8	-8.23	103.28	126.70
6	2	4623	OMG	C1'-N9-C4	8.22	150.91	126.50
6	2	4637	OMG	C1'-N9-C4	8.17	150.78	126.50
6	2	4494	OMG	C1'-N9-C8	-8.16	103.46	126.70
6	2	2050	OMG	C1'-N9-C4	8.09	150.54	126.50
6	2	4623	OMG	C1'-N9-C8	-8.07	103.71	126.70
6	2	2050	OMG	C1'-N9-C8	-8.06	103.75	126.70
6	2	4637	OMG	C1'-N9-C8	-8.02	103.87	126.70
6	2	1316	OMG	C1'-N9-C8	-7.99	103.97	126.70
6	2	2773	OMG	C1'-N9-C8	-7.97	104.02	126.70
6	2	1625	OMG	C1'-N9-C8	-7.97	104.02	126.70
6	2	1316	OMG	C1'-N9-C4	7.97	150.16	126.50
6	2	2364	OMG	C1'-N9-C4	7.96	150.13	126.50
6	2	2786	B9H	C6-N1-C2	-7.91	114.70	121.79
6	2	4370	OMG	C1'-N9-C4	7.91	149.99	126.50
6	2	1534	A2M	N6-C6-N1	-7.88	101.10	118.35
6	2	4370	OMG	C1'-N9-C8	-7.84	104.37	126.70
6	2	2364	OMG	C1'-N9-C8	-7.78	104.55	126.70
6	2	4083	5MU	C5-C6-N1	-7.75	115.37	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1883	OMG	C1'-N9-C8	-7.63	104.97	126.70
6	2	4472	B8W	C5-C4-N3	-7.56	118.69	127.19
6	2	373	OMG	C1'-N9-C8	-7.55	105.22	126.70
6	2	4355	E6G	N2-C2-N3	7.53	128.96	117.25
6	2	1883	OMG	C1'-N9-C4	7.44	148.60	126.50
6	2	4529	B8W	C5-C4-N3	-7.43	118.83	127.19
6	2	4083	5MU	C4-N3-C2	-7.40	117.77	127.35
6	2	4523	A2M	N6-C6-N1	-7.19	102.60	118.35
6	2	1517	2MG	C5-C4-N3	-7.19	116.79	128.46
6	2	373	OMG	C1'-N9-C4	7.19	147.85	126.50
6	2	237	B9B	C5-C4-N3	-7.18	119.11	127.19
6	2	398	A2M	N6-C6-N1	-7.04	102.94	118.35
6	2	4355	E6G	C5-C4-N3	-7.02	119.29	127.19
6	2	4571	A2M	N6-C6-N1	-6.99	103.05	118.35
6	2	4296	B8H	C4-N3-C2	-6.98	118.31	127.35
6	2	978	2MG	C2-N3-C4	6.98	120.69	112.04
6	2	1909	P7G	C4-C5-N7	6.97	110.35	106.67
6	2	4690	B8K	C72-C71-N7	6.92	129.26	118.86
6	2	1860	B8H	C4-N3-C2	-6.87	118.45	127.35
6	2	4185	B8W	C5-C4-N3	-6.87	119.47	127.19
6	2	2401	A2M	N6-C6-N1	-6.86	103.33	118.35
6	2	2380	B8W	C5-C4-N3	-6.84	119.50	127.19
6	2	729	2MG	C2-N3-C4	6.82	120.50	112.04
6	2	1524	A2M	N6-C6-N1	-6.80	103.46	118.35
6	2	4472	B8W	O6-C6-N1	6.79	128.38	119.01
6	2	1326	A2M	N6-C6-N1	-6.72	103.64	118.35
6	2	2363	A2M	N3-C2-N1	-6.70	118.13	128.60
6	2	4371	MHG	C2-N3-C4	6.69	120.34	112.04
6	2	4564	M7A	N3-C2-N1	-6.67	118.16	128.60
6	2	4529	B8W	N2-C2-N3	6.67	127.62	117.25
6	2	3718	A2M	N6-C6-N1	-6.67	103.75	118.35
6	2	2363	A2M	N6-C6-N1	-6.66	103.75	118.35
6	2	3867	A2M	N6-C6-N1	-6.63	103.84	118.35
6	2	1534	A2M	C5-C6-N6	6.56	137.71	123.43
6	2	1534	A2M	N3-C2-N1	-6.55	118.36	128.60
6	2	3899	BGH	C72-C71-N7	6.55	128.71	118.86
6	2	2401	A2M	N3-C2-N1	-6.53	118.38	128.60
6	2	4523	A2M	N3-C2-N1	-6.53	118.39	128.60
6	2	4571	A2M	N3-C2-N1	-6.50	118.43	128.60
6	2	1871	A2M	N3-C2-N1	-6.47	118.48	128.60
6	2	4220	6MZ	N1-C2-N3	-6.45	118.51	128.60
6	2	4690	B8K	C5-C6-N1	6.44	122.35	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	398	A2M	N3-C2-N1	-6.44	118.52	128.60
6	2	3897	B8K	C72-C71-N7	6.42	128.51	118.86
6	2	1524	A2M	N3-C2-N1	-6.39	118.61	128.60
6	2	1574	B9B	C5-C4-N3	-6.35	120.05	127.19
6	2	4872	2MG	C2-N3-C4	6.32	119.88	112.04
6	2	1871	A2M	N6-C6-N1	-6.32	104.52	118.35
6	2	4523	A2M	C5-C6-N6	6.28	137.10	123.43
6	2	4220	6MZ	C5-C4-N3	-6.21	118.65	126.75
6	2	2380	B8W	N2-C2-N3	6.14	126.81	117.25
6	2	729	2MG	C5-C4-N3	-6.13	118.51	128.46
6	2	3723	A2M	N3-C2-N1	-6.11	119.05	128.60
6	2	4355	E6G	O6-C6-N1	6.09	128.48	120.00
6	2	3723	A2M	N6-C6-N1	-6.07	105.05	118.35
6	2	1326	A2M	N3-C2-N1	-6.07	119.11	128.60
6	2	3867	A2M	N3-C2-N1	-6.07	119.11	128.60
6	2	3718	A2M	N3-C2-N1	-6.04	119.16	128.60
6	2	3718	A2M	C5-C6-N6	5.98	136.45	123.43
57	8	14	OMU	C4-N3-C2	-5.98	118.69	126.58
6	2	398	A2M	C5-C6-N6	5.97	136.43	123.43
6	2	4872	2MG	C2-N1-C6	-5.94	117.64	124.48
6	2	1326	A2M	C5-C6-N6	5.91	136.29	123.43
6	2	4296	B8H	N3-C2-N1	5.89	121.51	115.14
6	2	4472	B8W	N2-C2-N3	5.89	126.41	117.25
6	2	1871	A2M	N9-C8-N7	-5.88	105.87	113.91
6	2	4571	A2M	C5-C6-N6	5.88	136.22	123.43
6	2	2754	B9B	C5-C4-N3	-5.85	120.61	127.19
6	2	4523	A2M	N9-C8-N7	-5.82	105.95	113.91
6	2	3897	B8K	C5-C6-N1	5.79	121.20	110.99
6	2	4529	B8W	O6-C6-N1	5.73	126.92	119.01
6	2	2363	A2M	N9-C8-N7	-5.72	106.09	113.91
6	2	1860	B8H	N3-C2-N1	5.68	121.28	115.14
6	2	2401	A2M	N9-C8-N7	-5.68	106.14	113.91
6	2	1524	A2M	N9-C8-N7	-5.67	106.15	113.91
6	2	4571	A2M	N9-C8-N7	-5.67	106.16	113.91
6	2	3899	BGH	C5-C6-N1	5.66	120.97	110.99
6	2	1456	B8Q	C31-N3-C4	5.66	122.78	114.25
6	2	2401	A2M	C5-C6-N6	5.65	135.72	123.43
6	2	1524	A2M	C5-C6-N6	5.64	135.71	123.43
6	2	398	A2M	N9-C8-N7	-5.64	106.20	113.91
6	2	2363	A2M	C5-C6-N6	5.63	135.68	123.43
6	2	4472	B8W	N3-C4-N9	5.62	134.78	126.99
6	2	978	2MG	C5-C4-N3	-5.60	119.37	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	4872	2MG	C5-C4-N3	-5.60	119.38	128.46
6	2	1534	A2M	N9-C8-N7	-5.59	106.27	113.91
6	2	3867	A2M	C5-C6-N6	5.58	135.57	123.43
6	2	3867	A2M	N9-C8-N7	-5.58	106.28	113.91
6	2	3723	A2M	N9-C8-N7	-5.56	106.31	113.91
6	2	1456	B8Q	O2-C2-N3	-5.55	114.80	122.95
6	2	1322	1MA	C5-C4-N3	-5.54	119.00	127.26
6	2	3869	OMC	O2-C2-N3	-5.50	113.38	122.33
6	2	4371	MHG	C5-C6-N1	5.50	120.68	110.99
6	2	4306	OMU	C4-N3-C2	-5.49	119.34	126.58
6	2	3880	P7G	C4-C5-N7	5.48	109.56	106.67
6	2	237	B9B	N3-C4-N9	5.48	134.59	126.99
6	2	4620	OMU	C4-N3-C2	-5.43	119.41	126.58
6	2	4083	5MU	N3-C2-N1	5.40	122.06	114.89
6	2	1517	2MG	N9-C4-N3	5.38	136.73	125.94
6	2	1866	UR3	O3'-C3'-C2'	5.37	129.19	111.82
6	2	1871	A2M	C5-C6-N6	5.36	135.10	123.43
6	2	2297	E7G	C5-C6-N1	5.36	120.44	110.99
6	2	1517	2MG	C2-N1-C6	-5.34	118.33	124.48
6	2	2380	B8W	C61-O6-C6	-5.34	111.92	117.21
6	2	1797	E7G	C5-C6-N1	5.34	120.40	110.99
6	2	1456	B8Q	N3-C2-N1	5.34	123.40	117.13
6	2	1871	A2M	C4-N9-C8	5.33	111.50	105.73
6	2	1326	A2M	N9-C8-N7	-5.27	106.70	113.91
6	2	1866	UR3	C6-N1-C2	-5.21	117.12	121.79
6	2	4523	A2M	C4-N9-C8	5.18	111.34	105.73
6	2	4371	MHG	C4-C5-N7	5.17	109.51	104.91
6	2	4472	B8W	O6-C6-C5	-5.17	110.49	116.97
6	2	4494	OMG	C5-C4-N3	-5.16	120.08	128.46
6	2	3899	BGH	C2-N3-C4	5.16	121.49	112.30
6	2	729	2MG	C2-N1-C6	-5.14	118.56	124.48
6	2	4571	A2M	C4-N9-C8	5.13	111.29	105.73
6	2	1625	OMG	C5-C4-N3	-5.12	120.15	128.46
6	2	1797	E7G	C4-C5-N7	5.12	109.46	104.91
6	2	3723	A2M	C5-C6-N6	5.11	134.55	123.43
6	2	4185	B8W	N2-C2-N3	5.09	125.17	117.25
6	2	2786	B9H	C32-C31-N3	5.08	123.08	112.47
6	2	2363	A2M	C4-N9-C8	5.08	111.23	105.73
6	2	4529	B8W	N3-C4-N9	5.07	134.03	126.99
6	2	1605	7MG	C5-C6-N1	5.06	119.90	110.99
6	2	1524	A2M	C4-N9-C8	5.02	111.17	105.73
6	2	4690	B8K	C4-C5-N7	5.02	109.37	104.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	2297	E7G	C4-C5-N7	5.00	109.36	104.91
6	2	3899	BGH	N9-C8-N7	5.00	110.04	103.33
6	2	3723	A2M	C4-N9-C8	5.00	111.14	105.73
6	2	4872	2MG	CM2-N2-C2	-4.99	112.83	123.86
6	2	2773	OMG	C5-C4-N3	-4.99	120.37	128.46
6	2	1797	E7G	C2-N3-C4	4.99	121.18	112.30
6	2	4870	OMG	C5-C4-N3	-4.97	120.41	128.46
6	2	3718	A2M	N9-C8-N7	-4.95	107.14	113.91
6	2	1316	OMG	C5-C4-N3	-4.94	120.44	128.46
6	2	2401	A2M	C4-N9-C8	4.94	111.08	105.73
6	2	4083	5MU	C5M-C5-C6	-4.92	116.28	122.85
6	2	4690	B8K	C2-N3-C4	4.90	121.04	112.30
6	2	2401	A2M	C5-C4-N3	-4.87	120.39	126.75
6	2	3867	A2M	C4-N9-C8	4.87	111.00	105.73
6	2	1456	B8Q	C6-N1-C2	-4.83	117.47	121.79
6	2	2522	7MG	C5-C6-N1	4.82	119.48	110.99
6	2	4564	M7A	N3-C4-N9	4.81	132.95	126.87
6	2	4637	OMG	C5-C4-N3	-4.79	120.68	128.46
6	2	3897	B8K	C2-N3-C4	4.77	120.80	112.30
6	2	398	A2M	C4-N9-C8	4.77	110.90	105.73
6	2	2424	OMG	C5-C4-N3	-4.75	120.75	128.46
6	2	1322	1MA	N1-C2-N3	-4.71	120.39	126.00
6	2	237	B9B	N2-C2-N3	4.70	124.56	117.25
6	2	1326	A2M	C4-N9-C8	4.67	110.79	105.73
6	2	1534	A2M	C4-N9-C8	4.67	110.79	105.73
6	2	2364	OMG	C5-C4-N3	-4.65	120.91	128.46
6	2	2050	OMG	C5-C4-N3	-4.65	120.92	128.46
6	2	1574	B9B	N2-C2-N3	4.65	124.48	117.25
6	2	1574	B9B	N9-C8-N7	-4.63	107.58	113.91
6	2	3899	BGH	C5-C4-N9	4.63	112.35	106.35
6	2	978	2MG	C2-N1-C6	-4.62	119.16	124.48
6	2	1316	OMG	C2-N3-C4	4.60	120.50	112.30
6	2	2364	OMG	C2-N3-C4	4.58	120.47	112.30
6	2	3867	A2M	C5-C4-N3	-4.58	120.77	126.75
6	2	4550	7MG	C5-C6-N1	4.58	119.06	110.99
6	2	2363	A2M	C5-C4-N3	-4.57	120.78	126.75
6	2	1866	UR3	O3'-C3'-C4'	4.52	124.12	111.05
6	2	2754	B9B	N9-C8-N7	-4.52	107.73	113.91
6	2	4185	B8W	N9-C8-N7	-4.52	107.74	113.91
6	2	4494	OMG	C2-N3-C4	4.51	120.34	112.30
6	2	1605	7MG	C2-N3-C4	4.51	120.34	112.30
6	2	4530	UR3	C4-N3-C2	-4.49	120.34	124.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1909	P7G	N9-C8-N7	4.48	109.79	103.38
6	2	4083	5MU	O4-C4-C5	-4.48	119.70	124.90
6	2	2297	E7G	C2-N3-C4	4.48	120.28	112.30
6	2	4370	OMG	C5-C4-N3	-4.47	121.21	128.46
6	2	4370	OMG	C2-N3-C4	4.44	120.22	112.30
6	2	373	OMG	C2-N3-C4	4.44	120.21	112.30
6	2	2773	OMG	C2-N3-C4	4.44	120.21	112.30
6	2	4637	OMG	C2-N3-C4	4.44	120.21	112.30
6	2	3899	BGH	C4-C5-N7	4.43	108.85	104.91
6	2	4220	6MZ	C2-N3-C4	4.43	122.22	111.75
6	2	4870	OMG	C2-N3-C4	4.41	120.16	112.30
6	2	2754	B9B	N2-C2-N3	4.41	124.11	117.25
6	2	3897	B8K	C5-C4-N9	4.41	112.07	106.35
6	2	1326	A2M	C5-C4-N3	-4.40	121.01	126.75
6	2	1522	OMG	C5-C4-N3	-4.39	121.33	128.46
6	2	1522	OMG	C2-N3-C4	4.39	120.11	112.30
6	2	3867	A2M	C1'-N9-C8	-4.39	117.23	127.14
6	2	1625	OMG	C2-N3-C4	4.38	120.11	112.30
6	2	3869	OMC	C1'-N1-C2	4.37	128.17	118.42
