Full wwPDB EM Validation Report

Oct 13, 2024 – 10:53 am BST

PDB ID	:	8AAF
EMDB ID	:	EMD-15296
Title	:	Yeast RQC complex in state G
Authors	:	Tesina, P.; Buschauer, R.; Beckmann, R.
Deposited on	:	2022-07-01
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:

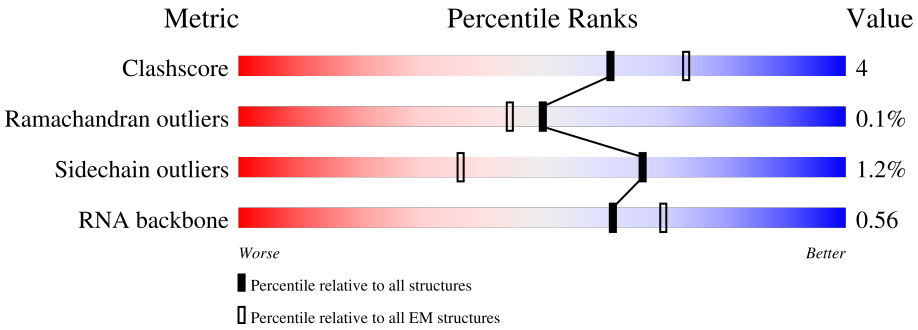
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	204	92% 8%
2	B	199	87% 12% ••
3	C	184	5% 87% 12% •
4	D	186	91% 8% •
5	E	189	5% 76% 7% 17%
6	F	172	87% 12% •
7	G	160	• 90% 9% •

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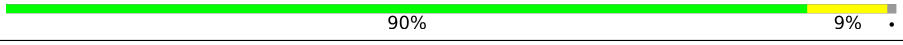
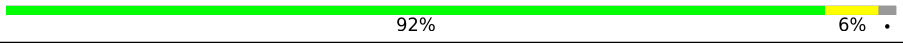
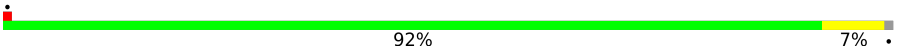
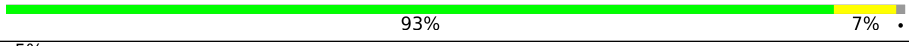
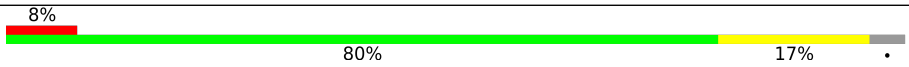
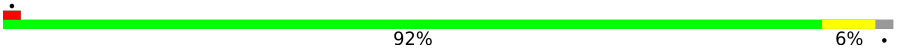
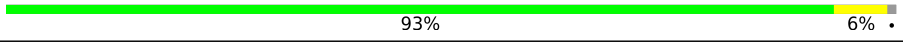
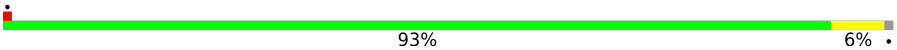
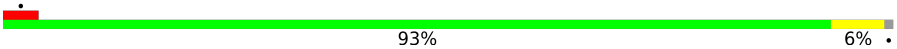
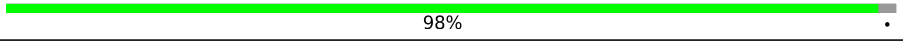
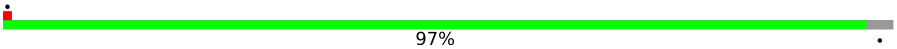
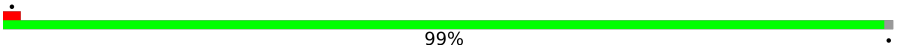
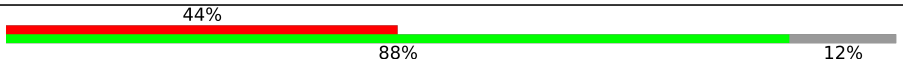
Mol	Chain	Length	Quality of chain
8	H	121	
9	I	137	
10	J	155	
11	K	142	
12	L	127	
13	M	136	
14	N	149	
15	O	59	
16	P	105	
17	Q	113	
18	R	130	
19	S	107	
20	T	121	
21	U	120	
22	V	100	
23	W	88	
24	X	78	
25	Y	51	
26	Z	128	
27	b	106	
28	c	92	
29	d	25	
30	f	3395	
31	h	121	
32	i	158	

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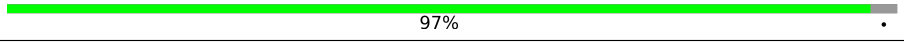
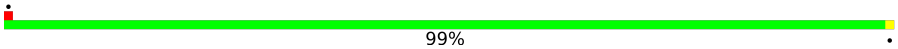
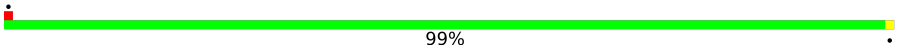
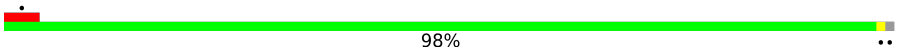
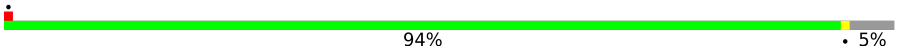
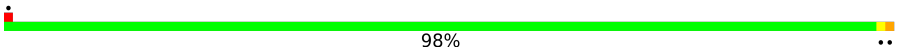
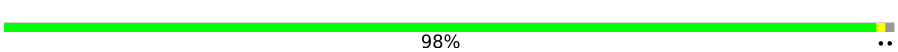
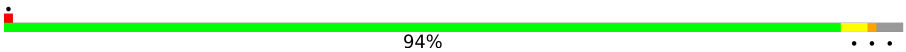
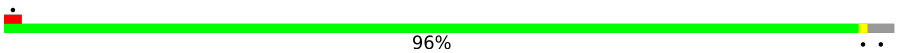
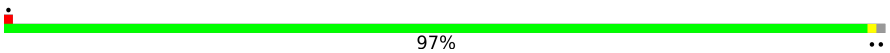
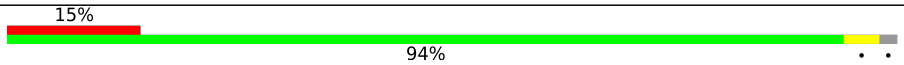
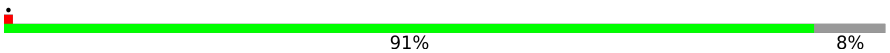
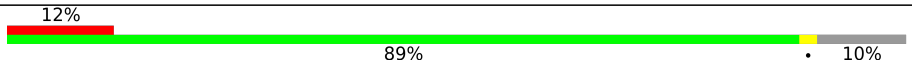
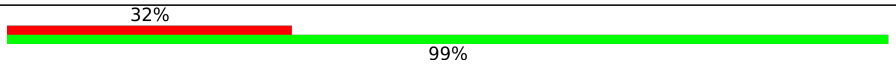
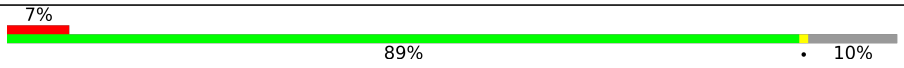
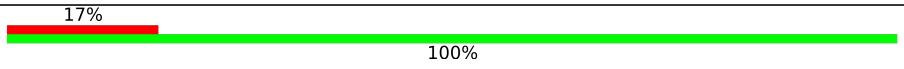
Mol	Chain	Length	Quality of chain
33	j	254	
34	k	387	
35	l	362	
36	m	297	
37	n	176	
38	o	244	
39	p	256	
40	q	191	
41	r	221	
42	s	174	
43	t	199	
44	u	138	
45	a	1038	
46	e	1562	
47	g	245	
48	v	157	
49	w	217	
50	x	76	
50	y	76	
51	z	165	
52	0	312	
53	1	18	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 151377 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 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	203	1720	1077	361	281	1	0	0

- Molecule 2 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	197	1555	1003	289	262	1	197	0

- Molecule 3 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	183	1416	879	284	253	0	0

- Molecule 4 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	185	1441	908	290	241	2	0	0

- Molecule 5 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	156	1258	781	265	212	0	0

- Molecule 6 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	171	1437	925	266	243	3	0	0

- Molecule 7 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	159	Total	C	N	O	S	0	0
			1272	802	245	221	4		

- Molecule 8 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 9 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 10 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	63	Total	C	N	O	S	0	0
			518	333	102	82	1		

- Molecule 11 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 12 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 13 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	135	Total	C	N	O	0	0
			1080	701	199	180		

- Molecule 14 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 15 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 16 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 17 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 18 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	127	Total	C	N	O	S	0	0
			1013	642	205	165	1		

- Molecule 19 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 20 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 21 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 22 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 23 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	77	Total	C	N	O	0	0
			612	391	115	106		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 26 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 27 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 28 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 29 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	22	Total	C	N	O	S	0	0
			207	127	56	23	1		

- Molecule 30 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	3216	Total	C	N	O	P	1	0
			68802	30732	12391	22462	3217		

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 32 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 33 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	246	Total	C	N	O	S	0	0
			1874	1168	380	325	1		

- Molecule 34 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 35 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 36 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 37 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	n	167	Total	C	N	O	0	0
			1307	843	234	230		

- Molecule 38 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 39 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 40 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 41 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	169	Total	C	N	O	S	0	0
			1346	843	252	247	4		

- Molecule 43 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	t	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 44 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	u	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 45 is a protein called Ribosome quality control complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	a	848	Total	C	N	O	S	0	0
			6582	4195	1142	1228	17		

- Molecule 46 is a protein called E3 ubiquitin-protein ligase listerin.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	e	1527	Total	C	N	O	S	0	0
			11509	7355	1936	2180	38		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	g	225	Total	C	N	O	S	0	0
			1651	1030	282	332	7		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	142	Total	C	N	O	S	0	0
			1085	676	183	217	9		

- Molecule 49 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	216	Total	C	N	O	S	0	0
			1709	1092	298	310	9		

- Molecule 50 is a RNA chain called Ala tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	74	Total	C	N	O	P	0	0
			1579	702	277	526	74		
50	y	73	Total	C	N	O	P	0	0
			1556	692	272	519	73		

- Molecule 51 is a protein called 60S ribosomal protein L12-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	z	148	Total	C	N	O	0	0
			734	438	148	148		

- Molecule 52 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	121	Total	C	N	O	S	0	0
			967	621	170	173	3		

- Molecule 53 is a protein called CAT-tailed nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	1	Total	Mg	0
			1	1	
54	C	1	Total	Mg	0
			1	1	
54	E	1	Total	Mg	0
			1	1	
54	I	1	Total	Mg	0
			1	1	
54	R	1	Total	Mg	0
			1	1	

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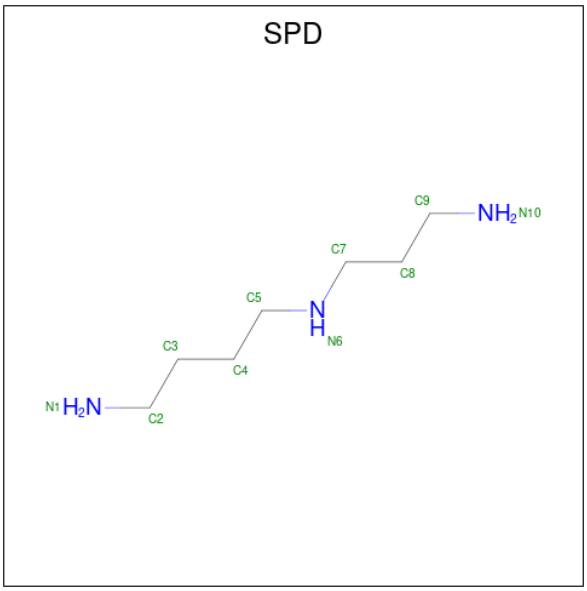
Mol	Chain	Residues	Atoms	AltConf
54	T	1	Total Mg 1 1	0
54	f	3	Total Mg 3 3	0
54	h	1	Total Mg 1 1	0
54	j	2	Total Mg 2 2	0
54	k	1	Total Mg 1 1	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
55	T	1	Total Zn 1 1	0
55	W	1	Total Zn 1 1	0
55	Z	1	Total Zn 1 1	0
55	b	1	Total Zn 1 1	0
55	c	1	Total Zn 1 1	0
55	e	2	Total Zn 2 2	0

- Molecule 56 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

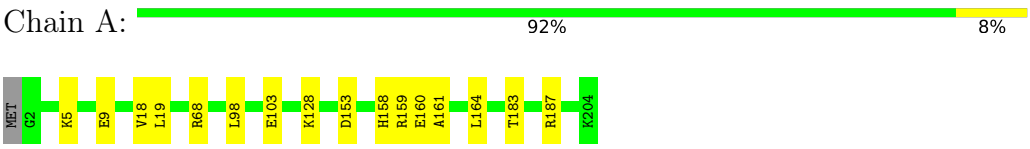


Mol	Chain	Residues	Atoms			AltConf
56	f	1	Total	C	N	0
			10	7	3	

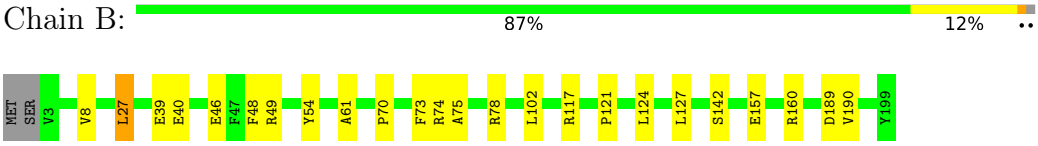
3 Residue-property plots (i)

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.

