



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 02:49 PM JST

PDB ID : 8IPX / pdb_00008ipx
EMDB ID : EMD-35649
Title : human nuclear pre-60S ribosomal particle - State C'
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-03-15
Resolution : 4.30 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

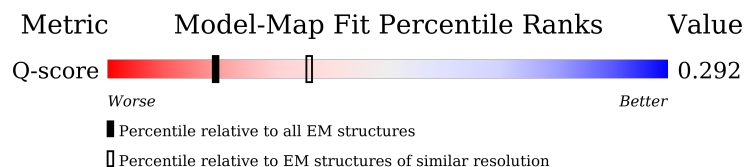
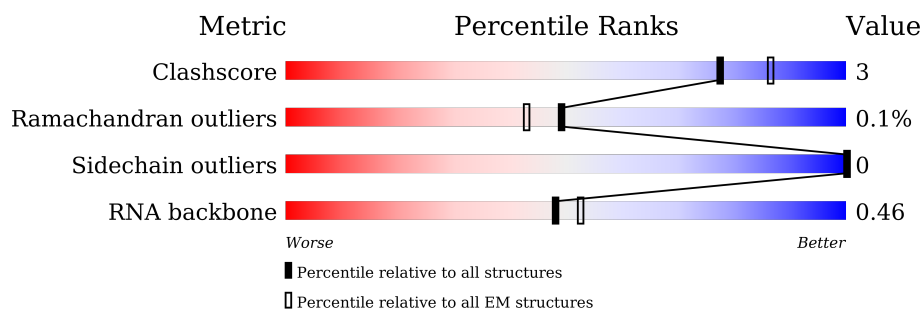
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

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	2	5054	34% 47% 18% • 31%
2	6	245	92% 88% 12%
3	7	163	66% 77% 6% • 17%

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Mol	Chain	Length	Quality of chain
4	8	156	
5	9	134	
6	A	159	
7	B	403	
8	D	427	
9	E	115	
10	G	266	
11	H	123	
12	I	192	
13	J	260	
14	L	148	
15	M	97	
16	P	51	
17	Q	211	
18	S	215	
19	U	204	
20	V	203	
21	X	92	
22	Z	188	
23	a	196	
24	b	176	
25	e	140	
26	h	145	
27	l	137	
28	m	257	

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Mol	Chain	Length	Quality of chain
29	n	110	
30	o	288	
31	p	248	
32	r	360	
33	u	549	
34	v	239	
35	w	731	
36	y	165	
37	z	129	
38	C	178	
39	R	297	
40	W	485	
41	T	160	
42	4	634	
43	Y	184	
44	k	135	
45	j	125	
46	d	128	
47	t	293	
48	x	60	
49	N	490	
50	1	255	
51	K	105	
52	F	117	
53	i	136	

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Mol	Chain	Length	Quality of chain
54	O	70	90% 94%
55	3	120	92% 63% 28%
56	q	588	69% 60% 9% 31%
57	g	156	67% 83% 10% 7%
58	f	478	54% 44% 10% 46%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 160786 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	3475	Total	C	N	O	P	0	0
			74602	33261	13645	24222	3474		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 3 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	135	Total	C	N	O	S	0	0
			1159	737	225	187	10		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 5 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	86	Total	C	N	O	S	0	0
			711	433	154	121	3		

- Molecule 6 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	45	Total	C	N	O	S	0	0
			352	221	76	52	3		

- Molecule 7 is a protein called 60S ribosomal protein L3.

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

- Molecule 8 is a protein called 60S ribosomal protein L4.

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

- Molecule 9 is a protein called 60S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L35.

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

- Molecule 12 is a protein called 60S ribosomal protein L9.

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

- Molecule 13 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	217	Total	C	N	O	S	0	0
			1772	1134	334	296	8		

- Molecule 14 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	112	Total	C	N	O	S	0	0
			877	557	172	145	3		

- Molecule 15 is a protein called 60S ribosomal protein L37.

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

- Molecule 16 is a protein called 60S ribosomal protein L39.

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

- Molecule 17 is a protein called 60S ribosomal protein L13.

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

- Molecule 18 is a protein called 60S ribosomal protein L14.

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

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

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

- Molecule 21 is a protein called 60S ribosomal protein L37a.

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

- Molecule 22 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 23 is a protein called 60S ribosomal protein L19.

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

- Molecule 24 is a protein called 60S ribosomal protein L18a.

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

- Molecule 25 is a protein called 60S ribosomal protein L23.

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

- Molecule 26 is a protein called 60S ribosomal protein L26.

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

- Molecule 27 is a protein called 60S ribosomal protein L28.

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

- Molecule 28 is a protein called 60S ribosomal protein L8.

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

- Molecule 29 is a protein called 60S ribosomal protein L35a.

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

- Molecule 30 is a protein called 60S ribosomal protein L6.

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

- Molecule 31 is a protein called 60S ribosomal protein L7.

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

- Molecule 32 is a protein called Coiled-coil domain-containing protein 86.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	r	82	Total	C	N	O	S	0	0
			723	442	158	121	2		

- Molecule 33 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	67	Total	C	N	O	S	0	0
			569	357	119	90	3		

- Molecule 34 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	v	217	Total	C	N	O	S	0	0
			1771	1129	311	320	11		

- Molecule 35 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	w	433	Total	C	N	O	S	0	0
			3472	2201	615	643	13		

- Molecule 36 is a protein called 60S ribosomal protein L12.

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

- Molecule 37 is a protein called Protein LLP homolog.

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

- Molecule 38 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	C	165	Total	C	N	O	S	0	0
			1319	836	245	233	5		

- Molecule 39 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 40 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	W	388	Total	C	N	O	S	0	0
			3018	1889	556	562	11		

- Molecule 41 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T	124	Total	C	N	O	S	0	0
			1001	632	194	171	4		

- Molecule 42 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	4	611	Total	C	N	O	S	0	0
			5016	3151	918	920	27		

- Molecule 43 is a protein called 60S ribosomal protein L17.

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

- Molecule 44 is a protein called 60S ribosomal protein L32.

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

- Molecule 45 is a protein called 60S ribosomal protein L31.

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

- Molecule 46 is a protein called 60S ribosomal protein L22.

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

- Molecule 47 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	111	Total	C	N	O	S	0	0
			928	601	157	167	3		

- Molecule 48 is a RNA chain called ITS2.

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

- Molecule 49 is a protein called Ribosomal L1 domain-containing protein 1.

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

- Molecule 50 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	230	Total	C	N	O	S	0	0
			1897	1226	357	310	4		

- Molecule 51 is a protein called 60S ribosomal protein L36.

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

- Molecule 52 is a protein called 60S ribosomal protein L34.

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

- Molecule 53 is a protein called 60S ribosomal protein L27.

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

- Molecule 54 is a protein called 60S ribosomal protein L38.

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

- Molecule 55 is a RNA chain called 5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	115	Total	C	N	O	P	0	0
			2453	1093	437	808	115		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	92	C	G	conflict	GB NR_023363
3	93	G	C	conflict	GB NR_023363
3	95	C	U	conflict	GB NR_023363
3	96	U	G	conflict	GB NR_023363

- Molecule 56 is a protein called Pescadillo homolog.

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

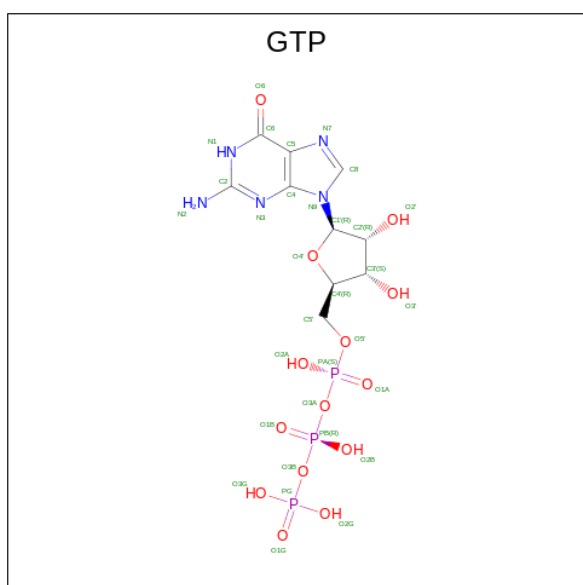
- Molecule 57 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	g	145	Total	C	N	O	S	0	0
			1170	750	222	197	1		

- Molecule 58 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	f	258	Total	C	N	O	S	0	0
			2137	1326	427	382	2		

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
59	w	1	Total	C	N	O	P	0
			32	10	5	14	3	

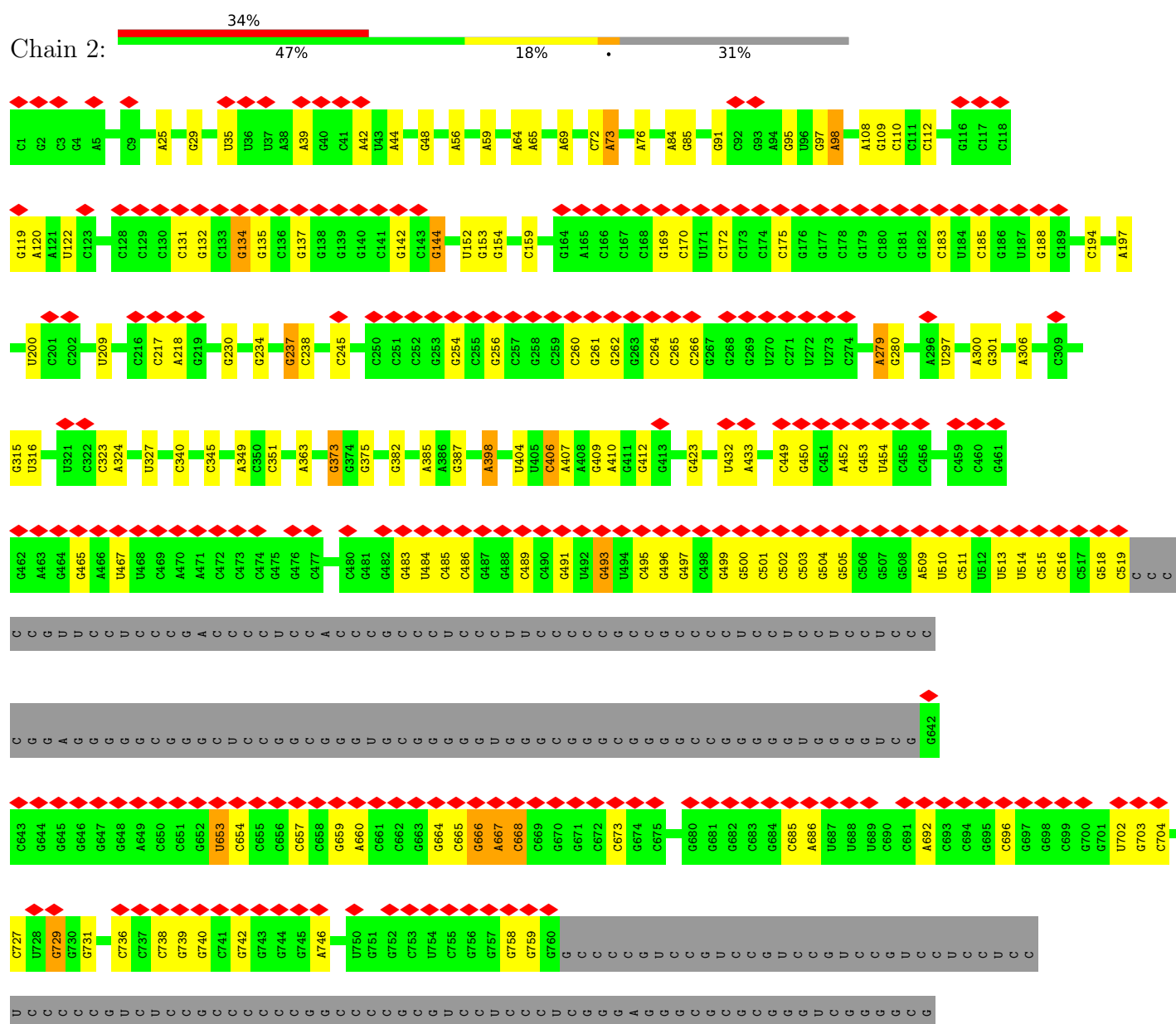
- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

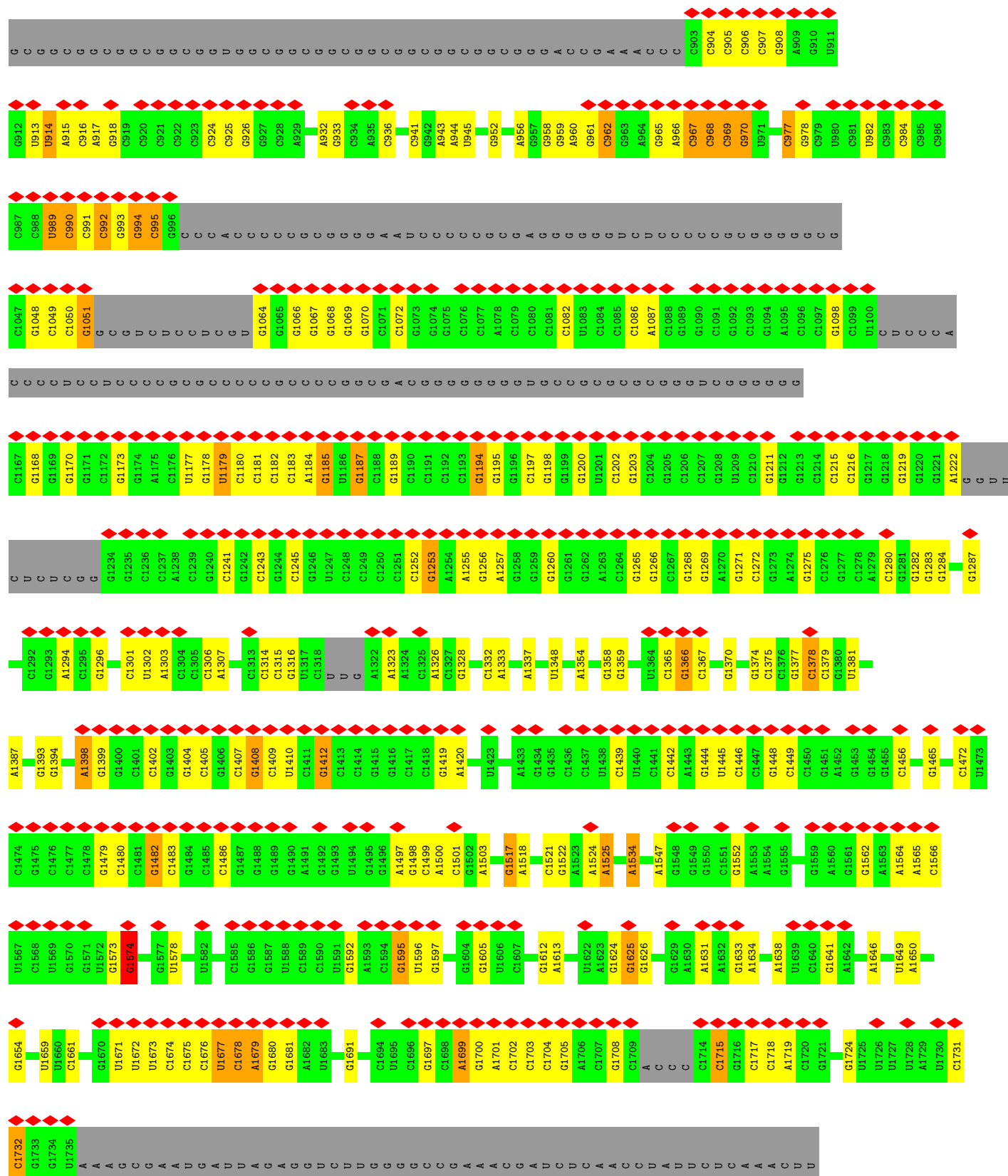
Mol	Chain	Residues	Atoms		AltConf
60	w	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

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

• Molecule 1: 28S rRNA

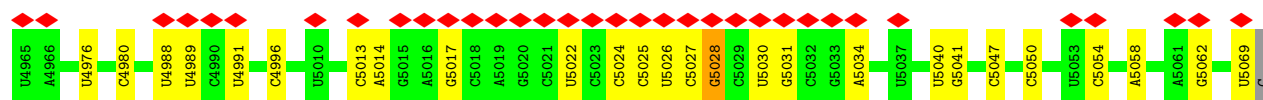




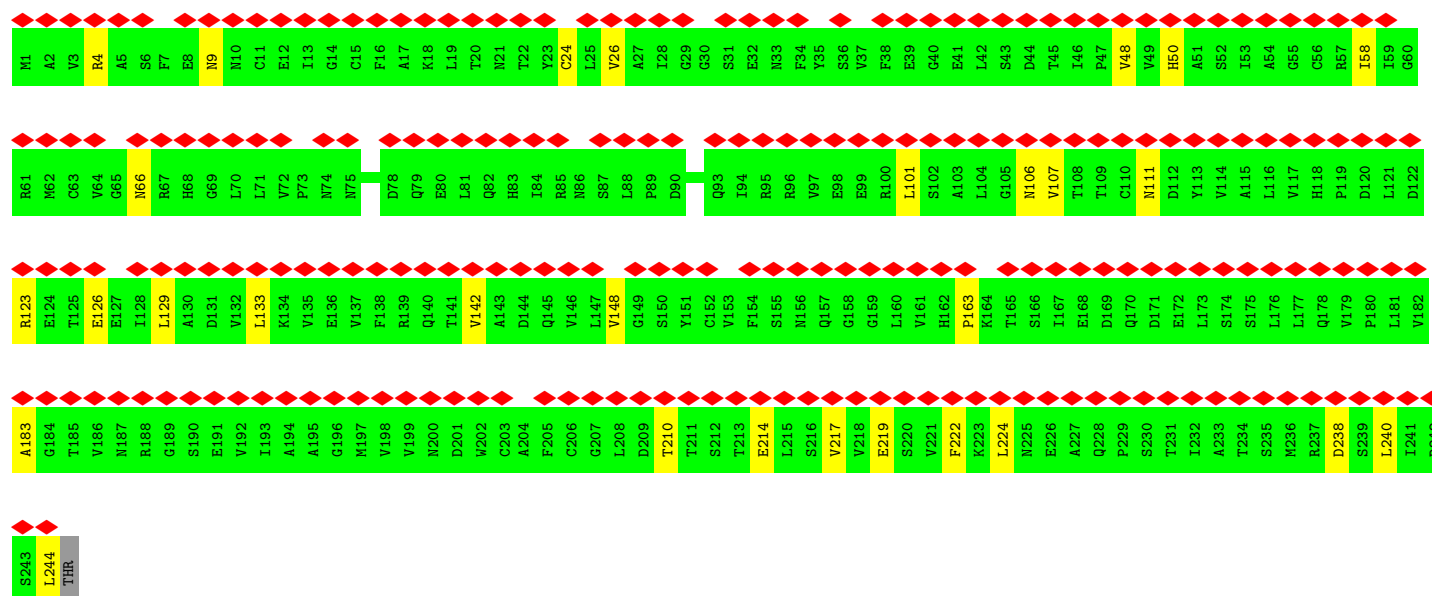
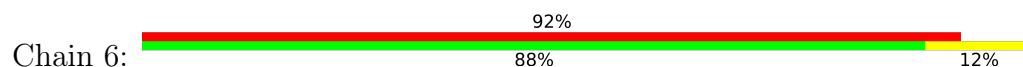




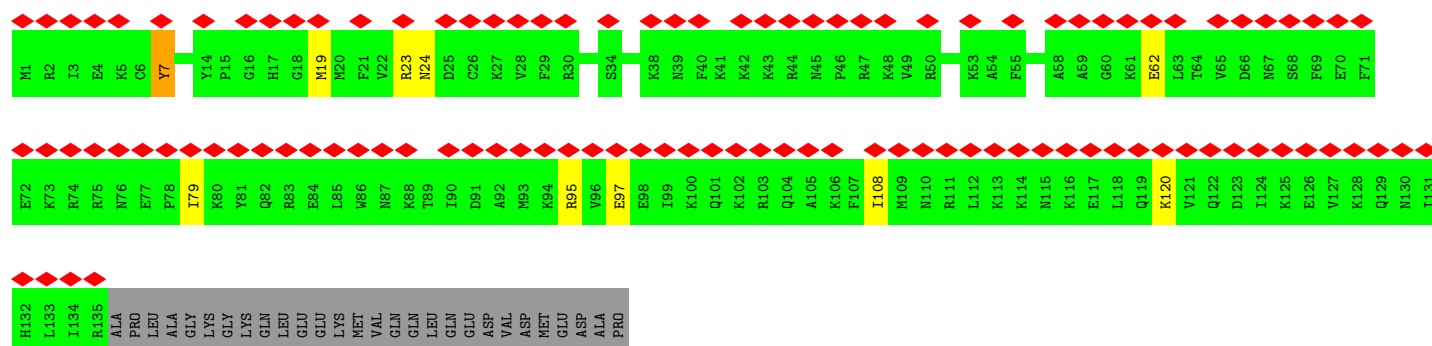




• Molecule 2: Eukaryotic translation initiation factor 6

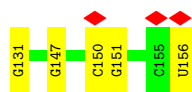


• Molecule 3: Probable ribosome biogenesis protein RLP24

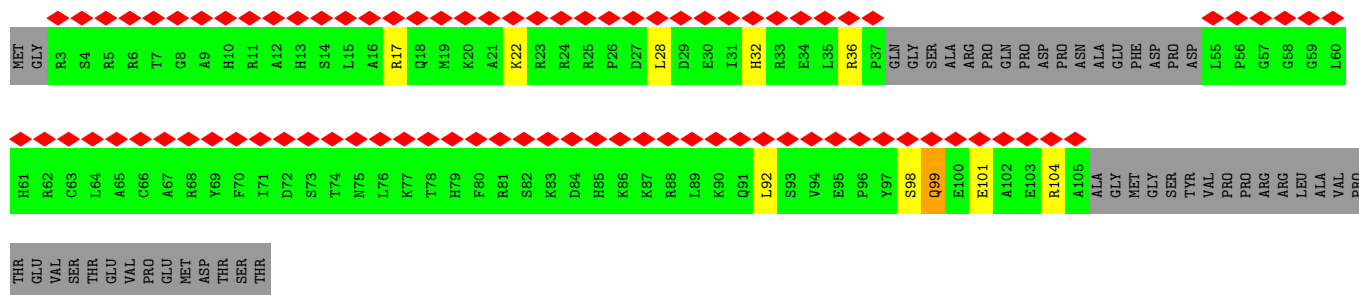


• Molecule 4: 5.8S rRNA

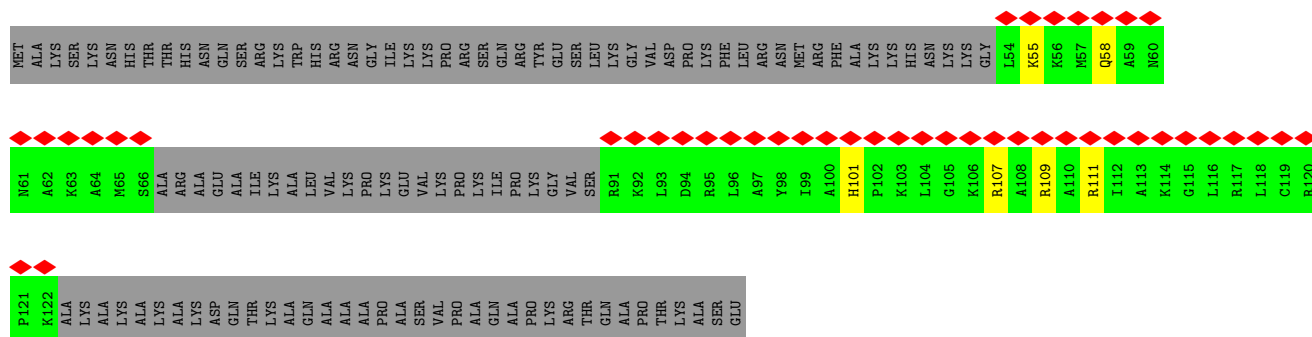




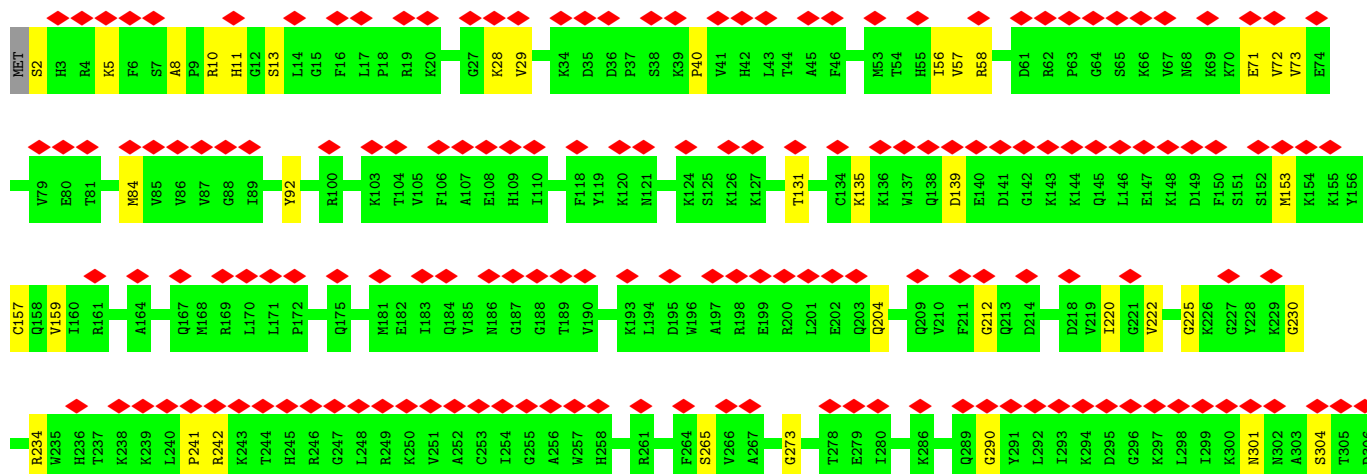
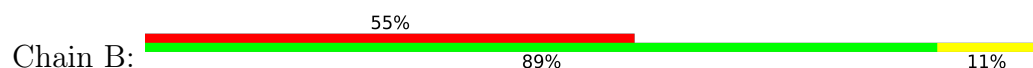
• Molecule 5: Zinc finger protein 593

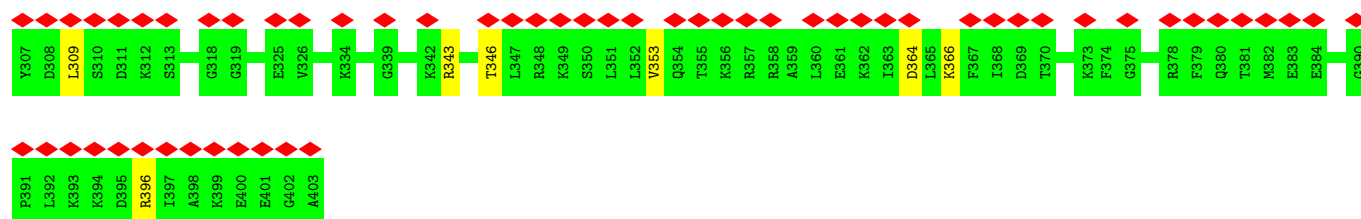


• Molecule 6: 60S ribosomal protein L29

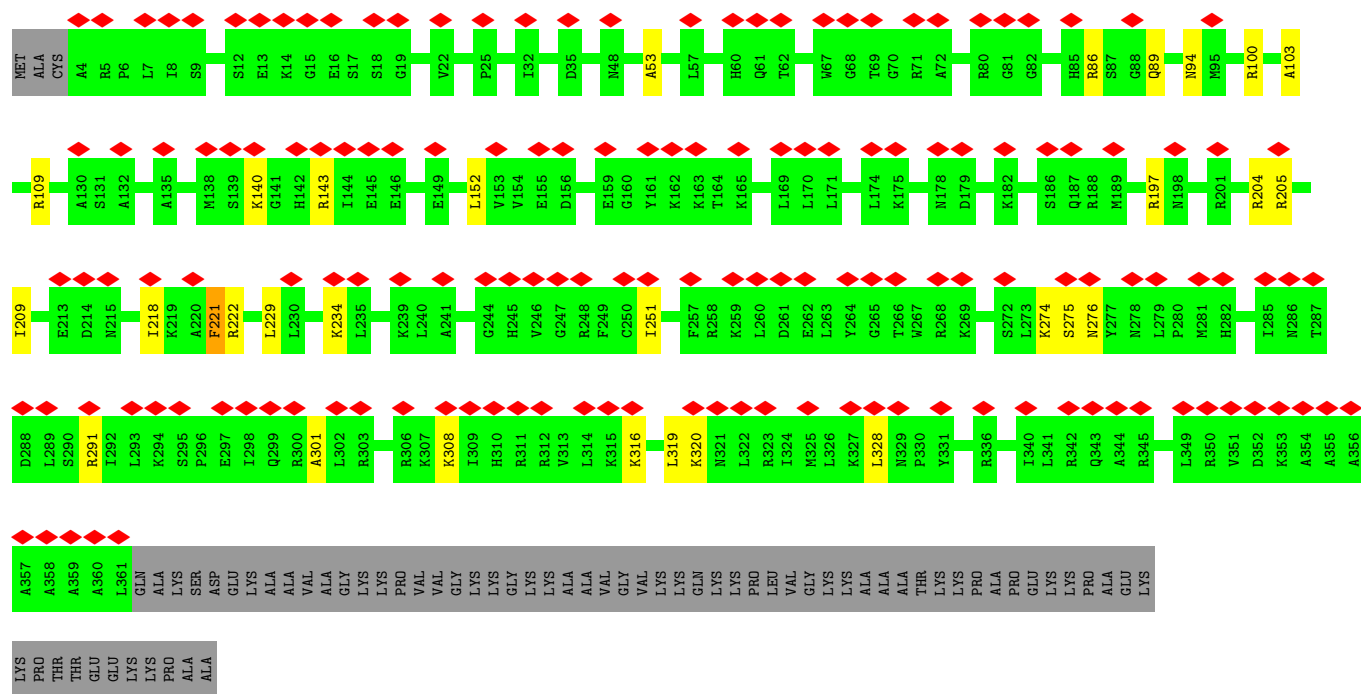
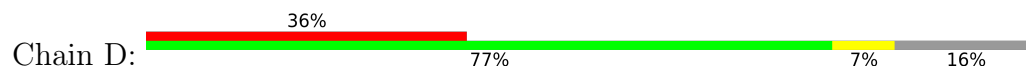


• Molecule 7: 60S ribosomal protein L3

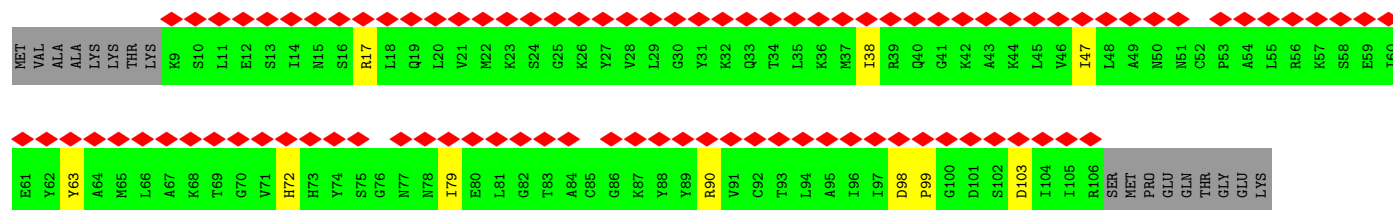
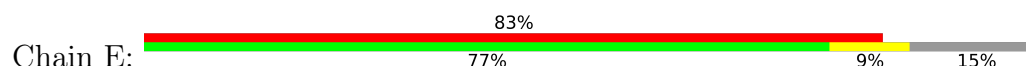




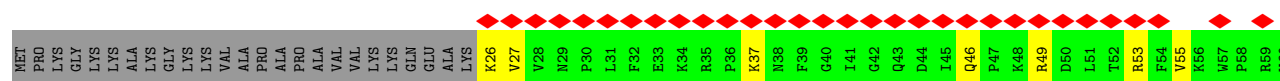
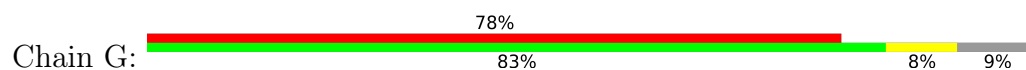
• Molecule 8: 60S ribosomal protein L4

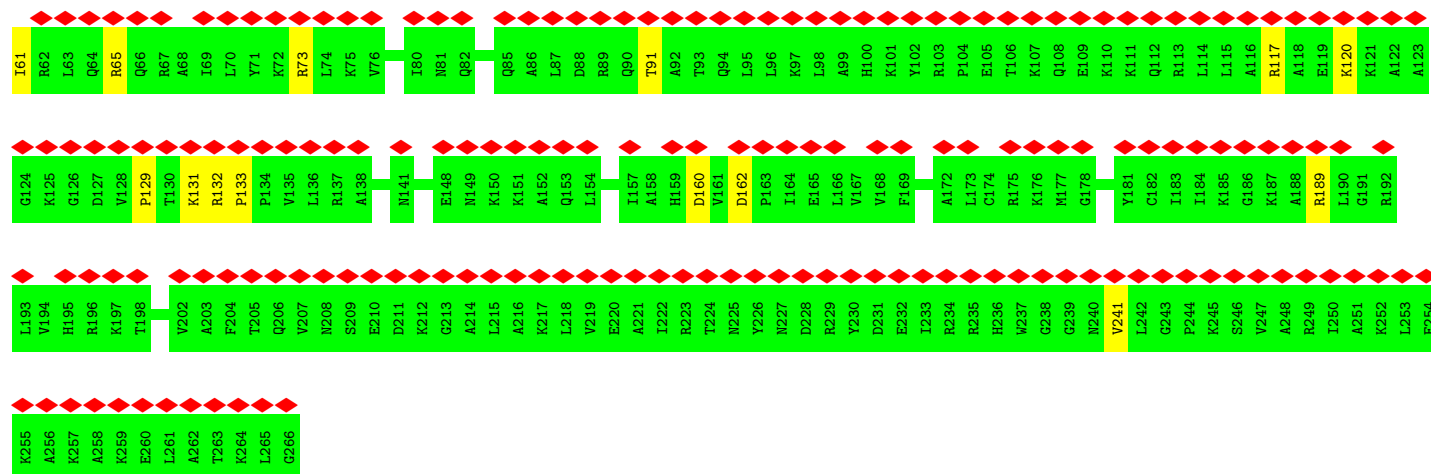


• Molecule 9: 60S ribosomal protein L30

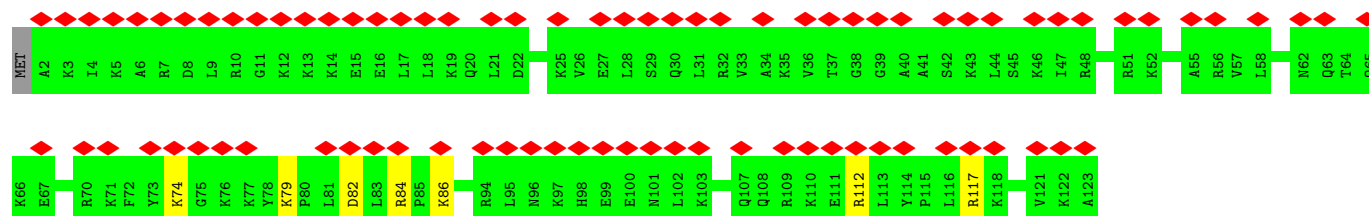
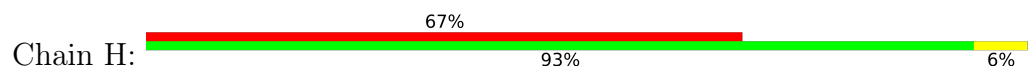


• Molecule 10: 60S ribosomal protein L7a

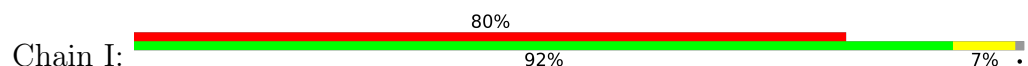




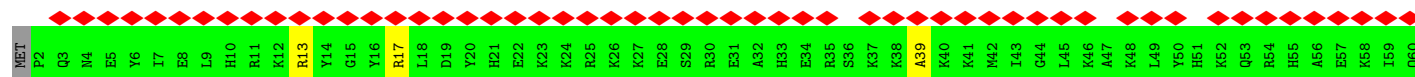
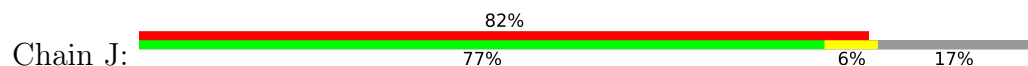
- Molecule 11: 60S ribosomal protein L35

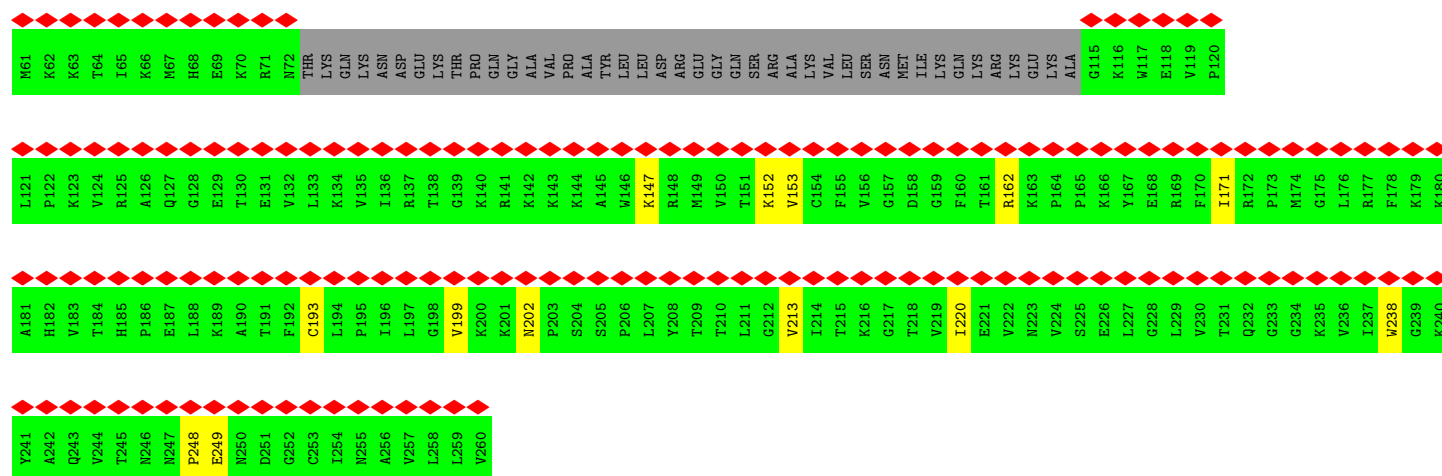


- Molecule 12: 60S ribosomal protein L9

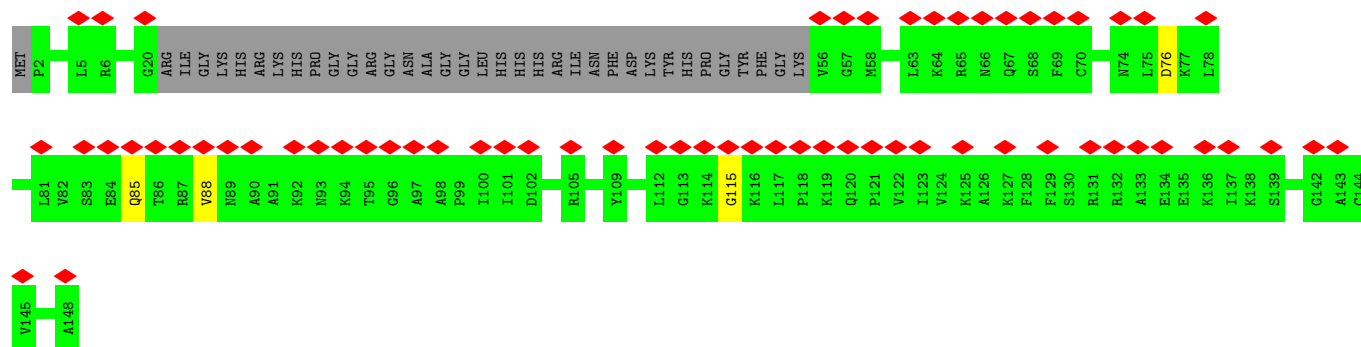
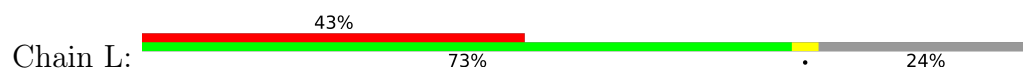


- Molecule 13: Ribosome biogenesis protein NSA2 homolog

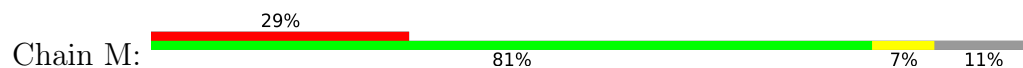




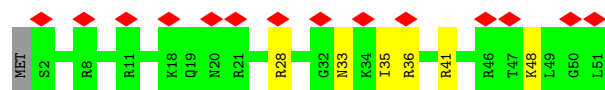
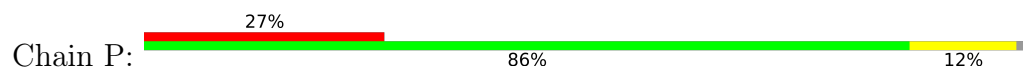
• Molecule 14: 60S ribosomal protein L27a



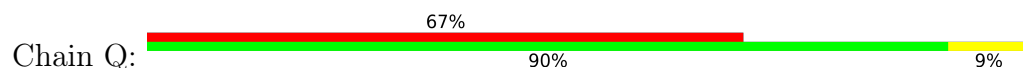
• Molecule 15: 60S ribosomal protein L37

