Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 04:43 AM EST

PDB ID	:	6AZ3
EMDB ID	:	EMD-7025
Title	:	Cryo-EM structure of of the large subunit of Leishmania ribosome bound to paromomycin
Authors	:	Shalev-Benami, M.; Zhang, Y.; Rozenberg, H.; Nobe, Y.; Taoka, M.; Matzov, D.; Zimmerman, E.; Bashan, A.; Isobe, T.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.
Deposited on	:	2017-09-09
Resolution	:	2.50 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:

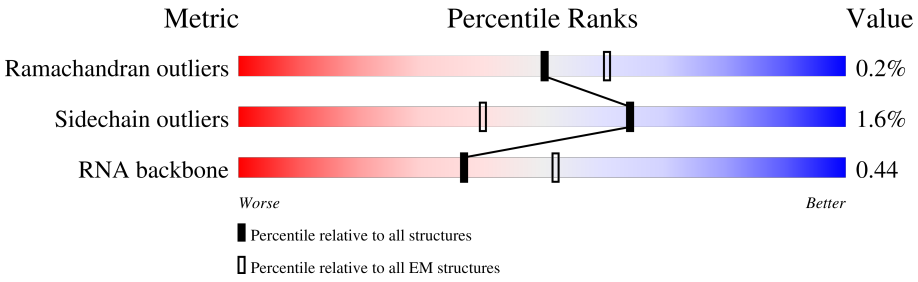
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	254	96%
2	B	402	98%
3	C	366	98%
4	D	168	22% 98%
5	E	186	100%
6	F	195	8% 69% 30%
7	G	348	61% 37%
8	H	221	6% 97%

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Mol	Chain	Length	Quality of chain
9	I	212	6% 97%
10	J	134	97%
11	K	149	11% 99%
12	L	144	98%
13	M	203	99%
14	N	213	15% 88% 11%
15	O	305	6% 81% 17%
16	P	197	97%
17	Q	189	14% 99%
18	R	178	99%
19	S	154	12% 97%
20	T	154	98%
21	U	121	13% 98%
22	V	118	6% 99%
23	W	121	98%
24	X	65	98%
25	Y	132	6% 99%
26	Z	140	96%
27	a	125	6% 100%
28	b	68	6% 97%
29	c	227	98%
30	d	92	9% 97%
31	e	119	7% 95% 5%
32	f	130	5% 97%
33	g	125	100%

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Mol	Chain	Length	Quality of chain
34	h	125	8% 98%
35	i	97	98%
36	j	80	99%
37	k	76	9% 97%
38	l	50	100%
39	m	50	94%
40	n	33	55% 100%
41	o	90	97%
42	p	96	97%
43	1	1778	61% 26% 9%
44	2	1526	47% 20% 29%
45	3	211	56% 25% 16%
46	4	183	65% 32%
47	5	133	43% 29% 27%
48	6	71	10% 46% 49%
49	7	171	63% 29% 5%
50	8	118	73% 24%

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 126561 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	254	1985	1235	412	327	11	7	0

- Molecule 2 is a protein called ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	402	3226	2036	644	533	13	10	0

- Molecule 3 is a protein called Ribosomal protein L1a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	366	2824	1761	563	485	15	2	0

- Molecule 4 is a protein called 60S ribosomal protein L11 (L5, L16).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	168	1220	774	229	209	8	0	0

- Molecule 5 is a protein called 60S ribosomal protein L9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	186	1448	917	268	257	6	0	0

- Molecule 6 is a protein called ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	137	1004	637	185	180	2	0	0

- Molecule 7 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	220	Total	C	N	O	S	2	0
			1746	1099	351	289	7		

- Molecule 8 is a protein called ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	221	Total	C	N	O	S	3	0
			1781	1128	360	286	7		

- Molecule 9 is a protein called ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	212	Total	C	N	O	S	0	0
			1647	1026	331	282	8		

- Molecule 10 is a protein called 60S ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	134	Total	C	N	O	S	0	0
			1001	634	190	171	6		

- Molecule 11 is a protein called Probable 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	149	Total	C	N	O	S	1	0
			1164	726	231	201	6		

- Molecule 12 is a protein called 60S ribosomal protein L27A/L29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	144	Total	C	N	O	S	0	0
			1126	708	226	186	6		

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	203	Total	C	N	O	S	0	0
			1714	1080	362	264	8		

- Molecule 14 is a protein called 60S ribosomal protein L10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	190	Total	C	N	O	S	0	0
			1454	924	285	233	12		

- Molecule 15 is a protein called 60S ribosomal protein L5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	252	Total	C	N	O	S	3	0
			1976	1259	376	336	5		

- Molecule 16 is a protein called 60S ribosomal protein L18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	197	Total	C	N	O	S	0	0
			1539	968	307	258	6		

- Molecule 17 is a protein called Ribosomal protein L19e family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	189	Total	C	N	O	S	0	0
			1452	899	313	235	5		

- Molecule 18 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	178	Total	C	N	O	S	0	0
			1454	927	280	242	5		

- Molecule 19 is a protein called 60S ribosomal protein L21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	154	Total	C	N	O	S	0	0
			1208	767	238	199	4		

- Molecule 20 is a protein called 60S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	154	Total	C	N	O	S	0	0
			1236	773	245	207	11		

- Molecule 21 is a protein called 60S ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	121	Total	C	N	O	S	0	0
			934	605	167	159	3		

- Molecule 22 is a protein called 60S ribosomal protein L23a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	118	Total	C	N	O	S	1	0
			928	590	173	162	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	27	ALA	-	expression tag	UNP A0A3S7WPH7

- Molecule 23 is a protein called ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	121	Total	C	N	O	S	0	0
			971	605	200	162	4		

- Molecule 24 is a protein called ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	65	Total	C	N	O	S	0	0
			553	363	107	79	4		

- Molecule 25 is a protein called Ribosomal L27e family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	132	Total	C	N	O	S	1	0
			1039	666	205	165	3		

- Molecule 26 is a protein called 60S ribosomal protein L28, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	140	Total	C	N	O	S	0	0
			1067	650	226	186	5		

- Molecule 27 is a protein called 60S_ribosomal_protein_L35_putative/GeneDB:LmjF.26.2330/GeneDB:LmjF.26.2340.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	125	Total	C	N	O	S	0	0
			985	615	205	163	2		

- Molecule 28 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	68	Total	C	N	O	S	0	0
			539	330	124	84	1		

- Molecule 29 is a protein called 60S ribosomal protein L7 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	227	Total	C	N	O	S	0	0
			1809	1152	349	297	11		

- Molecule 30 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	92	Total	C	N	O	S	0	0
			691	430	126	130	5		

- Molecule 31 is a protein called 60S ribosomal subunit protein L31, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	119	Total	C	N	O	S	0	0
			936	595	183	156	2		

- Molecule 32 is a protein called 60S_ribosomal_protein_L32/GeneDB:LmjF.21.1720.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	130	Total	C	N	O	S	1	0
			1048	659	210	175	4		

- Molecule 33 is a protein called Ribosomal protein L35Ae family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	125	Total	C	N	O	S	0	0
			998	623	209	161	5		

- Molecule 34 is a protein called 60S ribosomal protein L34, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	125	Total	C	N	O	S	1	0
			1010	623	221	160	6		

- Molecule 35 is a protein called 60S ribosomal protein L36, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	97	Total	C	N	O	S	0	0
			760	482	153	123	2		

- Molecule 36 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	80	Total	C	N	O	S	0	0
			663	403	152	102	6		

- Molecule 37 is a protein called Ribosomal L38e family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	76	Total	C	N	O	S	0	0
			575	361	110	101	3		

- Molecule 38 is a protein called 60S ribosomal protein L39, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	50	Total	C	N	O	S	0	0
			440	285	91	63	1		

- Molecule 39 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	50	Total	C	N	O	S	0	0
			393	248	80	58	7		

- Molecule 40 is a protein called ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	33	Total	C	N	O	S	0	0
			280	172	69	37	2		

- Molecule 41 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	90	Total	C	N	O	S	0	0
			696	432	144	114	6		

- Molecule 42 is a protein called 60S ribosomal protein L44, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	96	Total	C	N	O	S	0	0
			756	478	153	120	5		

- Molecule 43 is a RNA chain called rRNA alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1	1620	Total	C	N	O	P	0	0
			34631	15467	6334	11211	1619		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	A	deletion	GB 322500086
1	?	-	A	deletion	GB 322500086

- Molecule 44 is a RNA chain called rRNA beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2	1078	Total	C	N	O	P	0	0
			22996	10290	4137	7491	1078		

- Molecule 45 is a RNA chain called rRNA gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3	177	Total	C	N	O	P	0	0
			3751	1677	657	1240	177		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	U	deletion	GB 322500086
3	196	C	A	conflict	GB 322500086

- Molecule 46 is a RNA chain called rRNA delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	183	Total	C	N	O	P	0	0
			3906	1742	706	1275	183		

- Molecule 47 is a RNA chain called rRNA epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5	97	Total	C	N	O	P	0	0
			2075	925	379	674	97		

- Molecule 48 is a RNA chain called rRNA zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	6	71	Total	C	N	O	P	0	0
			1477	659	265	482	71		

- Molecule 49 is a RNA chain called rRNA 5.8S.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	163	Total	C	N	O	P	0	0
			3465	1552	616	1135	162		

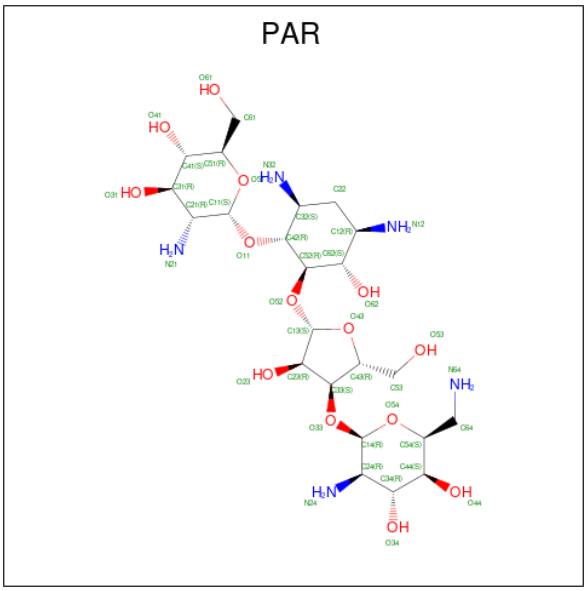
- Molecule 50 is a RNA chain called rRNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	118	Total	C	N	O	P	0	0
			2511	1123	448	822	118		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	14	U	C	conflict	GB 1229082190

- Molecule 51 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms	AltConf
51	1	1	Total C N O 210 115 25 70	0
51	1	1	Total C N O 210 115 25 70	0
51	1	1	Total C N O 210 115 25 70	0
51	1	1	Total C N O 210 115 25 70	0
51	1	1	Total C N O 210 115 25 70	0
51	2	1	Total C N O 168 92 20 56	0
51	2	1	Total C N O 168 92 20 56	0
51	2	1	Total C N O 168 92 20 56	0
51	2	1	Total C N O 168 92 20 56	0
51	7	1	Total C N O 42 23 5 14	0

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
52	1	21	Total Mg 21 21	0
52	2	8	Total Mg 8 8	0

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Mol	Chain	Residues	Atoms	AltConf
52	3	1	Total Mg 1 1	0
52	4	1	Total Mg 1 1	0
52	5	1	Total Mg 1 1	0
52	7	2	Total Mg 2 2	0

- Molecule 53 is water.

Mol	Chain	Residues	Atoms	AltConf
53	A	16	Total O 16 16	0
53	B	11	Total O 11 11	0
53	C	11	Total O 11 11	0
53	G	3	Total O 3 3	0
53	H	7	Total O 7 7	0
53	I	5	Total O 5 5	0
53	J	2	Total O 2 2	0
53	L	5	Total O 5 5	0
53	M	16	Total O 16 16	0
53	P	7	Total O 7 7	0
53	Q	5	Total O 5 5	0
53	R	2	Total O 2 2	0
53	S	4	Total O 4 4	0
53	T	3	Total O 3 3	0
53	V	4	Total O 4 4	0

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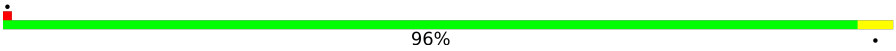
Mol	Chain	Residues	Atoms	AltConf
53	W	1	Total O 1 1	0
53	Y	1	Total O 1 1	0
53	a	1	Total O 1 1	0
53	c	2	Total O 2 2	0
53	e	1	Total O 1 1	0
53	f	3	Total O 3 3	0
53	g	5	Total O 5 5	0
53	h	5	Total O 5 5	0
53	i	1	Total O 1 1	0
53	j	8	Total O 8 8	0
53	l	3	Total O 3 3	0
53	p	6	Total O 6 6	0
53	1	442	Total O 442 442	0
53	2	278	Total O 278 278	0
53	3	26	Total O 26 26	0
53	4	47	Total O 47 47	0
53	5	27	Total O 27 27	0
53	6	2	Total O 2 2	0
53	7	45	Total O 45 45	0
53	8	14	Total O 14 14	0

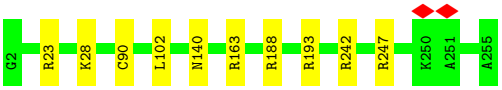
3 Residue-property plots (i)

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

• Molecule 1: ribosomal protein uL2

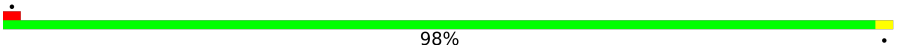
Chain A:

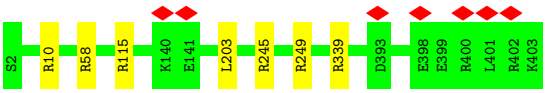




• Molecule 2: ribosomal protein uL3

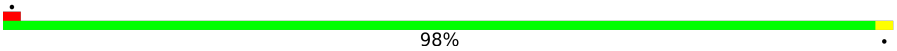
Chain B:

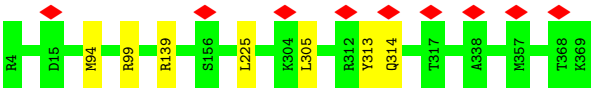




• Molecule 3: Ribosomal protein L1a, putative

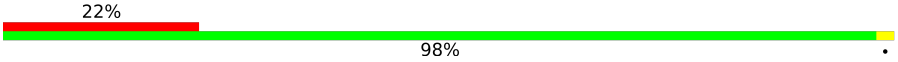
Chain C:

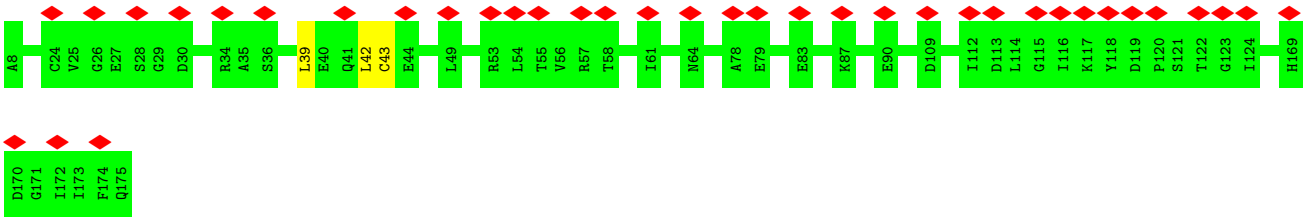




• Molecule 4: 60S ribosomal protein L11 (L5, L16)

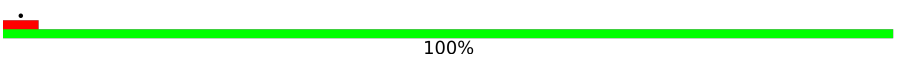
Chain D:

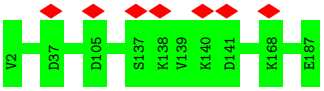




• Molecule 5: 60S ribosomal protein L9, putative

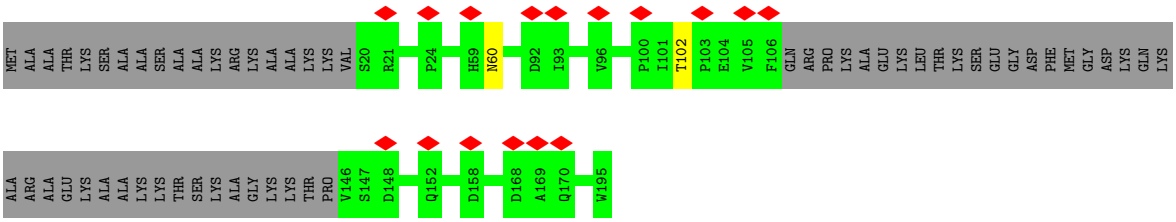
Chain E:





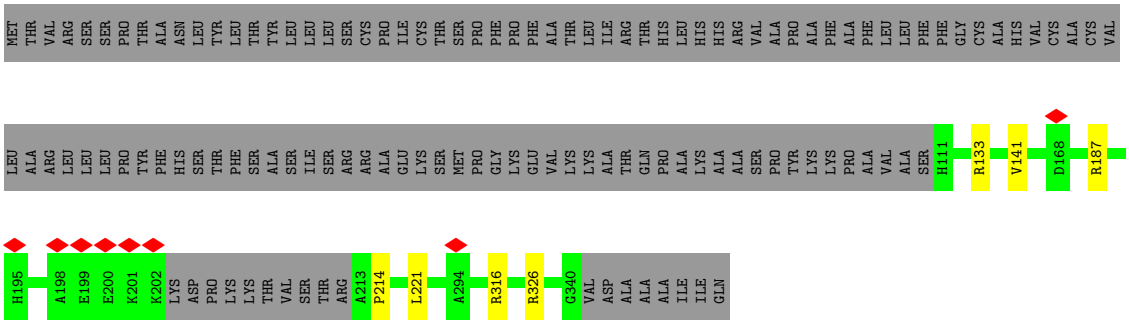
• Molecule 6: ribosomal protein eL6

Chain F:



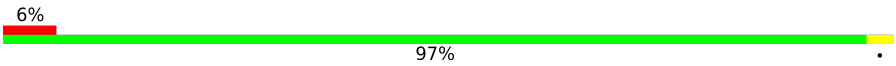
• Molecule 7: 60S ribosomal protein L7a

Chain G:



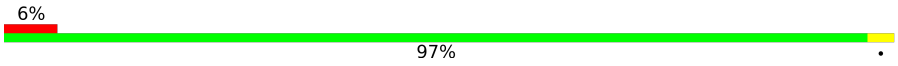
• Molecule 8: ribosomal protein uL13

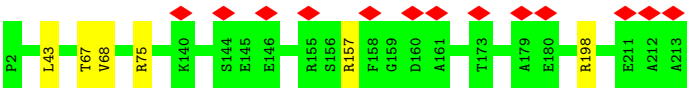
Chain H:



• Molecule 9: ribosomal protein eL13

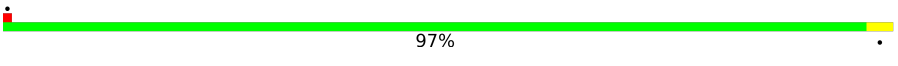
Chain I:





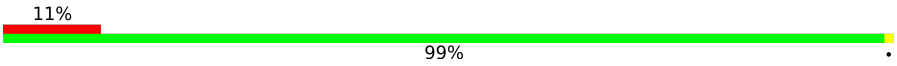
• Molecule 10: 60S ribosomal protein L23, putative

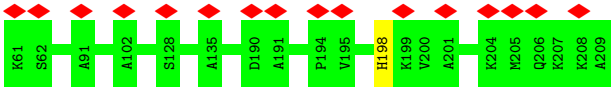
Chain J:



• Molecule 11: Probable 60S ribosomal protein L14

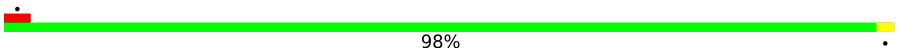
Chain K:

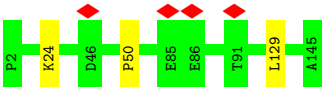




• Molecule 12: 60S ribosomal protein L27A/L29, putative

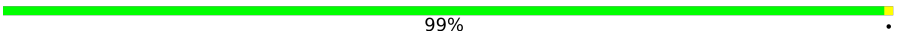
Chain L:

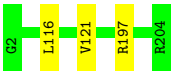




• Molecule 13: Ribosomal protein L15

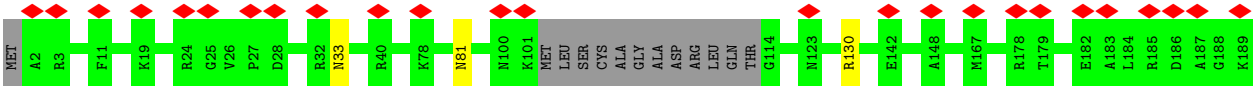
Chain M:

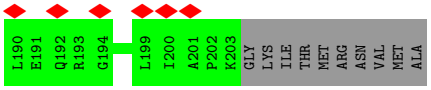




• Molecule 14: 60S ribosomal protein L10, putative

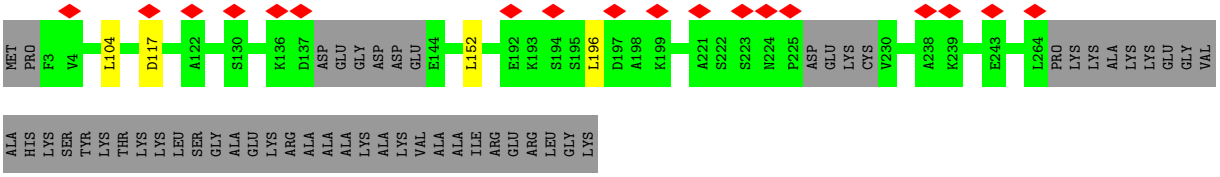
Chain N:





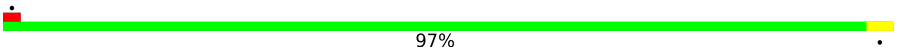
• Molecule 15: 60S ribosomal protein L5, putative

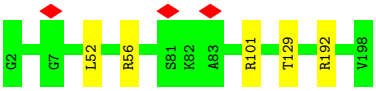
Chain O:



• Molecule 16: 60S ribosomal protein L18, putative

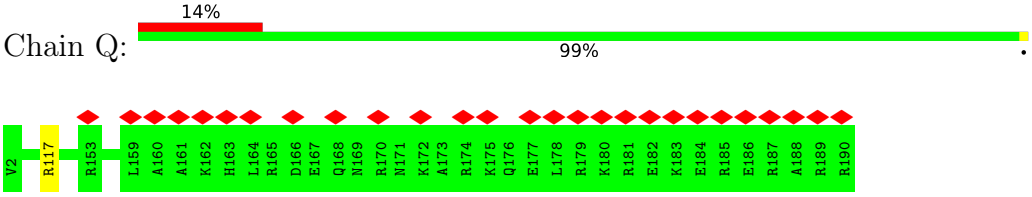
Chain P:





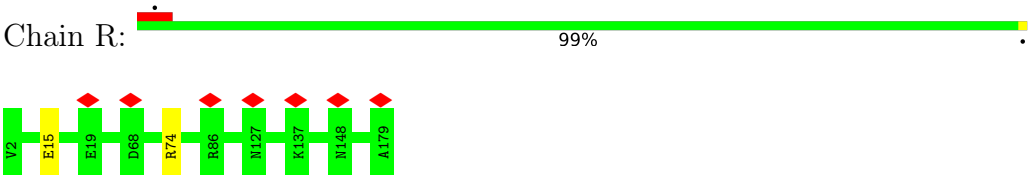
• Molecule 17: Ribosomal protein L19e family protein

Chain Q:



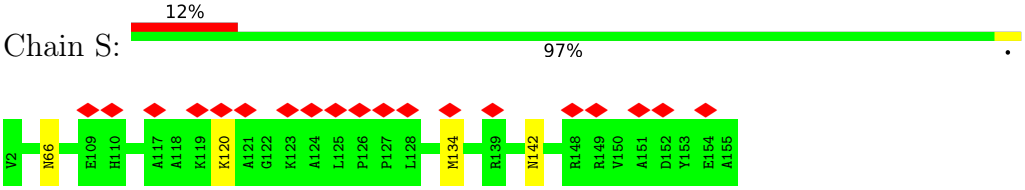
• Molecule 18: 60S ribosomal protein L18a

Chain R:



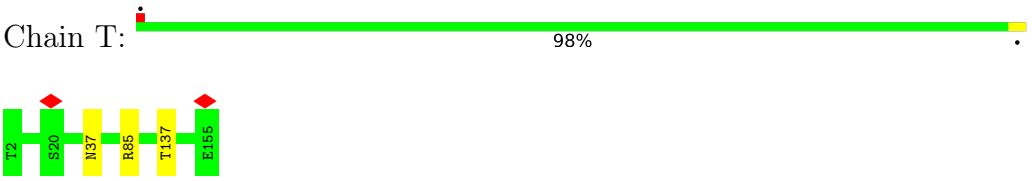
• Molecule 19: 60S ribosomal protein L21, putative

Chain S:



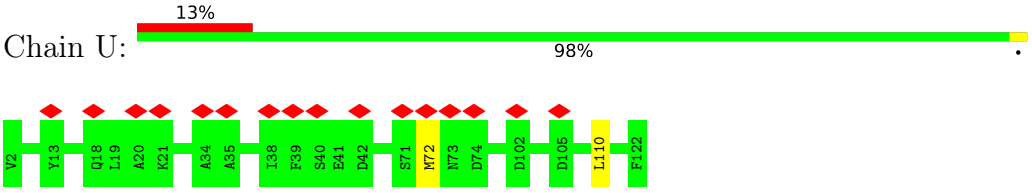
• Molecule 20: 60S ribosomal protein L17, putative

Chain T:



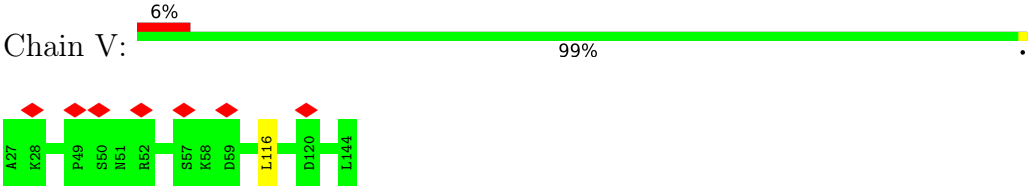
• Molecule 21: 60S ribosomal protein L22, putative

Chain U:



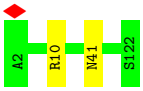
• Molecule 22: 60S ribosomal protein L23a, putative

Chain V:



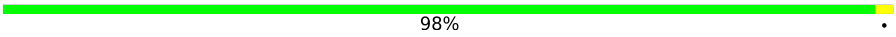
• Molecule 23: ribosomal protein uL24

Chain W:



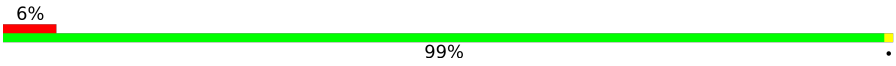
• Molecule 24: ribosomal protein eL24

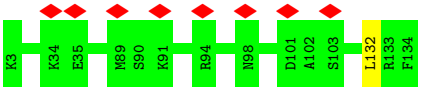
Chain X:



• Molecule 25: Ribosomal L27e family protein

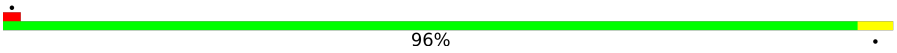
Chain Y:

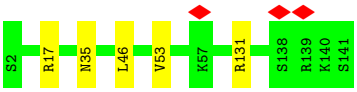




• Molecule 26: 60S ribosomal protein L28, putative

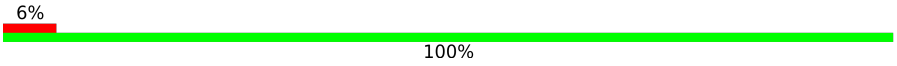
Chain Z:

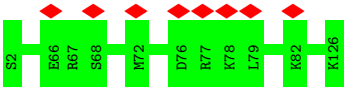




• Molecule 27: 60S_ribosomal_protein_L35_putative/GeneDB:LmjF.26.2330/GeneDB:LmjF.26.2340

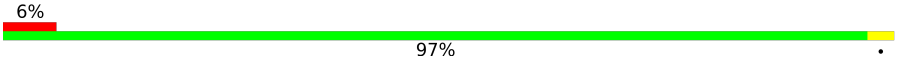
Chain a:

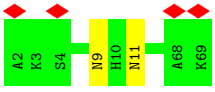




• Molecule 28: 60S ribosomal protein L29

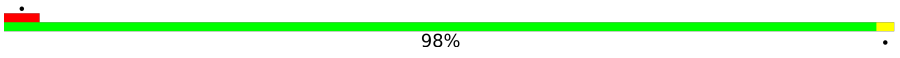
Chain b:

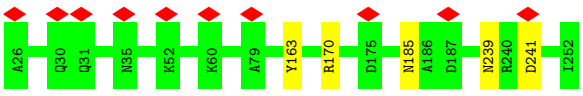




• Molecule 29: 60S ribosomal protein L7 family protein

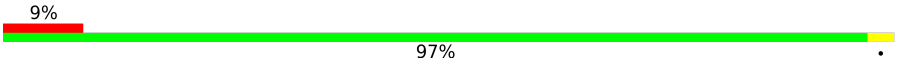
Chain c:

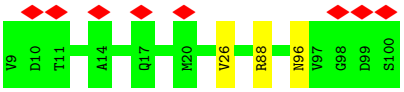




• Molecule 30: 60S ribosomal protein L30

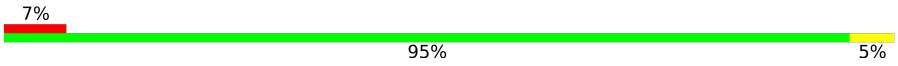
Chain d:

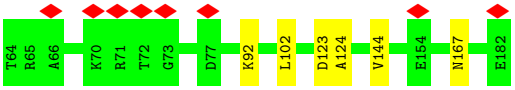




• Molecule 31: 60S ribosomal subunit protein L31, putative

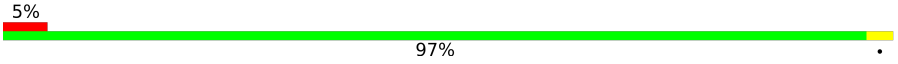
Chain e:

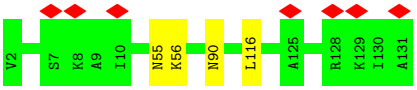




• Molecule 32: 60S_ribosomal_protein_L32/GeneDB:LmjF.21.1720

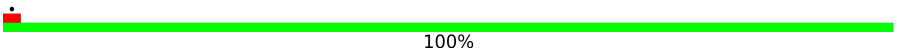
Chain f:

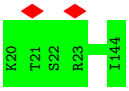




• Molecule 33: Ribosomal protein L35Ae family protein

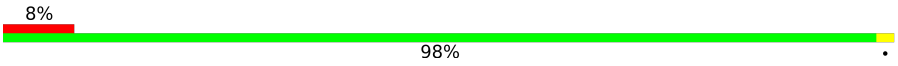
Chain g:

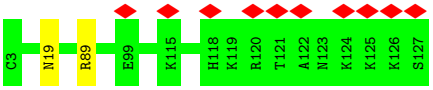




• Molecule 34: 60S ribosomal protein L34, putative

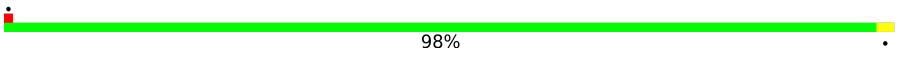
Chain h:

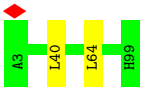




• Molecule 35: 60S ribosomal protein L36, putative

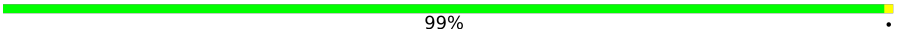
Chain i:





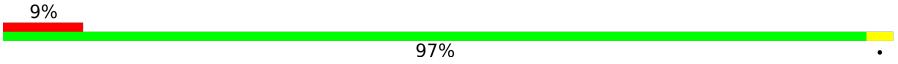
• Molecule 36: 60S ribosomal protein L37

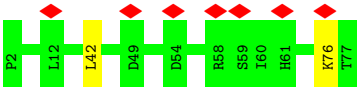
Chain j:



• Molecule 37: Ribosomal L38e family protein

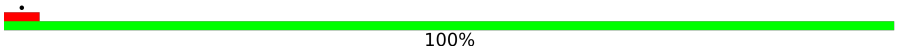
Chain k:

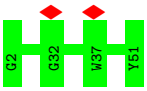




• Molecule 38: 60S ribosomal protein L39, putative

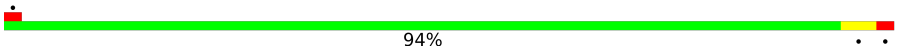
Chain l:

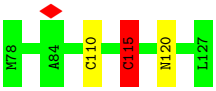




• Molecule 39: Ubiquitin-60S ribosomal protein L40

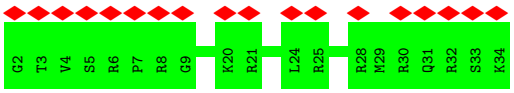
Chain m:





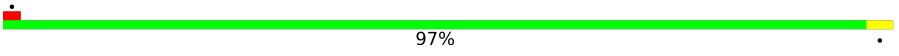
• Molecule 40: ribosomal protein eL41

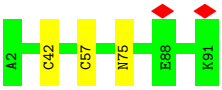
Chain n:



• Molecule 41: 60S ribosomal protein L37a

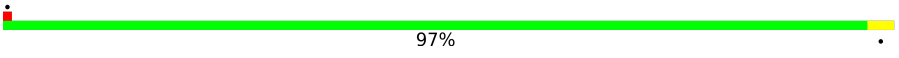
Chain o:

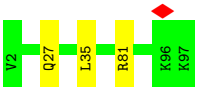




• Molecule 42: 60S ribosomal protein L44, putative

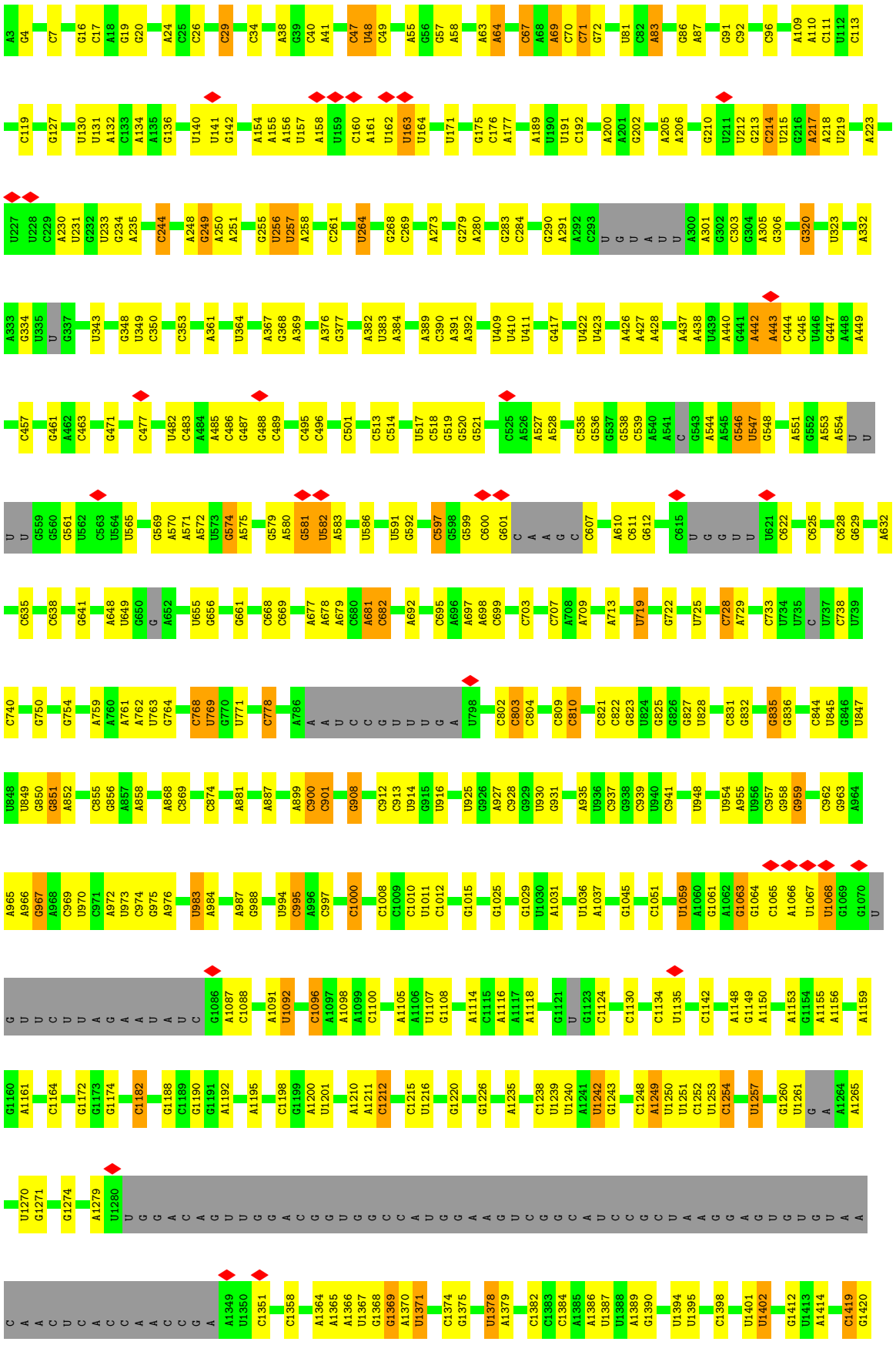
Chain p:

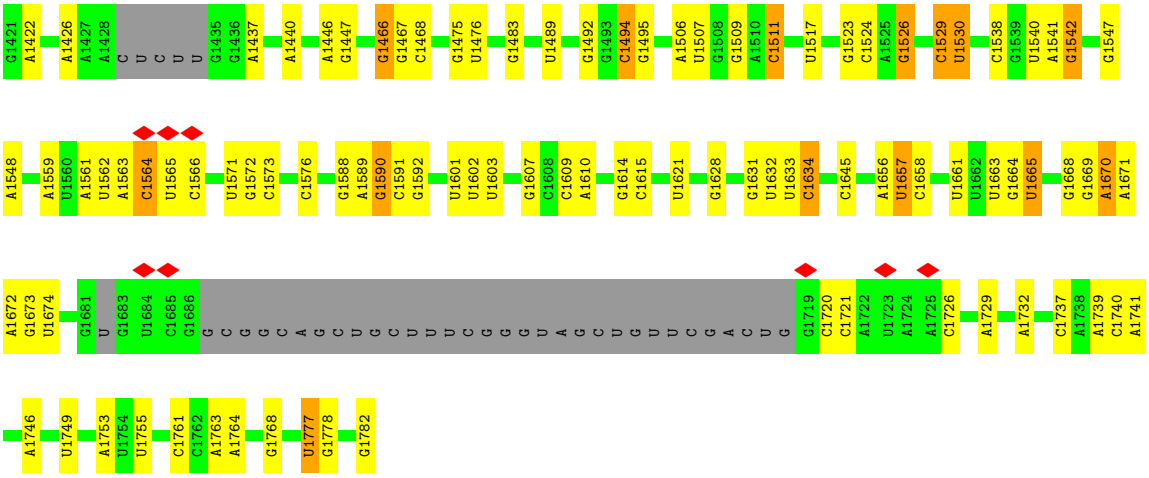




• Molecule 43: rRNA alpha

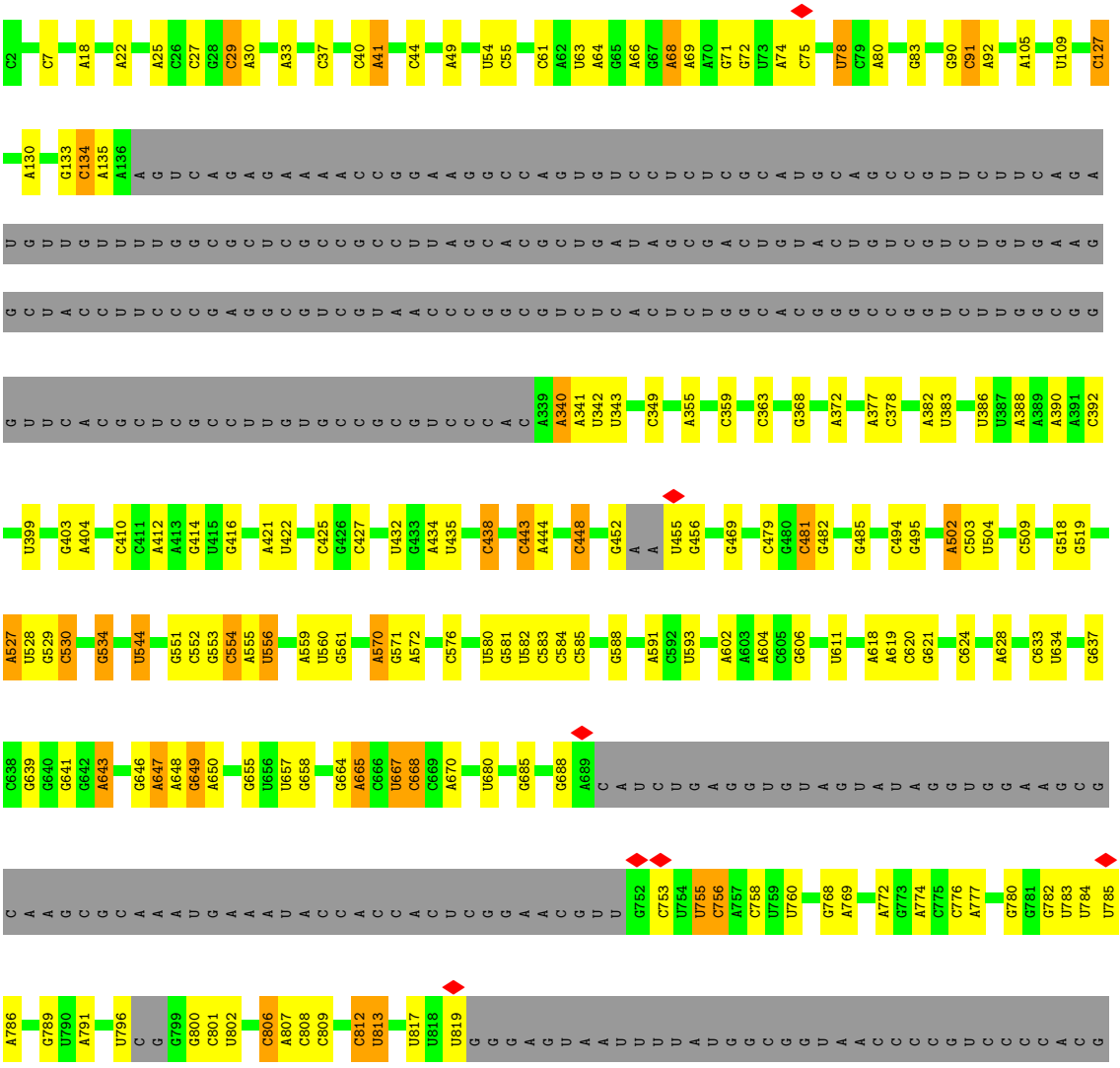
Chain 1:

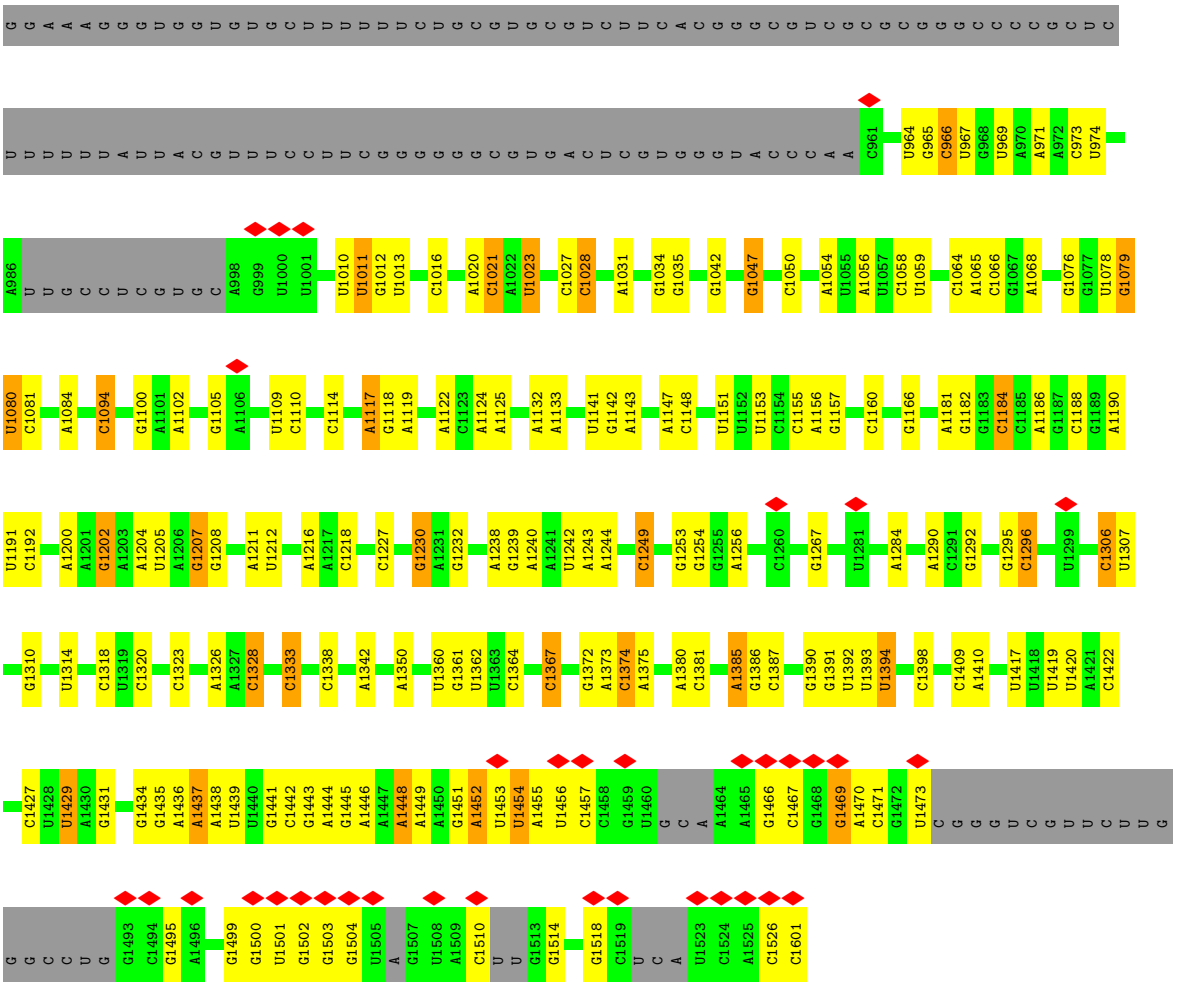




• Molecule 44: rRNA beta

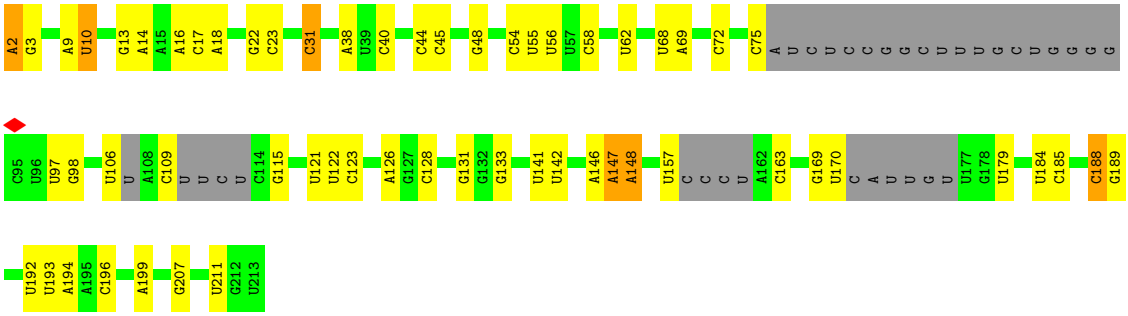
Chain 2:





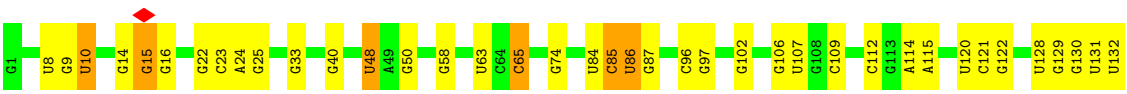
• Molecule 45: rRNA gamma

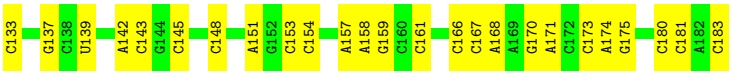
Chain 3:



• Molecule 46: rRNA delta

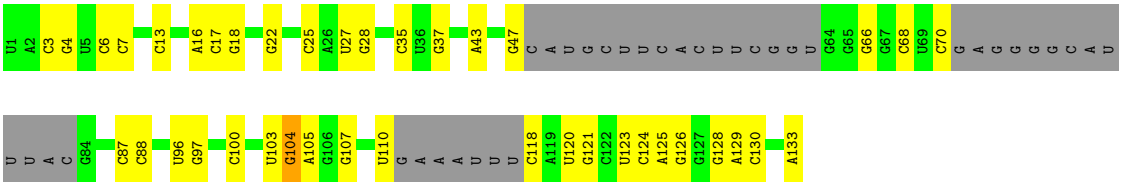
Chain 4:





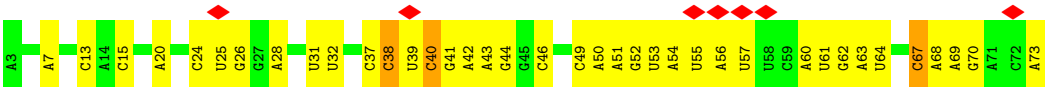
• Molecule 47: rRNA epsilon

Chain 5:



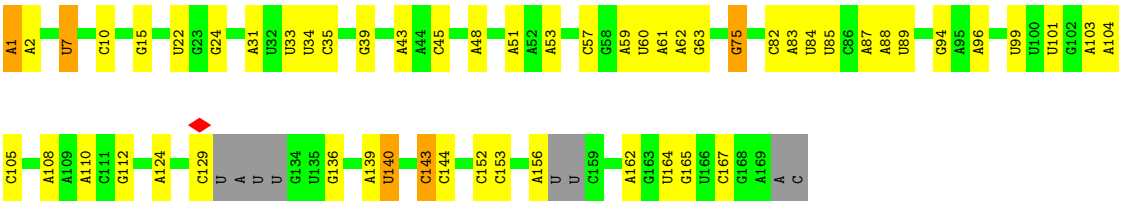
• Molecule 48: rRNA zeta

Chain 6:



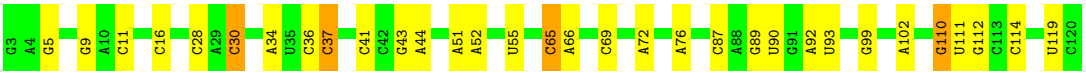
• Molecule 49: rRNA 5.8S

Chain 7:



• Molecule 50: rRNA 5S

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141028	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 ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	-0.407	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	391.68, 391.68, 391.68	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PAR, MG, OMC, A2M, OMG, OMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.54	0/2042	0.67	1/2735 (0.0%)
2	B	0.48	0/3313	0.68	1/4460 (0.0%)
3	C	0.46	0/2880	0.68	2/3879 (0.1%)
4	D	0.35	0/1242	0.60	0/1678
5	E	0.38	0/1468	0.61	0/1983
6	F	0.40	0/1024	0.63	0/1397
7	G	0.48	1/1777 (0.1%)	0.68	1/2390 (0.0%)
8	H	0.48	1/1825 (0.1%)	0.70	2/2452 (0.1%)
9	I	0.44	0/1680	0.63	1/2257 (0.0%)
10	J	0.49	0/1018	0.69	2/1373 (0.1%)
11	K	0.38	0/1184	0.60	0/1599
12	L	0.48	0/1153	0.68	1/1541 (0.1%)
13	M	0.52	1/1754 (0.1%)	0.67	1/2342 (0.0%)
14	N	0.35	0/1486	0.56	0/2006
15	O	0.41	0/2013	0.67	3/2703 (0.1%)
16	P	0.49	0/1564	0.68	1/2092 (0.0%)
17	Q	0.39	0/1470	0.54	0/1966
18	R	0.47	0/1488	0.64	0/2005
19	S	0.49	0/1235	0.67	0/1663
20	T	0.51	0/1260	0.62	0/1688
21	U	0.39	0/949	0.69	0/1271
22	V	0.44	0/946	0.67	1/1276 (0.1%)
23	W	0.41	0/985	0.65	0/1315
24	X	0.46	0/574	0.59	0/773
25	Y	0.44	0/1064	0.63	1/1430 (0.1%)
26	Z	0.41	0/1082	0.60	0/1452
27	a	0.38	0/996	0.63	0/1333
28	b	0.39	0/550	0.60	0/734
29	c	0.46	0/1842	0.65	1/2473 (0.0%)
30	d	0.39	0/701	0.64	0/953
31	e	0.42	0/951	0.70	1/1274 (0.1%)
32	f	0.50	0/1071	0.67	1/1434 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	g	0.51	0/1019	0.66	0/1372
34	h	0.48	0/1029	0.72	0/1370
35	i	0.38	0/774	0.63	2/1036 (0.2%)
36	j	0.52	0/677	0.70	0/904
37	k	0.42	0/583	0.60	1/787 (0.1%)
38	l	0.49	0/453	0.56	0/606
39	m	0.55	1/399 (0.3%)	0.83	2/531 (0.4%)
40	n	0.51	0/284	0.80	0/372
41	o	0.61	2/708 (0.3%)	0.77	1/944 (0.1%)
42	p	0.49	0/769	0.67	1/1021 (0.1%)
43	1	0.89	2/38135 (0.0%)	1.17	279/59442 (0.5%)
44	2	0.86	1/24785 (0.0%)	1.18	187/38608 (0.5%)
45	3	0.83	0/4162	1.21	34/6469 (0.5%)
46	4	0.84	0/4341	1.17	36/6767 (0.5%)
47	5	0.86	0/2317	1.21	26/3604 (0.7%)
48	6	0.64	0/1650	1.12	12/2568 (0.5%)
49	7	0.88	0/3770	1.23	39/5868 (0.7%)
50	8	0.72	0/2807	1.16	29/4371 (0.7%)
All	All	0.73	9/133249 (0.0%)	1.03	670/196567 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1
6	F	0	1
15	O	0	1
31	e	0	1
39	m	0	1
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	m	115	CYS	CB-SG	7.29	1.94	1.82
44	2	1601	C	C1'-N1	6.34	1.58	1.48
41	o	42	CYS	CB-SG	5.97	1.92	1.82
13	M	121	VAL	CB-CG2	-5.42	1.41	1.52
7	G	141	VAL	CB-CG2	-5.41	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	o	57	CYS	CB-SG	5.25	1.91	1.82
8	H	53	VAL	CB-CG1	-5.22	1.41	1.52
43	1	83	A	N9-C4	-5.02	1.34	1.37
43	1	908	G	N9-C4	-5.01	1.33	1.38