6	2	3723	A2M	C5-C4-N3	-4.36	121.06	126.75
6	2	2363	A2M	C1'-N9-C8	-4.35	117.31	127.14
6	2	398	A2M	C5-C4-N3	-4.34	121.08	126.75
6	2	729	2MG	N9-C4-N3	4.33	134.62	125.94
6	2	1797	E7G	C5-C4-N3	-4.31	119.92	128.13
6	2	4185	B8W	O6-C6-N1	4.30	124.94	119.01
6	2	3718	A2M	C4-N9-C8	4.29	110.38	105.73
6	2	237	B9B	N9-C8-N7	-4.29	108.04	113.91
6	2	1524	A2M	C5-C4-N3	-4.29	121.15	126.75
6	2	4623	OMG	C5-C4-N3	-4.28	121.52	128.46
6	2	1322	1MA	C2-N3-C4	4.27	120.80	112.41
6	2	2401	A2M	N3-C4-N9	4.27	134.11	127.08
6	2	1883	OMG	C2-N3-C4	4.26	119.90	112.30
6	2	1534	A2M	C5-C4-N3	-4.26	121.19	126.75
6	2	4220	6MZ	N3-C4-N9	4.25	134.09	127.08
6	2	1883	OMG	C5-C4-N3	-4.25	121.57	128.46
6	2	4355	E6G	N3-C4-N9	4.22	132.85	126.99
6	2	1326	A2M	C1'-N9-C8	-4.21	117.62	127.14
6	2	4571	A2M	C5-C4-N3	-4.21	121.26	126.75
6	2	4355	E6G	O6-C6-C5	-4.20	111.24	116.57
6	2	4690	B8K	N9-C8-N7	4.20	108.97	103.33
6	2	4620	OMU	N3-C2-N1	4.18	120.44	114.89
6	2	373	OMG	C5-C4-N3	-4.16	121.70	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	4523	A2M	C5-C4-N3	-4.16	121.32	126.75
6	2	2786	B9H	O3'-C3'-C2'	4.12	122.86	111.17
6	2	2424	OMG	C2-N3-C4	4.11	119.63	112.30
6	2	2380	B8W	N9-C8-N7	-4.09	108.32	113.91
6	2	1871	A2M	C5-C4-N3	-4.08	121.42	126.75
6	2	3723	A2M	N3-C4-N9	4.08	133.81	127.08
6	2	2363	A2M	N3-C4-N9	4.07	133.79	127.08
6	2	2401	A2M	C1'-N9-C8	-4.06	117.97	127.14
6	2	3867	A2M	N3-C4-N9	4.04	133.75	127.08
6	2	2422	OMC	O2-C2-N3	-4.04	115.76	122.33
6	2	1534	A2M	C2'-C1'-N9	4.02	120.30	113.53
6	2	4355	E6G	N9-C8-N7	-4.02	108.42	113.91
6	2	2050	OMG	C2-N3-C4	4.02	119.46	112.30
6	2	4571	A2M	C1'-N9-C8	-4.01	118.08	127.14
6	2	4690	B8K	C5-C4-N9	4.00	111.54	106.35
6	2	4355	E6G	N2-C2-N1	-4.00	111.04	117.25
6	2	1524	A2M	C1'-N9-C8	-3.98	118.14	127.14
6	2	3723	A2M	C1'-N9-C8	-3.97	118.17	127.14
6	2	1659	I4U	C5-C4-N3	-3.96	118.88	124.91
6	2	4472	B8W	N9-C8-N7	-3.96	108.50	113.91
6	2	4623	OMG	C2-N3-C4	3.94	119.32	112.30
6	2	4185	B8W	N3-C4-N9	3.94	132.45	126.99
6	2	4550	7MG	C2-N3-C4	3.92	119.29	112.30
6	2	2401	A2M	C2-N3-C4	3.92	121.01	111.75
6	2	4220	6MZ	N9-C8-N7	-3.90	108.58	113.91
6	2	2380	B8W	N3-C4-N9	3.86	132.35	126.99
6	2	1605	7MG	C5-C4-N9	3.85	111.34	106.35
6	2	4306	OMU	N3-C2-N1	3.84	119.99	114.89
6	2	3897	B8K	C4-C5-N7	3.84	108.32	104.91
6	2	2522	7MG	C5-C4-N9	3.82	111.31	106.35
57	8	14	OMU	N3-C2-N1	3.79	119.93	114.89
6	2	1534	A2M	C2-N3-C4	3.79	120.70	111.75
6	2	4083	5MU	C5M-C5-C4	3.78	122.92	118.77
6	2	1534	A2M	C1'-N9-C8	-3.77	118.62	127.14
6	2	1871	A2M	N3-C4-N9	3.77	133.29	127.08
6	2	1524	A2M	N3-C4-N9	3.76	133.28	127.08
6	2	1909	P7G	C71-N7-C5	3.76	133.42	124.52
6	2	3899	BGH	C5-C4-N3	-3.75	120.98	128.13
6	2	2363	A2M	C2-N3-C4	3.74	120.59	111.75
6	2	4523	A2M	C1'-N9-C8	-3.74	118.69	127.14
6	2	1574	B9B	N3-C4-N9	3.73	132.17	126.99
6	2	2804	OMC	O2-C2-N3	-3.72	116.28	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1326	A2M	N3-C4-N9	3.71	133.20	127.08
6	2	1524	A2M	C2-N3-C4	3.71	120.52	111.75
57	8	14	OMU	C5-C4-N3	3.71	120.39	114.84
6	2	4550	7MG	C5-C4-N9	3.71	111.16	106.35
6	2	1348	P4U	C5-C4-N3	-3.70	119.28	124.91
6	2	398	A2M	C2-N3-C4	3.69	120.47	111.75
6	2	398	A2M	N3-C4-N9	3.65	133.10	127.08
6	2	4185	B8W	N1-C2-N3	-3.65	119.69	125.42
6	2	4571	A2M	C2-N3-C4	3.65	120.38	111.75
6	2	4571	A2M	N3-C4-N9	3.65	133.10	127.08
6	2	2754	B9B	N3-C4-N9	3.64	132.04	126.99
6	2	2297	E7G	C5-C4-N3	-3.64	121.20	128.13
6	2	4296	B8H	C5-C4-N3	3.63	124.79	116.58
6	2	1860	B8H	C5-C4-N3	3.63	124.79	116.58
6	2	4523	A2M	C2-N3-C4	3.63	120.32	111.75
6	2	398	A2M	C1'-N9-C8	-3.62	118.95	127.14
6	2	1866	UR3	C4-N3-C2	-3.61	121.16	124.56
6	2	3897	B8K	N9-C8-N7	3.61	108.18	103.33
6	2	4371	MHG	C2-N1-C6	-3.61	120.33	124.48
6	2	2522	7MG	C2-N3-C4	3.60	118.70	112.30
6	2	1797	E7G	C5-C4-N9	3.59	111.01	106.35
6	2	4523	A2M	N3-C4-N9	3.58	132.98	127.08
6	2	1605	7MG	C5-C4-N3	-3.57	121.33	128.13
6	2	3867	A2M	C2-N3-C4	3.57	120.18	111.75
6	2	1574	B9B	N3-C2-N1	-3.54	119.87	125.42
6	2	1871	A2M	C2-N3-C4	3.53	120.10	111.75
57	8	14	OMU	CM2-O2'-C2'	3.53	123.78	114.52
6	2	2786	B9H	O2-C2-N1	-3.53	114.46	122.72
6	2	237	B9B	N3-C2-N1	-3.51	119.91	125.42
6	2	237	B9B	C61-O6-C6	-3.51	110.78	117.47
6	2	1871	A2M	C1'-N9-C8	-3.51	119.22	127.14
6	2	3718	A2M	C5-C4-N3	-3.50	122.18	126.75
6	2	4870	OMG	C2-N1-C6	-3.50	118.72	125.10
6	2	3723	A2M	C2-N3-C4	3.49	119.99	111.75
6	2	978	2MG	N9-C4-N3	3.49	132.94	125.94
6	2	4371	MHG	C5-C4-N3	-3.48	121.50	128.13
6	2	4306	OMU	C5-C4-N3	3.46	120.02	114.84
6	2	4529	B8W	O6-C6-C5	-3.46	112.63	116.97
6	2	2363	A2M	C5-N7-C8	3.46	108.43	103.51
6	2	4355	E6G	N3-C2-N1	-3.45	120.00	125.42
6	2	1326	A2M	C2-N3-C4	3.45	119.90	111.75
6	2	1534	A2M	N3-C4-N9	3.43	132.74	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	2786	B9H	C1'-N1-C6	3.42	128.30	120.84
6	2	4529	B8W	N2-C2-N1	-3.40	111.96	117.25
6	2	4220	6MZ	C4-C5-C6	3.38	119.42	116.81
6	2	1316	OMG	C2-N1-C6	-3.37	118.96	125.10
6	2	2424	OMG	C2-N1-C6	-3.36	118.96	125.10
6	2	2754	B9B	N3-C2-N1	-3.36	120.16	125.42
6	2	4637	OMG	C2-N1-C6	-3.35	118.98	125.10
6	2	4690	B8K	C6-C5-C4	-3.34	115.74	122.62
6	2	4564	M7A	C2-N3-C4	3.34	119.63	111.75
6	2	4523	A2M	C5-N7-C8	3.33	108.24	103.51
6	2	4620	OMU	C5-C4-N3	3.33	119.82	114.84
6	2	2380	B8W	N2-C2-N1	-3.32	112.09	117.25
6	2	1517	2MG	C5-C6-N1	3.32	121.62	113.19
6	2	2364	OMG	C2-N1-C6	-3.32	119.05	125.10
6	2	4597	UR3	C3U-N3-C2	3.31	123.12	117.31
6	2	4530	UR3	C6-N1-C2	-3.31	118.82	121.79
6	2	4083	5MU	C6-C5-C4	3.31	120.80	118.03
6	2	4371	MHG	C5-C4-N9	3.31	110.64	106.35
6	2	4690	B8K	C5-C4-N3	-3.30	121.85	128.13
6	2	2297	E7G	C5-C4-N9	3.29	110.62	106.35
6	2	4529	B8W	C6-C5-N7	-3.28	129.27	133.63
6	2	398	A2M	C5-N7-C8	3.27	108.16	103.51
6	2	4472	B8W	N1-C2-N3	-3.25	120.32	125.42
6	2	4472	B8W	C6-C5-N7	-3.24	129.34	133.63
6	2	2773	OMG	C2-N1-C6	-3.24	119.20	125.10
6	2	2401	A2M	C5-N7-C8	3.23	108.10	103.51
6	2	4623	OMG	C2-N1-C6	-3.23	119.20	125.10
6	2	4185	B8W	C5-N7-C8	3.23	108.10	103.51
6	2	2380	B8W	C5-N7-C8	3.22	108.09	103.51
6	2	3897	B8K	C5-C4-N3	-3.22	121.99	128.13
6	2	2380	B8W	O6-C6-N1	3.21	123.44	119.01
6	2	4494	OMG	C2-N1-C6	-3.20	119.27	125.10
6	2	4529	B8W	N1-C2-N3	-3.19	120.42	125.42
6	2	3899	BGH	O4'-C1'-N9	3.18	113.64	109.30
6	2	3867	A2M	C5-N7-C8	3.18	108.02	103.51
6	2	3869	OMC	O2-C2-N1	3.17	125.44	118.89
6	2	1574	B9B	C5-N7-C8	3.17	108.01	103.51
6	2	1883	OMG	C2'-C1'-N9	-3.15	108.10	114.22
6	2	373	OMG	C2-N1-C6	-3.15	119.36	125.10
6	2	1534	A2M	C5-N7-C8	3.15	107.98	103.51
6	2	2050	OMG	C2-N1-C6	-3.14	119.37	125.10
6	2	1517	2MG	O6-C6-C5	-3.13	118.30	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1522	OMG	C2-N1-C6	-3.13	119.40	125.10
6	2	1326	A2M	C5-N7-C8	3.12	107.94	103.51
6	2	1524	A2M	C5-N7-C8	3.12	107.94	103.51
6	2	3718	A2M	C2-N3-C4	3.11	119.11	111.75
6	2	4370	OMG	C2-N1-C6	-3.10	119.45	125.10
6	2	3897	B8K	C6-C5-C4	-3.10	116.23	122.62
6	2	4571	A2M	C5-N7-C8	3.09	107.90	103.51
6	2	4870	OMG	C5-C6-N1	3.08	121.02	113.19
6	2	2786	B9H	O3'-C3'-C4'	3.07	119.92	111.05
57	8	14	OMU	O4-C4-C5	-3.06	119.78	125.16
6	2	4690	B8K	C2-N1-C6	-3.05	119.54	125.10
6	2	1871	A2M	C5-N7-C8	3.04	107.83	103.51
6	2	1797	E7G	N9-C8-N7	3.04	107.73	103.38
6	2	373	OMG	N9-C8-N7	-3.04	107.67	113.39
6	2	1625	OMG	C2-N1-C6	-3.04	119.56	125.10
6	2	1316	OMG	C5-C6-N1	3.03	120.89	113.19
6	2	4483	B8T	O2-C2-N3	-3.02	117.41	122.33
6	2	4623	OMG	C5-C4-N9	3.02	111.11	105.63
6	2	4370	OMG	N2-C2-N1	3.01	123.13	116.71
6	2	1883	OMG	C2-N1-C6	-3.01	119.61	125.10
6	2	4220	6MZ	C5-N7-C8	3.01	107.78	103.51
6	2	3723	A2M	C5-N7-C8	2.99	107.76	103.51
6	2	2364	OMG	C5-C4-N9	2.98	111.03	105.63
6	2	4370	OMG	C5-C4-N9	2.97	111.02	105.63
6	2	1522	OMG	C5-C4-N9	2.97	111.02	105.63
6	2	1322	1MA	N9-C8-N7	-2.97	107.80	113.39
6	2	1871	A2M	C2'-C1'-N9	-2.95	108.56	113.53
6	2	373	OMG	C5-C6-N1	2.95	120.67	113.19
6	2	4494	OMG	O6-C6-C5	-2.94	118.80	126.60
6	2	1517	2MG	N1-C2-N3	-2.94	119.41	123.95
6	2	4335	5MC	CM5-C5-C6	-2.93	118.93	122.85
6	2	4550	7MG	C5-C4-N3	-2.93	122.54	128.13
6	2	1534	A2M	O4'-C1'-N9	-2.92	102.31	108.06
6	2	1866	UR3	O2'-C2'-C3'	2.91	121.24	111.82
6	2	2364	OMG	C5-C6-N1	2.90	120.56	113.19
6	2	237	B9B	C1'-N9-C8	-2.90	120.59	127.14
6	2	237	B9B	C4-N9-C8	2.88	108.85	105.73
6	2	2522	7MG	N9-C8-N7	2.88	107.49	103.38
6	2	4355	E6G	C5-N7-C8	2.87	107.58	103.51
6	2	4483	B8T	O3'-C3'-C4'	2.87	119.34	111.05
6	2	1322	1MA	N9-C4-N3	2.87	133.62	126.94
6	2	4371	MHG	N1-C2-N3	-2.86	119.53	123.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1860	B8H	O2-C2-N1	-2.85	119.66	122.87
6	2	4306	OMU	O4-C4-C5	-2.85	120.14	125.16
6	2	1625	OMG	C5-C4-N9	2.84	110.78	105.63
6	2	2522	7MG	C5-C4-N3	-2.84	122.72	128.13
6	2	1883	OMG	C5-C6-N1	2.84	120.40	113.19
6	2	2424	OMG	C5-C6-N1	2.84	120.40	113.19
6	2	978	2MG	C5-C6-N1	2.83	120.39	113.19
6	2	729	2MG	C5-C6-N1	2.83	120.39	113.19
6	2	4637	OMG	C5-C6-N1	2.83	120.38	113.19
6	2	1605	7MG	N9-C8-N7	2.83	107.42	103.38
6	2	3718	A2M	N3-C4-N9	2.83	131.74	127.08
6	2	2424	OMG	O6-C6-C5	-2.81	119.14	126.60
6	2	4637	OMG	C5-C4-N9	2.80	110.71	105.63
6	2	2773	OMG	C5-C6-N1	2.80	120.29	113.19
6	2	3899	BGH	C6-C5-C4	-2.79	116.86	122.62