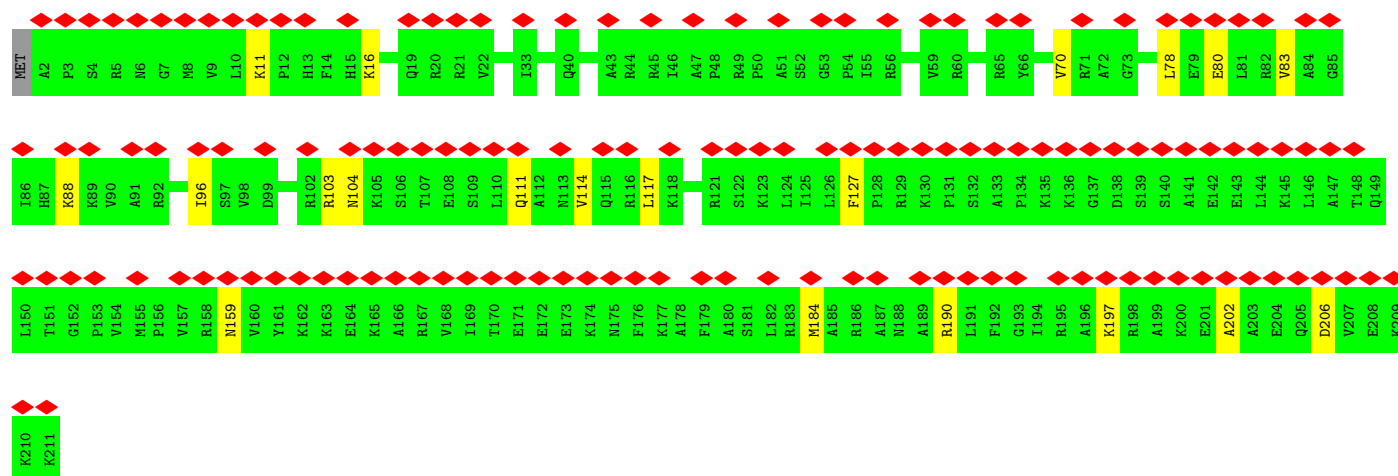


• Molecule 16: 60S ribosomal protein L39

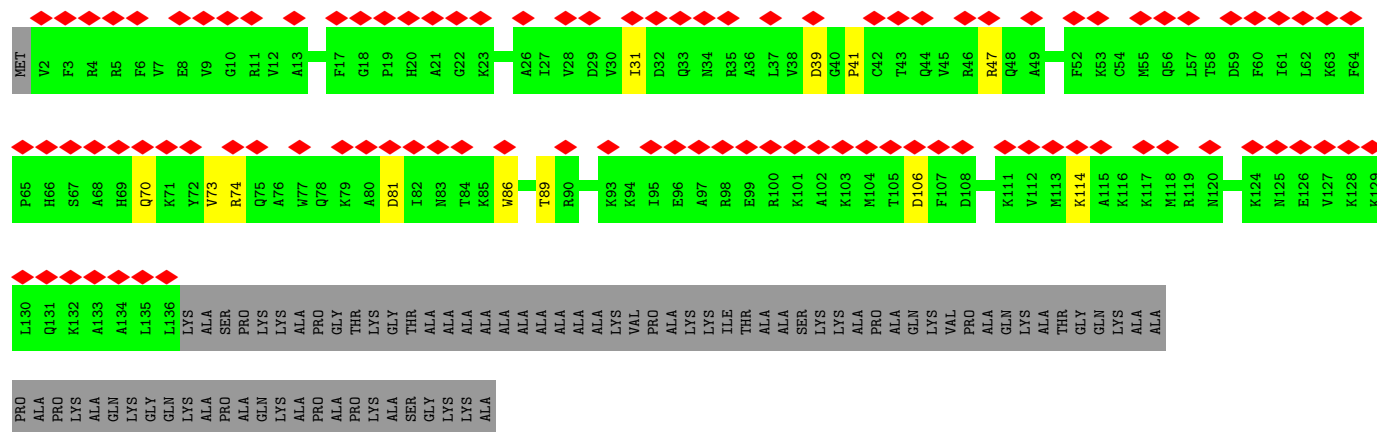


• Molecule 17: 60S ribosomal protein L13

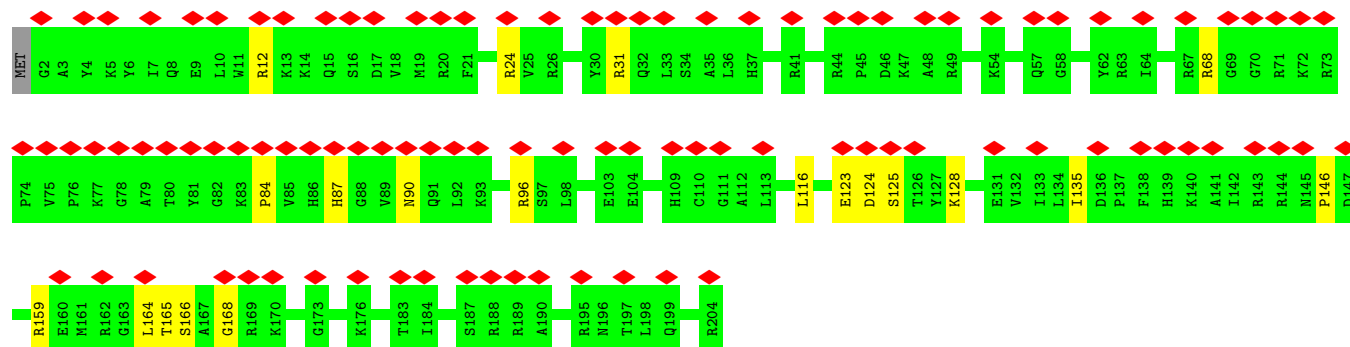
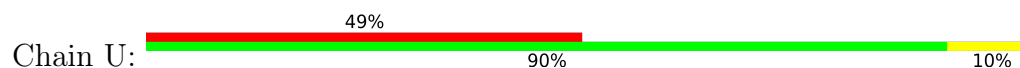




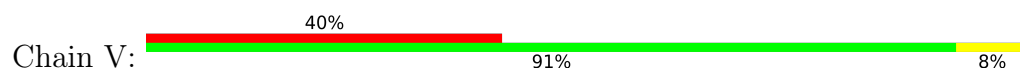
• Molecule 18: 60S ribosomal protein L14

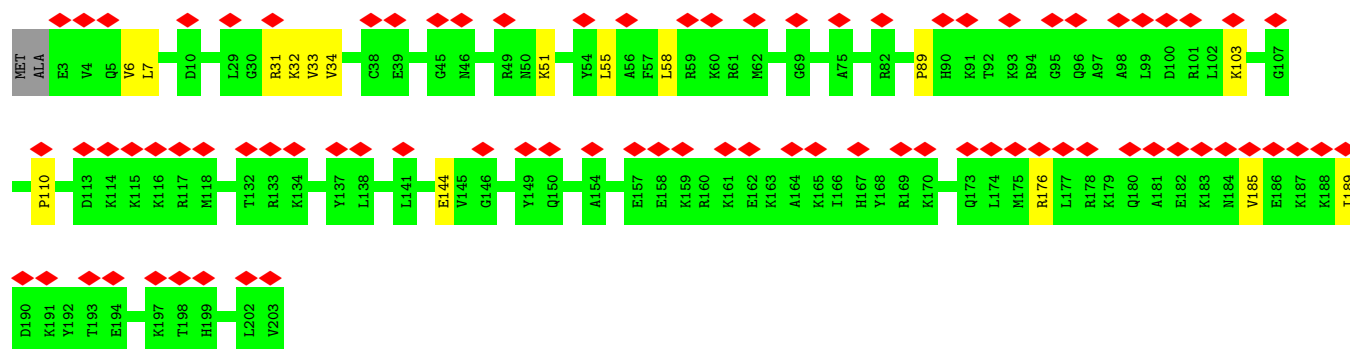


• Molecule 19: 60S ribosomal protein L15



• Molecule 20: 60S ribosomal protein L13a

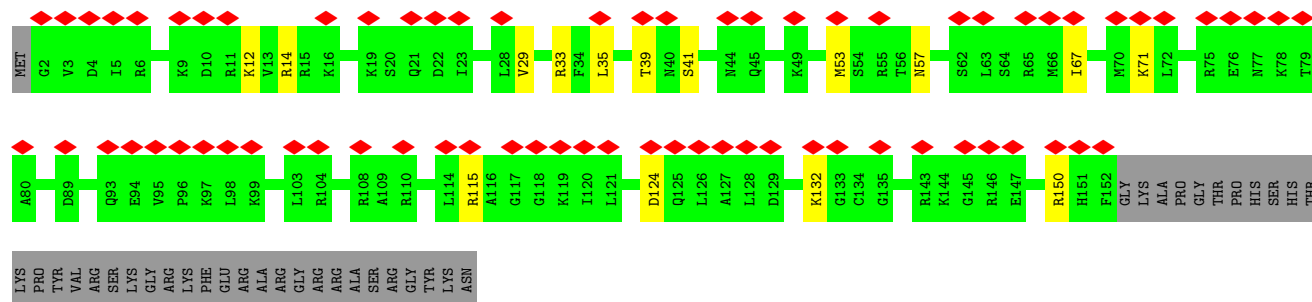




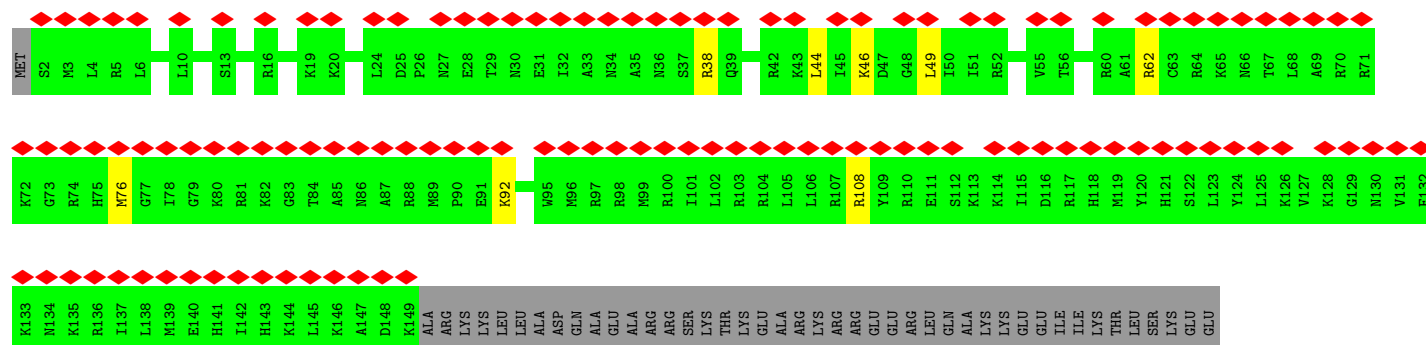
- Molecule 21: 60S ribosomal protein L37a



- Molecule 22: 60S ribosomal protein L18



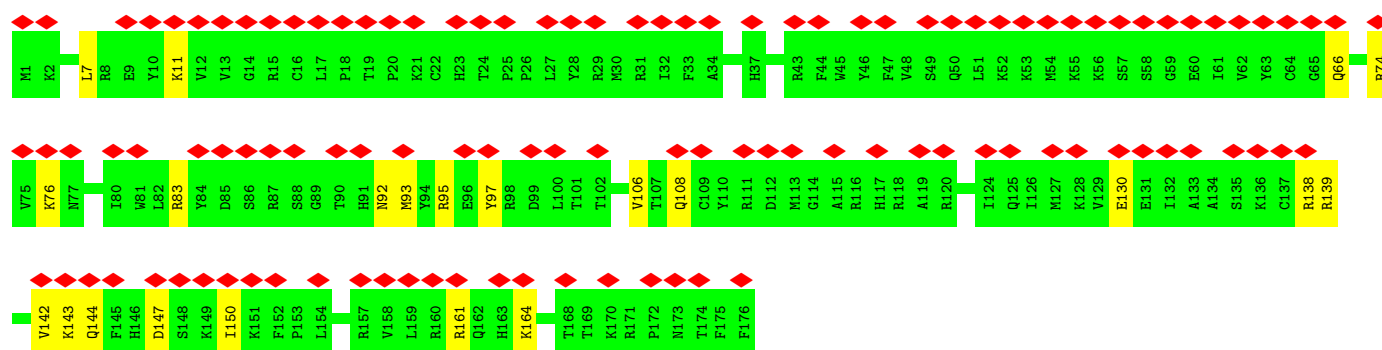
- Molecule 23: 60S ribosomal protein L19



GLU
THR
LYS
LYS

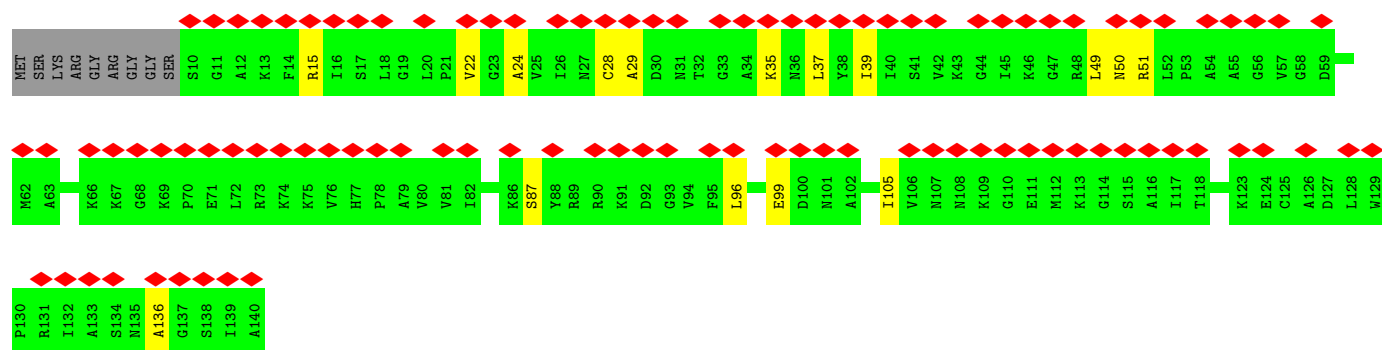
• Molecule 24: 60S ribosomal protein L18a

Chain b: 

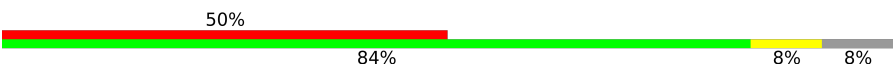


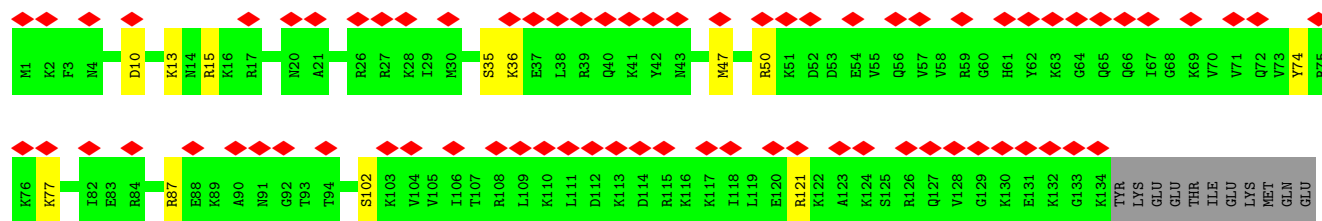
• Molecule 25: 60S ribosomal protein L23

Chain e: 



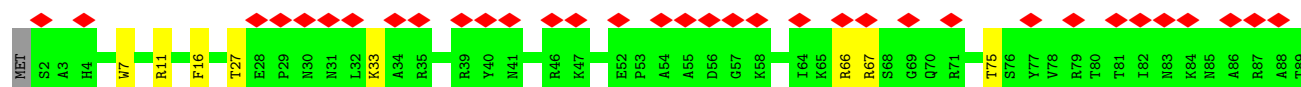
• Molecule 26: 60S ribosomal protein L26

Chain h: 

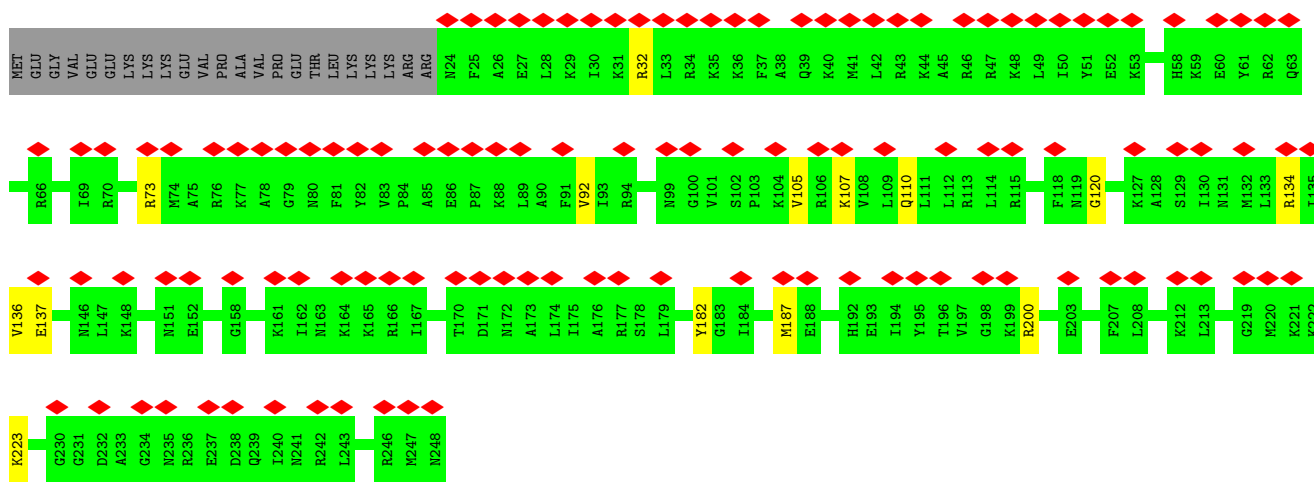
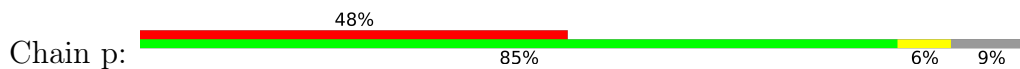


• Molecule 27: 60S ribosomal protein L28

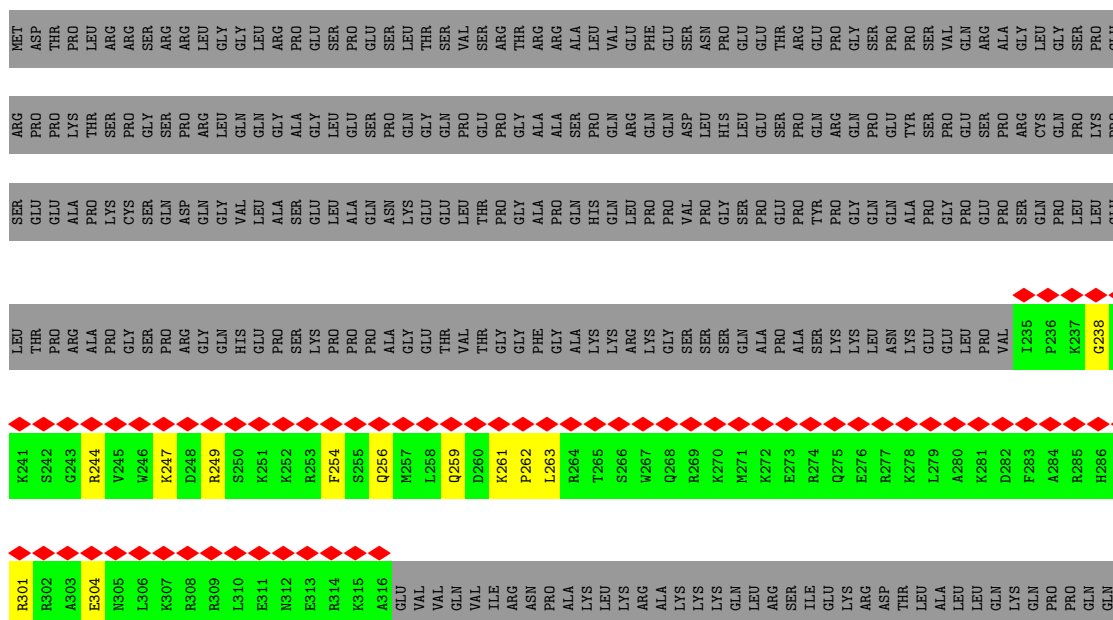
Chain l: 



- Molecule 31: 60S ribosomal protein L7

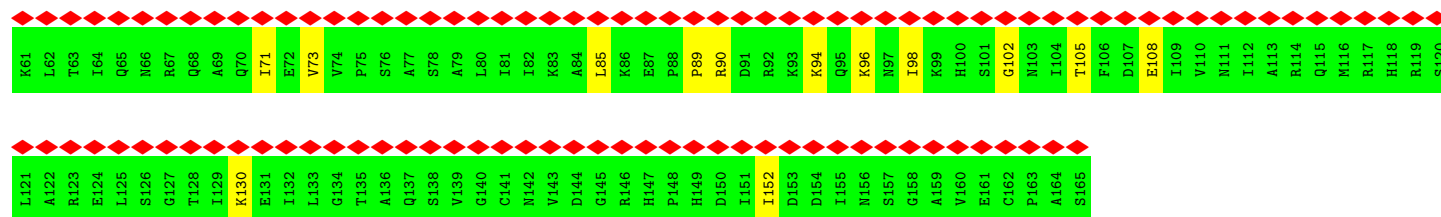


- Molecule 32: Coiled-coil domain-containing protein 86

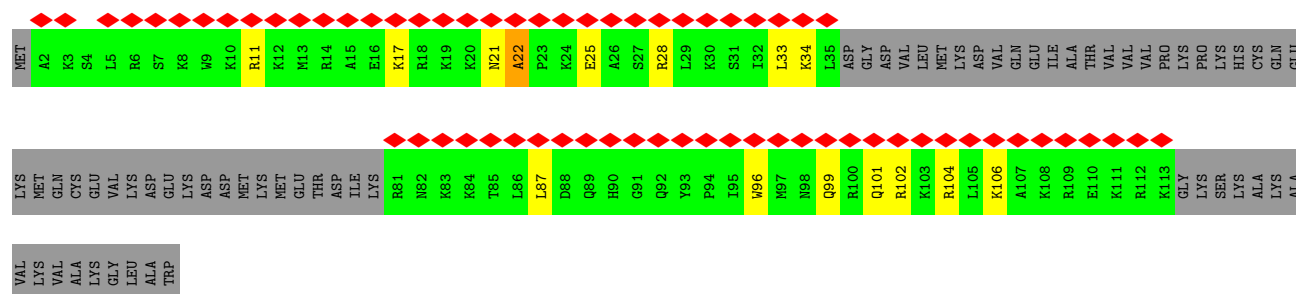
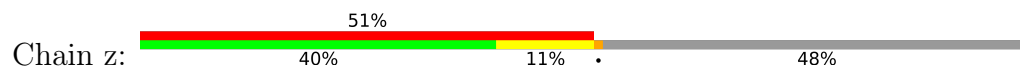


- Molecule 33: Guanine nucleotide-binding protein-like 3

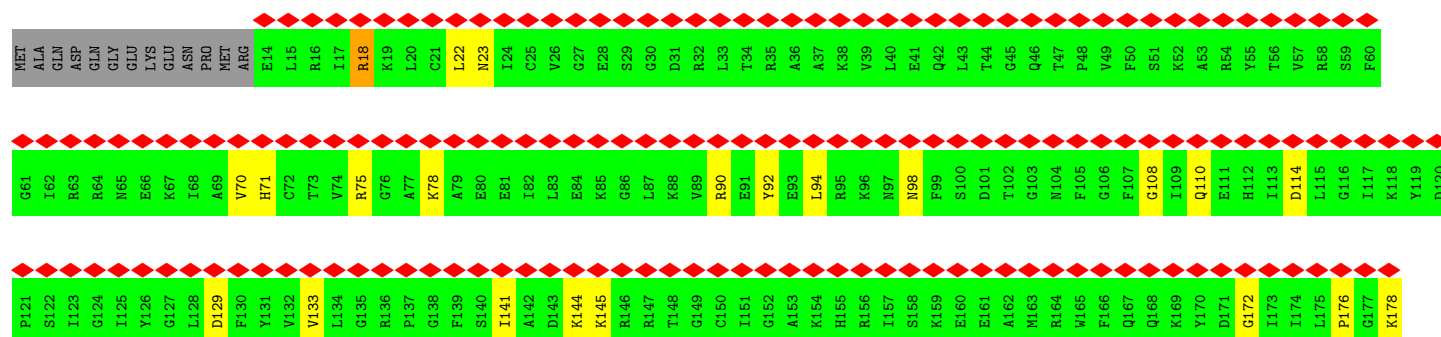
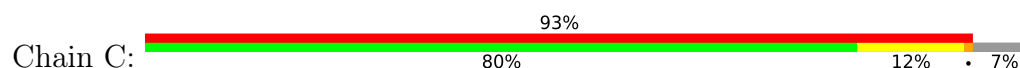
- Molecule 36: 60S ribosomal protein L12



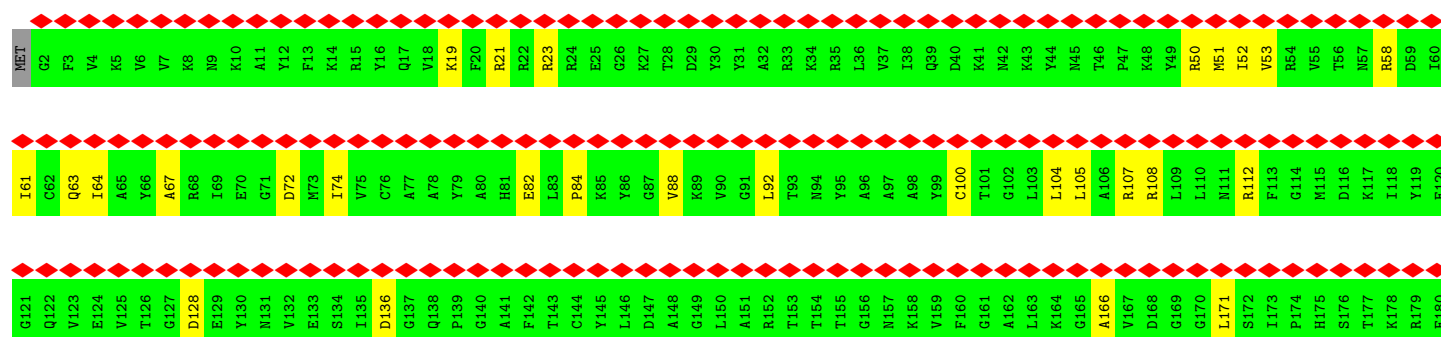
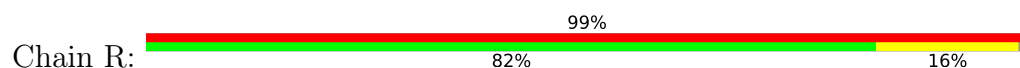
• Molecule 37: Protein LLP homolog



• Molecule 38: 60S ribosomal protein L11

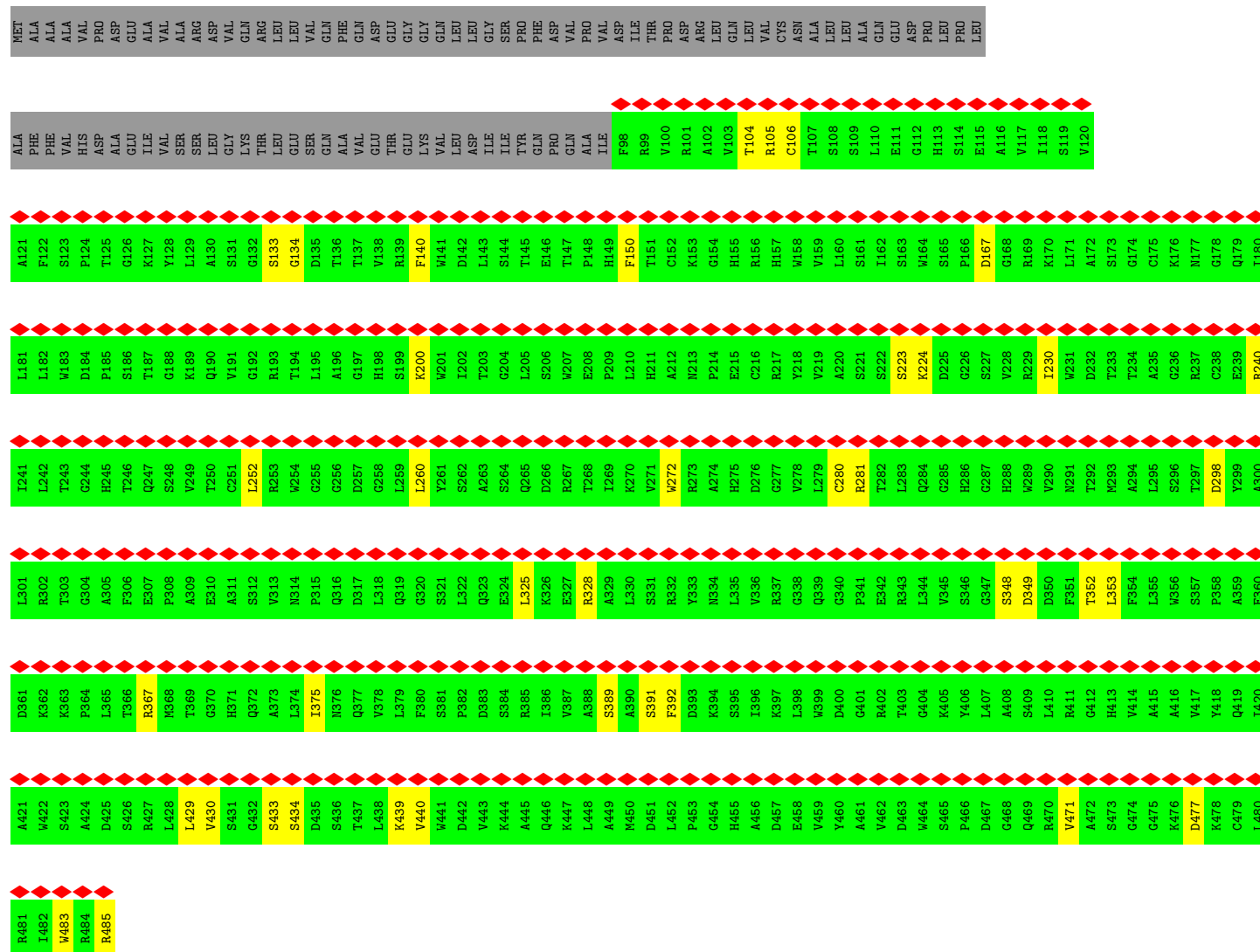
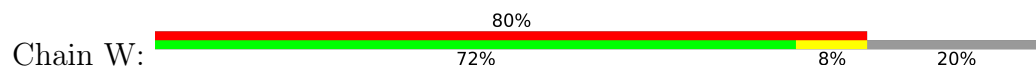


• Molecule 39: 60S ribosomal protein L5



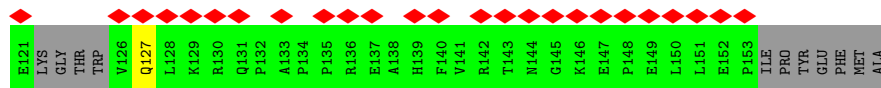
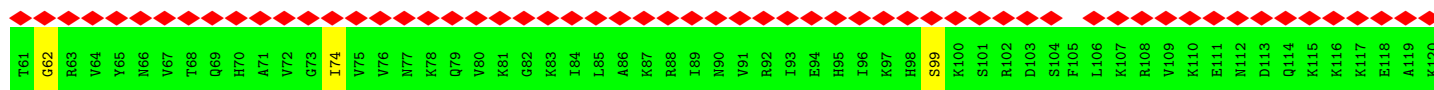


• Molecule 40: Notchless protein homolog 1

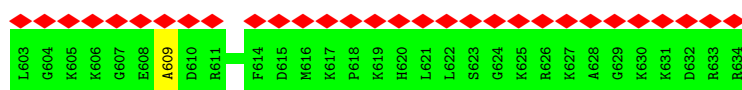
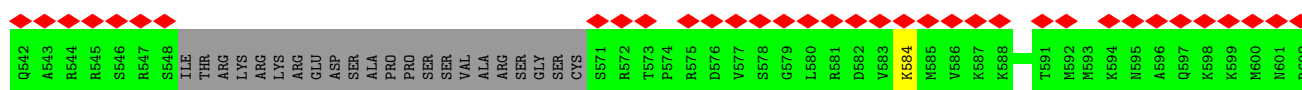
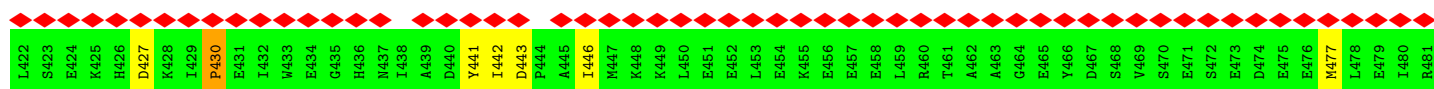
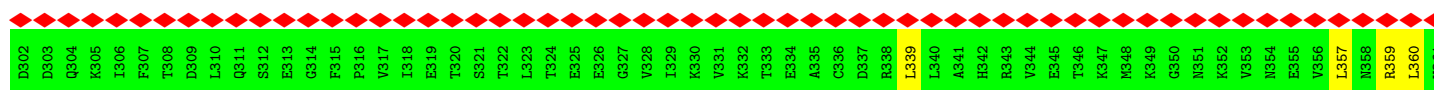
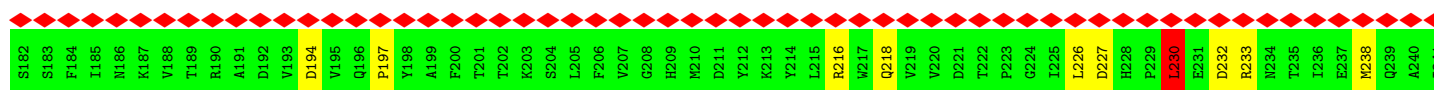
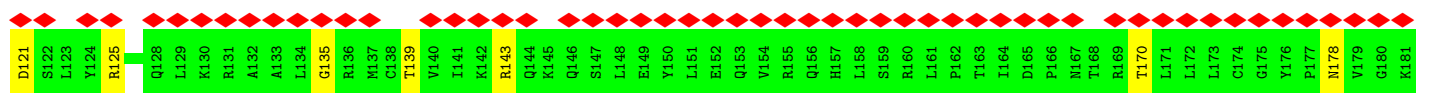
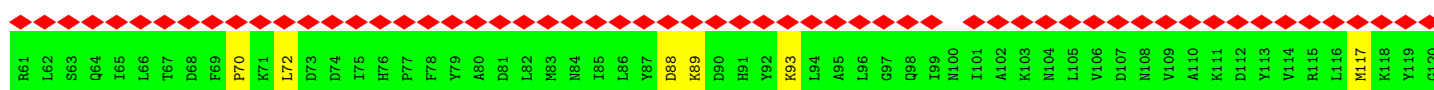
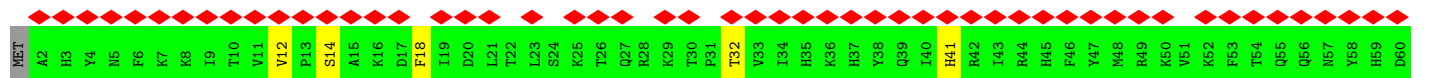
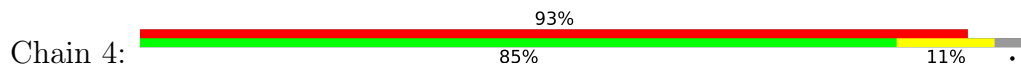


• Molecule 41: 60S ribosomal protein L21

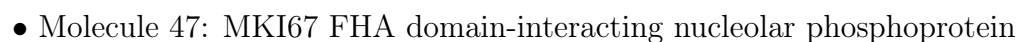
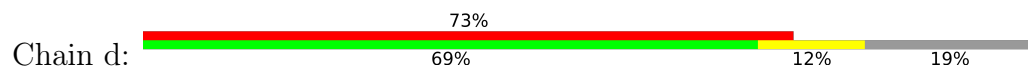
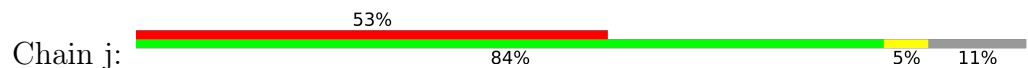
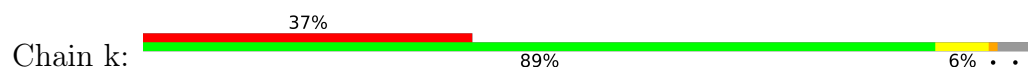




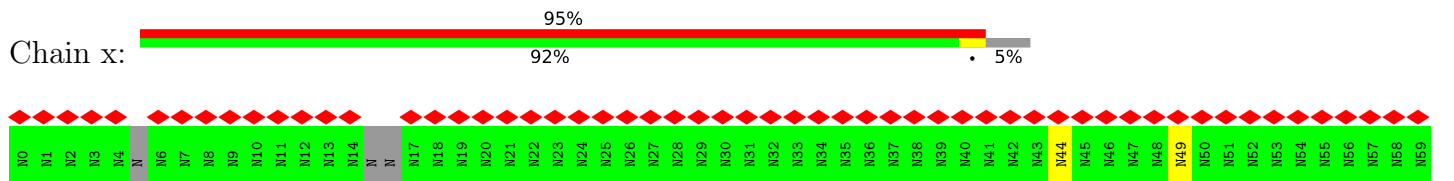
• Molecule 42: GTP-binding protein 4



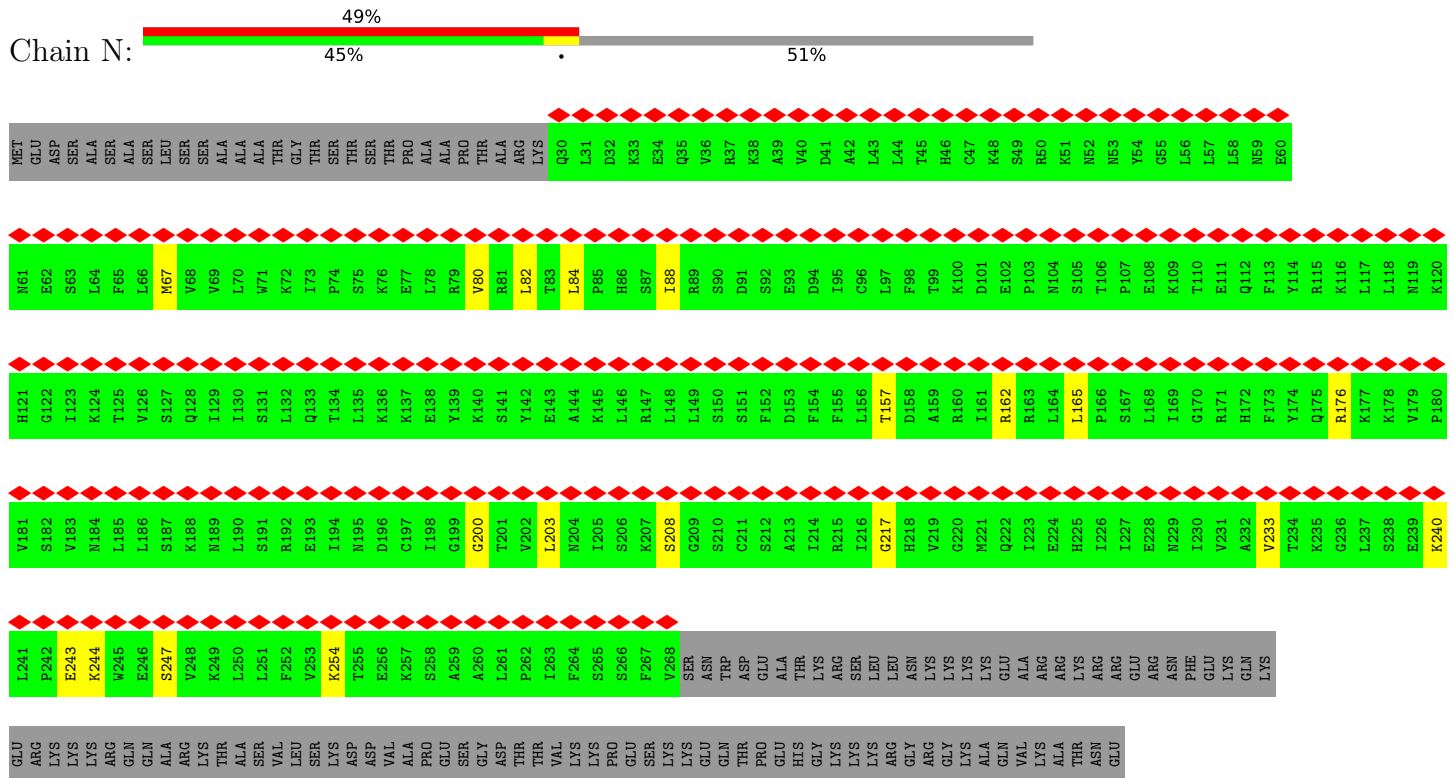
Chain Y: 39% 84% 7% 9%



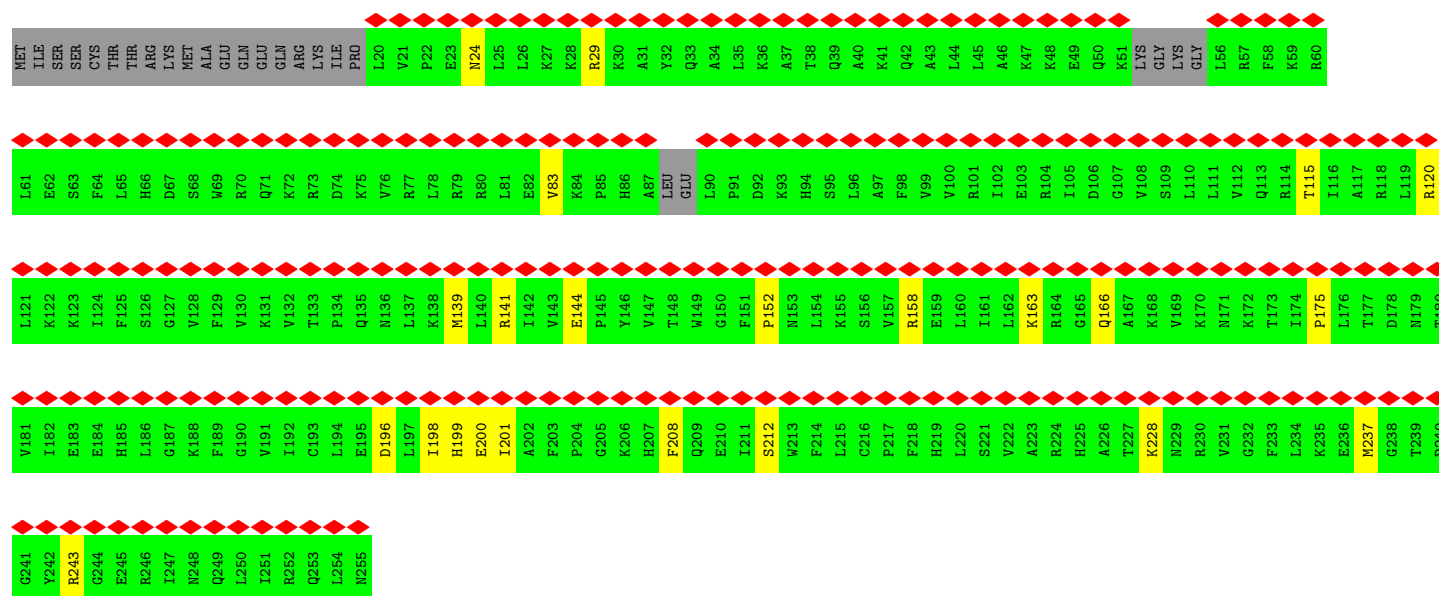
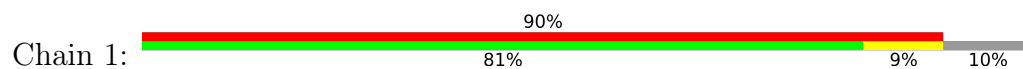
- Molecule 48: ITS2



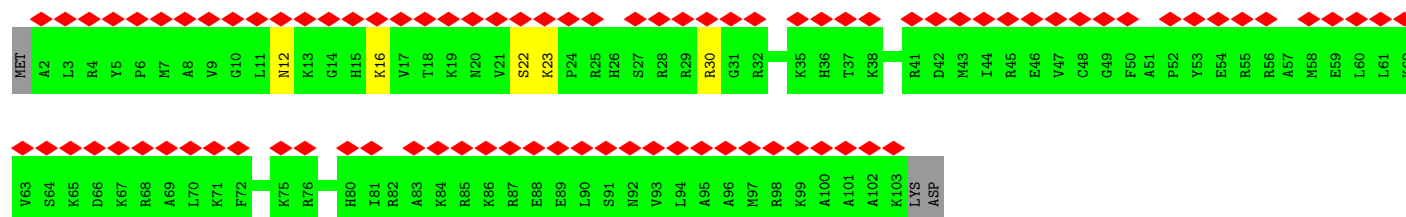
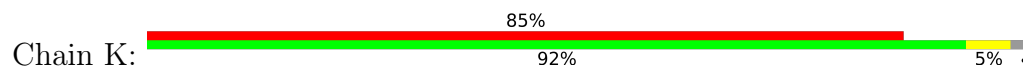
- Molecule 49: Ribosomal L1 domain-containing protein 1



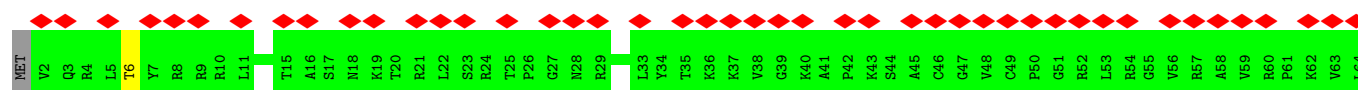
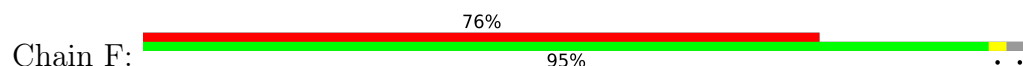
- Molecule 50: 60S ribosomal protein L7-like 1