All (670) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	966	C	N1-C2-O2	12.51	126.41	118.90
44	2	966	C	C2-N1-C1'	12.15	132.17	118.80
43	1	256	U	C2-N1-C1'	11.99	132.09	117.70
47	5	104	G	N7-C8-N9	11.16	118.68	113.10
43	1	778	C	N3-C2-O2	-11.06	114.16	121.90
46	4	132	U	O4'-C1'-N1	11.01	117.01	108.20
39	m	115	CYS	CA-CB-SG	10.89	133.60	114.00
44	2	966	C	N3-C2-O2	-10.89	114.28	121.90
44	2	667	OMU	OP1-P-O3'	-10.75	81.56	105.20
43	1	1012	C	N1-C2-O2	10.63	125.28	118.90
47	5	104	G	C8-N9-C4	-10.60	102.16	106.40
41	o	42	CYS	CA-CB-SG	10.58	133.05	114.00
43	1	1564	C	N1-C2-O2	10.52	125.21	118.90
43	1	1182	C	N1-C2-O2	10.49	125.20	118.90
43	1	778	C	N1-C2-O2	10.47	125.19	118.90
43	1	256	U	N1-C2-O2	10.27	129.99	122.80
48	6	57	U	N1-C2-O2	10.17	129.92	122.80
43	1	973	U	C2-N1-C1'	10.13	129.85	117.70
45	3	31	C	C2-N1-C1'	9.81	129.59	118.80
45	3	31	C	N1-C2-O2	9.71	124.73	118.90
44	2	91	C	N3-C2-O2	-9.57	115.20	121.90
48	6	57	U	C2-N1-C1'	9.57	129.19	117.70
45	3	31	C	N3-C2-O2	-9.53	115.23	121.90
45	3	185	C	C2-N1-C1'	9.46	129.20	118.80
43	1	256	U	N3-C2-O2	-9.42	115.61	122.20
44	2	667	OMU	OP2-P-O3'	-9.37	84.58	105.20
43	1	973	U	N1-C2-O2	9.32	129.33	122.80
43	1	1254	C	C2-N1-C1'	9.31	129.04	118.80
44	2	479	C	N1-C2-O2	9.30	124.48	118.90
50	8	65	C	N1-C2-O2	9.24	124.45	118.90
44	2	134	C	N1-C2-O2	9.22	124.43	118.90
43	1	1012	C	C2-N1-C1'	9.17	128.89	118.80
44	2	91	C	N1-C2-O2	9.13	124.38	118.90
45	3	72	C	N1-C2-O2	9.12	124.37	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1023	U	N1-C2-O2	9.10	129.17	122.80
45	3	185	C	N1-C2-O2	9.07	124.34	118.90
43	1	1494	C	O4'-C1'-N1	9.03	115.42	108.20
44	2	91	C	C2-N1-C1'	8.99	128.69	118.80
43	1	1012	C	N3-C2-O2	-8.98	115.61	121.90
44	2	479	C	C2-N1-C1'	8.93	128.63	118.80
44	2	1191	U	N3-C2-O2	-8.86	116.00	122.20
45	3	31	C	C6-N1-C2	-8.86	116.76	120.30
44	2	1023	U	C2-N1-C1'	8.84	128.30	117.70
46	4	112	C	C6-N1-C2	-8.83	116.77	120.30
45	3	128	C	C2-N1-C1'	8.78	128.46	118.80
50	8	11	C	N1-C2-O2	8.75	124.15	118.90
43	1	1564	C	C2-N1-C1'	8.71	128.38	118.80
48	6	57	U	N3-C2-O2	-8.70	116.11	122.20
44	2	966	C	C6-N1-C2	-8.70	116.82	120.30
43	1	973	U	N3-C2-O2	-8.67	116.13	122.20
43	1	1573	C	C2-N1-C1'	8.63	128.29	118.80
44	2	554	C	C6-N1-C2	-8.61	116.86	120.30
43	1	778	C	C2-N1-C1'	8.55	128.21	118.80
43	1	256	U	C6-N1-C1'	-8.54	109.24	121.20
50	8	90	U	N3-C2-O2	-8.54	116.22	122.20
43	1	447	G	O4'-C1'-N9	8.45	114.96	108.20
46	4	10	U	N3-C2-O2	-8.35	116.36	122.20
43	1	1254	C	N1-C2-O2	8.34	123.90	118.90
46	4	63	U	C2-N1-C1'	8.31	127.67	117.70
44	2	1064	C	C2-N1-C1'	8.24	127.87	118.80
44	2	649	G	O5'-P-OP2	-8.22	98.30	105.70
46	4	10	U	N1-C2-O2	8.21	128.55	122.80
44	2	966	C	C6-N1-C1'	-8.20	110.97	120.80
43	1	47	C	N1-C2-O2	8.17	123.81	118.90
43	1	1564	C	N3-C2-O2	-8.16	116.19	121.90
45	3	128	C	N1-C2-O2	8.16	123.80	118.90
47	5	3	C	N3-C2-O2	-8.16	116.19	121.90
49	7	35	C	C6-N1-C2	-8.15	117.04	120.30
44	2	1011	U	C2-N1-C1'	8.12	127.44	117.70
43	1	994	U	N3-C2-O2	-8.10	116.53	122.20
43	1	1466	G	C4-N9-C1'	8.09	137.02	126.50
44	2	1023	U	N3-C2-O2	-8.08	116.55	122.20
49	7	85	U	N1-C2-O2	8.03	128.42	122.80
47	5	104	G	C4-N9-C1'	8.01	136.92	126.50
43	1	582	U	C2-N1-C1'	8.00	127.30	117.70
43	1	1257	U	C2-N1-C1'	7.98	127.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	7	143	C	N1-C2-O2	7.97	123.68	118.90
44	2	812	C	C2-N1-C1'	7.96	127.56	118.80
43	1	916	U	C2-N1-C1'	7.96	127.25	117.70
50	8	87	C	N1-C2-O2	7.96	123.67	118.90
44	2	479	C	N3-C2-O2	-7.96	116.33	121.90
50	8	37	C	C2-N1-C1'	7.95	127.55	118.80
43	1	1466	G	C8-N9-C1'	-7.94	116.68	127.00
44	2	802	U	N3-C2-O2	-7.89	116.68	122.20
44	2	1011	U	N1-C2-O2	7.84	128.29	122.80
43	1	1092	U	O5'-P-OP1	7.82	120.08	110.70
44	2	812	C	N1-C2-O2	7.79	123.57	118.90
44	2	1191	U	C2-N1-C1'	7.74	126.99	117.70
43	1	1254	C	N3-C2-O2	-7.73	116.49	121.90
44	2	554	C	N3-C2-O2	-7.63	116.56	121.90
43	1	962	C	C6-N1-C2	-7.63	117.25	120.30
44	2	812	C	C6-N1-C2	-7.62	117.25	120.30
43	1	869	C	C6-N1-C2	-7.61	117.26	120.30
44	2	37	C	C6-N1-C2	-7.58	117.27	120.30
43	1	1182	C	C2-N3-C4	7.57	123.69	119.90
44	2	755	U	P-O3'-C3'	7.56	128.77	119.70
50	8	65	C	N3-C2-O2	-7.54	116.62	121.90
46	4	63	U	N3-C2-O2	-7.54	116.92	122.20
44	2	1011	U	N3-C2-O2	-7.53	116.93	122.20
50	8	90	U	C2-N1-C1'	7.52	126.73	117.70
2	B	203	LEU	CA-CB-CG	7.51	132.57	115.30
43	1	1761	C	N1-C2-O2	7.48	123.39	118.90
49	7	164	U	C2-N1-C1'	7.48	126.68	117.70
43	1	501	C	N1-C2-O2	7.47	123.38	118.90
50	8	65	C	C2-N1-C1'	7.43	126.97	118.80
49	7	85	U	N3-C2-O2	-7.42	117.00	122.20
44	2	1502	G	C4-N9-C1'	7.41	136.13	126.50
47	5	3	C	C2-N1-C1'	7.39	126.92	118.80
43	1	1242	U	C2-N1-C1'	7.38	126.56	117.70
49	7	85	U	C2-N1-C1'	7.37	126.55	117.70
43	1	1573	C	C6-N1-C2	-7.36	117.35	120.30
50	8	37	C	N1-C2-O2	7.35	123.31	118.90
43	1	682	C	C6-N1-C2	-7.34	117.36	120.30
43	1	1164	C	N1-C2-O2	7.32	123.29	118.90
44	2	29	C	P-O3'-C3'	7.31	128.47	119.70
44	2	134	C	N3-C2-O2	-7.31	116.78	121.90
43	1	1737	C	N1-C2-O2	7.30	123.28	118.90
43	1	607	C	C2-N1-C1'	7.29	126.81	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	217	A	P-O3'-C3'	7.27	128.43	119.70
45	3	185	C	C6-N1-C1'	-7.24	112.12	120.80
50	8	90	U	N1-C2-O2	7.23	127.86	122.80
45	3	147	A	N7-C8-N9	7.23	117.42	113.80
43	1	1242	U	N1-C2-O2	7.22	127.85	122.80
44	2	1502	G	N3-C4-N9	7.22	130.33	126.00
47	5	3	C	N1-C2-O2	7.21	123.22	118.90
44	2	812	C	N3-C2-O2	-7.21	116.86	121.90
44	2	18	A	C6-N1-C2	7.20	122.92	118.60
50	8	37	C	N3-C2-O2	-7.20	116.86	121.90
44	2	1526	C	OP2-P-O3'	7.19	121.02	105.20
43	1	916	U	N3-C2-O2	-7.18	117.17	122.20
46	4	181	C	N1-C2-O2	7.18	123.21	118.90
44	2	1502	G	N3-C4-C5	-7.17	125.02	128.60
44	2	1526	C	O3'-P-O5'	-7.17	90.38	104.00
46	4	10	U	C2-N1-C1'	7.17	126.30	117.70
49	7	99	U	N1-C2-O2	7.17	127.81	122.80
43	1	1466	G	N3-C4-N9	7.16	130.29	126.00
44	2	802	U	N1-C2-O2	7.15	127.80	122.80
43	1	962	C	C5-C6-N1	7.11	124.55	121.00
44	2	1192	C	C6-N1-C2	-7.09	117.46	120.30
46	4	148	C	N1-C2-O2	7.09	123.15	118.90
45	3	2	A	P-O3'-C3'	7.09	128.21	119.70
43	1	778	C	C6-N1-C2	-7.08	117.47	120.30
43	1	96	C	N1-C2-O2	7.07	123.14	118.90
43	1	1242	U	N3-C2-O2	-7.06	117.26	122.20
44	2	378	C	C6-N1-C2	-7.05	117.48	120.30
45	3	185	C	N3-C2-O2	-7.05	116.97	121.90
48	6	67	C	N1-C2-O2	7.05	123.13	118.90
43	1	1063	G	P-O3'-C3'	7.01	128.11	119.70
44	2	1064	C	N1-C2-O2	7.00	123.10	118.90
43	1	607	C	N1-C2-O2	6.98	123.09	118.90
50	8	11	C	N3-C2-O2	-6.97	117.02	121.90
43	1	941	C	N3-C2-O2	-6.96	117.03	121.90
44	2	668	C	OP1-P-OP2	6.96	130.04	119.60
46	4	63	U	N1-C2-O2	6.96	127.67	122.80
45	3	72	C	N3-C2-O2	-6.95	117.03	121.90
10	J	71	LEU	CA-CB-CG	6.94	131.27	115.30
45	3	128	C	N3-C2-O2	-6.93	117.05	121.90
44	2	432	U	N3-C2-O2	-6.93	117.35	122.20
46	4	86	U	N1-C2-O2	6.91	127.64	122.80
44	2	55	C	N1-C2-O2	6.90	123.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	1182	C	C5-C6-N1	6.88	124.44	121.00
49	7	99	U	C2-N1-C1'	6.87	125.95	117.70
45	3	54	C	C6-N1-C2	-6.87	117.55	120.30
46	4	86	U	C2-N1-C1'	6.85	125.92	117.70
49	7	164	U	N3-C2-O2	-6.83	117.42	122.20
43	1	1257	U	N1-C2-O2	6.83	127.58	122.80
44	2	1028	C	C6-N1-C2	-6.80	117.58	120.30
44	2	27	C	C6-N1-C2	-6.80	117.58	120.30
47	5	104	G	C5-N7-C8	-6.79	100.90	104.30
47	5	104	G	C6-C5-N7	-6.79	126.33	130.40
43	1	740	C	C6-N1-C2	-6.78	117.59	120.30
43	1	769	U	N3-C2-O2	-6.77	117.46	122.20
49	7	45	C	C6-N1-C2	-6.77	117.59	120.30
43	1	217	A	OP2-P-O3'	6.77	120.09	105.20
46	4	65	C	C6-N1-C2	-6.76	117.59	120.30
43	1	214	C	P-O3'-C3'	6.76	127.81	119.70
43	1	1511	C	N1-C2-O2	6.75	122.95	118.90
44	2	55	C	N3-C2-O2	-6.75	117.18	121.90
44	2	448	C	C6-N1-C2	-6.73	117.61	120.30
44	2	813	U	N3-C2-O2	-6.71	117.50	122.20
43	1	738	C	O5'-P-OP1	-6.70	99.67	105.70
44	2	134	C	C2-N1-C1'	6.70	126.17	118.80
44	2	509	C	C6-N1-C2	-6.70	117.62	120.30
49	7	164	U	N1-C2-O2	6.70	127.49	122.80
43	1	1212	C	N1-C2-O2	6.69	122.92	118.90
16	P	52	LEU	CA-CB-CG	6.69	130.69	115.30
47	5	17	C	C6-N1-C2	-6.69	117.62	120.30
43	1	582	U	N3-C2-O2	-6.69	117.52	122.20
49	7	35	C	C5-C6-N1	6.68	124.34	121.00
44	2	1394	U	N1-C2-O2	6.64	127.45	122.80
43	1	1164	C	C6-N1-C2	-6.63	117.65	120.30
43	1	916	U	N1-C2-O2	6.62	127.43	122.80
22	V	116	LEU	CA-CB-CG	6.62	130.51	115.30
43	1	768	C	P-O3'-C3'	6.62	127.64	119.70
44	2	1191	U	N1-C2-O2	6.61	127.43	122.80
44	2	1028	C	N1-C2-O2	6.60	122.86	118.90
44	2	813	U	C2-N1-C1'	6.58	125.60	117.70
44	2	813	U	N1-C2-O2	6.58	127.41	122.80
15	O	196	LEU	CA-CB-CG	6.58	130.43	115.30
43	1	1096	C	N1-C2-O2	6.57	122.84	118.90
43	1	1402	U	N3-C2-O2	-6.57	117.60	122.20
47	5	88	C	C6-N1-C2	-6.57	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	1369	G	P-O3'-C3'	6.56	127.57	119.70
43	1	244	C	C5-C6-N1	6.55	124.28	121.00
44	2	127	C	N1-C2-O2	6.55	122.83	118.90
46	4	181	C	N3-C2-O2	-6.55	117.32	121.90
44	2	91	C	C6-N1-C2	-6.54	117.69	120.30
48	6	57	U	C6-N1-C1'	-6.54	112.05	121.20
46	4	15	G	P-O3'-C3'	6.54	127.54	119.70
43	1	40	C	C6-N1-C2	-6.50	117.70	120.30
43	1	1254	C	C6-N1-C1'	-6.50	113.00	120.80
49	7	99	U	N3-C2-O2	-6.50	117.65	122.20
43	1	983	U	P-O3'-C3'	6.49	127.49	119.70
43	1	496	C	C6-N1-C2	-6.49	117.71	120.30
44	2	481	C	N1-C2-O2	6.48	122.79	118.90
43	1	638	C	C2-N1-C1'	6.47	125.92	118.80
31	e	102	LEU	CA-CB-CG	6.46	130.17	115.30
44	2	1184	C	N1-C2-O2	6.46	122.78	118.90
43	1	67	C	N1-C2-O2	6.45	122.77	118.90
43	1	966	A	C2-N3-C4	6.45	113.83	110.60
43	1	769	U	N1-C2-O2	6.44	127.31	122.80
43	1	445	C	N1-C2-O2	6.44	122.76	118.90
43	1	546	G	C2-N3-C4	6.44	115.12	111.90
43	1	1402	U	N1-C2-O2	6.43	127.30	122.80
49	7	82	C	N1-C2-O2	6.42	122.75	118.90
43	1	1164	C	C2-N1-C1'	6.41	125.85	118.80
49	7	143	C	N3-C2-O2	-6.40	117.42	121.90
13	M	116	LEU	CA-CB-CG	6.40	130.02	115.30
43	1	496	C	N1-C2-O2	6.40	122.74	118.90
43	1	1670	A	O4'-C1'-N9	6.37	113.29	108.20
43	1	1726	C	N1-C2-O2	6.37	122.72	118.90
44	2	1333	C	C6-N1-C2	-6.36	117.75	120.30
45	3	148	A	O4'-C1'-N9	6.36	113.28	108.20
45	3	128	C	C6-N1-C1'	-6.35	113.18	120.80
44	2	1419	U	C5-C6-N1	6.35	125.88	122.70
43	1	1590	G	O4'-C1'-N9	6.34	113.27	108.20
43	1	1012	C	C6-N1-C2	-6.34	117.77	120.30
43	1	607	C	N3-C2-O2	-6.33	117.47	121.90
43	1	1172	G	N3-C4-N9	6.33	129.80	126.00
43	1	869	C	C5-C6-N1	6.33	124.17	121.00
44	2	44	C	C6-N1-C2	-6.33	117.77	120.30
46	4	153	C	N1-C2-O2	6.33	122.70	118.90
44	2	1502	G	C8-N9-C1'	-6.32	118.78	127.00
43	1	973	U	C6-N1-C1'	-6.31	112.36	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1064	C	N3-C2-O2	-6.31	117.48	121.90
44	2	479	C	C6-N1-C1'	-6.31	113.23	120.80
43	1	939	C	C5-C6-N1	6.29	124.15	121.00
48	6	38	C	P-O3'-C3'	6.29	127.25	119.70
43	1	40	C	C5-C6-N1	6.29	124.14	121.00
43	1	682	C	C5-C6-N1	6.28	124.14	121.00
43	1	969	C	C6-N1-C2	-6.28	117.79	120.30
43	1	1576	C	N1-C2-O2	6.28	122.67	118.90
43	1	703	C	C6-N1-C2	-6.28	117.79	120.30
44	2	37	C	C5-C6-N1	6.27	124.14	121.00
43	1	997	C	C5-C6-N1	6.27	124.14	121.00
47	5	35	C	N1-C2-O2	6.26	122.66	118.90
43	1	973	U	C5-C6-N1	6.26	125.83	122.70
43	1	1564	C	C6-N1-C1'	-6.25	113.30	120.80
43	1	1737	C	N3-C2-O2	-6.25	117.53	121.90
44	2	966	C	C5-C6-N1	6.24	124.12	121.00
47	5	3	C	C6-N1-C2	-6.22	117.81	120.30
43	1	1012	C	C6-N1-C1'	-6.21	113.34	120.80
47	5	17	C	C5-C6-N1	6.20	124.10	121.00
43	1	29	C	N1-C2-O2	6.20	122.62	118.90
43	1	1602	U	C4-C5-C6	6.16	123.40	119.70
43	1	1254	C	C6-N1-C2	-6.15	117.84	120.30
43	1	1172	G	C4-N9-C1'	6.15	134.49	126.50
43	1	1632	U	N1-C2-O2	6.15	127.10	122.80
46	4	86	U	N3-C2-O2	-6.14	117.90	122.20
43	1	939	C	C6-N1-C2	-6.14	117.85	120.30
43	1	1573	C	N3-C2-O2	-6.13	117.61	121.90
44	2	1021	C	N1-C2-O2	6.13	122.58	118.90
43	1	1092	U	OP1-P-OP2	-6.09	110.46	119.60
43	1	364	U	N1-C2-O2	6.09	127.06	122.80
44	2	425	C	C2-N1-C1'	6.09	125.50	118.80
43	1	501	C	N3-C2-O2	-6.07	117.65	121.90
43	1	1576	C	N3-C2-O2	-6.07	117.65	121.90
44	2	576	C	C6-N1-C2	-6.06	117.88	120.30
50	8	69	C	C6-N1-C2	-6.06	117.88	120.30
43	1	47	C	N3-C2-O2	-6.05	117.66	121.90
44	2	1023	U	C6-N1-C1'	-6.05	112.73	121.20
44	2	68	A	P-O3'-C3'	6.05	126.96	119.70
43	1	582	U	N1-C2-O2	6.04	127.03	122.80
43	1	997	C	C6-N1-C2	-6.04	117.88	120.30
44	2	1080	U	N1-C2-O2	6.04	127.03	122.80
44	2	647	A	O4'-C1'-N9	6.04	113.03	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	91	C	C6-N1-C1'	-6.03	113.56	120.80
43	1	1254	C	O4'-C1'-N1	6.03	113.02	108.20
44	2	1437	A	P-O3'-C3'	6.03	126.93	119.70
43	1	963	G	N1-C6-O6	6.02	123.51	119.90
43	1	7	C	C6-N1-C2	-6.02	117.89	120.30
44	2	340	A	P-O3'-C3'	6.02	126.92	119.70
43	1	1164	C	N3-C2-O2	-6.00	117.70	121.90
43	1	901	C	N1-C2-O2	6.00	122.50	118.90
44	2	1027	C	N1-C2-O2	5.99	122.50	118.90
44	2	1394	U	N3-C2-O2	-5.98	118.02	122.20
43	1	1632	U	N3-C2-O2	-5.97	118.02	122.20
45	3	31	C	C6-N1-C1'	-5.97	113.64	120.80
43	1	1602	U	N1-C2-N3	5.96	118.48	114.90
49	7	35	C	N1-C2-O2	5.96	122.48	118.90
43	1	844	C	C6-N1-C2	-5.96	117.92	120.30
43	1	1374	C	C6-N1-C2	-5.96	117.92	120.30
43	1	1172	G	N3-C4-C5	-5.95	125.62	128.60
47	5	35	C	N3-C2-O2	-5.95	117.74	121.90
48	6	38	C	OP1-P-O3'	5.93	118.24	105.20
44	2	633	C	C6-N1-C2	-5.92	117.93	120.30
43	1	214	C	OP1-P-O3'	5.92	118.22	105.20
43	1	707	C	C6-N1-C2	-5.92	117.93	120.30
47	5	7	C	C6-N1-C2	-5.92	117.93	120.30
50	8	65	C	C6-N1-C2	-5.91	117.94	120.30
43	1	1358	C	C6-N1-C2	-5.90	117.94	120.30
43	1	719	U	O4'-C1'-N1	5.90	112.92	108.20
43	1	1059	U	N3-C2-O2	-5.90	118.07	122.20
44	2	1081	C	C6-N1-C2	-5.90	117.94	120.30
44	2	1202	G	N7-C8-N9	5.90	116.05	113.10
47	5	68	C	N3-C2-O2	-5.90	117.77	121.90
50	8	16	C	C6-N1-C2	-5.90	117.94	120.30
43	1	1517	U	N1-C2-O2	5.89	126.93	122.80
49	7	1	A	P-O3'-C3'	5.89	126.77	119.70
49	7	99	U	C5-C6-N1	5.89	125.64	122.70
43	1	1198	C	C6-N1-C2	-5.88	117.95	120.30
32	f	116	LEU	CA-CB-CG	5.88	128.82	115.30
50	8	87	C	N3-C2-O2	-5.88	117.78	121.90
45	3	179	U	C2-N1-C1'	5.87	124.75	117.70
50	8	87	C	C2-N1-C1'	5.87	125.26	118.80
44	2	1028	C	N3-C2-O2	-5.86	117.80	121.90
15	O	152	LEU	CA-CB-CG	5.86	128.77	115.30
43	1	113	C	C6-N1-C2	-5.86	117.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	1378	U	P-O3'-C3'	5.86	126.73	119.70
44	2	27	C	C5-C6-N1	5.85	123.93	121.00
44	2	41	A	O4'-C1'-N9	5.85	112.88	108.20
47	5	35	C	C6-N1-C2	-5.85	117.96	120.30
43	1	1384	C	N1-C2-O2	5.85	122.41	118.90
44	2	1064	C	C6-N1-C2	-5.85	117.96	120.30
49	7	112	G	C4-N9-C1'	5.85	134.10	126.50
43	1	1419	C	C6-N1-C2	-5.84	117.96	120.30
43	1	1257	U	C5-C6-N1	5.84	125.62	122.70
46	4	139	U	C5-C6-N1	5.83	125.61	122.70
43	1	1068	U	C2-N1-C1'	5.83	124.69	117.70
43	1	1212	C	C2-N1-C1'	5.82	125.21	118.80
44	2	1021	C	N3-C2-O2	-5.82	117.82	121.90
43	1	1351	C	N1-C2-O2	5.82	122.39	118.90
43	1	364	U	N3-C2-O2	-5.82	118.13	122.20
49	7	167	C	N1-C2-O2	5.82	122.39	118.90
44	2	554	C	C2-N1-C1'	5.81	125.19	118.80
12	L	129	LEU	CA-CB-CG	5.81	128.66	115.30
43	1	496	C	C5-C6-N1	5.81	123.91	121.00
47	5	118	C	N1-C2-O2	5.81	122.39	118.90
43	1	967	G	OP1-P-O3'	5.81	117.98	105.20
43	1	1172	G	C8-N9-C1'	-5.80	119.45	127.00
43	1	913	C	N1-C2-O2	5.80	122.38	118.90
49	7	153	C	C6-N1-C2	-5.80	117.98	120.30
44	2	1094	C	N1-C2-O2	5.79	122.37	118.90
43	1	1382	C	C6-N1-C2	-5.79	117.98	120.30
46	4	23	C	C6-N1-C2	-5.78	117.99	120.30
50	8	30	C	N1-C2-O2	5.78	122.37	118.90
44	2	54	U	N3-C2-O2	-5.78	118.16	122.20
43	1	941	C	C6-N1-C2	-5.77	117.99	120.30
44	2	438	C	N1-C2-O2	5.77	122.36	118.90
43	1	707	C	N1-C2-O2	5.77	122.36	118.90
44	2	1058	C	C6-N1-C2	-5.76	118.00	120.30
43	1	1100	C	C6-N1-C2	-5.76	118.00	120.30
43	1	1257	U	N3-C2-O2	-5.75	118.17	122.20
43	1	547	U	N1-C2-O2	5.75	126.83	122.80
46	4	153	C	N3-C2-O2	-5.75	117.88	121.90
47	5	130	C	N1-C2-O2	5.74	122.34	118.90
43	1	810	C	C6-N1-C2	-5.74	118.01	120.30
46	4	65	C	C5-C6-N1	5.74	123.87	121.00
43	1	963	G	C5-C6-O6	-5.73	125.16	128.60
46	4	48	U	O4'-C1'-N1	5.73	112.79	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	7	101	U	N1-C2-O2	5.73	126.81	122.80
39	m	110	CYS	CA-CB-SG	5.72	124.30	114.00
43	1	1365	A	O4'-C1'-N9	5.72	112.77	108.20
44	2	481	C	C6-N1-C2	-5.71	118.01	120.30
43	1	1402	U	C2-N1-C1'	5.71	124.55	117.70
1	A	102	LEU	CA-CB-CG	5.71	128.43	115.30
44	2	127	C	N3-C2-O2	-5.71	117.91	121.90
49	7	167	C	C2-N1-C1'	5.70	125.07	118.80
44	2	808	C	N1-C2-O2	5.70	122.32	118.90
45	3	147	A	C8-N9-C4	-5.69	103.52	105.80
43	1	1576	C	C2-N1-C1'	5.69	125.06	118.80
43	1	804	C	N1-C2-O2	5.68	122.31	118.90
44	2	1333	C	N1-C2-O2	5.68	122.31	118.90
43	1	249	G	P-O3'-C3'	5.68	126.52	119.70
43	1	1419	C	N1-C2-O2	5.68	122.31	118.90
44	2	134	C	P-O3'-C3'	5.68	126.51	119.70
45	3	23	C	N1-C2-O2	5.68	122.31	118.90
43	1	49	C	C6-N1-C2	-5.67	118.03	120.30
37	k	42	LEU	CA-CB-CG	5.66	128.33	115.30
43	1	442	A	O4'-C1'-N9	5.66	112.73	108.20
44	2	1117	A	C2-N3-C4	5.65	113.43	110.60
43	1	966	A	N1-C6-N6	-5.65	115.21	118.60
44	2	1333	C	C5-C6-N1	5.65	123.83	121.00
50	8	30	C	C6-N1-C2	-5.65	118.04	120.30
44	2	753	C	C6-N1-C2	-5.64	118.04	120.30
44	2	1192	C	C5-C6-N1	5.64	123.82	121.00
44	2	1429	U	N3-C2-O2	-5.64	118.25	122.20
43	1	1384	C	C6-N1-C2	-5.64	118.05	120.30
9	I	43	LEU	CA-CB-CG	5.63	128.25	115.30
50	8	11	C	C2-N1-C1'	5.63	125.00	118.80
44	2	54	U	N1-C2-O2	5.63	126.74	122.80
49	7	82	C	N3-C2-O2	-5.62	117.96	121.90
43	1	350	C	C6-N1-C2	-5.62	118.05	120.30
43	1	581	G	P-O3'-C3'	5.62	126.45	119.70
43	1	1000	C	C6-N1-C2	-5.62	118.05	120.30
43	1	1242	U	O4'-C1'-N1	5.61	112.69	108.20
44	2	1064	C	C6-N1-C1'	-5.61	114.07	120.80
43	1	67	C	N3-C2-O2	-5.61	117.98	121.90
48	6	40	C	P-O3'-C3'	5.60	126.42	119.70
43	1	1468	C	N1-C2-O2	5.60	122.26	118.90
43	1	1657	U	N3-C2-O2	-5.60	118.28	122.20
44	2	1469	G	P-O3'-C3'	5.59	126.41	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	7	57	C	C6-N1-C2	-5.59	118.06	120.30
43	1	638	C	N1-C2-O2	5.59	122.25	118.90
44	2	776	C	N3-C2-O2	-5.59	117.99	121.90
15	O	104	LEU	CA-CB-CG	5.58	128.15	115.30
43	1	851	G	C2-N3-C4	5.58	114.69	111.90
43	1	1674	U	N1-C2-O2	5.58	126.70	122.80
44	2	78	U	N3-C2-O2	-5.58	118.30	122.20
29	c	241	ASP	C-N-CA	5.58	135.64	121.70
43	1	1008	C	C6-N1-C2	-5.57	118.07	120.30
10	J	48	LEU	CA-CB-CG	5.57	128.12	115.30
44	2	410	C	N1-C2-O2	5.57	122.24	118.90
44	2	812	C	C5-C6-N1	5.57	123.78	121.00
49	7	57	C	C5-C6-N1	5.57	123.78	121.00
47	5	68	C	N1-C2-O2	5.56	122.24	118.90
44	2	556	U	N1-C2-O2	5.56	126.69	122.80
43	1	443	A	P-O3'-C3'	5.55	126.36	119.70
44	2	1184	C	C5-C6-N1	5.55	123.78	121.00
43	1	163	U	P-O3'-C3'	5.55	126.36	119.70
43	1	954	U	C2-N1-C1'	5.55	124.36	117.70
35	i	40	LEU	CA-CB-CG	5.54	128.05	115.30
43	1	1576	C	C6-N1-C2	-5.54	118.08	120.30
44	2	593	U	C2-N1-C1'	5.54	124.35	117.70
44	2	668	C	N1-C2-O2	5.54	122.22	118.90
43	1	1172	G	C2-N3-C4	5.53	114.67	111.90
44	2	756	C	C5-C6-N1	5.53	123.77	121.00
45	3	58	C	N1-C2-O2	5.52	122.21	118.90
46	4	112	C	C5-C6-N1	5.50	123.75	121.00
45	3	188	C	P-O3'-C3'	5.50	126.30	119.70
47	5	100	C	C6-N1-C2	-5.50	118.10	120.30
44	2	1202	G	C8-N9-C4	-5.50	104.20	106.40
43	1	607	C	C6-N1-C2	-5.49	118.10	120.30
43	1	638	C	N3-C2-O2	-5.48	118.06	121.90
43	1	1212	C	C5-C6-N1	5.48	123.74	121.00
50	8	37	C	C6-N1-C1'	-5.48	114.22	120.80
44	2	481	C	C2-N1-C1'	5.47	124.82	118.80
43	1	954	U	N1-C2-O2	5.47	126.63	122.80
44	2	432	U	N1-C2-O2	5.47	126.63	122.80
43	1	320	G	N3-C4-N9	5.46	129.28	126.00
44	2	448	C	C5-C6-N1	5.46	123.73	121.00
43	1	320	G	C8-N9-C1'	-5.46	119.90	127.00
43	1	574	G	N3-C4-C5	-5.46	125.87	128.60
43	1	738	C	C6-N1-C2	-5.45	118.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	634	U	N3-C2-O2	-5.45	118.38	122.20
43	1	1674	U	C2-N1-C1'	5.45	124.24	117.70
44	2	530	C	C6-N1-C2	-5.45	118.12	120.30
49	7	112	G	C8-N9-C1'	-5.45	119.92	127.00
44	2	435	U	N3-C2-O2	-5.45	118.39	122.20
43	1	1212	C	C6-N1-C2	-5.45	118.12	120.30
3	C	305	LEU	CA-CB-CG	5.45	127.82	115.30
43	1	1517	U	N3-C2-O2	-5.44	118.39	122.20
44	2	425	C	N3-C2-O2	-5.44	118.09	121.90
43	1	96	C	N3-C2-O2	-5.44	118.09	121.90
44	2	776	C	N1-C2-O2	5.44	122.16	118.90
43	1	71	C	C2-N1-C1'	5.43	124.78	118.80
43	1	1530	U	C5-C6-N1	5.43	125.42	122.70
45	3	179	U	N3-C2-O2	-5.43	118.40	122.20
43	1	320	G	C4-N9-C1'	5.42	133.54	126.50
46	4	86	U	C6-N1-C1'	-5.42	113.61	121.20
49	7	35	C	N3-C2-O2	-5.42	118.11	121.90
44	2	1207	G	P-O3'-C3'	5.41	126.19	119.70
43	1	269	C	N1-C2-O2	5.41	122.15	118.90
43	1	1634	C	N1-C2-O2	5.41	122.15	118.90
44	2	1184	C	C6-N1-C2	-5.41	118.14	120.30
46	4	109	C	C5-C6-N1	5.41	123.71	121.00
44	2	479	C	C6-N1-C2	-5.41	118.14	120.30
48	6	46	C	N1-C2-O2	5.41	122.14	118.90
44	2	1114	C	C6-N1-C2	-5.41	118.14	120.30
43	1	954	U	C5-C6-N1	5.40	125.40	122.70
44	2	399	U	C6-N1-C2	-5.40	117.76	121.00
44	2	1011	U	C6-N1-C1'	-5.40	113.64	121.20
43	1	769	U	C2-N1-C1'	5.40	124.18	117.70
43	1	802	C	C6-N1-C2	-5.40	118.14	120.30
43	1	778	C	C6-N1-C1'	-5.40	114.32	120.80
43	1	973	U	C6-N1-C2	-5.39	117.77	121.00
43	1	1164	C	C5-C6-N1	5.39	123.69	121.00
45	3	147	A	C5-N7-C8	-5.39	101.21	103.90
43	1	1249	A	C4-N9-C1'	5.38	135.99	126.30
43	1	34	C	N3-C2-O2	-5.38	118.13	121.90
43	1	244	C	C6-N1-C2	-5.38	118.15	120.30
43	1	810	C	N1-C2-O2	5.38	122.13	118.90
43	1	733	C	N1-C2-O2	5.38	122.13	118.90
43	1	855	C	C6-N1-C2	-5.37	118.15	120.30
44	2	1306	C	N1-C2-O2	5.37	122.12	118.90
43	1	728	C	P-O3'-C3'	5.37	126.15	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	1573	C	C6-N1-C1'	-5.37	114.35	120.80
44	2	481	C	N3-C2-O2	-5.37	118.14	121.90
48	6	57	U	C5-C6-N1	5.37	125.39	122.70
35	i	64	LEU	CA-CB-CG	5.37	127.65	115.30
43	1	995	C	N3-C2-O2	-5.37	118.14	121.90
43	1	163	U	OP1-P-O3'	5.37	117.01	105.20
50	8	41	C	N1-C2-O2	5.37	122.12	118.90
44	2	643	A	C2-N3-C4	5.36	113.28	110.60
44	2	1218	C	C6-N1-C2	-5.36	118.15	120.30
49	7	143	C	C6-N1-C2	-5.36	118.15	120.30
50	8	90	U	C6-N1-C2	-5.36	117.78	121.00
44	2	1011	U	O4'-C1'-N1	5.36	112.49	108.20
43	1	1674	U	N3-C2-O2	-5.36	118.45	122.20
44	2	809	C	N1-C2-O2	5.36	122.12	118.90
44	2	1452	A	P-O3'-C3'	5.36	126.13	119.70
43	1	707	C	N3-C2-O2	-5.36	118.15	121.90
43	1	1182	C	N3-C2-O2	-5.35	118.16	121.90
46	4	161	C	C6-N1-C2	-5.34	118.16	120.30
43	1	1761	C	N3-C2-O2	-5.34	118.16	121.90
44	2	1452	A	OP1-P-O3'	5.34	116.95	105.20
43	1	1645	C	N1-C2-O2	5.33	122.10	118.90
44	2	383	U	C4-C5-C6	5.33	122.90	119.70
44	2	378	C	C5-C6-N1	5.33	123.67	121.00
47	5	118	C	N3-C2-O2	-5.33	118.17	121.90
44	2	127	C	C2-N1-C1'	5.32	124.66	118.80
48	6	67	C	C2-N1-C1'	5.32	124.66	118.80
43	1	948	U	C5-C6-N1	5.32	125.36	122.70
49	7	153	C	O5'-P-OP1	-5.32	100.91	105.70
50	8	87	C	C6-N1-C2	-5.32	118.17	120.30
43	1	1059	U	N1-C2-O2	5.32	126.52	122.80
49	7	140	U	N3-C2-O2	-5.32	118.48	122.20
43	1	353	C	C6-N1-C2	-5.31	118.18	120.30
46	4	167	C	N1-C2-O2	5.31	122.09	118.90
43	1	622	C	C6-N1-C2	-5.31	118.18	120.30
43	1	913	C	C5-C6-N1	5.31	123.65	121.00
43	1	244	C	C2-N1-C1'	5.31	124.64	118.80
43	1	1634	C	N3-C2-O2	-5.30	118.19	121.90
43	1	1142	C	C6-N1-C2	-5.30	118.18	120.30
44	2	427	C	C6-N1-C2	-5.29	118.18	120.30
8	H	34	LEU	CA-CB-CG	5.29	127.46	115.30
46	4	63	U	C6-N1-C1'	-5.29	113.80	121.20
43	1	445	C	N3-C2-O2	-5.28	118.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	7	167	C	C6-N1-C2	-5.28	118.19	120.30
43	1	113	C	N1-C2-O2	5.28	122.07	118.90
44	2	383	U	C5-C6-N1	-5.28	120.06	122.70
44	2	530	C	N1-C2-O2	5.28	122.07	118.90
43	1	1378	U	OP2-P-O3'	5.28	116.81	105.20
43	1	1540	U	N3-C2-O2	-5.27	118.51	122.20
43	1	835	G	N3-C4-N9	5.27	129.16	126.00
43	1	966	A	C8-N9-C4	-5.27	103.69	105.80
44	2	593	U	C5-C6-N1	5.26	125.33	122.70
43	1	995	C	C6-N1-C2	-5.26	118.19	120.30
44	2	1188	C	C5-C6-N1	5.25	123.63	121.00
45	3	44	C	N1-C2-O2	5.25	122.05	118.90
49	7	140	U	N1-C2-O2	5.25	126.48	122.80
46	4	154	C	C6-N1-C2	-5.25	118.20	120.30
44	2	637	G	C5-C6-N1	5.25	114.12	111.50
50	8	110	G	O4'-C1'-N9	5.25	112.40	108.20
44	2	808	C	N3-C2-O2	-5.25	118.23	121.90
44	2	1212	U	C5-C6-N1	5.24	125.32	122.70
44	2	1125	A	C8-N9-C4	-5.24	103.71	105.80
47	5	88	C	C5-C6-N1	5.24	123.62	121.00
44	2	556	U	N3-C2-O2	-5.23	118.54	122.20
43	1	1777	U	N1-C2-O2	5.23	126.46	122.80
43	1	1777	U	N3-C2-O2	-5.23	118.54	122.20
7	G	221	LEU	CA-CB-CG	5.22	127.31	115.30
44	2	637	G	C2-N3-C4	5.22	114.51	111.90
50	8	37	C	C6-N1-C2	-5.21	118.21	120.30
43	1	803	C	N3-C2-O2	-5.21	118.25	121.90
49	7	45	C	C5-C6-N1	5.21	123.61	121.00
43	1	954	U	N3-C2-O2	-5.21	118.55	122.20
43	1	1215	C	N1-C2-O2	5.21	122.03	118.90
44	2	37	C	N1-C2-O2	5.21	122.03	118.90
43	1	113	C	C5-C6-N1	5.21	123.61	121.00
46	4	180	C	N1-C2-O2	5.21	122.03	118.90
44	2	383	U	N1-C2-N3	5.21	118.02	114.90
45	3	45	C	C6-N1-C2	-5.21	118.22	120.30
44	2	91	C	O4'-C1'-N1	5.20	112.36	108.20
46	4	166	C	C6-N1-C2	-5.20	118.22	120.30
43	1	527	A	O4'-C1'-N9	5.20	112.36	108.20
44	2	509	C	N1-C2-O2	5.20	122.02	118.90
43	1	1092	U	O5'-P-OP2	-5.19	101.03	105.70
44	2	18	A	N1-C2-N3	-5.19	126.70	129.30
43	1	908	G	N3-C2-N2	-5.19	116.27	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	4	63	U	O4'-C1'-N1	5.19	112.35	108.20
44	2	544	U	N3-C2-O2	-5.18	118.57	122.20
43	1	1254	C	C5-C6-N1	5.18	123.59	121.00
43	1	1419	C	N3-C2-O2	-5.18	118.28	121.90
44	2	1367	C	C6-N1-C2	-5.17	118.23	120.30
43	1	581	G	OP1-P-O3'	5.17	116.57	105.20
42	p	35	LEU	CA-CB-CG	5.17	127.19	115.30
43	1	17	C	C6-N1-C2	-5.17	118.23	120.30
43	1	1621	U	C2-N1-C1'	5.17	123.90	117.70
50	8	30	C	N3-C2-O2	-5.16	118.28	121.90
43	1	810	C	N3-C2-O2	-5.16	118.29	121.90
44	2	448	C	N1-C2-O2	5.16	122.00	118.90
44	2	584	C	C6-N1-C2	-5.16	118.24	120.30
47	5	104	G	C4-C5-N7	5.16	112.86	110.80
45	3	40	C	C6-N1-C2	-5.16	118.24	120.30
43	1	34	C	C6-N1-C2	-5.15	118.24	120.30
45	3	54	C	C5-C6-N1	5.15	123.58	121.00
43	1	257	U	C2-N1-C1'	5.15	123.88	117.70
43	1	900	C	C6-N1-C2	-5.15	118.24	120.30
43	1	1665	U	N1-C2-O2	5.15	126.40	122.80
43	1	914	U	C5-C6-N1	5.14	125.27	122.70
45	3	179	U	O4'-C1'-N1	5.14	112.31	108.20
48	6	67	C	N3-C2-O2	-5.14	118.30	121.90
50	8	16	C	C5-C6-N1	5.14	123.57	121.00
43	1	1096	C	N3-C2-O2	-5.14	118.30	121.90
44	2	776	C	C2-N1-C1'	5.13	124.44	118.80
44	2	1323	C	C5-C6-N1	5.13	123.57	121.00
43	1	19	G	O4'-C1'-N9	5.13	112.30	108.20
43	1	111	C	C6-N1-C2	-5.13	118.25	120.30
44	2	1374	C	C6-N1-C2	-5.13	118.25	120.30
44	2	806	C	N1-C2-O2	5.13	121.98	118.90
43	1	874	C	C6-N1-C2	-5.12	118.25	120.30
44	2	1080	U	N3-C2-O2	-5.12	118.62	122.20
44	2	40	C	C6-N1-C2	-5.12	118.25	120.30
25	Y	132	LEU	CA-CB-CG	5.12	127.07	115.30
44	2	1050	C	C6-N1-C2	-5.11	118.26	120.30
43	1	64	A	C4-C5-C6	-5.11	114.45	117.00
43	1	851	G	N3-C4-C5	-5.10	126.05	128.60
44	2	481	C	C5-C6-N1	5.10	123.55	121.00
46	4	85	C	C2-N1-C1'	5.10	124.41	118.80
43	1	501	C	C2-N1-C1'	5.10	124.41	118.80
49	7	82	C	C2-N1-C1'	5.10	124.41	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	1726	C	N3-C2-O2	-5.10	118.33	121.90
43	1	597	C	N1-C2-O2	5.10	121.96	118.90
44	2	1427	C	C5-C6-N1	5.09	123.55	121.00
44	2	1454	U	C5-C6-N1	5.09	125.25	122.70
49	7	101	U	C2-N1-C1'	5.09	123.81	117.70
44	2	1117	A	C4-N9-C1'	5.09	135.47	126.30
47	5	104	G	N3-C4-C5	-5.09	126.06	128.60
44	2	1151	U	N3-C2-O2	-5.08	118.64	122.20
46	4	10	U	C6-N1-C2	-5.08	117.95	121.00
44	2	509	C	C5-C6-N1	5.08	123.54	121.00
44	2	1066	C	N3-C2-O2	-5.08	118.35	121.90
43	1	514	C	C6-N1-C2	-5.07	118.27	120.30
44	2	809	C	N3-C2-O2	-5.07	118.35	121.90
8	H	29	LEU	CA-CB-CG	5.07	126.95	115.30
43	1	699	C	C6-N1-C2	-5.06	118.28	120.30
46	4	109	C	C6-N1-C2	-5.06	118.28	120.30
43	1	1573	C	O4'-C1'-N1	5.06	112.25	108.20
45	3	58	C	N3-C2-O2	-5.06	118.36	121.90
43	1	264	U	N3-C2-O2	-5.06	118.66	122.20
44	2	1448	A	O4'-C1'-N9	5.05	112.24	108.20
43	1	19	G	C4-N9-C1'	5.05	133.07	126.50
46	4	148	C	N3-C2-O2	-5.04	118.37	121.90
44	2	1320	C	C6-N1-C2	-5.04	118.28	120.30
43	1	809	C	C5-C6-N1	5.04	123.52	121.00
47	5	6	C	C6-N1-C2	-5.04	118.28	120.30
3	C	225	LEU	CA-CB-CG	5.04	126.89	115.30
43	1	928	C	N3-C2-O2	-5.04	118.37	121.90
43	1	26	C	C6-N1-C2	-5.04	118.29	120.30
45	3	148	A	N1-C6-N6	-5.04	115.58	118.60
44	2	1296	C	N1-C2-O2	5.03	121.92	118.90
43	1	1466	G	N9-C4-C5	-5.03	103.39	105.40
43	1	364	U	C5-C6-N1	5.03	125.22	122.70
43	1	119	C	N1-C2-O2	5.03	121.92	118.90
44	2	435	U	C2-N1-C1'	5.03	123.73	117.70
43	1	1507	U	N3-C2-O2	-5.02	118.69	122.20
43	1	546	G	N3-C4-C5	-5.02	126.09	128.60
43	1	901	C	C2-N1-C1'	5.02	124.32	118.80
43	1	937	C	C6-N1-C2	-5.02	118.29	120.30
44	2	1191	U	C6-N1-C2	-5.02	117.99	121.00
43	1	29	C	N3-C2-O2	-5.02	118.39	121.90
43	1	851	G	C4-N9-C1'	5.01	133.02	126.50
44	2	1328	C	N1-C2-O2	5.01	121.91	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	3	62	U	C5-C6-N1	5.01	125.21	122.70
49	7	152	C	C6-N1-C2	-5.01	118.30	120.30
49	7	143	C	C2-N1-C1'	5.01	124.31	118.80
44	2	1218	C	N1-C2-O2	5.01	121.90	118.90
49	7	10	C	C6-N1-C2	-5.01	118.30	120.30
50	8	36	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	115[B]	ARG	Mainchain
3	C	313	TYR	Peptide
6	F	102	THR	Peptide
15	O	117	ASP	Peptide
31	e	123	ASP	Peptide
39	m	115	CYS	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/254 (102%)	247 (95%)	13 (5%)	0	100	100
2	B	410/402 (102%)	387 (94%)	23 (6%)	0	100	100
3	C	366/366 (100%)	340 (93%)	25 (7%)	1 (0%)	41	61
4	D	166/168 (99%)	147 (89%)	17 (10%)	2 (1%)	13	24
5	E	184/186 (99%)	171 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	133/195 (68%)	120 (90%)	13 (10%)	0	100	100
7	G	218/348 (63%)	206 (94%)	11 (5%)	1 (0%)	29	48
8	H	222/221 (100%)	212 (96%)	10 (4%)	0	100	100
9	I	210/212 (99%)	188 (90%)	20 (10%)	2 (1%)	15	28
10	J	132/134 (98%)	119 (90%)	13 (10%)	0	100	100
11	K	148/149 (99%)	133 (90%)	15 (10%)	0	100	100
12	L	142/144 (99%)	127 (89%)	14 (10%)	1 (1%)	22	39
13	M	201/203 (99%)	195 (97%)	6 (3%)	0	100	100
14	N	186/213 (87%)	179 (96%)	7 (4%)	0	100	100
15	O	249/305 (82%)	232 (93%)	17 (7%)	0	100	100
16	P	195/197 (99%)	182 (93%)	13 (7%)	0	100	100
17	Q	187/189 (99%)	180 (96%)	7 (4%)	0	100	100
18	R	176/178 (99%)	153 (87%)	22 (12%)	1 (1%)	25	43
19	S	152/154 (99%)	138 (91%)	14 (9%)	0	100	100
20	T	152/154 (99%)	138 (91%)	14 (9%)	0	100	100
21	U	119/121 (98%)	103 (87%)	15 (13%)	1 (1%)	19	35
22	V	117/118 (99%)	109 (93%)	8 (7%)	0	100	100
23	W	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
24	X	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
25	Y	131/132 (99%)	128 (98%)	3 (2%)	0	100	100
26	Z	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
27	a	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
28	b	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
29	c	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
30	d	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
31	e	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	17	31
32	f	129/130 (99%)	123 (95%)	6 (5%)	0	100	100
33	g	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
34	h	124/125 (99%)	117 (94%)	7 (6%)	0	100	100
35	i	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
36	j	78/80 (98%)	77 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	k	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
38	l	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
39	m	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
40	n	31/33 (94%)	28 (90%)	3 (10%)	0	100	100
41	o	88/90 (98%)	79 (90%)	9 (10%)	0	100	100
42	p	94/96 (98%)	84 (89%)	9 (10%)	1 (1%)	14	26
All	All	6329/6652 (95%)	5911 (93%)	407 (6%)	11 (0%)	50	68