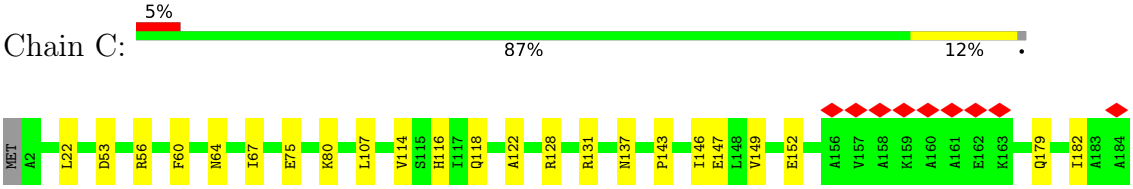
• Molecule 1: 60S ribosomal protein L15-A



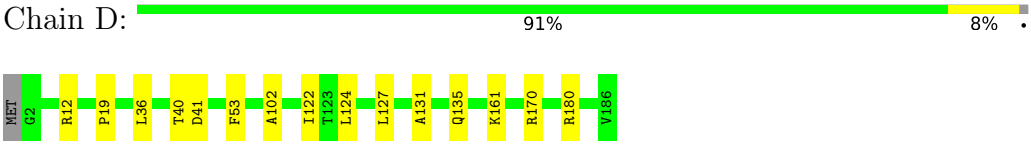
• Molecule 2: 60S ribosomal protein L16-A



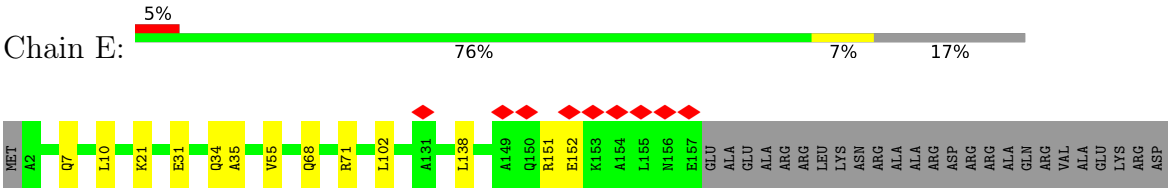
• Molecule 3: 60S ribosomal protein L17-A

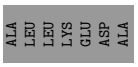


• Molecule 4: 60S ribosomal protein L18-A



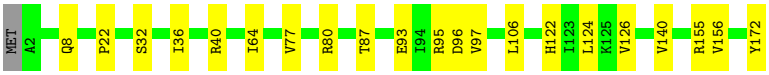
• Molecule 5: 60S ribosomal protein L19-A





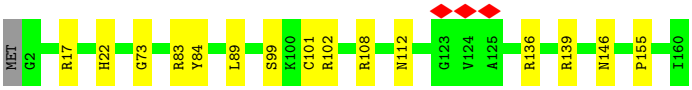
• Molecule 6: 60S ribosomal protein L20-A

Chain F:



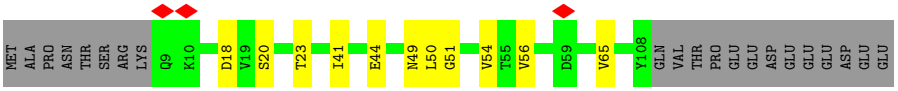
• Molecule 7: 60S ribosomal protein L21-A

Chain G:



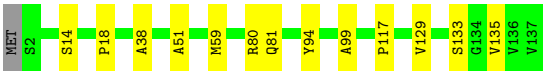
• Molecule 8: 60S ribosomal protein L22-A

Chain H:



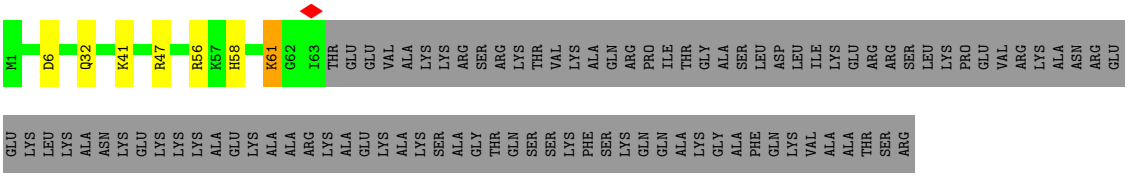
• Molecule 9: 60S ribosomal protein L23-A

Chain I:



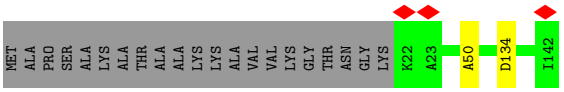
• Molecule 10: 60S ribosomal protein L24-A

Chain J:



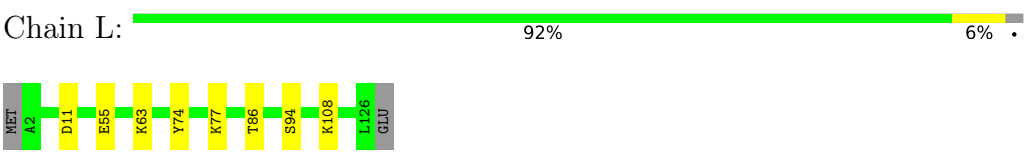
• Molecule 11: 60S ribosomal protein L25

Chain K:



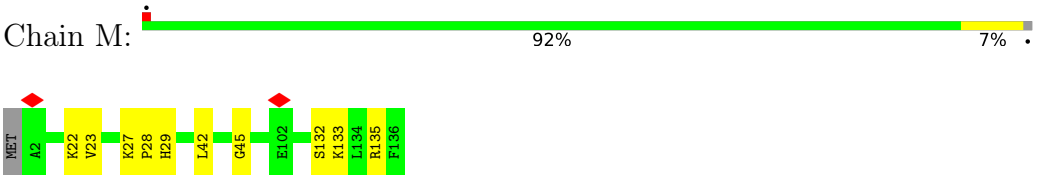
• Molecule 12: 60S ribosomal protein L26-A

Chain L:



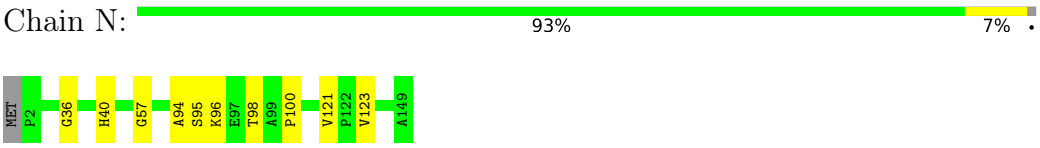
• Molecule 13: 60S ribosomal protein L27-A

Chain M:



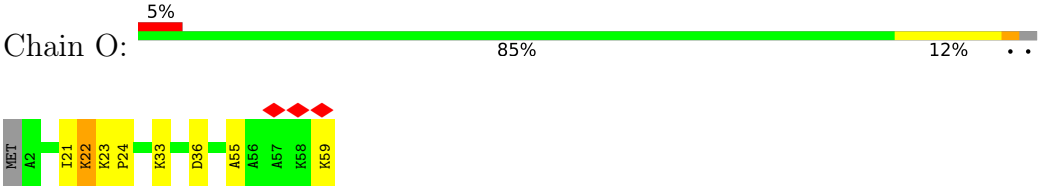
• Molecule 14: 60S ribosomal protein L28

Chain N:



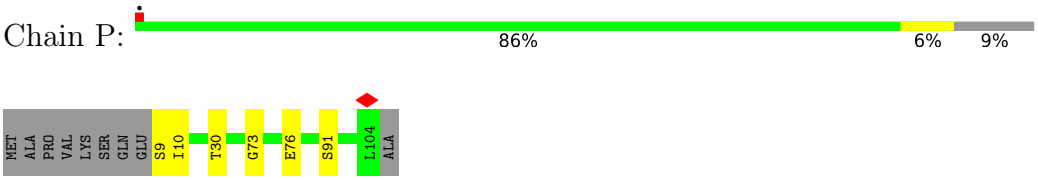
• Molecule 15: 60S ribosomal protein L29

Chain O:



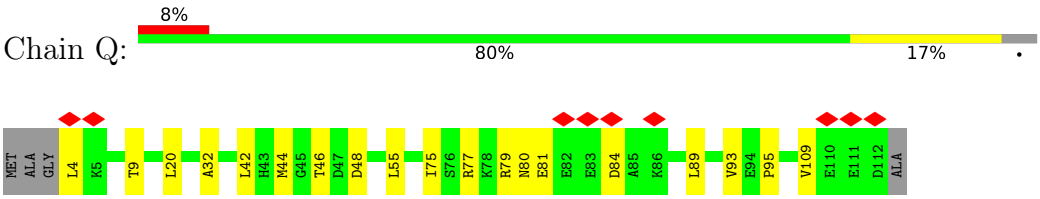
• Molecule 16: 60S ribosomal protein L30

Chain P:



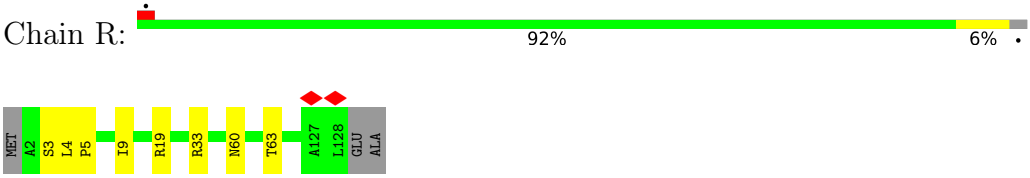
• Molecule 17: 60S ribosomal protein L31-A

Chain Q:



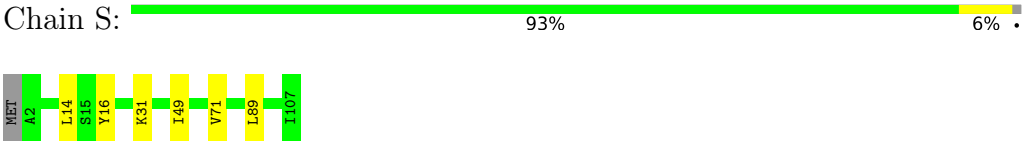
• Molecule 18: 60S ribosomal protein L32

Chain R:



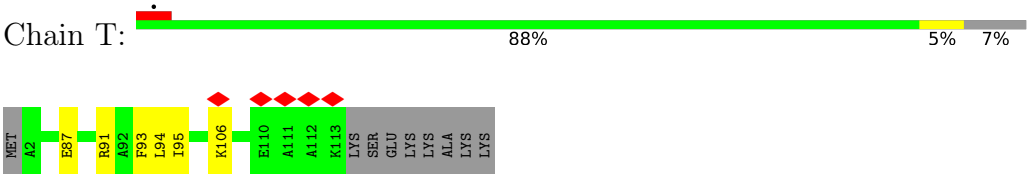
• Molecule 19: 60S ribosomal protein L33-A

Chain S:



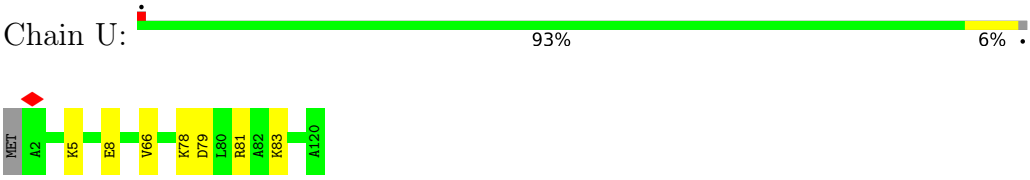
• Molecule 20: 60S ribosomal protein L34-A

Chain T:



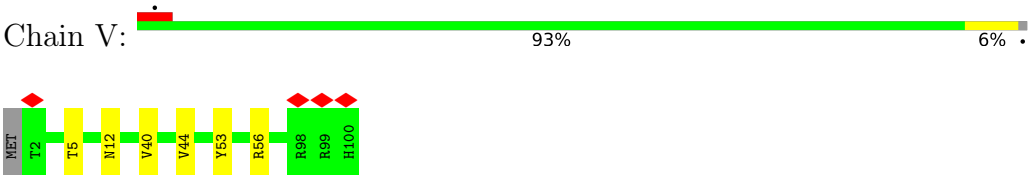
• Molecule 21: 60S ribosomal protein L35-A

Chain U:



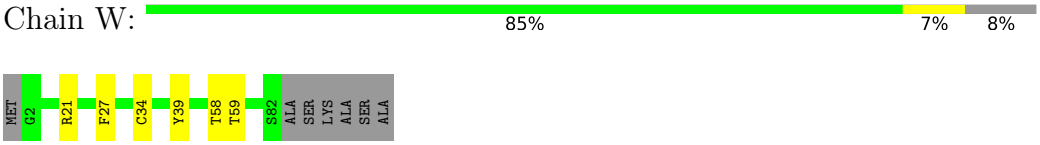
• Molecule 22: 60S ribosomal protein L36-A

Chain V:



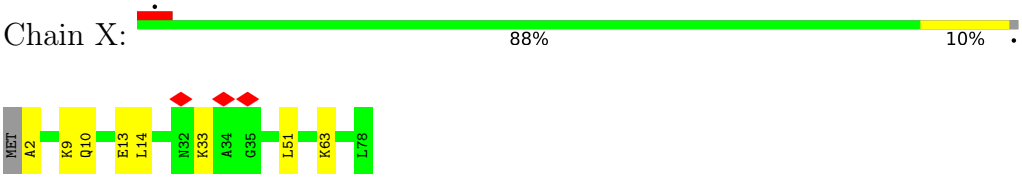
• Molecule 23: 60S ribosomal protein L37-A

Chain W:



• Molecule 24: 60S ribosomal protein L38

Chain X:

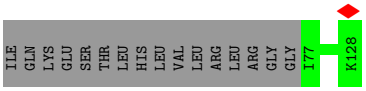


• Molecule 25: 60S ribosomal protein L39

Chain Y:

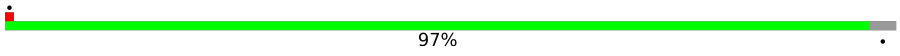
• Molecule 26: Ubiquitin-60S ribosomal protein L40

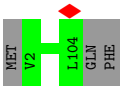
Chain Z:



• Molecule 27: 60S ribosomal protein L42-A

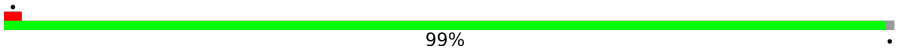
Chain b:

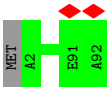




• Molecule 28: 60S ribosomal protein L43-A

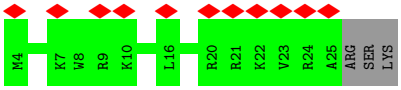
Chain c:





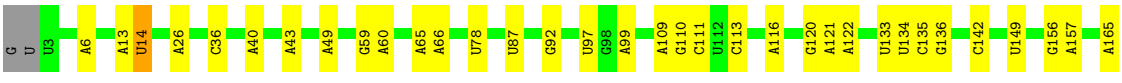
• Molecule 29: 60S ribosomal protein L41-A

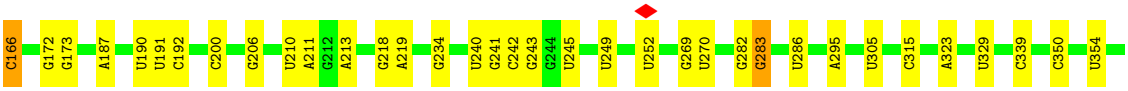
Chain d:

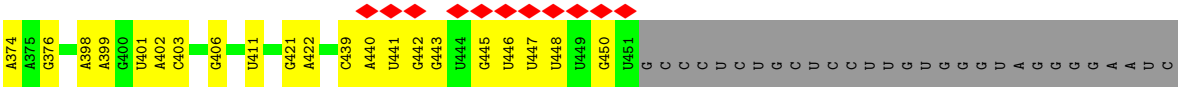


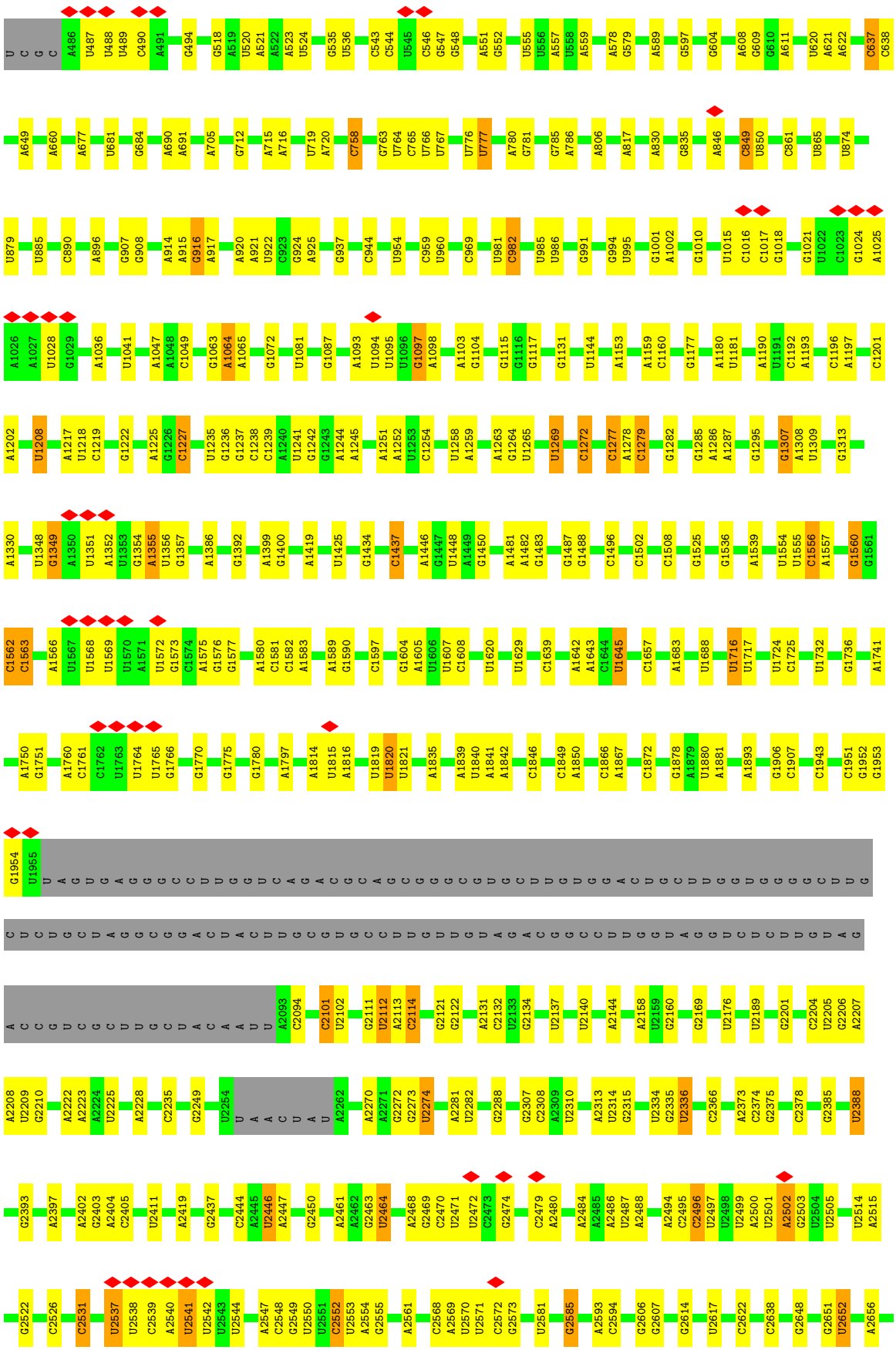
• Molecule 30: 25S rRNA

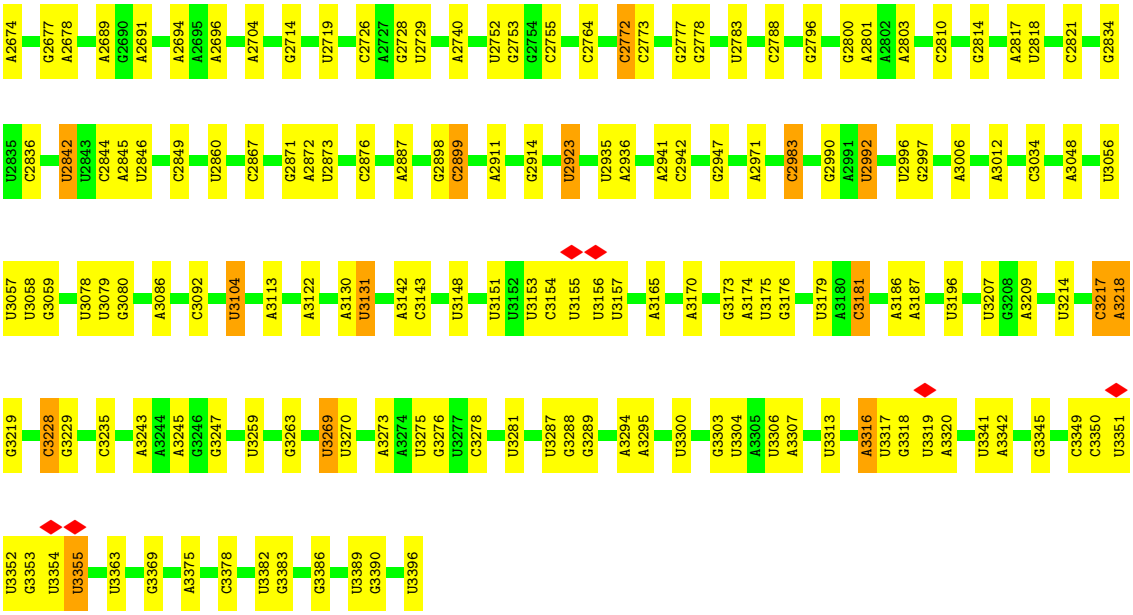
Chain f:





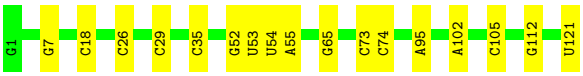






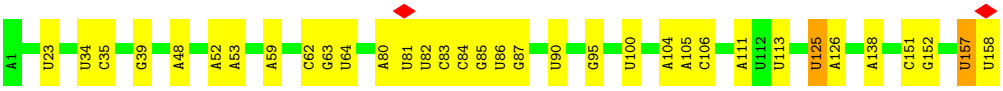
• Molecule 31: 5S rRNA

Chain h:



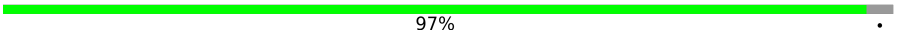
• Molecule 32: 5.8S rRNA

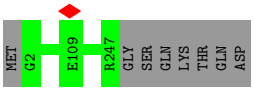
Chain i:



• Molecule 33: 60S ribosomal protein L2-A

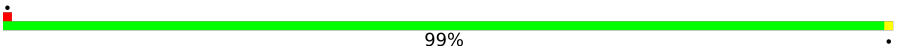
Chain j:

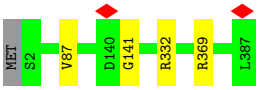




• Molecule 34: 60S ribosomal protein L3

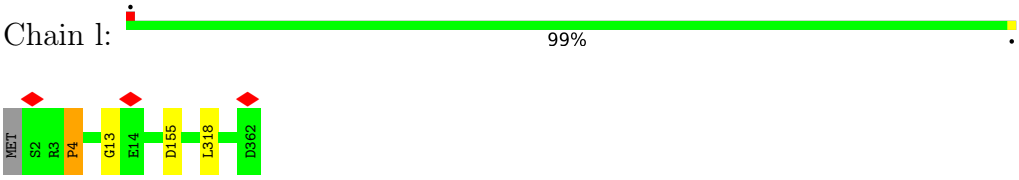
Chain k:





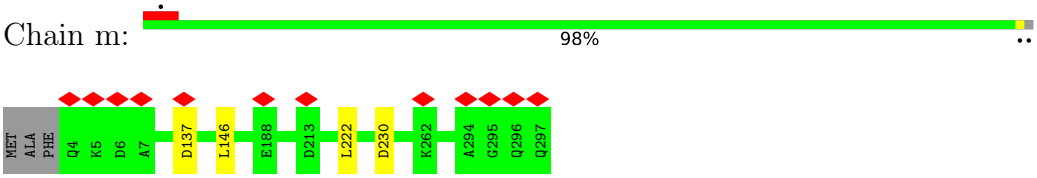
• Molecule 35: 60S ribosomal protein L4-A

Chain l:



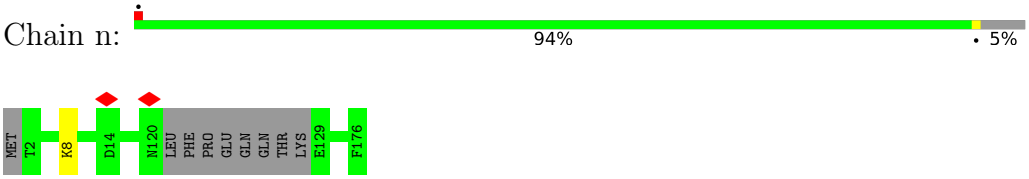
• Molecule 36: 60S ribosomal protein L5

Chain m:



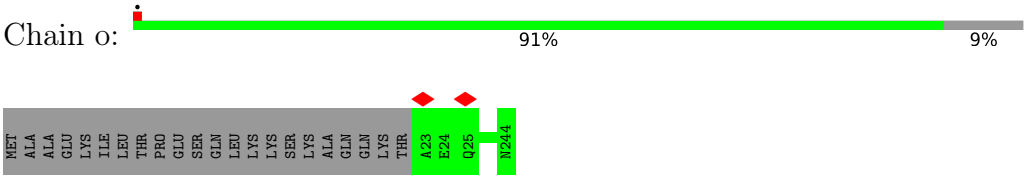
• Molecule 37: 60S ribosomal protein L6-B

Chain n:



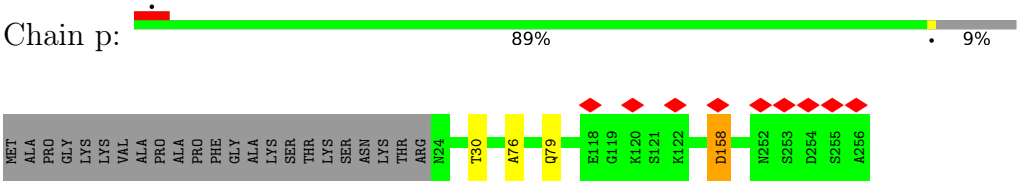
• Molecule 38: 60S ribosomal protein L7-A

Chain o:



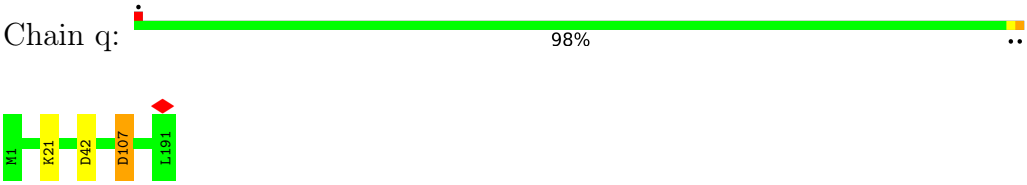
• Molecule 39: 60S ribosomal protein L8-A

Chain p:



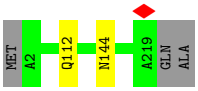
• Molecule 40: 60S ribosomal protein L9-A

Chain q:



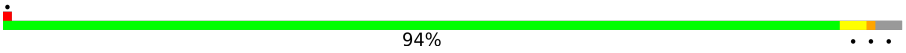
• Molecule 41: 60S ribosomal protein L10

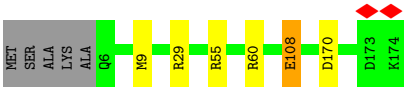
Chain r:



• Molecule 42: 60S ribosomal protein L11-A

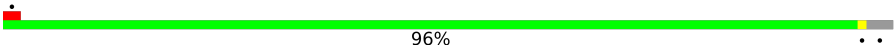
Chain s:

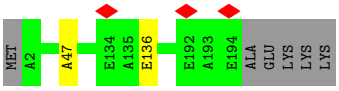




• Molecule 43: 60S ribosomal protein L13-A

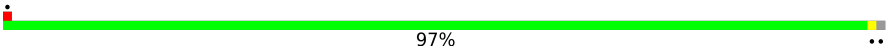
Chain t:

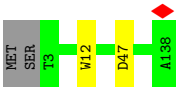




• Molecule 44: 60S ribosomal protein L14-A

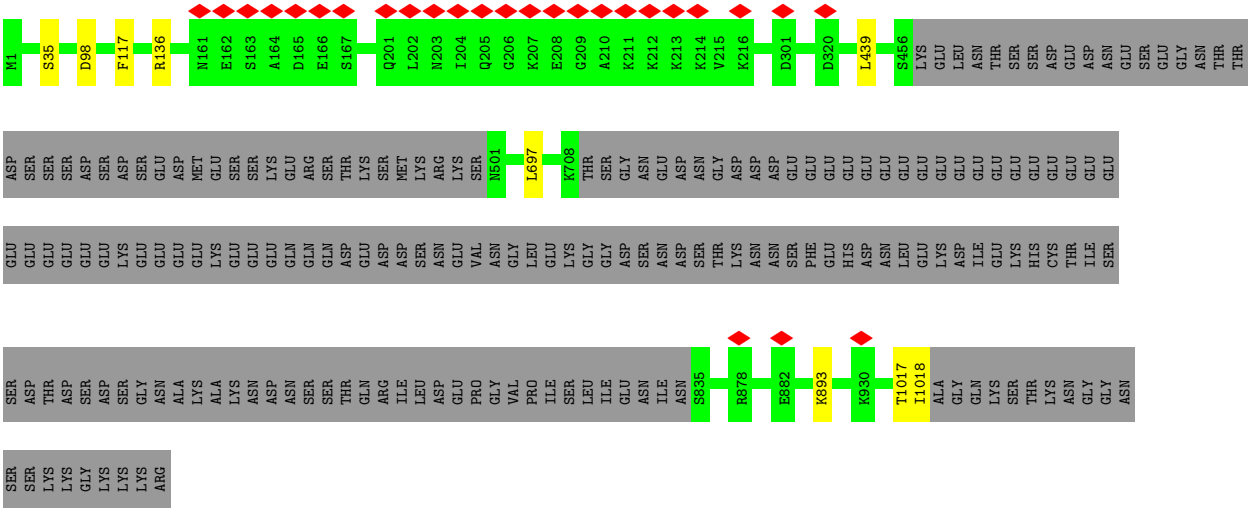
Chain u:





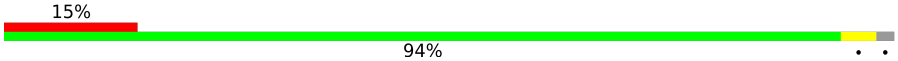
• Molecule 45: Ribosome quality control complex subunit 2

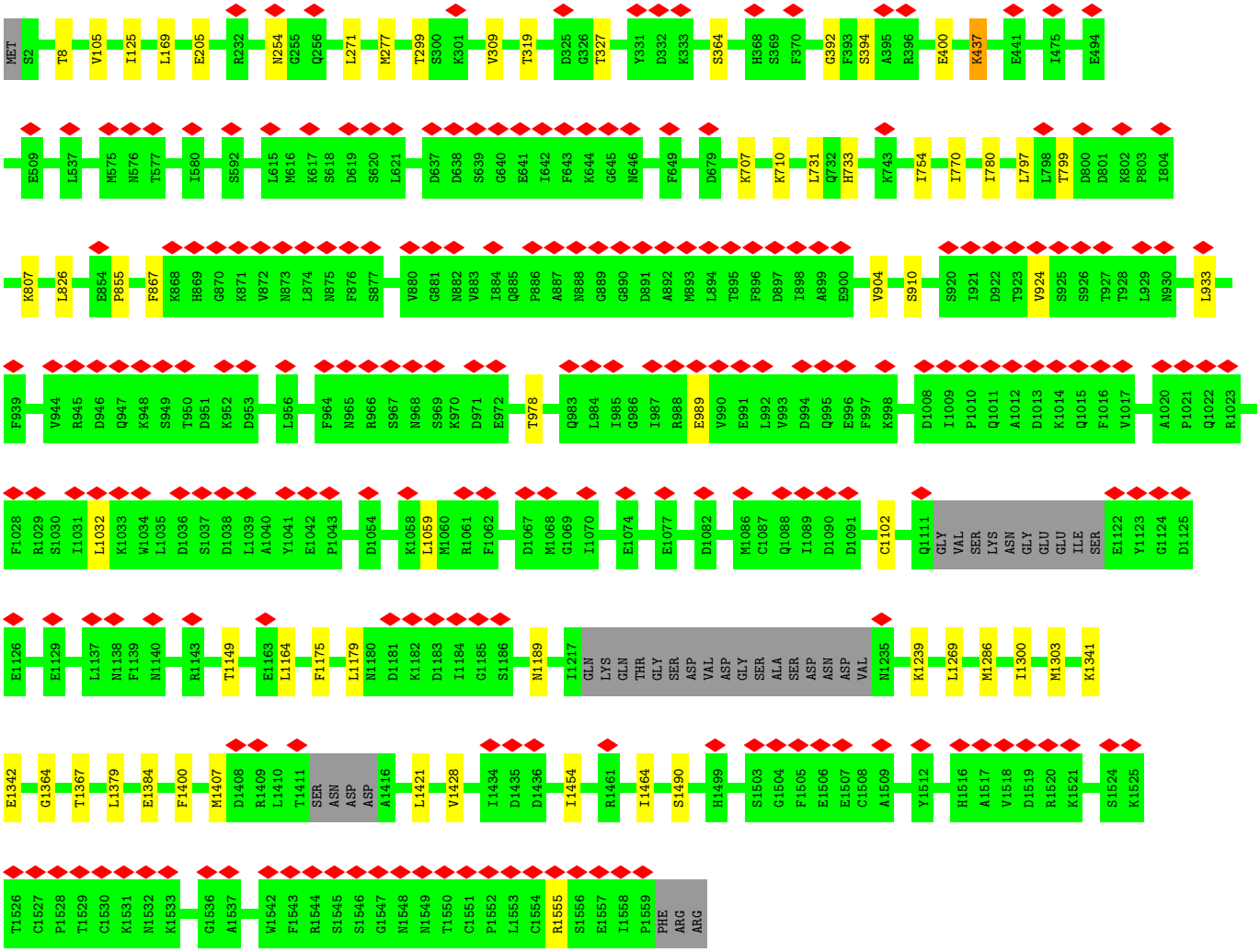
Chain a:



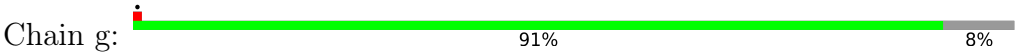
• Molecule 46: E3 ubiquitin-protein ligase listerin

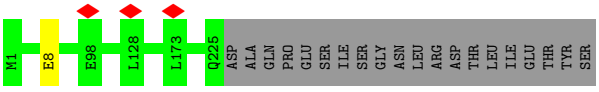
Chain e:



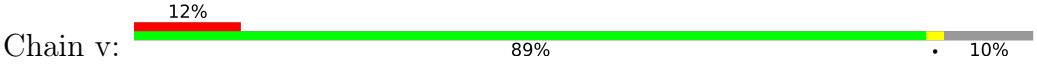


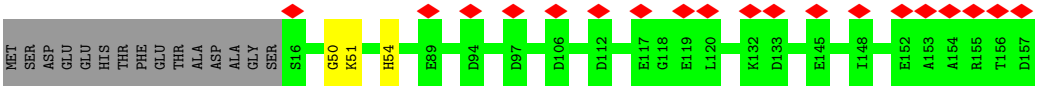
• Molecule 47: Eukaryotic translation initiation factor 6



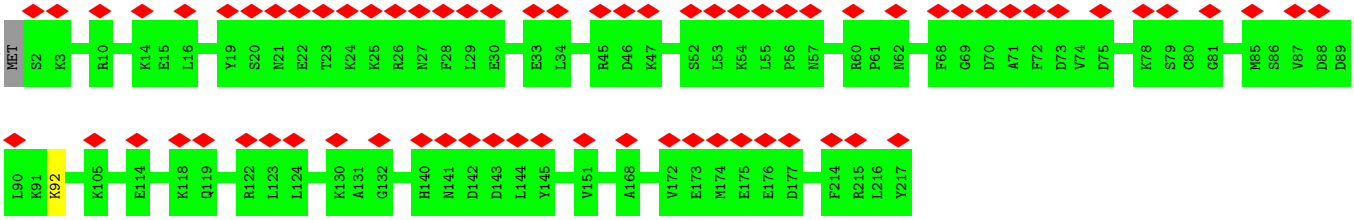


• Molecule 48: Eukaryotic translation initiation factor 5A-1

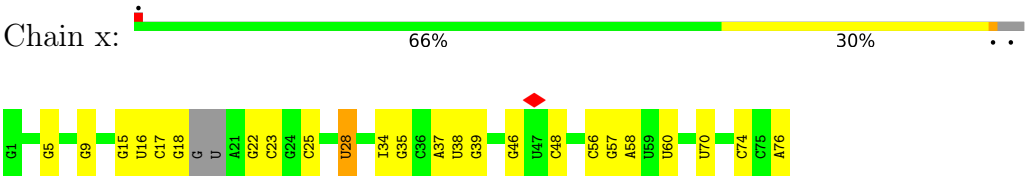




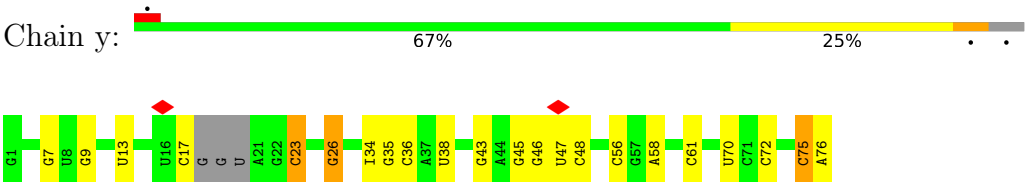
• Molecule 49: 60S ribosomal protein L1-A