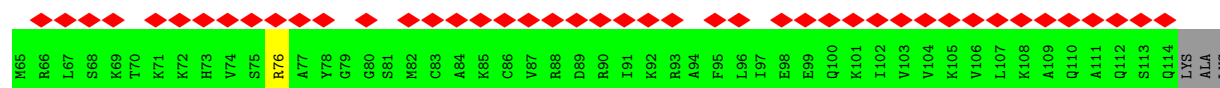


- Molecule 51: 60S ribosomal protein L36

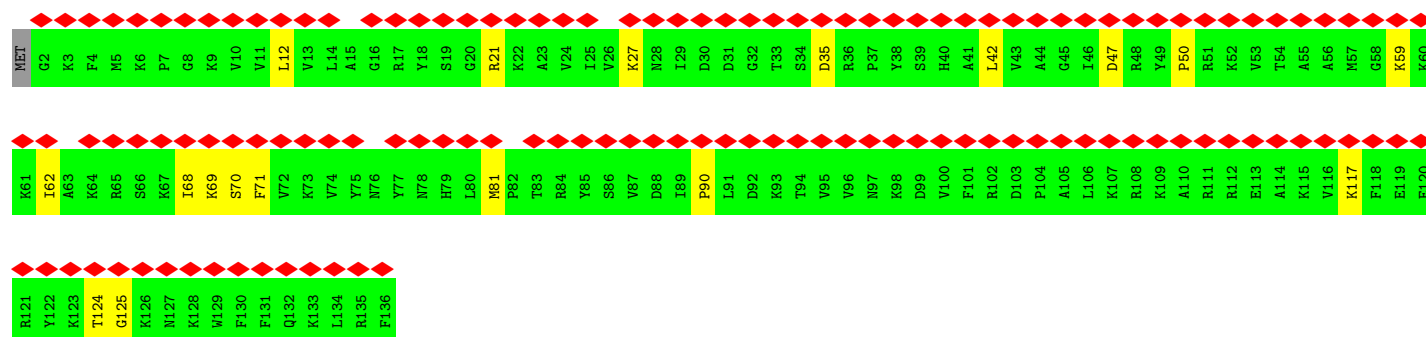
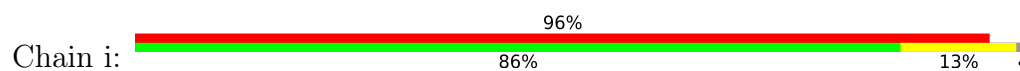


- Molecule 52: 60S ribosomal protein L34

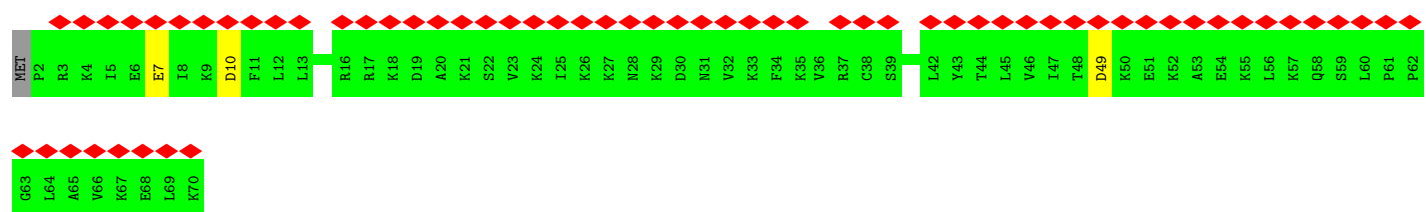




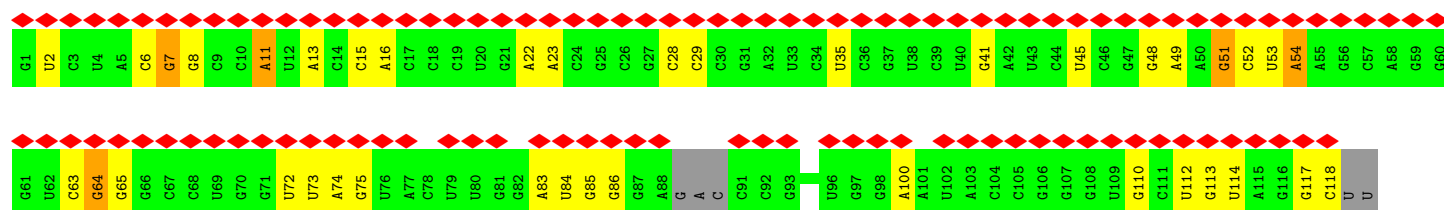
• Molecule 53: 60S ribosomal protein L27



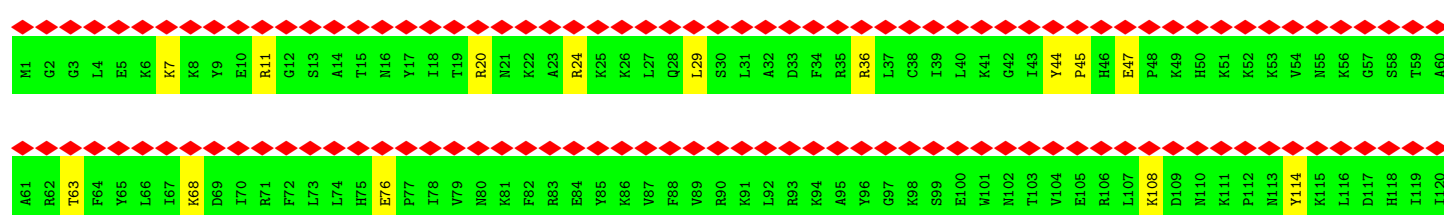
• Molecule 54: 60S ribosomal protein L38

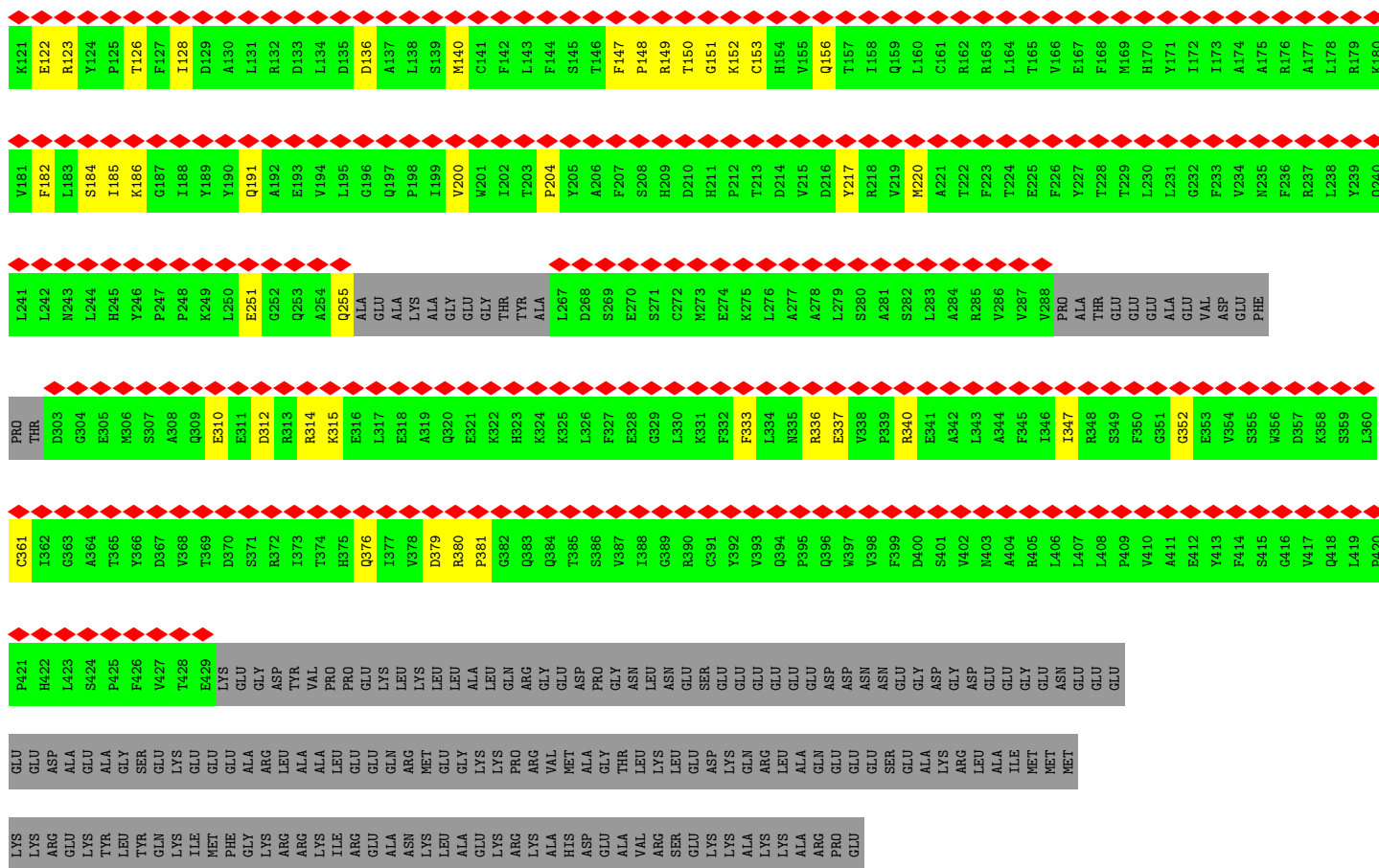


• Molecule 55: 5S RNA

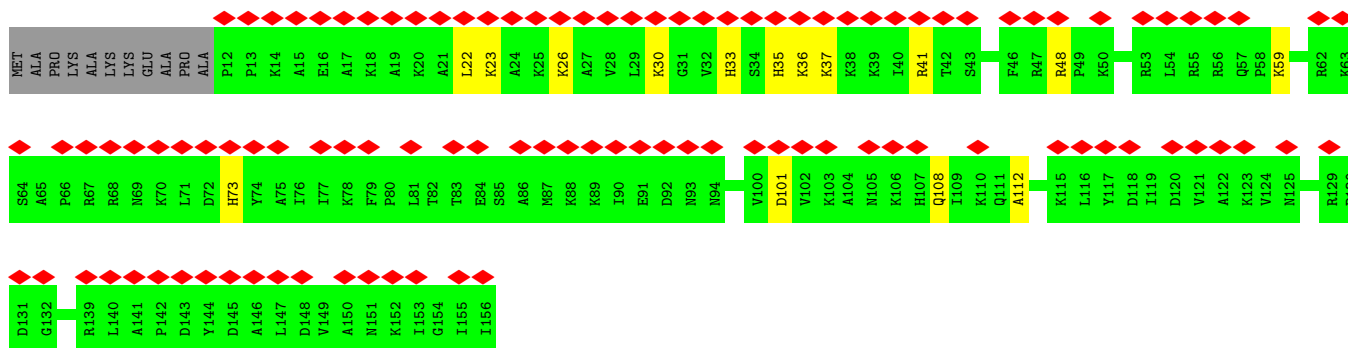
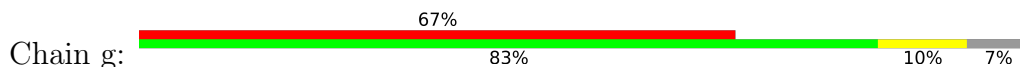


• Molecule 56: Pescadillo homolog

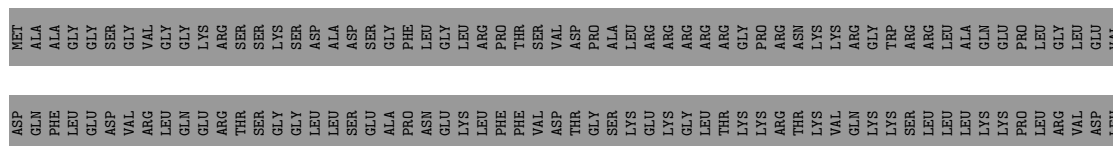
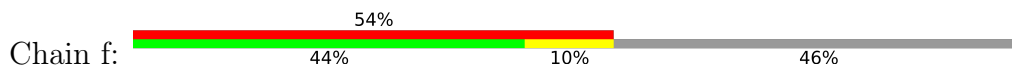




• Molecule 57: 60S ribosomal protein L23a



• Molecule 58: Ribosome biogenesis protein NOP53



S421	S422	E423	L424	T425	D426	S427	L428	R429	T430	L431	K432	P433	E434	G435	M436	L437	L438	R439	D440	R441	F442	K443	S444	F445	Q446	R447	R448	M449	M450	L451	E452	P453	R454	E455	R456	A457	K458	F459	K460	R461	K462	Y463	K464	V465	K466	L467	V468	E469	K470	R471	A472	F473	R474	E475	I476	Q477	L478			
A361	R362	L363	R364	R365	Q366	E367	L368	F369	R370	L371	R372	G373	I374	K375	A376	Q377	V378	A379	L380	R381	L382	A383	E384	L385	A386	R387	R388	Q389	R390	R391	R392	Q393	A394	R395	R396	E397	A398	E399	A400	D401	K402	P403	R404	R405	L406	G407	R408	L409	K410	Y411	Q412	A413	P414	D415	I416	D417	V418	Q419	L420	
L301	LEU	GLU	GLU	SER	ASP	GLY	GLU	GLY	PRO	GLY	GLN	GLU	GLY	PRO	GLU	ALA	ASP	GLY	ALA	GLU	VAL	CYS	PRO	THR	ALA	ARG	LEU	ALA	THR	E335	K336	K337	T338	E339	Q340	Q341	R342	R343	R344	E345	K346	A347	V348	H349	R350	L351	R352	V353	Q354	Q355	A356	A357	L358	R359	A360					
A241	P242	A243	G244	A245	S246	Y247	N248	P249	S250	F251	E252	D253	H254	Q255	T256	L257	L258	S259	A260	A261	H262	E263	V264	E265	Q267	R268	Q269	D210	E211	F212	F213	L214	E215	Q216	T217	K218	K219	K220	G221	V222	K223	R224	P225	A226	R227	L228	H229	T230	K231	P232	S233	Q234	A235	P236	A237	V238	E239	C298	E299	G300
ILE	LEU	GLU	ASN	THR	SER	LYS	VAL	PRO	ALA	PRO	LYS	ASP	VAL	LEU	ALA	HIS	GLN	VAL	PRO	ASN	LYS	LYS	LEU	LEU	ARG	ARG	LYS	GLU	GLN	TRP	GLU	LYS	LEU	ALA	LYS	GLN	GLY	LEU	PRO	ARG	GLU	VAL	ARG	ARG	ALA	GLN	ALA	ARG	LEU	LEU	ASN	PRO	SER	ALA	THR	ARG	ALA			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4919	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	0.152	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: B9B, OMG, GTP, B8W, 5MU, B9H, P4U, 2MG, M7A, OMU, 7MG, BGH, B8Q, A2M, OMC, B8K, P7G, MG, UR3, B8T, I4U, E7G

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	2	0.23	0/81689	0.44	21/127350 (0.0%)
2	6	0.26	0/1877	0.65	1/2554 (0.0%)
3	7	0.32	0/1181	0.64	2/1563 (0.1%)
4	8	0.23	0/3679	0.41	0/5732
5	9	0.29	0/723	0.75	3/961 (0.3%)
6	A	0.24	0/354	0.63	0/465
7	B	0.26	0/3315	0.63	4/4435 (0.1%)
8	D	0.25	0/2907	0.61	4/3905 (0.1%)
9	E	0.28	0/774	0.69	0/1038
10	G	0.31	0/1960	0.74	4/2637 (0.2%)
11	H	0.27	0/1023	0.57	0/1351
12	I	0.28	0/1537	0.66	1/2066 (0.0%)
13	J	0.20	0/1808	0.48	0/2414
14	L	0.21	0/893	0.52	0/1193
15	M	0.27	0/720	0.61	0/952
16	P	0.27	0/454	0.50	0/599
17	Q	0.28	0/1732	0.58	0/2315
18	S	0.31	0/1133	0.69	2/1516 (0.1%)
19	U	0.23	0/1746	0.55	2/2338 (0.1%)
20	V	0.29	0/1682	0.62	2/2250 (0.1%)
21	X	0.28	0/718	0.69	0/953
22	Z	0.24	0/1239	0.52	0/1658
23	a	0.28	0/1255	0.69	4/1662 (0.2%)
24	b	0.21	0/1501	0.46	0/2013
25	e	0.23	0/993	0.60	0/1332
26	h	0.25	0/1132	0.59	0/1504
27	l	0.26	0/1017	0.57	0/1364
28	m	0.26	0/1936	0.64	0/2596
29	n	0.25	0/895	0.66	3/1198 (0.3%)
30	o	0.27	0/1935	0.67	2/2596 (0.1%)
31	p	0.31	0/1916	0.60	0/2553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	r	0.37	0/732	0.82	1/960 (0.1%)
33	u	0.30	0/576	0.71	2/755 (0.3%)
34	v	0.26	0/1806	0.62	0/2420
35	w	0.26	0/3541	0.59	0/4775
36	y	0.30	0/1269	0.71	0/1712
37	z	0.35	1/587 (0.2%)	0.68	0/767
38	C	0.30	0/1341	0.73	2/1793 (0.1%)
39	R	0.30	0/2428	0.74	3/3252 (0.1%)
40	W	0.25	0/3093	0.63	0/4196
41	T	0.27	0/1018	0.67	1/1357 (0.1%)
42	4	0.33	0/5099	0.80	15/6840 (0.2%)
43	Y	0.25	0/1383	0.57	0/1856
44	k	0.23	0/1082	0.62	1/1443 (0.1%)
45	j	0.25	0/933	0.56	0/1256
46	d	0.27	0/864	0.75	2/1160 (0.2%)
47	t	0.29	0/955	0.68	0/1290
49	N	0.25	0/1956	0.58	1/2631 (0.0%)
50	l	0.28	1/1933 (0.1%)	0.65	2/2591 (0.1%)
51	K	0.29	0/843	0.67	0/1115
52	F	0.25	0/907	0.55	0/1209
53	i	0.27	0/1130	0.61	0/1507
54	O	0.32	0/575	0.79	0/761
55	3	0.24	0/2739	0.49	1/4266 (0.0%)
56	q	0.31	0/3395	0.69	0/4578
57	g	0.29	0/1191	0.61	0/1595
58	f	0.26	0/2169	0.65	2/2902 (0.1%)
All	All	0.25	2/169269 (0.0%)	0.54	88/246050 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	A	0	1
7	B	0	1
10	G	0	2
29	n	0	1
32	r	0	1
33	u	0	1
41	T	0	1
42	4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	Y	0	1
47	t	0	1
50	1	0	1
58	f	0	1
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	z	22	ALA	C-N	5.64	1.40	1.34
50	1	152	PRO	CG-CD	-5.28	1.32	1.50

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1871	A2M	OP2-P-O3'	-15.92	70.18	105.20
1	2	1871	A2M	OP1-P-O3'	14.70	137.55	105.20
1	2	1872	G	OP1-P-OP2	-13.63	78.71	119.60
1	2	1872	G	O5'-P-OP1	-9.23	80.30	108.00
50	1	152	PRO	N-CD-CG	-8.68	90.18	103.20
42	4	406	GLY	CA-C-N	7.77	136.38	121.54
42	4	406	GLY	C-N-CA	7.77	136.38	121.54
42	4	503	THR	CA-C-N	7.75	135.66	121.70
42	4	503	THR	C-N-CA	7.75	135.66	121.70
23	a	38	ARG	CA-C-N	7.27	135.42	121.54
23	a	38	ARG	C-N-CA	7.27	135.42	121.54
1	2	1872	G	O5'-P-OP2	6.89	128.67	108.00
42	4	41	HIS	CA-C-N	6.78	134.49	121.54
42	4	41	HIS	C-N-CA	6.78	134.49	121.54
58	f	202	LEU	CA-C-N	6.70	134.33	121.54
58	f	202	LEU	C-N-CA	6.70	134.33	121.54
23	a	76	MET	CA-C-N	6.68	134.50	121.41
23	a	76	MET	C-N-CA	6.68	134.50	121.41
42	4	70	PRO	N-CA-C	6.60	121.54	114.68
50	1	83	VAL	N-CA-C	-6.53	106.43	112.43
19	U	146	PRO	CA-C-N	6.42	133.81	121.54
19	U	146	PRO	C-N-CA	6.42	133.81	121.54
39	R	82	GLU	CA-C-N	6.39	127.67	120.06
39	R	82	GLU	C-N-CA	6.39	127.67	120.06
1	2	1678	C	P-O3'-C3'	6.31	129.67	120.20
18	S	31	ILE	CA-C-N	6.17	133.34	121.54
18	S	31	ILE	C-N-CA	6.17	133.34	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	2760	G	P-O3'-C3'	6.14	129.41	120.20
29	n	105	LEU	CA-C-N	6.11	136.72	121.80
29	n	105	LEU	C-N-CA	6.11	136.72	121.80
12	I	188	GLN	CA-CB-CG	6.11	126.31	114.10
42	4	230	LEU	CA-CB-CG	6.00	137.28	116.30
10	G	129	PRO	CA-C-N	5.92	130.80	122.46
10	G	129	PRO	C-N-CA	5.92	130.80	122.46
1	2	4228	G	P-O3'-C3'	5.88	129.02	120.20
42	4	391	GLU	CA-C-N	5.87	132.75	121.54
42	4	391	GLU	C-N-CA	5.87	132.75	121.54
1	2	914	U	P-O3'-C3'	5.86	128.99	120.20
42	4	430	PRO	CA-C-N	5.86	132.72	121.54
42	4	430	PRO	C-N-CA	5.86	132.72	121.54
1	2	3774	A	P-O3'-C3'	5.83	128.94	120.20
1	2	2486	G	P-O3'-C3'	5.72	128.78	120.20
3	7	7	TYR	CA-C-N	5.71	132.44	121.54
3	7	7	TYR	C-N-CA	5.71	132.44	121.54
1	2	406	C	C2'-C3'-O3'	5.70	122.24	113.70
7	B	304	SER	CA-C-N	5.68	132.38	121.54
7	B	304	SER	C-N-CA	5.68	132.38	121.54
5	9	98	SER	CA-C-N	5.60	132.24	121.54
5	9	98	SER	C-N-CA	5.60	132.24	121.54
41	T	127	GLN	CA-CB-CG	5.59	125.27	114.10
1	2	3905	A	P-O3'-C3'	5.57	128.55	120.20
2	6	58	ILE	N-CA-C	5.56	112.16	106.21
38	C	18	ARG	CA-C-N	5.56	128.73	120.90
38	C	18	ARG	C-N-CA	5.56	128.73	120.90
46	d	66	SER	CA-C-N	5.55	132.15	121.54
46	d	66	SER	C-N-CA	5.55	132.15	121.54
1	2	1980	U	P-O3'-C3'	5.55	128.52	120.20
42	4	257	LEU	CA-CB-CG	5.47	135.45	116.30
5	9	99	GLN	CA-CB-CG	5.45	125.00	114.10
55	3	51	G	C2'-C3'-O3'	5.43	121.84	113.70
1	2	2033	A	P-O3'-C3'	5.43	128.34	120.20
42	4	238	MET	CB-CG-SD	5.43	128.98	112.70
8	D	221	PHE	CA-C-N	5.42	131.90	121.54
8	D	221	PHE	C-N-CA	5.42	131.90	121.54
1	2	1931	C	P-O3'-C3'	5.40	128.30	120.20
39	R	235	MET	CA-CB-CG	5.38	124.85	114.10
32	r	261	LYS	CB-CG-CD	5.36	123.62	111.30
20	V	31	ARG	N-CA-C	5.35	117.17	110.91
30	o	127	SER	CA-C-N	5.33	130.93	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	o	127	SER	C-N-CA	5.33	130.93	122.61
1	2	1808	C	C2'-C3'-O3'	5.33	121.69	113.70
8	D	319	LEU	CA-CB-CG	5.27	134.76	116.30
1	2	406	C	P-O3'-C3'	5.26	128.09	120.20
33	u	4	PRO	CA-C-N	5.26	131.59	121.54
33	u	4	PRO	C-N-CA	5.26	131.59	121.54
42	4	12	VAL	CA-CB-CG1	5.25	119.33	110.40
7	B	29	VAL	CA-C-N	5.23	131.53	121.54
7	B	29	VAL	C-N-CA	5.23	131.53	121.54
1	2	4913	G	P-O3'-C3'	5.21	128.01	120.20
8	D	320	LYS	N-CA-C	-5.20	107.96	114.56
20	V	110	PRO	N-CA-C	5.19	117.03	110.70
49	N	244	LYS	CB-CA-C	5.13	120.64	110.42
10	G	131	LYS	CA-C-N	5.11	134.28	121.80
10	G	131	LYS	C-N-CA	5.11	134.28	121.80
44	k	90	MET	CB-CG-SD	5.10	128.00	112.70
1	2	1931	C	C2'-C3'-O3'	5.03	117.04	109.50
29	n	106	TYR	N-CA-C	5.02	120.91	109.81
1	2	1678	C	C2'-C3'-O3'	5.01	117.02	109.50