6	2	1522	OMG	C5-C6-N1	2.79	120.28	113.19
6	2	2773	OMG	C5-C4-N9	2.78	110.68	105.63
6	2	4083	5MU	O2-C2-N1	-2.78	119.09	122.79
6	2	4483	B8T	O3'-C3'-C2'	2.78	120.80	111.82
6	2	4296	B8H	O2-C2-N1	-2.77	119.75	122.87
6	2	978	2MG	N9-C8-N7	-2.77	108.18	113.39
6	2	3718	A2M	C1'-N9-C8	-2.76	120.90	127.14
6	2	2050	OMG	C5-C6-N1	2.76	120.20	113.19
6	2	2754	B9B	C5-N7-C8	2.76	107.43	103.51
6	2	2380	B8W	N1-C2-N3	-2.75	121.10	125.42
6	2	4872	2MG	C5-C6-N1	2.75	120.17	113.19
6	2	1797	E7G	C2-N1-C6	-2.74	120.10	125.10
6	2	4872	2MG	N9-C4-N3	2.74	131.44	125.94
6	2	4494	OMG	C5-C6-N1	2.74	120.14	113.19
6	2	2422	OMC	C1'-N1-C2	2.73	124.51	118.42
6	2	1883	OMG	O6-C6-C5	-2.73	119.37	126.60
6	2	373	OMG	C5-C4-N9	2.72	110.57	105.63
6	2	2401	A2M	C2'-C1'-N9	-2.72	108.95	113.53
6	2	4637	OMG	O4'-C1'-N9	2.72	114.58	108.36
6	2	3897	B8K	O6-C6-N1	-2.71	114.93	120.12
6	2	1860	B8H	O4-C4-N3	-2.71	114.93	120.12
6	2	1456	B8Q	C31-N3-C2	2.70	121.72	117.79
6	2	2754	B9B	C4-N9-C8	2.70	108.66	105.73
6	2	4536	OMC	O2-C2-N3	-2.69	117.96	122.33
6	2	2861	OMC	O2-C2-N3	-2.68	117.97	122.33
6	2	237	B9B	C5-N7-C8	2.68	107.32	103.51
6	2	4620	OMU	O4-C4-C5	-2.68	120.45	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	2522	7MG	C4-C5-N7	2.68	109.25	105.53
6	2	1534	A2M	O4'-C1'-C2'	-2.67	101.89	106.57
6	2	4335	5MC	C5-C6-N1	-2.66	120.60	123.34
6	2	3899	BGH	C2-N1-C6	-2.66	120.25	125.10
6	2	4550	7MG	C4-C5-N7	2.66	109.22	105.53
6	2	4671	B8T	C6-C5-C4	2.66	120.22	116.96
6	2	4370	OMG	C5-C6-N1	2.65	119.91	113.19
6	2	4220	6MZ	C5-C6-N1	2.65	121.02	118.20
6	2	4371	MHG	C71-C72-C73	-2.64	106.81	114.20
6	2	3897	B8K	C2-N1-C6	-2.64	120.29	125.10
6	2	729	2MG	N9-C8-N7	-2.63	108.43	113.39
6	2	4185	B8W	C2-N3-C4	2.63	121.16	113.89
6	2	4870	OMG	O6-C6-C5	-2.63	119.63	126.60
6	2	2754	B9B	C61-O6-C6	-2.62	112.47	117.47
6	2	2050	OMG	O6-C6-C5	-2.62	119.66	126.60
6	2	1625	OMG	C5-C6-N1	2.61	119.82	113.19
6	2	729	2MG	O6-C6-C5	-2.61	119.68	126.60
6	2	373	OMG	C4-C5-N7	-2.61	106.60	110.72
6	2	4370	OMG	C4-C5-N7	-2.60	106.61	110.72
6	2	2297	E7G	C2-N1-C6	-2.60	120.37	125.10
6	2	373	OMG	O4'-C1'-N9	2.59	114.29	108.36
6	2	1625	OMG	O6-C6-C5	-2.59	119.73	126.60
6	2	4872	2MG	N9-C8-N7	-2.58	108.52	113.39
6	2	4623	OMG	C5-C6-N1	2.58	119.75	113.19
6	2	3718	A2M	C5-N7-C8	2.58	107.18	103.51
6	2	4870	OMG	N9-C8-N7	-2.58	108.53	113.39
6	2	373	OMG	C6-C5-N7	2.58	135.04	130.25
6	2	1605	7MG	C4-C5-N7	2.57	109.10	105.53
6	2	729	2MG	CM2-N2-C2	-2.57	118.19	123.86
6	2	1316	OMG	O4'-C1'-N9	2.57	114.23	108.36
6	2	4472	B8W	N2-C2-N1	-2.56	113.27	117.25
6	2	373	OMG	C2'-C1'-N9	-2.56	109.25	114.22
6	2	2380	B8W	C4-N9-C1'	-2.56	120.50	126.59
6	2	3899	BGH	O6-C6-N1	-2.55	115.23	120.12
6	2	373	OMG	CM2-O2'-C2'	-2.55	107.84	114.52
6	2	4472	B8W	C5-N7-C8	2.54	107.12	103.51
6	2	3869	OMC	C6-N1-C2	-2.54	116.08	120.49
6	2	237	B9B	C2-N3-C4	2.53	120.89	113.89
6	2	1316	OMG	C5-C4-N9	2.51	110.19	105.63
6	2	1883	OMG	N9-C8-N7	-2.51	108.66	113.39
6	2	4296	B8H	O4-C4-N3	-2.51	115.31	120.12
6	2	2861	OMC	C1'-N1-C2	2.51	124.01	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	4623	OMG	C4-C5-N7	-2.50	106.76	110.72
6	2	1574	B9B	C2-N3-C4	2.49	120.78	113.89
6	2	1316	OMG	O6-C6-C5	-2.49	119.99	126.60
6	2	4494	OMG	C5-C4-N9	2.49	110.15	105.63
6	2	4355	E6G	C2-N1-C6	2.48	119.88	115.93
6	2	4185	B8W	C4-N9-C1'	-2.48	120.69	126.59
6	2	1605	7MG	C2-N1-C6	-2.46	120.61	125.10
6	2	1574	B9B	C4-N9-C8	2.45	108.39	105.73
6	2	978	2MG	N1-C2-N3	-2.45	120.16	123.95
6	2	2522	7MG	C2-N1-C6	-2.45	120.64	125.10
6	2	4637	OMG	C4-C5-N7	-2.44	106.86	110.72
6	2	2804	OMC	O2-C2-N1	2.44	123.92	118.89
6	2	2773	OMG	O6-C6-C5	-2.43	120.15	126.60
6	2	2364	OMG	C4-C5-N7	-2.43	106.88	110.72
6	2	2364	OMG	O6-C6-C5	-2.43	120.16	126.60
6	2	2050	OMG	O4'-C1'-N9	2.43	113.91	108.36
6	2	4483	B8T	C6-N1-C2	-2.42	116.29	120.49
6	2	4494	OMG	O4'-C1'-N9	2.42	113.91	108.36
6	2	4370	OMG	N9-C8-N7	-2.42	108.83	113.39
6	2	4371	MHG	C6-C5-C4	-2.42	117.63	122.62
6	2	2364	OMG	N2-C2-N1	2.42	121.86	116.71
6	2	4623	OMG	N2-C2-N1	2.41	121.85	116.71
6	2	1348	P4U	O2-C2-N3	-2.41	118.41	122.33
6	2	1797	E7G	N9-C4-N3	2.41	129.07	125.47
6	2	373	OMG	O6-C6-C5	-2.40	120.23	126.60
6	2	1522	OMG	O6-C6-C5	-2.40	120.24	126.60
6	2	1883	OMG	C5-C4-N9	2.40	109.98	105.63
6	2	4690	B8K	O6-C6-C5	-2.40	121.66	127.54
6	2	1316	OMG	N9-C8-N7	-2.40	108.88	113.39
6	2	3880	P7G	N9-C8-N7	2.39	106.80	103.38
6	2	1522	OMG	N2-C2-N1	2.38	121.79	116.71
6	2	4472	B8W	C2-N3-C4	2.37	120.45	113.89
6	2	2050	OMG	C5-C4-N9	2.37	109.93	105.63
6	2	1883	OMG	O4'-C1'-N9	2.37	113.78	108.36
6	2	2297	E7G	N9-C8-N7	2.37	106.76	103.38
6	2	4371	MHG	O6-C6-C5	-2.36	121.75	127.54
6	2	1524	A2M	C4'-O4'-C1'	-2.35	104.28	109.47
6	2	2364	OMG	O4'-C1'-N9	2.35	113.73	108.36
6	2	4597	UR3	C6-N1-C2	-2.35	119.68	121.79
6	2	4355	E6G	C2-N3-C4	2.35	120.37	113.89
6	2	3869	OMC	C1'-N1-C6	-2.34	115.73	120.84
6	2	1522	OMG	C4-C5-N7	-2.34	107.01	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1909	P7G	N2-C2-N3	2.33	121.68	116.71
6	2	1883	OMG	N2-C2-N1	2.33	121.68	116.71
6	2	2422	OMC	C6-N1-C2	-2.33	116.45	120.49
6	2	4550	7MG	C6-C5-C4	-2.33	117.82	122.62
6	2	4637	OMG	N2-C2-N1	2.33	121.67	116.71
6	2	4872	2MG	O6-C6-C5	-2.33	120.43	126.60
6	2	978	2MG	O6-C6-C5	-2.32	120.44	126.60
6	2	2522	7MG	C6-C5-C4	-2.30	117.87	122.62
6	2	978	2MG	CM2-N2-C2	-2.30	118.78	123.86
6	2	4370	OMG	O4'-C1'-N9	2.30	113.63	108.36
6	2	4597	UR3	C5-C6-N1	-2.30	117.95	121.81
6	2	4355	E6G	C5-C6-N1	-2.29	120.27	123.46
6	2	3887	OMC	O2-C2-N3	-2.29	118.60	122.33
6	2	4529	B8W	N9-C8-N7	-2.29	110.78	113.91
6	2	4564	M7A	C2-N1-C6	2.28	122.68	118.77
6	2	4597	UR3	C3U-N3-C4	2.28	121.15	117.89
6	2	3899	BGH	N2-C2-N1	2.27	121.54	116.71
6	2	4870	OMG	C5-C4-N9	2.26	109.72	105.63
6	2	2297	E7G	C6-C5-C4	-2.25	117.99	122.62
6	2	2522	7MG	O6-C6-C5	-2.24	122.04	127.54
6	2	4185	B8W	C5-C6-N1	-2.24	120.34	123.46
6	2	4597	UR3	O2-C2-N1	-2.24	117.47	122.72
6	2	4637	OMG	O6-C6-C5	-2.24	120.66	126.60
6	2	1456	B8Q	C1'-N1-C2	2.24	120.77	116.99
6	2	3880	P7G	C71-N7-C5	2.23	129.80	124.52
6	2	4370	OMG	O6-C6-C5	-2.23	120.69	126.60
6	2	2804	OMC	C1'-N1-C2	2.23	123.39	118.42
6	2	373	OMG	N2-C2-N1	2.23	121.45	116.71
6	2	373	OMG	C8-N7-C5	2.22	108.25	104.24
6	2	1522	OMG	N9-C8-N7	-2.21	109.22	113.39
6	2	2424	OMG	O4'-C1'-N9	2.21	113.42	108.36
6	2	1522	OMG	O4'-C1'-N9	2.20	113.40	108.36
6	2	4185	B8W	C2-N1-C6	2.20	119.43	115.93
6	2	4185	B8W	C4-N9-C8	2.20	108.11	105.73
6	2	4637	OMG	N9-C8-N7	-2.20	109.25	113.39
6	2	4623	OMG	O4'-C1'-N9	2.20	113.38	108.36
6	2	4529	B8W	C2-N3-C4	2.19	119.95	113.89
6	2	2380	B8W	C4-C5-N7	-2.19	107.95	110.62
6	2	2364	OMG	N9-C8-N7	-2.19	109.27	113.39
6	2	1866	UR3	C2'-C1'-N1	2.19	119.41	113.22
6	2	2754	B9B	C2-N3-C4	2.18	119.92	113.89
6	2	4185	B8W	C4-C5-N7	-2.18	107.96	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	4529	B8W	C5-C6-N1	-2.17	120.44	123.46
6	2	4623	OMG	O6-C6-C5	-2.17	120.84	126.60
6	2	1517	2MG	N9-C8-N7	-2.17	109.30	113.39
6	2	3867	A2M	C4-N9-C1'	2.16	131.75	126.59
6	2	2773	OMG	C4-C5-N7	-2.16	107.30	110.72
6	2	1625	OMG	O4'-C1'-N9	2.15	113.29	108.36
6	2	2424	OMG	C5-C4-N9	2.15	109.54	105.63
6	2	4690	B8K	O6-C6-N1	-2.15	115.99	120.12
6	2	4623	OMG	N9-C8-N7	-2.15	109.34	113.39
6	2	4472	B8W	C4-N9-C8	2.15	108.05	105.73
6	2	4597	UR3	O2-C2-N3	-2.14	118.32	121.34
6	2	4370	OMG	C6-C5-N7	2.14	134.23	130.25
6	2	2380	B8W	C1'-N9-C8	2.14	131.96	127.14
6	2	2364	OMG	C6-C5-N7	2.13	134.22	130.25
6	2	1605	7MG	C6-C5-C4	-2.13	118.22	122.62
6	2	3869	OMC	C6-C5-C4	2.13	120.93	117.50
6	2	1522	OMG	C6-C5-N7	2.11	134.18	130.25
6	2	2297	E7G	O6-C6-C5	-2.10	122.39	127.54
6	2	2380	B8W	C2-N3-C4	2.10	119.69	113.89
6	2	1322	1MA	C8-N7-C5	2.09	108.03	104.24
6	2	4550	7MG	N1-C2-N3	-2.09	119.42	123.32
6	2	4529	B8W	C2-N1-C6	2.09	119.25	115.93
6	2	4536	OMC	C1'-N1-C2	2.09	123.08	118.42
6	2	1797	E7G	O6-C6-C5	-2.09	122.42	127.54
6	2	4370	OMG	C8-N7-C5	2.08	108.00	104.24
6	2	4550	7MG	N9-C8-N7	2.07	106.34	103.38
6	2	1316	OMG	C4-C5-N7	-2.07	107.44	110.72
6	2	1326	A2M	C4-N9-C1'	2.07	131.53	126.59
6	2	3899	BGH	N1-C2-N3	-2.07	119.46	123.32
6	2	1326	A2M	O3'-C3'-C2'	-2.07	105.30	111.17
6	2	1909	P7G	N3-C2-N1	-2.06	119.47	123.32
6	2	4083	5MU	O4-C4-N3	-2.06	116.17	120.12
6	2	2773	OMG	O4'-C1'-N9	2.06	113.07	108.36
6	2	3897	B8K	N1-C2-N3	-2.06	119.48	123.32
6	2	4690	B8K	N1-C2-N3	-2.05	119.49	123.32
6	2	2050	OMG	N9-C8-N7	-2.05	109.53	113.39
6	2	2422	OMC	O2-C2-N1	2.05	123.12	118.89
6	2	4870	OMG	C4-C5-N7	-2.05	107.48	110.72
6	2	2363	A2M	C4-N9-C1'	2.04	131.46	126.59
6	2	4371	MHG	C21-N2-C2	-2.04	119.35	123.86
6	2	4371	MHG	N9-C8-N7	2.04	106.30	103.38
6	2	4306	OMU	O2-C2-N1	-2.04	120.08	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	3867	A2M	O4'-C4'-C3'	-2.04	101.08	105.11
6	2	4564	M7A	C5-C4-N3	-2.03	121.85	126.62
6	2	2380	B8W	C5-C4-N9	2.03	108.15	105.78
6	2	978	2MG	C8-N7-C5	2.03	107.92	104.24
6	2	4370	OMG	C2'-C1'-N9	-2.03	110.28	114.22
6	2	4494	OMG	N2-C2-N1	2.03	121.03	116.71
6	2	2773	OMG	N2-C2-N1	2.02	121.02	116.71
6	2	2380	B8W	C5-C6-N1	-2.02	120.65	123.46
6	2	4623	OMG	C6-C5-N7	2.01	133.99	130.25
6	2	1605	7MG	O6-C6-C5	-2.00	122.63	127.54