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	43	CYS
9	I	68	VAL
31	e	124	ALA
3	C	314	GLN
4	D	42	LEU
42	p	27	GLN
9	I	67	THR
18	R	15	GLU
21	U	72	MET
7	G	214	PRO
12	L	50	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/198 (103%)	191 (94%)	13 (6%)	17	33
2	B	333/340 (98%)	325 (98%)	8 (2%)	49	74
3	C	291/297 (98%)	287 (99%)	4 (1%)	67	86
4	D	114/146 (78%)	113 (99%)	1 (1%)	78	92
5	E	160/169 (95%)	160 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	100/154 (65%)	99 (99%)	1 (1%)	76 90
7	G	178/292 (61%)	173 (97%)	5 (3%)	43 70
8	H	184/187 (98%)	179 (97%)	5 (3%)	44 71
9	I	167/175 (95%)	164 (98%)	3 (2%)	59 81
10	J	105/107 (98%)	103 (98%)	2 (2%)	57 80
11	K	116/125 (93%)	114 (98%)	2 (2%)	60 82
12	L	114/114 (100%)	113 (99%)	1 (1%)	78 92
13	M	179/179 (100%)	178 (99%)	1 (1%)	86 95
14	N	138/179 (77%)	135 (98%)	3 (2%)	52 77
15	O	193/242 (80%)	193 (100%)	0	100 100
16	P	163/163 (100%)	159 (98%)	4 (2%)	47 73
17	Q	130/166 (78%)	129 (99%)	1 (1%)	81 93
18	R	156/157 (99%)	155 (99%)	1 (1%)	86 95
19	S	123/128 (96%)	119 (97%)	4 (3%)	38 64
20	T	130/133 (98%)	127 (98%)	3 (2%)	50 76
21	U	91/106 (86%)	90 (99%)	1 (1%)	73 89
22	V	97/102 (95%)	97 (100%)	0	100 100
23	W	105/105 (100%)	103 (98%)	2 (2%)	57 80
24	X	58/60 (97%)	57 (98%)	1 (2%)	60 82
25	Y	104/113 (92%)	104 (100%)	0	100 100
26	Z	108/113 (96%)	103 (95%)	5 (5%)	27 50
27	a	98/115 (85%)	98 (100%)	0	100 100
28	b	54/56 (96%)	52 (96%)	2 (4%)	34 60
29	c	180/189 (95%)	176 (98%)	4 (2%)	52 77
30	d	77/81 (95%)	74 (96%)	3 (4%)	32 57
31	e	101/104 (97%)	98 (97%)	3 (3%)	41 68
32	f	108/111 (97%)	105 (97%)	3 (3%)	43 70
33	g	101/103 (98%)	101 (100%)	0	100 100
34	h	104/108 (96%)	102 (98%)	2 (2%)	57 80
35	i	77/81 (95%)	77 (100%)	0	100 100
36	j	67/68 (98%)	66 (98%)	1 (2%)	65 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	k	60/69 (87%)	59 (98%)	1 (2%)	60 82
38	l	44/46 (96%)	44 (100%)	0	100 100
39	m	41/44 (93%)	39 (95%)	2 (5%)	25 47
40	n	28/31 (90%)	28 (100%)	0	100 100
41	o	70/72 (97%)	69 (99%)	1 (1%)	67 86
42	p	77/83 (93%)	76 (99%)	1 (1%)	69 87
All	All	5128/5611 (91%)	5034 (98%)	94 (2%)	64 81

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23[A]	ARG
1	A	23[B]	ARG
1	A	28[A]	LYS
1	A	28[B]	LYS
1	A	28[C]	LYS
1	A	90[A]	CYS
1	A	90[B]	CYS
1	A	140	ASN
1	A	163	ARG
1	A	188	ARG
1	A	193	ARG
1	A	242	ARG
1	A	247	ARG
2	B	10	ARG
2	B	58[A]	ARG
2	B	58[B]	ARG
2	B	245[A]	ARG
2	B	245[B]	ARG
2	B	249[A]	ARG
2	B	249[B]	ARG
2	B	339	ARG
3	C	94	MET
3	C	99[A]	ARG
3	C	99[B]	ARG
3	C	139	ARG
4	D	39	LEU
6	F	60	ASN
7	G	133	ARG
7	G	187[A]	ARG

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Mol	Chain	Res	Type
7	G	187[B]	ARG
7	G	316	ARG
7	G	326	ARG
8	H	54	VAL
8	H	79	ARG
8	H	108	ARG
8	H	112[A]	ARG
8	H	112[B]	ARG
9	I	75	ARG
9	I	157	ARG
9	I	198	ARG
10	J	12	ARG
10	J	82	ARG
11	K	198[A]	HIS
11	K	198[B]	HIS
12	L	24	LYS
13	M	197	ARG
14	N	33	ASN
14	N	81	ASN
14	N	130	ARG
16	P	56	ARG
16	P	101	ARG
16	P	129	THR
16	P	192	ARG
17	Q	117	ARG
18	R	74	ARG
19	S	66	ASN
19	S	120	LYS
19	S	134	MET
19	S	142	ASN
20	T	37	ASN
20	T	85	ARG
20	T	137	THR
21	U	110	LEU
23	W	10	ARG
23	W	41	ASN
24	X	22	VAL
26	Z	17	ARG
26	Z	35	ASN
26	Z	46	LEU
26	Z	53	VAL
26	Z	131	ARG

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Mol	Chain	Res	Type
28	b	9	ASN
28	b	11	ASN
29	c	163	TYR
29	c	170	ARG
29	c	185	ASN
29	c	239	ASN
30	d	26	VAL
30	d	88	ARG
30	d	96	ASN
31	e	92	LYS
31	e	144	VAL
31	e	167	ASN
32	f	55	ASN
32	f	56	LYS
32	f	90	ASN
34	h	19	ASN
34	h	89	ARG
36	j	57	ARG
37	k	76	LYS
39	m	115	CYS
39	m	120	ASN
41	o	75	ASN
42	p	81	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	21	HIS
1	A	140	ASN
1	A	194	ASN
1	A	209	HIS
1	A	228	HIS
2	B	24	GLN
2	B	55	HIS
2	B	174	HIS
2	B	282	GLN
2	B	284	ASN
2	B	299	ASN
2	B	352	GLN
3	C	46	ASN
3	C	61	HIS

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Mol	Chain	Res	Type
3	C	115	ASN
3	C	118	GLN
3	C	197	ASN
3	C	243	HIS
4	D	154	HIS
5	E	75	HIS
6	F	60	ASN
7	G	111	HIS
7	G	144	GLN
7	G	258	ASN
7	G	335	HIS
8	H	68	ASN
8	H	186	HIS
8	H	190	GLN
9	I	12	HIS
9	I	16	HIS
9	I	23	GLN
9	I	36	GLN
9	I	70	HIS
9	I	108	ASN
10	J	100	ASN
11	K	126	ASN
12	L	34	ASN
12	L	41	HIS
12	L	74	ASN
12	L	114	HIS
13	M	196	ASN
14	N	33	ASN
14	N	71	GLN
14	N	81	ASN
14	N	192	GLN
14	N	196	HIS
15	O	35	GLN
17	Q	118	HIS
17	Q	141	HIS
18	R	10	GLN
18	R	75	ASN
18	R	116	HIS
18	R	145	HIS
18	R	155	GLN
19	S	66	ASN
19	S	111	GLN

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Mol	Chain	Res	Type
19	S	142	ASN
20	T	37	ASN
20	T	97	ASN
20	T	110	ASN
22	V	34	GLN
22	V	114	ASN
23	W	41	ASN
23	W	97	HIS
24	X	14	HIS
26	Z	35	ASN
26	Z	37	ASN
28	b	7	HIS
28	b	9	ASN
28	b	11	ASN
28	b	17	HIS
28	b	19	ASN
28	b	30	HIS
28	b	51	ASN
29	c	109	GLN
29	c	239	ASN
30	d	96	ASN
31	e	120	ASN
31	e	132	HIS
31	e	167	ASN
32	f	55	ASN
32	f	99	HIS
33	g	25	ASN
33	g	49	GLN
33	g	111	HIS
34	h	19	ASN
34	h	62	HIS
34	h	87	GLN
36	j	10	GLN
36	j	28	HIS
39	m	109	ASN
39	m	120	ASN
41	o	75	ASN
42	p	20	HIS
42	p	73	GLN
42	p	82	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
43	1	1603/1778 (90%)	438 (27%)	18 (1%)
44	2	1067/1526 (69%)	287 (26%)	17 (1%)
45	3	172/211 (81%)	45 (26%)	3 (1%)
46	4	182/183 (99%)	47 (25%)	2 (1%)
47	5	93/133 (69%)	30 (32%)	0
48	6	70/71 (98%)	34 (48%)	4 (5%)
49	7	161/171 (94%)	39 (24%)	2 (1%)
50	8	117/118 (99%)	25 (21%)	1 (0%)
All	All	3465/4191 (82%)	945 (27%)	47 (1%)

All (945) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
43	1	4	G
43	1	16	G
43	1	20	G
43	1	24	A
43	1	29	C
43	1	38	A
43	1	41	A
43	1	47	C
43	1	48	OMU
43	1	55	A
43	1	57	G
43	1	58	A
43	1	63	A
43	1	64	A
43	1	67	C
43	1	69	A2M
43	1	70	C
43	1	71	C
43	1	72	G
43	1	81	U
43	1	83	A
43	1	86	G
43	1	87	A
43	1	91	G
43	1	92	C
43	1	109	A
43	1	110	A
43	1	127	G
43	1	130	U
43	1	131	U

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Mol	Chain	Res	Type
43	1	132	A
43	1	134	A
43	1	136	G
43	1	140	U
43	1	141	U
43	1	142	G
43	1	154	A
43	1	155	A
43	1	156	A
43	1	157	U
43	1	158	A
43	1	160	C
43	1	161	A
43	1	162	U
43	1	163	U
43	1	164	U
43	1	171	U
43	1	175	G
43	1	176	C
43	1	177	A
43	1	189	A
43	1	191	U
43	1	192	C
43	1	200	A
43	1	202	G
43	1	205	A
43	1	206	A
43	1	210	G
43	1	212	U
43	1	213	G
43	1	215	U
43	1	217	A
43	1	218	A
43	1	219	U
43	1	223	A
43	1	230	A
43	1	231	U
43	1	233	U
43	1	234	G
43	1	244	C
43	1	248	A
43	1	249	G

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Mol	Chain	Res	Type
43	1	250	A
43	1	251	A
43	1	255	G
43	1	256	U
43	1	257	U
43	1	258	A
43	1	261	C
43	1	264	U
43	1	268	G
43	1	273	A
43	1	279	G
43	1	280	A
43	1	283	G
43	1	284	C
43	1	290	G
43	1	291	A
43	1	301	A
43	1	303	C
43	1	305	A
43	1	306	G
43	1	320	G
43	1	323	U
43	1	332	A
43	1	334	G
43	1	343	U
43	1	348	G
43	1	349	U
43	1	361	A
43	1	367	A
43	1	368	G
43	1	369	A
43	1	376	A
43	1	377	G
43	1	382	A
43	1	383	U
43	1	384	A
43	1	389	A
43	1	390	C
43	1	391	A
43	1	392	A
43	1	409	U
43	1	410	U

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Mol	Chain	Res	Type
43	1	411	U
43	1	417	G
43	1	422	U
43	1	423	U
43	1	426	A
43	1	427	A
43	1	428	A
43	1	438	A
43	1	440	A
43	1	442	A
43	1	443	A
43	1	444	C
43	1	449	A
43	1	457	C
43	1	461	G
43	1	463	C
43	1	471	G
43	1	477	C
43	1	482	U
43	1	483	C
43	1	485	A
43	1	486	C
43	1	487	G
43	1	488	G
43	1	489	C
43	1	495	C
43	1	513	C
43	1	517	U
43	1	518	C
43	1	519	G
43	1	520	G
43	1	521	G
43	1	528	A
43	1	535	C
43	1	536	G
43	1	538	G
43	1	539	C
43	1	544	A
43	1	546	G
43	1	547	U
43	1	548	G
43	1	551	A

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Mol	Chain	Res	Type
43	1	553	A
43	1	554	A
43	1	561	G
43	1	565	U
43	1	569	G
43	1	570	A
43	1	571	A
43	1	572	A
43	1	574	G
43	1	575	A
43	1	579	G
43	1	580	A
43	1	581	G
43	1	582	U
43	1	583	A
43	1	586	U
43	1	591	U
43	1	592	G
43	1	597	C
43	1	599	G
43	1	600	C
43	1	601	G
43	1	610	A
43	1	611	C
43	1	612	G
43	1	625	C
43	1	628	C
43	1	629	G
43	1	632	A
43	1	635	C
43	1	641	G
43	1	648	A
43	1	649	U
43	1	655	U
43	1	656	G
43	1	661	G
43	1	668	C
43	1	669	C
43	1	677	A
43	1	679	A
43	1	681	A2M
43	1	682	C

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Mol	Chain	Res	Type
43	1	692	A
43	1	698	A
43	1	709	A
43	1	713	A
43	1	719	U
43	1	722	G
43	1	725	U
43	1	729	A
43	1	750	G
43	1	754	G
43	1	759	A
43	1	761	A
43	1	762	A
43	1	763	U
43	1	764	G
43	1	769	U
43	1	771	U
43	1	778	C
43	1	803	C
43	1	810	C
43	1	821	C
43	1	822	C
43	1	823	G
43	1	825	G
43	1	827	G
43	1	828	U
43	1	831	C
43	1	832	G
43	1	835	G
43	1	836	G
43	1	849	U
43	1	850	G
43	1	851	G
43	1	852	A
43	1	868	A
43	1	881	A
43	1	887	A
43	1	899	A
43	1	900	C
43	1	901	C
43	1	908	G
43	1	912	C

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Mol	Chain	Res	Type
43	1	925	U
43	1	930	U
43	1	931	G
43	1	935	A
43	1	957	C
43	1	958	G
43	1	959	OMG
43	1	965	A
43	1	967	G
43	1	970	U
43	1	972	A
43	1	974	C
43	1	975	G
43	1	976	A
43	1	983	U
43	1	984	A
43	1	987	A
43	1	988	G
43	1	995	C
43	1	1000	C
43	1	1010	C
43	1	1011	U
43	1	1015	G
43	1	1025	G
43	1	1029	G
43	1	1031	A
43	1	1036	U
43	1	1037	A
43	1	1045	G
43	1	1051	C
43	1	1059	U
43	1	1061	G
43	1	1063	G
43	1	1064	G
43	1	1065	C
43	1	1066	A
43	1	1067	U
43	1	1068	U
43	1	1087	A
43	1	1088	C
43	1	1091	A
43	1	1092	U

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Mol	Chain	Res	Type
43	1	1096	C
43	1	1098	A
43	1	1105	A
43	1	1108	G
43	1	1114	A
43	1	1116	A
43	1	1118	A
43	1	1124	C
43	1	1130	C
43	1	1134	C
43	1	1135	U
43	1	1148	A
43	1	1149	G
43	1	1150	A
43	1	1153	A
43	1	1155	A
43	1	1156	A
43	1	1159	A
43	1	1161	A
43	1	1174	G
43	1	1182	C
43	1	1188	G
43	1	1192	A
43	1	1195	A
43	1	1200	A
43	1	1201	U
43	1	1210	A
43	1	1211	A
43	1	1212	C
43	1	1216	U
43	1	1220	G
43	1	1226	G
43	1	1235	A
43	1	1238	C
43	1	1239	U
43	1	1240	U
43	1	1242	U
43	1	1243	G
43	1	1248	C
43	1	1249	A
43	1	1250	U
43	1	1251	U