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	1	200	GLU	Peptide
42	4	294	LYS	Peptide
42	4	503	THR	Peptide
6	A	107	ARG	Sidechain
7	B	241	PRO	Peptide
10	G	162	ASP	Peptide
10	G	189	ARG	Sidechain
41	T	53	PRO	Peptide
43	Y	131	ARG	Peptide
58	f	204	ARG	Peptide
29	n	106	TYR	Peptide
32	r	254	PHE	Peptide
47	t	142	SER	Peptide
33	u	54	ALA	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	2	74602	0	37551	265	0
2	6	1852	0	1828	17	0
3	7	1159	0	1224	9	0
4	8	3315	0	1684	8	0
5	9	711	0	724	7	0
6	A	352	0	398	3	0
7	B	3244	0	3389	28	0
8	D	2853	0	3028	22	0
9	E	764	0	804	5	0
10	G	1927	0	2074	13	0
11	H	1015	0	1148	6	0
12	I	1518	0	1601	8	0
13	J	1772	0	1892	11	0
14	L	877	0	938	3	0
15	M	705	0	741	5	0
16	P	444	0	483	5	0
17	Q	1701	0	1818	16	0
18	S	1111	0	1174	8	0
19	U	1701	0	1749	13	0
20	V	1650	0	1794	8	0
21	X	708	0	760	6	0
22	Z	1223	0	1330	10	0
23	a	1239	0	1363	10	0
24	b	1461	0	1502	17	0
25	e	979	0	1039	12	0
26	h	1115	0	1205	10	0
27	l	1002	0	1068	9	0
28	m	1898	0	1993	8	0
29	n	876	0	912	3	0
30	o	1897	0	2046	19	0
31	p	1878	0	2009	9	0
32	r	723	0	770	9	0
33	u	569	0	635	2	0
34	v	1771	0	1810	12	0
35	w	3472	0	3527	23	0
36	y	1250	0	1305	12	0
37	z	581	0	656	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C	1319	0	1358	14	0
39	R	2382	0	2410	31	0
40	W	3018	0	2959	24	0
41	T	1001	0	1064	5	0
42	4	5016	0	5153	45	0
43	Y	1355	0	1389	9	0
44	k	1064	0	1160	7	0
45	j	918	0	964	5	0
46	d	850	0	868	9	0
47	t	928	0	906	9	0
48	x	684	0	456	2	0
49	N	1924	0	2027	12	0
50	1	1897	0	2029	12	0
51	K	832	0	917	3	0
52	F	897	0	989	2	0
53	i	1107	0	1182	19	0
54	O	569	0	635	5	0
55	3	2453	0	1243	15	0
56	q	3317	0	3368	62	0
57	g	1170	0	1283	36	0
58	f	2137	0	2201	111	0
59	w	32	0	12	0	0
60	w	1	0	0	0	0
All	All	160786	0	124545	799	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 (799) 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)
57:g:30:LYS:HE3	58:f:473:PHE:CE1	1.24	1.70
1:2:4083:5MU:C5	1:2:4083:5MU:C4	1.79	1.68
56:q:186:LYS:NZ	58:f:417:ASP:HB2	1.41	1.34
57:g:37:LYS:HE2	58:f:465:VAL:CG2	1.59	1.33
57:g:33:HIS:HB2	58:f:473:PHE:CZ	1.63	1.32
57:g:30:LYS:CE	58:f:473:PHE:HE1	1.44	1.30
57:g:33:HIS:HB2	58:f:473:PHE:CE2	1.66	1.29
57:g:30:LYS:CE	58:f:473:PHE:CE1	2.17	1.24
54:O:7:GLU:OE1	58:f:364:ARG:NH1	1.76	1.17
54:O:49:ASP:OD1	58:f:365:HIS:CE1	2.00	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:g:37:LYS:HE2	58:f:465:VAL:HG21	1.18	1.13
57:g:37:LYS:CE	58:f:465:VAL:HG21	1.79	1.11
56:q:156:GLN:HG3	58:f:188:VAL:CG2	1.85	1.07
1:2:2763:U:H2'	58:f:391:ARG:NH2	1.71	1.06
23:a:108:ARG:CZ	58:f:339:GLU:OE1	2.03	1.05
1:2:2763:U:H2'	58:f:391:ARG:CZ	1.86	1.04
56:q:204:PRO:HB3	58:f:437:ILE:CD1	1.89	1.03
57:g:33:HIS:CB	58:f:473:PHE:CZ	2.43	1.01
57:g:33:HIS:CB	58:f:473:PHE:CE2	2.45	0.99
56:q:156:GLN:HG3	58:f:188:VAL:HG22	1.42	0.98
1:2:4297:G:N1	1:2:4313:A:H2	1.63	0.95
56:q:186:LYS:HE3	58:f:417:ASP:OD2	1.66	0.95
56:q:186:LYS:HZ2	58:f:417:ASP:HB2	1.21	0.95
1:2:4321:U:H3	1:2:4326:G:H1	0.99	0.94
56:q:186:LYS:HZ1	58:f:417:ASP:HB2	1.11	0.94
57:g:30:LYS:HE3	58:f:473:PHE:CD1	2.03	0.92
54:O:49:ASP:OD1	58:f:365:HIS:NE2	2.01	0.91
56:q:20:ARG:NH1	58:f:454:ARG:HH22	1.67	0.90
1:2:4745:G:H1	1:2:4955:A:H61	1.20	0.90
57:g:22:LEU:HD21	58:f:478:LEU:OXT	1.71	0.90
57:g:33:HIS:HB2	58:f:473:PHE:HZ	1.31	0.89
1:2:4297:G:N1	1:2:4313:A:C2	2.36	0.89
56:q:186:LYS:NZ	58:f:417:ASP:CB	2.34	0.88
56:q:68:LYS:HB2	58:f:227:ARG:NH2	1.88	0.87
1:2:2763:U:O2'	58:f:391:ARG:NE	2.09	0.86
53:i:125:GLY:HA3	58:f:288:ALA:HB2	1.58	0.83
1:2:2592:U:H3	1:2:4126:C:H42	1.22	0.83
1:2:2592:U:H3	1:2:4126:C:N4	1.78	0.81
56:q:156:GLN:HG3	58:f:188:VAL:HG23	1.62	0.81
1:2:2763:U:H2'	58:f:391:ARG:NE	1.96	0.80
1:2:2845:A:H61	1:2:3843:C:H42	1.26	0.80
1:2:4297:G:H1	1:2:4313:A:H2	0.89	0.80
57:g:33:HIS:HB2	58:f:473:PHE:HE2	1.39	0.80
53:i:125:GLY:HA3	58:f:288:ALA:CB	2.12	0.80
57:g:33:HIS:CG	58:f:473:PHE:HZ	2.01	0.79
57:g:33:HIS:CB	58:f:473:PHE:HE2	1.95	0.78
57:g:30:LYS:HB3	58:f:473:PHE:CE1	2.19	0.78
53:i:125:GLY:C	58:f:288:ALA:HB2	2.09	0.78
1:2:2007:G:H21	1:2:2012:A:H62	1.31	0.77
57:g:33:HIS:CB	58:f:473:PHE:HZ	1.90	0.76
23:a:108:ARG:NH1	58:f:339:GLU:CD	2.45	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:108:ARG:NH2	58:f:339:GLU:OE1	2.19	0.75
56:q:186:LYS:HZ1	58:f:417:ASP:CB	1.93	0.75
1:2:2763:U:C2'	58:f:391:ARG:NE	2.51	0.74
53:i:125:GLY:CA	58:f:288:ALA:HB2	2.17	0.74
55:3:7:G:H1	55:3:112:U:H3	1.33	0.74
56:q:184:SER:OG	58:f:245:ALA:O	2.04	0.74
56:q:123:ARG:HG2	58:f:224:ARG:HH12	1.52	0.74
1:2:2452:G:H21	1:2:2507:A:H62	1.34	0.74
56:q:204:PRO:HB3	58:f:437:ILE:HD11	1.71	0.73
57:g:37:LYS:CE	58:f:465:VAL:CG2	2.47	0.72
57:g:59:LYS:HA	58:f:216:GLN:HE22	1.53	0.72
23:a:108:ARG:NH1	58:f:339:GLU:OE1	2.21	0.72
1:2:2763:U:C2'	58:f:391:ARG:HE	2.05	0.69
56:q:20:ARG:HH12	58:f:454:ARG:HH22	1.40	0.69
56:q:63:THR:HG21	58:f:452:GLU:OE1	1.93	0.69
1:2:2763:U:H2'	58:f:391:ARG:HH21	1.55	0.69
56:q:204:PRO:HB3	58:f:437:ILE:HD12	1.75	0.68
57:g:37:LYS:HE2	58:f:465:VAL:HG22	1.69	0.67
22:Z:67:ILE:O	22:Z:71:LYS:HB2	1.94	0.66
56:q:156:GLN:CG	58:f:188:VAL:HG22	2.21	0.65
57:g:22:LEU:O	57:g:26:LYS:HB2	1.97	0.65
1:2:1939:A:N6	1:2:4401:G:N1	2.44	0.65
1:2:2679:G:OP1	58:f:342:ARG:NH2	2.30	0.65
35:w:348:TRP:HA	35:w:361:ASP:O	1.98	0.64
1:2:2763:U:C2'	58:f:391:ARG:NH2	2.58	0.64
56:q:186:LYS:HZ2	58:f:417:ASP:CB	2.04	0.64
1:2:1098:G:H1	1:2:1197:C:H42	1.44	0.63
1:2:2845:A:N6	1:2:3843:C:H42	1.97	0.63
56:q:45:PRO:HG2	58:f:406:LEU:HD12	1.79	0.63
57:g:22:LEU:CD2	58:f:478:LEU:OXT	2.45	0.63
1:2:2845:A:H61	1:2:3843:C:N4	1.96	0.62
40:W:260:LEU:HB2	40:W:272:TRP:HB2	1.81	0.62
38:C:18:ARG:HB3	38:C:133:VAL:HG23	1.82	0.62
46:d:22:THR:O	46:d:109:SER:HA	2.01	0.61
1:2:2007:G:N2	1:2:2012:A:H62	1.98	0.61
1:2:2557:G:H1	1:2:2570:U:H3	1.48	0.61
53:i:125:GLY:O	58:f:288:ALA:HB2	2.01	0.61
25:e:87:SER:HA	25:e:96:LEU:O	2.01	0.60
53:i:59:LYS:HD2	58:f:279:LEU:CD1	2.32	0.60
56:q:63:THR:HG22	58:f:407:GLY:HA2	1.84	0.60
56:q:136:ASP:OD1	58:f:237:ALA:HB1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:e:28:CYS:SG	25:e:29:ALA:N	2.73	0.60
1:2:4745:G:H1	1:2:4955:A:N6	1.95	0.60
1:2:1939:A:H61	1:2:4401:G:H1	1.50	0.59
42:4:371:LYS:HB3	42:4:373:ARG:HE	1.68	0.59
37:z:17:LYS:O	37:z:21:ASN:HB2	2.03	0.59
1:2:4929:C:H5''	18:S:114:LYS:HD2	1.83	0.59
20:V:34:VAL:HG12	20:V:103:LYS:HB2	1.84	0.59
1:2:2362:U:H2'	1:2:2363:A2M:H8	1.84	0.59
41:T:28:ALA:O	41:T:32:ARG:NH1	2.36	0.59
49:N:80:VAL:HB	49:N:203:LEU:HB3	1.85	0.59
56:q:380:ARG:HD2	58:f:429:ARG:HH12	1.69	0.58
1:2:4235:G:O6	1:2:4288:C:N4	2.37	0.58
4:8:83:C:N3	26:h:50:ARG:NH2	2.52	0.58
36:y:60:VAL:HG22	36:y:73:VAL:HG12	1.86	0.58
40:W:471:VAL:HB	40:W:483:TRP:HB2	1.86	0.57
23:a:108:ARG:NH1	58:f:339:GLU:OE2	2.37	0.57
22:Z:35:LEU:O	22:Z:39:THR:HB	2.03	0.57
32:r:244:ARG:HD3	32:r:247:LYS:HD3	1.86	0.57
30:o:173:LEU:HB2	30:o:189:THR:O	2.04	0.57
1:2:967:C:H2'	30:o:110:ARG:HH22	1.69	0.56
1:2:3776:G:H5'	35:w:292:GLY:H	1.70	0.56
8:D:218:ILE:O	8:D:222:ARG:HB3	2.05	0.56
1:2:2452:G:N2	1:2:2507:A:H62	2.04	0.56
34:v:121:GLU:HB2	34:v:200:PHE:HB3	1.87	0.56
1:2:3697:U:H5''	1:2:3698:G:H5'	1.88	0.56
1:2:4539:U:H5''	35:w:352:THR:HG23	1.86	0.56
38:C:22:LEU:O	38:C:71:HIS:HA	2.05	0.56
55:3:28:C:H1'	55:3:54:A:H61	1.69	0.56
40:W:280:CYS:SG	40:W:281:ARG:NH1	2.78	0.56
56:q:340:ARG:NH1	56:q:361:CYS:SG	2.78	0.56
9:E:47:ILE:HG12	9:E:72:HIS:HB3	1.86	0.56
49:N:157:THR:HG21	49:N:165:LEU:HD11	1.86	0.56
57:g:37:LYS:HE3	58:f:465:VAL:HG21	1.81	0.56
1:2:1939:A:N6	1:2:4401:G:H1	2.01	0.56
57:g:36:LYS:HG3	58:f:470:LYS:HG2	1.87	0.56
1:2:1187:G:N7	39:R:275:GLN:NE2	2.55	0.55
1:2:4434:C:HO2'	13:J:193:CYS:HG	1.51	0.55
50:1:163:LYS:HB3	56:q:148:PRO:HB3	1.88	0.55
40:W:375:ILE:HD13	40:W:391:SER:HB2	1.89	0.55
42:4:170:THR:HG22	42:4:218:GLN:HB2	1.89	0.55
49:N:82:LEU:O	49:N:200:GLY:HA3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:T:41:ASP:HA	41:T:60:LYS:O	2.07	0.54
1:2:2020:U:H2'	1:2:2021:G:H8	1.72	0.54
1:2:73:A:N7	17:Q:103:ARG:NH2	2.55	0.54
56:q:20:ARG:HH11	58:f:454:ARG:HH22	1.51	0.54
56:q:333:PHE:HB3	56:q:376:GLN:HG3	1.90	0.54
1:2:1268:G:N7	6:A:111:ARG:NH2	2.55	0.54
1:2:1552:G:O2'	1:2:1574:B9B:N2	2.41	0.54
35:w:210:LEU:HD22	35:w:365:VAL:HG11	1.89	0.54
58:f:452:GLU:OE2	58:f:454:ARG:NH2	2.41	0.54
39:R:268:ARG:NH2	39:R:271:MET:SD	2.81	0.54
45:j:46:LEU:HD11	45:j:64:ILE:HG21	1.90	0.54
56:q:68:LYS:HB2	58:f:227:ARG:HH21	1.72	0.54
3:7:62:GLU:HG3	3:7:108:ILE:HD11	1.90	0.53
58:f:337:LYS:HD2	58:f:342:ARG:HE	1.73	0.53
8:D:328:LEU:HD12	31:p:187:MET:HG3	1.91	0.53
12:I:152:GLU:O	12:I:156:ASN:HB2	2.08	0.53
1:2:2572:C:OP1	58:f:277:ARG:HD2	2.08	0.53
35:w:50:ARG:HG2	35:w:56:ILE:HA	1.89	0.53
1:2:3937:C:H1'	19:U:125:SER:HB2	1.91	0.53
5:9:101:GLU:HA	5:9:104:ARG:HG2	1.91	0.53
53:i:62:ILE:HG22	58:f:279:LEU:HD22	1.90	0.53
49:N:67:MET:HE3	49:N:254:LYS:HD3	1.90	0.53
1:2:4472:B8W:N2	1:2:4483:B8T:O2	2.41	0.53
2:6:163:PRO:HA	2:6:183:ALA:HB1	1.91	0.53
27:l:16:PHE:HB3	27:l:27:THR:H	1.74	0.53
56:q:68:LYS:CB	58:f:227:ARG:NH2	2.68	0.53
35:w:219:VAL:HB	35:w:313:VAL:HG22	1.91	0.53
22:Z:12:LYS:HD2	22:Z:14:ARG:HH21	1.73	0.53
1:2:29:G:O2'	19:U:96:ARG:NH1	2.42	0.53
1:2:667:A:N7	8:D:291:ARG:NH1	2.57	0.53
1:2:1702:C:H4'	8:D:308:LYS:HD3	1.91	0.53
7:B:57:VAL:HG12	7:B:73:VAL:HG12	1.91	0.53
20:V:7:LEU:HB3	20:V:33:VAL:HG12	1.89	0.53
27:l:94:ARG:HH12	30:o:112:MET:HE2	1.73	0.53
1:2:4421:C:N4	1:2:4424:A:N7	2.51	0.52
1:2:375:G:N7	15:M:56:ARG:NH2	2.56	0.52
1:2:2763:U:C2'	58:f:391:ARG:HH21	2.17	0.52
1:2:3722:G:H2'	1:2:3723:A2M:H8	1.91	0.52
43:Y:50:ASP:HB3	43:Y:55:LYS:HB2	1.91	0.52
1:2:2678:A:H4'	58:f:336:LYS:HG2	1.91	0.52
56:q:63:THR:CG2	58:f:452:GLU:OE1	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:230:GLY:O	7:B:234:ARG:HB2	2.10	0.52
19:U:165:THR:HG23	19:U:168:GLY:H	1.74	0.52
45:j:32:ARG:HB3	45:j:48:GLU:HG2	1.92	0.52
1:2:2343:G:OP2	8:D:109:ARG:NH2	2.43	0.52
1:2:4236:G:N2	1:2:4289:U:O2	2.42	0.52
12:I:8:GLN:OE1	32:r:256:GLN:NE2	2.43	0.52
7:B:222:VAL:O	7:B:343:ARG:NH1	2.43	0.52
35:w:267:ARG:HH21	35:w:464:ASN:HB3	1.74	0.52
1:2:2420:A:OP2	43:Y:127:ARG:NH1	2.43	0.52
1:2:4602:A:H62	1:2:4609:G:H21	1.58	0.52
35:w:18:SER:HB2	35:w:33:ARG:HH12	1.75	0.52
1:2:4297:G:O6	1:2:4313:A:N1	2.43	0.52
2:6:24:CYS:HB3	2:6:48:VAL:HG12	1.91	0.52
42:4:178:ASN:ND2	42:4:197:PRO:O	2.43	0.52
42:4:269:LEU:O	42:4:273:GLN:NE2	2.43	0.51
31:p:107:LYS:HD2	31:p:110:GLN:HE21	1.74	0.51
39:R:108:ARG:O	39:R:112:ARG:HB2	2.11	0.51
39:R:23:ARG:O	39:R:23:ARG:NH1	2.43	0.51
40:W:140:PHE:HB2	40:W:150:PHE:HB2	1.90	0.51
1:2:4596:C:OP1	2:6:9:ASN:ND2	2.42	0.51
1:2:2549:G:H5'	58:f:388:ARG:NH2	2.25	0.51
22:Z:29:VAL:O	22:Z:33:ARG:HB2	2.10	0.51
24:b:138:ARG:NH2	33:u:55:PRO:O	2.41	0.51
1:2:493:G:O6	1:2:660:A:N1	2.44	0.51
57:g:30:LYS:CB	58:f:473:PHE:CE1	2.92	0.51
1:2:3641:U:OP2	1:2:3646:A:N6	2.44	0.51
6:A:101:HIS:O	6:A:109:ARG:NH2	2.44	0.51
22:Z:124:ASP:OD1	22:Z:124:ASP:N	2.43	0.51
35:w:312:SER:HB2	35:w:360:ILE:HD11	1.93	0.51
42:4:227:ASP:N	42:4:227:ASP:OD1	2.44	0.51
56:q:76:GLU:CD	58:f:220:LYS:HE3	2.35	0.51
56:q:312:ASP:OD1	56:q:315:LYS:NZ	2.42	0.51
2:6:163:PRO:HB3	42:4:359:ARG:HD2	1.92	0.51
7:B:84:MET:O	7:B:204:GLN:HA	2.11	0.51
30:o:157:HIS:HB3	30:o:160:LYS:HD2	1.92	0.51
42:4:443:ASP:HB3	42:4:446:ILE:HB	1.91	0.51
56:q:147:PHE:HZ	58:f:438:LEU:HD11	1.76	0.51
1:2:1708:G:O2'	1:2:1715:C:N4	2.44	0.51
18:S:81:ASP:OD1	18:S:81:ASP:N	2.43	0.51
31:p:92:VAL:O	31:p:120:GLY:HA2	2.10	0.51
56:q:184:SER:OG	56:q:185:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:2300:A:N7	8:D:143:ARG:NH1	2.59	0.50
50:1:237:MET:O	50:1:243:ARG:NH2	2.44	0.50
1:2:5040:U:OP2	7:B:396:ARG:NH2	2.44	0.50
17:Q:78:LEU:HD11	17:Q:88:LYS:HD3	1.94	0.50
18:S:106:ASP:OD2	30:o:161:ARG:NH2	2.44	0.50
42:4:14:SER:O	42:4:18:PHE:HB2	2.11	0.50
50:1:166:GLN:HA	50:1:175:PRO:HA	1.94	0.50
1:2:1914:C:H4'	20:V:89:PRO:HD3	1.93	0.50
1:2:2391:G:OP2	42:4:504:GLN:NE2	2.45	0.50
30:o:69:TYR:O	30:o:72:LYS:NZ	2.44	0.50
1:2:1374:G:H1'	8:D:234:LYS:HG2	1.93	0.50
1:2:2335:C:H2'	1:2:2336:G:H8	1.77	0.50
39:R:208:MET:HA	39:R:211:LEU:HD23	1.93	0.50
47:t:141:PRO:HG2	47:t:144:PRO:HG3	1.93	0.50
1:2:2856:C:O2	7:B:242:ARG:NH2	2.45	0.50
1:2:4241:C:OP2	38:C:145:LYS:NZ	2.45	0.50
1:2:4769:G:OP1	20:V:176:ARG:NH1	2.44	0.50
42:4:121:ASP:H	42:4:125:ARG:HD3	1.77	0.50
42:4:230:LEU:O	42:4:233:ARG:NH1	2.44	0.50
56:q:122:GLU:HG3	58:f:224:ARG:HH11	1.76	0.50
1:2:264:C:O2	11:H:112:ARG:NH1	2.45	0.50
1:2:4673:U:OP2	25:e:15:ARG:NH2	2.45	0.50
40:W:252:LEU:HD11	40:W:260:LEU:HD12	1.92	0.50
1:2:245:C:H41	1:2:1366:G:H22	1.59	0.50
39:R:50:ARG:NH2	55:3:6:C:O2'	2.45	0.50
56:q:36:ARG:NH2	56:q:114:TYR:OH	2.44	0.50
1:2:1677:U:O2	1:2:1679:A:N6	2.44	0.50
1:2:2562:G:N2	1:2:2565:A:OP2	2.45	0.50
1:2:2583:C:OP2	52:F:76:ARG:NH1	2.45	0.50
1:2:2845:A:O3'	5:9:22:LYS:NZ	2.45	0.50
2:6:219:GLU:HG3	2:6:224:LEU:HD12	1.93	0.50
40:W:430:VAL:HA	40:W:439:LYS:O	2.12	0.50
50:1:115:THR:HB	50:1:139:MET:HE1	1.93	0.50
1:2:3865:A:N3	44:k:27:ARG:NH2	2.60	0.50
30:o:161:ARG:O	30:o:182:ASN:ND2	2.45	0.50
35:w:221:VAL:HG22	35:w:251:ILE:HB	1.94	0.50
24:b:97:TYR:HB3	24:b:108:GLN:HE21	1.76	0.49
42:4:534:LYS:NZ	46:d:31:ASP:O	2.42	0.49
56:q:140:MET:HE1	56:q:220:MET:HG2	1.93	0.49
1:2:4358:U:H4'	17:Q:197:LYS:HD2	1.94	0.49
2:6:238:ASP:OD1	2:6:238:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:C:129:ASP:OD1	38:C:129:ASP:N	2.45	0.49
57:g:33:HIS:CG	58:f:473:PHE:CZ	2.86	0.49
1:2:968:C:OP2	30:o:110:ARG:NH1	2.44	0.49
1:2:1393:G:O2'	17:Q:190:ARG:NH2	2.45	0.49
1:2:1853:G:N2	1:2:1853:G:OP2	2.45	0.49
1:2:2400:G:H21	52:F:6:THR:HG22	1.76	0.49
42:4:517:ARG:NH2	42:4:534:LYS:O	2.44	0.49
1:2:194:C:O2	26:h:121:ARG:NH1	2.46	0.49
1:2:994:G:N7	1:2:1050:C:N4	2.61	0.49
1:2:4265:U:O4	39:R:19:LYS:NZ	2.46	0.49
39:R:21:ARG:NH2	55:3:8:G:O6	2.45	0.49
1:2:2483:G:OP2	56:q:20:ARG:NH2	2.44	0.49
1:2:977:C:OP2	30:o:59:ARG:NH2	2.46	0.49
1:2:1517:2MG:HN2	8:D:103:ALA:HA	1.77	0.49
1:2:4088:C:OP1	28:m:37:ARG:NH1	2.45	0.49
1:2:667:A:OP1	27:l:67:ARG:NH2	2.45	0.49
1:2:1378:C:N4	17:Q:159:ASN:OD1	2.45	0.49
32:r:238:GLY:O	32:r:249:ARG:NH2	2.45	0.49
1:2:1445:U:H3	1:2:2103:G:H22	1.60	0.49
1:2:2521:G:H2'	1:2:2522:7MG:H82	1.95	0.49
7:B:58:ARG:O	7:B:71:GLU:HA	2.13	0.49
35:w:425:LEU:HD22	35:w:443:VAL:HG13	1.94	0.49
42:4:503:THR:O	42:4:507:ARG:NH2	2.45	0.49
53:i:21:ARG:NH1	53:i:47:ASP:O	2.45	0.49
56:q:186:LYS:CE	58:f:417:ASP:OD2	2.51	0.49
1:2:970:G:OP1	30:o:123:ARG:NH1	2.46	0.49
8:D:301:ALA:HB1	22:Z:132:LYS:HD3	1.94	0.49
40:W:391:SER:OG	40:W:392:PHE:N	2.46	0.49
56:q:191:GLN:HG2	56:q:200:VAL:HG22	1.95	0.49
1:2:300:A:H2'	1:2:301:G:H8	1.77	0.48
1:2:3620:G:OP1	1:2:3622:C:N4	2.45	0.48
13:J:199:VAL:HA	13:J:220:ILE:HG22	1.94	0.48
53:i:12:LEU:HB2	53:i:81:MET:HB3	1.95	0.48
1:2:97:G:OP1	17:Q:16:LYS:NZ	2.45	0.48
38:C:114:ASP:OD1	38:C:114:ASP:N	2.46	0.48
47:t:62:PHE:O	47:t:66:SER:HB2	2.13	0.48
49:N:88:ILE:HG23	49:N:217:GLY:HA2	1.94	0.48
1:2:1179:U:O4	39:R:289:ARG:NH1	2.47	0.48
1:2:1521:C:OP1	8:D:100:ARG:NH2	2.46	0.48
1:2:4126:C:OP1	10:G:37:LYS:NZ	2.46	0.48
5:9:36:ARG:HH22	5:9:92:LEU:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:238:TRP:HB3	35:w:85:ARG:HB2	1.96	0.48
47:t:148:ARG:NH2	48:x:44:N:O2'	2.46	0.48
55:3:112:U:H2'	55:3:113:G:H8	1.78	0.48
1:2:2875:C:OP1	21:X:23:ARG:NH1	2.46	0.48
4:8:126:C:O2'	4:8:128:C:N4	2.41	0.48
1:2:423:G:OP1	43:Y:62:ARG:NH1	2.47	0.48
1:2:1398:A:N6	1:2:1419:G:O2'	2.47	0.48
1:2:2712:G:O6	23:a:46:LYS:NZ	2.45	0.48
7:B:40:PRO:HB2	37:z:34:LYS:HE3	1.94	0.48
30:o:178:PRO:HB2	30:o:181:LEU:HD23	1.94	0.48
31:p:182:TYR:HB3	31:p:200:ARG:HG3	1.94	0.48
49:N:162:ARG:HA	49:N:165:LEU:HG	1.95	0.48
1:2:382:G:N1	1:2:385:A:OP2	2.45	0.48
1:2:665:C:H4'	1:2:666:G:H5'	1.95	0.48
1:2:2686:G:O2'	1:2:2688:G:N7	2.45	0.48
7:B:92:TYR:HB2	7:B:159:VAL:HB	1.95	0.48
19:U:84:PRO:O	19:U:87:HIS:ND1	2.45	0.48
37:z:101:GLN:HA	37:z:104:ARG:HD3	1.95	0.48
39:R:58:ARG:HH12	55:3:28:C:H41	1.60	0.48
40:W:433:SER:OG	40:W:434:SER:N	2.47	0.48
7:B:131:THR:O	7:B:135:LYS:NZ	2.46	0.48
24:b:144:GLN:HA	32:r:262:PRO:HD3	1.95	0.48
34:v:40:LEU:HD11	34:v:102:LEU:HD22	1.95	0.48
1:2:992:C:N4	1:2:995:C:O2'	2.46	0.48
1:2:1306:C:H2'	1:2:1307:A:H8	1.79	0.48
1:2:3838:U:H5'	5:9:17:ARG:HD2	1.96	0.48
39:R:51:MET:HA	39:R:63:GLN:O	2.14	0.48
58:f:219:LYS:HE3	58:f:221:GLY:HA3	1.96	0.48
2:6:66:ASN:ND2	2:6:111:ASN:O	2.47	0.48
9:E:17:ARG:HD3	9:E:103:ASP:HA	1.94	0.48
18:S:41:PRO:HB3	18:S:70:GLN:HE21	1.78	0.48
36:y:89:PRO:O	36:y:94:LYS:NZ	2.47	0.48
40:W:200:LYS:HB3	40:W:224:LYS:HB3	1.96	0.48
48:x:49:N:OP2	49:N:176:ARG:NH1	2.46	0.48
49:N:84:LEU:HD21	49:N:233:VAL:HG23	1.96	0.48
53:i:59:LYS:HD2	58:f:279:LEU:HD13	1.95	0.48
1:2:758:G:H5''	12:I:52:LYS:HG3	1.95	0.47
1:2:4163:U:OP2	10:G:53:ARG:NH1	2.45	0.47
1:2:4516:G:OP2	7:B:2:SER:N	2.47	0.47
54:O:7:GLU:HB2	54:O:10:ASP:HB2	1.96	0.47
1:2:134:G:OP2	11:H:74:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:2625:U:OP2	42:4:510:ARG:NH2	2.47	0.47
20:V:185:VAL:HG12	20:V:189:ILE:HG12	1.96	0.47
22:Z:53:MET:HE3	22:Z:57:ASN:HB3	1.95	0.47
36:y:130:LYS:HG2	36:y:152:ILE:HG12	1.95	0.47
49:N:243:GLU:HB3	49:N:247:SER:HB2	1.96	0.47
56:q:7:LYS:O	56:q:11:ARG:NH2	2.46	0.47
57:g:30:LYS:NZ	58:f:473:PHE:CE1	2.79	0.47
1:2:3855:C:H2'	1:2:3856:A:H8	1.80	0.47
7:B:10:ARG:NH1	7:B:11:HIS:O	2.47	0.47
10:G:26:LYS:HG3	10:G:27:VAL:HG13	1.96	0.47
35:w:164:ILE:HD11	42:4:278:LEU:HA	1.96	0.47
39:R:197:LYS:HG3	39:R:202:GLN:HB2	1.95	0.47
40:W:325:LEU:HD23	40:W:328:ARG:HH11	1.79	0.47
42:4:232:ASP:OD1	42:4:232:ASP:N	2.46	0.47
1:2:4570:G:H2'	1:2:4571:A2M:H8	1.95	0.47
3:7:19:MET:SD	3:7:19:MET:N	2.87	0.47
34:v:208:TRP:HB2	34:v:215:PHE:HD1	1.79	0.47
44:k:26:ASP:OD1	44:k:26:ASP:N	2.44	0.47
56:q:136:ASP:OD1	58:f:441:ARG:NH2	2.48	0.47
1:2:727:C:OP1	31:p:73:ARG:NH2	2.47	0.47
7:B:153:MET:O	7:B:157:CYS:HB2	2.15	0.47
34:v:208:TRP:HA	34:v:214:ARG:O	2.15	0.47
36:y:45:ASP:HB3	36:y:71:ILE:HD11	1.96	0.47
38:C:75:ARG:O	38:C:78:LYS:NZ	2.47	0.47
38:C:92:TYR:HB3	38:C:172:GLY:HA2	1.96	0.47
38:C:141:ILE:HA	38:C:144:LYS:HE2	1.97	0.47
42:4:244:LEU:O	42:4:282:LYS:NZ	2.47	0.47
9:E:38:ILE:HG21	9:E:63:TYR:HB3	1.97	0.47
12:I:94:SER:HB2	12:I:142:ASP:HB3	1.97	0.47
14:L:85:GLN:HA	14:L:88:VAL:HG22	1.97	0.47
37:z:99:GLN:HA	37:z:102:ARG:HD2	1.96	0.47
56:q:68:LYS:CB	58:f:227:ARG:HH21	2.27	0.47
1:2:2092:G:O2'	1:2:2262:G:N2	2.48	0.47
1:2:2705:G:O6	23:a:46:LYS:NZ	2.48	0.47
1:2:4370:G:N2	1:2:4371:G:N2	2.63	0.47
34:v:125:ALA:HB2	34:v:197:MET:HB3	1.97	0.47
40:W:223:SER:OG	40:W:224:LYS:N	2.47	0.47
49:N:82:LEU:O	49:N:200:GLY:CA	2.63	0.47
1:2:1921:C:N3	24:b:161:ARG:NH2	2.63	0.47
24:b:139:ARG:O	24:b:143:LYS:HB2	2.15	0.47
39:R:74:ILE:O	55:3:114:U:O2'	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:4:294:LYS:HG3	42:4:299:LEU:HD22	1.96	0.47
55:3:2:U:H3	55:3:117:G:H1	1.62	0.47
1:2:3688:U:OP2	28:m:198:ARG:NH2	2.48	0.47
13:J:152:LYS:NZ	13:J:249:GLU:OE2	2.46	0.47
1:2:1906:U:H2'	1:2:1907:A:H8	1.79	0.47
1:2:4419:U:H5'	1:2:4424:A:H61	1.79	0.47
11:H:79:LYS:O	11:H:84:ARG:NH2	2.47	0.47
19:U:123:GLU:HG3	19:U:128:LYS:HG3	1.97	0.47
37:z:25:GLU:OE1	37:z:28:ARG:NH2	2.47	0.47
39:R:223:PHE:HB3	39:R:226:TYR:HB2	1.96	0.47
57:g:35:HIS:HB3	58:f:468:VAL:O	2.15	0.47
1:2:962:C:O3'	31:p:32:ARG:NH1	2.48	0.46
1:2:2101:C:H2'	1:2:2102:G:H2'	1.97	0.46
7:B:225:GLY:HA2	7:B:273:GLY:HA3	1.97	0.46
7:B:364:ASP:OD1	7:B:364:ASP:N	2.48	0.46
11:H:82:ASP:OD1	11:H:82:ASP:N	2.47	0.46
18:S:41:PRO:HG3	18:S:73:VAL:HG13	1.96	0.46
31:p:105:VAL:HG13	31:p:136:VAL:HG12	1.97	0.46
36:y:39:PRO:HD2	42:4:259:GLU:HB3	1.95	0.46
42:4:250:ALA:HB2	42:4:339:LEU:HB2	1.96	0.46
1:2:4620:OMU:OP1	25:e:51:ARG:NH1	2.48	0.46
3:7:24:ASN:ND2	25:e:99:GLU:OE2	2.49	0.46
16:P:28:ARG:NH1	16:P:36:ARG:O	2.45	0.46
45:j:64:ILE:HG23	45:j:68:LEU:HD23	1.96	0.46
47:t:148:ARG:NH2	49:N:208:SER:OG	2.48	0.46
1:2:404:U:O3'	26:h:87:ARG:NH2	2.48	0.46
1:2:2476:G:N7	57:g:48:ARG:NH2	2.64	0.46
38:C:94:LEU:HD22	38:C:98:ASN:HD21	1.81	0.46
44:k:6:PRO:HG3	44:k:73:GLY:HA3	1.96	0.46
8:D:86:ARG:NH1	8:D:89:GLN:OE1	2.49	0.46
12:I:180:TYR:OH	13:J:17:ARG:NH1	2.49	0.46
20:V:6:VAL:HG12	20:V:32:LYS:HG3	1.98	0.46
21:X:38:THR:HG22	21:X:45:THR:HG22	1.98	0.46
41:T:41:ASP:H	41:T:99:SER:HB2	1.80	0.46
46:d:56:LEU:HD23	46:d:61:VAL:HB	1.98	0.46
1:2:1573:G:OP1	23:a:92:LYS:NZ	2.44	0.46
1:2:1992:U:H5'	1:2:1993:C:H5'	1.96	0.46
1:2:5024:C:H5	1:2:5028:G:H21	1.64	0.46
11:H:117:ARG:NH2	17:Q:127:PHE:O	2.49	0.46
1:2:1253:G:O2'	1:2:1257:A:N6	2.49	0.46
10:G:117:ARG:HD3	10:G:120:LYS:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:116:LEU:HD22	19:U:135:ILE:HD11	1.97	0.46
56:q:310:GLU:OE2	56:q:314:ARG:NH2	2.49	0.46
1:2:1896:A:OP1	31:p:223:LYS:NZ	2.47	0.46
16:P:41:ARG:HG2	42:4:609:ALA:HB2	1.97	0.46
28:m:116:LEU:HB3	28:m:126:LEU:HB2	1.96	0.46
34:v:207:MET:O	34:v:215:PHE:HA	2.16	0.46
42:4:72:LEU:HD13	42:4:89:LYS:HG3	1.98	0.46
1:2:1332:C:H2'	1:2:1333:A:H8	1.80	0.46
1:2:1562:G:N2	1:2:1565:A:OP2	2.49	0.46
12:I:111:LEU:HD21	12:I:125:ARG:HB2	1.98	0.46
39:R:64:ILE:HG23	39:R:105:LEU:HD21	1.97	0.46
39:R:88:VAL:HG13	39:R:239:MET:HE1	1.97	0.46
40:W:477:ASP:OD1	40:W:477:ASP:N	2.47	0.46
42:4:226:LEU:O	42:4:233:ARG:NH2	2.49	0.46
57:g:23:LYS:HD2	58:f:478:LEU:HA	1.98	0.46
1:2:1499:C:OP1	22:Z:150:ARG:NH2	2.49	0.46
7:B:290:GLY:O	7:B:301:ASN:ND2	2.48	0.46
35:w:307:ASP:N	35:w:307:ASP:OD1	2.47	0.46
39:R:211:LEU:HG	39:R:219:TYR:HB2	1.98	0.46
39:R:292:GLU:OE2	39:R:293:ARG:NH1	2.49	0.46
1:2:1951:G:O2'	24:b:95:ARG:NH2	2.49	0.45
1:2:4996:C:OP1	45:j:32:ARG:NH1	2.46	0.45
4:8:47:C:H1'	4:8:61:A:H2'	1.98	0.45
35:w:305:HIS:HB2	35:w:311:ILE:HD11	1.98	0.45
40:W:230:ILE:HB	40:W:240:ARG:HB2	1.98	0.45
42:4:170:THR:HA	42:4:218:GLN:O	2.15	0.45
1:2:4457:U:OP1	25:e:50:ASN:ND2	2.49	0.45
4:8:75:G:OP2	26:h:74:TYR:OH	2.35	0.45
13:J:147:LYS:HD3	13:J:171:ILE:HD11	1.96	0.45
21:X:30:GLU:OE1	21:X:33:GLN:NE2	2.46	0.45
28:m:20:VAL:HA	28:m:23:ARG:HG3	1.98	0.45
47:t:58:GLU:HB2	47:t:74:PHE:HE2	1.81	0.45
1:2:1185:G:O4'	39:R:282:GLN:NE2	2.49	0.45
8:D:152:LEU:HD23	8:D:251:ILE:HG12	1.98	0.45
14:L:76:ASP:HB3	14:L:115:GLY:HA3	1.99	0.45
27:l:66:ARG:NH1	27:l:75:THR:O	2.49	0.45
43:Y:94:MET:HG2	43:Y:148:MET:HE2	1.97	0.45
55:3:11:A:O2'	55:3:13:A:OP2	2.34	0.45
1:2:95:G:OP2	17:Q:11:LYS:NZ	2.49	0.45
12:I:4:ILE:HB	32:r:259:GLN:HG3	1.98	0.45
55:3:15:C:H2'	55:3:16:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:2562:G:N2	1:2:2566:G:N7	2.65	0.45
13:J:202:ASN:ND2	13:J:213:VAL:O	2.49	0.45
38:C:176:PRO:HG2	38:C:178:LYS:HG2	1.98	0.45
46:d:48:LYS:HG2	46:d:53:ALA:HB2	1.98	0.45
1:2:2112:G:OP1	1:2:2251:G:N1	2.49	0.45
1:2:2431:A:OP1	16:P:41:ARG:NH1	2.48	0.45
1:2:3774:A:N7	1:2:3776:G:N2	2.64	0.45
1:2:4244:A:H62	1:2:4264:G:H21	1.64	0.45
20:V:51:LYS:HE3	20:V:144:GLU:HB3	1.99	0.45
46:d:74:SER:OG	46:d:75:GLU:N	2.50	0.45
47:t:144:PRO:HA	47:t:147:LYS:HB2	1.98	0.45
56:q:44:TYR:CE1	58:f:450:MET:HG2	2.51	0.45
1:2:238:C:O2	26:h:102:SER:OG	2.35	0.45
1:2:969:C:O2'	1:2:970:G:N2	2.50	0.45
1:2:2601:A:N6	1:2:2744:A:OP2	2.45	0.45
8:D:275:SER:OG	8:D:276:ASN:N	2.46	0.45
47:t:143:TYR:HA	47:t:144:PRO:HD3	1.87	0.45
1:2:990:C:N4	1:2:1051:G:O2'	2.42	0.45
1:2:1282:G:OP2	8:D:316:LYS:NZ	2.49	0.45
7:B:57:VAL:HA	7:B:72:VAL:O	2.17	0.45
53:i:50:PRO:HD3	53:i:68:ILE:HG13	1.99	0.45
1:2:260:C:H2'	1:2:261:G:H8	1.82	0.45
1:2:664:G:N2	1:2:666:G:O6	2.49	0.45
1:2:4496:A:H61	1:2:4504:C:H42	1.65	0.45
56:q:220:MET:HE1	58:f:442:PHE:HB2	1.99	0.45
1:2:1480:C:O2'	1:2:1482:G:OP2	2.35	0.44
1:2:3928:A:OP1	19:U:90:ASN:ND2	2.46	0.44
9:E:79:ILE:HG22	9:E:90:ARG:HB3	1.97	0.44
17:Q:96:ILE:HD12	17:Q:117:LEU:HD11	1.99	0.44
24:b:130:GLU:OE2	33:u:62:ARG:NH2	2.50	0.44
25:e:37:LEU:HD21	25:e:105:ILE:HD11	1.99	0.44
29:n:36:ARG:NH1	29:n:79:GLY:O	2.50	0.44
35:w:25:GLN:HB3	35:w:32:MET:HG2	1.97	0.44
1:2:375:G:OP2	15:M:52:LYS:NZ	2.45	0.44
1:2:989:U:O2	1:2:1064:G:O6	2.34	0.44
1:2:4741:C:OP1	1:2:4900:C:N4	2.45	0.44
3:7:97:GLU:OE2	42:4:441:TYR:OH	2.35	0.44
35:w:210:LEU:HB2	35:w:365:VAL:HG21	1.99	0.44
10:G:61:ILE:HG22	10:G:65:ARG:HE	1.81	0.44
10:G:160:ASP:OD1	10:G:160:ASP:N	2.47	0.44
32:r:290:GLU:HB3	32:r:294:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:T:62:GLY:HA3	41:T:74:ILE:HG23	1.99	0.44
1:2:85:G:N2	1:2:98:A:OP2	2.44	0.44
1:2:2459:G:N2	1:2:2462:C:OP2	2.47	0.44
1:2:4105:A:N3	1:2:4106:G:N1	2.64	0.44
2:6:240:LEU:O	2:6:244:LEU:HB2	2.18	0.44
5:9:28:LEU:O	5:9:32:HIS:ND1	2.50	0.44
8:D:140:LYS:O	8:D:204:ARG:NH2	2.50	0.44
36:y:28:LEU:HB3	36:y:32:ILE:HD12	1.99	0.44
38:C:23:ASN:HA	38:C:70:VAL:O	2.17	0.44
39:R:100:CYS:O	39:R:104:LEU:HB2	2.18	0.44
1:2:1988:G:OP1	35:w:147:LYS:NZ	2.47	0.44
1:2:4302:U:O2'	1:2:4308:C:N4	2.51	0.44
1:2:4670:C:O2'	1:2:4672:A:OP2	2.34	0.44
25:e:35:LYS:HD2	25:e:35:LYS:HA	1.84	0.44
50:1:228:LYS:H	50:1:228:LYS:HG2	1.62	0.44
1:2:1732:C:H42	1:2:1797:G:H1	1.65	0.44
1:2:1939:A:N1	1:2:4401:G:C2	2.85	0.44
1:2:3892:U:O2'	43:Y:80:GLN:OE1	2.35	0.44
7:B:212:GLY:HA3	37:z:33:LEU:HD11	2.00	0.44
39:R:166:ALA:HB1	39:R:171:LEU:HD12	1.98	0.44
40:W:352:THR:HG21	40:W:367:ARG:HH11	1.81	0.44
42:4:381:VAL:HG23	42:4:382:VAL:HG23	2.00	0.44
1:2:4251:A:H5''	38:C:108:GLY:HA3	2.00	0.44
6:A:55:LYS:HA	6:A:58:GLN:HG2	2.00	0.44
24:b:74:ARG:O	24:b:76:LYS:NZ	2.49	0.44
39:R:53:VAL:HA	39:R:61:ILE:O	2.18	0.44
42:4:243:ALA:O	42:4:247:LEU:HB2	2.18	0.44
50:1:196:ASP:OD2	56:q:380:ARG:NH1	2.49	0.44
53:i:27:LYS:HB3	53:i:42:LEU:HB3	2.00	0.44
1:2:952:G:H4'	29:n:75:THR:HG23	2.00	0.44
7:B:353:VAL:HG11	37:z:22:ALA:HB2	1.98	0.44
53:i:47:ASP:HB3	53:i:69:LYS:HB3	2.00	0.44
54:O:49:ASP:OD1	58:f:365:HIS:HE1	1.84	0.44
56:q:150:THR:HG23	56:q:153:CYS:H	1.83	0.44
1:2:35:U:H4'	1:2:1525:A:H2	1.83	0.44
23:a:44:LEU:HD22	23:a:49:LEU:HD22	2.00	0.44
35:w:136:ASP:OD1	35:w:136:ASP:N	2.48	0.44
39:R:67:ALA:HA	39:R:72:ASP:HA	2.00	0.44
42:4:503:THR:H	42:4:507:ARG:HH21	1.66	0.44
53:i:62:ILE:HG22	58:f:279:LEU:CD2	2.48	0.44
1:2:2295:C:H2'	1:2:2296:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:10:ARG:NH2	7:B:265:SER:O	2.51	0.43
28:m:30:ARG:NH1	28:m:36:GLU:OE2	2.50	0.43
42:4:135:GLY:O	42:4:139:THR:OG1	2.35	0.43
56:q:47:GLU:OE2	58:f:404:ARG:HB3	2.17	0.43
1:2:1994:C:H4'	36:y:130:LYS:HB3	1.99	0.43
1:2:2592:U:N3	1:2:4126:C:N4	2.51	0.43
1:2:4980:C:N3	43:Y:69:ARG:NH2	2.63	0.43
7:B:139:ASP:OD2	37:z:96:TRP:NE1	2.46	0.43
8:D:209:ILE:HB	8:D:229:LEU:HD13	2.00	0.43
40:W:200:LYS:HD2	40:W:200:LYS:HA	1.79	0.43
1:2:1646:A:O2'	15:M:49:TRP:O	2.36	0.43
1:2:4077:A:H62	1:2:4169:G:H21	1.66	0.43
1:2:4236:G:HO2'	1:2:4328:G:HO2'	1.63	0.43
10:G:73:ARG:NH1	10:G:241:VAL:O	2.46	0.43
17:Q:111:GLN:HA	17:Q:114:VAL:HG12	2.00	0.43
22:Z:39:THR:HG22	22:Z:41:SER:H	1.83	0.43
30:o:150:LEU:O	30:o:161:ARG:HA	2.19	0.43
55:3:35:U:O2	55:3:45:U:O2'	2.32	0.43
27:l:94:ARG:HG3	27:l:111:ILE:HD11	1.99	0.43
30:o:153:LEU:HD11	30:o:195:ILE:HG13	2.01	0.43
44:k:106:LYS:HB3	44:k:106:LYS:HE2	1.85	0.43
1:2:327:U:O2'	51:K:30:ARG:NH1	2.51	0.43
2:6:129:LEU:O	2:6:133:LEU:HB2	2.18	0.43
8:D:94:ASN:OD1	8:D:94:ASN:N	2.52	0.43
31:p:134:ARG:HA	31:p:137:GLU:HG3	2.00	0.43
40:W:348:SER:OG	40:W:349:ASP:N	2.52	0.43
51:K:22:SER:OG	51:K:23:LYS:N	2.51	0.43
53:i:35:ASP:OD1	53:i:35:ASP:N	2.49	0.43
3:7:79:ILE:HD12	42:4:442:ILE:HG22	1.99	0.43
26:h:10:ASP:HB3	26:h:13:LYS:HB2	2.00	0.43
39:R:52:ILE:HD13	55:3:6:C:H4'	2.00	0.43
46:d:106:SER:OG	46:d:107:LYS:N	2.51	0.43
50:1:120:ARG:NH2	50:1:212:SER:O	2.50	0.43
50:1:199:HIS:CE1	56:q:336:ARG:HE	2.36	0.43
56:q:381:PRO:HD3	58:f:429:ARG:HH22	1.82	0.43
3:7:120:LYS:HG3	42:4:477:MET:HE1	2.00	0.43
10:G:91:THR:HG22	47:t:110:LEU:HD13	2.00	0.43
30:o:277:LEU:HA	30:o:281:ILE:HD11	2.01	0.43
39:R:84:PRO:HG3	39:R:92:LEU:HD11	2.01	0.43
39:R:136:ASP:OD1	39:R:136:ASP:N	2.49	0.43
1:2:1375:C:OP1	8:D:274:LYS:NZ	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:2262:G:OP2	27:l:98:ARG:NH2	2.47	0.43
1:2:2489:C:H41	56:q:149:ARG:HG3	1.83	0.43
1:2:3917:A:H2'	1:2:3918:G:H8	1.84	0.43
1:2:4162:C:H5	10:G:73:ARG:HH12	1.67	0.43
7:B:220:ILE:HB	7:B:346:THR:HB	1.99	0.43
1:2:702:U:H5'	30:o:121:VAL:HG11	2.01	0.43
1:2:1945:G:N2	13:J:39:ALA:O	2.47	0.43
1:2:2026:A:H5''	32:r:263:LEU:HD13	2.01	0.43
1:2:4078:C:OP1	19:U:31:ARG:NH1	2.52	0.43
4:8:39:G:OP1	11:H:86:LYS:NZ	2.46	0.43
10:G:132:ARG:HA	10:G:133:PRO:HD3	1.85	0.43
13:J:13:ARG:NH2	42:4:194:ASP:OD1	2.52	0.43
15:M:20:ARG:NH2	15:M:39:TYR:OH	2.50	0.43
34:v:27:ILE:HG12	34:v:76:ALA:HB2	1.99	0.43
41:T:52:MET:HA	41:T:53:PRO:HD3	1.87	0.43
51:K:12:ASN:O	51:K:16:LYS:NZ	2.49	0.43
53:i:124:THR:HG23	58:f:282:PRO:HD2	2.01	0.43
1:2:4266:G:O2'	1:2:4269:G:O6	2.36	0.43
43:Y:94:MET:HE3	43:Y:94:MET:HB2	1.97	0.43
47:t:78:ARG:HA	47:t:85:SER:HA	2.00	0.43
50:1:141:ARG:HA	50:1:144:GLU:HG3	2.00	0.43
56:q:126:THR:HG22	56:q:128:ILE:H	1.84	0.43
1:2:4092:G:H3'	1:2:4093:G:H21	1.84	0.42
1:2:4464:A:H62	42:4:32:THR:HB	1.84	0.42
7:B:56:ILE:O	7:B:73:VAL:HA	2.19	0.42
16:P:33:ASN:ND2	16:P:35:ILE:O	2.52	0.42
40:W:133:SER:OG	40:W:134:GLY:N	2.51	0.42
1:2:1500:A:H5''	1:2:1501:C:H5''	2.02	0.42
1:2:3870:C:H2'	1:2:3871:A:H8	1.84	0.42
2:6:123:ARG:HA	2:6:126:GLU:HG2	2.00	0.42
12:I:86:LEU:HD23	12:I:186:THR:HG21	2.02	0.42
20:V:55:LEU:HD23	20:V:58:LEU:HD12	2.00	0.42
37:z:87:LEU:HD21	37:z:106:LYS:HZ3	1.85	0.42
1:2:279:A:N7	19:U:12:ARG:NH1	2.67	0.42
1:2:2045:G:N2	1:2:2046:G:N7	2.67	0.42
1:2:2764:A:H2'	1:2:2765:A:H8	1.83	0.42
7:B:309:LEU:HD11	42:4:430:PRO:HB3	2.01	0.42
8:D:218:ILE:O	8:D:221:PHE:C	2.61	0.42
19:U:24:ARG:HE	19:U:24:ARG:HB3	1.64	0.42
40:W:105:ARG:HE	40:W:106:CYS:H	1.66	0.42
40:W:167:ASP:OD1	40:W:167:ASP:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:161:ARG:HH11	24:b:164:LYS:HD3	1.84	0.42
34:v:164:ARG:HA	34:v:164:ARG:HD3	1.84	0.42
39:R:236:MET:HA	39:R:239:MET:HG3	2.01	0.42
56:q:337:GLU:HG3	56:q:379:ASP:HB2	2.01	0.42
57:g:101:ASP:OD1	57:g:101:ASP:N	2.46	0.42
1:2:958:G:O2'	30:o:123:ARG:O	2.35	0.42
1:2:2406:G:O2'	16:P:48:LYS:NZ	2.52	0.42
1:2:4265:U:O5'	1:2:4279:A:N6	2.52	0.42
15:M:58:THR:OG1	15:M:59:THR:N	2.53	0.42
24:b:11:LYS:HE3	24:b:11:LYS:HB2	1.89	0.42
1:2:1069:G:OP2	30:o:65:ARG:NH2	2.51	0.42
1:2:2418:A:N1	1:2:2429:A:O2'	2.51	0.42
1:2:2621:A:OP1	46:d:80:LYS:NZ	2.52	0.42
1:2:3717:A:H2'	1:2:3718:A2M:H8	2.01	0.42
1:2:4476:C:O2'	1:2:4478:G:OP2	2.36	0.42
1:2:4761:G:H2'	1:2:4762:A:H8	1.84	0.42
42:4:584:LYS:HB3	42:4:584:LYS:HE3	1.86	0.42
55:3:23:A:N3	55:3:118:C:O2'	2.50	0.42
57:g:33:HIS:HB3	58:f:473:PHE:CE2	2.46	0.42
1:2:2519:U:O2'	1:2:2530:U:O2	2.35	0.42
1:2:4467:A:O2'	1:2:4510:A:N3	2.46	0.42
1:2:4678:G:H5''	37:z:11:ARG:HD3	2.02	0.42
4:8:131:G:H5''	57:g:108:GLN:HE21	1.85	0.42
34:v:96:LEU:HD23	34:v:96:LEU:HA	1.94	0.42
56:q:347:ILE:O	56:q:352:GLY:N	2.52	0.42
1:2:4606:G:O3'	42:4:216:ARG:NH2	2.49	0.42
17:Q:70:VAL:H	17:Q:159:ASN:HD21	1.66	0.42
18:S:86:TRP:O	18:S:89:THR:OG1	2.38	0.42
53:i:70:SER:OG	53:i:71:PHE:N	2.53	0.42
1:2:351:C:OP2	8:D:197:ARG:NH1	2.45	0.42
1:2:1408:G:O2'	1:2:1412:G:O6	2.37	0.42
1:2:4321:U:O4	1:2:4326:G:O6	2.37	0.42
34:v:69:LYS:HD3	34:v:69:LYS:HA	1.82	0.42
24:b:139:ARG:HB2	24:b:142:VAL:HG22	2.01	0.42
27:l:7:TRP:O	27:l:11:ARG:HB2	2.20	0.42
1:2:653:U:OP1	22:Z:115:ARG:NH1	2.53	0.41
1:2:2411:C:H2'	1:2:2412:A:H8	1.84	0.41
1:2:4100:C:N4	1:2:4109:G:OP2	2.47	0.41
1:2:4494:OMG:HM21	25:e:22:VAL:HG11	2.02	0.41
36:y:105:THR:OG1	36:y:108:GLU:OE1	2.35	0.41
39:R:107:ARG:HA	39:R:107:ARG:HD2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:W:429:LEU:O	40:W:440:VAL:HA	2.20	0.41
53:i:90:PRO:O	53:i:117:LYS:NZ	2.53	0.41
53:i:125:GLY:HA3	58:f:288:ALA:HB3	1.97	0.41
1:2:385:A:OP1	26:h:77:LYS:NZ	2.52	0.41
1:2:1952:G:H4'	24:b:93:MET:HE3	2.02	0.41
9:E:98:ASP:HA	9:E:99:PRO:HD3	1.93	0.41
13:J:162:ARG:HB3	35:w:216:SER:HA	2.02	0.41
35:w:37:THR:HG23	35:w:40:ARG:HH21	1.85	0.41
39:R:236:MET:O	39:R:240:TYR:CB	2.68	0.41
43:Y:168:LYS:HA	43:Y:168:LYS:HD3	1.92	0.41
1:2:1086:C:H2'	1:2:1087:A:H8	1.86	0.41
1:2:1810:G:H2'	1:2:1811:G:H8	1.85	0.41
1:2:4498:U:H4'	1:2:4500:U:H4'	2.03	0.41
1:2:4912:G:N7	1:2:4913:G:N2	2.69	0.41
2:6:214:GLU:HA	2:6:217:VAL:HG12	2.01	0.41
19:U:159:ARG:HB3	19:U:164:LEU:HB2	2.03	0.41
26:h:47:MET:HE3	26:h:47:MET:HB3	1.91	0.41
40:W:298:ASP:OD1	40:W:298:ASP:N	2.52	0.41
42:4:357:LEU:HD23	42:4:360:LEU:HD12	2.03	0.41
1:2:736:C:OP1	18:S:74:ARG:NH1	2.47	0.41
1:2:4940:C:OP1	30:o:156:ARG:NH1	2.49	0.41
2:6:4:ARG:NH1	2:6:210:THR:O	2.54	0.41
4:8:27:U:H4'	8:D:53:ALA:HB3	2.03	0.41
13:J:153:VAL:HG11	13:J:248:PRO:HB2	2.00	0.41
36:y:16:ARG:HA	36:y:58:ILE:O	2.20	0.41
38:C:90:ARG:HD2	38:C:90:ARG:HA	1.90	0.41
42:4:117:MET:HE2	42:4:117:MET:HB2	1.96	0.41
1:2:667:A:H5''	1:2:668:C:H5''	2.03	0.41
1:2:2111:G:N7	1:2:2251:G:O2'	2.49	0.41
1:2:3687:A:O2'	28:m:236:GLY:N	2.53	0.41
1:2:4394:A:N6	1:2:4395:U:O4	2.54	0.41
1:2:4645:C:OP2	23:a:62:ARG:NH1	2.54	0.41
10:G:46:GLN:OE1	10:G:49:ARG:NH2	2.54	0.41
28:m:27:ALA:O	28:m:128:ARG:NH2	2.43	0.41
28:m:116:LEU:O	28:m:126:LEU:N	2.53	0.41
39:R:128:ASP:OD1	39:R:128:ASP:N	2.54	0.41
45:j:95:ASP:OD1	45:j:95:ASP:N	2.52	0.41
58:f:452:GLU:HA	58:f:453:PRO:HD3	1.91	0.41
1:2:729:2MG:N2	24:b:66:GLN:O	2.41	0.41
1:2:2611:A:H5'	1:2:2688:G:H4'	2.03	0.41
1:2:4582:C:OP2	7:B:28:LYS:NZ	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:117:ARG:HA	10:G:120:LYS:HG2	2.03	0.41
24:b:147:ASP:HB3	24:b:150:ILE:HB	2.03	0.41
25:e:24:ALA:HB3	25:e:39:ILE:HD12	2.02	0.41
32:r:292:GLU:HA	32:r:295:ARG:HG2	2.03	0.41
36:y:90:ARG:HG3	36:y:98:ILE:HD11	2.02	0.41
56:q:24:ARG:NH1	56:q:29:LEU:O	2.53	0.41
56:q:150:THR:OG1	56:q:151:GLY:N	2.53	0.41
1:2:1168:G:O6	1:2:1194:G:N2	2.48	0.41
1:2:2490:U:OP2	56:q:108:LYS:NZ	2.45	0.41
1:2:4251:A:H1'	38:C:110:GLN:HG3	2.03	0.41
2:6:106:ASN:ND2	25:e:136:ALA:O	2.53	0.41
4:8:14:OMU:H1'	4:8:14:OMU:HM23	1.68	0.41
32:r:301:ARG:HH21	32:r:304:GLU:HG2	1.86	0.41
42:4:357:LEU:HA	42:4:360:LEU:HD12	2.02	0.41
46:d:84:LYS:HE3	46:d:102:VAL:HB	2.03	0.41
1:2:73:A:H62	17:Q:103:ARG:HH22	1.69	0.41
1:2:153:G:H2'	1:2:154:G:H8	1.85	0.41
1:2:323:C:H2'	1:2:324:A:H8	1.86	0.41
1:2:1595:G:H1'	1:2:1597:G:H21	1.85	0.41
1:2:1884:C:H2'	1:2:1885:G:H8	1.84	0.41
3:7:95:ARG:HD2	3:7:95:ARG:HA	1.86	0.41
7:B:8:ALA:HB2	25:e:49:LEU:HD22	2.03	0.41
17:Q:80:GLU:OE2	17:Q:104:ASN:ND2	2.54	0.41
21:X:3:LYS:HD2	21:X:3:LYS:HA	1.93	0.41
1:2:230:G:OP1	26:h:15:ARG:NH1	2.48	0.41
1:2:1479:G:H21	17:Q:184:MET:HE1	1.86	0.41
14:L:76:ASP:OD1	14:L:76:ASP:N	2.54	0.41
18:S:39:ASP:HB3	18:S:47:ARG:HG2	2.02	0.41
19:U:68:ARG:NH1	19:U:124:ASP:O	2.51	0.41
35:w:213:VAL:HG21	35:w:362:CYS:HB3	2.02	0.41
35:w:431:LYS:HA	35:w:431:LYS:HD3	1.95	0.41
36:y:96:LYS:H	36:y:96:LYS:HG2	1.58	0.41
40:W:353:LEU:HD11	40:W:389:SER:HB3	2.02	0.41
46:d:60:VAL:HG23	46:d:61:VAL:HG23	2.01	0.41
50:1:29:ARG:NH1	58:f:265:GLU:OE2	2.54	0.41
56:q:251:GLU:OE2	56:q:255:GLN:NE2	2.48	0.41
1:2:2652:G:N2	21:X:61:MET:SD	2.91	0.41
1:2:3664:G:H2'	1:2:3665:G:H8	1.86	0.41
1:2:4439:U:H1'	42:4:93:LYS:HB3	2.02	0.41
2:6:26:VAL:O	2:6:50:HIS:HA	2.21	0.41
2:6:142:VAL:HG23	2:6:148:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:165:THR:OG1	19:U:166:SER:N	2.53	0.41
21:X:38:THR:HA	21:X:45:THR:HA	2.03	0.41
27:l:105:ASP:OD1	27:l:105:ASP:N	2.46	0.41
34:v:39:TYR:O	34:v:104:PHE:HA	2.20	0.41
50:1:201:ILE:HA	50:1:208:PHE:HE1	1.86	0.41
1:2:1699:A:OP1	1:2:2085:G:O2'	2.37	0.40
1:2:2017:A:O2'	1:2:2018:C:O4'	2.38	0.40
1:2:2486:G:OP2	58:f:456:ARG:HD3	2.21	0.40
1:2:4154:G:H5''	58:f:464:LYS:HZ1	1.86	0.40
3:7:23:ARG:HH11	5:9:28:LEU:HD12	1.86	0.40
24:b:76:LYS:HE2	24:b:76:LYS:HB2	1.91	0.40
24:b:83:ARG:HG2	24:b:92:ASN:HB3	2.03	0.40
26:h:35:SER:OG	26:h:36:LYS:N	2.55	0.40
27:l:33:LYS:HA	44:k:90:MET:HG3	2.03	0.40
34:v:96:LEU:HD21	34:v:102:LEU:HD21	2.03	0.40
36:y:85:LEU:HD11	36:y:102:GLY:HA3	2.03	0.40
55:3:64:G:H2'	55:3:65:G:H8	1.85	0.40
1:2:2302:C:O2'	44:k:102:ASN:O	2.37	0.40
1:2:2763:U:C3'	58:f:391:ARG:HH21	2.33	0.40
1:2:4432:C:H2'	1:2:4433:G:H8	1.86	0.40
2:6:101:LEU:HD13	2:6:107:VAL:HG21	2.04	0.40
2:6:219:GLU:O	2:6:222:PHE:O	2.38	0.40
3:7:7:TYR:HD2	5:9:99:GLN:HG2	1.87	0.40
7:B:57:VAL:HG23	7:B:366:LYS:HB3	2.03	0.40
30:o:245:GLN:NE2	30:o:249:ASP:OD2	2.49	0.40
44:k:89:LEU:HD13	44:k:118:LEU:HD22	2.02	0.40
55:3:7:G:O6	55:3:112:U:O4	2.39	0.40
56:q:152:LYS:HD2	56:q:217:TYR:HD2	1.86	0.40
1:2:4436:U:H5	42:4:143:ARG:HD3	1.85	0.40
24:b:7:LEU:HD12	24:b:106:VAL:HG12	2.03	0.40
39:R:208:MET:HE2	39:R:233:PRO:HG3	2.03	0.40
40:W:104:THR:OG1	40:W:485:ARG:O	2.39	0.40
42:4:247:LEU:HD23	42:4:247:LEU:HA	1.96	0.40
42:4:272:PHE:O	42:4:276:ARG:HB2	2.22	0.40
1:2:907:C:H2'	1:2:908:G:H8	1.87	0.40
1:2:1328:G:O2'	1:2:2349:A:OP1	2.39	0.40
1:2:1870:C:H2'	1:2:1871:A2M:H8	2.04	0.40
1:2:4622:A:H4'	7:B:13:SER:HB2	2.03	0.40
8:D:204:ARG:NH1	8:D:205:ARG:O	2.54	0.40
10:G:55:VAL:HG21	57:g:41:ARG:HD2	2.02	0.40
17:Q:83:VAL:HG12	17:Q:114:VAL:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Y:47:TYR:OH	43:Y:57:CYS:O	2.38	0.40
49:N:240:LYS:HD3	49:N:240:LYS:HA	1.89	0.40
50:1:158:ARG:HG2	50:1:198:ILE:HD13	2.03	0.40
56:q:182:PHE:CZ	58:f:246:SER:HB3	2.56	0.40
57:g:73:HIS:HD2	57:g:112:ALA:HA	1.86	0.40
1:2:142:G:O2'	1:2:144:G:OP1	2.35	0.40
1:2:4753:U:OP1	29:n:100:ARG:NH1	2.54	0.40
17:Q:202:ALA:O	17:Q:206:ASP:HB2	2.21	0.40
42:4:412:ASP:HB3	42:4:415:LYS:HE3	2.03	0.40
58:f:235:ALA:HB3	58:f:448:ARG:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	6	242/245 (99%)	227 (94%)	15 (6%)	0	100	100
3	7	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
5	9	82/134 (61%)	71 (87%)	11 (13%)	0	100	100
6	A	41/159 (26%)	39 (95%)	2 (5%)	0	100	100
7	B	401/403 (100%)	382 (95%)	18 (4%)	1 (0%)	43	77
8	D	356/427 (83%)	334 (94%)	22 (6%)	0	100	100
9	E	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
10	G	239/266 (90%)	225 (94%)	14 (6%)	0	100	100
11	H	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
12	I	188/192 (98%)	179 (95%)	9 (5%)	0	100	100
13	J	213/260 (82%)	207 (97%)	6 (3%)	0	100	100
14	L	108/148 (73%)	101 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	M	84/97 (87%)	80 (95%)	4 (5%)	0	100	100
16	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
17	Q	208/211 (99%)	200 (96%)	8 (4%)	0	100	100
18	S	133/215 (62%)	127 (96%)	6 (4%)	0	100	100
19	U	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
20	V	199/203 (98%)	192 (96%)	7 (4%)	0	100	100
21	X	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
22	Z	149/188 (79%)	147 (99%)	2 (1%)	0	100	100
23	a	146/196 (74%)	142 (97%)	4 (3%)	0	100	100
24	b	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
25	e	129/140 (92%)	118 (92%)	11 (8%)	0	100	100
26	h	132/145 (91%)	126 (96%)	6 (4%)	0	100	100
27	l	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
28	m	246/257 (96%)	221 (90%)	25 (10%)	0	100	100
29	n	107/110 (97%)	102 (95%)	5 (5%)	0	100	100
30	o	231/288 (80%)	220 (95%)	11 (5%)	0	100	100
31	p	224/248 (90%)	216 (96%)	8 (4%)	0	100	100
32	r	80/360 (22%)	77 (96%)	3 (4%)	0	100	100
33	u	63/549 (12%)	58 (92%)	4 (6%)	1 (2%)	7	37
34	v	215/239 (90%)	206 (96%)	9 (4%)	0	100	100
35	w	427/731 (58%)	406 (95%)	19 (4%)	2 (0%)	24	62
36	y	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
37	z	63/129 (49%)	60 (95%)	3 (5%)	0	100	100
38	C	163/178 (92%)	145 (89%)	18 (11%)	0	100	100
39	R	291/297 (98%)	273 (94%)	17 (6%)	1 (0%)	36	71
40	W	386/485 (80%)	365 (95%)	21 (5%)	0	100	100
41	T	120/160 (75%)	112 (93%)	8 (7%)	0	100	100
42	4	607/634 (96%)	555 (91%)	47 (8%)	5 (1%)	16	52
43	Y	165/184 (90%)	158 (96%)	7 (4%)	0	100	100
44	k	127/135 (94%)	120 (94%)	7 (6%)	0	100	100
45	j	109/125 (87%)	103 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	d	102/128 (80%)	95 (93%)	7 (7%)	0	100	100
47	t	109/293 (37%)	105 (96%)	4 (4%)	0	100	100
49	N	237/490 (48%)	231 (98%)	6 (2%)	0	100	100
50	1	224/255 (88%)	216 (96%)	7 (3%)	1 (0%)	30	66
51	K	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
52	F	111/117 (95%)	109 (98%)	2 (2%)	0	100	100
53	i	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
54	O	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
56	q	398/588 (68%)	382 (96%)	16 (4%)	0	100	100
57	g	143/156 (92%)	135 (94%)	8 (6%)	0	100	100
58	f	254/478 (53%)	236 (93%)	17 (7%)	1 (0%)	30	66
All	All	9699/12780 (76%)	9184 (95%)	503 (5%)	12 (0%)	49	83