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	8	14	OMU	C1'-C2'-O2'-CM2
6	2	237	B9B	C5-C6-O6-C61
6	2	237	B9B	N1-C6-O6-C61
6	2	237	B9B	C3'-C4'-C5'-O5'
6	2	398	A2M	O4'-C4'-C5'-O5'
6	2	1348	P4U	N3-C4-O4-C41
6	2	1574	B9B	C5-C6-O6-C61
6	2	1574	B9B	N1-C6-O6-C61
6	2	1625	OMG	C3'-C4'-C5'-O5'
6	2	1797	E7G	C3'-C4'-C5'-O5'
6	2	1797	E7G	O4'-C4'-C5'-O5'
6	2	1866	UR3	O4'-C4'-C5'-O5'
6	2	1866	UR3	C3'-C4'-C5'-O5'
6	2	1883	OMG	C3'-C4'-C5'-O5'
6	2	2364	OMG	O4'-C4'-C5'-O5'
6	2	2380	B8W	C5-C6-O6-C61
6	2	2380	B8W	N1-C6-O6-C61
6	2	2424	OMG	O4'-C4'-C5'-O5'
6	2	2424	OMG	C3'-C4'-C5'-O5'
6	2	2754	B9B	C5-C6-O6-C61
6	2	2754	B9B	N1-C6-O6-C61
6	2	2786	B9H	C32-C31-N3-C2
6	2	2786	B9H	C32-C31-N3-C4
6	2	3723	A2M	O4'-C4'-C5'-O5'
6	2	3867	A2M	O4'-C4'-C5'-O5'
6	2	3867	A2M	C3'-C4'-C5'-O5'
6	2	3869	OMC	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
6	2	3869	OMC	O4'-C1'-N1-C6
6	2	3880	P7G	O4'-C4'-C5'-O5'
6	2	3897	B8K	O4'-C4'-C5'-O5'
6	2	4185	B8W	C5-C6-O6-C61
6	2	4185	B8W	N1-C6-O6-C61
6	2	4220	6MZ	N1-C6-N6-C9
6	2	4355	E6G	C5-C6-O6-C61
6	2	4355	E6G	N1-C6-O6-C61
6	2	4371	MHG	C71-C72-C73-C75
6	2	4637	OMG	O4'-C4'-C5'-O5'
6	2	4637	OMG	C1'-C2'-O2'-CM2
6	2	4870	OMG	C3'-C4'-C5'-O5'
6	2	237	B9B	O4'-C4'-C5'-O5'
6	2	398	A2M	C3'-C4'-C5'-O5'
6	2	1883	OMG	O4'-C4'-C5'-O5'
6	2	2364	OMG	C3'-C4'-C5'-O5'
6	2	3723	A2M	C3'-C4'-C5'-O5'
6	2	3880	P7G	C3'-C4'-C5'-O5'
6	2	3897	B8K	C3'-C4'-C5'-O5'
6	2	4637	OMG	C3'-C4'-C5'-O5'
6	2	4870	OMG	O4'-C4'-C5'-O5'
6	2	1625	OMG	O4'-C4'-C5'-O5'
6	2	1909	P7G	O4'-C4'-C5'-O5'
6	2	4523	A2M	O4'-C4'-C5'-O5'
6	2	4523	A2M	C3'-C4'-C5'-O5'
6	2	4872	2MG	O4'-C4'-C5'-O5'
6	2	4872	2MG	C3'-C4'-C5'-O5'
6	2	4529	B8W	C5-C6-O6-C61
6	2	4296	B8H	C3'-C4'-C5'-O5'
6	2	4296	B8H	O4'-C4'-C5'-O5'
6	2	4371	MHG	C2'-C1'-N9-C8
6	2	4371	MHG	C71-C72-C73-C74
6	2	2297	E7G	C72-C71-N7-C8
6	2	4870	OMG	C4'-C5'-O5'-P
6	2	1605	7MG	O4'-C4'-C5'-O5'
6	2	1909	P7G	C3'-C4'-C5'-O5'
6	2	1524	A2M	C3'-C2'-O2'-CM'
6	2	2401	A2M	C3'-C2'-O2'-CM'
6	2	3869	OMC	C3'-C2'-O2'-CM2
6	2	3701	OMC	C2'-C1'-N1-C6
6	2	1326	A2M	C4'-C5'-O5'-P
6	2	4335	5MC	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
6	2	3899	BGH	O4'-C4'-C5'-O5'
6	2	373	OMG	C4'-C5'-O5'-P
6	2	3887	OMC	C4'-C5'-O5'-P
6	2	4523	A2M	C4'-C5'-O5'-P
6	2	4371	MHG	O4'-C4'-C5'-O5'
6	2	4529	B8W	N1-C6-O6-C61
6	2	3897	B8K	C4'-C5'-O5'-P
6	2	729	2MG	O4'-C4'-C5'-O5'
6	2	1797	E7G	C72-C71-N7-C8
6	2	4296	B8H	O4'-C1'-C5-C4
6	2	3869	OMC	C2'-C1'-N1-C6
6	2	3701	OMC	O4'-C1'-N1-C6
6	2	4371	MHG	O4'-C1'-N9-C8
6	2	1909	P7G	C72-C71-N7-C8
6	2	2297	E7G	C3'-C4'-C5'-O5'
6	2	3718	A2M	O4'-C4'-C5'-O5'
6	2	4306	OMU	C1'-C2'-O2'-CM2
6	2	1524	A2M	O4'-C1'-N9-C8
6	2	3701	OMC	C2'-C1'-N1-C2
6	2	3701	OMC	O4'-C1'-N1-C2
6	2	1534	A2M	O4'-C4'-C5'-O5'
6	2	4371	MHG	C72-C71-N7-C8
6	2	4371	MHG	N7-C71-C72-C73
6	2	1659	I4U	C42-C41-O4-C4
6	2	1659	I4U	C43-C41-O4-C4
6	2	3867	A2M	C4'-C5'-O5'-P
6	2	1605	7MG	C3'-C4'-C5'-O5'
6	2	2422	OMC	O4'-C4'-C5'-O5'
6	2	3880	P7G	N7-C71-C72-C73