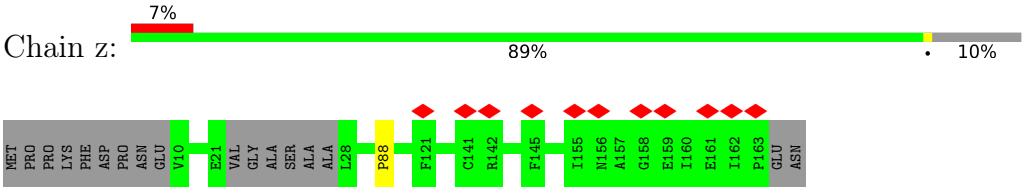
• Molecule 50: Ala tRNA



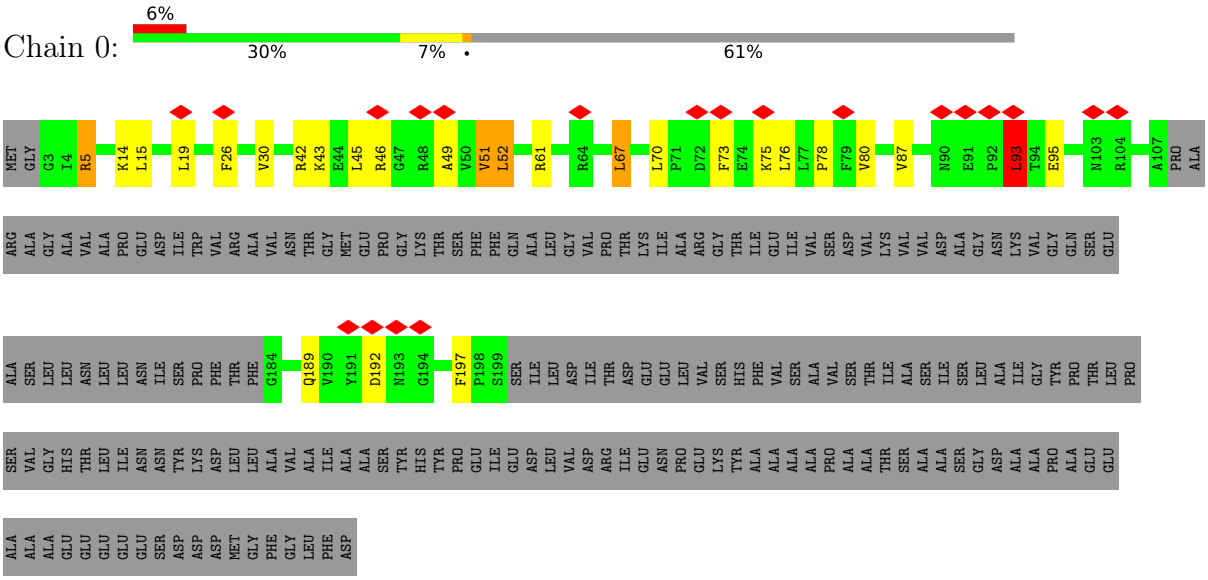
• Molecule 50: Ala tRNA



• Molecule 51: 60S ribosomal protein L12-B

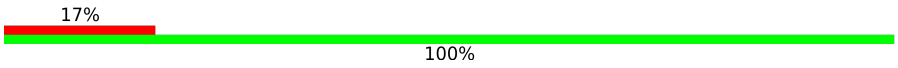


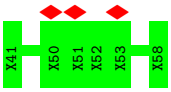
• Molecule 52: 60S acidic ribosomal protein P0



• Molecule 53: CAT-tailed nascent peptide

Chain 1:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56884	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 ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.510	Depositor
Minimum map value	-1.743	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	476.55002, 476.55002, 476.55002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, ZN, 5CT, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/1757	0.70	1/2354 (0.0%)
2	B	0.39	0/1585	0.64	1/2128 (0.0%)
3	C	0.37	0/1439	0.71	2/1938 (0.1%)
4	D	0.34	0/1465	0.67	1/1965 (0.1%)
5	E	0.37	0/1275	0.67	1/1702 (0.1%)
6	F	0.38	0/1473	0.65	0/1980
7	G	0.36	0/1296	0.62	0/1739
8	H	0.37	0/812	0.73	3/1099 (0.3%)
9	I	0.35	0/1018	0.64	0/1369
10	J	0.36	0/530	0.63	0/703
11	K	0.41	0/979	0.69	1/1321 (0.1%)
12	L	0.35	0/995	0.67	1/1329 (0.1%)
13	M	0.36	0/1106	0.61	0/1485
14	N	0.40	0/1200	0.62	0/1607
15	O	0.33	0/473	0.69	1/629 (0.2%)
16	P	0.35	0/745	0.67	0/1001
17	Q	0.39	0/890	0.77	2/1196 (0.2%)
18	R	0.32	0/1034	0.59	0/1385
19	S	0.38	0/868	0.61	0/1168
20	T	0.35	0/890	0.67	0/1189
21	U	0.34	0/978	0.65	1/1301 (0.1%)
22	V	0.34	0/772	0.66	0/1026
23	W	0.39	0/660	0.69	0/875
24	X	0.33	0/618	0.78	1/826 (0.1%)
25	Y	0.33	0/443	0.65	0/588
26	Z	0.33	0/416	0.70	0/553
27	b	0.36	0/836	0.66	0/1104
28	c	0.36	0/701	0.66	0/934
29	d	0.26	0/208	0.84	0/267
30	f	0.61	0/77011	1.03	296/120065 (0.2%)
31	h	0.53	0/2883	0.98	8/4491 (0.2%)
32	i	0.60	0/3746	0.96	7/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	j	0.37	0/1908	0.67	0/2564
34	k	0.36	0/3146	0.64	1/4228 (0.0%)
35	l	0.36	0/2800	0.64	2/3790 (0.1%)
36	m	0.34	0/2400	0.67	4/3239 (0.1%)
37	n	0.36	0/1329	0.67	0/1794
38	o	0.37	0/1821	0.61	0/2451
39	p	0.34	0/1836	0.62	2/2481 (0.1%)
40	q	0.37	0/1529	0.68	2/2060 (0.1%)
41	r	0.33	0/1801	0.64	0/2416
42	s	0.36	0/1367	0.70	3/1834 (0.2%)
43	t	0.36	0/1568	0.69	1/2106 (0.0%)
44	u	0.34	0/1068	0.66	1/1438 (0.1%)
45	a	0.31	0/6692	0.57	3/9027 (0.0%)
46	e	0.39	0/11708	0.55	2/15899 (0.0%)
47	g	0.32	0/1672	0.63	0/2281
48	v	0.31	0/1084	0.62	1/1456 (0.1%)
49	w	0.33	0/1736	0.65	0/2332
50	x	0.61	3/1760 (0.2%)	1.18	14/2738 (0.5%)
50	y	0.40	0/1734	1.10	7/2697 (0.3%)
51	z	0.38	0/733	0.60	0/1015
52	0	0.33	0/982	0.55	0/1320
All	All	0.50	3/161776 (0.0%)	0.88	370/236315 (0.2%)

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
21	U	0	1
34	k	0	1
35	l	0	2
39	p	0	3
40	q	0	1
44	u	0	1
46	e	0	1
47	g	0	1
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	x	34	I	P-OP1	18.99	1.86	1.48
50	x	34	I	C6-O6	7.65	1.38	1.23
50	x	76	A	C3'-O3'	5.80	1.50	1.42

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	x	34	I	O5'-P-OP2	28.59	145.01	110.70
30	f	3217	C	N1-C2-O2	12.11	126.17	118.90
30	f	3217	C	C2-N1-C1'	11.31	131.24	118.80
50	y	75	C	C6-N1-C2	-10.32	116.17	120.30
30	f	3217	C	N3-C2-O2	-9.73	115.09	121.90
11	K	134	ASP	CB-CG-OD1	9.67	127.01	118.30
17	Q	84	ASP	CB-CG-OD1	9.29	126.66	118.30
30	f	922	U	C2-N1-C1'	9.29	128.84	117.70
50	y	75	C	C5-C6-N1	9.09	125.55	121.00
30	f	2531	C	N1-C2-O2	8.89	124.24	118.90
30	f	922	U	N1-C2-O2	8.85	128.99	122.80
30	f	3278	C	N1-C2-O2	8.71	124.12	118.90
30	f	3181	C	N1-C2-O2	8.68	124.11	118.90
30	f	3181	C	C2-N1-C1'	8.49	128.14	118.80
50	x	34	I	OP1-P-OP2	-8.39	94.72	119.90
30	f	2836	C	N3-C2-O2	-8.32	116.07	121.90
30	f	1279	C	C5-C6-N1	8.27	125.14	121.00
30	f	2836	C	C2-N1-C1'	8.20	127.82	118.80
36	m	230	ASP	CB-CG-OD1	8.10	125.59	118.30
30	f	1496	C	C2-N1-C1'	8.09	127.70	118.80
30	f	922	U	N3-C2-O2	-8.01	116.60	122.20
30	f	406	G	O4'-C1'-N9	7.93	114.55	108.20
30	f	1645	U	N3-C2-O2	-7.90	116.67	122.20
30	f	2205	U	N1-C2-O2	7.85	128.29	122.80
30	f	2444	C	C2-N1-C1'	7.80	127.39	118.80
30	f	3217	C	C6-N1-C2	-7.79	117.18	120.30
4	D	41	ASP	CB-CG-OD1	7.79	125.31	118.30
30	f	1208	U	N1-C2-O2	7.78	128.25	122.80
30	f	3217	C	C6-N1-C1'	-7.76	111.49	120.80
30	f	2983	C	C2-N1-C1'	7.75	127.32	118.80
30	f	3306	U	N3-C2-O2	-7.67	116.83	122.20
30	f	2652	U	N3-C2-O2	-7.65	116.85	122.20
30	f	3278	C	N3-C2-O2	-7.58	116.60	121.90
30	f	3306	U	C2-N1-C1'	7.56	126.78	117.70
30	f	2541	U	P-O3'-C3'	7.54	128.75	119.70
30	f	3278	C	C2-N1-C1'	7.54	127.10	118.80