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	u	55	PRO
50	1	24	ASN
58	f	203	ASP
39	R	270	LYS
42	4	88	ASP
35	w	132	VAL
42	4	230	LEU
42	4	407	ASP
35	w	323	LYS
42	4	427	ASP
42	4	366	THR
7	B	5	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	
2	6	212/213 (100%)	212 (100%)	0	100	100
3	7	126/149 (85%)	126 (100%)	0	100	100
5	9	74/114 (65%)	74 (100%)	0	100	100
6	A	34/126 (27%)	34 (100%)	0	100	100
7	B	349/349 (100%)	349 (100%)	0	100	100
8	D	298/348 (86%)	298 (100%)	0	100	100
9	E	83/97 (86%)	83 (100%)	0	100	100
10	G	203/223 (91%)	203 (100%)	0	100	100
11	H	109/110 (99%)	109 (100%)	0	100	100
12	I	169/171 (99%)	169 (100%)	0	100	100
13	J	191/228 (84%)	191 (100%)	0	100	100
14	L	94/121 (78%)	94 (100%)	0	100	100
15	M	73/80 (91%)	73 (100%)	0	100	100
16	P	47/48 (98%)	47 (100%)	0	100	100
17	Q	176/177 (99%)	176 (100%)	0	100	100
18	S	115/161 (71%)	115 (100%)	0	100	100
19	U	171/172 (99%)	171 (100%)	0	100	100
20	V	173/174 (99%)	173 (100%)	0	100	100
21	X	74/75 (99%)	74 (100%)	0	100	100
22	Z	136/165 (82%)	136 (100%)	0	100	100
23	a	133/175 (76%)	133 (100%)	0	100	100
24	b	157/157 (100%)	157 (100%)	0	100	100
25	e	101/107 (94%)	101 (100%)	0	100	100
26	h	124/135 (92%)	124 (100%)	0	100	100
27	l	109/121 (90%)	109 (100%)	0	100	100
28	m	190/199 (96%)	190 (100%)	0	100	100
29	n	88/89 (99%)	88 (100%)	0	100	100
30	o	208/252 (82%)	208 (100%)	0	100	100
31	p	195/215 (91%)	195 (100%)	0	100	100
32	r	76/312 (24%)	76 (100%)	0	100	100
33	u	61/485 (13%)	61 (100%)	0	100	100
34	v	194/214 (91%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	w	385/654 (59%)	385 (100%)	0	100	100
36	y	137/137 (100%)	137 (100%)	0	100	100
37	z	61/115 (53%)	61 (100%)	0	100	100
38	C	138/149 (93%)	138 (100%)	0	100	100
39	R	246/250 (98%)	246 (100%)	0	100	100
40	W	322/404 (80%)	322 (100%)	0	100	100
41	T	109/140 (78%)	109 (100%)	0	100	100
42	4	554/574 (96%)	554 (100%)	0	100	100
43	Y	147/163 (90%)	147 (100%)	0	100	100
44	k	115/121 (95%)	115 (100%)	0	100	100
45	j	101/110 (92%)	101 (100%)	0	100	100
46	d	94/115 (82%)	94 (100%)	0	100	100
47	t	103/274 (38%)	103 (100%)	0	100	100
49	N	222/437 (51%)	222 (100%)	0	100	100
50	1	206/228 (90%)	206 (100%)	0	100	100
51	K	86/89 (97%)	86 (100%)	0	100	100
52	F	97/100 (97%)	97 (100%)	0	100	100
53	i	117/118 (99%)	117 (100%)	0	100	100
54	O	64/65 (98%)	64 (100%)	0	100	100
56	q	359/509 (70%)	359 (100%)	0	100	100
57	g	126/133 (95%)	126 (100%)	0	100	100
58	f	222/402 (55%)	222 (100%)	0	100	100
All	All	8554/11049 (77%)	8554 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
2	6	82	GLN
2	6	86	ASN
2	6	156	ASN
3	7	24	ASN
3	7	130	ASN

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Mol	Chain	Res	Type
3	7	132	HIS
5	9	99	GLN
7	B	121	ASN
7	B	167	GLN
8	D	60	HIS
8	D	310	HIS
8	D	317	ASN
8	D	329	ASN
9	E	15	ASN
9	E	72	HIS
12	I	8	GLN
12	I	98	HIS
12	I	116	ASN
12	I	138	GLN
13	J	4	ASN
13	J	55	HIS
13	J	247	ASN
16	P	17	GLN
17	Q	15	HIS
17	Q	149	GLN
17	Q	205	GLN
18	S	20	HIS
18	S	66	HIS
18	S	70	GLN
18	S	78	GLN
18	S	120	ASN
19	U	37	HIS
19	U	149	GLN
19	U	156	HIS
20	V	180	GLN
20	V	184	ASN
22	Z	7	HIS
23	a	39	GLN
23	a	134	ASN
23	a	141	HIS
25	e	108	ASN
27	l	21	ASN
28	m	187	HIS
28	m	216	HIS
29	n	99	HIS
30	o	157	HIS
31	p	110	GLN

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Mol	Chain	Res	Type
32	r	256	GLN
32	r	312	ASN
34	v	62	HIS
34	v	106	ASN
34	v	186	GLN
35	w	149	GLN
35	w	222	GLN
35	w	255	ASN
36	y	66	ASN
36	y	149	HIS
37	z	89	GLN
37	z	92	GLN
37	z	98	ASN
38	C	98	ASN
39	R	63	GLN
39	R	111	ASN
39	R	225	GLN
40	W	469	GLN
41	T	77	ASN
42	4	41	HIS
42	4	84	ASN
42	4	196	GLN
42	4	538	HIS
44	k	57	ASN
44	k	63	ASN
45	j	34	HIS
47	t	67	GLN
50	1	94	HIS
50	1	185	HIS
50	1	229	ASN
51	K	20	ASN
56	q	197	GLN
56	q	211	HIS
56	q	240	GLN
56	q	335	ASN
56	q	403	ASN
56	q	422	HIS
57	g	33	HIS
58	f	216	GLN
58	f	248	ASN
58	f	286	GLN
58	f	341	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	3451/5054 (68%)	818 (23%)	21 (0%)
4	8	155/156 (99%)	29 (18%)	0
48	x	0/60	-	-
55	3	113/120 (94%)	23 (20%)	2 (1%)
All	All	3719/5390 (68%)	870 (23%)	23 (0%)

All (870) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	25	A
1	2	39	A
1	2	42	A
1	2	44	A
1	2	48	G
1	2	56	A
1	2	59	A
1	2	64	A
1	2	65	A
1	2	69	A
1	2	72	C
1	2	73	A
1	2	76	A
1	2	84	A
1	2	91	G
1	2	98	A
1	2	108	A
1	2	109	G
1	2	110	C
1	2	112	C
1	2	119	G
1	2	120	A
1	2	122	U
1	2	131	C
1	2	132	G
1	2	134	G
1	2	135	G
1	2	137	G
1	2	144	G
1	2	152	U
1	2	159	C
1	2	169	G

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Mol	Chain	Res	Type
1	2	170	C
1	2	172	C
1	2	175	C
1	2	183	C
1	2	185	C
1	2	188	G
1	2	197	A
1	2	200	U
1	2	209	U
1	2	217	C
1	2	218	A
1	2	234	G
1	2	237	B9B
1	2	254	G
1	2	256	G
1	2	262	G
1	2	265	C
1	2	266	C
1	2	279	A
1	2	280	G
1	2	297	U
1	2	306	A
1	2	315	G
1	2	316	U
1	2	340	C
1	2	345	C
1	2	349	A
1	2	363	A
1	2	373	OMG
1	2	387	G
1	2	398	A2M
1	2	407	A
1	2	409	G
1	2	410	A
1	2	412	G
1	2	432	U
1	2	433	A
1	2	449	C
1	2	450	G
1	2	452	A
1	2	453	G
1	2	454	U

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Mol	Chain	Res	Type
1	2	465	G
1	2	467	U
1	2	483	G
1	2	484	U
1	2	485	C
1	2	486	C
1	2	489	C
1	2	491	G
1	2	493	G
1	2	495	C
1	2	496	G
1	2	497	G
1	2	499	G
1	2	500	G
1	2	501	C
1	2	502	C
1	2	503	C
1	2	504	G
1	2	505	G
1	2	509	A
1	2	510	U
1	2	511	C
1	2	513	U
1	2	514	U
1	2	515	C
1	2	516	C
1	2	518	G
1	2	519	C
1	2	653	U
1	2	654	C
1	2	657	C
1	2	659	G
1	2	666	G
1	2	667	A
1	2	668	C
1	2	673	C
1	2	685	C
1	2	686	A
1	2	692	A
1	2	696	C
1	2	703	G
1	2	704	C

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Mol	Chain	Res	Type
1	2	731	G
1	2	738	C
1	2	739	G
1	2	740	G
1	2	742	G
1	2	746	A
1	2	759	G
1	2	904	C
1	2	905	C
1	2	906	C
1	2	913	U
1	2	914	U
1	2	915	A
1	2	916	C
1	2	917	A
1	2	918	G
1	2	924	C
1	2	925	C
1	2	926	G
1	2	932	A
1	2	933	G
1	2	936	C
1	2	941	C
1	2	943	A
1	2	944	A
1	2	945	U
1	2	956	A
1	2	959	G
1	2	960	A
1	2	961	G
1	2	962	C
1	2	965	G
1	2	966	A
1	2	967	C
1	2	968	C
1	2	969	C
1	2	970	G
1	2	977	C
1	2	982	U
1	2	984	C
1	2	989	U
1	2	990	C

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Mol	Chain	Res	Type
1	2	991	C
1	2	992	C
1	2	993	G
1	2	994	G
1	2	995	C
1	2	1048	G
1	2	1049	C
1	2	1051	G
1	2	1066	G
1	2	1067	G
1	2	1068	G
1	2	1070	G
1	2	1072	C
1	2	1082	C
1	2	1170	G
1	2	1173	G
1	2	1177	U
1	2	1178	G
1	2	1179	U
1	2	1180	C
1	2	1181	C
1	2	1182	C
1	2	1183	C
1	2	1184	A
1	2	1185	G
1	2	1187	G
1	2	1189	G
1	2	1194	G
1	2	1195	G
1	2	1198	G
1	2	1200	G
1	2	1202	C
1	2	1203	G
1	2	1211	G
1	2	1215	C
1	2	1216	C
1	2	1219	G
1	2	1222	A
1	2	1241	C
1	2	1243	C
1	2	1245	C
1	2	1252	C

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Mol	Chain	Res	Type
1	2	1253	G
1	2	1255	A
1	2	1256	G
1	2	1260	G
1	2	1265	G
1	2	1266	G
1	2	1269	G
1	2	1271	G
1	2	1272	C
1	2	1275	G
1	2	1280	C
1	2	1283	G
1	2	1284	G
1	2	1287	G
1	2	1294	A
1	2	1296	G
1	2	1301	C
1	2	1302	U
1	2	1303	A
1	2	1314	C
1	2	1315	C
1	2	1323	A
1	2	1337	A
1	2	1354	A
1	2	1358	G
1	2	1359	G
1	2	1365	C
1	2	1366	G
1	2	1367	C
1	2	1370	G
1	2	1377	G
1	2	1378	C
1	2	1379	C
1	2	1381	U
1	2	1387	A
1	2	1394	G
1	2	1398	A
1	2	1399	G
1	2	1402	C
1	2	1404	G
1	2	1405	C
1	2	1407	C

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Mol	Chain	Res	Type
1	2	1408	G
1	2	1409	C
1	2	1410	U
1	2	1412	G
1	2	1420	A
1	2	1439	C
1	2	1442	C
1	2	1444	G
1	2	1446	C
1	2	1448	G
1	2	1449	C
1	2	1465	G
1	2	1472	C
1	2	1482	G
1	2	1483	C
1	2	1486	C
1	2	1497	A
1	2	1498	G
1	2	1503	A
1	2	1518	A
1	2	1525	A
1	2	1534	A2M
1	2	1547	A
1	2	1564	A
1	2	1566	C
1	2	1574	B9B
1	2	1578	U
1	2	1592	G
1	2	1595	G
1	2	1596	U
1	2	1612	G
1	2	1613	A
1	2	1624	G
1	2	1625	OMG
1	2	1626	G
1	2	1631	A
1	2	1633	G
1	2	1634	A
1	2	1638	A
1	2	1641	G
1	2	1649	U
1	2	1650	A

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Mol	Chain	Res	Type
1	2	1654	G
1	2	1661	C
1	2	1671	U
1	2	1672	U
1	2	1673	U
1	2	1674	C
1	2	1675	C
1	2	1676	C
1	2	1677	U
1	2	1679	A
1	2	1680	G
1	2	1681	G
1	2	1691	G
1	2	1697	G
1	2	1699	A
1	2	1700	G
1	2	1701	A
1	2	1703	C
1	2	1704	C
1	2	1705	G
1	2	1715	C
1	2	1717	C
1	2	1718	C
1	2	1719	A
1	2	1724	G
1	2	1731	C
1	2	1732	C
1	2	1796	U
1	2	1797	G
1	2	1803	G
1	2	1804	A
1	2	1806	G
1	2	1809	C
1	2	1810	G
1	2	1815	G
1	2	1816	C
1	2	1821	G
1	2	1822	U
1	2	1832	C
1	2	1834	U
1	2	1836	G
1	2	1837	A

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Mol	Chain	Res	Type
1	2	1842	G
1	2	1854	G
1	2	1855	G
1	2	1856	C
1	2	1861	U
1	2	1862	U
1	2	1865	G
1	2	1869	G
1	2	1870	C
1	2	1871	A2M
1	2	1882	U
1	2	1883	OMG
1	2	1888	A
1	2	1897	A
1	2	1916	G
1	2	1918	U
1	2	1919	G
1	2	1920	C
1	2	1921	C
1	2	1922	G
1	2	1931	C
1	2	1932	A
1	2	1935	C
1	2	1939	A
1	2	1940	G
1	2	1942	A
1	2	1943	A
1	2	1944	A
1	2	1948	G
1	2	1956	A
1	2	1959	U
1	2	1960	A
1	2	1966	C
1	2	1972	G
1	2	1974	U
1	2	1979	A
1	2	1980	U
1	2	1981	G
1	2	1984	A
1	2	1985	G
1	2	1990	A
1	2	1997	U

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Mol	Chain	Res	Type
1	2	2001	G
1	2	2002	A
1	2	2003	G
1	2	2004	U
1	2	2010	A
1	2	2011	C
1	2	2017	A
1	2	2018	C
1	2	2025	A
1	2	2026	A
1	2	2033	A
1	2	2034	G
1	2	2040	A
1	2	2044	U
1	2	2046	G
1	2	2048	U
1	2	2055	G
1	2	2056	G
1	2	2069	A
1	2	2084	C
1	2	2085	G
1	2	2092	G
1	2	2093	A
1	2	2095	A
1	2	2096	G
1	2	2098	G
1	2	2101	C
1	2	2102	G
1	2	2104	G
1	2	2105	A
1	2	2110	C
1	2	2111	G
1	2	2112	G
1	2	2113	C
1	2	2252	G
1	2	2253	A
1	2	2255	C
1	2	2256	C
1	2	2258	C
1	2	2259	G
1	2	2260	C
1	2	2263	A

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Mol	Chain	Res	Type
1	2	2268	A
1	2	2289	C
1	2	2300	A
1	2	2301	G
1	2	2306	G
1	2	2313	A
1	2	2331	G
1	2	2333	G
1	2	2348	G
1	2	2351	C
1	2	2360	A
1	2	2364	OMG
1	2	2395	A
1	2	2410	C
1	2	2416	G
1	2	2417	A
1	2	2418	A
1	2	2422	OMC
1	2	2424	OMG
1	2	2425	U
1	2	2439	G
1	2	2441	C
1	2	2450	G
1	2	2465	C
1	2	2471	G
1	2	2474	G
1	2	2475	G
1	2	2476	G
1	2	2477	A
1	2	2478	C
1	2	2484	A
1	2	2486	G
1	2	2487	G
1	2	2488	C
1	2	2489	C
1	2	2490	U
1	2	2497	C
1	2	2507	A
1	2	2511	A
1	2	2512	A
1	2	2513	A
1	2	2518	G

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Mol	Chain	Res	Type
1	2	2519	U
1	2	2529	A
1	2	2543	A
1	2	2544	G
1	2	2545	U
1	2	2546	G
1	2	2547	G
1	2	2554	U
1	2	2555	G
1	2	2559	G
1	2	2560	C
1	2	2566	G
1	2	2567	G
1	2	2583	C
1	2	2587	A
1	2	2589	C
1	2	2601	A
1	2	2618	G
1	2	2627	C
1	2	2638	G
1	2	2653	C
1	2	2661	U
1	2	2662	G
1	2	2669	C
1	2	2670	C
1	2	2675	G
1	2	2687	U
1	2	2694	G
1	2	2695	A
1	2	2696	A
1	2	2707	U
1	2	2708	U
1	2	2709	C
1	2	2710	C
1	2	2711	G
1	2	2719	C
1	2	2721	G
1	2	2723	U
1	2	2724	G
1	2	2725	A
1	2	2726	G
1	2	2739	C

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Mol	Chain	Res	Type
1	2	2742	G
1	2	2743	A
1	2	2753	G
1	2	2754	B9B
1	2	2758	G
1	2	2761	U
1	2	2763	U
1	2	2769	U
1	2	2770	C
1	2	2772	C
1	2	2787	A
1	2	2788	U
1	2	2790	U
1	2	2799	G
1	2	2814	C
1	2	2815	A
1	2	2826	U
1	2	2827	G
1	2	2842	G
1	2	2855	G
1	2	2875	C
1	2	2901	G
1	2	2902	G
1	2	2904	U
1	2	2905	C
1	2	2906	G
1	2	2908	U
1	2	2909	C
1	2	3585	G
1	2	3588	C
1	2	3591	C
1	2	3594	C
1	2	3595	U
1	2	3596	A
1	2	3597	G
1	2	3606	U
1	2	3615	G
1	2	3616	U
1	2	3626	G
1	2	3635	A
1	2	3644	U
1	2	3662	A

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Mol	Chain	Res	Type
1	2	3663	A
1	2	3672	G
1	2	3673	C
1	2	3679	U
1	2	3680	U
1	2	3682	A
1	2	3691	G
1	2	3696	C
1	2	3702	A
1	2	3710	G
1	2	3711	A
1	2	3712	A
1	2	3713	U
1	2	3714	G
1	2	3722	G
1	2	3729	U
1	2	3735	G
1	2	3736	A
1	2	3748	A
1	2	3750	G
1	2	3753	G
1	2	3773	U
1	2	3775	A
1	2	3776	G
1	2	3833	C
1	2	3838	U
1	2	3839	G
1	2	3840	U
1	2	3867	A2M
1	2	3875	G
1	2	3876	A
1	2	3877	A
1	2	3879	G
1	2	3897	B8K
1	2	3903	A
1	2	3904	G
1	2	3905	A
1	2	3906	A
1	2	3914	U
1	2	3915	U
1	2	3924	C
1	2	3938	G

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Mol	Chain	Res	Type
1	2	4076	G
1	2	4084	G
1	2	4085	A
1	2	4095	G
1	2	4097	G
1	2	4099	G
1	2	4100	C
1	2	4101	C
1	2	4102	C
1	2	4103	C
1	2	4104	G
1	2	4105	A
1	2	4107	G
1	2	4108	G
1	2	4111	U
1	2	4112	C
1	2	4114	C
1	2	4115	G
1	2	4116	C
1	2	4117	U
1	2	4119	C
1	2	4121	G
1	2	4127	A
1	2	4133	C
1	2	4139	G
1	2	4140	C
1	2	4141	G
1	2	4142	C
1	2	4143	G
1	2	4144	C
1	2	4146	G
1	2	4147	G
1	2	4149	C
1	2	4157	A
1	2	4158	C
1	2	4162	C
1	2	4163	U
1	2	4170	A
1	2	4183	G
1	2	4184	G
1	2	4207	C
1	2	4211	C

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Mol	Chain	Res	Type
1	2	4223	C
1	2	4226	G
1	2	4228	G
1	2	4229	U
1	2	4230	C
1	2	4231	C
1	2	4233	A
1	2	4234	A
1	2	4235	G
1	2	4236	G
1	2	4242	U
1	2	4251	A
1	2	4254	G
1	2	4255	A
1	2	4258	C
1	2	4265	U
1	2	4266	G
1	2	4267	G
1	2	4268	A
1	2	4271	A
1	2	4273	A
1	2	4274	A
1	2	4275	G
1	2	4278	C
1	2	4279	A
1	2	4280	A
1	2	4281	A
1	2	4286	C
1	2	4288	C
1	2	4290	U
1	2	4291	G
1	2	4292	A
1	2	4297	G
1	2	4302	U
1	2	4313	A
1	2	4315	A
1	2	4319	C
1	2	4321	U
1	2	4323	A
1	2	4329	G
1	2	4330	G
1	2	4332	C

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Mol	Chain	Res	Type
1	2	4340	U
1	2	4341	C
1	2	4342	C
1	2	4343	U
1	2	4347	G
1	2	4348	A
1	2	4349	C
1	2	4350	C
1	2	4368	G
1	2	4370	G
1	2	4371	G
1	2	4372	U
1	2	4387	C
1	2	4395	U
1	2	4396	A
1	2	4401	G
1	2	4413	C
1	2	4414	A
1	2	4416	G
1	2	4417	C
1	2	4418	G
1	2	4419	U
1	2	4420	U
1	2	4421	C
1	2	4422	A
1	2	4423	U
1	2	4424	A
1	2	4425	G
1	2	4426	C
1	2	4427	G
1	2	4428	A
1	2	4433	G
1	2	4436	U
1	2	4437	U
1	2	4438	U
1	2	4440	G
1	2	4441	A
1	2	4446	U
1	2	4447	C
1	2	4449	A
1	2	4450	U
1	2	4451	G

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Mol	Chain	Res	Type
1	2	4452	U
1	2	4453	C
1	2	4464	A
1	2	4466	C
1	2	4475	G
1	2	4476	C
1	2	4484	A
1	2	4498	U
1	2	4499	G
1	2	4500	U
1	2	4502	C
1	2	4503	A
1	2	4512	U
1	2	4513	A
1	2	4518	A
1	2	4519	C
1	2	4524	G
1	2	4529	B8W
1	2	4543	G
1	2	4545	G
1	2	4548	A
1	2	4550	7MG
1	2	4555	U
1	2	4556	U
1	2	4557	U
1	2	4558	U
1	2	4560	C
1	2	4567	G
1	2	4584	A
1	2	4589	A
1	2	4590	A
1	2	4599	A
1	2	4600	G
1	2	4601	U
1	2	4607	A
1	2	4608	G
1	2	4635	A
1	2	4636	U
1	2	4637	OMG
1	2	4656	A
1	2	4670	C
1	2	4672	A

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Mol	Chain	Res	Type
1	2	4678	G
1	2	4684	A
1	2	4694	G
1	2	4695	C
1	2	4708	A
1	2	4709	U
1	2	4719	G
1	2	4730	C
1	2	4731	G
1	2	4732	G
1	2	4733	C
1	2	4734	A
1	2	4740	G
1	2	4741	C
1	2	4742	G
1	2	4745	G
1	2	4751	G
1	2	4754	G
1	2	4757	C
1	2	4759	C
1	2	4761	G
1	2	4765	G
1	2	4771	C
1	2	4773	C
1	2	4776	G
1	2	4870	OMG
1	2	4871	C
1	2	4872	2MG
1	2	4875	G
1	2	4877	G
1	2	4882	U
1	2	4883	C
1	2	4889	G
1	2	4893	A
1	2	4895	C
1	2	4896	G
1	2	4899	G
1	2	4900	C
1	2	4901	G
1	2	4910	G
1	2	4912	G
1	2	4914	C

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Mol	Chain	Res	Type
1	2	4916	G
1	2	4927	G
1	2	4928	C
1	2	4938	A
1	2	4940	C
1	2	4941	G
1	2	4943	A
1	2	4949	G
1	2	4976	U
1	2	4988	U
1	2	4989	U
1	2	4991	U
1	2	5013	C
1	2	5014	A
1	2	5017	G
1	2	5022	U
1	2	5025	C
1	2	5026	U
1	2	5027	C
1	2	5028	G
1	2	5030	U
1	2	5031	G
1	2	5034	A
1	2	5041	G
1	2	5047	C
1	2	5050	C
1	2	5054	C
1	2	5058	A
1	2	5062	G
1	2	5069	U
4	8	25	G
4	8	34	U
4	8	35	C
4	8	39	G
4	8	48	A
4	8	52	A
4	8	59	A
4	8	62	A
4	8	63	U
4	8	80	A
4	8	82	A
4	8	84	A

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Mol	Chain	Res	Type
4	8	85	U
4	8	103	A
4	8	104	A
4	8	105	C
4	8	108	A
4	8	110	U
4	8	114	G
4	8	123	U
4	8	124	U
4	8	125	C
4	8	126	C
4	8	127	U
4	8	128	C
4	8	147	G
4	8	150	C
4	8	151	G
4	8	156	U
55	3	7	G
55	3	11	A
55	3	22	A
55	3	29	C
55	3	41	G
55	3	48	G
55	3	49	A
55	3	51	G
55	3	52	C
55	3	53	U
55	3	54	A
55	3	63	C
55	3	64	G
55	3	72	U
55	3	73	U
55	3	74	A
55	3	75	G
55	3	83	A
55	3	84	U
55	3	85	G
55	3	86	G
55	3	100	A
55	3	110	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	406	C
1	2	914	U
1	2	1184	A
1	2	1633	G
1	2	1678	C
1	2	1808	C
1	2	1931	C
1	2	1980	U
1	2	2033	A
1	2	2486	G
1	2	2487	G
1	2	2496	G
1	2	2760	G
1	2	3701	OMC
1	2	3774	A
1	2	3875	G
1	2	3905	A
1	2	4228	G
1	2	4555	U
1	2	4636	U
1	2	4913	G
55	3	51	G
55	3	72	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	2	398	1	22,25,26	3.20	9 (40%)	31,36,39	2.94	10 (32%)
1	B8T	2	4483	1	19,22,23	3.66	8 (42%)	26,31,34	1.37	6 (23%)
1	UR3	2	4597	1	19,22,23	2.82	6 (31%)	26,32,35	1.88	3 (11%)
1	B8Q	2	1456	1	17,22,23	2.96	5 (29%)	22,32,35	2.21	6 (27%)
1	B8T	2	4671	1	19,22,23	3.61	8 (42%)	26,31,34	0.93	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	2	2050	1	23,26,27	2.65	8 (34%)	33,38,41	2.72	11 (33%)
1	7MG	2	2522	1	22,26,27	3.76	10 (45%)	29,39,42	1.97	10 (34%)
1	OMC	2	3909	1	19,22,23	3.13	8 (42%)	26,31,34	1.85	7 (26%)
1	A2M	2	3718	1	22,25,26	3.20	9 (40%)	31,36,39	2.92	10 (32%)
1	BGH	2	3899	1	25,29,30	4.60	17 (68%)	31,43,46	2.58	11 (35%)
1	7MG	2	4550	1	22,26,27	3.85	10 (45%)	29,39,42	1.98	7 (24%)
1	OMG	2	2424	1	23,26,27	2.72	8 (34%)	33,38,41	2.91	10 (30%)
1	M7A	2	4564	1	20,25,26	2.02	3 (15%)	28,37,40	3.91	7 (25%)
1	A2M	2	1534	1	22,25,26	3.18	9 (40%)	31,36,39	2.99	10 (32%)
1	OMU	2	4620	1	19,22,23	2.97	8 (42%)	26,31,34	1.74	5 (19%)
1	B9B	2	1574	1	25,28,29	1.73	5 (20%)	35,40,43	5.15	11 (31%)
1	A2M	2	4523	1	22,25,26	3.16	9 (40%)	31,36,39	3.00	10 (32%)
1	OMG	2	2364	1	23,26,27	2.66	8 (34%)	33,38,41	2.73	11 (33%)
1	A2M	2	3723	1	22,25,26	3.17	9 (40%)	31,36,39	3.01	10 (32%)
1	A2M	2	3867	1	22,25,26	3.16	9 (40%)	31,36,39	2.98	10 (32%)
1	7MG	2	1605	1	22,26,27	3.87	10 (45%)	29,39,42	2.00	8 (27%)
1	P4U	2	1348	1	21,24,25	3.61	8 (38%)	27,33,36	1.06	2 (7%)
1	A2M	2	2401	1	22,25,26	3.20	9 (40%)	31,36,39	3.03	11 (35%)
1	A2M	2	1871	1	22,25,26	3.19	10 (45%)	31,36,39	2.97	11 (35%)
1	OMG	2	1625	1	23,26,27	2.71	8 (34%)	33,38,41	2.76	10 (30%)
1	OMC	2	3887	1	19,22,23	3.05	8 (42%)	26,31,34	1.01	1 (3%)
1	B8W	2	4472	1	23,26,27	2.74	5 (21%)	33,38,41	2.47	15 (45%)
1	2MG	2	1517	1	23,26,27	2.99	8 (34%)	32,38,41	2.35	8 (25%)
1	P7G	2	1909	1	24,28,29	4.09	11 (45%)	27,41,44	1.55	3 (11%)
1	A2M	2	2363	1	22,25,26	3.19	9 (40%)	31,36,39	2.98	11 (35%)
1	OMC	2	2422	1	19,22,23	3.03	8 (42%)	26,31,34	1.00	2 (7%)
1	OMG	2	4494	1	23,26,27	2.71	8 (34%)	33,38,41	2.81	10 (30%)
1	B8W	2	4185	1	23,26,27	2.75	6 (26%)	33,38,41	2.61	13 (39%)
1	B8W	2	4529	1	23,26,27	2.78	5 (21%)	33,38,41	2.58	13 (39%)
1	A2M	2	1524	1	22,25,26	3.20	9 (40%)	31,36,39	2.99	11 (35%)
1	OMG	2	4637	1	23,26,27	2.66	8 (34%)	33,38,41	2.74	11 (33%)
1	OMG	2	1522	1	23,26,27	2.68	8 (34%)	33,38,41	2.81	10 (30%)
1	B8K	2	4690	1	24,28,29	3.30	12 (50%)	30,42,45	2.67	11 (36%)
1	OMG	2	4870	1	23,26,27	2.70	8 (34%)	33,38,41	3.00	10 (30%)
1	A2M	2	3825	1	22,25,26	3.19	9 (40%)	31,36,39	3.01	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	E7G	2	2297	1	24,27,28	4.04	11 (45%)	30,40,43	2.12	9 (30%)
1	B8W	2	2380	1	23,26,27	2.71	5 (21%)	33,38,41	2.57	14 (42%)
1	OMG	2	1316	1	23,26,27	2.68	8 (34%)	33,38,41	2.74	11 (33%)
1	2MG	2	978	1	23,26,27	3.03	8 (34%)	32,38,41	2.20	9 (28%)
1	2MG	2	729	1	23,26,27	2.97	8 (34%)	32,38,41	2.31	8 (25%)
1	OMG	2	373	1	23,26,27	2.68	8 (34%)	33,38,41	2.71	13 (39%)
1	OMC	2	4536	1	19,22,23	3.04	8 (42%)	26,31,34	1.12	3 (11%)
1	B9B	2	237	1	25,28,29	1.74	6 (24%)	35,40,43	5.18	12 (34%)
1	B8K	2	3897	1	24,28,29	3.44	11 (45%)	30,42,45	2.53	11 (36%)
1	A2M	2	4571	1	22,25,26	3.16	9 (40%)	31,36,39	2.94	11 (35%)
1	OMG	2	2773	1	23,26,27	2.70	8 (34%)	33,38,41	2.78	9 (27%)
1	2MG	2	4872	1	23,26,27	2.93	8 (34%)	32,38,41	2.27	11 (34%)
1	OMC	2	2365	1	19,22,23	2.99	8 (42%)	26,31,34	0.74	0
4	OMU	8	14	1,4	19,22,23	2.96	8 (42%)	26,31,34	1.79	6 (23%)
1	OMC	2	3701	1	19,22,23	3.01	8 (42%)	26,31,34	0.74	0
1	5MU	2	4083	1	19,22,23	7.22	8 (42%)	28,32,35	3.37	10 (35%)
1	B9H	2	2786	1	20,25,26	3.24	3 (15%)	22,35,38	1.95	5 (22%)
1	OMC	2	2804	1	19,22,23	2.98	8 (42%)	26,31,34	0.76	0
1	A2M	2	1326	1	22,25,26	3.18	9 (40%)	31,36,39	2.95	10 (32%)
1	OMC	2	3869	1	19,22,23	3.02	8 (42%)	26,31,34	0.90	1 (3%)
1	I4U	2	1659	1	21,24,25	3.56	9 (42%)	27,34,37	1.11	2 (7%)
1	B9B	2	2754	1	25,28,29	1.73	5 (20%)	35,40,43	5.23	11 (31%)
1	UR3	2	4530	1	19,22,23	2.89	6 (31%)	26,32,35	1.26	2 (7%)
1	P7G	2	3880	1	24,28,29	4.19	11 (45%)	27,41,44	1.37	2 (7%)
1	OMC	2	2861	1	19,22,23	3.04	8 (42%)	26,31,34	1.10	3 (11%)
1	OMG	2	4623	1	23,26,27	2.67	8 (34%)	33,38,41	2.76	12 (36%)
1	OMG	2	1883	1	23,26,27	2.72	8 (34%)	33,38,41	2.75	11 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	2	398	1	-	2/9/27/28	0/3/3/3
1	B8T	2	4483	1	-	0/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	2	4597	1	-	0/7/25/26	0/2/2/2
1	B8Q	2	1456	1	-	0/7/42/43	0/2/2/2
1	B8T	2	4671	1	-	0/7/27/28	0/2/2/2
1	OMG	2	2050	1	-	0/9/27/28	0/3/3/3
1	7MG	2	2522	1	-	0/7/37/38	0/3/3/3
1	OMC	2	3909	1	-	2/9/27/28	0/2/2/2
1	A2M	2	3718	1	-	0/9/27/28	0/3/3/3
1	BGH	2	3899	1	-	1/13/43/44	0/3/3/3
1	7MG	2	4550	1	-	2/7/37/38	0/3/3/3
1	OMG	2	2424	1	-	2/9/27/28	0/3/3/3
1	M7A	2	4564	1	-	0/7/37/38	0/3/3/3
1	A2M	2	1534	1	-	2/9/27/28	0/3/3/3
1	OMU	2	4620	1	-	0/9/27/28	0/2/2/2
1	B9B	2	1574	1	-	3/11/29/30	0/3/3/3
1	A2M	2	4523	1	-	1/9/27/28	0/3/3/3
1	OMG	2	2364	1	-	3/9/27/28	0/3/3/3
1	A2M	2	3723	1	-	0/9/27/28	0/3/3/3
1	A2M	2	3867	1	-	3/9/27/28	0/3/3/3
1	7MG	2	1605	1	-	0/7/37/38	0/3/3/3
1	P4U	2	1348	1	-	1/10/29/30	0/2/2/2
1	A2M	2	2401	1	-	0/9/27/28	0/3/3/3
1	A2M	2	1871	1	-	2/9/27/28	0/3/3/3
1	OMG	2	1625	1	-	3/9/27/28	0/3/3/3
1	OMC	2	3887	1	-	1/9/27/28	0/2/2/2
1	B8W	2	4472	1	-	2/9/27/28	0/3/3/3
1	2MG	2	1517	1	-	1/9/27/28	0/3/3/3
1	P7G	2	1909	1	-	3/10/40/41	0/3/3/3
1	A2M	2	2363	1	-	0/9/27/28	0/3/3/3
1	OMC	2	2422	1	-	1/9/27/28	0/2/2/2
1	OMG	2	4494	1	-	0/9/27/28	0/3/3/3
1	B8W	2	4185	1	-	2/9/27/28	0/3/3/3
1	B8W	2	4529	1	-	2/9/27/28	0/3/3/3
1	A2M	2	1524	1	-	2/9/27/28	0/3/3/3
1	OMG	2	4637	1	-	4/9/27/28	0/3/3/3
1	OMG	2	1522	1	-	0/9/27/28	0/3/3/3
1	B8K	2	4690	1	-	0/11/41/42	0/3/3/3
1	OMG	2	4870	1	-	3/9/27/28	0/3/3/3
1	A2M	2	3825	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	E7G	2	2297	1	-	1/9/39/40	0/3/3/3
1	B8W	2	2380	1	-	2/9/27/28	0/3/3/3
1	OMG	2	1316	1	-	0/9/27/28	0/3/3/3
1	2MG	2	978	1	-	0/9/27/28	0/3/3/3
1	2MG	2	729	1	-	1/9/27/28	0/3/3/3
1	OMG	2	373	1	-	1/9/27/28	0/3/3/3
1	OMC	2	4536	1	-	0/9/27/28	0/2/2/2
1	B9B	2	237	1	-	6/11/29/30	0/3/3/3
1	B8K	2	3897	1	-	3/11/41/42	0/3/3/3
1	A2M	2	4571	1	-	0/9/27/28	0/3/3/3
1	OMG	2	2773	1	-	0/9/27/28	0/3/3/3
1	2MG	2	4872	1	-	2/9/27/28	0/3/3/3
1	OMC	2	2365	1	-	0/9/27/28	0/2/2/2
4	OMU	8	14	1,4	-	1/9/27/28	0/2/2/2
1	OMC	2	3701	1	-	2/9/27/28	0/2/2/2
1	5MU	2	4083	1	-	0/7/25/26	0/2/2/2
1	B9H	2	2786	1	-	1/12/47/48	0/2/2/2
1	OMC	2	2804	1	-	0/9/27/28	0/2/2/2
1	A2M	2	1326	1	-	0/9/27/28	0/3/3/3
1	OMC	2	3869	1	-	0/9/27/28	0/2/2/2
1	I4U	2	1659	1	-	1/9/29/30	0/2/2/2
1	B9B	2	2754	1	-	4/11/29/30	0/3/3/3
1	UR3	2	4530	1	-	0/7/25/26	0/2/2/2
1	P7G	2	3880	1	-	2/10/40/41	0/3/3/3
1	OMC	2	2861	1	-	0/9/27/28	0/2/2/2
1	OMG	2	4623	1	-	0/9/27/28	0/3/3/3
1	OMG	2	1883	1	-	2/9/27/28	0/3/3/3