There are no ring outliers.

18 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	2	1574	B9B	1	0
6	2	4306	OMU	1	0
57	8	14	OMU	1	0
6	2	729	2MG	1	0
6	2	4296	B8H	1	0
6	2	4371	MHG	1	0
6	2	1860	B8H	1	0
6	2	1866	UR3	1	0

Continued on next page...

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	2	4083	5MU	2	0
6	2	2363	A2M	1	0
6	2	2364	OMG	2	0
6	2	2754	B9B	1	0
6	2	1871	A2M	1	0
6	2	4620	OMU	1	0
6	2	2773	OMG	1	0
6	2	4872	2MG	2	0
6	2	4623	OMG	1	0
6	2	4637	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	GDP	A	801	64,63	28,30,30	1.27	3 (10%)	44,47,47	1.91	9 (20%)

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
62	GDP	A	801	64,63	-	2/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	A	801	GDP	C6-N1	-3.31	1.32	1.38
62	A	801	GDP	C5-N7	-2.51	1.34	1.39
62	A	801	GDP	C5-C4	2.34	1.45	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	A	801	GDP	C5-C4-N3	-6.17	118.45	128.46
62	A	801	GDP	C2-N3-C4	4.98	121.17	112.30
62	A	801	GDP	N9-C4-N3	4.62	135.22	125.94
62	A	801	GDP	PA-O3A-PB	-3.52	120.74	132.83
62	A	801	GDP	C6-C5-N7	3.09	136.00	130.25
62	A	801	GDP	C4-C5-N7	-2.54	106.70	110.72
62	A	801	GDP	O3B-PB-O2B	2.35	116.63	107.64
62	A	801	GDP	C3'-C2'-C1'	2.35	105.89	101.43
62	A	801	GDP	O6-C6-C5	-2.14	120.91	126.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

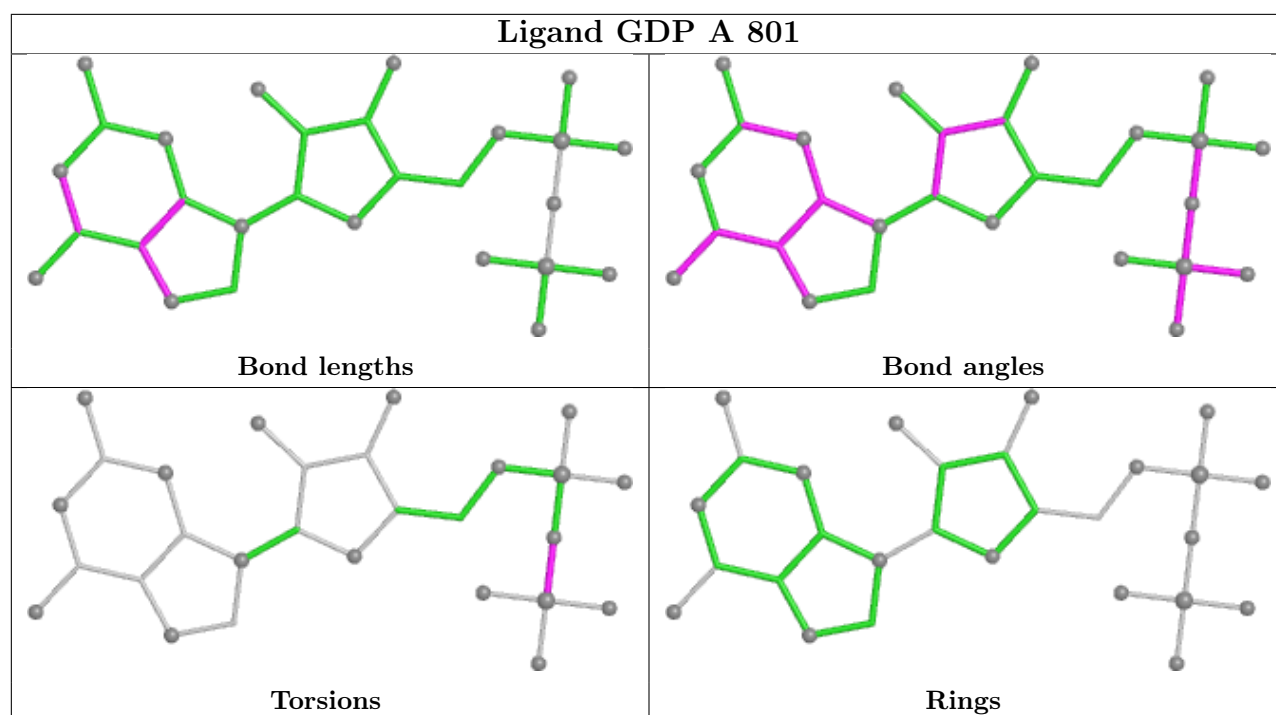
Mol	Chain	Res	Type	Atoms
62	A	801	GDP	PA-O3A-PB-O2B
62	A	801	GDP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	A	801	GDP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

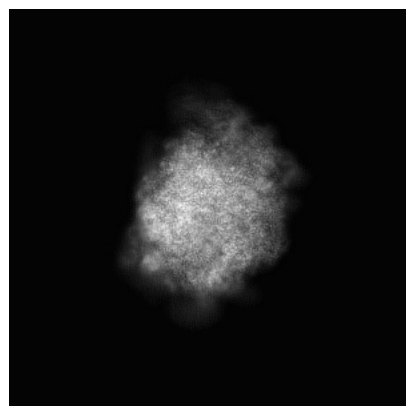
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35597. These allow visual inspection of the internal detail of the map and identification of artifacts.

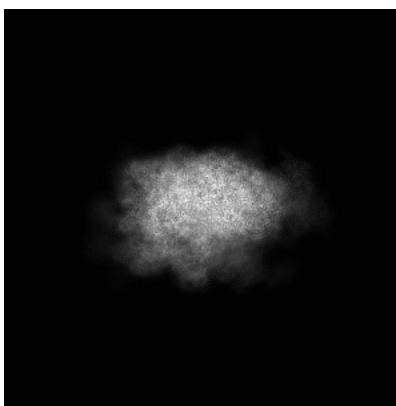
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

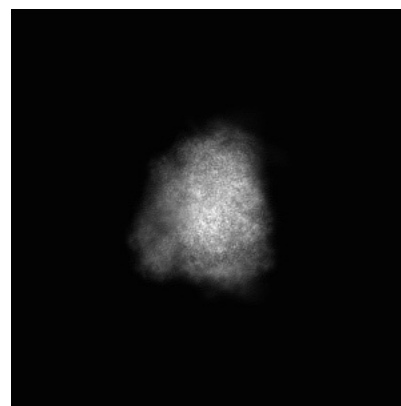
6.1.1 Primary map



X

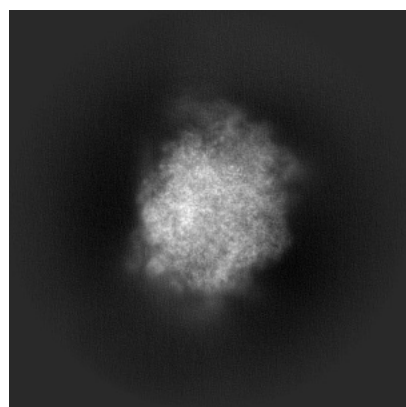


Y

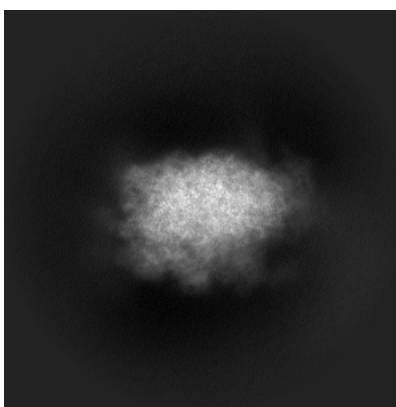


Z

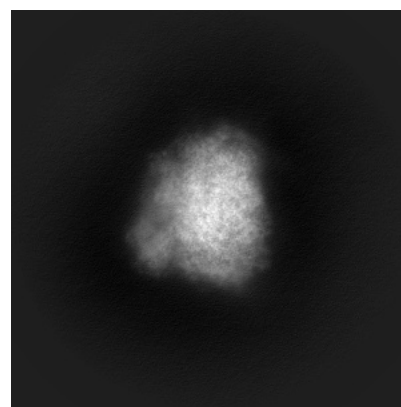
6.1.2 Raw map



X



Y

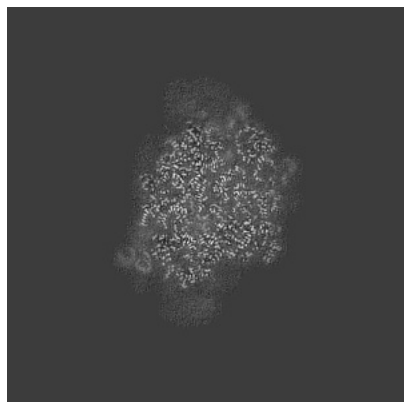


Z

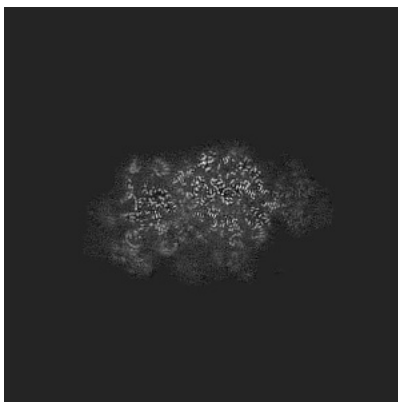
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