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Mol	Chain	Res	Type
43	1	1252	C
43	1	1253	OMU
43	1	1254	C
43	1	1257	U
43	1	1260	G
43	1	1261	U
43	1	1265	A
43	1	1270	U
43	1	1271	G
43	1	1274	G
43	1	1279	A
43	1	1364	A
43	1	1366	A
43	1	1367	U
43	1	1368	G
43	1	1369	G
43	1	1370	A
43	1	1371	OMU
43	1	1375	G
43	1	1378	U
43	1	1379	A
43	1	1386	A
43	1	1387	U
43	1	1389	A
43	1	1390	G
43	1	1394	U
43	1	1395	U
43	1	1398	C
43	1	1401	U
43	1	1402	U
43	1	1412	G
43	1	1414	A
43	1	1419	C
43	1	1420	G
43	1	1422	A
43	1	1426	A
43	1	1437	A
43	1	1440	A
43	1	1446	A
43	1	1447	G
43	1	1466	G
43	1	1467	G

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Mol	Chain	Res	Type
43	1	1475	G
43	1	1476	U
43	1	1483	G
43	1	1489	U
43	1	1492	G
43	1	1494	C
43	1	1495	G
43	1	1506	A
43	1	1509	G
43	1	1511	C
43	1	1523	G
43	1	1524	C
43	1	1526	OMG
43	1	1529	OMC
43	1	1530	U
43	1	1538	C
43	1	1542	OMG
43	1	1547	G
43	1	1548	A
43	1	1559	A
43	1	1561	A
43	1	1562	U
43	1	1563	A
43	1	1564	C
43	1	1565	U
43	1	1566	C
43	1	1571	U
43	1	1572	G
43	1	1588	G
43	1	1589	A
43	1	1590	G
43	1	1591	C
43	1	1592	G
43	1	1601	U
43	1	1603	U
43	1	1607	G
43	1	1609	C
43	1	1610	A
43	1	1614	G
43	1	1615	C
43	1	1631	G
43	1	1633	U

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Mol	Chain	Res	Type
43	1	1634	C
43	1	1656	A
43	1	1657	U
43	1	1658	C
43	1	1663	U
43	1	1664	G
43	1	1665	U
43	1	1668	G
43	1	1669	G
43	1	1670	A
43	1	1671	A
43	1	1672	A
43	1	1673	G
43	1	1720	C
43	1	1721	C
43	1	1729	A
43	1	1732	A
43	1	1739	A
43	1	1740	C
43	1	1741	A
43	1	1746	A
43	1	1749	U
43	1	1753	A
43	1	1755	U
43	1	1763	A
43	1	1764	A
43	1	1768	G
43	1	1777	U
43	1	1778	G
43	1	1782	G
44	2	7	C
44	2	22	A
44	2	25	A
44	2	29	C
44	2	30	A
44	2	33	A
44	2	41	A
44	2	49	A
44	2	61	C
44	2	63	U
44	2	64	A
44	2	66	A

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Mol	Chain	Res	Type
44	2	68	A
44	2	69	A
44	2	72	G
44	2	74	A
44	2	75	C
44	2	78	U
44	2	80	A
44	2	83	G
44	2	90	G
44	2	91	C
44	2	92	A
44	2	105	A
44	2	109	U
44	2	127	C
44	2	130	A
44	2	133	G
44	2	134	C
44	2	135	A
44	2	340	A
44	2	341	A
44	2	342	U
44	2	343	U
44	2	349	C
44	2	355	A
44	2	363	C
44	2	368	G
44	2	372	A
44	2	377	A
44	2	386	U
44	2	388	A
44	2	390	A
44	2	392	C
44	2	403	G
44	2	404	A
44	2	412	A
44	2	414	G
44	2	416	G
44	2	421	A
44	2	422	U
44	2	434	A
44	2	438	C
44	2	444	A

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Mol	Chain	Res	Type
44	2	448	C
44	2	452	G
44	2	456	G
44	2	469	G
44	2	481	C
44	2	482	G
44	2	485	G
44	2	494	C
44	2	495	G
44	2	502	A2M
44	2	503	C
44	2	504	U
44	2	518	G
44	2	519	G
44	2	527	A2M
44	2	528	U
44	2	529	G
44	2	530	C
44	2	534	OMG
44	2	544	U
44	2	551	G
44	2	552	C
44	2	553	G
44	2	554	C
44	2	555	A
44	2	556	U
44	2	559	A
44	2	561	G
44	2	570	A2M
44	2	571	G
44	2	580	U
44	2	581	G
44	2	582	U
44	2	585	C
44	2	588	G
44	2	602	A
44	2	606	G
44	2	611	U
44	2	618	A
44	2	619	A
44	2	620	C
44	2	621	G

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Mol	Chain	Res	Type
44	2	624	C
44	2	639	G
44	2	643	A
44	2	647	A
44	2	648	A
44	2	649	G
44	2	650	A
44	2	657	U
44	2	658	G
44	2	664	G
44	2	665	A2M
44	2	667	OMU
44	2	668	C
44	2	670	A
44	2	680	U
44	2	685	G
44	2	688	G
44	2	755	U
44	2	756	C
44	2	758	C
44	2	760	U
44	2	768	G
44	2	769	A
44	2	772	A
44	2	774	A
44	2	777	A
44	2	780	G
44	2	782	G
44	2	783	U
44	2	784	U
44	2	785	U
44	2	786	A
44	2	789	G
44	2	791	A
44	2	796	U
44	2	800	G
44	2	801	C
44	2	806	C
44	2	807	A
44	2	812	C
44	2	813	U
44	2	817	U

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Mol	Chain	Res	Type
44	2	819	U
44	2	964	U
44	2	965	G
44	2	966	C
44	2	967	U
44	2	969	U
44	2	971	A
44	2	973	C
44	2	974	U
44	2	1010	U
44	2	1011	U
44	2	1012	G
44	2	1013	U
44	2	1016	C
44	2	1020	A
44	2	1021	C
44	2	1023	U
44	2	1028	C
44	2	1031	A
44	2	1034	G
44	2	1035	G
44	2	1042	G
44	2	1047	OMG
44	2	1054	A
44	2	1056	A
44	2	1059	U
44	2	1065	A
44	2	1076	G
44	2	1079	OMG
44	2	1080	U
44	2	1084	A
44	2	1094	C
44	2	1100	G
44	2	1102	A
44	2	1105	G
44	2	1109	U
44	2	1110	C
44	2	1117	A
44	2	1118	G
44	2	1119	A
44	2	1122	A
44	2	1124	A

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Mol	Chain	Res	Type
44	2	1132	A
44	2	1133	A
44	2	1141	U
44	2	1142	G
44	2	1143	A
44	2	1147	A
44	2	1148	C
44	2	1155	C
44	2	1156	A
44	2	1157	G
44	2	1166	G
44	2	1181	A
44	2	1182	G
44	2	1184	C
44	2	1190	A
44	2	1200	A
44	2	1202	G
44	2	1204	A
44	2	1205	U
44	2	1207	G
44	2	1208	G
44	2	1211	A
44	2	1216	A
44	2	1227	C
44	2	1230	OMG
44	2	1238	A
44	2	1239	G
44	2	1240	A
44	2	1242	U
44	2	1243	A
44	2	1244	A
44	2	1249	OMC
44	2	1253	G
44	2	1256	A
44	2	1267	G
44	2	1284	A
44	2	1290	A
44	2	1292	G
44	2	1295	G
44	2	1296	C
44	2	1306	C
44	2	1307	U

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Mol	Chain	Res	Type
44	2	1310	G
44	2	1314	U
44	2	1326	A
44	2	1328	C
44	2	1333	C
44	2	1338	C
44	2	1342	A
44	2	1350	A
44	2	1362	U
44	2	1364	C
44	2	1367	C
44	2	1372	G
44	2	1374	C
44	2	1375	A
44	2	1380	A
44	2	1381	C
44	2	1385	A2M
44	2	1386	G
44	2	1387	C
44	2	1390	G
44	2	1391	G
44	2	1392	U
44	2	1393	U
44	2	1394	U
44	2	1409	C
44	2	1410	A
44	2	1417	U
44	2	1422	C
44	2	1429	U
44	2	1431	G
44	2	1434	G
44	2	1435	G
44	2	1436	A
44	2	1437	A
44	2	1438	A
44	2	1439	U
44	2	1441	G
44	2	1442	C
44	2	1443	G
44	2	1444	A
44	2	1445	G
44	2	1446	A

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Mol	Chain	Res	Type
44	2	1448	A
44	2	1449	A
44	2	1451	G
44	2	1452	A
44	2	1453	U
44	2	1454	U
44	2	1455	A
44	2	1456	U
44	2	1457	C
44	2	1466	G
44	2	1467	C
44	2	1470	A
44	2	1471	C
44	2	1473	U
44	2	1495	G
44	2	1499	G
44	2	1500	G
44	2	1501	U
44	2	1503	G
44	2	1504	G
44	2	1510	C
44	2	1514	G
44	2	1518	G
45	3	3	G
45	3	9	A
45	3	10	OMU
45	3	13	G
45	3	14	A
45	3	16	A
45	3	17	C
45	3	18	A
45	3	22	G
45	3	31	C
45	3	38	A
45	3	48	G
45	3	55	U
45	3	56	U
45	3	68	U
45	3	69	A
45	3	75	C
45	3	97	U
45	3	98	G

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Mol	Chain	Res	Type
45	3	106	U
45	3	109	C
45	3	115	G
45	3	121	U
45	3	122	U
45	3	123	C
45	3	126	A
45	3	131	G
45	3	133	G
45	3	142	U
45	3	146	A
45	3	147	A
45	3	148	A
45	3	157	U
45	3	163	C
45	3	169	G
45	3	170	U
45	3	184	U
45	3	189	G
45	3	192	U
45	3	193	U
45	3	194	A
45	3	196	C
45	3	199	A
45	3	207	G
45	3	211	U
46	4	8	U
46	4	9	G
46	4	10	U
46	4	14	G
46	4	16	G
46	4	22	G
46	4	24	A
46	4	25	G
46	4	33	G
46	4	40	G
46	4	48	U
46	4	50	G
46	4	58	G
46	4	65	C
46	4	84	U
46	4	85	C

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Mol	Chain	Res	Type
46	4	86	U
46	4	87	G
46	4	96	C
46	4	97	G
46	4	102	G
46	4	107	U
46	4	114	A
46	4	115	A
46	4	120	U
46	4	121	C
46	4	122	G
46	4	128	U
46	4	129	G
46	4	130	G
46	4	131	U
46	4	133	C
46	4	137	G
46	4	142	A
46	4	143	C
46	4	145	C
46	4	151	A
46	4	157	A
46	4	158	A
46	4	159	G
46	4	168	A
46	4	170	G
46	4	171	A
46	4	173	C
46	4	174	A
46	4	175	G
46	4	183	C
47	5	4	G
47	5	13	C
47	5	16	A
47	5	18	G
47	5	22	G
47	5	25	C
47	5	27	U
47	5	28	G
47	5	37	G
47	5	43	A
47	5	47	G

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Mol	Chain	Res	Type
47	5	66	G
47	5	70	C
47	5	87	C
47	5	96	U
47	5	97	G
47	5	103	U
47	5	104	G
47	5	105	A
47	5	107	G
47	5	110	U
47	5	120	U
47	5	121	G
47	5	123	U
47	5	124	C
47	5	125	A
47	5	126	G
47	5	128	G
47	5	129	A
47	5	133	A
48	6	7	A
48	6	13	C
48	6	15	C
48	6	20	A
48	6	24	C
48	6	25	U
48	6	26	G
48	6	28	A
48	6	31	U
48	6	32	U
48	6	37	C
48	6	39	U
48	6	40	C
48	6	41	G
48	6	42	A
48	6	43	A
48	6	44	G
48	6	49	C
48	6	50	A
48	6	51	A
48	6	52	G
48	6	53	U
48	6	54	A

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Mol	Chain	Res	Type
48	6	55	U
48	6	56	A
48	6	60	A
48	6	62	G
48	6	63	A
48	6	64	U
48	6	67	C
48	6	68	A
48	6	69	A
48	6	70	G
48	6	73	A
49	7	2	A
49	7	7	OMU
49	7	15	G
49	7	22	U
49	7	24	G
49	7	31	A
49	7	33	U
49	7	34	U
49	7	39	G
49	7	48	A
49	7	51	A
49	7	53	A
49	7	59	A
49	7	60	U
49	7	61	A
49	7	62	A
49	7	63	G
49	7	75	OMG
49	7	83	A
49	7	84	U
49	7	87	A
49	7	88	A
49	7	89	U
49	7	94	G
49	7	96	A
49	7	103	A
49	7	104	A
49	7	105	C
49	7	108	A
49	7	110	A
49	7	124	A

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Mol	Chain	Res	Type
49	7	129	C
49	7	136	G
49	7	139	A
49	7	140	U
49	7	143	C
49	7	144	C
49	7	156	A
49	7	165	G
50	8	5	G
50	8	9	G
50	8	28	C
50	8	30	C
50	8	34	A
50	8	37	C
50	8	43	G
50	8	44	A
50	8	51	A
50	8	52	A
50	8	55	U
50	8	65	C
50	8	66	A
50	8	72	A
50	8	76	A
50	8	89	G
50	8	92	A
50	8	93	U
50	8	99	G
50	8	102	A
50	8	110	G
50	8	111	U
50	8	112	G
50	8	114	C
50	8	119	U

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
43	1	141	U
43	1	154	A
43	1	162	U
43	1	163	U
43	1	191	U

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Mol	Chain	Res	Type
43	1	214	C
43	1	217	A
43	1	249	G
43	1	443	A
43	1	581	G
43	1	648	A
43	1	728	C
43	1	768	C
43	1	983	U
43	1	1063	G
43	1	1369	G
43	1	1378	U
43	1	1526	OMG
44	2	29	C
44	2	68	A
44	2	134	C
44	2	340	A
44	2	443	OMC
44	2	455	U
44	2	551	G
44	2	552	C
44	2	618	A
44	2	646	G
44	2	648	A
44	2	755	U
44	2	973	C
44	2	1207	G
44	2	1437	A
44	2	1452	A
44	2	1469	G
45	3	2	A
45	3	141	U
45	3	188	C
46	4	15	G
46	4	106	G
48	6	38	C
48	6	40	C
48	6	51	A
48	6	61	U
49	7	1	A
49	7	60	U
50	8	43	G

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

68 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	$\#\|Z\| > 2$
44	OMC	2	1398	44	19,22,23	0.93	1 (5%)	26,31,34	1.06	2 (7%)
44	OMG	2	1254	44	18,26,27	1.22	2 (11%)	19,38,41	1.64	5 (26%)
43	OMC	1	695	43	19,22,23	0.83	0	26,31,34	0.97	1 (3%)
43	OMC	1	1529	43	19,22,23	1.03	2 (10%)	26,31,34	1.12	3 (11%)
44	A2M	2	628	44	18,25,26	1.63	1 (5%)	18,36,39	1.04	2 (11%)
43	OMU	1	845	43	19,22,23	0.56	0	26,31,34	0.93	1 (3%)
43	OMU	1	1107	43	19,22,23	0.68	0	26,31,34	0.97	2 (7%)
44	OMG	2	1232	44	18,26,27	1.27	2 (11%)	19,38,41	1.40	3 (15%)
44	OMC	2	1249	44	19,22,23	1.04	1 (5%)	26,31,34	1.17	2 (7%)
46	OMG	4	74	46	18,26,27	1.24	2 (11%)	19,38,41	1.56	4 (21%)
43	A2M	1	678	43,44	18,25,26	1.63	2 (11%)	18,36,39	1.05	2 (11%)
43	A2M	1	697	43	18,25,26	1.61	3 (16%)	18,36,39	1.24	2 (11%)
43	OMG	1	856	43	18,26,27	1.26	2 (11%)	19,38,41	1.66	3 (15%)
43	OMG	1	1190	43	18,26,27	1.43	3 (16%)	19,38,41	1.61	2 (10%)
44	OMU	2	73	44	19,22,23	0.64	0	26,31,34	0.85	0
44	OMU	2	1420	44	19,22,23	0.54	0	26,31,34	0.86	2 (7%)
44	OMC	2	359	44	19,22,23	1.05	1 (5%)	26,31,34	1.09	4 (15%)
43	OMU	1	1371	43	19,22,23	1.16	1 (5%)	26,31,34	1.68	6 (23%)
44	OMC	2	583	44	19,22,23	0.99	1 (5%)	26,31,34	1.05	2 (7%)
44	OMU	2	1078	44	19,22,23	0.64	1 (5%)	26,31,34	1.05	2 (7%)
44	OMC	2	1160	44	19,22,23	0.95	1 (5%)	26,31,34	1.13	3 (11%)
44	OMG	2	71	44	18,26,27	1.38	2 (11%)	19,38,41	1.48	3 (15%)
44	OMU	2	560	44	19,22,23	0.60	0	26,31,34	1.02	2 (7%)
43	OMU	1	1661	43	19,22,23	0.63	0	26,31,34	0.84	1 (3%)
44	OMG	2	1047	44	18,26,27	1.29	2 (11%)	19,38,41	1.46	2 (10%)
44	OMG	2	1079	44	18,26,27	1.24	2 (11%)	19,38,41	1.65	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
44	A2M	2	1385	44	18,25,26	1.54	2 (11%)	18,36,39	1.22	3 (16%)
44	A2M	2	572	44	18,25,26	1.50	1 (5%)	18,36,39	1.16	2 (11%)
43	A2M	1	235	43	18,25,26	1.66	2 (11%)	18,36,39	1.02	1 (5%)
49	OMU	7	7	43,49	19,22,23	0.51	0	26,31,34	1.00	2 (7%)
43	A2M	1	437	43	18,25,26	1.42	1 (5%)	18,36,39	1.00	0
43	OMU	1	48	43	19,22,23	0.71	0	26,31,34	1.01	2 (7%)
43	A2M	1	681	43	18,25,26	1.64	2 (11%)	18,36,39	1.03	2 (11%)
43	A2M	1	1541	43,44	18,25,26	1.69	2 (11%)	18,36,39	1.00	1 (5%)
43	OMU	1	1253	43	19,22,23	0.64	0	26,31,34	0.77	0
43	OMG	1	959	43	18,26,27	1.27	2 (11%)	19,38,41	1.39	4 (21%)
44	OMC	2	443	44	19,22,23	0.84	0	26,31,34	1.22	4 (15%)
44	A2M	2	1186	44	18,25,26	1.74	3 (16%)	18,36,39	1.08	0
43	OMG	1	1526	43	18,26,27	1.40	2 (11%)	19,38,41	1.42	5 (26%)
44	OMC	2	1318	44	19,22,23	0.99	2 (10%)	26,31,34	1.25	3 (11%)
43	A2M	1	955	43	18,25,26	1.74	2 (11%)	18,36,39	1.22	2 (11%)
49	A2M	7	43	49	18,25,26	1.52	2 (11%)	18,36,39	1.23	1 (5%)
44	A2M	2	570	43,44	18,25,26	1.51	1 (5%)	18,36,39	1.45	2 (11%)
44	A2M	2	665	44	18,25,26	1.86	3 (16%)	18,36,39	1.12	2 (11%)
44	A2M	2	1068	44	18,25,26	1.50	3 (16%)	18,36,39	1.17	1 (5%)
44	OMU	2	1360	44	19,22,23	0.51	0	26,31,34	0.98	2 (7%)
43	A2M	1	858	43	18,25,26	1.74	2 (11%)	18,36,39	1.06	1 (5%)
44	OMU	2	1153	44	19,22,23	0.58	0	26,31,34	0.83	2 (7%)
44	OMG	2	1361	44	18,26,27	1.36	2 (11%)	19,38,41	1.54	4 (21%)
44	OMG	2	655	44	18,26,27	1.38	2 (11%)	19,38,41	1.51	3 (15%)
44	OMU	2	667	44	19,22,23	0.63	0	26,31,34	1.18	2 (7%)
44	OMG	2	534	44	18,26,27	1.31	2 (11%)	19,38,41	1.53	4 (21%)
43	A2M	1	927	43	18,25,26	1.71	2 (11%)	18,36,39	1.11	1 (5%)
44	OMG	2	641	44	18,26,27	1.45	2 (11%)	19,38,41	1.53	5 (26%)
43	OMG	1	1542	43,44	18,26,27	1.26	2 (11%)	19,38,41	1.52	2 (10%)
44	A2M	2	502	44	18,25,26	0.93	1 (5%)	18,36,39	1.45	3 (16%)
44	OMG	2	1230	44	18,26,27	1.45	2 (11%)	19,38,41	1.24	2 (10%)
43	OMG	1	1628	43	18,26,27	1.27	2 (11%)	19,38,41	1.61	5 (26%)
43	A2M	1	69	43	18,25,26	1.59	3 (16%)	18,36,39	1.27	1 (5%)
44	A2M	2	527	44	18,25,26	1.78	3 (16%)	18,36,39	1.41	4 (22%)
43	OMU	1	847	43	19,22,23	0.51	0	26,31,34	1.02	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	A2M	2	591	44	18,25,26	1.68	3 (16%)	18,36,39	1.00	1 (5%)
44	A2M	2	604	43,44	18,25,26	1.52	2 (11%)	18,36,39	1.00	0
44	A2M	2	1373	44	18,25,26	1.72	2 (11%)	18,36,39	0.96	0
49	OMG	7	75	49	18,26,27	1.24	2 (11%)	19,38,41	1.58	6 (31%)
49	A2M	7	162	43,49	18,25,26	1.67	2 (11%)	18,36,39	1.01	1 (5%)
45	OMU	3	10	45	19,22,23	0.68	0	26,31,34	1.01	1 (3%)
44	A2M	2	382	44	18,25,26	0.92	0	18,36,39	1.12	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	OMC	2	1398	44	-	0/9/27/28	0/2/2/2
44	OMG	2	1254	44	-	0/5/27/28	0/3/3/3
43	OMC	1	695	43	-	0/9/27/28	0/2/2/2
43	OMC	1	1529	43	-	2/9/27/28	0/2/2/2
44	A2M	2	628	44	-	0/5/27/28	0/3/3/3
43	OMU	1	845	43	-	0/9/27/28	0/2/2/2
43	OMU	1	1107	43	-	0/9/27/28	0/2/2/2
44	OMG	2	1232	44	-	0/5/27/28	0/3/3/3
44	OMC	2	1249	44	-	1/9/27/28	0/2/2/2
46	OMG	4	74	46	-	0/5/27/28	0/3/3/3
43	A2M	1	678	43,44	-	1/5/27/28	0/3/3/3
43	A2M	1	697	43	-	0/5/27/28	0/3/3/3
43	OMG	1	856	43	-	0/5/27/28	0/3/3/3
43	OMG	1	1190	43	-	0/5/27/28	0/3/3/3
44	OMU	2	73	44	-	0/9/27/28	0/2/2/2
44	OMU	2	1420	44	-	0/9/27/28	0/2/2/2
44	OMC	2	359	44	-	0/9/27/28	0/2/2/2
43	OMU	1	1371	43	-	5/9/27/28	0/2/2/2
44	OMC	2	583	44	-	0/9/27/28	0/2/2/2
44	OMU	2	1078	44	-	0/9/27/28	0/2/2/2
44	OMC	2	1160	44	-	0/9/27/28	0/2/2/2
44	OMG	2	71	44	-	0/5/27/28	0/3/3/3
44	OMU	2	560	44	-	1/9/27/28	0/2/2/2
43	OMU	1	1661	43	-	0/9/27/28	0/2/2/2
44	OMG	2	1047	44	-	2/5/27/28	0/3/3/3
44	OMG	2	1079	44	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A2M	2	1385	44	-	2/5/27/28	0/3/3/3
44	A2M	2	572	44	-	0/5/27/28	0/3/3/3
43	A2M	1	235	43	-	1/5/27/28	0/3/3/3
49	OMU	7	7	43,49	-	2/9/27/28	0/2/2/2
43	A2M	1	437	43	-	0/5/27/28	0/3/3/3
43	OMU	1	48	43	-	2/9/27/28	0/2/2/2
43	A2M	1	681	43	-	3/5/27/28	0/3/3/3
43	A2M	1	1541	43,44	-	0/5/27/28	0/3/3/3
43	OMU	1	1253	43	-	2/9/27/28	0/2/2/2
43	OMG	1	959	43	-	2/5/27/28	0/3/3/3
44	OMC	2	443	44	-	5/9/27/28	0/2/2/2
44	A2M	2	1186	44	-	0/5/27/28	0/3/3/3
43	OMG	1	1526	43	-	0/5/27/28	0/3/3/3
44	OMC	2	1318	44	-	0/9/27/28	0/2/2/2
43	A2M	1	955	43	-	0/5/27/28	0/3/3/3
49	A2M	7	43	49	-	0/5/27/28	0/3/3/3
44	A2M	2	570	43,44	-	1/5/27/28	0/3/3/3
44	A2M	2	665	44	-	2/5/27/28	0/3/3/3
44	A2M	2	1068	44	-	0/5/27/28	0/3/3/3
44	OMU	2	1360	44	-	0/9/27/28	0/2/2/2
43	A2M	1	858	43	-	1/5/27/28	0/3/3/3
44	OMU	2	1153	44	-	0/9/27/28	0/2/2/2
44	OMG	2	1361	44	-	0/5/27/28	0/3/3/3
44	OMG	2	655	44	-	0/5/27/28	0/3/3/3
44	OMU	2	667	44	-	2/9/27/28	0/2/2/2
44	OMG	2	534	44	-	2/5/27/28	0/3/3/3
43	A2M	1	927	43	-	0/5/27/28	0/3/3/3
44	OMG	2	641	44	-	2/5/27/28	0/3/3/3
43	OMG	1	1542	43,44	-	2/5/27/28	0/3/3/3
44	A2M	2	502	44	-	2/5/27/28	0/3/3/3
44	OMG	2	1230	44	-	2/5/27/28	0/3/3/3
43	OMG	1	1628	43	-	0/5/27/28	0/3/3/3
43	A2M	1	69	43	-	0/5/27/28	0/3/3/3
44	A2M	2	527	44	-	0/5/27/28	0/3/3/3
43	OMU	1	847	43	-	0/9/27/28	0/2/2/2
44	A2M	2	591	44	-	0/5/27/28	0/3/3/3
44	A2M	2	604	43,44	-	0/5/27/28	0/3/3/3
44	A2M	2	1373	44	-	0/5/27/28	0/3/3/3
49	OMG	7	75	49	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	A2M	7	162	43,49	-	0/5/27/28	0/3/3/3
45	OMU	3	10	45	-	1/9/27/28	0/2/2/2
44	A2M	2	382	44	-	1/5/27/28	0/3/3/3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	665	A2M	O5'-C5'	-5.54	1.31	1.44
44	2	1186	A2M	O5'-C5'	-5.51	1.31	1.44
43	1	681	A2M	O5'-C5'	-5.45	1.31	1.44
43	1	927	A2M	O5'-C5'	-5.43	1.31	1.44
44	2	570	A2M	O5'-C5'	-5.31	1.31	1.44
44	2	628	A2M	O5'-C5'	-5.28	1.31	1.44
44	2	527	A2M	O5'-C5'	-5.25	1.31	1.44
43	1	678	A2M	O5'-C5'	-5.21	1.32	1.44
43	1	955	A2M	O5'-C5'	-5.21	1.32	1.44
43	1	697	A2M	O5'-C5'	-5.18	1.32	1.44
43	1	858	A2M	O5'-C5'	-5.08	1.32	1.44
43	1	235	A2M	O5'-C5'	-5.07	1.32	1.44
44	2	591	A2M	O5'-C5'	-5.07	1.32	1.44
44	2	572	A2M	O5'-C5'	-5.06	1.32	1.44
43	1	1541	A2M	O5'-C5'	-5.02	1.32	1.44
44	2	1373	A2M	O5'-C5'	-4.98	1.32	1.44
49	7	162	A2M	O5'-C5'	-4.93	1.32	1.44
43	1	69	A2M	O5'-C5'	-4.89	1.32	1.44
43	1	437	A2M	O5'-C5'	-4.85	1.32	1.44
49	7	43	A2M	O5'-C5'	-4.75	1.33	1.44
44	2	1068	A2M	O5'-C5'	-4.71	1.33	1.44
44	2	1385	A2M	O5'-C5'	-4.66	1.33	1.44
44	2	604	A2M	O5'-C5'	-4.65	1.33	1.44
43	1	1371	OMU	C2-N1	4.61	1.45	1.38
44	2	1230	OMG	C6-N1	4.15	1.44	1.37
43	1	1526	OMG	C6-N1	4.12	1.44	1.37
44	2	1361	OMG	C6-N1	4.11	1.44	1.37
44	2	655	OMG	C6-N1	4.00	1.43	1.37
44	2	1047	OMG	C6-N1	3.89	1.43	1.37
44	2	641	OMG	C6-N1	3.83	1.43	1.37
49	7	75	OMG	C6-N1	3.75	1.43	1.37
44	2	71	OMG	C6-N1	3.73	1.43	1.37
43	1	856	OMG	C6-N1	3.72	1.43	1.37
44	2	534	OMG	C6-N1	3.64	1.43	1.37
43	1	1628	OMG	C6-N1	3.55	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1	1542	OMG	C6-N1	3.54	1.43	1.37
44	2	1079	OMG	C6-N1	3.51	1.43	1.37
44	2	1232	OMG	C6-N1	3.48	1.43	1.37
46	4	74	OMG	C6-N1	3.48	1.43	1.37
43	1	959	OMG	C6-N1	3.44	1.43	1.37
49	7	162	A2M	O4'-C4'	-3.36	1.37	1.45
43	1	1190	OMG	C5-C6	-3.35	1.40	1.47
44	2	1254	OMG	C6-N1	3.28	1.42	1.37
43	1	927	A2M	O4'-C4'	-3.27	1.37	1.45
44	2	1230	OMG	C5-C6	-3.22	1.40	1.47
43	1	858	A2M	O4'-C4'	-3.09	1.38	1.45
44	2	359	OMC	C2-N1	3.09	1.46	1.40
44	2	1249	OMC	C2-N1	3.09	1.46	1.40
44	2	655	OMG	C5-C6	-2.91	1.41	1.47
44	2	1186	A2M	O4'-C4'	-2.90	1.38	1.45
44	2	71	OMG	C5-C6	-2.89	1.41	1.47
44	2	641	OMG	C5-C6	-2.84	1.41	1.47
43	1	1529	OMC	C2-N1	2.83	1.46	1.40
44	2	534	OMG	C5-C6	-2.83	1.41	1.47
43	1	1541	A2M	O4'-C4'	-2.83	1.38	1.45
44	2	1373	A2M	O4'-C4'	-2.82	1.38	1.45
44	2	591	A2M	O4'-C4'	-2.81	1.38	1.45
43	1	1190	OMG	C6-N1	2.80	1.42	1.37
44	2	1385	A2M	O4'-C4'	-2.79	1.38	1.45
43	1	959	OMG	C5-C6	-2.78	1.41	1.47
46	4	74	OMG	C5-C6	-2.76	1.41	1.47
43	1	1190	OMG	C2-N2	2.76	1.40	1.34
44	2	665	A2M	O3'-C3'	-2.76	1.36	1.43
44	2	1232	OMG	C5-C6	-2.75	1.41	1.47
43	1	1526	OMG	C5-C6	-2.75	1.41	1.47
43	1	235	A2M	O4'-C4'	-2.73	1.38	1.45
43	1	955	A2M	O3'-C3'	-2.72	1.36	1.43
44	2	1254	OMG	C5-C6	-2.70	1.41	1.47
44	2	527	A2M	C3'-C2'	2.70	1.59	1.52
44	2	665	A2M	O4'-C4'	-2.69	1.39	1.45
43	1	1542	OMG	C5-C6	-2.69	1.41	1.47
44	2	1361	OMG	C5-C6	-2.67	1.42	1.47
43	1	678	A2M	O4'-C4'	-2.64	1.39	1.45
43	1	1628	OMG	C5-C6	-2.59	1.42	1.47
44	2	1079	OMG	C5-C6	-2.55	1.42	1.47
43	1	69	A2M	O4'-C1'	-2.53	1.37	1.41
44	2	1047	OMG	C5-C6	-2.50	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1160	OMC	C2-N1	2.47	1.45	1.40
43	1	856	OMG	C5-C6	-2.46	1.42	1.47
44	2	583	OMC	C2-N1	2.43	1.45	1.40
49	7	75	OMG	C5-C6	-2.39	1.42	1.47
44	2	527	A2M	O3'-C3'	2.39	1.48	1.43
44	2	1318	OMC	C4-N3	-2.38	1.29	1.34
49	7	43	A2M	O4'-C4'	-2.34	1.39	1.45
43	1	69	A2M	C5'-C4'	2.26	1.58	1.51
44	2	1068	A2M	O4'-C4'	-2.25	1.40	1.45
44	2	1068	A2M	O3'-C3'	-2.25	1.37	1.43
44	2	1318	OMC	C2-N1	2.17	1.44	1.40
44	2	604	A2M	O4'-C4'	-2.15	1.40	1.45
43	1	1529	OMC	C4-N3	-2.15	1.30	1.34
44	2	502	A2M	C5-C4	2.13	1.46	1.40
43	1	681	A2M	O4'-C4'	-2.11	1.40	1.45
44	2	1186	A2M	O4'-C1'	-2.08	1.38	1.41
44	2	1078	OMU	C2-N1	2.05	1.41	1.38
43	1	697	A2M	O4'-C4'	-2.05	1.40	1.45
43	1	697	A2M	O3'-C3'	-2.04	1.38	1.43
44	2	1398	OMC	C2-N1	2.01	1.44	1.40
44	2	591	A2M	O3'-C3'	-2.01	1.38	1.43