All (546) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	4083	5MU	C4-C5	20.78	1.79	1.44
1	2	4083	5MU	C6-N1	16.00	1.65	1.38
1	2	4083	5MU	C6-C5	-11.45	1.15	1.34
1	2	4083	5MU	C4-N3	-11.05	1.18	1.38
1	2	1659	I4U	C4-N3	10.65	1.45	1.31
1	2	1348	P4U	C4-N3	10.59	1.45	1.31
1	2	2786	B9H	C2-N3	9.82	1.49	1.37
1	2	2297	E7G	C5-N7	9.67	1.46	1.35
1	2	3880	P7G	C5-N7	9.64	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	3880	P7G	C8-N9	9.43	1.51	1.46
1	2	1909	P7G	C5-N7	9.38	1.46	1.35
1	2	1909	P7G	C8-N9	9.28	1.51	1.46
1	2	3897	B8K	C8-N9	9.27	1.51	1.46
1	2	1605	7MG	C8-N9	9.11	1.51	1.46
1	2	2297	E7G	C8-N9	9.07	1.51	1.46
1	2	4550	7MG	C8-N9	9.03	1.51	1.46
1	2	3899	BGH	O4'-C1'	8.98	1.63	1.42
1	2	4472	B8W	O6-C6	8.90	1.49	1.35
1	2	1871	A2M	C3'-C4'	-8.89	1.30	1.53
1	2	1524	A2M	C3'-C4'	-8.86	1.30	1.53
1	2	3825	A2M	C3'-C4'	-8.81	1.30	1.53
1	2	1326	A2M	C3'-C4'	-8.81	1.30	1.53
1	2	3723	A2M	C3'-C4'	-8.81	1.30	1.53
1	2	398	A2M	C3'-C4'	-8.78	1.30	1.53
1	2	1605	7MG	C5-N7	8.77	1.45	1.35
1	2	4529	B8W	O6-C6	8.77	1.49	1.35
1	2	2363	A2M	C3'-C4'	-8.76	1.30	1.53
1	2	2401	A2M	C3'-C4'	-8.75	1.30	1.53
1	2	3899	BGH	C2'-C1'	-8.75	1.30	1.53
1	2	1534	A2M	C3'-C4'	-8.75	1.30	1.53
1	2	2522	7MG	C5-N7	8.73	1.45	1.35
1	2	3718	A2M	C3'-C4'	-8.72	1.30	1.53
1	2	4571	A2M	C3'-C4'	-8.72	1.30	1.53
1	2	4550	7MG	C5-N7	8.70	1.45	1.35
1	2	3867	A2M	C3'-C4'	-8.70	1.30	1.53
1	2	4523	A2M	C3'-C4'	-8.63	1.30	1.53
1	2	4185	B8W	O6-C6	8.59	1.48	1.35
1	2	2522	7MG	C8-N9	8.57	1.50	1.46
1	2	2380	B8W	O6-C6	8.47	1.48	1.35
1	2	4690	B8K	C8-N9	8.38	1.50	1.46
1	2	1456	B8Q	C6-C5	8.37	1.52	1.33
1	2	3899	BGH	C8-N9	8.36	1.50	1.46
1	2	978	2MG	C2-N3	8.10	1.47	1.31
1	2	4185	B8W	C2-N2	8.05	1.50	1.33
1	2	4529	B8W	C2-N2	8.02	1.49	1.33
1	2	2380	B8W	C2-N2	7.95	1.49	1.33
1	2	729	2MG	C2-N3	7.88	1.47	1.31
1	2	1517	2MG	C2-N3	7.88	1.47	1.31
1	2	4472	B8W	C2-N2	7.84	1.49	1.33
1	2	4872	2MG	C2-N3	7.79	1.46	1.31
1	2	398	A2M	O4'-C4'	7.74	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	3718	A2M	O4'-C4'	7.73	1.62	1.45
1	2	1871	A2M	O4'-C4'	7.69	1.62	1.45
1	2	2401	A2M	O4'-C4'	7.66	1.62	1.45
1	2	2363	A2M	O4'-C4'	7.65	1.62	1.45
1	2	3825	A2M	O4'-C4'	7.64	1.62	1.45
1	2	1534	A2M	O4'-C4'	7.63	1.62	1.45
1	2	1326	A2M	O4'-C4'	7.61	1.62	1.45
1	2	4523	A2M	O4'-C4'	7.58	1.61	1.45
1	2	4571	A2M	O4'-C4'	7.52	1.61	1.45
1	2	3723	A2M	O4'-C4'	7.51	1.61	1.45
1	2	4483	B8T	C2-N3	7.50	1.51	1.36
1	2	3899	BGH	O4'-C4'	-7.48	1.28	1.45
1	2	1524	A2M	O4'-C4'	7.47	1.61	1.45
1	2	3867	A2M	O4'-C4'	7.42	1.61	1.45
1	2	4671	B8T	C2-N3	7.27	1.51	1.36
1	2	4671	B8T	C4-N3	7.10	1.45	1.32
1	2	2786	B9H	C2-N1	7.07	1.48	1.38
1	2	4483	B8T	C4-N3	7.04	1.45	1.32
4	8	14	OMU	C2-N1	7.04	1.49	1.38
1	2	2786	B9H	C6-C5	6.99	1.49	1.33
1	2	4620	OMU	C2-N1	6.94	1.49	1.38
1	2	4671	B8T	C6-C5	6.92	1.51	1.35
1	2	978	2MG	C2-N2	6.86	1.48	1.33
1	2	1517	2MG	C2-N2	6.84	1.48	1.33
1	2	4530	UR3	C6-C5	6.84	1.51	1.35
1	2	729	2MG	C4-N3	6.84	1.50	1.34
1	2	4530	UR3	C2-N1	6.82	1.48	1.38
1	2	4483	B8T	C6-C5	6.82	1.50	1.35
1	2	4597	UR3	C6-C5	6.81	1.50	1.35
1	2	978	2MG	C4-N3	6.69	1.50	1.34
1	2	1517	2MG	C4-N3	6.67	1.50	1.34
1	2	1456	B8Q	C2-N3	6.66	1.46	1.35
1	2	4690	B8K	C2-N3	6.66	1.49	1.33
1	2	729	2MG	C2-N2	6.65	1.48	1.33
1	2	3897	B8K	C2-N3	6.62	1.49	1.33
1	2	4620	OMU	C2-N3	6.60	1.49	1.38
4	8	14	OMU	C2-N3	6.58	1.49	1.38
1	2	3909	OMC	C6-C5	6.55	1.50	1.35
1	2	2297	E7G	C8-N7	6.54	1.52	1.45
1	2	4872	2MG	C2-N2	6.53	1.47	1.33
1	2	3880	P7G	C8-N7	6.43	1.51	1.45
1	2	1909	P7G	C4-N9	6.43	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	3869	OMC	C2-N3	6.42	1.49	1.36
1	2	4536	OMC	C2-N3	6.42	1.49	1.36
1	2	2424	OMG	C2-N3	6.39	1.48	1.33
1	2	3880	P7G	C4-N9	6.39	1.44	1.35
1	2	3899	BGH	C4-N9	6.37	1.45	1.37
1	2	3887	OMC	C2-N3	6.37	1.49	1.36
1	2	2422	OMC	C2-N3	6.35	1.49	1.36
1	2	3880	P7G	C4-N3	6.35	1.48	1.37
1	2	4483	B8T	C4-N4	6.34	1.48	1.35
1	2	2861	OMC	C2-N3	6.34	1.49	1.36
1	2	2365	OMC	C2-N3	6.32	1.49	1.36
1	2	1625	OMG	C2-N3	6.31	1.48	1.33
1	2	4671	B8T	C4-N4	6.31	1.48	1.35
1	2	4597	UR3	C2-N3	6.30	1.51	1.39
1	2	1909	P7G	C4-N3	6.30	1.48	1.37
1	2	1883	OMG	C2-N3	6.30	1.48	1.33
1	2	3701	OMC	C2-N3	6.30	1.49	1.36
1	2	4494	OMG	C2-N3	6.29	1.48	1.33
1	2	1659	I4U	C2-N3	6.25	1.49	1.36
1	2	1625	OMG	C4-N3	6.25	1.49	1.34
1	2	2424	OMG	C4-N3	6.25	1.49	1.34
1	2	4870	OMG	C4-N3	6.24	1.49	1.34
1	2	1883	OMG	C4-N3	6.23	1.49	1.34
1	2	2804	OMC	C2-N3	6.23	1.49	1.36
1	2	2773	OMG	C2-N3	6.23	1.48	1.33
1	2	4870	OMG	C2-N3	6.22	1.48	1.33
1	2	4872	2MG	C4-N3	6.22	1.49	1.34
1	2	1348	P4U	C2-N3	6.22	1.49	1.36
1	2	4494	OMG	C4-N3	6.20	1.49	1.34
1	2	2773	OMG	C4-N3	6.17	1.48	1.34
1	2	1348	P4U	C6-C5	6.14	1.49	1.35
1	2	1316	OMG	C4-N3	6.12	1.48	1.34
1	2	373	OMG	C2-N3	6.11	1.47	1.33
1	2	1316	OMG	C2-N3	6.11	1.47	1.33
1	2	1659	I4U	C6-C5	6.11	1.49	1.35
1	2	1522	OMG	C2-N3	6.09	1.47	1.33
1	2	1883	OMG	C2-N2	6.07	1.48	1.34
1	2	2424	OMG	C2-N2	6.07	1.48	1.34
1	2	1522	OMG	C4-N3	6.07	1.48	1.34
1	2	2364	OMG	C4-N3	6.06	1.48	1.34
1	2	4870	OMG	C2-N2	6.06	1.48	1.34
1	2	373	OMG	C4-N3	6.05	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	3701	OMC	C6-C5	6.05	1.49	1.35
1	2	1522	OMG	C2-N2	6.04	1.48	1.34
1	2	2364	OMG	C2-N3	6.04	1.47	1.33
1	2	4597	UR3	C2-N1	6.03	1.47	1.38
1	2	2773	OMG	C2-N2	6.03	1.48	1.34
1	2	1625	OMG	C2-N2	6.02	1.48	1.34
1	2	373	OMG	C2-N2	6.02	1.48	1.34
1	2	4494	OMG	C2-N2	6.00	1.48	1.34
1	2	3887	OMC	C6-C5	6.00	1.49	1.35
1	2	2365	OMC	C6-C5	6.00	1.49	1.35
1	2	2050	OMG	C4-N3	5.99	1.48	1.34
1	2	4623	OMG	C2-N3	5.98	1.47	1.33
1	2	2050	OMG	C2-N3	5.98	1.47	1.33
1	2	4623	OMG	C2-N2	5.97	1.48	1.34
1	2	2861	OMC	C6-C5	5.97	1.48	1.35
1	2	2422	OMC	C6-C5	5.96	1.48	1.35
1	2	4637	OMG	C2-N3	5.96	1.47	1.33
1	2	4623	OMG	C4-N3	5.96	1.48	1.34
1	2	4536	OMC	C6-C5	5.95	1.48	1.35
1	2	1316	OMG	C2-N2	5.95	1.48	1.34
1	2	4637	OMG	C4-N3	5.95	1.48	1.34
1	2	3880	P7G	C2-N2	5.93	1.48	1.34
1	2	1909	P7G	C2-N2	5.93	1.48	1.34
1	2	2050	OMG	C2-N2	5.92	1.48	1.34
1	2	4637	OMG	C2-N2	5.92	1.48	1.34
1	2	2804	OMC	C6-C5	5.91	1.48	1.35
1	2	3869	OMC	C6-C5	5.89	1.48	1.35
1	2	2364	OMG	C2-N2	5.88	1.48	1.34
1	2	4564	M7A	C4-N9	5.86	1.49	1.38
1	2	4550	7MG	C2-N3	5.82	1.47	1.33
1	2	3897	B8K	C4-N9	5.81	1.44	1.37
1	2	3899	BGH	C4-N3	5.79	1.48	1.34
1	2	1605	7MG	C2-N3	5.77	1.47	1.33
1	2	3899	BGH	C2-N3	5.74	1.47	1.33
1	2	4530	UR3	C2-N3	5.74	1.50	1.39
1	2	2297	E7G	C4-N9	5.73	1.44	1.37
1	2	237	B9B	C2-N2	5.73	1.45	1.33
1	2	2754	B9B	C2-N2	5.73	1.45	1.33
1	2	3909	OMC	C2-N3	5.70	1.47	1.36
1	2	2297	E7G	C4-N3	5.68	1.47	1.34
1	2	2522	7MG	C2-N3	5.67	1.46	1.33
1	2	1909	P7G	C8-N7	5.67	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	2297	E7G	C2-N3	5.66	1.46	1.33
1	2	1574	B9B	C2-N2	5.62	1.45	1.33
1	2	4550	7MG	C4-N3	5.61	1.47	1.34
1	2	1605	7MG	C4-N3	5.57	1.47	1.34
1	2	3909	OMC	C2-N1	5.56	1.52	1.40
1	2	4620	OMU	C6-C5	5.54	1.47	1.35
1	2	4550	7MG	C4-N9	5.52	1.44	1.37
1	2	1605	7MG	C4-N9	5.48	1.44	1.37
1	2	2522	7MG	C4-N3	5.48	1.47	1.34
1	2	3909	OMC	C4-N4	5.44	1.46	1.33
1	2	4690	B8K	C4-N9	5.34	1.43	1.37
1	2	3880	P7G	C2-N1	5.33	1.46	1.33
4	8	14	OMU	C6-C5	5.30	1.47	1.35
1	2	1909	P7G	C2-N1	5.24	1.45	1.33
1	2	2522	7MG	C4-N9	5.24	1.43	1.37
1	2	3701	OMC	C4-N3	5.16	1.44	1.34
1	2	2297	E7G	C2-N2	5.16	1.46	1.34
1	2	4536	OMC	C4-N3	5.14	1.44	1.34
1	2	4483	B8T	C2-N1	5.13	1.51	1.40
1	2	3869	OMC	C4-N3	5.12	1.44	1.34
1	2	3887	OMC	C4-N3	5.12	1.44	1.34
1	2	2365	OMC	C4-N3	5.11	1.44	1.34
1	2	2804	OMC	C4-N3	5.10	1.44	1.34
1	2	2861	OMC	C2-N1	5.08	1.51	1.40
1	2	2422	OMC	C4-N3	5.06	1.44	1.34
1	2	2861	OMC	C4-N3	5.06	1.44	1.34
1	2	3887	OMC	C2-N1	4.98	1.50	1.40
1	2	4536	OMC	C2-N1	4.97	1.50	1.40
1	2	3701	OMC	C4-N4	4.89	1.45	1.33
1	2	2861	OMC	C4-N4	4.89	1.45	1.33
1	2	3887	OMC	C4-N4	4.88	1.45	1.33
1	2	2422	OMC	C2-N1	4.88	1.50	1.40
1	2	3899	BGH	C2-N2	4.87	1.45	1.34
1	2	2422	OMC	C4-N4	4.87	1.45	1.33
1	2	4536	OMC	C4-N4	4.87	1.45	1.33
1	2	3867	A2M	O4'-C1'	-4.86	1.30	1.42
1	2	2804	OMC	C4-N4	4.84	1.45	1.33
1	2	2365	OMC	C4-N4	4.84	1.45	1.33
1	2	3869	OMC	C4-N4	4.83	1.45	1.33
1	2	1605	7MG	C2-N2	4.79	1.45	1.34
1	2	2522	7MG	C2-N2	4.77	1.45	1.34
1	2	3869	OMC	C2-N1	4.76	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	4550	7MG	C2-N2	4.76	1.45	1.34
1	2	1456	B8Q	C2-N1	4.73	1.45	1.38
1	2	1348	P4U	O4-C4	4.71	1.40	1.35
1	2	1326	A2M	O4'-C1'	-4.61	1.31	1.42
1	2	1524	A2M	O4'-C1'	-4.61	1.31	1.42
1	2	4671	B8T	C2-N1	4.61	1.50	1.40
1	2	398	A2M	O4'-C1'	-4.60	1.31	1.42
1	2	3909	OMC	C4-N3	4.58	1.43	1.34
1	2	1659	I4U	C5-C4	4.58	1.49	1.43
1	2	4523	A2M	C6-N6	4.57	1.45	1.34
1	2	3825	A2M	C6-N6	4.57	1.45	1.34
1	2	3718	A2M	O4'-C1'	-4.56	1.31	1.42
1	2	1524	A2M	C6-N6	4.56	1.45	1.34
1	2	1871	A2M	C6-N6	4.55	1.45	1.34
1	2	3899	BGH	C5-N7	4.55	1.47	1.39
1	2	3718	A2M	C6-N6	4.55	1.45	1.34
1	2	2401	A2M	O4'-C1'	-4.54	1.31	1.42
1	2	1326	A2M	C6-N6	4.53	1.45	1.34
1	2	3723	A2M	C6-N6	4.53	1.45	1.34
1	2	4571	A2M	C6-N6	4.52	1.45	1.34
1	2	2401	A2M	C6-N6	4.52	1.45	1.34
1	2	4523	A2M	O4'-C1'	-4.52	1.31	1.42
1	2	4571	A2M	O4'-C1'	-4.52	1.31	1.42
1	2	2363	A2M	O4'-C1'	-4.52	1.31	1.42
1	2	2804	OMC	C2-N1	4.52	1.49	1.40
1	2	3723	A2M	O4'-C1'	-4.52	1.31	1.42
1	2	2363	A2M	C6-N6	4.51	1.45	1.34
1	2	3825	A2M	O4'-C1'	-4.51	1.31	1.42
1	2	1534	A2M	O4'-C1'	-4.50	1.31	1.42
1	2	3867	A2M	C6-N6	4.50	1.45	1.34
1	2	398	A2M	C6-N6	4.49	1.45	1.34
1	2	4083	5MU	C2-N3	4.49	1.46	1.38
1	2	1534	A2M	C6-N6	4.48	1.45	1.34
1	2	1348	P4U	C5-C4	4.47	1.48	1.43
1	2	4690	B8K	C4-N3	4.45	1.44	1.34
1	2	1348	P4U	C2-N1	4.45	1.49	1.40
1	2	3701	OMC	C2-N1	4.42	1.49	1.40
1	2	3897	B8K	C4-N3	4.41	1.44	1.34
1	2	1659	I4U	C2-N1	4.40	1.49	1.40
1	2	2365	OMC	C2-N1	4.36	1.49	1.40
1	2	4564	M7A	C6-N6	4.36	1.45	1.34
1	2	1871	A2M	O4'-C1'	-4.34	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	3897	B8K	C5-C6	4.33	1.54	1.43
1	2	3899	BGH	C5-C6	4.31	1.54	1.43
1	2	978	2MG	C2-N1	4.30	1.43	1.36
1	2	3897	B8K	C5-N7	4.29	1.47	1.39
1	2	4872	2MG	C2-N1	4.29	1.43	1.36
1	2	1517	2MG	C2-N1	4.27	1.43	1.36
1	2	729	2MG	C2-N1	4.15	1.43	1.36
1	2	4690	B8K	C5-N7	4.10	1.46	1.39
4	8	14	OMU	C4-N3	4.02	1.45	1.38
1	2	4671	B8T	C5-C4	3.93	1.49	1.40
1	2	4620	OMU	C4-N3	3.93	1.45	1.38
1	2	4564	M7A	C5-N7	3.90	1.48	1.39
1	2	4690	B8K	C5-C6	3.90	1.53	1.43
1	2	1625	OMG	C5-N7	-3.90	1.31	1.39
1	2	1605	7MG	C5-C6	3.88	1.53	1.43
1	2	4494	OMG	C5-N7	-3.87	1.31	1.39
1	2	4550	7MG	C5-C6	3.86	1.53	1.43
1	2	1883	OMG	C5-N7	-3.83	1.31	1.39
1	2	2297	E7G	C5-C6	3.81	1.53	1.43
1	2	3880	P7G	C2-N3	3.81	1.47	1.37
1	2	1909	P7G	C2-N3	3.79	1.47	1.37
1	2	2424	OMG	C5-N7	-3.78	1.31	1.39
1	2	2364	OMG	C5-N7	-3.77	1.31	1.39
1	2	3880	P7G	C6-N1	3.77	1.44	1.38
1	2	4637	OMG	C5-N7	-3.76	1.31	1.39
1	2	1522	OMG	C5-N7	-3.75	1.31	1.39
1	2	1316	OMG	C5-N7	-3.73	1.31	1.39
1	2	3899	BGH	O2'-C2'	3.71	1.52	1.42
1	2	2773	OMG	C5-N7	-3.68	1.31	1.39
1	2	2050	OMG	C5-N7	-3.68	1.31	1.39
1	2	1605	7MG	C2-N1	3.67	1.46	1.37
1	2	4483	B8T	C5-C4	3.63	1.48	1.40
1	2	3909	OMC	C6-N1	3.62	1.46	1.38
1	2	3897	B8K	C6-N1	3.62	1.45	1.38
1	2	4690	B8K	C6-N1	3.62	1.45	1.38
1	2	2522	7MG	C5-C6	3.61	1.52	1.43
1	2	4550	7MG	C2-N1	3.61	1.46	1.37
1	2	373	OMG	C5-N7	-3.60	1.32	1.39
1	2	4870	OMG	C5-N7	-3.60	1.32	1.39
1	2	3899	BGH	C71-N7	3.58	1.47	1.39
1	2	4623	OMG	C5-N7	-3.57	1.32	1.39
1	2	2754	B9B	O6-C6	3.57	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	2297	E7G	C2-N1	3.57	1.46	1.37
1	2	3897	B8K	C2-N2	3.56	1.42	1.34
1	2	2522	7MG	C2-N1	3.54	1.46	1.37
1	2	1909	P7G	C6-N1	3.53	1.44	1.38
1	2	4690	B8K	C71-N7	3.51	1.47	1.39
1	2	4690	B8K	C2-N2	3.50	1.42	1.34
1	2	3897	B8K	C71-N7	3.49	1.47	1.39
1	2	1574	B9B	O6-C6	3.47	1.40	1.35
1	2	4530	UR3	C6-N1	3.46	1.46	1.38
1	2	4483	B8T	C6-N1	3.44	1.46	1.38
1	2	3869	OMC	C6-N1	3.39	1.46	1.38
1	2	237	B9B	O6-C6	3.39	1.40	1.35
1	2	1348	P4U	C6-N1	3.39	1.46	1.38
1	2	4083	5MU	C2-N1	3.37	1.43	1.38
1	2	3899	BGH	C6-N1	3.34	1.45	1.38
1	2	1909	P7G	C5-C4	3.34	1.44	1.37
1	2	2522	7MG	C6-N1	3.33	1.45	1.38
1	2	3897	B8K	C2-N1	3.33	1.45	1.37
1	2	3887	OMC	C6-N1	3.33	1.46	1.38
1	2	1605	7MG	C6-N1	3.32	1.45	1.38
1	2	4550	7MG	C6-N1	3.32	1.45	1.38
1	2	4690	B8K	C2-N1	3.31	1.45	1.37
1	2	1659	I4U	C6-N1	3.28	1.45	1.38
1	2	2297	E7G	C6-N1	3.27	1.44	1.38
1	2	4623	OMG	C6-N1	3.27	1.44	1.38
1	2	3880	P7G	C5-C4	3.27	1.43	1.37
1	2	2422	OMC	C6-N1	3.27	1.45	1.38
1	2	4536	OMC	C6-N1	3.27	1.45	1.38
1	2	3899	BGH	C2-N1	3.27	1.45	1.37
1	2	2365	OMC	C6-N1	3.25	1.45	1.38
1	2	2861	OMC	C6-N1	3.24	1.45	1.38
1	2	4671	B8T	C6-N1	3.22	1.45	1.38
1	2	1316	OMG	C6-N1	3.22	1.44	1.38
1	2	4637	OMG	C6-N1	3.20	1.44	1.38
1	2	4597	UR3	C6-N1	3.20	1.45	1.38
1	2	1909	P7G	O6-C6	-3.19	1.18	1.23
1	2	2364	OMG	C6-N1	3.19	1.44	1.38
1	2	1883	OMG	C6-N1	3.19	1.44	1.38
1	2	2773	OMG	C6-N1	3.18	1.44	1.38
1	2	3701	OMC	C6-N1	3.15	1.45	1.38
1	2	373	OMG	C6-N1	3.14	1.44	1.38
1	2	1883	OMG	O6-C6	-3.12	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	4623	OMG	O6-C6	-3.12	1.17	1.23
1	2	4637	OMG	O6-C6	-3.12	1.17	1.23
1	2	1625	OMG	C6-N1	3.12	1.44	1.38
1	2	4870	OMG	O6-C6	-3.11	1.17	1.23
1	2	1316	OMG	O6-C6	-3.11	1.17	1.23
1	2	4494	OMG	C6-N1	3.10	1.44	1.38
1	2	1522	OMG	C6-N1	3.10	1.44	1.38
1	2	373	OMG	O6-C6	-3.10	1.17	1.23
1	2	2050	OMG	O6-C6	-3.09	1.17	1.23
1	2	2364	OMG	O6-C6	-3.09	1.17	1.23
1	2	4870	OMG	C6-N1	3.08	1.44	1.38
1	2	2050	OMG	C6-N1	3.08	1.44	1.38
1	2	2424	OMG	C6-N1	3.07	1.44	1.38
1	2	2804	OMC	C6-N1	3.07	1.45	1.38
1	2	4494	OMG	O6-C6	-3.07	1.17	1.23
1	2	3880	P7G	O6-C6	-3.06	1.18	1.23
1	2	2424	OMG	O6-C6	-3.05	1.17	1.23
1	2	1522	OMG	O6-C6	-3.04	1.17	1.23
1	2	4529	B8W	C5-N7	-3.03	1.33	1.39
1	2	1517	2MG	C5-N7	-3.02	1.33	1.39
1	2	2773	OMG	O6-C6	-3.01	1.17	1.23
1	2	729	2MG	C5-N7	-2.99	1.33	1.39
1	2	1574	B9B	C5-C4	-2.96	1.33	1.39
4	8	14	OMU	O4-C4	-2.96	1.18	1.24
1	2	4620	OMU	O4-C4	-2.96	1.18	1.24
1	2	2401	A2M	O3'-C3'	2.95	1.49	1.43
1	2	1625	OMG	O6-C6	-2.95	1.18	1.23
1	2	3867	A2M	O3'-C3'	2.95	1.49	1.43
1	2	3718	A2M	O3'-C3'	2.92	1.49	1.43
1	2	1524	A2M	O3'-C3'	2.92	1.49	1.43
1	2	4083	5MU	O4-C4	-2.92	1.18	1.23
1	2	1534	A2M	O3'-C3'	2.91	1.49	1.43
1	2	398	A2M	O3'-C3'	2.90	1.49	1.43
1	2	3897	B8K	C5-C4	2.90	1.47	1.38
1	2	2380	B8W	C5-C4	-2.87	1.33	1.39
1	2	3899	BGH	O3'-C3'	-2.87	1.36	1.43
1	2	1659	I4U	O4-C41	-2.86	1.40	1.47
1	2	4571	A2M	O3'-C3'	2.86	1.49	1.43
1	2	3825	A2M	O3'-C3'	2.86	1.49	1.43
1	2	2363	A2M	O3'-C3'	2.85	1.49	1.43
1	2	978	2MG	C5-N7	-2.84	1.33	1.39
1	2	4523	A2M	O3'-C3'	2.83	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1326	A2M	O3'-C3'	2.83	1.49	1.43
1	2	1871	A2M	O3'-C3'	2.82	1.49	1.43
1	2	3723	A2M	O3'-C3'	2.82	1.49	1.43
1	2	4690	B8K	C5-C4	2.82	1.47	1.38
1	2	4185	B8W	C5-N7	-2.82	1.33	1.39
1	2	4185	B8W	C5-C4	-2.79	1.33	1.39
1	2	4483	B8T	O2-C2	-2.79	1.18	1.23
1	2	4872	2MG	C5-N7	-2.79	1.33	1.39
1	2	4872	2MG	C5-C6	2.79	1.54	1.44
1	2	237	B9B	C5-C4	-2.78	1.33	1.39
1	2	237	B9B	C5-N7	-2.78	1.33	1.39
1	2	2754	B9B	C5-C4	-2.77	1.33	1.39
1	2	2380	B8W	C5-N7	-2.77	1.33	1.39
1	2	4671	B8T	O2-C2	-2.75	1.18	1.23
1	2	4620	OMU	C6-N1	2.75	1.44	1.38
1	2	978	2MG	C5-C6	2.74	1.54	1.44
1	2	3909	OMC	C5-C4	2.74	1.49	1.42
1	2	2804	OMC	O2-C2	-2.73	1.18	1.23
1	2	2422	OMC	O2-C2	-2.73	1.18	1.23
1	2	729	2MG	C5-C6	2.73	1.54	1.44
1	2	4529	B8W	C5-C4	-2.73	1.33	1.39
1	2	1659	I4U	O2-C2	-2.72	1.18	1.23
1	2	2365	OMC	O2-C2	-2.72	1.18	1.23
1	2	1517	2MG	C5-C6	2.71	1.54	1.44
1	2	1348	P4U	O2-C2	-2.71	1.18	1.23
1	2	2401	A2M	C5-C4	-2.71	1.33	1.39
4	8	14	OMU	C6-N1	2.69	1.44	1.38
1	2	2363	A2M	O2'-C2'	-2.69	1.35	1.42
1	2	3899	BGH	O6-C6	-2.69	1.18	1.23
1	2	1534	A2M	C5-C4	-2.69	1.34	1.39
1	2	3867	A2M	C5-C4	-2.68	1.34	1.39
1	2	1524	A2M	O2'-C2'	-2.68	1.35	1.42
1	2	4472	B8W	C5-C4	-2.68	1.34	1.39
1	2	3723	A2M	C5-C4	-2.67	1.34	1.39
1	2	3825	A2M	C5-C4	-2.67	1.34	1.39
1	2	1534	A2M	O2'-C2'	-2.66	1.35	1.42
1	2	2363	A2M	C5-C4	-2.66	1.34	1.39
1	2	398	A2M	C5-C4	-2.65	1.34	1.39
1	2	1574	B9B	C5-N7	-2.65	1.34	1.39
1	2	2773	OMG	C5-C6	2.64	1.54	1.44
1	2	1326	A2M	C5-C4	-2.64	1.34	1.39
1	2	4872	2MG	C6-N1	2.64	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1871	A2M	C5-C4	-2.63	1.34	1.39
1	2	2754	B9B	C5-N7	-2.62	1.34	1.39
1	2	1524	A2M	C5-C4	-2.62	1.34	1.39
1	2	3718	A2M	C5-C4	-2.62	1.34	1.39
1	2	4571	A2M	C5-C4	-2.62	1.34	1.39
1	2	2401	A2M	O2'-C2'	-2.62	1.35	1.42
1	2	2363	A2M	C8-N9	-2.62	1.32	1.37
1	2	4083	5MU	O2-C2	-2.62	1.18	1.23
1	2	4523	A2M	O2'-C2'	-2.61	1.35	1.42
1	2	398	A2M	O2'-C2'	-2.61	1.35	1.42
1	2	3869	OMC	O2-C2	-2.61	1.18	1.23
1	2	4523	A2M	C5-C4	-2.61	1.34	1.39
1	2	3701	OMC	O2-C2	-2.60	1.18	1.23
1	2	1316	OMG	C5-C6	2.60	1.54	1.44
1	2	2050	OMG	C5-C6	2.60	1.54	1.44
1	2	1625	OMG	C5-C6	2.60	1.54	1.44
1	2	3825	A2M	O2'-C2'	-2.60	1.36	1.42
1	2	3718	A2M	O2'-C2'	-2.59	1.36	1.42
1	2	4623	OMG	C5-C6	2.59	1.54	1.44
1	2	4472	B8W	C5-N7	-2.59	1.34	1.39
1	2	3701	OMC	C5-C4	2.59	1.48	1.42
1	2	4637	OMG	C5-C6	2.57	1.53	1.44
1	2	2522	7MG	O6-C6	-2.57	1.18	1.23
1	2	1659	I4U	O4-C4	2.57	1.40	1.35
1	2	4870	OMG	C5-C6	2.56	1.53	1.44
1	2	2861	OMC	O2-C2	-2.56	1.19	1.23
1	2	1522	OMG	C5-C6	2.55	1.53	1.44
1	2	4536	OMC	O2-C2	-2.55	1.19	1.23
1	2	4494	OMG	C5-C6	2.54	1.53	1.44
1	2	3887	OMC	O2-C2	-2.54	1.19	1.23
1	2	1517	2MG	C6-N1	2.54	1.43	1.38
1	2	2424	OMG	C5-C6	2.54	1.53	1.44
1	2	2364	OMG	C5-C6	2.54	1.53	1.44
1	2	373	OMG	C5-C6	2.53	1.53	1.44
1	2	978	2MG	C6-N1	2.53	1.43	1.38
1	2	4637	OMG	C2-N1	2.52	1.43	1.37
1	2	373	OMG	C2-N1	2.52	1.43	1.37
1	2	1605	7MG	O6-C6	-2.51	1.18	1.23
1	2	2773	OMG	C2-N1	2.51	1.43	1.37
1	2	4623	OMG	C2-N1	2.51	1.43	1.37
1	2	3723	A2M	O2'-C2'	-2.50	1.36	1.42
1	2	4550	7MG	O6-C6	-2.50	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	4529	B8W	C8-N9	-2.50	1.33	1.37
1	2	1871	A2M	O2'-C2'	-2.50	1.36	1.42
1	2	3867	A2M	O2'-C2'	-2.50	1.36	1.42
1	2	2050	OMG	C2-N1	2.49	1.43	1.37
1	2	1522	OMG	C2-N1	2.49	1.43	1.37
1	2	4494	OMG	C2-N1	2.49	1.43	1.37
1	2	2424	OMG	C2-N1	2.49	1.43	1.37
1	2	1625	OMG	C2-N1	2.49	1.43	1.37
1	2	2364	OMG	C2-N1	2.48	1.43	1.37
1	2	4870	OMG	C2-N1	2.47	1.43	1.37
1	2	1316	OMG	C2-N1	2.47	1.43	1.37
1	2	4571	A2M	O2'-C2'	-2.47	1.36	1.42
1	2	1883	OMG	C2-N1	2.46	1.43	1.37
1	2	4571	A2M	C8-N9	-2.46	1.33	1.37
1	2	2297	E7G	O6-C6	-2.45	1.18	1.23
4	8	14	OMU	O2-C2	-2.45	1.18	1.23
1	2	2401	A2M	C8-N9	-2.43	1.33	1.37
1	2	1883	OMG	C5-C6	2.43	1.53	1.44
1	2	2861	OMC	C5-C4	2.43	1.48	1.42
1	2	3718	A2M	C8-N9	-2.43	1.33	1.37
1	2	2422	OMC	C5-C4	2.42	1.48	1.42
1	2	1456	B8Q	C6-N1	2.41	1.43	1.38
1	2	3887	OMC	C5-C4	2.41	1.48	1.42
1	2	2804	OMC	C5-C4	2.41	1.48	1.42
1	2	4523	A2M	C8-N9	-2.41	1.33	1.37
1	2	1534	A2M	C8-N9	-2.40	1.33	1.37
1	2	4620	OMU	O2-C2	-2.39	1.18	1.23
1	2	2365	OMC	C5-C4	2.39	1.48	1.42
1	2	3723	A2M	C8-N9	-2.39	1.33	1.37
1	2	3825	A2M	C8-N9	-2.38	1.33	1.37
1	2	4872	2MG	C4-N9	-2.37	1.31	1.38
1	2	4571	A2M	C5-N7	-2.37	1.34	1.39
1	2	1326	A2M	O2'-C2'	-2.36	1.36	1.42
1	2	1326	A2M	C8-N9	-2.36	1.33	1.37
1	2	4620	OMU	C5-C4	2.36	1.48	1.43
4	8	14	OMU	C5-C4	2.35	1.48	1.43
1	2	729	2MG	C6-N1	2.34	1.43	1.38
1	2	4530	UR3	C4-N3	2.34	1.46	1.40
1	2	1524	A2M	C8-N9	-2.33	1.33	1.37
1	2	4597	UR3	C5-C4	2.33	1.49	1.43
1	2	3718	A2M	C5-N7	-2.33	1.34	1.39
1	2	398	A2M	C8-N9	-2.32	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1524	A2M	C5-N7	-2.30	1.34	1.39
1	2	3869	OMC	C5-C4	2.30	1.48	1.42
1	2	3867	A2M	C8-N9	-2.29	1.33	1.37
1	2	4536	OMC	C5-C4	2.29	1.48	1.42
1	2	2363	A2M	C5-N7	-2.28	1.34	1.39
1	2	3909	OMC	O2-C2	-2.28	1.19	1.23
1	2	1326	A2M	C5-N7	-2.28	1.34	1.39
1	2	398	A2M	C5-N7	-2.25	1.34	1.39
1	2	4530	UR3	C5-C4	2.24	1.49	1.43
1	2	3867	A2M	C5-N7	-2.21	1.34	1.39
1	2	2401	A2M	C5-N7	-2.20	1.34	1.39
1	2	4597	UR3	C4-N3	2.19	1.45	1.40
1	2	3899	BGH	C5-C4	2.18	1.45	1.38
1	2	237	B9B	C5-C6	-2.18	1.37	1.41
1	2	1871	A2M	C5-N7	-2.17	1.34	1.39
1	2	237	B9B	C8-N9	-2.17	1.33	1.37
1	2	3825	A2M	C5-N7	-2.17	1.34	1.39
1	2	2380	B8W	C8-N9	-2.14	1.33	1.37
1	2	1871	A2M	C8-N9	-2.13	1.33	1.37
1	2	4185	B8W	C4-N3	2.12	1.37	1.34
1	2	3723	A2M	C5-N7	-2.12	1.35	1.39
1	2	1534	A2M	C5-N7	-2.12	1.35	1.39
1	2	4523	A2M	C5-N7	-2.11	1.35	1.39
1	2	4185	B8W	C8-N9	-2.11	1.33	1.37
1	2	4690	B8K	O6-C6	-2.08	1.19	1.23
1	2	4472	B8W	C8-N9	-2.08	1.33	1.37
1	2	978	2MG	C4-N9	-2.07	1.32	1.38
1	2	1574	B9B	C8-N9	-2.07	1.33	1.37
1	2	2754	B9B	C8-N9	-2.03	1.33	1.37
1	2	1456	B8Q	O2-C2	-2.02	1.18	1.22
1	2	1871	A2M	O5'-C5'	-2.01	1.39	1.44
1	2	729	2MG	O6-C6	-2.01	1.19	1.23
1	2	1517	2MG	O6-C6	-2.01	1.19	1.23