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	x	34	I	O5'-P-OP1	7.51	119.72	110.70
30	f	2205	U	N3-C2-O2	-7.50	116.95	122.20
50	x	76	A	C2'-C3'-O3'	7.47	125.93	109.50
30	f	758	C	C2-N1-C1'	7.46	127.00	118.80
30	f	1645	U	N1-C2-O2	7.42	128.00	122.80
30	f	2836	C	N1-C2-O2	7.42	123.35	118.90
30	f	2502	A	OP2-P-O3'	7.39	121.46	105.20
30	f	1277	C	C2-N1-C1'	7.38	126.92	118.80
30	f	3181	C	N3-C2-O2	-7.34	116.76	121.90
30	f	2235	C	C2-N1-C1'	7.32	126.86	118.80
15	O	36	ASP	CB-CG-OD1	7.25	124.82	118.30
30	f	1239	C	C2-N1-C1'	7.23	126.75	118.80
30	f	1556	C	N1-C2-O2	7.22	123.23	118.90
30	f	2531	C	C2-N1-C1'	7.18	126.70	118.80
42	s	170	ASP	CB-CG-OD1	7.18	124.76	118.30
30	f	1349	G	N3-C4-C5	-7.16	125.02	128.60
30	f	1277	C	N1-C2-O2	7.14	123.19	118.90
30	f	2502	A	P-O3'-C3'	7.13	128.26	119.70
30	f	2923	U	N1-C2-O2	7.12	127.78	122.80
30	f	1227	C	C2-N1-C1'	7.11	126.62	118.80
30	f	2205	U	C2-N1-C1'	7.11	126.23	117.70
39	p	158	ASP	CB-CG-OD1	7.11	124.70	118.30
30	f	1815	U	P-O3'-C3'	7.08	128.19	119.70
30	f	1227	C	N1-C2-O2	7.08	123.14	118.90
30	f	78	U	N3-C2-O2	-7.07	117.25	122.20
30	f	982	C	C2-N1-C1'	7.06	126.57	118.80
30	f	1307	G	P-O3'-C3'	7.06	128.17	119.70
30	f	36	C	N1-C2-O2	7.04	123.12	118.90
30	f	1604	G	C4-N9-C1'	7.04	135.65	126.50
30	f	14	U	O5'-P-OP2	-7.03	99.37	105.70
30	f	1645	U	C2-N1-C1'	7.02	126.12	117.70
30	f	1872	C	N1-C2-O2	6.97	123.08	118.90
30	f	2405	C	C6-N1-C2	-6.97	117.51	120.30
30	f	1349	G	C4-N9-C1'	6.95	135.54	126.50
30	f	1272	C	N1-C2-O2	6.94	123.06	118.90
30	f	1208	U	C2-N1-C1'	6.92	126.00	117.70
30	f	3217	C	C5-C6-N1	6.90	124.45	121.00
50	x	25	C	N3-C2-O2	-6.90	117.07	121.90
30	f	3275	U	OP1-P-O3'	6.86	120.30	105.20
30	f	3306	U	N1-C2-O2	6.86	127.60	122.80
30	f	3235	C	C2-N1-C1'	6.83	126.32	118.80
30	f	2846	U	C2-N1-C1'	6.80	125.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	1227	C	C5-C6-N1	6.79	124.39	121.00
30	f	2923	U	N3-C2-O2	-6.78	117.45	122.20
30	f	2846	U	N3-C2-O2	-6.78	117.45	122.20
12	L	11	ASP	CB-CG-OD1	6.72	124.35	118.30
30	f	270	U	N1-C2-O2	6.72	127.51	122.80
30	f	1227	C	C6-N1-C2	-6.72	117.61	120.30
30	f	2836	C	C6-N1-C2	-6.70	117.62	120.30
50	x	28	U	N3-C4-O4	6.68	124.08	119.40
30	f	2983	C	N3-C2-O2	-6.67	117.23	121.90
30	f	270	U	N3-C2-O2	-6.67	117.53	122.20
30	f	2537	U	P-O3'-C3'	6.66	127.69	119.70
30	f	2531	C	N3-C2-O2	-6.65	117.25	121.90
31	h	26	C	N1-C2-O2	6.64	122.89	118.90
30	f	2112	U	OP2-P-O3'	6.61	119.75	105.20
30	f	1239	C	N1-C2-O2	6.60	122.86	118.90
30	f	3058	U	C2-N1-C1'	6.59	125.61	117.70
30	f	2189	U	N1-C2-O2	6.58	127.40	122.80
30	f	1208	U	N3-C2-O2	-6.56	117.61	122.20
30	f	3214	U	C2-N1-C1'	6.53	125.54	117.70
2	B	27[A]	LEU	CB-CG-CD2	-6.52	99.91	111.00
32	i	64	U	N3-C2-O2	-6.52	117.64	122.20
30	f	2235	C	C6-N1-C2	-6.48	117.71	120.30
30	f	3034	C	N1-C2-O2	6.47	122.78	118.90
30	f	2101	C	P-O3'-C3'	6.47	127.46	119.70
30	f	2189	U	N3-C2-O2	-6.46	117.68	122.20
31	h	105	C	N1-C2-O2	6.45	122.77	118.90
30	f	524	U	N1-C2-O2	6.45	127.32	122.80
30	f	2112	U	P-O3'-C3'	6.44	127.42	119.70
30	f	2550	U	N3-C2-O2	-6.42	117.71	122.20
30	f	2274	U	N1-C2-O2	6.38	127.27	122.80
35	l	155	ASP	CB-CG-OD1	6.38	124.04	118.30
44	u	47	ASP	CB-CG-OD1	6.38	124.04	118.30
30	f	1269	U	C2-N1-C1'	6.38	125.35	117.70
30	f	2983	C	N1-C2-O2	6.37	122.72	118.90
30	f	986	U	N3-C2-O2	-6.35	117.75	122.20
30	f	1269	U	N1-C2-O2	6.34	127.24	122.80
30	f	524	U	N3-C2-O2	-6.33	117.77	122.20
30	f	865	U	N3-C2-O2	-6.32	117.78	122.20
21	U	79	ASP	CB-CG-OD1	6.31	123.98	118.30
30	f	1556	C	N3-C2-O2	-6.30	117.49	121.90
30	f	3058	U	N1-C2-O2	6.30	127.21	122.80
30	f	2726	C	N3-C2-O2	-6.29	117.50	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	m	137	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	153	ASP	CB-CG-OD1	6.29	123.96	118.30
30	f	2464	U	C2-N1-C1'	6.29	125.24	117.70
30	f	2617	U	N3-C2-O2	-6.28	117.81	122.20
30	f	36	C	N3-C2-O2	-6.27	117.51	121.90
30	f	922	U	C6-N1-C1'	-6.26	112.43	121.20
30	f	1496	C	C6-N1-C2	-6.26	117.80	120.30
45	a	697	LEU	CA-CB-CG	6.24	129.66	115.30
30	f	2726	C	C2-N1-C1'	6.24	125.66	118.80
30	f	1716	U	P-O3'-C3'	6.22	127.16	119.70
40	q	42	ASP	CB-CG-OD1	6.22	123.89	118.30
30	f	192	C	C2-N1-C1'	6.21	125.64	118.80
30	f	1269	U	N3-C2-O2	-6.21	117.85	122.20
30	f	1097	G	P-O3'-C3'	6.21	127.15	119.70
46	e	437	LYS	N-CA-C	-6.21	94.25	111.00
30	f	3104	U	N1-C2-O2	6.19	127.13	122.80
30	f	1878	G	C4-N9-C1'	6.17	134.52	126.50
30	f	2444	C	C6-N1-C2	-6.16	117.84	120.30
30	f	1349	G	N3-C4-N9	6.14	129.68	126.00
30	f	637	C	P-O3'-C3'	6.14	127.07	119.70
30	f	3104	U	N3-C2-O2	-6.14	117.90	122.20
30	f	2846	U	N1-C2-O2	6.12	127.08	122.80
30	f	915	A	C2-N3-C4	6.11	113.65	110.60
30	f	2550	U	C2-N1-C1'	6.11	125.03	117.70
30	f	1115	G	C4-N9-C1'	6.09	134.42	126.50
30	f	2923	U	C2-N1-C1'	6.08	125.00	117.70
30	f	2553	U	C2-N1-C1'	6.08	124.99	117.70
30	f	1064	A	P-O3'-C3'	6.07	126.99	119.70
30	f	995	U	N1-C2-O2	6.06	127.05	122.80
30	f	2388	U	N3-C2-O2	-6.06	117.96	122.20
30	f	2132	C	C6-N1-C2	-6.06	117.88	120.30
30	f	1907	C	N1-C2-O2	6.05	122.53	118.90
30	f	2842	U	N1-C2-O2	6.05	127.03	122.80
30	f	2132	C	N3-C2-O2	-6.03	117.68	121.90
30	f	3131	U	C2-N1-C1'	6.03	124.93	117.70
30	f	1872	C	N3-C2-O2	-6.02	117.69	121.90
30	f	1604	G	N3-C4-N9	6.01	129.61	126.00
30	f	969	C	C6-N1-C2	-6.01	117.90	120.30
30	f	1604	G	C8-N9-C1'	-6.00	119.20	127.00
30	f	3300	U	N3-C2-O2	-5.99	118.00	122.20
30	f	2274	U	C2-N1-C1'	5.99	124.89	117.70
30	f	3181	C	C6-N1-C1'	-5.98	113.62	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	985	U	N3-C2-O2	-5.98	118.01	122.20
30	f	2405	C	N3-C2-O2	-5.98	117.71	121.90
30	f	1556	C	C2-N1-C1'	5.96	125.36	118.80
8	H	51	GLY	C-N-CA	5.95	136.58	121.70
30	f	1279	C	C6-N1-C2	-5.94	117.92	120.30
34	k	87	VAL	CG1-CB-CG2	-5.93	101.40	110.90
8	H	18	ASP	CB-CG-OD1	5.93	123.64	118.30
30	f	1425	U	N3-C2-O2	-5.93	118.05	122.20
31	h	26	C	C6-N1-C2	-5.93	117.93	120.30
30	f	2204	C	C6-N1-C2	-5.92	117.93	120.30
30	f	1355	A	P-O3'-C3'	5.91	126.80	119.70
30	f	1604	G	N3-C4-C5	-5.91	125.65	128.60
30	f	865	U	N1-C2-O2	5.89	126.92	122.80
30	f	2652	U	N1-C2-O2	5.89	126.92	122.80
30	f	2585	G	N3-C4-C5	-5.89	125.66	128.60
32	i	100	U	C2-N1-C1'	5.88	124.75	117.70
30	f	1562	C	P-O3'-C3'	5.88	126.75	119.70
30	f	1820	U	P-O3'-C3'	5.87	126.75	119.70
30	f	1272	C	N3-C2-O2	-5.86	117.80	121.90
30	f	1525	G	C4-N9-C1'	5.85	134.10	126.50
30	f	2531	C	C6-N1-C2	-5.85	117.96	120.30
30	f	3048	A	O4'-C1'-N9	5.84	112.88	108.20
30	f	1437	C	C2-N1-C1'	5.83	125.22	118.80
30	f	142	C	N1-C2-O2	5.83	122.40	118.90
30	f	2638	C	N1-C2-O2	5.83	122.40	118.90
30	f	3214	U	N3-C2-O2	-5.83	118.12	122.20
30	f	835	G	O4'-C1'-N9	5.83	112.86	108.20
30	f	2622	C	N1-C2-O2	5.83	122.39	118.90
30	f	1577	G	N1-C6-O6	-5.81	116.41	119.90
30	f	2274	U	N3-C2-O2	-5.81	118.13	122.20
30	f	3316	A	P-O3'-C3'	5.80	126.66	119.70
50	x	34	I	O6-C6-C5	5.79	137.37	120.00
30	f	3350	C	C6-N1-C2	-5.79	117.98	120.30
42	s	9	MET	CA-CB-CG	5.78	123.12	113.30
30	f	2531	C	C5-C6-N1	5.77	123.88	121.00
30	f	270	U	C2-N1-C1'	5.76	124.61	117.70
30	f	3228	C	P-O3'-C3'	5.74	126.59	119.70
30	f	2992	U	N3-C2-O2	-5.72	118.19	122.20
45	a	117	PHE	N-CA-CB	-5.72	100.30	110.60
30	f	3218	A	P-O3'-C3'	5.72	126.56	119.70
30	f	97	U	N3-C2-O2	-5.71	118.20	122.20
30	f	1190	A	C4-N9-C1'	5.71	136.58	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	758	C	C6-N1-C2	-5.71	118.02	120.30
30	f	2204	C	C5-C6-N1	5.71	123.85	121.00
30	f	354	U	N1-C2-O2	5.69	126.78	122.80
46	e	1364	GLY	N-CA-C	5.69	127.31	113.10
32	i	64	U	N1-C2-O2	5.68	126.78	122.80
30	f	2899	C	N3-C2-O2	-5.67	117.93	121.90
30	f	2132	C	N1-C2-O2	5.67	122.30	118.90
30	f	3034	C	N3-C2-O2	-5.67	117.93	121.90
30	f	282	G	P-O3'-C3'	5.67	126.50	119.70
30	f	2553	U	C6-N1-C1'	-5.67	113.26	121.20
30	f	2899	C	C2-N1-C1'	5.67	125.03	118.80
8	H	50	LEU	CA-CB-CG	5.67	128.33	115.30
30	f	1448	U	N3-C2-O2	-5.66	118.24	122.20
30	f	916	G	P-O3'-C3'	5.66	126.49	119.70
30	f	1277	C	N3-C2-O2	-5.65	117.94	121.90
30	f	2366	C	C2-N1-C1'	5.65	125.01	118.80
30	f	3058	U	N3-C2-O2	-5.62	118.26	122.20
30	f	2378	C	C2-N1-C1'	5.62	124.98	118.80
30	f	2137	U	C2-N1-C1'	5.61	124.44	117.70
30	f	1349	G	C8-N9-C1'	-5.61	119.71	127.00
30	f	142	C	C6-N1-C2	-5.61	118.06	120.30
30	f	113	C	C2-N1-C1'	5.60	124.96	118.80
31	h	26	C	N3-C2-O2	-5.59	117.99	121.90
30	f	1496	C	C5-C6-N1	5.58	123.79	121.00
30	f	777	U	N3-C2-O2	-5.58	118.30	122.20
30	f	2842	U	N3-C2-O2	-5.57	118.30	122.20
30	f	2983	C	C6-N1-C2	-5.57	118.07	120.30
30	f	3057	U	N3-C2-O2	-5.56	118.31	122.20
30	f	3269	U	P-O3'-C3'	5.56	126.37	119.70
50	x	25	C	N1-C2-O2	5.55	122.23	118.90
30	f	2764	C	N1-C2-O2	5.55	122.23	118.90
3	C	53	ASP	CB-CG-OD1	5.54	123.29	118.30
30	f	1496	C	N1-C2-O2	5.54	122.23	118.90
40	q	107	ASP	CB-CG-OD1	5.54	123.28	118.30