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	856	OMG	O6-C6-N1	-4.41	115.44	120.65
43	1	1371	OMU	O2-C2-N1	4.03	128.14	122.79
43	1	1371	OMU	C1'-N1-C2	4.02	124.85	117.57
43	1	1190	OMG	O6-C6-C5	3.92	132.03	124.37
44	2	1254	OMG	O6-C6-N1	-3.89	116.06	120.65
44	2	1047	OMG	O6-C6-N1	-3.81	116.15	120.65
43	1	856	OMG	O6-C6-C5	3.78	131.75	124.37
44	2	1079	OMG	O6-C6-N1	-3.73	116.25	120.65
43	1	1190	OMG	O6-C6-N1	-3.70	116.28	120.65
43	1	1542	OMG	O6-C6-N1	-3.69	116.29	120.65
49	7	75	OMG	O6-C6-N1	-3.69	116.29	120.65
46	4	74	OMG	O6-C6-C5	3.57	131.34	124.37
46	4	74	OMG	O6-C6-N1	-3.54	116.46	120.65
44	2	1361	OMG	O6-C6-C5	3.51	131.23	124.37
43	1	1628	OMG	O6-C6-C5	3.46	131.13	124.37
44	2	1361	OMG	O6-C6-N1	-3.46	116.57	120.65
44	2	502	A2M	N3-C2-N1	-3.44	123.30	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1047	OMG	O6-C6-C5	3.44	131.09	124.37
44	2	1318	OMC	CM2-O2'-C2'	-3.40	105.59	114.52
44	2	1254	OMG	O6-C6-C5	3.40	131.02	124.37
43	1	1542	OMG	O6-C6-C5	3.39	131.00	124.37
49	7	75	OMG	O6-C6-C5	3.38	130.97	124.37
43	1	1628	OMG	O6-C6-N1	-3.36	116.68	120.65
44	2	667	OMU	CM2-O2'-C2'	-3.35	105.73	114.52
44	2	1079	OMG	O6-C6-C5	3.33	130.88	124.37
44	2	443	OMC	C5-C4-N3	3.30	126.95	121.33
44	2	534	OMG	O6-C6-C5	3.26	130.73	124.37
44	2	1232	OMG	O6-C6-C5	3.22	130.67	124.37
44	2	534	OMG	O6-C6-N1	-3.20	116.87	120.65
44	2	655	OMG	O6-C6-C5	3.18	130.58	124.37
43	1	959	OMG	O6-C6-N1	-3.12	116.96	120.65
44	2	1318	OMC	C5-C4-N3	3.10	126.60	121.33
43	1	959	OMG	O6-C6-C5	3.05	130.34	124.37
44	2	560	OMU	CM2-O2'-C2'	-3.05	106.52	114.52
44	2	359	OMC	C5-C4-N3	3.00	126.44	121.33
44	2	1232	OMG	O6-C6-N1	-3.00	117.11	120.65
44	2	570	A2M	O2'-C2'-C1'	2.99	115.03	109.09
44	2	534	OMG	CM2-O2'-C2'	-2.92	106.86	114.52
44	2	1398	OMC	C5-C4-N3	2.91	126.27	121.33
49	7	43	A2M	C3'-C2'-C1'	-2.89	97.47	102.89
44	2	1160	OMC	C5-C4-N3	2.88	126.23	121.33
44	2	655	OMG	O6-C6-N1	-2.88	117.25	120.65
43	1	1371	OMU	O2-C2-N3	-2.88	116.14	121.50
43	1	1529	OMC	C5-C4-N3	2.87	126.22	121.33
44	2	1249	OMC	C5-C4-N3	2.86	126.19	121.33
44	2	1385	A2M	C3'-C2'-C1'	-2.85	97.52	102.89
44	2	1249	OMC	CM2-O2'-C2'	-2.85	107.05	114.52
44	2	71	OMG	O6-C6-N1	-2.84	117.30	120.65
43	1	69	A2M	O4'-C1'-C2'	-2.80	101.72	106.59
44	2	641	OMG	O6-C6-C5	2.79	129.82	124.37
44	2	1318	OMC	N4-C4-N3	-2.78	113.09	117.97
44	2	583	OMC	C5-C4-N3	2.78	126.05	121.33
43	1	1526	OMG	O6-C6-C5	2.77	129.78	124.37
44	2	1254	OMG	CM2-O2'-C2'	-2.76	107.29	114.52
43	1	955	A2M	C3'-C2'-C1'	-2.74	97.74	102.89
44	2	1078	OMU	CM2-O2'-C2'	-2.74	107.34	114.52
44	2	641	OMG	CM2-O2'-C2'	-2.73	107.35	114.52
43	1	1526	OMG	N2-C2-N3	-2.71	114.47	119.74
44	2	382	A2M	C4-C5-N7	-2.70	106.58	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	1529	OMC	CM2-O2'-C2'	-2.69	107.47	114.52
44	2	527	A2M	C4-C5-N7	2.68	112.19	109.40
43	1	695	OMC	C5-C4-N3	2.67	125.88	121.33
44	2	655	OMG	CM2-O2'-C2'	-2.64	107.60	114.52
44	2	641	OMG	O6-C6-N1	-2.63	117.54	120.65
44	2	527	A2M	O3'-C3'-C4'	2.63	118.65	111.05
44	2	1230	OMG	O6-C6-C5	2.61	129.46	124.37
44	2	502	A2M	C4-C5-N7	-2.60	106.69	109.40
43	1	1661	OMU	CM2-O2'-C2'	-2.59	107.73	114.52
44	2	1079	OMG	N2-C2-N3	-2.55	114.78	119.74
44	2	1360	OMU	C4-N3-C2	-2.52	123.25	126.58
44	2	382	A2M	N3-C2-N1	-2.52	124.73	128.68
43	1	1371	OMU	CM2-O2'-C2'	-2.50	107.95	114.52
44	2	443	OMC	CM2-O2'-C2'	-2.47	108.05	114.52
44	2	71	OMG	O6-C6-C5	2.46	129.18	124.37
43	1	48	OMU	CM2-O2'-C2'	-2.45	108.08	114.52
44	2	1360	OMU	CM2-O2'-C2'	-2.45	108.10	114.52
44	2	359	OMC	CM2-O2'-C2'	-2.39	108.26	114.52
44	2	71	OMG	C2-N1-C6	-2.37	120.72	125.10
44	2	527	A2M	O3'-C3'-C2'	2.37	117.89	111.17
44	2	1420	OMU	CM2-O2'-C2'	-2.36	108.32	114.52
44	2	1160	OMC	C4-N3-C2	-2.36	116.45	120.25
44	2	560	OMU	C4-N3-C2	-2.35	123.48	126.58
43	1	1541	A2M	C4-C5-N7	2.34	111.83	109.40
44	2	1361	OMG	N2-C2-N3	-2.33	115.19	119.74
43	1	1371	OMU	C1'-N1-C6	-2.33	115.75	120.84
43	1	1628	OMG	N1-C2-N3	2.33	127.67	123.32
45	3	10	OMU	CM2-O2'-C2'	-2.33	108.41	114.52
44	2	1254	OMG	N1-C2-N3	2.33	127.67	123.32
44	2	443	OMC	C4-N3-C2	-2.33	116.50	120.25
43	1	1107	OMU	C4-N3-C2	-2.32	123.52	126.58
44	2	527	A2M	C2-N1-C6	-2.31	114.80	118.75
44	2	583	OMC	CM2-O2'-C2'	-2.30	108.48	114.52
49	7	7	OMU	C4-N3-C2	-2.30	123.55	126.58
44	2	572	A2M	C4-C5-N7	2.30	111.79	109.40
44	2	665	A2M	C4-C5-N7	2.29	111.79	109.40
43	1	678	A2M	C4-C5-N7	2.28	111.77	109.40
43	1	1628	OMG	N2-C2-N3	-2.26	115.33	119.74
43	1	847	OMU	CM2-O2'-C2'	-2.26	108.60	114.52
44	2	667	OMU	C4-N3-C2	-2.26	123.61	126.58
44	2	443	OMC	N4-C4-N3	-2.25	114.01	117.97
44	2	628	A2M	C4-C5-N7	2.25	111.75	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1254	OMG	C2-N1-C6	-2.25	120.95	125.10
44	2	1079	OMG	C2-N1-C6	-2.25	120.95	125.10
44	2	1153	OMU	CM2-O2'-C2'	-2.25	108.62	114.52
43	1	1526	OMG	O6-C6-N1	-2.24	118.00	120.65
43	1	1371	OMU	C2'-C1'-N1	-2.24	109.87	114.22
43	1	845	OMU	CM2-O2'-C2'	-2.24	108.64	114.52
49	7	162	A2M	C4-C5-N7	2.24	111.73	109.40
43	1	697	A2M	C4-C5-N7	2.23	111.72	109.40
43	1	681	A2M	C4-C5-N7	2.23	111.72	109.40
43	1	48	OMU	C4-N3-C2	-2.22	123.65	126.58
43	1	858	A2M	C4-C5-N7	2.21	111.71	109.40
43	1	697	A2M	C3'-C2'-C1'	-2.21	98.73	102.89
44	2	1068	A2M	C3'-C2'-C1'	-2.20	98.76	102.89
43	1	681	A2M	C2'-C3'-C4'	-2.19	97.23	101.99
44	2	570	A2M	O3'-C3'-C2'	-2.19	104.94	111.17
43	1	1107	OMU	CM2-O2'-C2'	-2.19	108.78	114.52
43	1	959	OMG	N1-C2-N3	2.19	127.40	123.32
44	2	359	OMC	C4-N3-C2	-2.18	116.74	120.25
44	2	1160	OMC	CM2-O2'-C2'	-2.17	108.82	114.52
46	4	74	OMG	N1-C2-N3	2.16	127.36	123.32
49	7	75	OMG	N1-C2-N3	2.15	127.33	123.32
46	4	74	OMG	CM2-O2'-C2'	-2.14	108.90	114.52
43	1	1526	OMG	N1-C2-N3	2.14	127.31	123.32
49	7	75	OMG	C2-N1-C6	-2.13	121.18	125.10
44	2	1079	OMG	N1-C2-N3	2.13	127.29	123.32
44	2	1385	A2M	C1'-N9-C4	-2.12	122.91	126.64
44	2	572	A2M	C3'-C2'-C1'	-2.12	98.90	102.89
43	1	1526	OMG	C2-N1-C6	-2.12	121.20	125.10
44	2	641	OMG	C2-N1-C6	-2.11	121.20	125.10
43	1	235	A2M	C2-N1-C6	-2.11	115.14	118.75
43	1	1628	OMG	CM2-O2'-C2'	-2.11	108.98	114.52
44	2	502	A2M	O3'-C3'-C2'	-2.11	105.18	111.17
43	1	927	A2M	C4-C5-N7	2.11	111.59	109.40
44	2	534	OMG	N1-C2-N3	2.10	127.25	123.32
44	2	1153	OMU	C4-N3-C2	-2.10	123.81	126.58
43	1	678	A2M	C2-N1-C6	-2.09	115.18	118.75
44	2	1385	A2M	C4-C5-N7	2.08	111.56	109.40
49	7	75	OMG	CM2-O2'-C2'	-2.07	109.08	114.52
44	2	591	A2M	C3'-C2'-C1'	-2.07	98.99	102.89
43	1	1529	OMC	N4-C4-N3	-2.06	114.34	117.97
43	1	959	OMG	C2-N1-C6	-2.06	121.30	125.10
44	2	1078	OMU	C4-N3-C2	-2.06	123.87	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	628	A2M	C2-N1-C6	-2.06	115.23	118.75
44	2	641	OMG	N2-C2-N3	-2.06	115.74	119.74
43	1	955	A2M	C2-N1-C6	-2.05	115.24	118.75
44	2	1398	OMC	C4-N3-C2	-2.05	116.94	120.25
44	2	1230	OMG	O6-C6-N1	-2.05	118.23	120.65
44	2	359	OMC	N4-C4-N3	-2.04	114.38	117.97
44	2	1361	OMG	CM2-O2'-C2'	-2.04	109.17	114.52
49	7	7	OMU	CM2-O2'-C2'	-2.03	109.20	114.52
44	2	1232	OMG	CM2-O2'-C2'	-2.02	109.22	114.52
43	1	856	OMG	N2-C2-N3	-2.02	115.81	119.74
43	1	847	OMU	C4-N3-C2	-2.01	123.93	126.58
49	7	75	OMG	N2-C2-N3	-2.01	115.83	119.74
44	2	665	A2M	C2-N1-C6	-2.00	115.33	118.75
44	2	1420	OMU	C4-N3-C2	-2.00	123.94	126.58

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1	48	OMU	C3'-C4'-C5'-O5'
43	1	48	OMU	O4'-C4'-C5'-O5'
43	1	681	A2M	O4'-C4'-C5'-O5'
43	1	959	OMG	O4'-C4'-C5'-O5'
43	1	959	OMG	C3'-C4'-C5'-O5'
43	1	1253	OMU	C3'-C4'-C5'-O5'
43	1	1253	OMU	O4'-C4'-C5'-O5'
43	1	1371	OMU	O4'-C1'-N1-C2
43	1	1371	OMU	O4'-C1'-N1-C6
43	1	1542	OMG	O4'-C4'-C5'-O5'
43	1	1542	OMG	C3'-C4'-C5'-O5'
44	2	382	A2M	C1'-C2'-O2'-CM'
44	2	443	OMC	C2'-C1'-N1-C6
44	2	534	OMG	O4'-C4'-C5'-O5'
44	2	534	OMG	C3'-C4'-C5'-O5'
44	2	570	A2M	C1'-C2'-O2'-CM'
44	2	665	A2M	O4'-C4'-C5'-O5'
44	2	665	A2M	C3'-C4'-C5'-O5'
44	2	667	OMU	C3'-C4'-C5'-O5'
44	2	667	OMU	O4'-C4'-C5'-O5'
44	2	1047	OMG	O4'-C4'-C5'-O5'
44	2	1230	OMG	O4'-C4'-C5'-O5'
44	2	1230	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
49	7	75	OMG	O4'-C4'-C5'-O5'
49	7	75	OMG	C3'-C4'-C5'-O5'
44	2	443	OMC	C2'-C1'-N1-C2
43	1	681	A2M	C3'-C4'-C5'-O5'
43	1	1371	OMU	C3'-C4'-C5'-O5'
44	2	502	A2M	O4'-C4'-C5'-O5'
44	2	641	OMG	C3'-C4'-C5'-O5'
44	2	1047	OMG	C3'-C4'-C5'-O5'
44	2	1385	A2M	O4'-C4'-C5'-O5'
44	2	502	A2M	C3'-C4'-C5'-O5'
44	2	641	OMG	O4'-C4'-C5'-O5'
49	7	7	OMU	C3'-C4'-C5'-O5'
44	2	1385	A2M	C3'-C4'-C5'-O5'
43	1	1371	OMU	O4'-C4'-C5'-O5'
44	2	1079	OMG	O4'-C4'-C5'-O5'
49	7	7	OMU	O4'-C4'-C5'-O5'
44	2	1079	OMG	C3'-C4'-C5'-O5'
44	2	1249	OMC	C4'-C5'-O5'-P
43	1	235	A2M	C3'-C2'-O2'-CM'
44	2	560	OMU	C4'-C5'-O5'-P
44	2	443	OMC	O4'-C1'-N1-C2
45	3	10	OMU	C3'-C4'-C5'-O5'
44	2	443	OMC	O4'-C1'-N1-C6
43	1	858	A2M	C3'-C2'-O2'-CM'
43	1	1371	OMU	C4'-C5'-O5'-P
43	1	1529	OMC	C3'-C2'-O2'-CM2
44	2	443	OMC	C4'-C5'-O5'-P
43	1	678	A2M	O4'-C4'-C5'-O5'
43	1	1529	OMC	O4'-C4'-C5'-O5'
43	1	681	A2M	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 34 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
51	PAR	1	1802	-	45,45,45	3.53	9 (20%)	64,67,67	1.17	7 (10%)
51	PAR	1	1804	-	45,45,45	3.64	9 (20%)	64,67,67	1.56	11 (17%)
51	PAR	2	1702	-	45,45,45	3.55	8 (17%)	64,67,67	1.43	7 (10%)
51	PAR	7	201	-	45,45,45	3.53	9 (20%)	64,67,67	1.76	17 (26%)
51	PAR	2	1705	-	45,45,45	3.55	9 (20%)	64,67,67	1.63	14 (21%)
51	PAR	1	1803	43	45,45,45	3.54	8 (17%)	64,67,67	1.35	7 (10%)
51	PAR	1	1805	-	45,45,45	3.48	8 (17%)	64,67,67	1.57	13 (20%)
51	PAR	2	1704	-	45,45,45	3.58	8 (17%)	64,67,67	1.26	8 (12%)
51	PAR	2	1703	-	45,45,45	3.58	10 (22%)	64,67,67	1.97	17 (26%)
51	PAR	1	1801	-	45,45,45	3.55	8 (17%)	64,67,67	1.34	9 (14%)

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
51	PAR	1	1802	-	-	6/18/94/94	0/4/4/4
51	PAR	1	1804	-	-	7/18/94/94	0/4/4/4
51	PAR	2	1702	-	-	4/18/94/94	0/4/4/4
51	PAR	7	201	-	-	8/18/94/94	0/4/4/4
51	PAR	2	1705	-	-	12/18/94/94	0/4/4/4
51	PAR	1	1803	43	-	7/18/94/94	0/4/4/4
51	PAR	1	1805	-	-	8/18/94/94	0/4/4/4
51	PAR	2	1704	-	-	6/18/94/94	0/4/4/4
51	PAR	2	1703	-	-	9/18/94/94	0/4/4/4
51	PAR	1	1801	-	-	8/18/94/94	0/4/4/4

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	1	1804	PAR	C13-C23	-16.87	1.31	1.52
51	2	1704	PAR	C13-C23	-16.59	1.31	1.52
51	1	1803	PAR	C13-C23	-16.56	1.31	1.52
51	1	1802	PAR	C13-C23	-16.40	1.31	1.52
51	1	1801	PAR	C13-C23	-16.37	1.32	1.52
51	7	201	PAR	C13-C23	-16.15	1.32	1.52
51	1	1805	PAR	C13-C23	-16.12	1.32	1.52
51	2	1702	PAR	C13-C23	-16.11	1.32	1.52
51	2	1705	PAR	C13-C23	-16.02	1.32	1.52
51	2	1703	PAR	C13-C23	-15.93	1.32	1.52
51	1	1804	PAR	O43-C13	12.69	1.64	1.41
51	1	1801	PAR	O43-C13	12.64	1.64	1.41
51	2	1702	PAR	O43-C13	12.56	1.64	1.41
51	2	1705	PAR	O43-C13	12.46	1.64	1.41
51	1	1802	PAR	O43-C13	12.44	1.64	1.41
51	2	1704	PAR	O43-C13	12.37	1.63	1.41
51	2	1703	PAR	O43-C13	12.26	1.63	1.41
51	1	1805	PAR	O43-C13	12.26	1.63	1.41
51	1	1803	PAR	O43-C13	11.99	1.63	1.41
51	7	201	PAR	O43-C13	11.92	1.63	1.41
51	7	201	PAR	O43-C43	-7.23	1.28	1.45
51	1	1803	PAR	O43-C43	-6.91	1.29	1.45
51	2	1703	PAR	O43-C43	-6.87	1.29	1.45
51	2	1702	PAR	O43-C43	-6.76	1.29	1.45
51	1	1801	PAR	O43-C43	-6.73	1.29	1.45
51	2	1705	PAR	O43-C43	-6.73	1.30	1.45
51	2	1704	PAR	O43-C43	-6.58	1.30	1.45
51	1	1804	PAR	O43-C43	-6.48	1.30	1.45
51	1	1802	PAR	O43-C43	-6.47	1.30	1.45
51	1	1805	PAR	O43-C43	-6.41	1.30	1.45
51	2	1703	PAR	C31-C21	-6.16	1.45	1.53
51	2	1704	PAR	C31-C21	-4.83	1.47	1.53
51	1	1804	PAR	C34-C24	-4.72	1.47	1.53
51	1	1804	PAR	C31-C21	-4.60	1.47	1.53
51	1	1805	PAR	C34-C24	-4.56	1.47	1.53
51	2	1702	PAR	C31-C21	-4.56	1.47	1.53
51	7	201	PAR	C31-C21	-4.53	1.47	1.53
51	2	1705	PAR	C34-C24	-4.53	1.47	1.53
51	1	1801	PAR	C31-C21	-4.31	1.48	1.53
51	2	1705	PAR	O54-C14	4.27	1.52	1.41
51	1	1803	PAR	C34-C24	-4.16	1.48	1.53
51	2	1703	PAR	O54-C14	4.11	1.52	1.41
51	1	1803	PAR	C31-C21	-4.10	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	2	1702	PAR	O54-C14	4.06	1.52	1.41
51	7	201	PAR	C34-C24	-4.02	1.48	1.53
51	1	1805	PAR	O54-C14	3.92	1.51	1.41
51	2	1702	PAR	C34-C24	-3.90	1.48	1.53
51	2	1704	PAR	O54-C14	3.89	1.51	1.41
51	1	1802	PAR	C31-C21	-3.88	1.48	1.53
51	2	1705	PAR	C31-C21	-3.80	1.48	1.53
51	1	1802	PAR	C34-C24	-3.80	1.48	1.53
51	2	1704	PAR	C34-C24	-3.79	1.48	1.53
51	1	1804	PAR	O54-C14	3.79	1.51	1.41
51	7	201	PAR	O54-C14	3.70	1.51	1.41
51	1	1803	PAR	O54-C14	3.66	1.51	1.41
51	1	1802	PAR	O54-C14	3.61	1.51	1.41
51	1	1801	PAR	O54-C14	3.55	1.50	1.41
51	2	1703	PAR	C34-C24	-3.54	1.49	1.53
51	1	1801	PAR	C34-C24	-3.52	1.49	1.53
51	7	201	PAR	O33-C33	-3.31	1.35	1.43
51	2	1702	PAR	O33-C33	-3.18	1.35	1.43
51	1	1805	PAR	C31-C21	-3.10	1.49	1.53
51	2	1703	PAR	O51-C11	3.06	1.49	1.41
51	1	1801	PAR	O33-C33	-3.05	1.35	1.43
51	1	1802	PAR	O33-C33	-2.98	1.36	1.43
51	2	1703	PAR	O33-C33	-2.93	1.36	1.43
51	2	1705	PAR	O33-C33	-2.92	1.36	1.43
51	1	1805	PAR	O33-C33	-2.92	1.36	1.43
51	1	1803	PAR	O33-C33	-2.87	1.36	1.43
51	2	1705	PAR	O51-C11	2.84	1.49	1.41
51	2	1704	PAR	O33-C33	-2.84	1.36	1.43
51	2	1704	PAR	O51-C11	2.82	1.49	1.41
51	1	1804	PAR	O33-C33	-2.81	1.36	1.43
51	1	1801	PAR	O51-C11	2.79	1.48	1.41
51	7	201	PAR	O51-C11	2.78	1.48	1.41
51	1	1802	PAR	O51-C11	2.67	1.48	1.41
51	1	1804	PAR	O51-C11	2.57	1.48	1.41
51	2	1705	PAR	C64-C54	2.55	1.55	1.52
51	2	1702	PAR	O51-C11	2.51	1.48	1.41
51	1	1803	PAR	O51-C11	2.46	1.48	1.41
51	1	1805	PAR	O51-C11	2.40	1.48	1.41
51	2	1703	PAR	C21-N21	-2.26	1.43	1.47
51	1	1804	PAR	O51-C51	2.24	1.49	1.44
51	2	1703	PAR	O51-C51	2.22	1.49	1.44
51	1	1802	PAR	C64-C54	2.05	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	7	201	PAR	C22-C12	-2.01	1.49	1.53