All (543) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	2754	B9B	O6-C6-C5	21.33	143.58	116.57
1	2	1574	B9B	O6-C6-C5	21.25	143.47	116.57
1	2	237	B9B	O6-C6-C5	20.95	143.10	116.57
1	2	2754	B9B	O6-C6-N1	-18.29	94.52	120.00
1	2	1574	B9B	O6-C6-N1	-18.08	94.82	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	237	B9B	O6-C6-N1	-18.04	94.87	120.00
1	2	4564	M7A	C5-C6-N6	13.86	147.40	123.74
1	2	4564	M7A	N6-C6-N1	-11.73	92.66	118.35
1	2	4083	5MU	C5-C4-N3	10.26	124.07	115.31
1	2	4870	OMG	C1'-N9-C8	-10.01	98.21	126.70
1	2	4870	OMG	C1'-N9-C4	9.74	155.45	126.50
1	2	2424	OMG	C1'-N9-C4	9.29	154.10	126.50
1	2	2424	OMG	C1'-N9-C8	-9.04	100.95	126.70
1	2	1522	OMG	C1'-N9-C4	8.82	152.71	126.50
1	2	4494	OMG	C1'-N9-C4	8.78	152.57	126.50
1	2	2773	OMG	C1'-N9-C4	8.70	152.35	126.50
1	2	1522	OMG	C1'-N9-C8	-8.64	102.09	126.70
1	2	1625	OMG	C1'-N9-C4	8.63	152.12	126.50
1	2	2050	OMG	C1'-N9-C4	8.47	151.66	126.50
1	2	2364	OMG	C1'-N9-C4	8.45	151.60	126.50
1	2	2773	OMG	C1'-N9-C8	-8.43	102.70	126.70
1	2	4494	OMG	C1'-N9-C8	-8.33	102.98	126.70
1	2	4637	OMG	C1'-N9-C4	8.31	151.18	126.50
1	2	1316	OMG	C1'-N9-C4	8.29	151.13	126.50
1	2	1883	OMG	C1'-N9-C4	8.27	151.07	126.50
1	2	4623	OMG	C1'-N9-C4	8.23	150.96	126.50
1	2	4623	OMG	C1'-N9-C8	-8.23	103.28	126.70
1	2	2050	OMG	C1'-N9-C8	-8.22	103.29	126.70
1	2	1625	OMG	C1'-N9-C8	-8.13	103.56	126.70
1	2	1883	OMG	C1'-N9-C8	-8.12	103.59	126.70
1	2	1316	OMG	C1'-N9-C8	-8.08	103.69	126.70
1	2	4637	OMG	C1'-N9-C8	-8.08	103.69	126.70
1	2	2364	OMG	C1'-N9-C8	-8.06	103.75	126.70
1	2	4083	5MU	C5-C6-N1	-7.94	115.17	123.34
1	2	373	OMG	C1'-N9-C4	7.87	149.87	126.50
1	2	373	OMG	C1'-N9-C8	-7.87	104.30	126.70
1	2	4597	UR3	C4-N3-C2	-7.43	117.57	124.56
1	2	1517	2MG	C2-N3-C4	7.31	121.10	112.04
1	2	729	2MG	C2-N3-C4	7.12	120.87	112.04
1	2	237	B9B	C5-C4-N3	-7.11	119.19	127.19
1	2	4185	B8W	C5-C4-N3	-7.01	119.30	127.19
1	2	1534	A2M	N6-C6-N1	-6.99	103.05	118.35
1	2	4083	5MU	C4-N3-C2	-6.99	118.31	127.35
1	2	4529	B8W	C5-C4-N3	-6.87	119.46	127.19
1	2	2363	A2M	N6-C6-N1	-6.87	103.30	118.35
1	2	1871	A2M	N6-C6-N1	-6.87	103.31	118.35
1	2	2754	B9B	C5-C4-N3	-6.84	119.50	127.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	3825	A2M	N6-C6-N1	-6.84	103.37	118.35
1	2	4523	A2M	N6-C6-N1	-6.83	103.40	118.35
1	2	4472	B8W	C5-C4-N3	-6.80	119.54	127.19
1	2	3723	A2M	N6-C6-N1	-6.79	103.47	118.35
1	2	398	A2M	N6-C6-N1	-6.79	103.49	118.35
1	2	2401	A2M	N6-C6-N1	-6.78	103.51	118.35
1	2	3867	A2M	N6-C6-N1	-6.74	103.60	118.35
1	2	1326	A2M	N6-C6-N1	-6.72	103.64	118.35
1	2	4571	A2M	N6-C6-N1	-6.71	103.66	118.35
1	2	3718	A2M	N6-C6-N1	-6.69	103.69	118.35
1	2	1524	A2M	N6-C6-N1	-6.68	103.72	118.35
1	2	978	2MG	C2-N3-C4	6.64	120.28	112.04
1	2	4690	B8K	C72-C71-N7	6.55	128.72	118.86
1	2	2380	B8W	C5-C4-N3	-6.51	119.86	127.19
1	2	4872	2MG	C2-N3-C4	6.43	120.02	112.04
1	2	4185	B8W	N2-C2-N3	6.41	127.22	117.25
1	2	1574	B9B	C5-C4-N3	-6.35	120.05	127.19
1	2	2380	B8W	N2-C2-N3	6.35	127.12	117.25
1	2	3723	A2M	N3-C2-N1	-6.32	118.72	128.60
1	2	2401	A2M	N3-C2-N1	-6.29	118.77	128.60
1	2	1534	A2M	N3-C2-N1	-6.28	118.78	128.60
1	2	1871	A2M	N3-C2-N1	-6.28	118.78	128.60
1	2	3825	A2M	N3-C2-N1	-6.27	118.79	128.60
1	2	398	A2M	N3-C2-N1	-6.26	118.82	128.60
1	2	4523	A2M	N3-C2-N1	-6.24	118.83	128.60
1	2	1326	A2M	N3-C2-N1	-6.22	118.87	128.60
1	2	729	2MG	C5-C4-N3	-6.20	118.41	128.46
1	2	3867	A2M	N3-C2-N1	-6.18	118.93	128.60
1	2	2401	A2M	N9-C8-N7	-6.16	105.49	113.91
1	2	1524	A2M	N3-C2-N1	-6.16	118.97	128.60
1	2	4571	A2M	N3-C2-N1	-6.15	118.98	128.60
1	2	2363	A2M	N3-C2-N1	-6.13	119.01	128.60
1	2	4564	M7A	N3-C2-N1	-6.13	119.01	128.60
1	2	3718	A2M	N3-C2-N1	-6.12	119.03	128.60
1	2	4529	B8W	N2-C2-N3	6.12	126.77	117.25
1	2	1517	2MG	C5-C4-N3	-6.10	118.57	128.46
1	2	3899	BGH	C72-C71-N7	6.07	127.99	118.86
1	2	3825	A2M	N9-C8-N7	-6.06	105.62	113.91
1	2	3723	A2M	N9-C8-N7	-6.05	105.63	113.91
1	2	3897	B8K	C72-C71-N7	6.02	127.92	118.86
1	2	4690	B8K	C5-C6-N1	6.02	121.59	110.99
1	2	1534	A2M	N9-C8-N7	-5.99	105.72	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	4523	A2M	N9-C8-N7	-5.97	105.75	113.91
1	2	1534	A2M	C5-C6-N6	5.93	136.34	123.43
1	2	1871	A2M	C5-C6-N6	5.92	136.31	123.43
1	2	4523	A2M	C5-C6-N6	5.89	136.24	123.43
1	2	3867	A2M	N9-C8-N7	-5.87	105.89	113.91
1	2	398	A2M	N9-C8-N7	-5.86	105.90	113.91
1	2	3825	A2M	C5-C6-N6	5.85	136.16	123.43
1	2	398	A2M	C5-C6-N6	5.84	136.15	123.43
1	2	1524	A2M	N9-C8-N7	-5.84	105.92	113.91
1	2	2363	A2M	C5-C6-N6	5.84	136.13	123.43
1	2	1871	A2M	N9-C8-N7	-5.83	105.94	113.91
1	2	3723	A2M	C5-C6-N6	5.83	136.11	123.43
1	2	4472	B8W	N2-C2-N3	5.79	126.26	117.25
1	2	2401	A2M	C5-C6-N6	5.79	136.02	123.43
1	2	1524	A2M	C5-C6-N6	5.78	136.01	123.43
1	2	3718	A2M	C5-C6-N6	5.78	136.01	123.43
1	2	3867	A2M	C5-C6-N6	5.78	136.00	123.43
1	2	1326	A2M	N9-C8-N7	-5.77	106.02	113.91
1	2	4571	A2M	C5-C6-N6	5.74	135.92	123.43
1	2	1326	A2M	C5-C6-N6	5.73	135.91	123.43
1	2	3718	A2M	N9-C8-N7	-5.73	106.07	113.91
1	2	3899	BGH	C5-C6-N1	5.72	121.06	110.99
1	2	2363	A2M	N9-C8-N7	-5.71	106.10	113.91
1	2	3897	B8K	C5-C6-N1	5.67	120.98	110.99
1	2	1456	B8Q	N3-C2-N1	5.63	123.75	117.13
1	2	4529	B8W	O6-C6-N1	5.60	126.74	119.01
1	2	2786	B9H	C31-N3-C2	5.57	124.17	117.21
1	2	4571	A2M	N9-C8-N7	-5.57	106.30	113.91
1	2	3909	OMC	O2-C2-N3	-5.53	113.34	122.33
1	2	1625	OMG	C5-C4-N3	-5.52	119.50	128.46
1	2	2424	OMG	C5-C4-N3	-5.52	119.51	128.46
1	2	4494	OMG	C5-C4-N3	-5.51	119.52	128.46
1	2	2401	A2M	C4-N9-C8	5.48	111.67	105.73
1	2	978	2MG	C5-C4-N3	-5.41	119.68	128.46
1	2	1909	P7G	C4-C5-N7	5.40	109.52	106.67
4	8	14	OMU	C4-N3-C2	-5.38	119.48	126.58
1	2	3723	A2M	C4-N9-C8	5.36	111.54	105.73
1	2	4523	A2M	C4-N9-C8	5.28	111.45	105.73
1	2	1534	A2M	C4-N9-C8	5.23	111.40	105.73
1	2	4620	OMU	C4-N3-C2	-5.23	119.68	126.58
1	2	1883	OMG	C5-C4-N3	-5.22	120.00	128.46
1	2	3825	A2M	C4-N9-C8	5.21	111.38	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	2773	OMG	C5-C4-N3	-5.19	120.04	128.46
1	2	4872	2MG	C5-C4-N3	-5.19	120.04	128.46
1	2	1524	A2M	C4-N9-C8	5.16	111.32	105.73
1	2	2364	OMG	C5-C4-N3	-5.14	120.12	128.46
1	2	3899	BGH	C2-N3-C4	5.12	121.43	112.30
1	2	3867	A2M	C4-N9-C8	5.12	111.28	105.73
1	2	2754	B9B	N2-C2-N3	5.11	125.20	117.25
1	2	1316	OMG	C5-C4-N3	-5.10	120.19	128.46
1	2	1522	OMG	C5-C4-N3	-5.10	120.19	128.46
1	2	1456	B8Q	C31-N3-C4	5.09	121.91	114.25
1	2	398	A2M	C4-N9-C8	5.08	111.23	105.73
1	2	2297	E7G	C5-C6-N1	5.06	119.90	110.99
1	2	4870	OMG	C5-C4-N3	-5.04	120.28	128.46
1	2	237	B9B	N2-C2-N3	5.02	125.06	117.25
1	2	1605	7MG	C5-C6-N1	4.98	119.77	110.99
1	2	4564	M7A	N3-C4-N9	4.98	133.16	126.87
1	2	2363	A2M	C4-N9-C8	4.97	111.11	105.73
1	2	2050	OMG	C5-C4-N3	-4.97	120.40	128.46
1	2	4637	OMG	C5-C4-N3	-4.95	120.44	128.46
1	2	4690	B8K	C4-C5-N7	4.94	109.30	104.91
1	2	1326	A2M	C4-N9-C8	4.93	111.07	105.73
1	2	2297	E7G	C4-C5-N7	4.93	109.29	104.91
1	2	4872	2MG	C2-N1-C6	-4.92	118.81	124.48
1	2	237	B9B	N3-C4-N9	4.92	133.81	126.99
1	2	3897	B8K	C2-N3-C4	4.92	121.06	112.30
1	2	3718	A2M	C4-N9-C8	4.90	111.03	105.73
1	2	1871	A2M	C4-N9-C8	4.88	111.01	105.73
1	2	2522	7MG	C5-C6-N1	4.87	119.58	110.99
1	2	4550	7MG	C5-C6-N1	4.87	119.57	110.99
1	2	3880	P7G	C4-C5-N7	4.85	109.23	106.67
1	2	1517	2MG	C2-N1-C6	-4.83	118.92	124.48
1	2	373	OMG	C5-C4-N3	-4.80	120.67	128.46
1	2	4571	A2M	C4-N9-C8	4.80	110.93	105.73
1	2	2786	B9H	C6-N1-C2	-4.79	117.50	121.79
1	2	4083	5MU	N3-C2-N1	4.77	121.22	114.89
1	2	4623	OMG	C5-C4-N3	-4.76	120.73	128.46
1	2	4690	B8K	C2-N3-C4	4.76	120.78	112.30
1	2	2363	A2M	C5-C4-N3	-4.70	120.62	126.75
1	2	4571	A2M	C5-C4-N3	-4.67	120.65	126.75
1	2	729	2MG	C2-N1-C6	-4.63	119.16	124.48
1	2	4083	5MU	C5M-C5-C6	-4.62	116.68	122.85
1	2	1326	A2M	C5-C4-N3	-4.62	120.73	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1456	B8Q	O2-C2-N3	-4.59	116.20	122.95
1	2	1625	OMG	C2-N3-C4	4.59	120.48	112.30
1	2	4530	UR3	C4-N3-C2	-4.59	120.24	124.56
1	2	4690	B8K	N9-C8-N7	4.58	109.47	103.33
1	2	4494	OMG	C2-N3-C4	4.57	120.44	112.30
1	2	3718	A2M	C5-C4-N3	-4.57	120.79	126.75
1	2	2424	OMG	C2-N3-C4	4.56	120.43	112.30
1	2	3867	A2M	C5-C4-N3	-4.55	120.82	126.75
1	2	3825	A2M	C5-C4-N3	-4.54	120.82	126.75
1	2	2773	OMG	C2-N3-C4	4.52	120.36	112.30
1	2	4529	B8W	N3-C4-N9	4.52	133.26	126.99
1	2	1883	OMG	C2-N3-C4	4.51	120.34	112.30
1	2	4185	B8W	N3-C4-N9	4.50	133.23	126.99
1	2	1316	OMG	C2-N3-C4	4.49	120.30	112.30
1	2	2364	OMG	C2-N3-C4	4.48	120.28	112.30
1	2	1534	A2M	C5-C4-N3	-4.47	120.92	126.75
1	2	2297	E7G	C2-N3-C4	4.47	120.26	112.30
1	2	1522	OMG	C2-N3-C4	4.47	120.25	112.30
1	2	373	OMG	C2-N3-C4	4.46	120.25	112.30
1	2	1605	7MG	C2-N3-C4	4.46	120.25	112.30
1	2	3723	A2M	C5-C4-N3	-4.46	120.94	126.75
1	2	4623	OMG	C2-N3-C4	4.46	120.24	112.30
1	2	1574	B9B	N2-C2-N3	4.45	124.18	117.25
1	2	4637	OMG	C2-N3-C4	4.43	120.20	112.30
1	2	2754	B9B	N3-C4-N9	4.43	133.13	126.99
1	2	4550	7MG	C2-N3-C4	4.41	120.16	112.30
1	2	2401	A2M	C5-C4-N3	-4.38	121.03	126.75
1	2	4870	OMG	C2-N3-C4	4.37	120.09	112.30
1	2	398	A2M	C5-C4-N3	-4.35	121.07	126.75
1	2	1871	A2M	C5-C4-N3	-4.34	121.09	126.75
1	2	3897	B8K	C5-C4-N9	4.33	111.97	106.35
1	2	4523	A2M	C5-C4-N3	-4.33	121.11	126.75
1	2	2363	A2M	C1'-N9-C8	-4.33	117.37	127.14
1	2	978	2MG	C2-N1-C6	-4.32	119.51	124.48
1	2	2522	7MG	C2-N3-C4	4.31	119.98	112.30
1	2	2050	OMG	C2-N3-C4	4.31	119.98	112.30
1	2	3867	A2M	C1'-N9-C8	-4.28	117.47	127.14
1	2	2380	B8W	N9-C8-N7	-4.28	108.06	113.91
1	2	729	2MG	N9-C4-N3	4.25	134.48	125.94
1	2	4472	B8W	N9-C8-N7	-4.25	108.10	113.91
1	2	4185	B8W	O6-C6-N1	4.24	124.86	119.01
1	2	1524	A2M	C5-C4-N3	-4.24	121.22	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1574	B9B	N9-C8-N7	-4.23	108.13	113.91
1	2	4571	A2M	C1'-N9-C8	-4.23	117.59	127.14
1	2	3909	OMC	O2-C2-N1	4.14	127.43	118.89
1	2	3899	BGH	C4-C5-N7	4.13	108.58	104.91
1	2	4185	B8W	N9-C8-N7	-4.12	108.28	113.91
1	2	3899	BGH	N9-C8-N7	4.11	108.85	103.33
1	2	4083	5MU	O4-C4-C5	-4.06	120.19	124.90
1	2	1517	2MG	N9-C4-N3	4.05	134.07	125.94
1	2	2754	B9B	N9-C8-N7	-4.05	108.38	113.91
1	2	3899	BGH	C5-C4-N9	4.04	111.60	106.35
1	2	237	B9B	N9-C8-N7	-4.03	108.40	113.91
1	2	3723	A2M	C1'-N9-C8	-4.01	118.07	127.14
1	2	3867	A2M	N3-C4-N9	4.00	133.68	127.08
1	2	2363	A2M	N3-C4-N9	4.00	133.67	127.08
1	2	4571	A2M	N3-C4-N9	3.98	133.65	127.08
1	2	1326	A2M	C1'-N9-C8	-3.97	118.17	127.14
1	2	3718	A2M	C1'-N9-C8	-3.96	118.20	127.14
1	2	1326	A2M	N3-C4-N9	3.95	133.60	127.08
1	2	1524	A2M	C1'-N9-C8	-3.93	118.26	127.14
1	2	3723	A2M	N3-C4-N9	3.91	133.52	127.08
1	2	2401	A2M	C1'-N9-C8	-3.91	118.32	127.14
1	2	3825	A2M	C1'-N9-C8	-3.90	118.32	127.14
1	2	4523	A2M	C1'-N9-C8	-3.90	118.33	127.14
1	2	4690	B8K	C5-C4-N9	3.85	111.34	106.35
1	2	3825	A2M	N3-C4-N9	3.84	133.41	127.08
1	2	2401	A2M	N3-C4-N9	3.84	133.41	127.08
1	2	3718	A2M	N3-C4-N9	3.84	133.40	127.08
1	2	1659	I4U	C5-C4-N3	-3.81	119.11	124.91
1	2	1534	A2M	N3-C4-N9	3.81	133.36	127.08
1	2	3897	B8K	C4-C5-N7	3.79	108.28	104.91
1	2	4472	B8W	N3-C4-N9	3.78	132.24	126.99
1	2	1534	A2M	C1'-N9-C8	-3.78	118.60	127.14
1	2	3897	B8K	N9-C8-N7	3.78	108.40	103.33
1	2	4620	OMU	N3-C2-N1	3.77	119.90	114.89
1	2	4872	2MG	CM2-N2-C2	-3.77	115.54	123.86
1	2	398	A2M	N3-C4-N9	3.76	133.28	127.08
1	2	2380	B8W	C61-O6-C6	-3.75	113.50	117.21
1	2	4523	A2M	N3-C4-N9	3.75	133.25	127.08
1	2	2380	B8W	N3-C4-N9	3.74	132.18	126.99
1	2	1574	B9B	N3-C4-N9	3.74	132.18	126.99
1	2	1605	7MG	C5-C4-N3	-3.73	121.03	128.13
1	2	2297	E7G	C5-C4-N3	-3.73	121.03	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1524	A2M	N3-C4-N9	3.71	133.19	127.08
1	2	4550	7MG	C5-C4-N3	-3.70	121.08	128.13
1	2	3825	A2M	C5-N7-C8	3.70	108.77	103.51
1	2	3899	BGH	C5-C4-N3	-3.70	121.08	128.13
1	2	1456	B8Q	C6-N1-C2	-3.69	118.48	121.79
1	2	398	A2M	C1'-N9-C8	-3.69	118.80	127.14
1	2	1534	A2M	C2-N3-C4	3.68	120.45	111.75
1	2	1605	7MG	C5-C4-N9	3.68	111.12	106.35
1	2	3825	A2M	C2-N3-C4	3.67	120.42	111.75
1	2	4571	A2M	C2-N3-C4	3.67	120.42	111.75
1	2	3723	A2M	C2-N3-C4	3.67	120.41	111.75
1	2	2380	B8W	O6-C6-N1	3.66	124.06	119.01
1	2	2363	A2M	C2-N3-C4	3.66	120.39	111.75
1	2	1326	A2M	C2-N3-C4	3.66	120.39	111.75
1	2	4083	5MU	C5M-C5-C4	3.64	122.77	118.77
1	2	2401	A2M	C2-N3-C4	3.63	120.33	111.75
1	2	2401	A2M	C5-N7-C8	3.62	108.65	103.51
1	2	1871	A2M	C2-N3-C4	3.61	120.28	111.75
1	2	3723	A2M	C5-N7-C8	3.61	108.63	103.51
1	2	3867	A2M	C2-N3-C4	3.60	120.26	111.75
1	2	3718	A2M	C2-N3-C4	3.59	120.24	111.75
1	2	1871	A2M	N3-C4-N9	3.59	133.00	127.08
1	2	4523	A2M	C2-N3-C4	3.57	120.19	111.75
1	2	398	A2M	C2-N3-C4	3.57	120.19	111.75
1	2	1534	A2M	C5-N7-C8	3.56	108.57	103.51
1	2	4523	A2M	C5-N7-C8	3.55	108.55	103.51
4	8	14	OMU	N3-C2-N1	3.53	119.57	114.89
1	2	1326	A2M	C5-N7-C8	3.53	108.52	103.51
1	2	4550	7MG	C5-C4-N9	3.52	110.92	106.35
1	2	4564	M7A	C2-N3-C4	3.52	120.07	111.75
1	2	2363	A2M	C5-N7-C8	3.51	108.50	103.51
1	2	398	A2M	C5-N7-C8	3.51	108.50	103.51
1	2	1871	A2M	C5-N7-C8	3.51	108.50	103.51
1	2	2297	E7G	C5-C4-N9	3.50	110.89	106.35
1	2	1524	A2M	C2-N3-C4	3.50	120.02	111.75
1	2	1348	P4U	C5-C4-N3	-3.50	119.59	124.91
1	2	237	B9B	N3-C2-N1	-3.49	119.94	125.42
4	8	14	OMU	C5-C4-N3	3.48	120.05	114.84
1	2	3867	A2M	C5-N7-C8	3.48	108.45	103.51
1	2	4472	B8W	N1-C2-N3	-3.47	119.97	125.42
1	2	2754	B9B	N3-C2-N1	-3.46	119.99	125.42
1	2	3718	A2M	C5-N7-C8	3.46	108.42	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	2522	7MG	C5-C4-N3	-3.45	121.56	128.13
1	2	2522	7MG	C5-C4-N9	3.44	110.81	106.35
1	2	4185	B8W	N1-C2-N3	-3.41	120.08	125.42
1	2	2380	B8W	N1-C2-N3	-3.38	120.11	125.42
1	2	4620	OMU	C5-C4-N3	3.38	119.89	114.84
1	2	4529	B8W	N9-C8-N7	-3.38	109.30	113.91
1	2	978	2MG	N9-C4-N3	3.37	132.71	125.94
1	2	4472	B8W	C5-N7-C8	3.36	108.29	103.51
1	2	1524	A2M	C5-N7-C8	3.36	108.28	103.51
1	2	4571	A2M	C5-N7-C8	3.35	108.27	103.51
1	2	1574	B9B	N3-C2-N1	-3.34	120.17	125.42
1	2	1871	A2M	C1'-N9-C8	-3.29	119.71	127.14
1	2	4690	B8K	C6-C5-C4	-3.25	115.93	122.62
1	2	4529	B8W	N1-C2-N3	-3.24	120.34	125.42
1	2	2050	OMG	C2-N1-C6	-3.20	119.27	125.10
1	2	2364	OMG	C2-N1-C6	-3.19	119.28	125.10
1	2	3897	B8K	C5-C4-N3	-3.19	122.05	128.13
1	2	1909	P7G	N9-C8-N7	3.17	107.92	103.38
1	2	3897	B8K	C6-C5-C4	-3.17	116.08	122.62
1	2	4637	OMG	C2-N1-C6	-3.16	119.33	125.10
1	2	1883	OMG	C2-N1-C6	-3.15	119.35	125.10
1	2	2424	OMG	C2-N1-C6	-3.14	119.37	125.10
1	2	4494	OMG	C2-N1-C6	-3.13	119.39	125.10
1	2	4529	B8W	O6-C6-C5	-3.13	113.05	116.97
1	2	2861	OMC	O2-C2-N3	-3.12	117.25	122.33
1	2	4536	OMC	O2-C2-N3	-3.11	117.27	122.33
1	2	1316	OMG	C2-N1-C6	-3.11	119.43	125.10
1	2	4690	B8K	C5-C4-N3	-3.10	122.22	128.13
1	2	1625	OMG	C2-N1-C6	-3.10	119.44	125.10
1	2	4623	OMG	C2-N1-C6	-3.09	119.47	125.10
1	2	4472	B8W	O6-C6-N1	3.08	123.27	119.01
1	2	2380	B8W	C5-N7-C8	3.07	107.87	103.51
1	2	373	OMG	C2-N1-C6	-3.06	119.51	125.10
1	2	2522	7MG	N9-C8-N7	3.04	107.72	103.38
1	2	1522	OMG	C2-N1-C6	-3.02	119.59	125.10
1	2	4083	5MU	C6-C5-C4	3.01	120.55	118.03
4	8	14	OMU	O4-C4-C5	-3.01	119.87	125.16
1	2	2380	B8W	C4-N9-C1'	-3.01	119.43	126.59
1	2	2773	OMG	C2-N1-C6	-3.00	119.62	125.10
1	2	4185	B8W	C5-N7-C8	3.00	107.77	103.51
1	2	4870	OMG	C2-N1-C6	-2.98	119.67	125.10
1	2	4872	2MG	N9-C8-N7	-2.94	107.85	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1574	B9B	C5-N7-C8	2.93	107.67	103.51
1	2	4185	B8W	N2-C2-N1	-2.92	112.71	117.25
1	2	4597	UR3	C6-N1-C2	-2.92	119.17	121.79
1	2	4483	B8T	O2-C2-N3	-2.91	117.60	122.33
1	2	978	2MG	N9-C8-N7	-2.89	107.94	113.39
1	2	3899	BGH	C6-C5-C4	-2.89	116.66	122.62
1	2	2380	B8W	N2-C2-N1	-2.89	112.76	117.25
1	2	2522	7MG	C4-C5-N7	2.89	109.54	105.53
1	2	3887	OMC	O2-C2-N3	-2.87	117.66	122.33
1	2	4185	B8W	C61-O6-C6	-2.87	114.37	117.21
1	2	4872	2MG	N9-C4-N3	2.86	131.68	125.94
1	2	1883	OMG	O6-C6-C5	-2.85	119.04	126.60
1	2	4620	OMU	O4-C4-C5	-2.84	120.17	125.16
1	2	1517	2MG	C5-C6-N1	2.83	120.36	113.19
1	2	4483	B8T	O3'-C3'-C2'	2.82	120.94	111.82
1	2	1524	A2M	C4'-O4'-C1'	-2.82	103.26	109.47
1	2	1605	7MG	N9-C8-N7	2.81	107.40	103.38
1	2	2401	A2M	C2'-C1'-N9	-2.81	108.80	113.53
1	2	1574	B9B	C61-O6-C6	-2.81	112.12	117.47
1	2	237	B9B	C5-N7-C8	2.81	107.50	103.51
1	2	4529	B8W	N2-C2-N1	-2.80	112.89	117.25
1	2	1883	OMG	C5-C6-N1	2.80	120.31	113.19
1	2	2754	B9B	C5-N7-C8	2.80	107.49	103.51
1	2	3909	OMC	C5-C4-N4	2.80	124.98	120.57
1	2	373	OMG	C5-C6-N1	2.80	120.29	113.19
1	2	3899	BGH	O6-C6-N1	-2.77	114.81	120.12
1	2	729	2MG	C5-C6-N1	2.75	120.19	113.19
1	2	4671	B8T	C6-C5-C4	2.75	120.32	116.96
1	2	2422	OMC	O2-C2-N3	-2.74	117.87	122.33
1	2	2424	OMG	C5-C6-N1	2.74	120.14	113.19
1	2	978	2MG	C5-C6-N1	2.73	120.12	113.19
1	2	4597	UR3	C3U-N3-C2	2.72	122.09	117.31
1	2	4870	OMG	C5-C6-N1	2.71	120.08	113.19
1	2	2364	OMG	C5-C6-N1	2.71	120.06	113.19
1	2	1909	P7G	C71-N7-C5	2.71	130.93	124.52
1	2	4623	OMG	C5-C6-N1	2.70	120.05	113.19
1	2	4872	2MG	C5-C6-N1	2.70	120.04	113.19
1	2	1316	OMG	C5-C6-N1	2.69	120.01	113.19
1	2	2364	OMG	C5-C4-N9	2.69	110.50	105.63
1	2	4472	B8W	C4-N9-C1'	-2.68	120.20	126.59
1	2	4623	OMG	C5-C4-N9	2.68	110.49	105.63
1	2	3897	B8K	O6-C6-N1	-2.68	114.98	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	2297	E7G	N9-C8-N7	2.68	107.20	103.38
1	2	4637	OMG	C5-C6-N1	2.67	119.97	113.19
1	2	4637	OMG	O4'-C1'-N9	2.67	114.47	108.36
1	2	4494	OMG	C5-C6-N1	2.67	119.97	113.19
1	2	2050	OMG	C5-C6-N1	2.67	119.96	113.19
1	2	1625	OMG	C5-C6-N1	2.66	119.95	113.19
1	2	2050	OMG	C5-C4-N9	2.66	110.45	105.63
1	2	1522	OMG	C5-C6-N1	2.65	119.93	113.19
1	2	1316	OMG	C5-C4-N9	2.65	110.44	105.63
1	2	1517	2MG	O6-C6-C5	-2.65	119.56	126.60
1	2	2773	OMG	C5-C6-N1	2.65	119.92	113.19
1	2	4637	OMG	C5-C4-N9	2.65	110.43	105.63
1	2	4083	5MU	O2-C2-N1	-2.63	119.29	122.79
1	2	4690	B8K	C2-N1-C6	-2.61	120.34	125.10
1	2	4550	7MG	C4-C5-N7	2.59	109.12	105.53
1	2	1605	7MG	C4-C5-N7	2.59	109.12	105.53
1	2	3909	OMC	C4-N3-C2	2.58	124.42	120.25
1	2	4550	7MG	N9-C8-N7	2.58	107.07	103.38
1	2	3909	OMC	C1'-N1-C2	2.58	124.18	118.42
1	2	373	OMG	O6-C6-C5	-2.56	119.80	126.60
1	2	2773	OMG	C5-C4-N9	2.56	110.28	105.63
1	2	1625	OMG	C5-C4-N9	2.56	110.27	105.63
1	2	2364	OMG	O6-C6-C5	-2.55	119.85	126.60
1	2	4472	B8W	C2-N1-C6	2.53	119.95	115.93
1	2	2424	OMG	O6-C6-C5	-2.53	119.89	126.60
1	2	1522	OMG	O6-C6-C5	-2.53	119.89	126.60
1	2	1625	OMG	O6-C6-C5	-2.53	119.89	126.60
1	2	237	B9B	C2-N3-C4	2.52	120.86	113.89
1	2	4494	OMG	O6-C6-C5	-2.52	119.91	126.60
1	2	729	2MG	N9-C8-N7	-2.51	108.66	113.39
1	2	373	OMG	C5-C4-N9	2.51	110.19	105.63
1	2	4529	B8W	C5-N7-C8	2.51	107.08	103.51
1	2	4637	OMG	O6-C6-C5	-2.50	119.96	126.60
1	2	4494	OMG	C5-C4-N9	2.50	110.17	105.63
1	2	4872	2MG	O6-C6-C5	-2.50	119.97	126.60
1	2	729	2MG	O6-C6-C5	-2.50	119.97	126.60
1	2	1522	OMG	C5-C4-N9	2.50	110.16	105.63
1	2	1316	OMG	O6-C6-C5	-2.48	120.01	126.60
1	2	1605	7MG	C2-N1-C6	-2.48	120.57	125.10
1	2	978	2MG	O6-C6-C5	-2.48	120.03	126.60
1	2	237	B9B	C61-O6-C6	-2.48	112.76	117.47
1	2	2297	E7G	C2-N1-C6	-2.48	120.58	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	4472	B8W	C2-N3-C4	2.48	120.73	113.89
1	2	4623	OMG	O6-C6-C5	-2.47	120.04	126.60
1	2	1517	2MG	N9-C8-N7	-2.47	108.74	113.39
1	2	978	2MG	N1-C2-N3	-2.47	120.14	123.95
1	2	373	OMG	O4'-C1'-N9	2.46	113.99	108.36
1	2	2754	B9B	C2-N3-C4	2.46	120.69	113.89
1	2	2050	OMG	O6-C6-C5	-2.46	120.08	126.60
1	2	2380	B8W	C1'-N9-C8	2.45	132.68	127.14
1	2	2773	OMG	O6-C6-C5	-2.45	120.10	126.60
1	2	4564	M7A	C5-C4-N3	-2.44	120.90	126.62
1	2	4494	OMG	O4'-C1'-N9	2.44	113.94	108.36
1	2	2786	B9H	O3'-C3'-C4'	2.43	118.09	111.05
1	2	4870	OMG	O6-C6-C5	-2.43	120.14	126.60
1	2	4472	B8W	C5-C6-N1	-2.43	120.08	123.46
1	2	4623	OMG	O4'-C1'-N9	2.43	113.92	108.36
1	2	3880	P7G	N9-C8-N7	2.43	106.85	103.38
1	2	2861	OMC	C1'-N1-C2	2.42	123.82	118.42
1	2	1316	OMG	O4'-C1'-N9	2.42	113.89	108.36
1	2	1517	2MG	N1-C2-N3	-2.41	120.23	123.95
1	2	3909	OMC	C5-C4-N3	-2.41	117.23	121.33
1	2	3869	OMC	O2-C2-N3	-2.40	118.43	122.33
1	2	4529	B8W	C6-C5-N7	-2.40	130.45	133.63
1	2	2754	B9B	C61-O6-C6	-2.39	112.91	117.47
1	2	1871	A2M	C2'-C1'-N9	-2.39	109.51	113.53
1	2	4472	B8W	C4-C5-N7	-2.38	107.72	110.62
1	2	2786	B9H	O2-C2-N1	-2.38	117.15	122.72
1	2	4185	B8W	C2-N3-C4	2.37	120.45	113.89
1	2	2364	OMG	O4'-C1'-N9	2.37	113.79	108.36
1	2	4483	B8T	O3'-C3'-C4'	2.37	117.90	111.05
1	2	1456	B8Q	C31-N3-C2	2.36	121.22	117.79
1	2	3897	B8K	C2-N1-C6	-2.36	120.80	125.10
1	2	1574	B9B	C2-N3-C4	2.36	120.40	113.89
1	2	3899	BGH	N1-C2-N3	-2.35	118.94	123.32
1	2	2380	B8W	C2-N1-C6	2.35	119.66	115.93
1	2	2424	OMG	N9-C4-N3	2.35	130.65	125.94
1	2	3899	BGH	C2-N1-C6	-2.34	120.83	125.10
1	2	4529	B8W	C5-C6-N1	-2.34	120.21	123.46
1	2	4550	7MG	C2-N1-C6	-2.32	120.86	125.10
1	2	2424	OMG	C5-C4-N9	2.32	109.84	105.63
1	2	237	B9B	C1'-N9-C8	-2.32	121.90	127.14
1	2	4623	OMG	C4-C5-N7	-2.32	107.06	110.72
1	2	1883	OMG	C2'-C1'-N9	-2.31	109.73	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	4185	B8W	C4-N9-C1'	-2.31	121.09	126.59
1	2	729	2MG	N1-C2-N3	-2.31	120.39	123.95
1	2	3897	B8K	N1-C2-N3	-2.30	119.03	123.32
1	2	1883	OMG	O4'-C1'-N9	2.30	113.61	108.36
1	2	4623	OMG	N9-C8-N7	-2.29	109.07	113.39
1	2	4623	OMG	N2-C2-N1	2.29	121.59	116.71
1	2	4083	5MU	O4-C4-N3	-2.28	115.74	120.12
1	2	1625	OMG	O4'-C1'-N9	2.28	113.58	108.36
1	2	4530	UR3	C6-N1-C2	-2.28	119.74	121.79
1	2	237	B9B	C4-N9-C8	2.28	108.20	105.73
1	2	373	OMG	N9-C8-N7	-2.27	109.11	113.39
4	8	14	OMU	C1'-N1-C2	2.27	121.68	117.57
1	2	4529	B8W	C2-N1-C6	2.27	119.53	115.93
1	2	2380	B8W	C2-N3-C4	2.26	120.14	113.89
1	2	1456	B8Q	C1'-N1-C2	2.26	120.80	116.99
1	2	4564	M7A	C4-N9-C1'	-2.25	121.25	126.60
1	2	4870	OMG	N9-C8-N7	-2.25	109.15	113.39
1	2	4637	OMG	N2-C2-N1	2.25	121.50	116.71
1	2	373	OMG	C2'-C1'-N9	-2.24	109.86	114.22
1	2	1883	OMG	C5-C4-N9	2.24	109.70	105.63
1	2	2050	OMG	O4'-C1'-N9	2.24	113.49	108.36
1	2	4690	B8K	N1-C2-N3	-2.24	119.14	123.32
1	2	4472	B8W	N2-C2-N1	-2.24	113.77	117.25
1	2	3909	OMC	C6-N1-C2	-2.23	116.62	120.49
1	2	4870	OMG	N9-C4-N3	2.23	130.41	125.94
1	2	1316	OMG	C4-C5-N7	-2.22	107.20	110.72
4	8	14	OMU	CM2-O2'-C2'	2.22	120.35	114.52
1	2	4185	B8W	C2-N1-C6	2.22	119.46	115.93
1	2	4690	B8K	O6-C6-C5	-2.22	122.10	127.54
1	2	4472	B8W	C1'-N9-C8	2.21	132.13	127.14
1	2	2522	7MG	C2-N1-C6	-2.21	121.07	125.10
1	2	4637	OMG	C4-C5-N7	-2.20	107.25	110.72
1	2	4494	OMG	N9-C4-N3	2.18	130.31	125.94
1	2	4529	B8W	C2-N3-C4	2.18	119.91	113.89
1	2	1883	OMG	N9-C4-N3	2.17	130.31	125.94
1	2	373	OMG	C4-C5-N7	-2.17	107.29	110.72
1	2	4536	OMC	C1'-N1-C2	2.17	123.26	118.42
1	2	2424	OMG	O4'-C1'-N9	2.16	113.29	108.36
1	2	1522	OMG	O4'-C1'-N9	2.15	113.28	108.36
1	2	1574	B9B	C4-N9-C8	2.15	108.06	105.73
1	2	1625	OMG	N9-C4-N3	2.14	130.23	125.94
1	2	4872	2MG	C1'-N9-C4	-2.14	120.15	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	2754	B9B	C4-N9-C8	2.13	108.03	105.73
1	2	4483	B8T	C6-C5-C4	2.12	119.56	116.96
1	2	978	2MG	C8-N7-C5	2.12	108.08	104.24
1	2	2522	7MG	C6-C5-C4	-2.12	118.25	122.62
1	2	2380	B8W	C5-C6-N1	-2.11	120.52	123.46
1	2	2050	OMG	C4-C5-N7	-2.10	107.39	110.72
1	2	4872	2MG	C8-N7-C5	2.10	108.04	104.24
1	2	4472	B8W	C5-C4-N9	2.10	108.22	105.78
1	2	1659	I4U	O2-C2-N3	-2.09	118.93	122.33
1	2	4483	B8T	C5-C4-N3	-2.09	119.23	122.59
1	2	2786	B9H	C21-O2'-C2'	2.08	119.98	114.52
1	2	2522	7MG	O6-C6-C5	-2.08	122.44	127.54
1	2	4620	OMU	O2-C2-N1	-2.07	120.03	122.79
1	2	2861	OMC	O2-C2-N1	2.07	123.17	118.89
1	2	2422	OMC	C1'-N1-C2	2.07	123.04	118.42
1	2	4536	OMC	O2-C2-N1	2.07	123.16	118.89
1	2	2363	A2M	C4-N9-C1'	2.07	131.52	126.59
1	2	1605	7MG	O6-C6-C5	-2.06	122.49	127.54
1	2	2773	OMG	C4-C5-N7	-2.05	107.47	110.72
1	2	2297	E7G	C6-C5-C4	-2.05	118.39	122.62
1	2	4483	B8T	C6-N1-C2	-2.05	116.94	120.49
1	2	4185	B8W	C5-C6-N1	-2.03	120.63	123.46
1	2	1348	P4U	O2-C2-N3	-2.03	119.03	122.33
1	2	4870	OMG	C5-C4-N9	2.03	109.31	105.63
1	2	2364	OMG	C4-C5-N7	-2.03	107.51	110.72
1	2	2364	OMG	N2-C2-N1	2.02	121.01	116.71
1	2	2297	E7G	O6-C6-C5	-2.02	122.59	127.54
1	2	2522	7MG	N1-C2-N3	-2.02	119.56	123.32
1	2	4571	A2M	C4-N9-C1'	2.02	131.40	126.59
1	2	373	OMG	N2-C2-N1	2.02	121.00	116.71
1	2	1522	OMG	C4-C5-N7	-2.01	107.54	110.72
1	2	1316	OMG	N2-C2-N1	2.01	120.98	116.71
1	2	4872	2MG	N1-C2-N3	-2.00	120.85	123.95
1	2	2050	OMG	N2-C2-N1	2.00	120.98	116.71

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	8	14	OMU	C1'-C2'-O2'-CM2
1	2	237	B9B	C5-C6-O6-C61
1	2	237	B9B	N1-C6-O6-C61

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Mol	Chain	Res	Type	Atoms
1	2	237	B9B	C3'-C4'-C5'-O5'
1	2	237	B9B	O4'-C4'-C5'-O5'
1	2	398	A2M	O4'-C4'-C5'-O5'
1	2	1348	P4U	N3-C4-O4-C41
1	2	1574	B9B	C5-C6-O6-C61
1	2	1574	B9B	N1-C6-O6-C61
1	2	1574	B9B	C62-C61-O6-C6
1	2	1625	OMG	C3'-C4'-C5'-O5'
1	2	1871	A2M	O4'-C4'-C5'-O5'
1	2	1871	A2M	C3'-C4'-C5'-O5'
1	2	1883	OMG	C3'-C4'-C5'-O5'
1	2	2364	OMG	C1'-C2'-O2'-CM2
1	2	2380	B8W	C5-C6-O6-C61
1	2	2380	B8W	N1-C6-O6-C61
1	2	2424	OMG	O4'-C4'-C5'-O5'
1	2	2424	OMG	C3'-C4'-C5'-O5'
1	2	2754	B9B	C5-C6-O6-C61
1	2	2754	B9B	N1-C6-O6-C61
1	2	2754	B9B	C62-C61-O6-C6
1	2	2786	B9H	C1'-C2'-O2'-C21
1	2	4185	B8W	C5-C6-O6-C61
1	2	4472	B8W	C5-C6-O6-C61
1	2	4472	B8W	N1-C6-O6-C61
1	2	4550	7MG	O4'-C4'-C5'-O5'
1	2	4550	7MG	C3'-C4'-C5'-O5'
1	2	4637	OMG	O4'-C4'-C5'-O5'
1	2	4637	OMG	C1'-C2'-O2'-CM2
1	2	4870	OMG	O4'-C4'-C5'-O5'
1	2	4870	OMG	C3'-C4'-C5'-O5'
1	2	4872	2MG	O4'-C4'-C5'-O5'
1	2	398	A2M	C3'-C4'-C5'-O5'
1	2	1883	OMG	O4'-C4'-C5'-O5'
1	2	2364	OMG	O4'-C4'-C5'-O5'
1	2	3867	A2M	C3'-C4'-C5'-O5'
1	2	3897	B8K	O4'-C4'-C5'-O5'
1	2	4529	B8W	C3'-C4'-C5'-O5'
1	2	4529	B8W	O4'-C4'-C5'-O5'
1	2	4637	OMG	C3'-C4'-C5'-O5'
1	2	4872	2MG	C3'-C4'-C5'-O5'
1	2	237	B9B	O6-C61-C62-C63
1	2	1625	OMG	O4'-C4'-C5'-O5'
1	2	1909	P7G	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	2	2364	OMG	C3'-C4'-C5'-O5'
1	2	3867	A2M	O4'-C4'-C5'-O5'
1	2	3897	B8K	C3'-C4'-C5'-O5'
1	2	3880	P7G	O4'-C4'-C5'-O5'
1	2	1909	P7G	C3'-C4'-C5'-O5'
1	2	3701	OMC	C3'-C4'-C5'-O5'
1	2	3701	OMC	O4'-C4'-C5'-O5'
1	2	3880	P7G	C3'-C4'-C5'-O5'
1	2	1524	A2M	O4'-C1'-N9-C4
1	2	2297	E7G	C72-C71-N7-C8
1	2	2754	B9B	O6-C61-C62-C63
1	2	1534	A2M	C4'-C5'-O5'-P
1	2	237	B9B	C62-C61-O6-C6
1	2	4185	B8W	N1-C6-O6-C61
1	2	3867	A2M	C4'-C5'-O5'-P
1	2	373	OMG	C4'-C5'-O5'-P
1	2	3887	OMC	C4'-C5'-O5'-P
1	2	4523	A2M	C4'-C5'-O5'-P
1	2	1524	A2M	O4'-C1'-N9-C8
1	2	1625	OMG	C4'-C5'-O5'-P
1	2	4637	OMG	C4'-C5'-O5'-P
1	2	3897	B8K	C4'-C5'-O5'-P
1	2	2422	OMC	O4'-C4'-C5'-O5'
1	2	4870	OMG	C4'-C5'-O5'-P
1	2	1909	P7G	C72-C71-N7-C8
1	2	1517	2MG	C4'-C5'-O5'-P
1	2	3909	OMC	O4'-C4'-C5'-O5'
1	2	729	2MG	O4'-C4'-C5'-O5'
1	2	1534	A2M	O4'-C4'-C5'-O5'
1	2	3909	OMC	C2'-C1'-N1-C2
1	2	1659	I4U	C43-C41-O4-C4
1	2	3899	BGH	O4'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	4483	B8T	1	0
1	2	2522	7MG	1	0
1	2	3718	A2M	1	0
1	2	4620	OMU	1	0
1	2	1574	B9B	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	3723	A2M	1	0
1	2	1871	A2M	1	0
1	2	4472	B8W	1	0
1	2	1517	2MG	1	0
1	2	2363	A2M	1	0
1	2	4494	OMG	1	0
1	2	729	2MG	1	0
1	2	4571	A2M	1	0
4	8	14	OMU	1	0
1	2	4083	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
59	GTP	w	801	60	30,34,34	0.83	1 (3%)	46,54,54	1.77	11 (23%)

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
59	GTP	w	801	60	-	5/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	w	801	GTP	C2-N3	2.13	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	w	801	GTP	C5-C4-N3	-5.20	120.02	128.46
59	w	801	GTP	C2-N3-C4	4.68	120.63	112.30
59	w	801	GTP	N9-C4-N3	3.39	132.76	125.94
59	w	801	GTP	PA-O3A-PB	-3.29	121.53	132.83
59	w	801	GTP	C2-N1-C6	-2.95	119.73	125.10
59	w	801	GTP	PB-O3B-PG	-2.70	123.56	132.83
59	w	801	GTP	C5-C6-N1	2.59	119.76	113.19
59	w	801	GTP	N9-C8-N7	-2.59	108.52	113.39
59	w	801	GTP	C8-N7-C5	2.54	108.83	104.24
59	w	801	GTP	O6-C6-C5	-2.40	120.24	126.60
59	w	801	GTP	C3'-C2'-C1'	2.00	105.23	101.43

There are no chirality outliers.