50	y	70	U	N1-C2-O2	5.54	126.68	122.80
50	x	28	U	C5-C4-O4	-5.54	122.58	125.90
32	i	125	U	C2-N1-C1'	5.53	124.34	117.70
50	x	70	U	N1-C2-O2	5.53	126.67	122.80
30	f	2366	C	C5-C6-N1	5.53	123.76	121.00
50	x	25	C	C6-N1-C2	-5.53	118.09	120.30
30	f	995	U	N3-C2-O2	-5.52	118.34	122.20
30	f	2552	C	N1-C2-O2	5.51	122.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	2726	C	N1-C2-O2	5.51	122.20	118.90
31	h	35	C	N1-C2-O2	5.51	122.20	118.90
31	h	52	G	P-O3'-C3'	5.49	126.29	119.70
30	f	1554	U	P-O3'-C3'	5.49	126.28	119.70
30	f	982	C	N1-C2-O2	5.48	122.19	118.90
30	f	3214	U	N1-C2-O2	5.48	126.64	122.80
30	f	1688	U	N3-C2-O2	-5.48	118.37	122.20
30	f	315	C	C2-N1-C1'	5.48	124.82	118.80
30	f	2210	G	N3-C4-C5	-5.48	125.86	128.60
30	f	2444	C	N1-C2-O2	5.47	122.18	118.90
30	f	283	G	C4-N9-C1'	5.47	133.61	126.50
30	f	283	G	N3-C4-N9	5.47	129.28	126.00
24	X	14	LEU	CA-CB-CG	5.46	127.85	115.30
30	f	3355	U	C2-N1-C1'	5.45	124.25	117.70
30	f	411	U	N3-C2-O2	-5.43	118.40	122.20
30	f	2585	G	N3-C4-N9	5.43	129.26	126.00
30	f	986	U	N1-C2-O2	5.43	126.60	122.80
50	y	72	C	C2-N1-C1'	5.42	124.76	118.80
30	f	982	C	C6-N1-C2	-5.42	118.13	120.30
30	f	3153	U	C2-N1-C1'	5.42	124.20	117.70
45	a	439	LEU	CA-CB-CG	-5.41	102.86	115.30
30	f	1878	G	C8-N9-C1'	-5.41	119.97	127.00
30	f	3350	C	P-O3'-C3'	5.41	126.19	119.70
30	f	2726	C	C6-N1-C2	-5.40	118.14	120.30
30	f	2552	C	C2-N1-C1'	5.40	124.74	118.80
30	f	3057	U	N1-C2-O2	5.39	126.57	122.80
30	f	2783	U	N3-C2-O2	-5.39	118.43	122.20
30	f	1732	U	N1-C2-O2	5.38	126.57	122.80
30	f	2622	C	N3-C2-O2	-5.38	118.13	121.90
30	f	78	U	N1-C2-O2	5.38	126.57	122.80
3	C	114	VAL	CG1-CB-CG2	-5.38	102.30	110.90
30	f	1437	C	C6-N1-C2	-5.37	118.15	120.30
30	f	1349	G	C2-N3-C4	5.36	114.58	111.90
30	f	3278	C	C6-N1-C1'	-5.36	114.37	120.80
30	f	915	A	C4-N9-C1'	5.35	135.93	126.30
30	f	1496	C	C6-N1-C1'	-5.35	114.38	120.80
30	f	982	C	C5-C6-N1	5.35	123.67	121.00
30	f	2500	A	P-O3'-C3'	5.34	126.11	119.70
30	f	1425	U	N1-C2-O2	5.34	126.54	122.80
30	f	142	C	N3-C2-O2	-5.32	118.18	121.90
30	f	2336	U	N3-C2-O2	-5.32	118.48	122.20
30	f	3235	C	N1-C2-O2	5.32	122.09	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	1907	C	N3-C2-O2	-5.32	118.18	121.90
30	f	890	C	N1-C2-O2	5.31	122.09	118.90
30	f	1277	C	C6-N1-C2	-5.31	118.17	120.30
30	f	1525	G	C8-N9-C1'	-5.31	120.09	127.00
30	f	1115	G	C8-N9-C1'	-5.30	120.11	127.00
30	f	2836	C	C6-N1-C1'	-5.30	114.44	120.80
30	f	1190	A	C2-N3-C4	5.30	113.25	110.60
30	f	1732	U	N3-C2-O2	-5.29	118.50	122.20
30	f	1608	C	C2-N1-C1'	5.28	124.61	118.80
43	t	136	GLU	CA-CB-CG	5.28	125.02	113.40
30	f	2497	U	N3-C2-O2	-5.28	118.50	122.20
30	f	2235	C	N1-C2-O2	5.28	122.07	118.90
30	f	2366	C	C6-N1-C2	-5.28	118.19	120.30
30	f	2444	C	C5-C6-N1	5.27	123.64	121.00
30	f	1560	G	N3-C4-N9	-5.27	122.84	126.00
50	y	26	G	N3-C4-N9	5.27	129.16	126.00
30	f	2114	C	C6-N1-C2	-5.27	118.19	120.30
31	h	105	C	N3-C2-O2	-5.26	118.21	121.90
32	i	125	U	N1-C2-O2	5.26	126.48	122.80
30	f	2568	C	O4'-C1'-N1	5.26	112.41	108.20
48	v	50	GLY	N-CA-C	-5.25	99.97	113.10
30	f	3349	C	C6-N1-C2	-5.24	118.20	120.30
50	x	34	I	N1-C6-O6	-5.24	104.28	120.00
30	f	915	A	C8-N9-C4	-5.24	103.70	105.80
42	s	108	GLU	CA-CB-CG	5.24	124.92	113.40
30	f	3181	C	C6-N1-C2	-5.24	118.21	120.30
30	f	192	C	C6-N1-C2	-5.23	118.21	120.30
30	f	3148	U	N3-C2-O2	-5.23	118.54	122.20
30	f	2405	C	N1-C2-O2	5.22	122.03	118.90
30	f	2496	C	C2-N1-C1'	5.22	124.54	118.80
30	f	1239	C	C6-N1-C1'	-5.21	114.54	120.80
30	f	2622	C	C6-N1-C2	-5.21	118.22	120.30
30	f	1608	C	C5-C6-N1	5.20	123.60	121.00
30	f	2585	G	C4-N9-C1'	5.20	133.26	126.50
30	f	954	U	N3-C2-O2	-5.19	118.57	122.20
30	f	890	C	N3-C2-O2	-5.18	118.27	121.90
30	f	2235	C	C5-C6-N1	5.18	123.59	121.00
30	f	1237	G	N3-C4-N9	5.18	129.11	126.00
50	y	23	C	C6-N1-C2	-5.18	118.23	120.30
30	f	2899	C	N1-C2-O2	5.17	122.00	118.90
30	f	2983	C	C6-N1-C1'	-5.17	114.59	120.80
50	x	23	C	C6-N1-C2	-5.17	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	h	18	C	C2-N1-C1'	5.17	124.49	118.80
30	f	2446	U	O4'-C1'-N1	5.17	112.33	108.20
50	x	70	U	N3-C2-O2	-5.17	118.58	122.20
30	f	637	C	OP1-P-O3'	5.16	116.55	105.20
32	i	100	U	N1-C2-O2	5.16	126.41	122.80
30	f	849	C	P-O3'-C3'	5.15	125.88	119.70
30	f	1563	C	C6-N1-C1'	5.14	126.97	120.80
30	f	1608	C	C6-N1-C2	-5.14	118.24	120.30
30	f	166	C	C2-N1-C1'	5.14	124.46	118.80
30	f	758	C	N1-C2-O2	5.13	121.98	118.90
30	f	2405	C	C2-N1-C1'	5.13	124.44	118.80
30	f	2772	C	N1-C2-O2	5.12	121.97	118.90
30	f	149	U	N3-C2-O2	-5.12	118.62	122.20
30	f	1951	C	C2-N1-C1'	5.12	124.43	118.80
30	f	87	U	N1-C2-O2	5.10	126.37	122.80
30	f	969	C	N3-C2-O2	-5.10	118.33	121.90
50	y	70	U	N3-C2-O2	-5.10	118.63	122.20
30	f	1597	C	C5-C6-N1	5.09	123.55	121.00
36	m	222	LEU	CA-CB-CG	5.09	127.01	115.30
35	l	4	PRO	C-N-CA	5.08	134.41	121.70
30	f	2550	U	N1-C2-O2	5.08	126.36	122.80
30	f	2638	C	N3-C2-O2	-5.08	118.34	121.90
30	f	2444	C	C6-N1-C1'	-5.08	114.71	120.80
30	f	1097	G	OP2-P-O3'	5.07	116.36	105.20
32	i	157	U	N1-C2-O2	5.07	126.35	122.80
30	f	2873	U	C2-N1-C1'	5.07	123.79	117.70
17	Q	42	LEU	CA-CB-CG	5.07	126.96	115.30
30	f	1272	C	C6-N1-C2	-5.04	118.28	120.30
30	f	1820	U	OP2-P-O3'	5.03	116.28	105.20
36	m	146	LEU	CB-CG-CD1	-5.03	102.44	111.00
39	p	79	GLN	CA-CB-CG	5.03	124.47	113.40
30	f	354	U	N3-C2-O2	-5.03	118.68	122.20
30	f	885	U	N3-C2-O2	-5.03	118.68	122.20
30	f	3355	U	N1-C2-O2	5.02	126.31	122.80
5	E	10	LEU	CB-CG-CD1	5.02	119.53	111.00
30	f	3363	U	N3-C2-O2	-5.02	118.69	122.20
30	f	1562	C	N3-C2-O2	-5.01	118.39	121.90
30	f	2836	C	O4'-C1'-N1	5.01	112.21	108.20
30	f	282	G	C2'-C3'-O3'	5.00	121.70	113.70
30	f	1355	A	OP2-P-O3'	5.00	116.20	105.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	U	83	LYS	Peptide
46	e	392	GLY	Peptide
47	g	8	GLU	Peptide
34	k	141	GLY	Peptide
35	l	13	GLY	Peptide
35	l	318	LEU	Peptide
39	p	158	ASP	Peptide
39	p	30	THR	Peptide
39	p	76	ALA	Peptide
40	q	21	LYS	Peptide
44	u	12	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1720	0	1779	9	0
2	B	1555	0	1659	13	0
3	C	1416	0	1433	11	0
4	D	1441	0	1543	8	0
5	E	1258	0	1342	6	0
6	F	1437	0	1475	15	0
7	G	1272	0	1312	9	0
8	H	796	0	812	4	0
9	I	1003	0	1048	7	0
10	J	518	0	542	4	0
11	K	964	0	1025	1	0
12	L	984	0	1075	4	0
13	M	1080	0	1122	5	0
14	N	1169	0	1211	6	0
15	O	462	0	491	4	0
16	P	737	0	792	3	0
17	Q	876	0	912	9	0
18	R	1013	0	1077	5	0
19	S	850	0	880	3	0
20	T	880	0	942	3	0
21	U	969	0	1078	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	766	0	844	4	0
23	W	645	0	645	3	0
24	X	612	0	682	3	0
25	Y	436	0	475	0	0
26	Z	410	0	442	0	0
27	b	824	0	888	0	0
28	c	694	0	734	0	0
29	d	207	0	250	0	0
30	f	68802	0	34573	0	0
31	h	2579	0	1304	0	0
32	i	3353	0	1695	0	0
33	j	1874	0	1943	0	0
34	k	3075	0	3142	0	0
35	l	2748	0	2859	0	0
36	m	2351	0	2294	0	0
37	n	1307	0	1377	0	0
38	o	1784	0	1862	0	0
39	p	1804	0	1877	0	0
40	q	1508	0	1572	0	0
41	r	1764	0	1804	0	0
42	s	1346	0	1370	0	0
43	t	1543	0	1608	0	0
44	u	1053	0	1149	0	0
45	a	6582	0	6484	0	0
46	e	11509	0	10768	0	0
47	g	1651	0	1613	0	0
48	v	1085	0	1086	0	0
49	w	1709	0	1799	0	0
50	x	1579	0	798	0	0
50	y	1556	0	788	0	0
51	z	734	0	344	0	0
52	0	967	0	990	13	0
53	1	90	0	20	0	0
54	A	1	0	0	0	0
54	C	1	0	0	0	0
54	E	1	0	0	0	0
54	I	1	0	0	0	0
54	R	1	0	0	0	0
54	T	1	0	0	0	0
54	f	3	0	0	0	0
54	h	1	0	0	0	0
54	j	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	k	1	0	0	0	0
55	T	1	0	0	0	0
55	W	1	0	0	0	0
55	Z	1	0	0	0	0
55	b	1	0	0	0	0
55	c	1	0	0	0	0
55	e	2	0	0	0	0
56	f	10	0	19	0	0
All	All	151377	0	113648	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:21:ARG:HE	23:W:39:TYR:HB2	1.58	0.69
52:0:26:PHE:HB2	52:0:87:VAL:HB	1.73	0.69
2:B:46[A]:GLU:HB3	2:B:49[A]:ARG:HG3	1.75	0.68
7:G:84:TYR:HB2	15:O:24:PRO:HD3	1.78	0.64
2:B:27[A]:LEU:HD21	2:B:102[A]:LEU:HB2	1.80	0.63
13:M:27:LYS:HB3	13:M:42:LEU:HB2	1.81	0.62
9:I:14:SER:O	9:I:81:GLN:NE2	2.33	0.62
6:F:80:ARG:HH21	6:F:87:THR:HG21	1.66	0.60
6:F:8:GLN:HB3	6:F:64:ILE:HD11	1.85	0.59
52:0:192:ASP:HB2	52:0:197:PHE:HE2	1.67	0.59
1:A:183:THR:HG22	1:A:187:ARG:HB2	1.85	0.59
21:U:5:LYS:HB2	21:U:8:GLU:HG2	1.84	0.58
6:F:77:VAL:HG22	6:F:126:VAL:HG23	1.85	0.58
52:0:43:LYS:HA	52:0:46:ARG:HG2	1.87	0.57
11:K:50:ALA:HB1	21:U:66:VAL:HG11	1.86	0.57
17:Q:4:LEU:O	17:Q:79:ARG:NH2	2.38	0.56
17:Q:55:LEU:HB2	17:Q:95:PRO:HD3	1.86	0.56
10:J:56:ARG:HA	10:J:61:LYS:HG3	1.88	0.56
20:T:87:GLU:OE2	20:T:91:ARG:NH1	2.39	0.55
18:R:19:ARG:HD3	18:R:33:ARG:HB2	1.89	0.55
52:0:42:ARG:HG2	52:0:51:VAL:HG11	1.89	0.55
2:B:157[A]:GLU:OE2	2:B:160[A]:ARG:NH2	2.40	0.54
17:Q:9:THR:HG23	17:Q:109:VAL:HG23	1.88	0.54
14:N:95:SER:OG	14:N:98:THR:OG1	2.25	0.54
8:H:56:VAL:HG12	8:H:65:VAL:HG22	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:17:ARG:HG2	7:G:22:HIS:HA	1.90	0.53
2:B:75[A]:ALA:HB3	2:B:78[A]:ARG:HG2	1.90	0.53