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	2	1703	PAR	O52-C13-O43	-5.59	105.38	111.43
51	1	1805	PAR	C41-C31-C21	5.03	119.72	111.07
51	2	1703	PAR	C22-C12-C62	4.81	117.30	110.04
51	7	201	PAR	C44-C34-C24	4.68	119.11	111.07
51	1	1804	PAR	O51-C51-C41	4.52	117.91	109.69
51	7	201	PAR	O52-C52-C62	4.43	119.06	107.28
51	7	201	PAR	O52-C13-O43	4.38	116.17	111.43
51	2	1705	PAR	C13-C23-C33	4.23	107.19	102.10
51	2	1702	PAR	C44-C34-C24	4.17	118.25	111.07
51	2	1703	PAR	O52-C52-C42	4.14	117.99	107.48
51	1	1804	PAR	C14-O33-C33	-4.04	107.97	117.96
51	1	1801	PAR	C14-O33-C33	-3.97	108.15	117.96
51	1	1804	PAR	C31-C41-C51	3.73	116.89	110.24
51	1	1803	PAR	O54-C54-C44	3.68	116.37	109.69
51	2	1705	PAR	O52-C13-O43	-3.57	107.57	111.43
51	2	1703	PAR	O52-C13-C23	3.50	115.22	107.96
51	2	1702	PAR	C14-O33-C33	-3.49	109.33	117.96
51	2	1703	PAR	O51-C51-C41	3.48	116.02	109.69
51	1	1805	PAR	C52-C62-C12	3.48	118.12	109.63
51	2	1703	PAR	C32-C22-C12	3.48	118.32	111.18
51	1	1803	PAR	C44-C34-C24	3.47	117.04	111.07
51	1	1804	PAR	O33-C14-C24	3.46	114.17	108.22
51	1	1805	PAR	C14-O33-C33	-3.44	109.45	117.96
51	1	1803	PAR	C34-C44-C54	3.42	116.34	110.24
51	2	1705	PAR	C14-O54-C54	3.40	120.36	113.69
51	1	1805	PAR	C62-C52-C42	3.37	119.37	111.66
51	7	201	PAR	O62-C62-C12	-3.33	103.70	109.81
51	2	1703	PAR	C11-O51-C51	3.32	120.21	113.69
51	2	1705	PAR	O54-C14-C24	3.29	117.47	110.06
51	2	1703	PAR	C11-O11-C42	-3.24	109.95	117.96
51	2	1703	PAR	C61-C51-C41	-3.23	105.45	113.00
51	7	201	PAR	C14-O33-C33	-3.22	109.99	117.96
51	2	1705	PAR	C34-C24-N24	-3.19	104.52	111.05
51	2	1703	PAR	C64-C54-C44	-3.18	106.85	113.10
51	1	1802	PAR	C11-O11-C42	-3.14	110.20	117.96
51	1	1801	PAR	C13-O52-C52	-3.13	110.22	117.96
51	1	1804	PAR	C22-C12-C62	3.04	114.62	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	2	1703	PAR	O11-C42-C52	3.03	115.18	107.48
51	2	1705	PAR	O52-C52-C62	3.01	115.29	107.28
51	1	1801	PAR	C44-C34-C24	2.99	116.22	111.07
51	2	1703	PAR	C62-C52-C42	-2.99	104.83	111.66
51	1	1805	PAR	C13-O52-C52	-2.99	110.57	117.96
51	2	1705	PAR	O33-C14-C24	2.95	113.31	108.22
51	7	201	PAR	C14-C24-C34	2.95	117.94	110.21
51	1	1804	PAR	C52-C62-C12	2.95	116.82	109.63
51	2	1705	PAR	C14-O33-C33	-2.91	110.75	117.96
51	1	1801	PAR	O51-C11-C21	2.90	116.59	110.06
51	2	1704	PAR	C14-O33-C33	-2.90	110.78	117.96
51	2	1702	PAR	O54-C14-C24	2.85	116.47	110.06
51	1	1803	PAR	C13-C23-C33	2.84	105.52	102.10
51	1	1805	PAR	C22-C12-C62	2.81	114.28	110.04
51	1	1803	PAR	C14-O33-C33	-2.77	111.10	117.96
51	1	1805	PAR	C11-C21-C31	2.74	117.39	110.21
51	2	1702	PAR	C13-C23-C33	2.72	105.38	102.10
51	7	201	PAR	C52-C42-C32	2.71	116.22	111.16
51	2	1702	PAR	O51-C51-C41	2.70	114.59	109.69
51	7	201	PAR	C34-C44-C54	2.67	115.00	110.24
51	2	1704	PAR	C61-C51-C41	-2.66	106.77	113.00
51	1	1804	PAR	C13-O52-C52	-2.64	111.42	117.96
51	1	1803	PAR	O11-C11-C21	2.64	112.77	108.22
51	1	1805	PAR	C11-O11-C42	-2.64	111.43	117.96
51	2	1704	PAR	O51-C51-C41	2.60	114.41	109.69
51	7	201	PAR	O52-C52-C42	-2.53	101.05	107.48
51	7	201	PAR	C13-O52-C52	2.52	124.21	117.96
51	1	1802	PAR	C44-C34-C24	2.52	115.40	111.07
51	1	1803	PAR	C11-O11-C42	-2.48	111.83	117.96
51	1	1805	PAR	C13-C23-C33	2.47	105.07	102.10
51	1	1802	PAR	C32-C22-C12	2.45	116.20	111.18
51	2	1704	PAR	C14-C24-C34	2.38	116.45	110.21
51	7	201	PAR	O52-C13-C23	2.38	112.89	107.96
51	1	1804	PAR	C61-C51-C41	-2.38	107.44	113.00
51	1	1801	PAR	C11-O51-C51	2.37	118.34	113.69
51	2	1703	PAR	C52-C42-C32	-2.37	106.75	111.16
51	2	1703	PAR	C53-C43-C33	-2.35	107.36	114.85
51	2	1705	PAR	O52-C13-C23	2.33	112.78	107.96
51	2	1705	PAR	C14-C24-N24	2.32	114.38	110.20
51	2	1704	PAR	C44-C34-C24	2.32	115.05	111.07
51	1	1805	PAR	C11-C21-N21	-2.31	106.03	110.20
51	7	201	PAR	C11-O11-C42	-2.29	112.31	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	1	1801	PAR	C13-C23-C33	2.28	104.84	102.10
51	2	1702	PAR	C64-C54-C44	-2.27	108.64	113.10
51	7	201	PAR	O34-C34-C24	-2.26	106.16	110.22
51	1	1805	PAR	C52-C42-C32	2.25	115.37	111.16
51	1	1801	PAR	C61-C51-C41	-2.25	107.74	113.00
51	2	1704	PAR	C13-O52-C52	-2.25	112.41	117.96
51	2	1703	PAR	C13-O52-C52	-2.24	112.41	117.96
51	7	201	PAR	C13-C23-C33	2.24	104.80	102.10
51	7	201	PAR	C22-C32-C42	2.21	115.11	109.53
51	1	1804	PAR	C11-O51-C51	2.19	117.99	113.69
51	1	1802	PAR	C13-C23-C33	2.17	104.71	102.10
51	2	1702	PAR	C11-O51-C51	2.16	117.92	113.69
51	2	1703	PAR	O54-C54-C64	2.15	110.01	106.01
51	1	1802	PAR	C62-C12-N12	-2.14	106.73	110.97
51	1	1801	PAR	O33-C14-C24	2.13	111.88	108.22
51	2	1705	PAR	C11-O11-C42	-2.12	112.72	117.96
51	2	1704	PAR	C31-C41-C51	2.11	114.00	110.24
51	2	1705	PAR	O62-C62-C12	-2.11	105.95	109.81
51	1	1805	PAR	C31-C41-C51	2.11	114.00	110.24
51	1	1801	PAR	C11-C21-C31	2.10	115.71	110.21
51	7	201	PAR	C64-C54-C44	-2.10	108.97	113.10
51	1	1802	PAR	C22-C32-C42	2.10	114.83	109.53
51	1	1802	PAR	C62-C52-C42	-2.07	106.94	111.66
51	1	1804	PAR	C34-C24-N24	-2.06	106.83	111.05
51	2	1705	PAR	C41-C31-C21	2.06	114.61	111.07
51	1	1804	PAR	O34-C34-C24	-2.03	106.57	110.22
51	2	1703	PAR	C22-C32-C42	2.02	114.64	109.53
51	2	1704	PAR	C11-O51-C51	2.02	117.65	113.69
51	1	1805	PAR	C64-C54-C44	-2.02	109.14	113.10
51	7	201	PAR	C34-C24-N24	-2.01	106.93	111.05
51	2	1705	PAR	O51-C11-C21	2.01	114.58	110.06

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	1	1801	PAR	C23-C13-O52-C52
51	1	1802	PAR	C33-C43-C53-O53
51	1	1803	PAR	O54-C54-C64-N64
51	1	1804	PAR	C23-C13-O52-C52
51	1	1805	PAR	C44-C54-C64-N64
51	1	1805	PAR	O54-C54-C64-N64

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Mol	Chain	Res	Type	Atoms
51	2	1703	PAR	C23-C13-O52-C52
51	2	1703	PAR	O43-C13-O52-C52
51	2	1705	PAR	C23-C13-O52-C52
51	2	1705	PAR	O43-C13-O52-C52
51	2	1705	PAR	C24-C14-O33-C33
51	2	1705	PAR	O54-C54-C64-N64
51	7	201	PAR	C23-C13-O52-C52
51	7	201	PAR	O43-C13-O52-C52
51	2	1705	PAR	C62-C52-O52-C13
51	1	1801	PAR	O43-C43-C53-O53
51	2	1703	PAR	O43-C43-C53-O53
51	1	1801	PAR	C33-C43-C53-O53
51	1	1803	PAR	C33-C43-C53-O53
51	1	1801	PAR	O51-C11-O11-C42
51	1	1803	PAR	C41-C51-C61-O61
51	1	1802	PAR	O43-C43-C53-O53
51	1	1804	PAR	O43-C43-C53-O53
51	2	1705	PAR	O43-C43-C53-O53
51	1	1804	PAR	C33-C43-C53-O53
51	1	1803	PAR	O54-C14-O33-C33
51	1	1803	PAR	O43-C43-C53-O53
51	1	1802	PAR	O54-C14-O33-C33
51	2	1703	PAR	C33-C43-C53-O53
51	1	1803	PAR	O51-C51-C61-O61
51	2	1704	PAR	C33-C43-C53-O53
51	2	1705	PAR	C33-C43-C53-O53
51	2	1702	PAR	O51-C11-O11-C42
51	7	201	PAR	O51-C51-C61-O61
51	2	1703	PAR	C41-C51-C61-O61
51	1	1805	PAR	C41-C51-C61-O61
51	7	201	PAR	C62-C52-O52-C13
51	7	201	PAR	C41-C51-C61-O61
51	7	201	PAR	C42-C52-O52-C13
51	7	201	PAR	O54-C14-O33-C33
51	2	1704	PAR	O43-C43-C53-O53
51	1	1805	PAR	O51-C51-C61-O61
51	2	1702	PAR	O51-C51-C61-O61
51	1	1801	PAR	O51-C51-C61-O61
51	1	1804	PAR	O43-C13-O52-C52
51	2	1704	PAR	O43-C13-O52-C52
51	2	1703	PAR	O51-C51-C61-O61
51	1	1804	PAR	O51-C51-C61-O61

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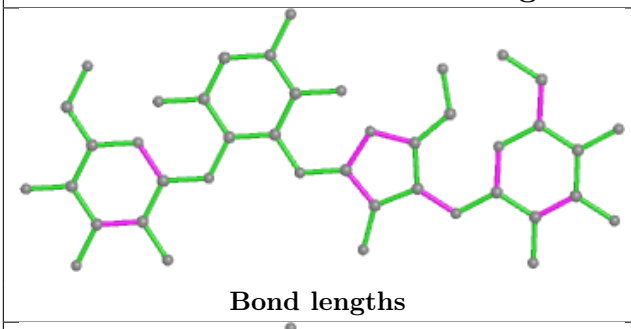
Mol	Chain	Res	Type	Atoms
51	2	1703	PAR	O54-C14-O33-C33
51	1	1805	PAR	C24-C14-O33-C33
51	2	1705	PAR	C41-C51-C61-O61
51	1	1801	PAR	O43-C13-O52-C52
51	1	1805	PAR	C33-C43-C53-O53
51	2	1704	PAR	C23-C13-O52-C52
51	2	1705	PAR	O51-C51-C61-O61
51	2	1704	PAR	O51-C11-O11-C42
51	2	1704	PAR	O54-C14-O33-C33
51	1	1801	PAR	O54-C54-C64-N64
51	1	1803	PAR	C43-C33-O33-C14
51	1	1802	PAR	C21-C11-O11-C42
51	2	1703	PAR	C21-C11-O11-C42
51	1	1805	PAR	C62-C52-O52-C13
51	2	1705	PAR	O54-C14-O33-C33
51	1	1801	PAR	O54-C14-O33-C33
51	1	1805	PAR	C23-C13-O52-C52
51	1	1802	PAR	O51-C51-C61-O61
51	1	1802	PAR	C23-C33-O33-C14
51	1	1804	PAR	C23-C33-O33-C14
51	1	1804	PAR	C43-C33-O33-C14
51	2	1702	PAR	C23-C33-O33-C14
51	2	1702	PAR	C43-C33-O33-C14
51	2	1703	PAR	C23-C33-O33-C14
51	2	1705	PAR	C23-C33-O33-C14
51	2	1705	PAR	C44-C54-C64-N64
51	7	201	PAR	C23-C33-O33-C14

There are no ring outliers.

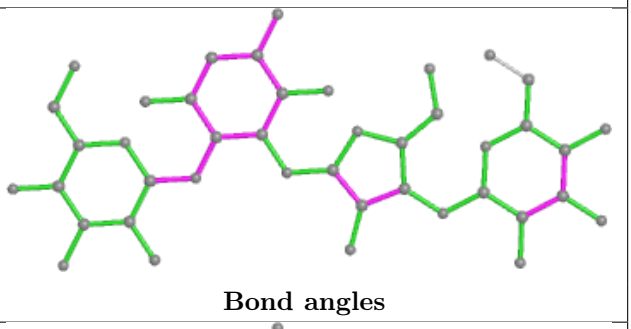
No monomer is involved in short contacts.

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 then 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.

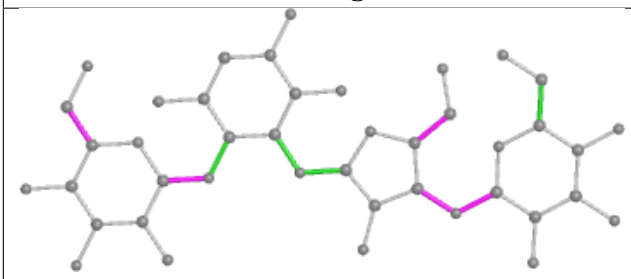
Ligand PAR 1 1802



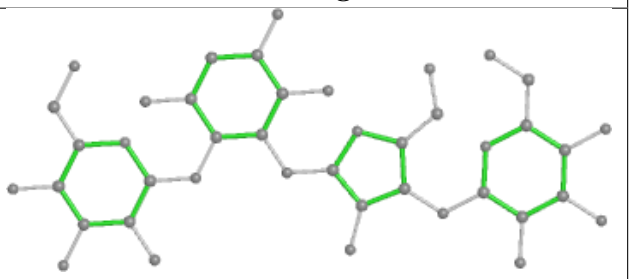
Bond lengths



Bond angles

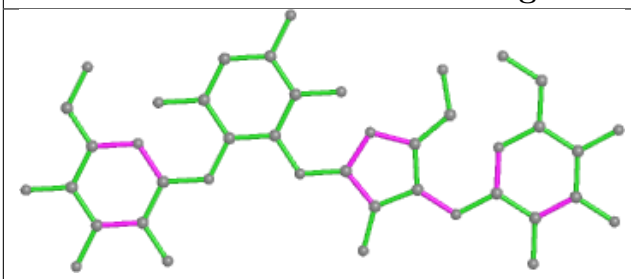


Torsions

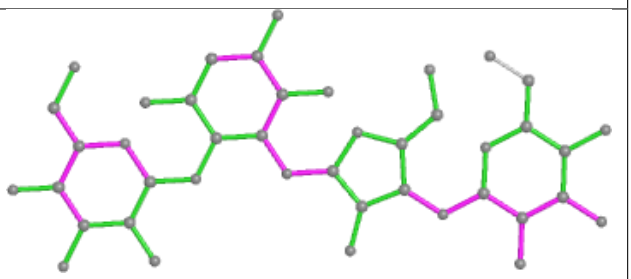


Rings

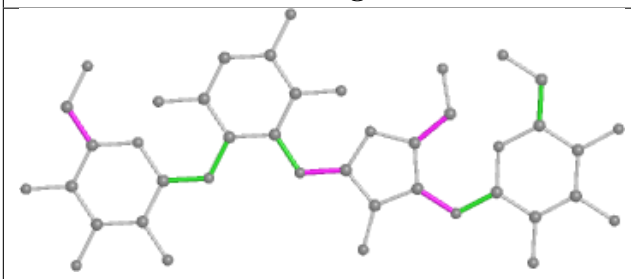
Ligand PAR 1 1804



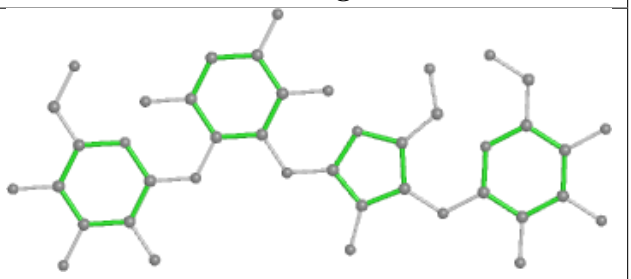
Bond lengths



Bond angles

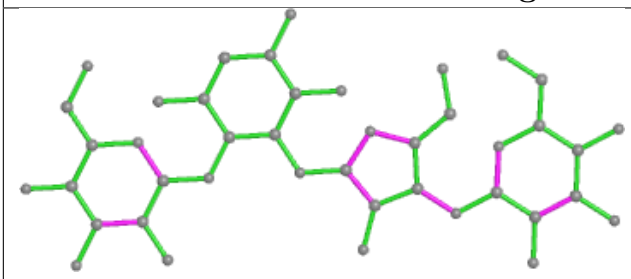


Torsions

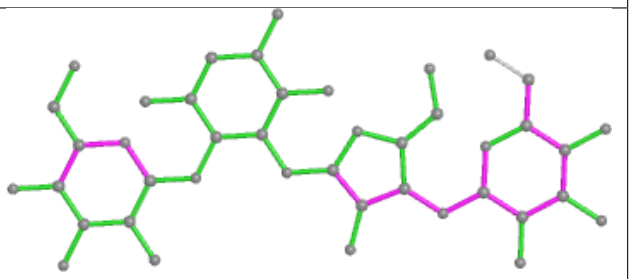


Rings

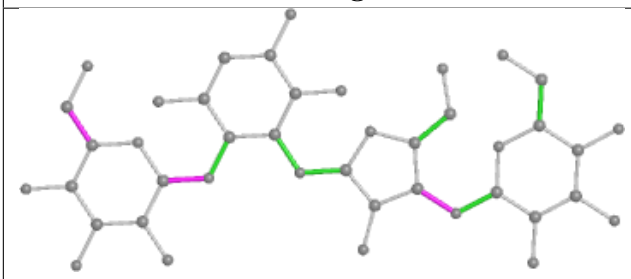
Ligand PAR 2 1702



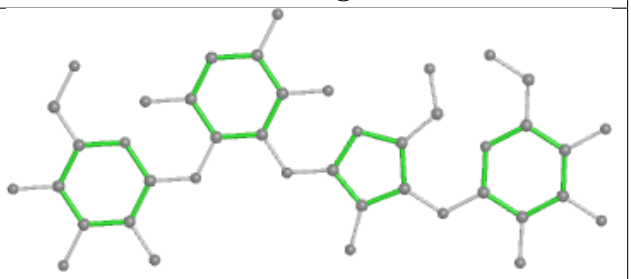
Bond lengths



Bond angles

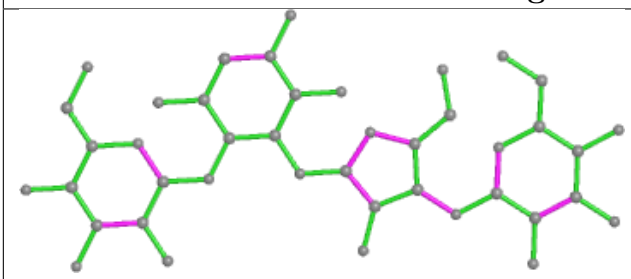


Torsions

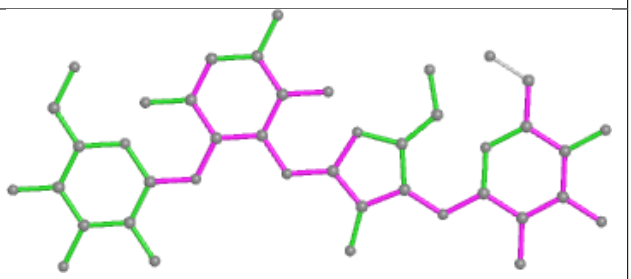


Rings

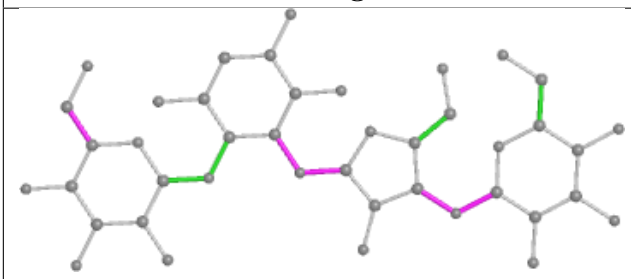
Ligand PAR 7 201



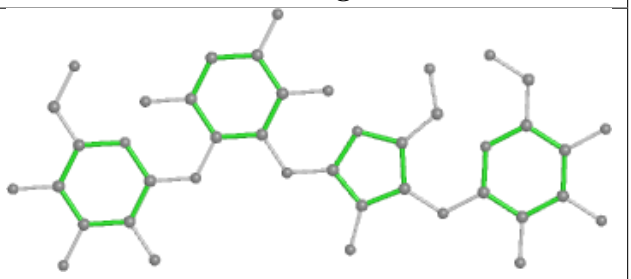
Bond lengths



Bond angles

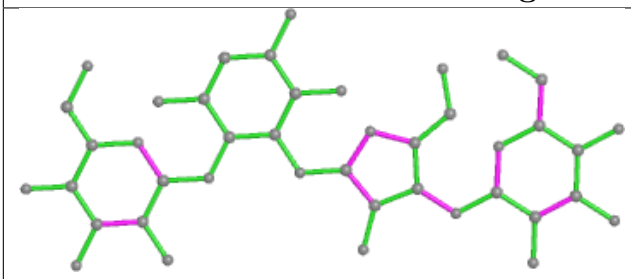


Torsions

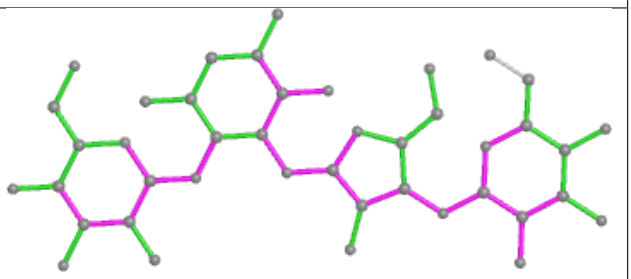


Rings

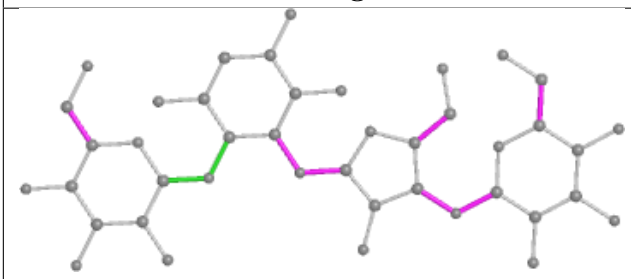
Ligand PAR 2 1705



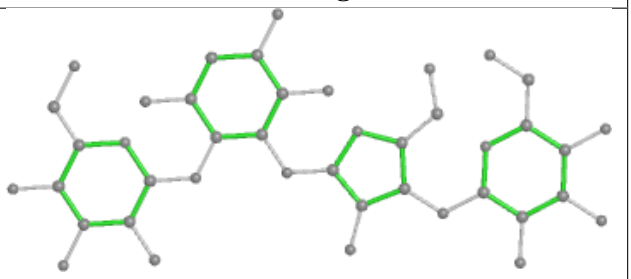
Bond lengths



Bond angles

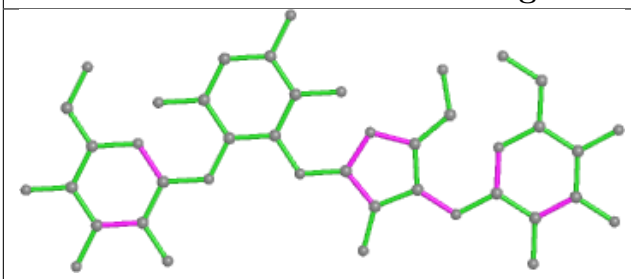


Torsions

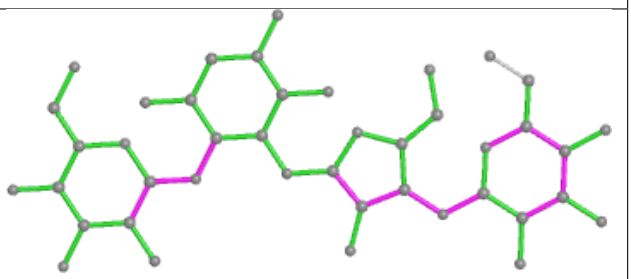


Rings

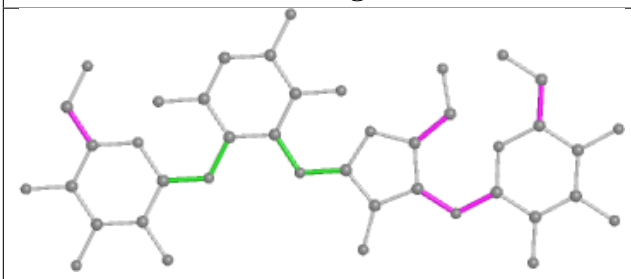
Ligand PAR 1 1803



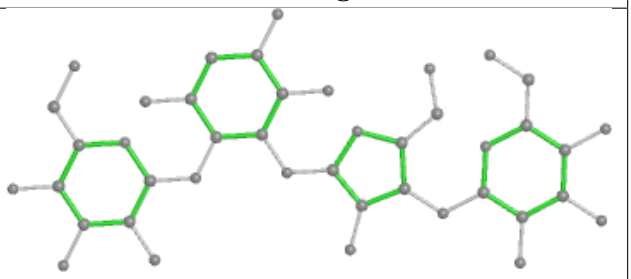
Bond lengths



Bond angles

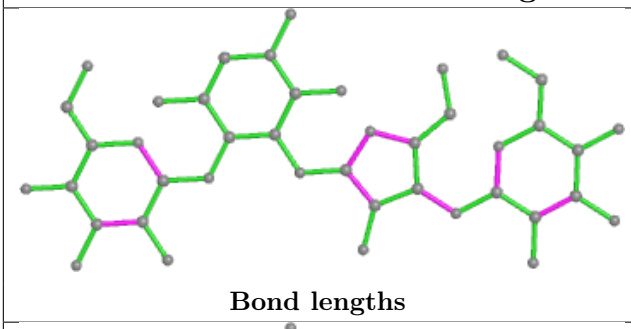


Torsions

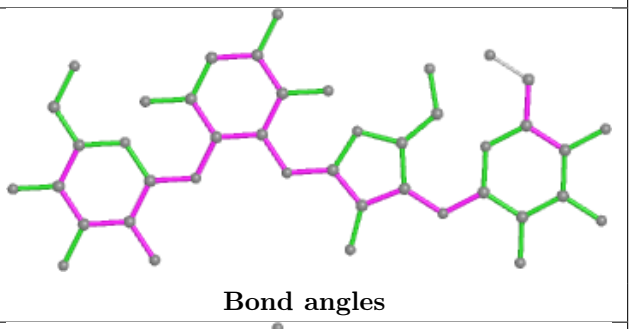


Rings

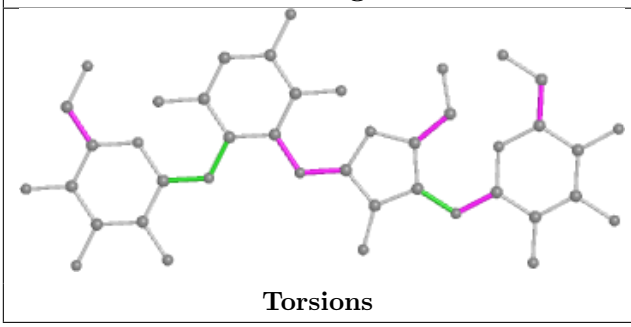
Ligand PAR 1 1805



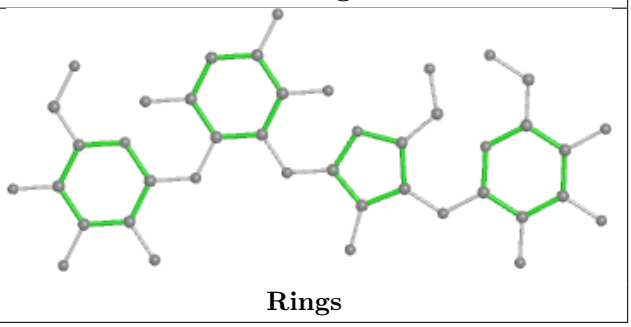
Bond lengths



Bond angles

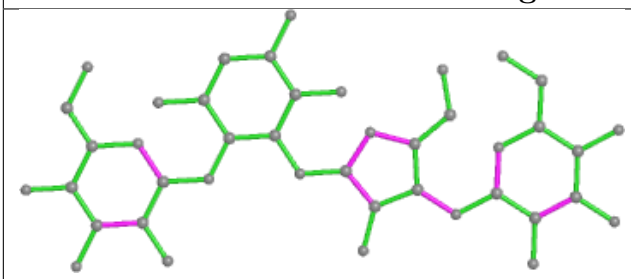


Torsions

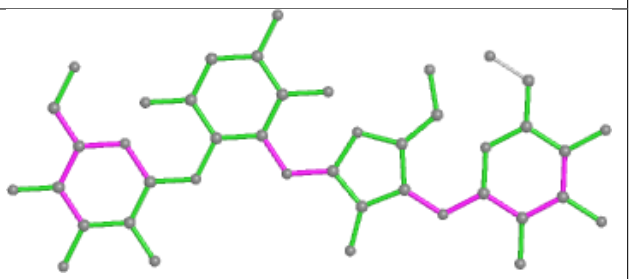


Rings

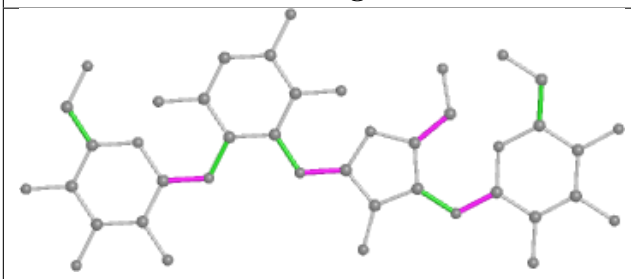
Ligand PAR 2 1704



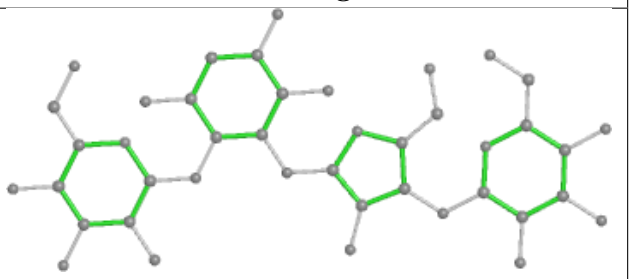
Bond lengths



Bond angles

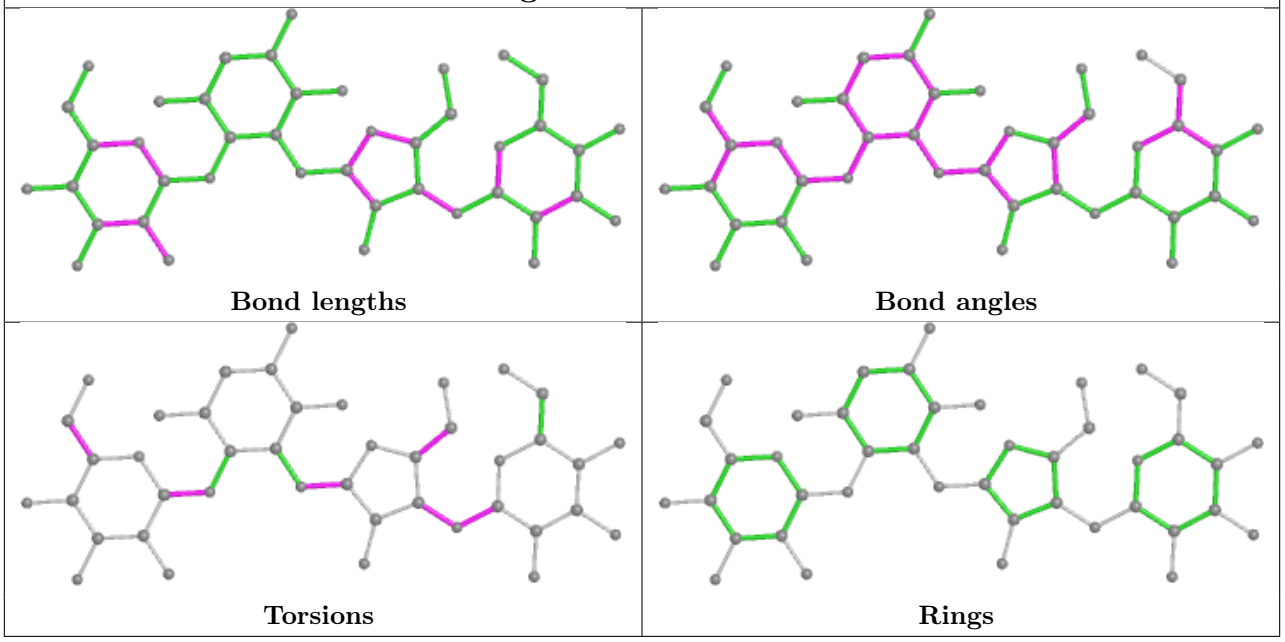


Torsions

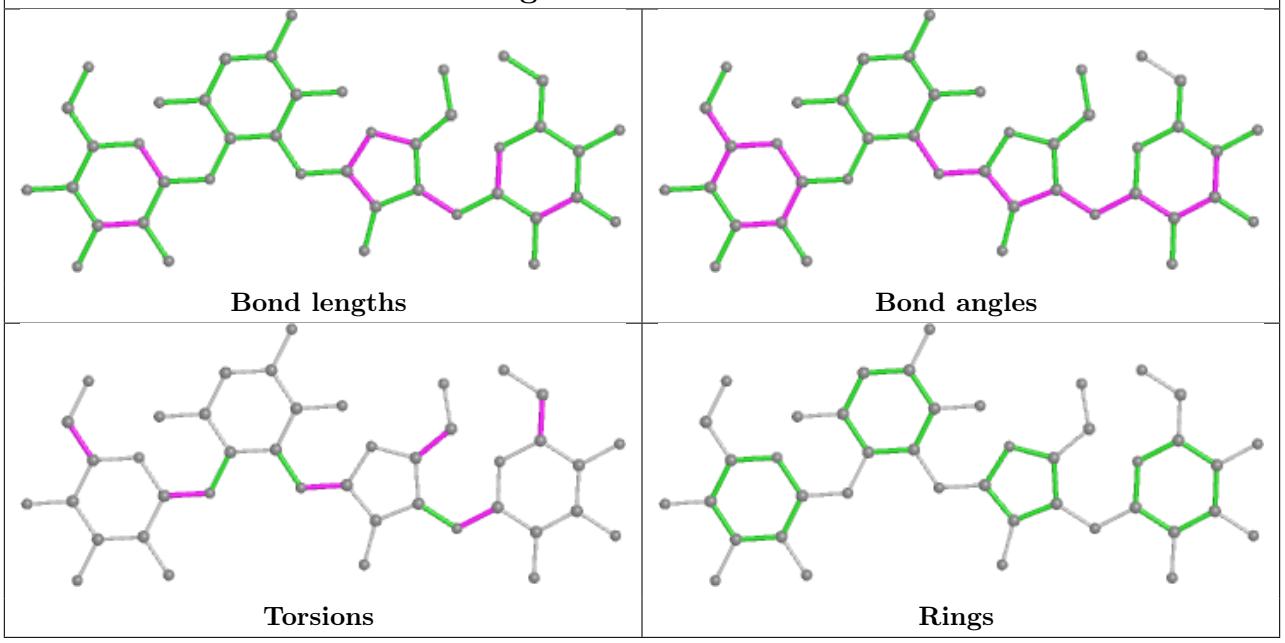


Rings

Ligand PAR 2 1703



Ligand PAR 1 1801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

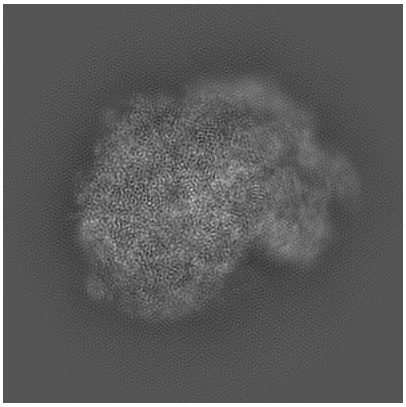
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7025. These allow visual inspection of the internal detail of the map and identification of artifacts.