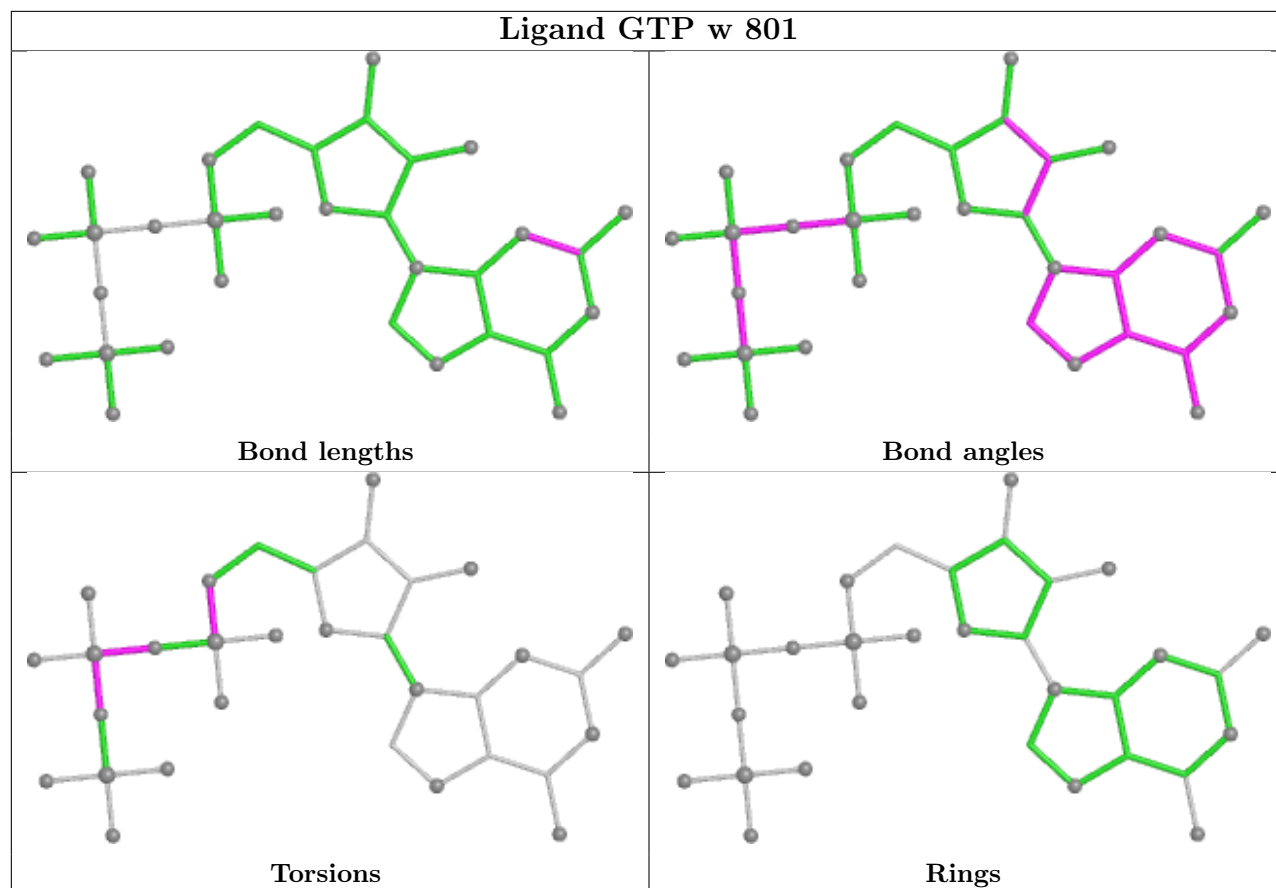
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	w	801	GTP	C5'-O5'-PA-O3A
59	w	801	GTP	PA-O3A-PB-O1B
59	w	801	GTP	C5'-O5'-PA-O2A
59	w	801	GTP	PG-O3B-PB-O3A
59	w	801	GTP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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.

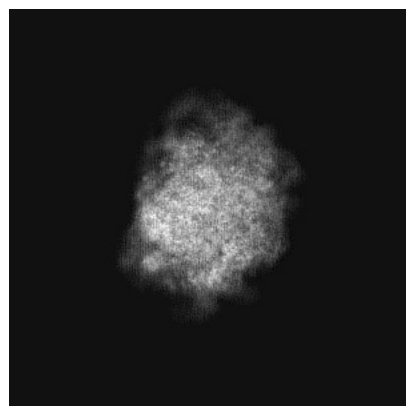
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35649. These allow visual inspection of the internal detail of the map and identification of artifacts.

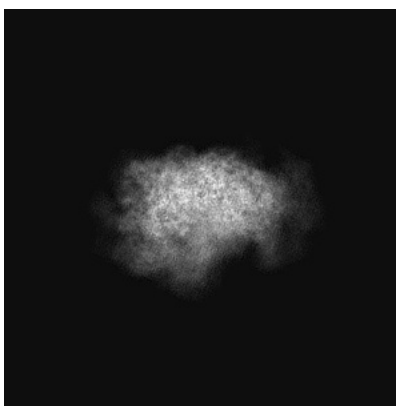
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

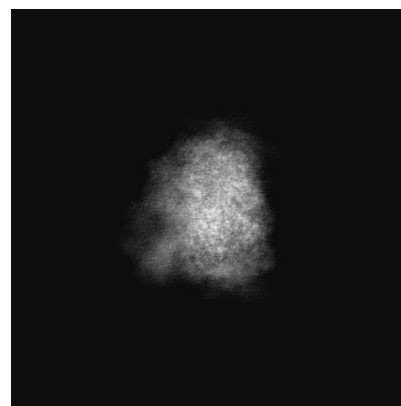
6.1.1 Primary map



X

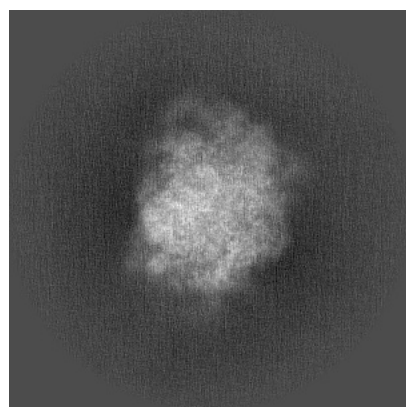


Y

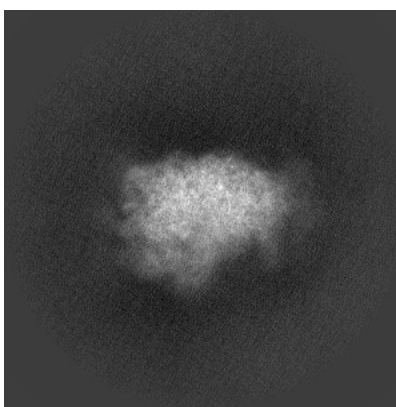


Z

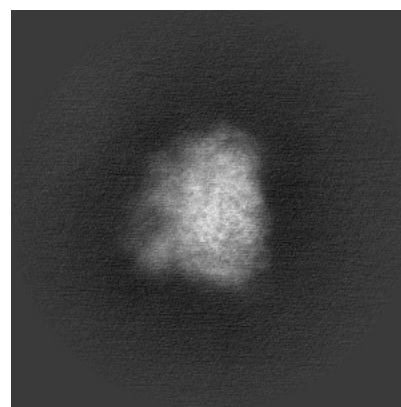
6.1.2 Raw map



X



Y

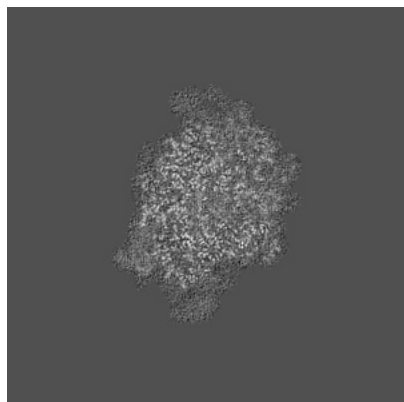


Z

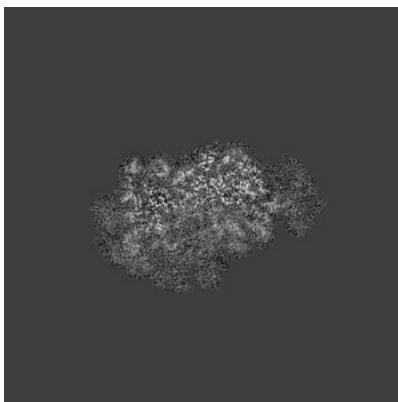
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

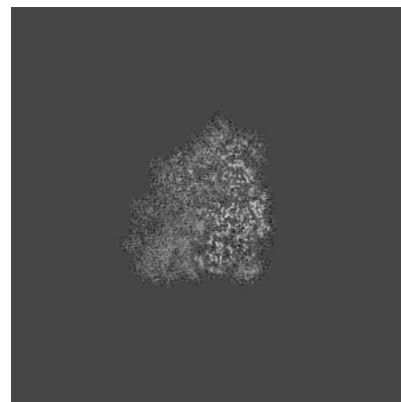
6.2.1 Primary map



X Index: 200

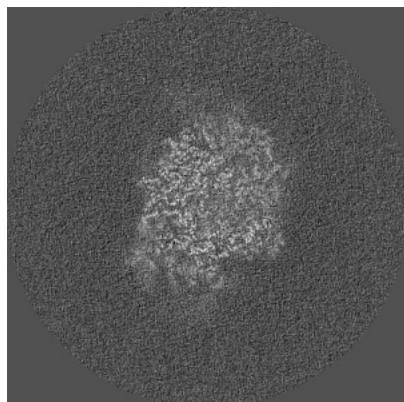


Y Index: 200

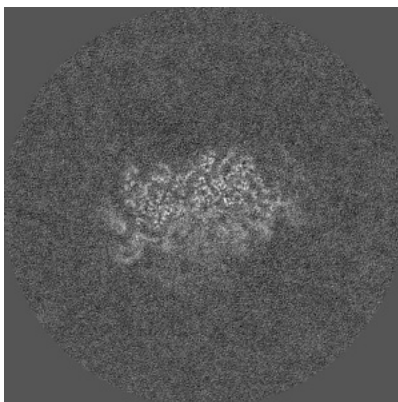


Z Index: 200

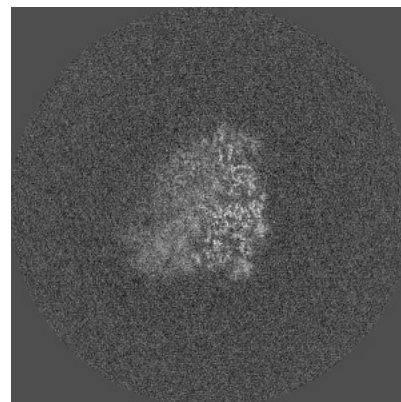
6.2.2 Raw map



X Index: 200



Y Index: 200

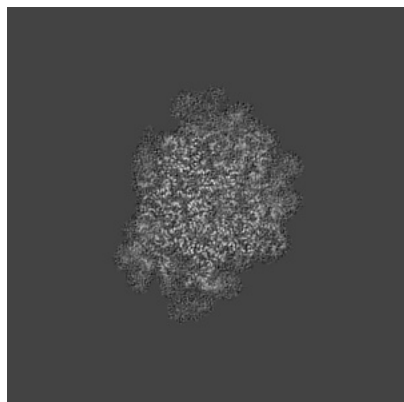


Z Index: 200

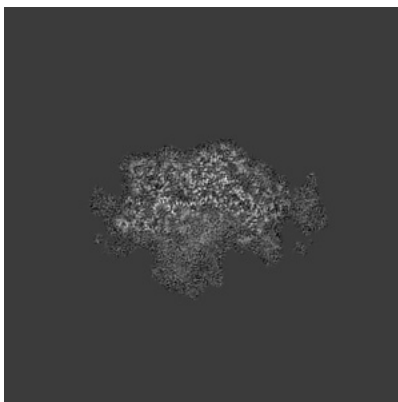
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

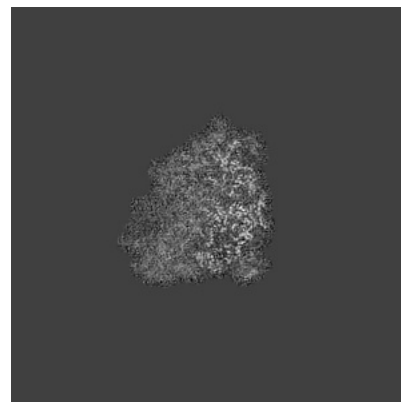
6.3.1 Primary map



X Index: 207

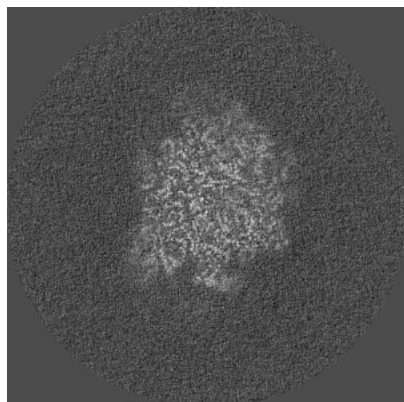


Y Index: 181

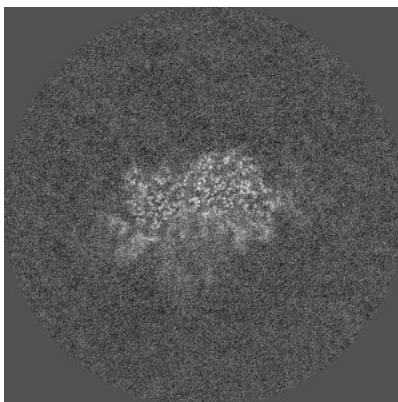


Z Index: 198

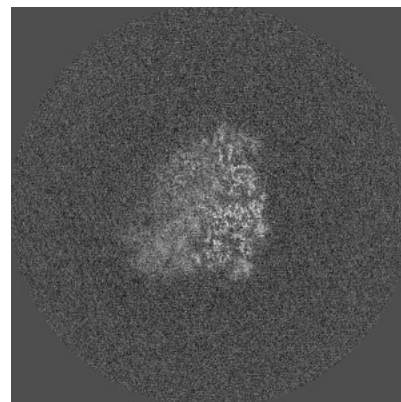
6.3.2 Raw map



X Index: 205



Y Index: 199

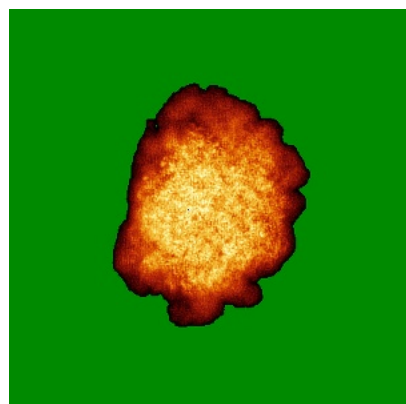


Z Index: 200

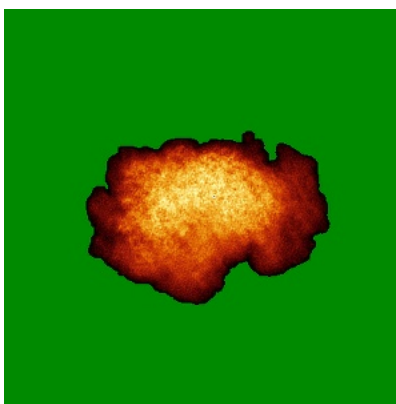
The images above show the largest variance slices of the map in three orthogonal directions.

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

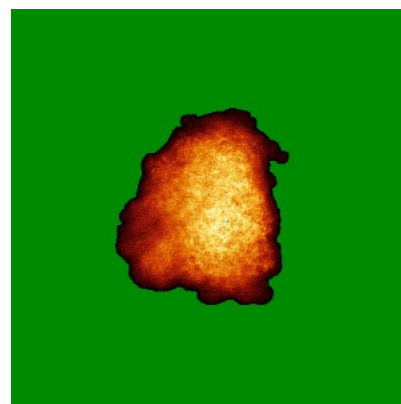
6.4.1 Primary map



X

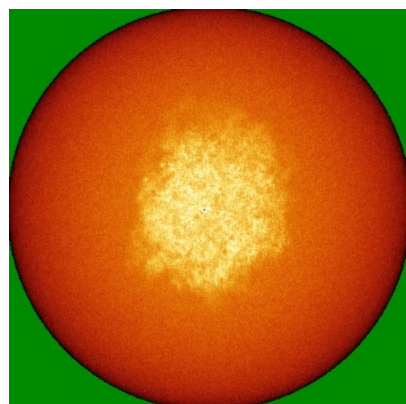


Y

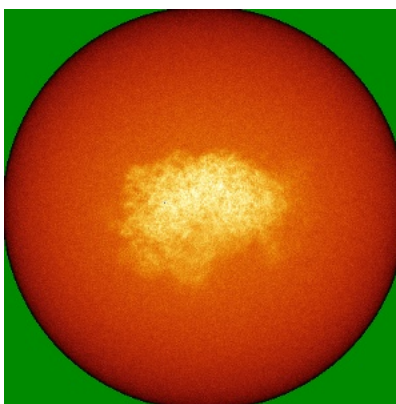


Z

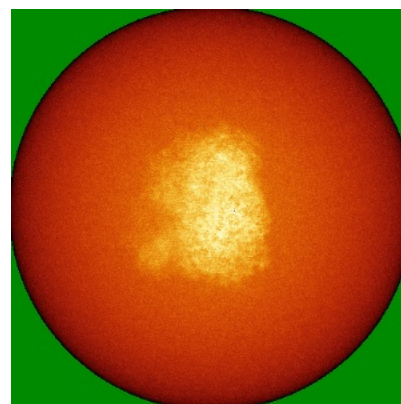
6.4.2 Raw map



X



Y

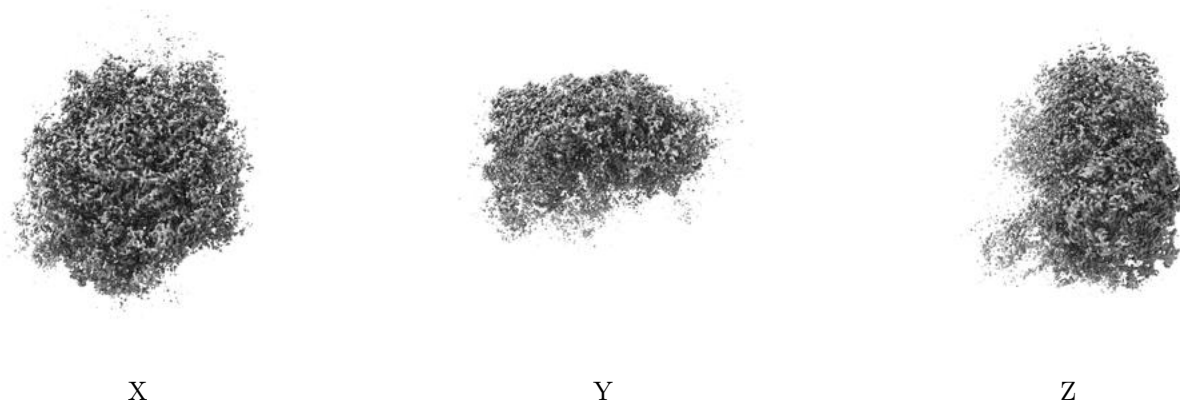


Z

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.

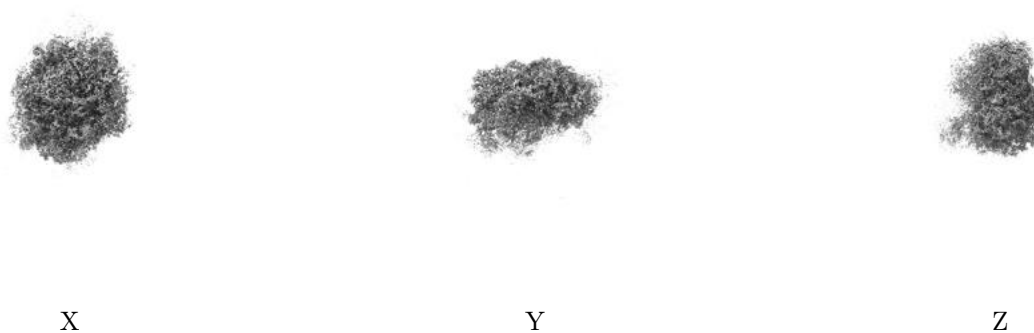
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

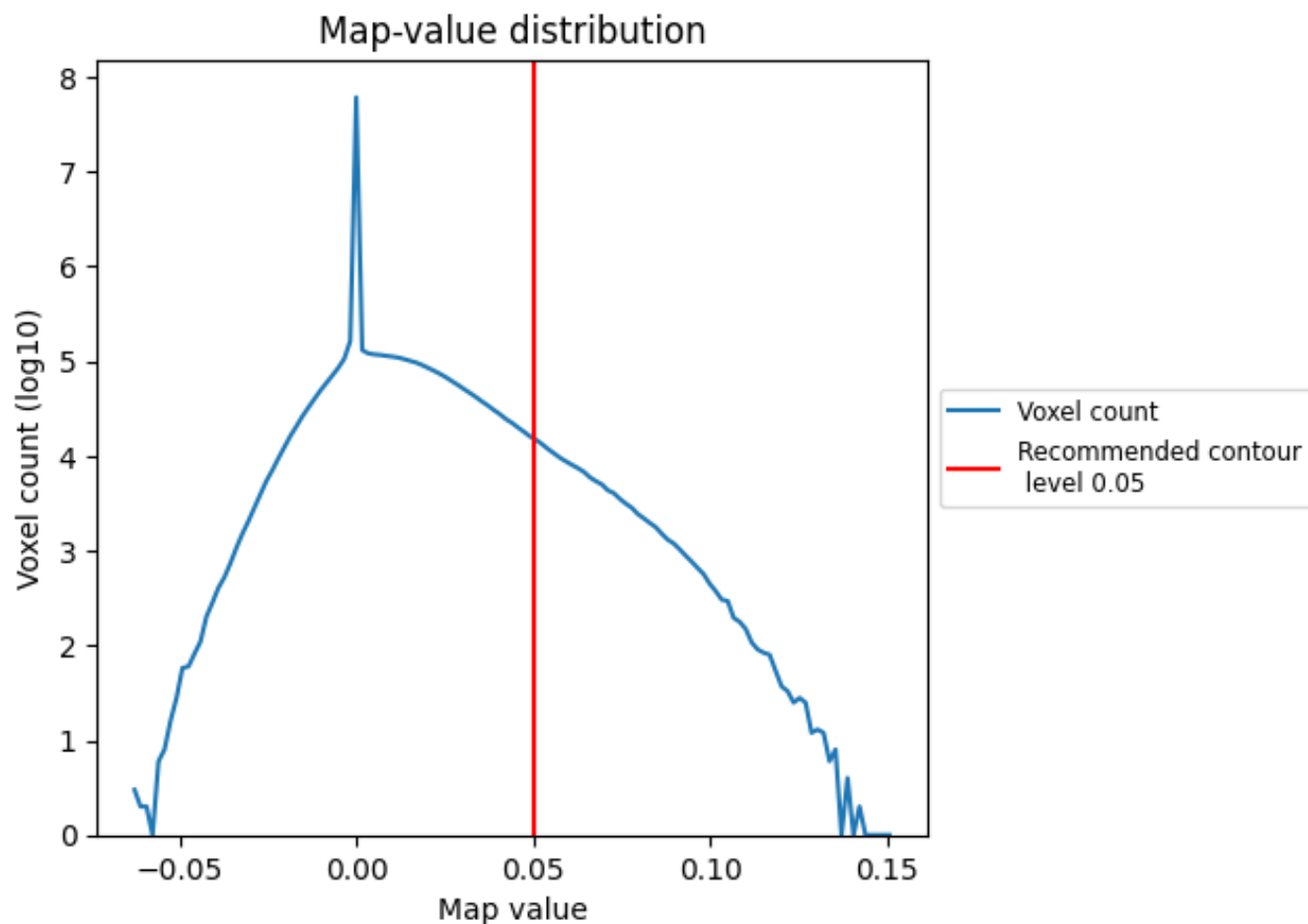
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

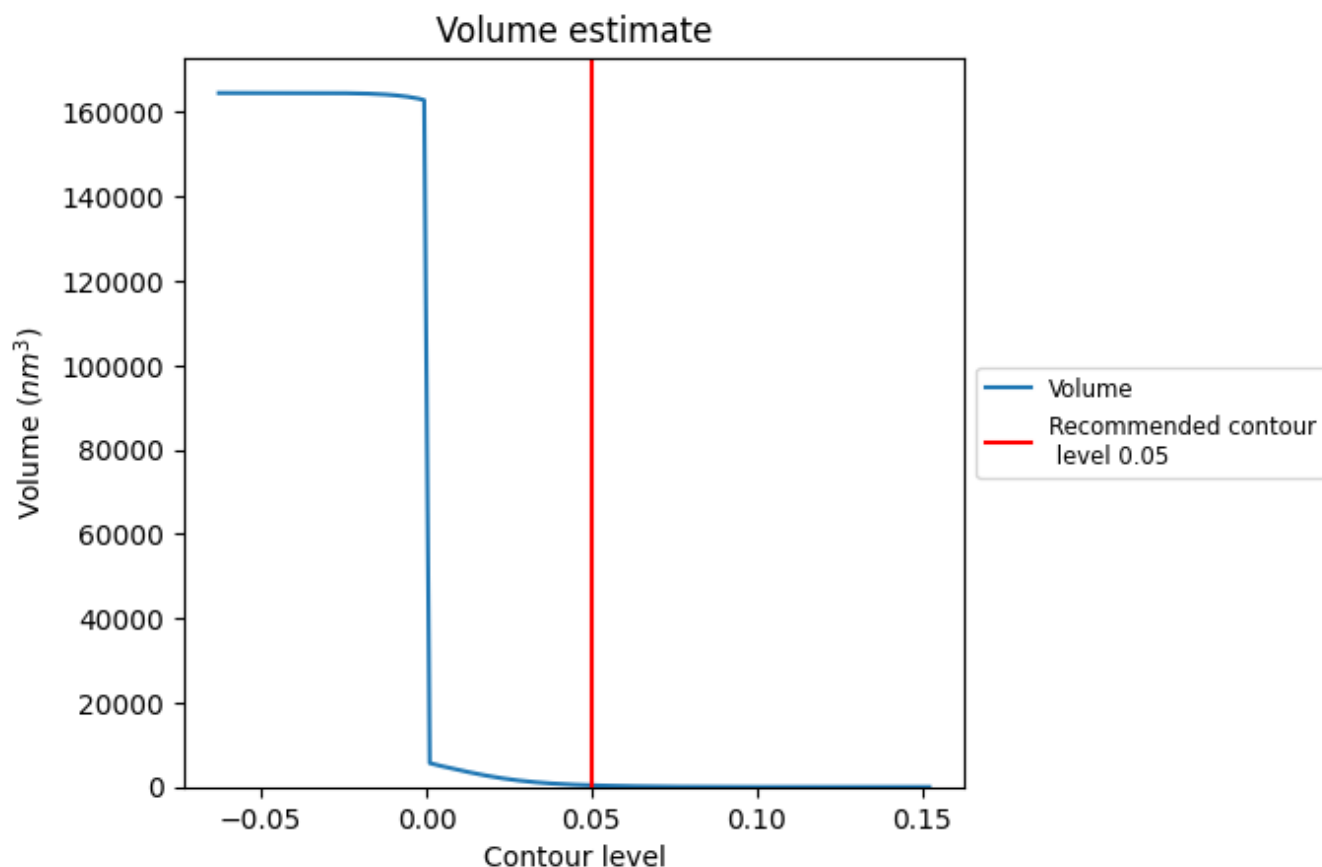
This section contains the results of statistical analysis of the map.

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.

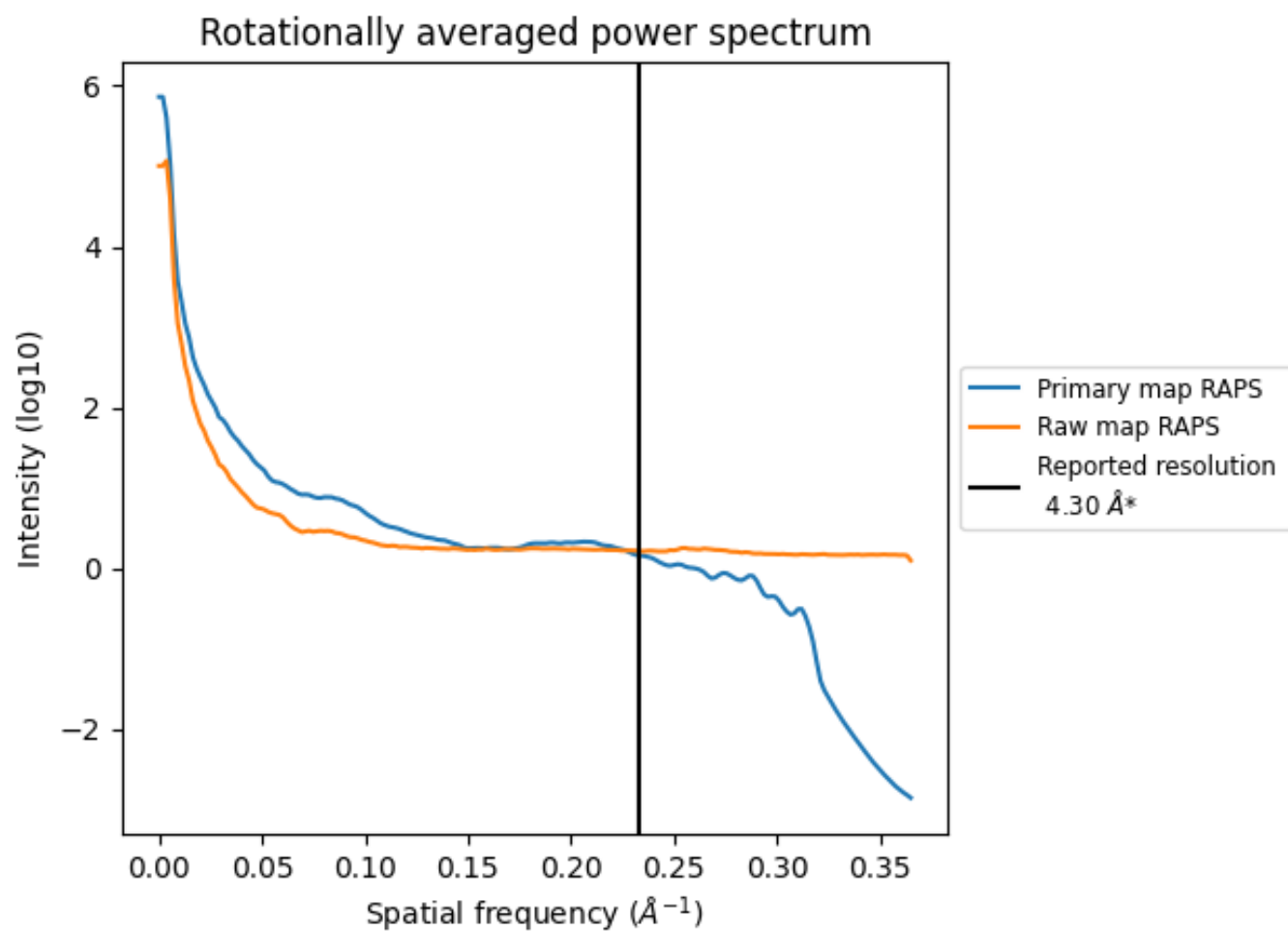
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 388 nm^3 ; this corresponds to an approximate mass of 351 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 ⓘ

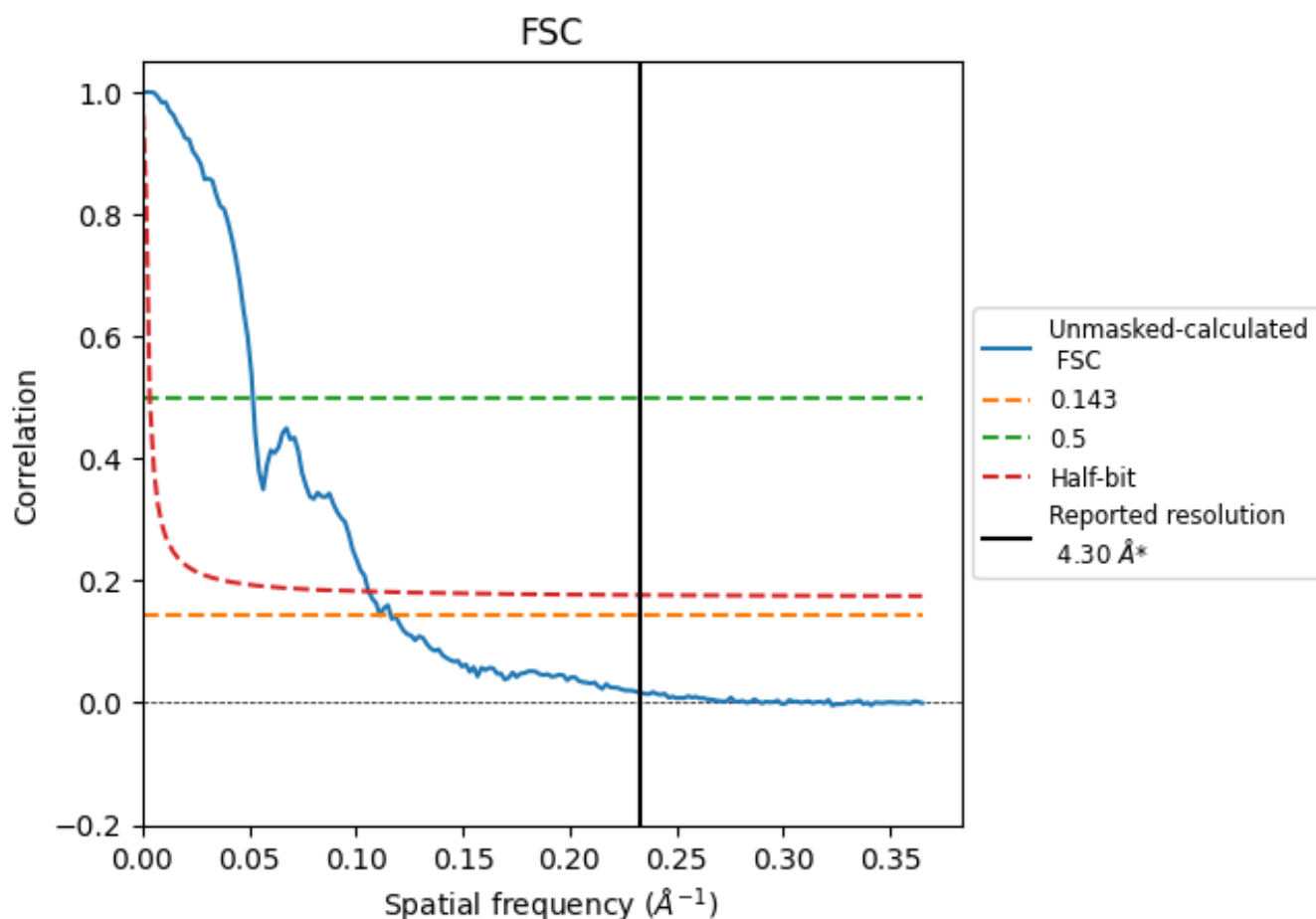


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

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 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

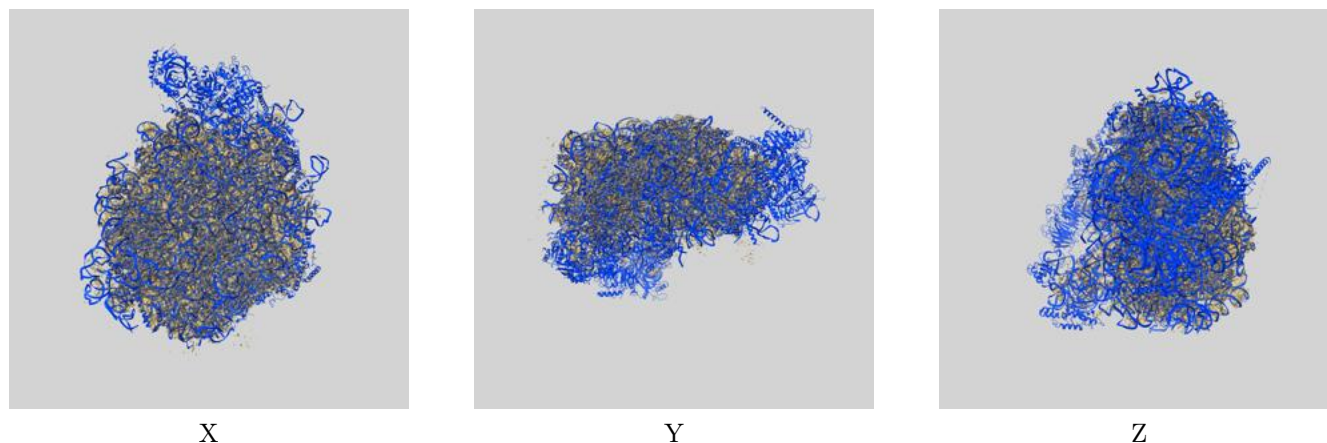
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.98	19.31	9.43

*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 8.98 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

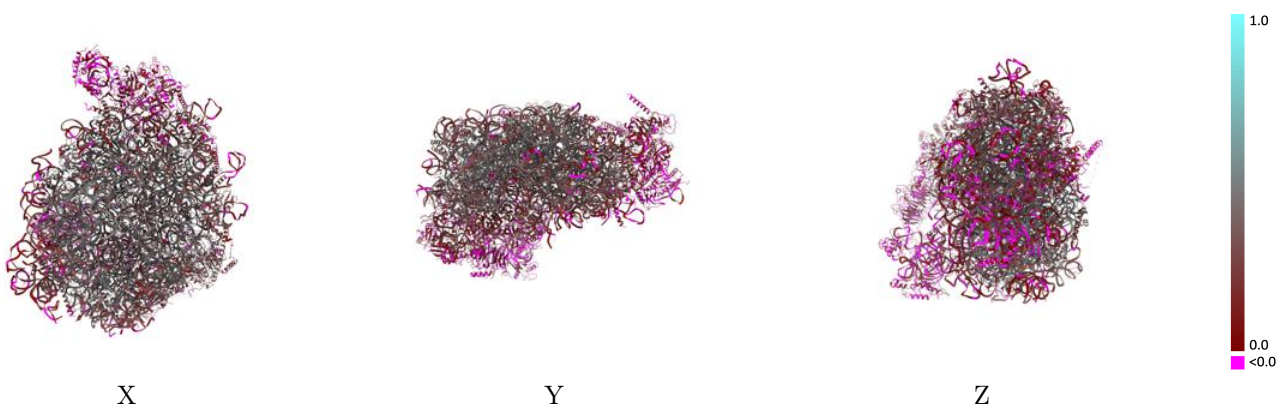
This section contains information regarding the fit between EMDB map EMD-35649 and PDB model 8IPX. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



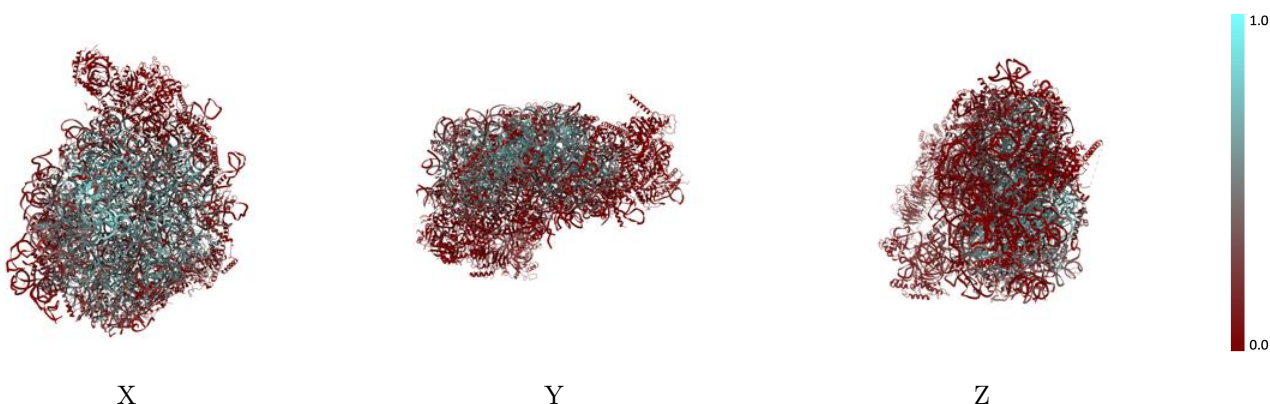
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



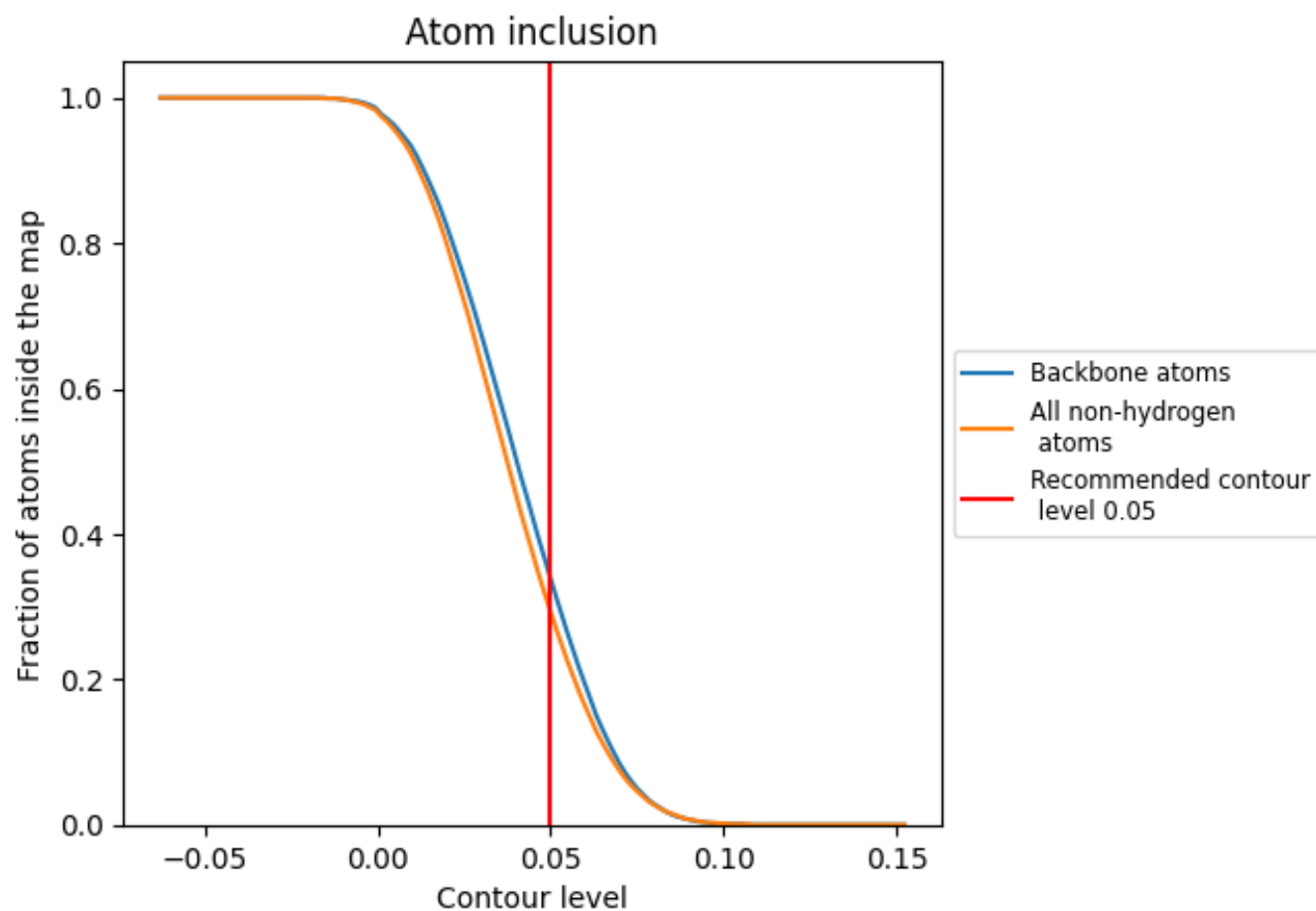
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 29% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2920	 0.2920
1	 0.0010	 0.1020
2	 0.3950	 0.3190
3	 0.0950	 0.1160
4	 0.1000	 0.2600
6	 0.1430	 0.2940
7	 0.2360	 0.3640
8	 0.5910	 0.4070
9	 0.0220	 0.1700
A	 0.0470	 0.2120
B	 0.3730	 0.4160
C	 0.0010	 0.0130
D	 0.4580	 0.4280
E	 0.0670	 0.2370
F	 0.2420	 0.3550
G	 0.1610	 0.2710
H	 0.3360	 0.3750
I	 0.2290	 0.3480
J	 0.0340	 0.2070
K	 0.2470	 0.3340
L	 0.3710	 0.4000
M	 0.5040	 0.4210
N	 0.0000	 0.0090
O	 0.1290	 0.2870
P	 0.4820	 0.4440
Q	 0.3040	 0.3510
R	 0.0030	 0.0200
S	 0.3320	 0.3800
T	 0.0700	 0.1290
U	 0.4170	 0.4160
V	 0.4510	 0.4200
W	 0.0000	 0.0380
X	 0.1380	 0.2790
Y	 0.4360	 0.4010
Z	 0.4340	 0.4410



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Chain	Atom inclusion	Q-score
a	 0.2390	 0.3490
b	 0.3490	 0.4060
d	 0.1830	 0.3170
e	 0.2930	 0.3910
f	 0.0020	 0.1560
g	 0.2730	 0.3340
h	 0.4110	 0.3970
i	 0.0780	 0.2720
j	 0.3390	 0.3860
k	 0.4790	 0.4390
l	 0.4290	 0.4270
m	 0.0950	 0.2830
n	 0.4890	 0.4640
o	 0.2200	 0.3260
p	 0.4030	 0.4040
q	 0.0140	 0.1640
r	 0.0000	 0.0710
t	 0.0010	 0.0740
u	 0.0220	 0.1340
v	 0.0090	 0.1390
w	 0.0350	 0.2120
x	 0.0000	 0.0240
y	 0.0060	 0.0830
z	 0.0650	 0.2300