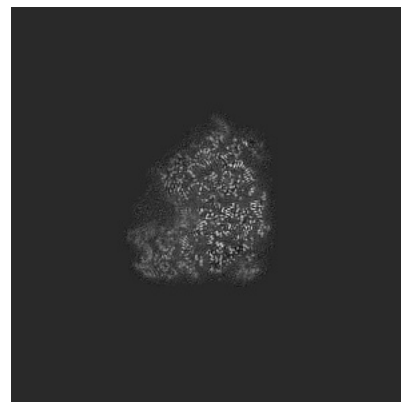
6.2.1 Primary map



X Index: 200

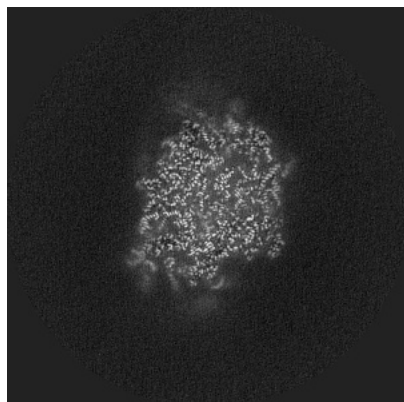


Y Index: 200

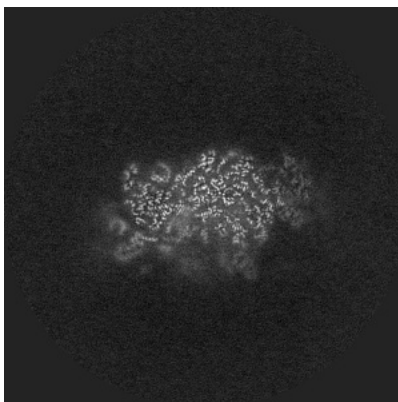


Z Index: 200

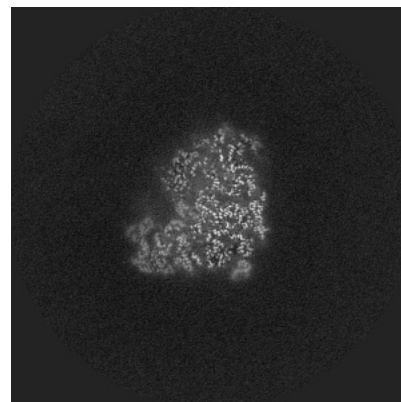
6.2.2 Raw map



X Index: 200



Y Index: 200

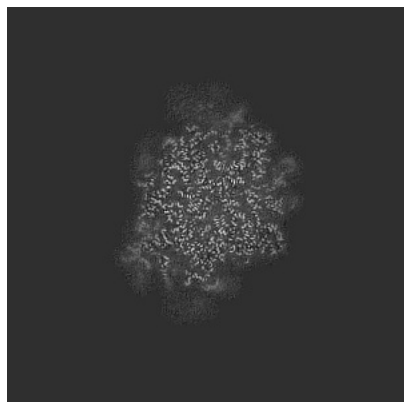


Z Index: 200

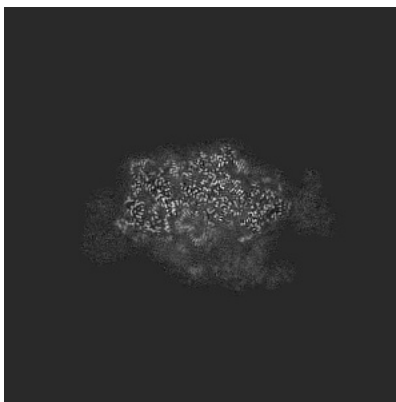
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

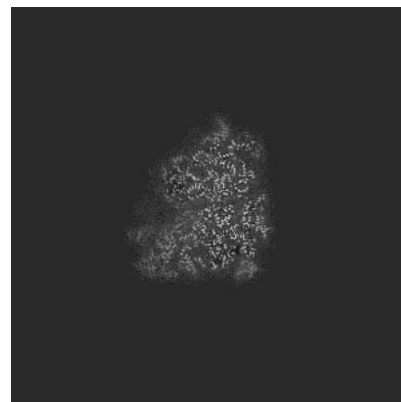
6.3.1 Primary map



X Index: 206

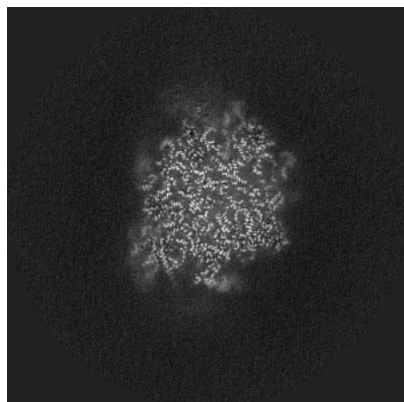


Y Index: 182

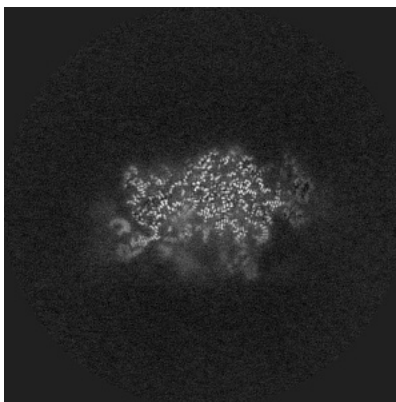


Z Index: 202

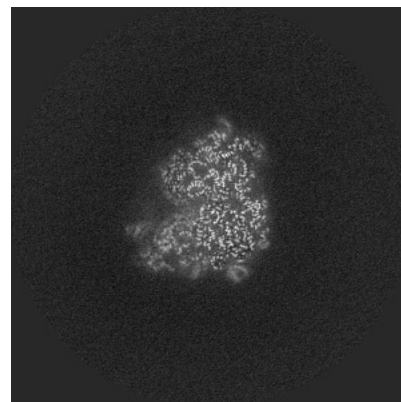
6.3.2 Raw map



X Index: 205



Y Index: 198

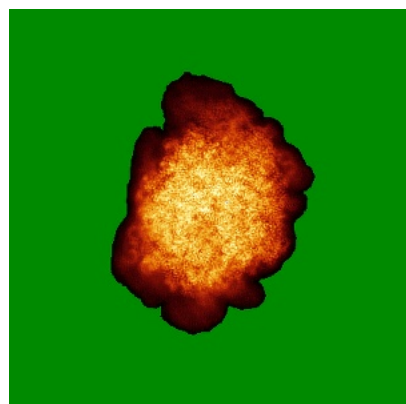


Z Index: 205

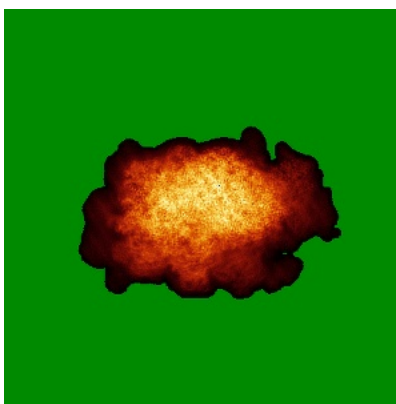
The images above show the largest variance slices of the map in three orthogonal directions.

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

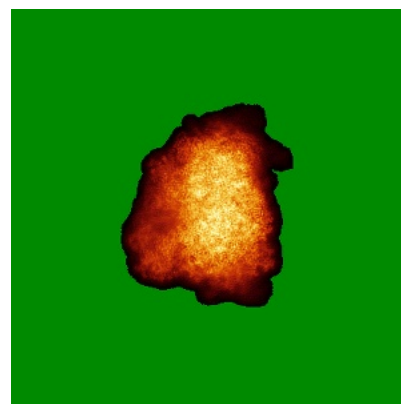
6.4.1 Primary map



X

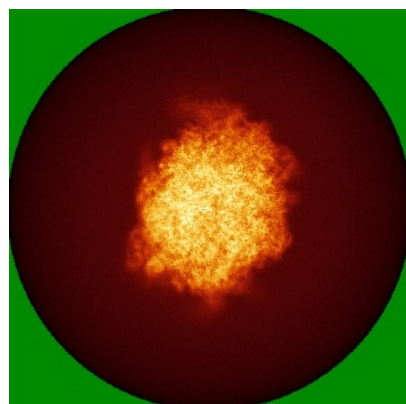


Y

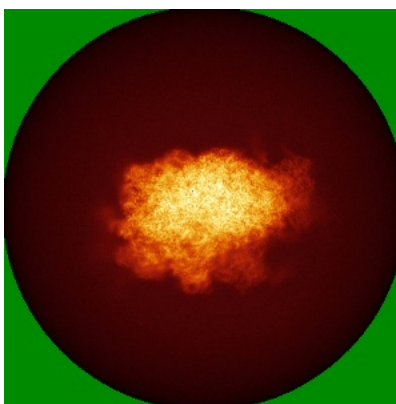


Z

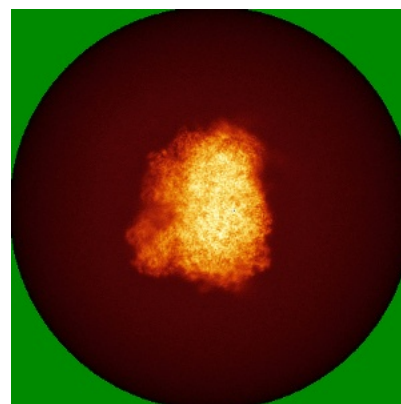
6.4.2 Raw map



X



Y

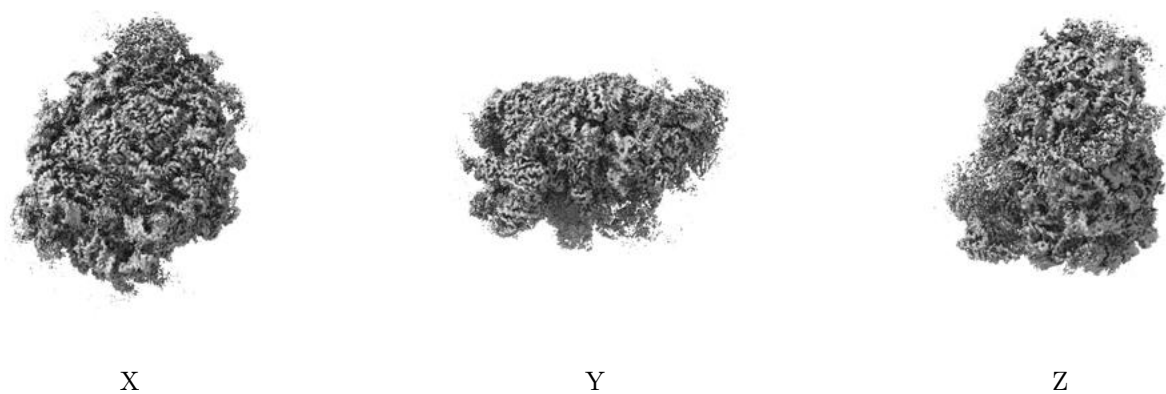


Z

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

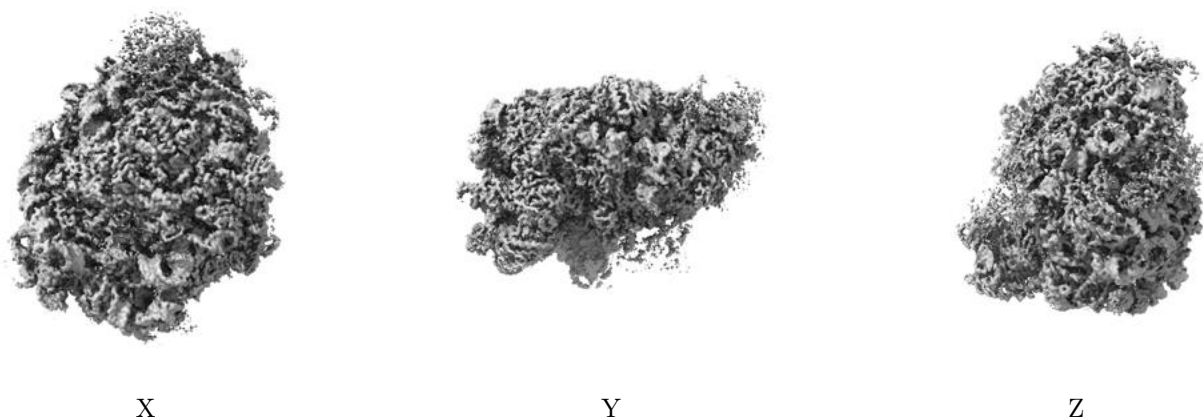
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