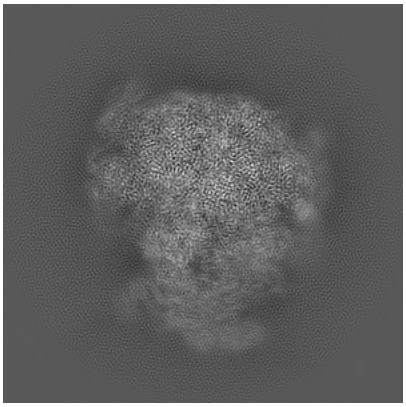
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

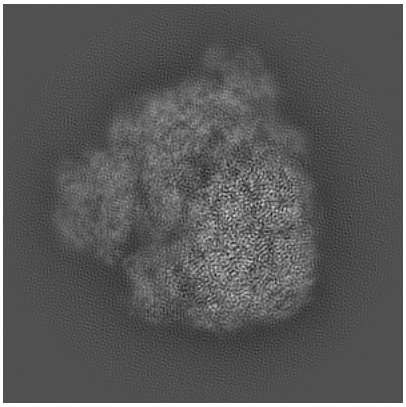
6.1.1 Primary map



X



Y

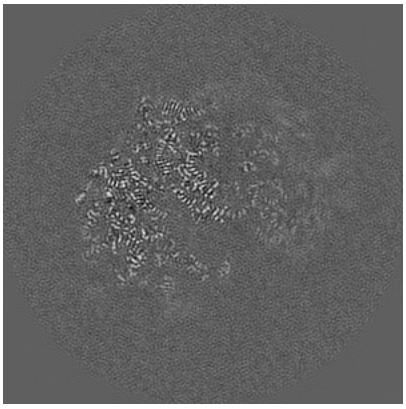


Z

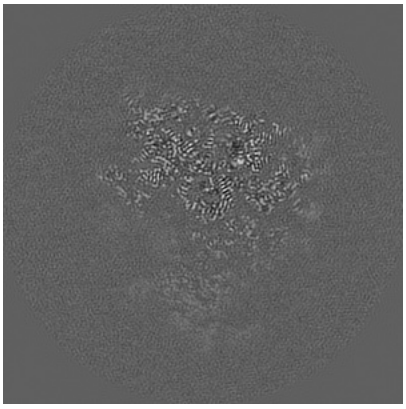
The images above show the map projected in three orthogonal directions.

6.2 Central slices

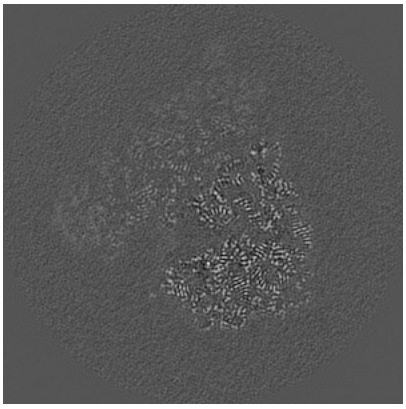
6.2.1 Primary map



X Index: 192



Y Index: 192

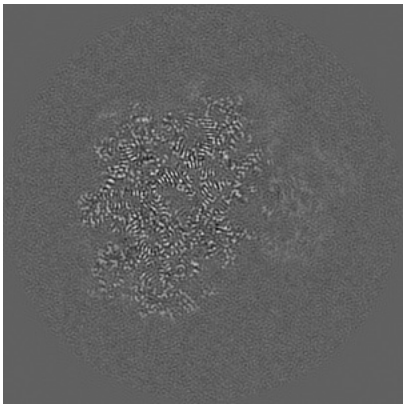


Z Index: 192

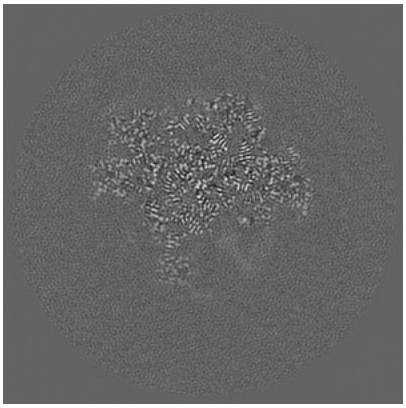
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

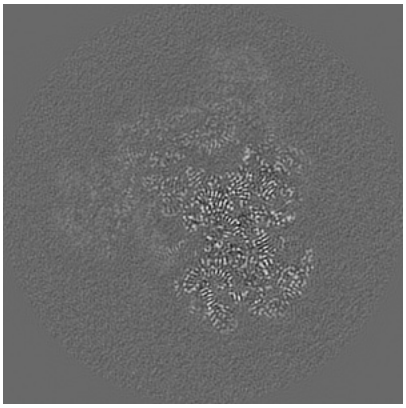
6.3.1 Primary map



X Index: 228



Y Index: 133

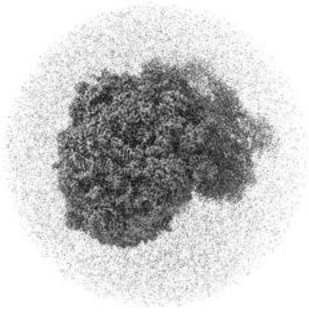


Z Index: 211

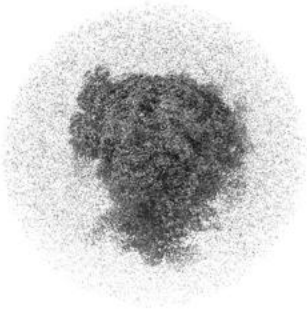
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

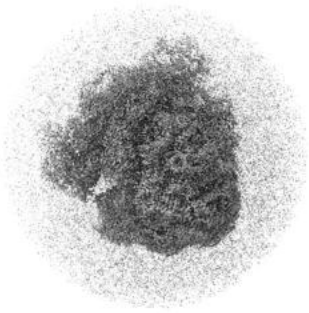
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

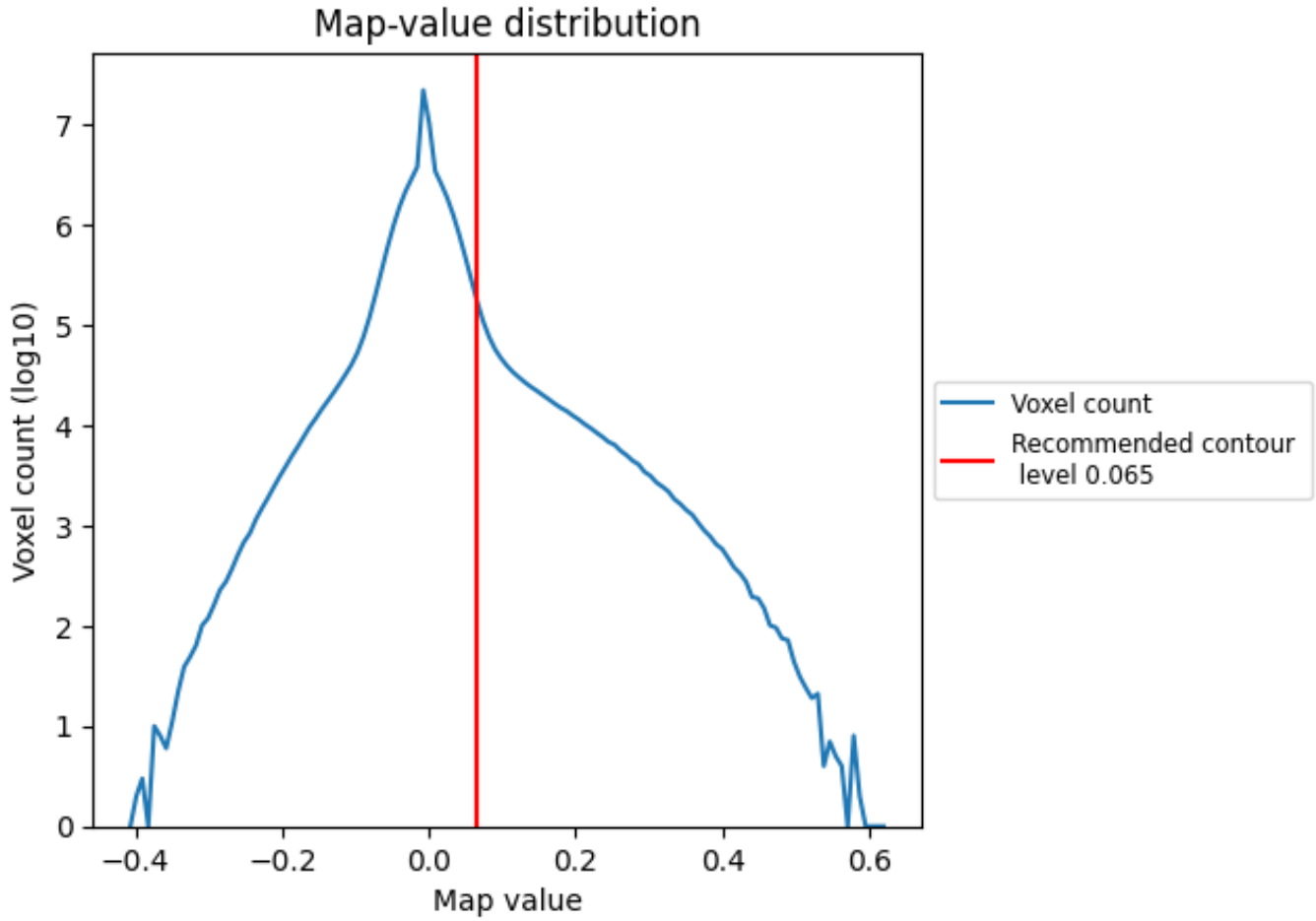
6.5 Mask visualisation (i)

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

7 Map analysis

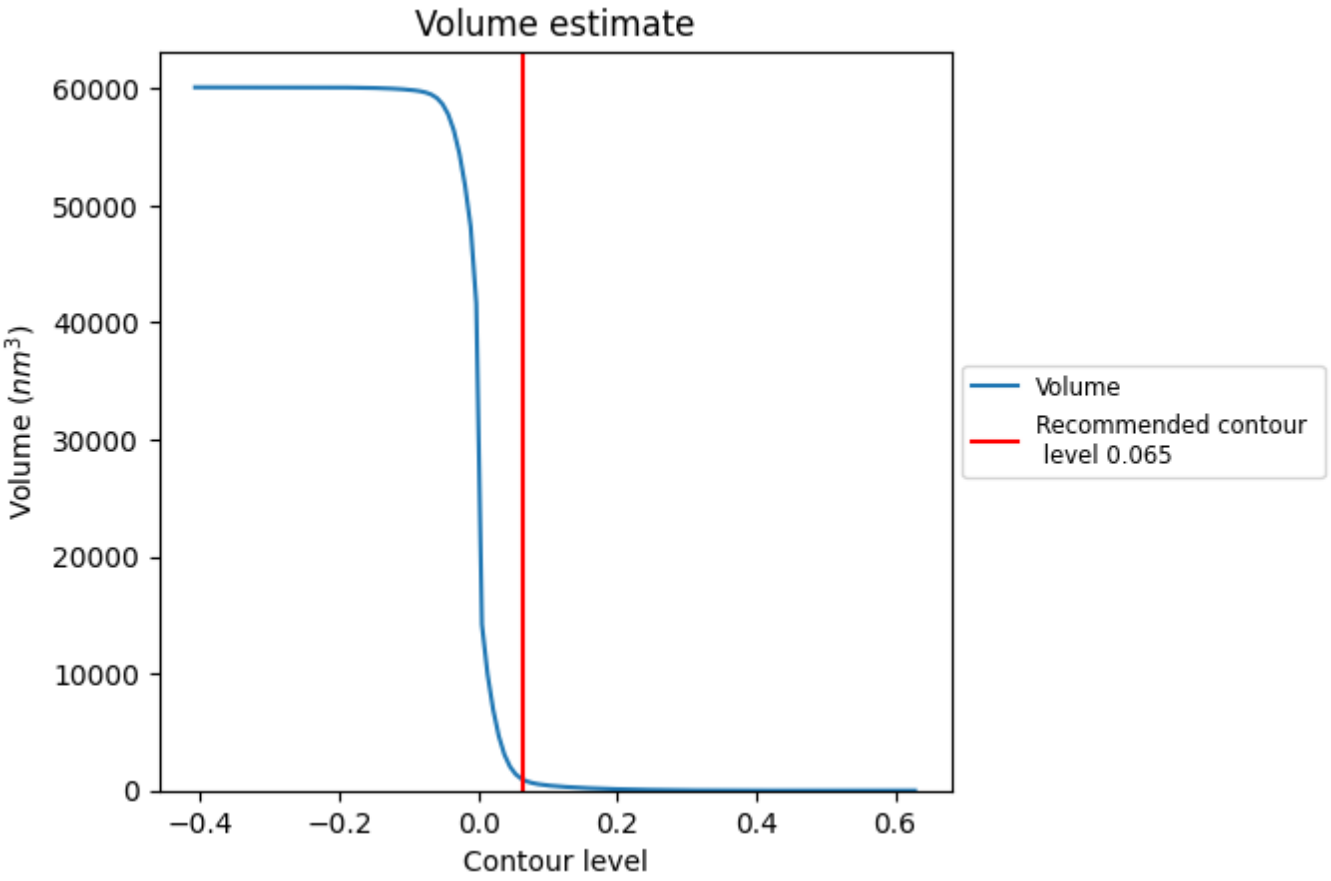
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

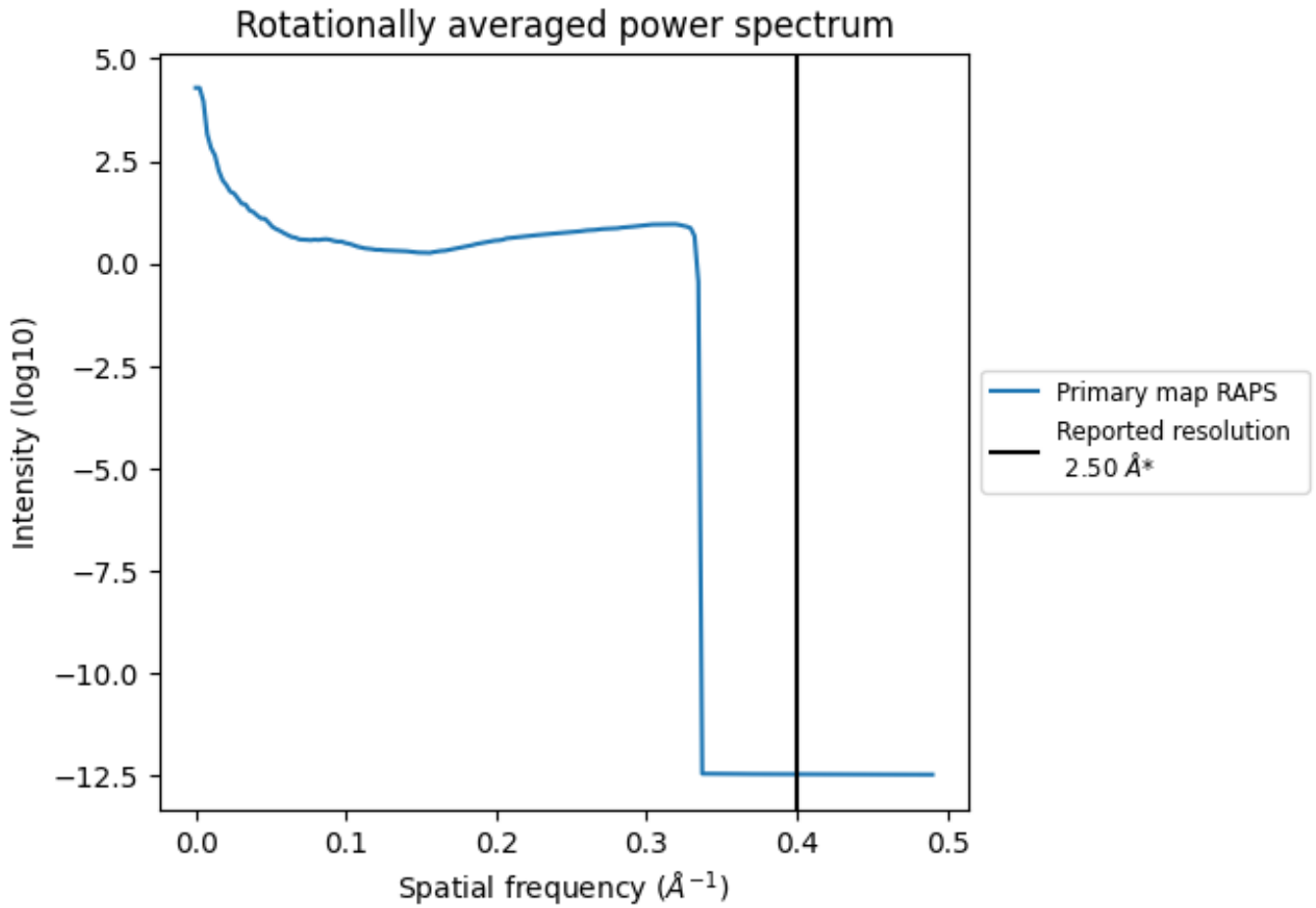
7.2 Volume estimate



The volume at the recommended contour level is 933 nm^3; this corresponds to an approximate mass of 843 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.400 $Å^{-1}$

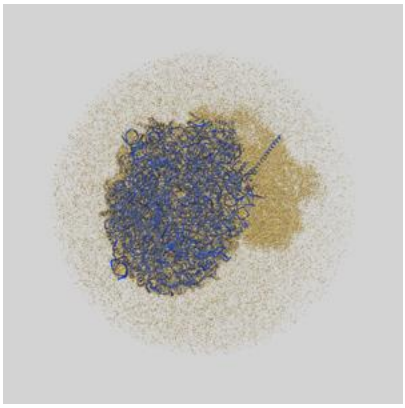
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

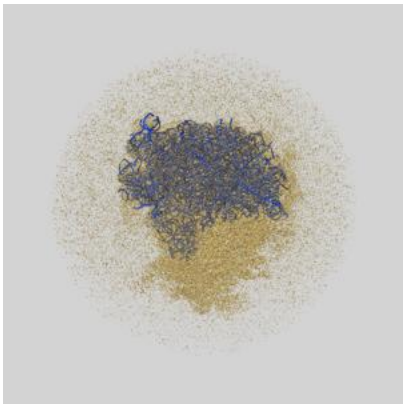
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7025 and PDB model 6AZ3. Per-residue inclusion information can be found in section 3 on page 16.

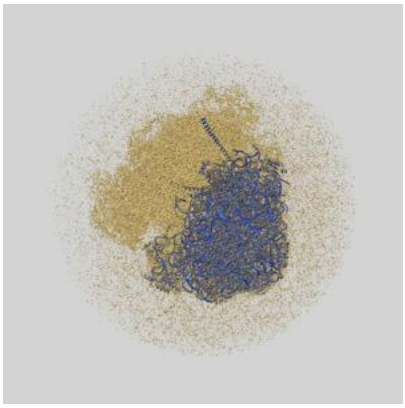
9.1 Map-model overlay



X



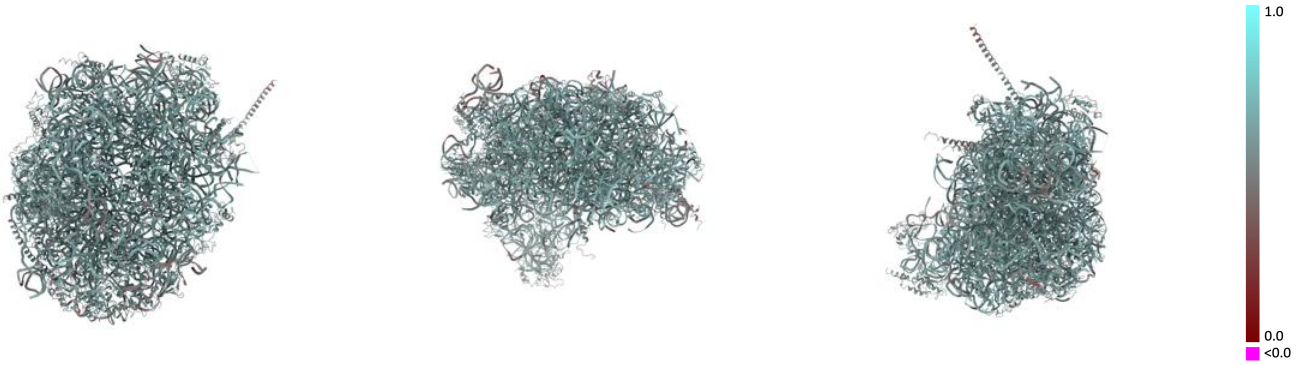
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065 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.

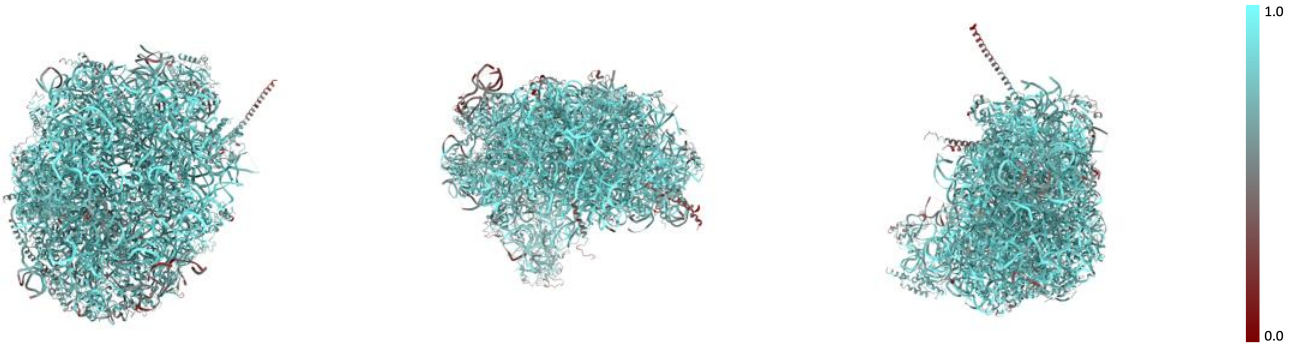
9.2 Q-score mapped to coordinate model



X Y Z

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

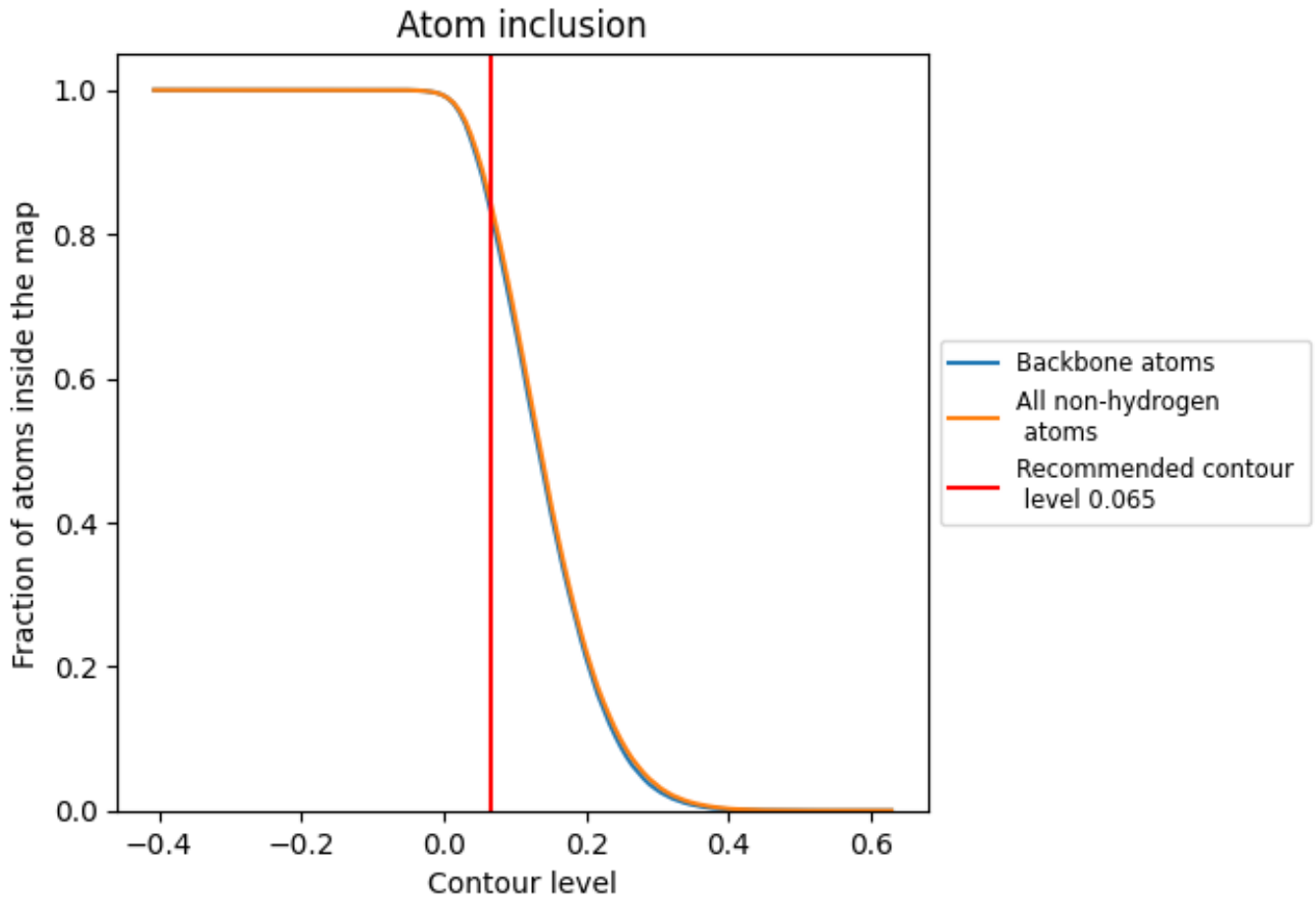
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 85% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8463	0.5990
1	0.8894	0.6060
2	0.8715	0.6030
3	0.8774	0.6030
4	0.8938	0.6070
5	0.9037	0.6110
6	0.7847	0.5640
7	0.9176	0.6160
8	0.8881	0.6020
A	0.8647	0.6180
B	0.8466	0.6060
C	0.8128	0.5930
D	0.6276	0.5280
E	0.7475	0.5770
F	0.6963	0.5560
G	0.7880	0.5850
H	0.8081	0.5990
I	0.8119	0.5880
J	0.8241	0.6040
K	0.7175	0.5670
L	0.8687	0.6140
M	0.9132	0.6250
N	0.6676	0.5660
O	0.7545	0.5720
P	0.8612	0.6080
Q	0.7428	0.5830
R	0.7872	0.5890
S	0.7543	0.5800
T	0.8656	0.6140
U	0.6525	0.5300
V	0.7960	0.5880
W	0.8419	0.6010
X	0.8399	0.5990
Y	0.7645	0.5850
Z	0.7879	0.5770

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Chain	Atom inclusion	Q-score
a	0.7958	0.5870
b	0.8161	0.6050
c	0.8079	0.5960
d	0.7179	0.5780
e	0.7881	0.5880
f	0.8348	0.5970
g	0.8705	0.6160
h	0.7775	0.5850
i	0.7761	0.5800
j	0.9101	0.6240
k	0.7424	0.5850
l	0.8548	0.6110
m	0.7842	0.5930
n	0.4330	0.4860
o	0.8219	0.6070
p	0.8370	0.6050