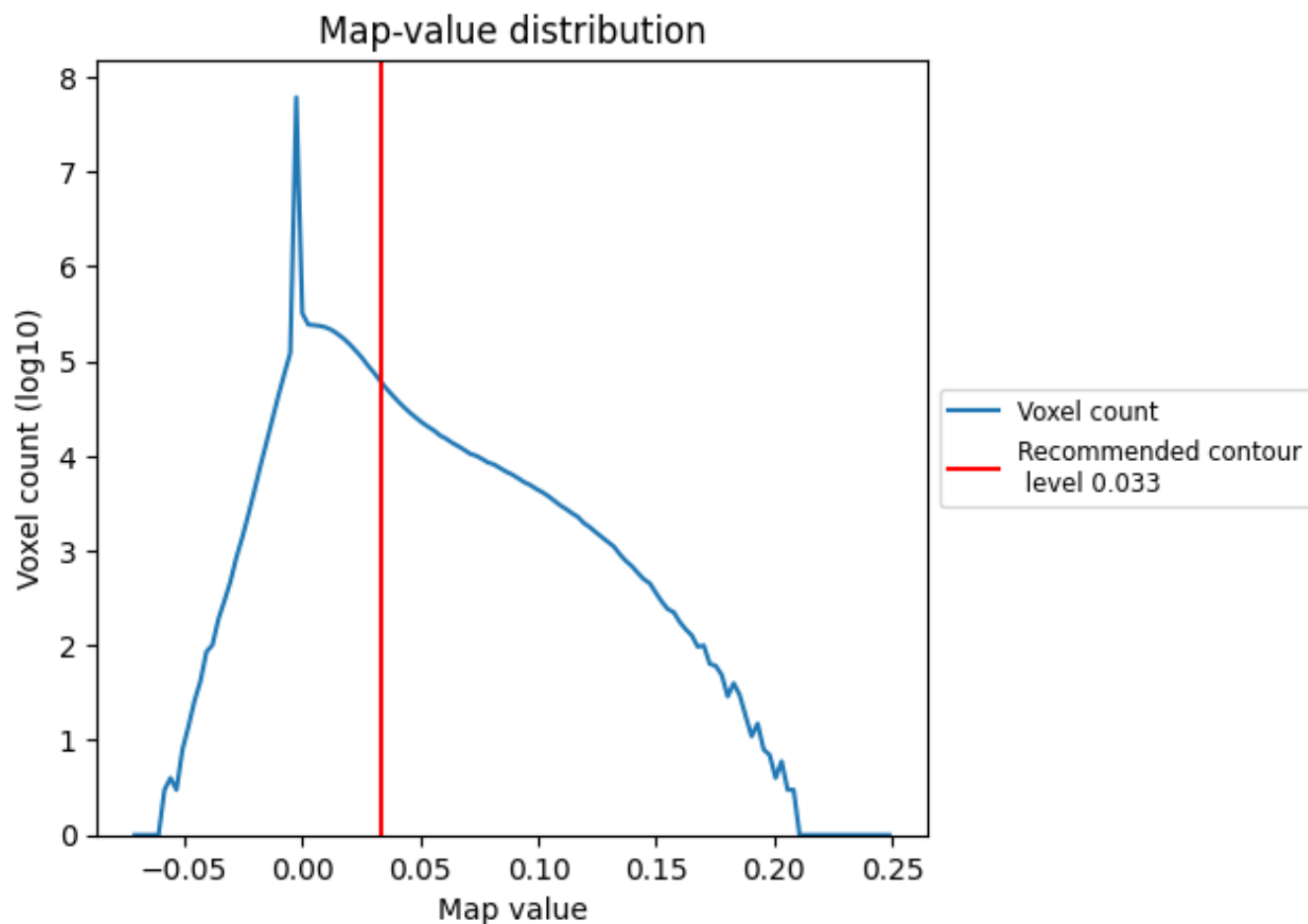
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

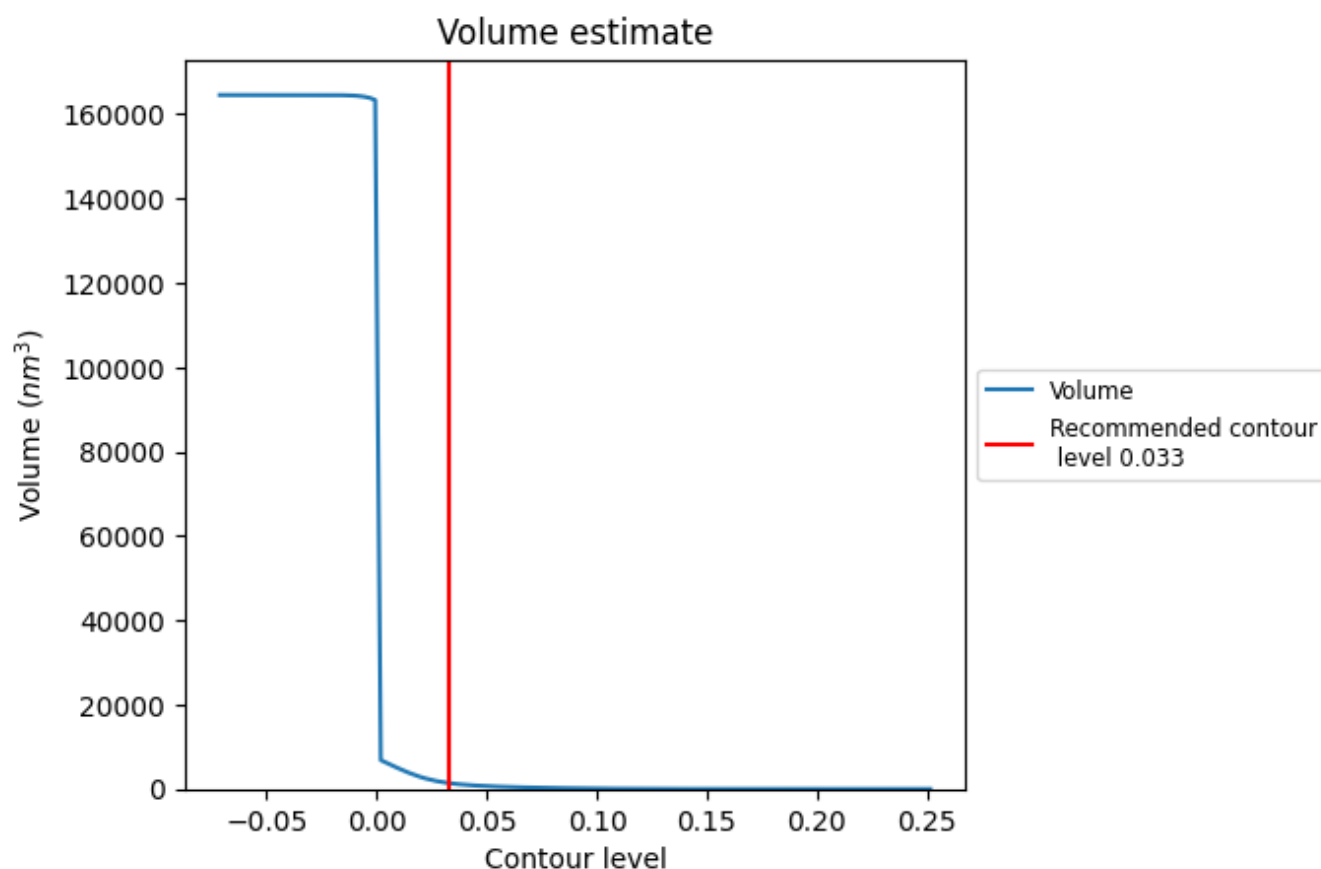
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

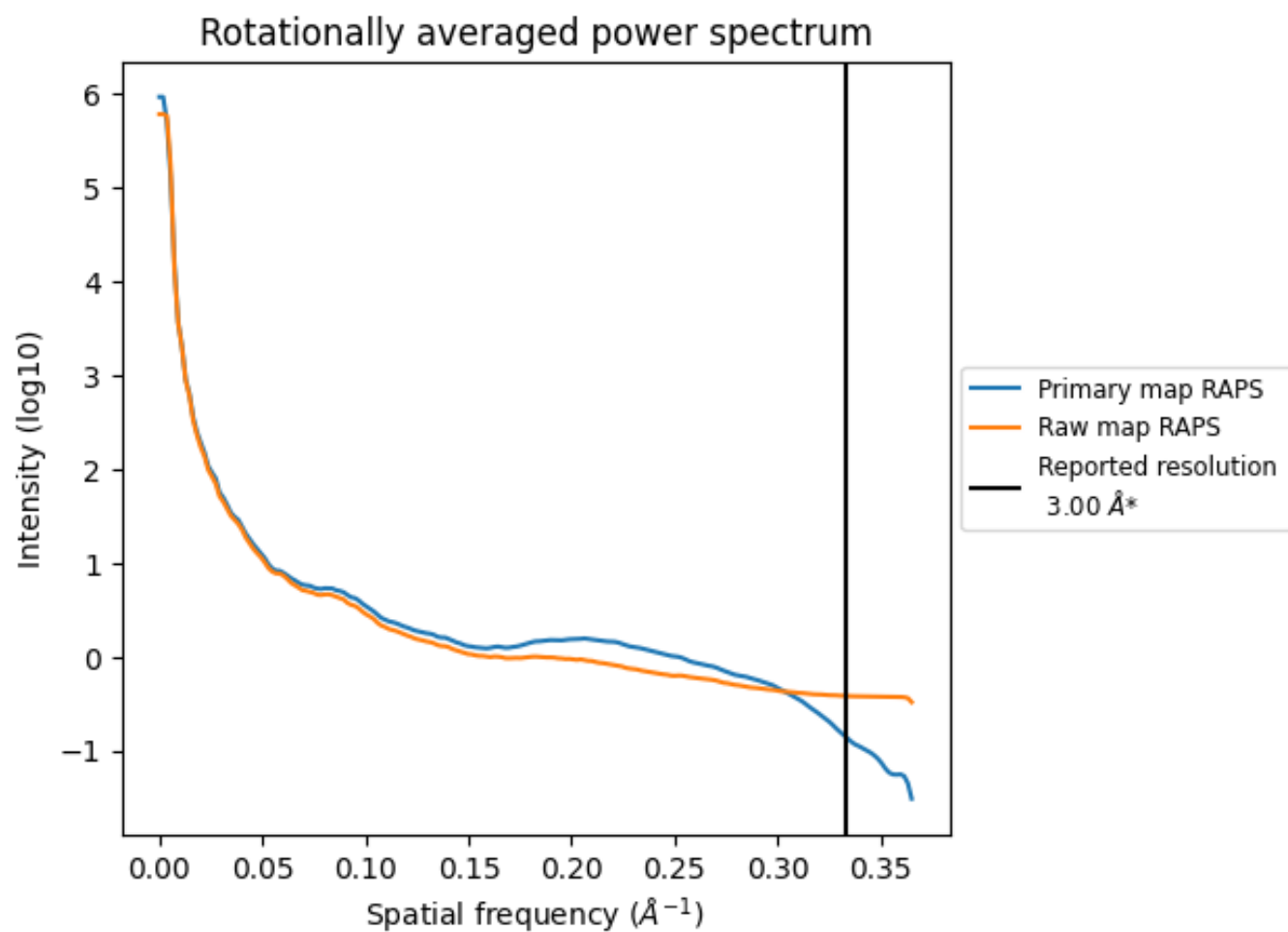
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1388 nm^3 ; this corresponds to an approximate mass of 1254 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 ⓘ

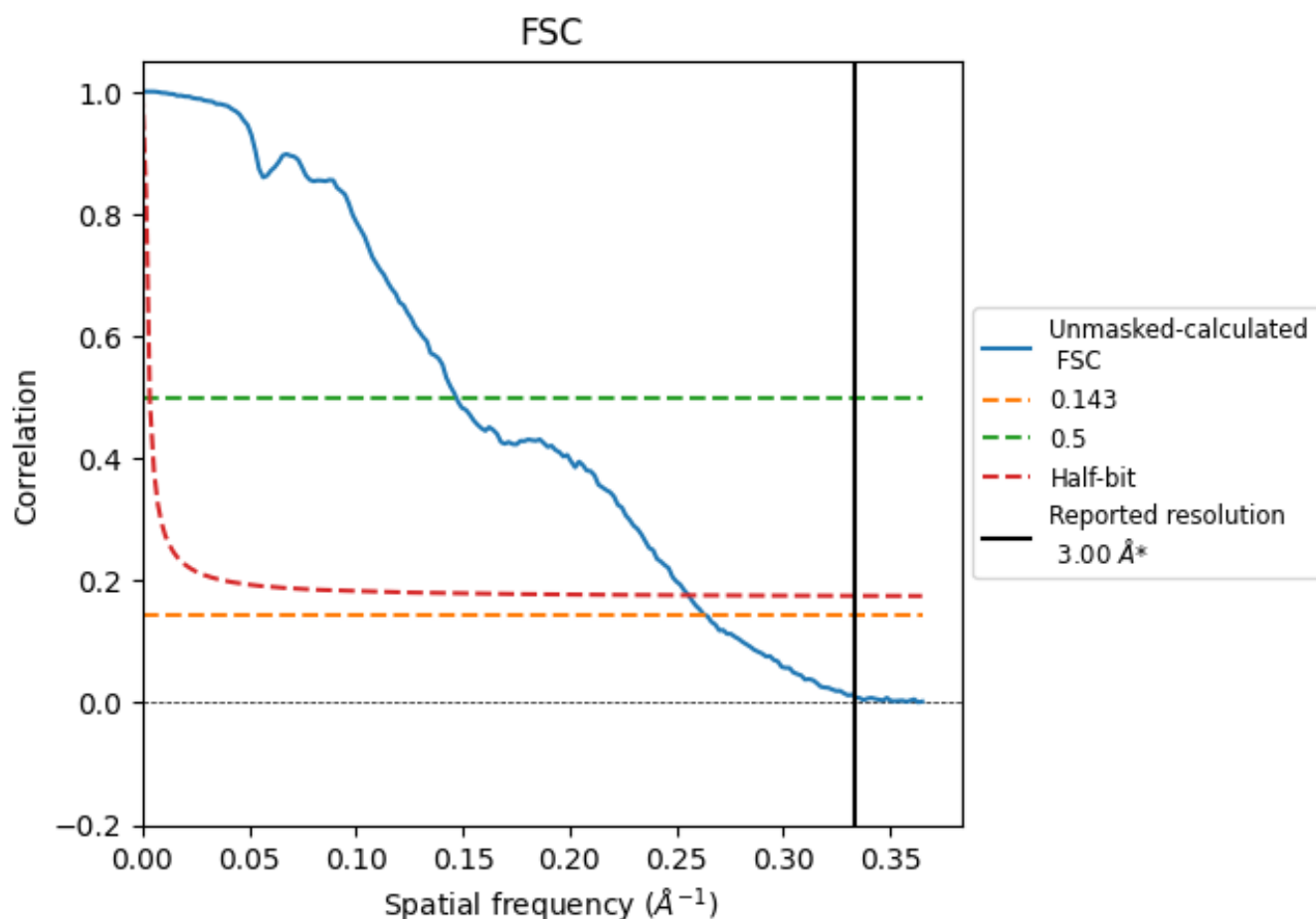


*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

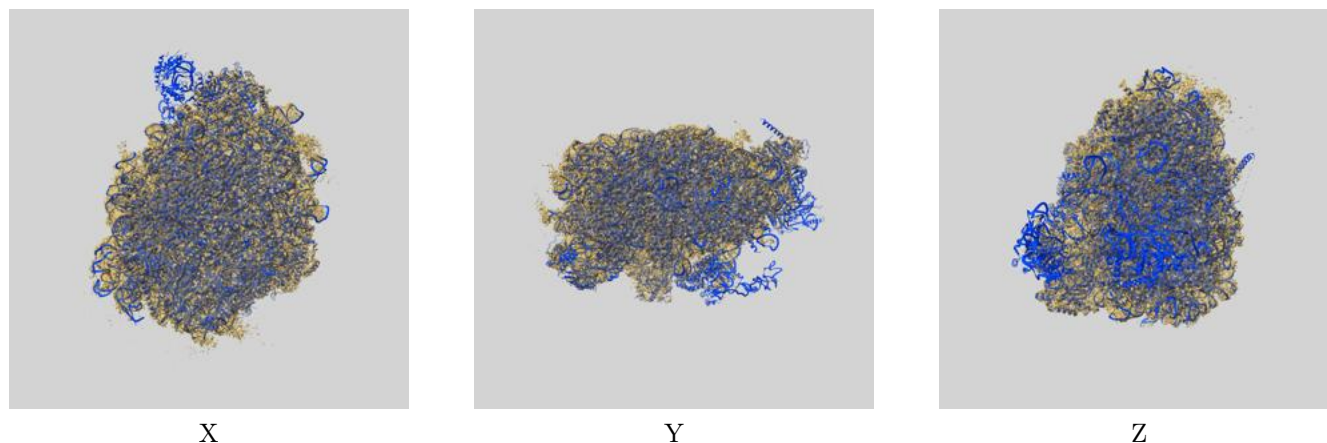
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	6.81	3.91

*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 3.80 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

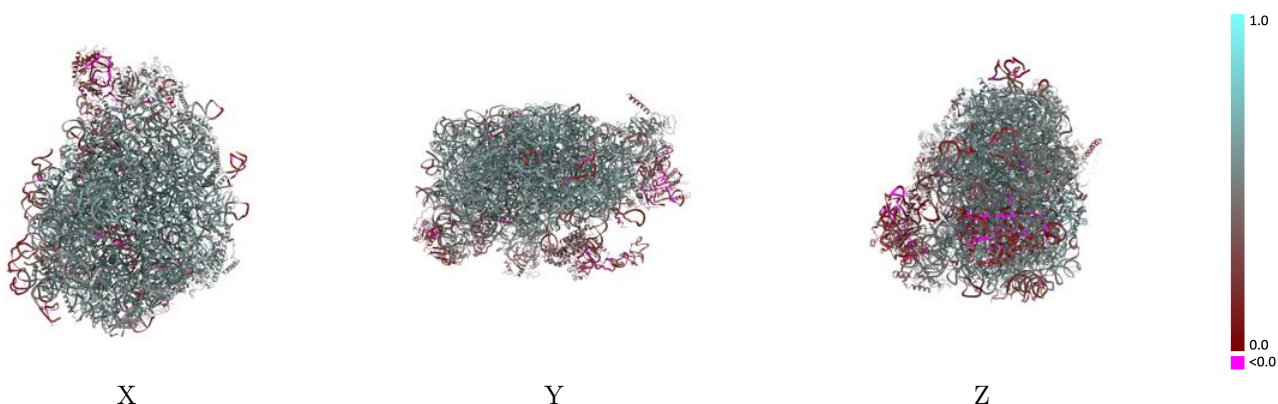
This section contains information regarding the fit between EMDB map EMD-35597 and PDB model 8INF. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



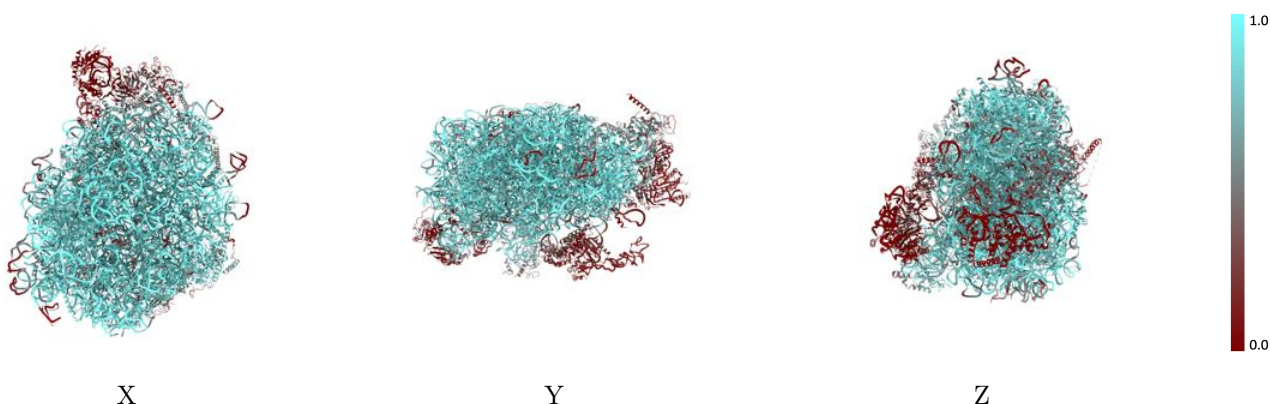
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



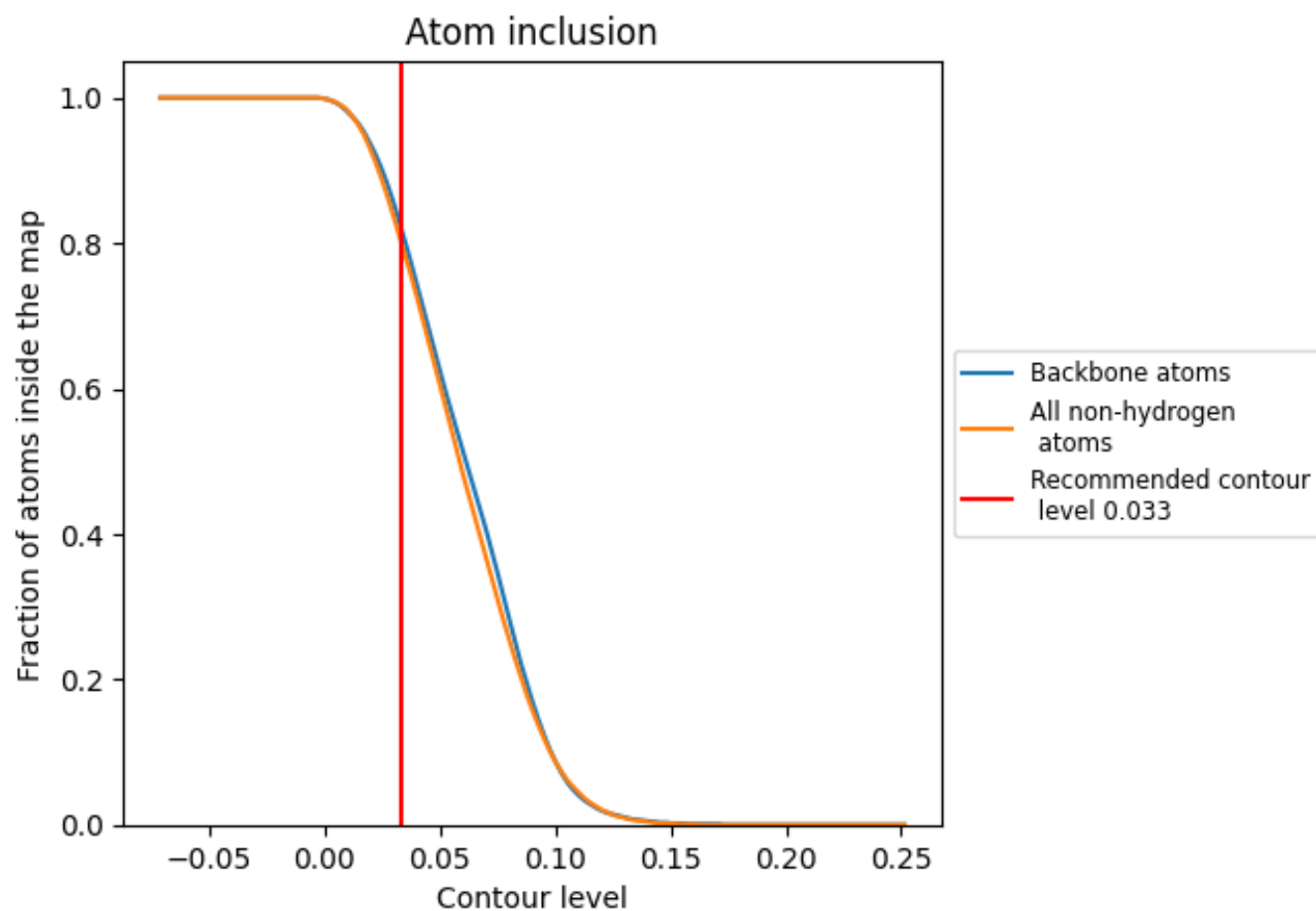
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.033).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8040	 0.4970
1	 0.3460	 0.1860
2	 0.9000	 0.5130
3	 0.3430	 0.4380
4	 0.7470	 0.4840
5	 0.9450	 0.4750
6	 0.8180	 0.5320
7	 0.8770	 0.5580
8	 0.9580	 0.5610
9	 0.7650	 0.5080
A	 0.7790	 0.5190
B	 0.9370	 0.5810
C	 0.8490	 0.4790
D	 0.9640	 0.5840
E	 0.8180	 0.5300
F	 0.9050	 0.5670
G	 0.7940	 0.5180
H	 0.9220	 0.5630
I	 0.8800	 0.5460
J	 0.2110	 0.2000
K	 0.8720	 0.5360
L	 0.9550	 0.5850
M	 0.9870	 0.5970
N	 0.4820	 0.3080
O	 0.8130	 0.5250
P	 0.9910	 0.6020
Q	 0.8820	 0.5440
R	 0.5440	 0.4360
S	 0.9470	 0.5660
T	 0.6860	 0.4410
U	 0.9860	 0.5950
V	 0.9490	 0.5740
W	 0.8000	 0.5140
X	 0.8630	 0.5580
Y	 0.8900	 0.5620



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Chain	Atom inclusion	Q-score
Z	 0.9760	 0.5950
a	 0.9340	 0.5640
b	 0.9680	 0.5920
c	 0.9210	 0.5430
d	 0.8460	 0.5410
e	 0.9390	 0.5730
f	 0.2480	 0.3250
g	 0.8650	 0.5530
h	 0.9120	 0.5640
i	 0.8830	 0.5550
j	 0.8840	 0.5640
k	 0.9810	 0.5950
l	 0.9640	 0.5830
m	 0.9590	 0.5840
n	 0.9770	 0.5990
o	 0.8220	 0.5070
p	 0.9510	 0.5700
q	 0.0240	 0.2150
r	 0.6910	 0.4200
s	 0.2260	 0.2200
t	 0.1190	 0.2660
u	 0.0010	 0.1820
v	 0.5240	 0.4780
w	 0.4000	 0.4070
x	 0.0030	 0.0540
y	 0.1950	 0.2480
z	 0.7100	 0.4730