10:J:6:ASP:OD1	10:J:32:GLN:N	2.40	0.53
8:H:44:GLU:OE2	8:H:49:ASN:ND2	2.41	0.52
10:J:47:ARG:HH21	10:J:58:HIS:HB2	1.73	0.52
2:B:61[A]:ALA:HA	2:B:70[A]:PRO:HD2	1.90	0.52
3:C:118:GLN:NE2	3:C:147:GLU:OE2	2.39	0.52
6:F:77:VAL:HG11	6:F:106:LEU:HD22	1.92	0.52
6:F:96:ASP:OD1	6:F:97:VAL:N	2.38	0.52
4:D:36:LEU:O	4:D:40:THR:OG1	2.27	0.52
6:F:80:ARG:HB2	6:F:122:HIS:HB2	1.91	0.52
7:G:136:ARG:HD2	7:G:139:ARG:HH12	1.74	0.51
9:I:94:TYR:OH	10:J:41:LYS:NZ	2.39	0.51
14:N:100:PRO:HG2	14:N:123:VAL:HG23	1.92	0.51
7:G:99:SER:HG	7:G:101:CYS:HG	1.57	0.51
1:A:103:GLU:HG3	1:A:160:GLU:HB2	1.93	0.50
15:O:23:LYS:HG3	15:O:24:PRO:HD2	1.93	0.50
2:B:74[A]:ARG:O	2:B:142[A]:SER:OG	2.23	0.50
3:C:107:LEU:HD12	3:C:152:GLU:HG3	1.92	0.50
3:C:60:PHE:HB3	3:C:64:ASN:HB3	1.93	0.49
17:Q:77:ARG:HD2	17:Q:89:LEU:HD13	1.94	0.49
16:P:9:SER:OG	16:P:10:ILE:N	2.39	0.49
2:B:46[A]:GLU:HG3	2:B:48[A]:PHE:H	1.77	0.49
16:P:30:THR:HG23	16:P:91:SER:HB2	1.95	0.49
6:F:155:ARG:HB2	6:F:172:TYR:HD1	1.77	0.49
7:G:108:ARG:O	7:G:112:ASN:HB2	2.12	0.49
14:N:94:ALA:HA	14:N:121:VAL:HG23	1.95	0.48
4:D:131:ALA:HB1	4:D:135:GLN:H	1.78	0.48
17:Q:80:ASN:OD1	17:Q:81:GLU:N	2.45	0.48
52:0:5:ARG:HA	52:0:5:ARG:HD3	1.47	0.48
13:M:133:LYS:HE3	13:M:135:ARG:HD3	1.95	0.48
19:S:49:ILE:HD11	19:S:71:VAL:HG22	1.96	0.48
4:D:102:ALA:HA	4:D:122:ILE:O	2.14	0.48
6:F:93:GLU:HG3	6:F:140:VAL:HG11	1.95	0.48
3:C:22:LEU:HD12	3:C:146:ILE:HD12	1.97	0.47
13:M:23:VAL:HG12	13:M:45:GLY:HA3	1.94	0.47
4:D:19:PRO:HB3	4:D:53:PHE:HA	1.96	0.47
17:Q:75:ILE:HG12	17:Q:93:VAL:HG22	1.96	0.47
9:I:18:PRO:HA	9:I:51:ALA:HA	1.97	0.47
52:0:26:PHE:HZ	52:0:93:LEU:HA	1.80	0.47
5:E:21:LYS:HE3	5:E:55:VAL:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:151:ARG:NH2	5:E:152:GLU:OE2	2.45	0.47
1:A:5:LYS:HE2	22:V:40:VAL:HG21	1.97	0.47
4:D:170:ARG:HD2	14:N:57:GLY:HA3	1.97	0.47
5:E:68:GLN:OE1	5:E:71:ARG:NH2	2.43	0.46
15:O:55:ALA:O	15:O:59:LYS:HB3	2.16	0.46
3:C:67:ILE:HD11	3:C:80:LYS:HB3	1.97	0.46
13:M:28:PRO:O	13:M:29:HIS:ND1	2.48	0.46
12:L:55:GLU:HB2	12:L:108:LYS:HB3	1.98	0.46
12:L:74:TYR:HB3	12:L:77:LYS:HB2	1.98	0.46
2:B:39[A]:GLU:HG2	2:B:40[A]:GLU:HG2	1.97	0.46
18:R:9:ILE:HG12	18:R:63:THR:HG23	1.97	0.46
14:N:96:LYS:HB2	14:N:96:LYS:HE2	1.70	0.46
18:R:60:ASN:HB3	18:R:63:THR:HB	1.97	0.46
1:A:159:ARG:HB3	1:A:164:LEU:HB2	1.98	0.45
17:Q:44:MET:O	17:Q:77:ARG:NH1	2.49	0.45
19:S:14:LEU:HD11	19:S:31:LYS:HB2	1.98	0.45
13:M:22:LYS:NZ	13:M:132:SER:O	2.47	0.45
6:F:22:PRO:O	7:G:146:ASN:ND2	2.38	0.45
22:V:53:TYR:HA	22:V:56:ARG:HG2	1.99	0.45
9:I:38:ALA:HB3	9:I:59:MET:HB2	1.99	0.44
24:X:10:GLN:HA	24:X:13:GLU:HG2	1.99	0.44
6:F:80:ARG:HG3	6:F:124:LEU:HD21	1.99	0.44
9:I:129:VAL:O	9:I:133:SER:HB3	2.17	0.44
2:B:127[A]:LEU:HD22	6:F:156:VAL:HG13	2.00	0.44
4:D:161:LYS:HA	4:D:161:LYS:HD3	1.82	0.44
6:F:80:ARG:HD2	7:G:155:PRO:HA	2.00	0.44
14:N:36:GLY:HA3	14:N:40:HIS:CE1	2.53	0.44
17:Q:46:THR:HG22	17:Q:48:ASP:H	1.82	0.43
52:0:45:LEU:HB3	52:0:49:ALA:HB3	1.99	0.43
8:H:20:SER:HA	8:H:23:THR:HG22	2.00	0.43
20:T:95:ILE:HG21	20:T:95:ILE:HD13	1.81	0.43
9:I:117:PRO:HA	9:I:135:VAL:HG13	2.00	0.43
52:0:15:LEU:O	52:0:19:LEU:HG	2.18	0.43
23:W:58:THR:OG1	23:W:59:THR:N	2.51	0.43
1:A:158:HIS:HB3	1:A:161:ALA:HB3	2.00	0.43
23:W:27:PHE:HA	23:W:34:CYS:HA	2.01	0.43
1:A:68:ARG:HA	1:A:98:LEU:HD21	2.01	0.43
4:D:124:LEU:HD13	4:D:127:LEU:HD23	2.01	0.43
52:0:75:LYS:O	52:0:78:PRO:HD2	2.19	0.43
3:C:56:ARG:NH2	3:C:75:GLU:OE2	2.51	0.43
5:E:102:LEU:HD22	5:E:138:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:2:ALA:N	24:X:51:LEU:O	2.52	0.43
18:R:3:SER:OG	18:R:4:LEU:N	2.51	0.43
2:B:54[A]:TYR:OH	2:B:73[A]:PHE:O	2.37	0.42
9:I:80:ARG:HB2	9:I:99:ALA:HB3	2.00	0.42
12:L:86:THR:OG1	12:L:94:SER:OG	2.36	0.42
15:O:21:ILE:O	15:O:22:LYS:C	2.57	0.42
3:C:179:GLN:HA	3:C:182:ILE:HG22	2.00	0.42
6:F:95:ARG:HB2	6:F:140:VAL:HG23	2.00	0.42
52:0:67:LEU:HD22	52:0:67:LEU:HA	1.85	0.42
24:X:33:LYS:HA	24:X:33:LYS:HD3	1.84	0.42
52:0:70:LEU:HB3	52:0:73:PHE:CD1	2.55	0.42
21:U:78:LYS:HA	21:U:81:ARG:HG2	2.00	0.42
52:0:14:LYS:HE3	52:0:52:LEU:HD11	2.00	0.42
52:0:61:ARG:HA	52:0:61:ARG:HD2	1.92	0.42
6:F:32:SER:HB2	6:F:36:ILE:HD12	2.01	0.42
8:H:41:ILE:HG21	8:H:54:VAL:HG21	2.02	0.42
7:G:102:ARG:HD2	7:G:102:ARG:HA	1.76	0.41
3:C:116:HIS:HB3	3:C:149:VAL:HB	2.02	0.41
3:C:182:ILE:HD12	3:C:182:ILE:HA	1.85	0.41
16:P:73:GLY:N	16:P:76:GLU:OE1	2.42	0.41
19:S:16:TYR:OH	19:S:89:LEU:O	2.31	0.41
1:A:98:LEU:HD22	1:A:128:LYS:HD2	2.02	0.41
12:L:63:LYS:HA	12:L:63:LYS:HD3	1.92	0.41
2:B:8[A]:VAL:HG12	2:B:117[A]:ARG:HG3	2.03	0.41
3:C:131:ARG:HG3	3:C:137:ASN:ND2	2.36	0.41
22:V:5:THR:HG23	22:V:12:ASN:HB2	2.03	0.41
1:A:9:GLU:HG3	22:V:44:VAL:HG21	2.03	0.41
3:C:122:ALA:HB3	3:C:143:PRO:HB2	2.02	0.41
5:E:7:GLN:NE2	5:E:35:ALA:O	2.53	0.41
2:B:121[A]:PRO:HA	2:B:124[A]:LEU:HD12	2.03	0.40
2:B:189[A]:ASP:OD1	2:B:190[A]:VAL:N	2.53	0.40
6:F:40:ARG:HA	6:F:40:ARG:HD2	1.84	0.40
17:Q:20:LEU:HD11	17:Q:32:ALA:HB2	2.03	0.40
1:A:18:VAL:HG13	1:A:19:LEU:HD12	2.01	0.40
4:D:180:ARG:HE	4:D:180:ARG:HB2	1.62	0.40
5:E:31:GLU:HA	5:E:34:GLN:HB2	2.03	0.40
18:R:4:LEU:HD12	18:R:5:PRO:HD2	2.01	0.40
20:T:93:PHE:HD2	20:T:94:LEU:HD22	1.86	0.40
7:G:73:GLY:HA2	7:G:89:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
2	B	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
3	C	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
4	D	183/186 (98%)	176 (96%)	7 (4%)	0	100	100
5	E	154/189 (82%)	151 (98%)	3 (2%)	0	100	100
6	F	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
7	G	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
8	H	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
9	I	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
10	J	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
11	K	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
12	L	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
13	M	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
14	N	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
15	O	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	7	12
16	P	94/105 (90%)	93 (99%)	1 (1%)	0	100	100
17	Q	107/113 (95%)	98 (92%)	9 (8%)	0	100	100
18	R	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
19	S	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
20	T	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
21	U	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
22	V	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
23	W	79/88 (90%)	75 (95%)	4 (5%)	0	100	100
24	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
25	Y	48/51 (94%)	46 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
27	b	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
28	c	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
29	d	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
33	j	244/254 (96%)	226 (93%)	18 (7%)	0	100	100
34	k	384/387 (99%)	364 (95%)	20 (5%)	0	100	100
35	l	359/362 (99%)	329 (92%)	29 (8%)	1 (0%)	37	56
36	m	292/297 (98%)	277 (95%)	15 (5%)	0	100	100
37	n	163/176 (93%)	154 (94%)	9 (6%)	0	100	100
38	o	220/244 (90%)	207 (94%)	13 (6%)	0	100	100
39	p	231/256 (90%)	220 (95%)	11 (5%)	0	100	100
40	q	189/191 (99%)	174 (92%)	14 (7%)	1 (0%)	25	44
41	r	216/221 (98%)	206 (95%)	10 (5%)	0	100	100
42	s	167/174 (96%)	161 (96%)	5 (3%)	1 (1%)	22	39
43	t	191/199 (96%)	174 (91%)	16 (8%)	1 (0%)	25	44
44	u	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
45	a	842/1038 (81%)	825 (98%)	16 (2%)	1 (0%)	48	69
46	e	1519/1562 (97%)	1496 (98%)	21 (1%)	2 (0%)	48	69
47	g	223/245 (91%)	215 (96%)	8 (4%)	0	100	100
48	v	139/157 (88%)	139 (100%)	0	0	100	100
49	w	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
51	z	144/165 (87%)	135 (94%)	8 (6%)	1 (1%)	19	35
52	0	117/312 (38%)	116 (99%)	0	1 (1%)	14	28
All	All	9314/10279 (91%)	8951 (96%)	353 (4%)	10 (0%)	50	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	z	88	PRO
46	e	437	LYS
15	O	22	LYS
45	a	35	SER
46	e	855	PRO
35	l	4	PRO

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Mol	Chain	Res	Type
40	q	107	ASP
42	s	108	GLU
52	0	93	LEU
43	t	47	ALA

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	175/176 (99%)	175 (100%)	0	100	100
2	B	160/162 (99%)	160 (100%)	0	100	100
3	C	138/146 (94%)	137 (99%)	1 (1%)	81	93
4	D	150/151 (99%)	149 (99%)	1 (1%)	81	93
5	E	129/154 (84%)	129 (100%)	0	100	100
6	F	155/156 (99%)	155 (100%)	0	100	100
7	G	135/137 (98%)	134 (99%)	1 (1%)	81	93
8	H	87/107 (81%)	87 (100%)	0	100	100
9	I	104/105 (99%)	104 (100%)	0	100	100
10	J	54/129 (42%)	53 (98%)	1 (2%)	52	77
11	K	104/118 (88%)	104 (100%)	0	100	100
12	L	108/110 (98%)	108 (100%)	0	100	100
13	M	112/116 (97%)	112 (100%)	0	100	100
14	N	117/119 (98%)	117 (100%)	0	100	100
15	O	46/47 (98%)	45 (98%)	1 (2%)	47	73
16	P	81/88 (92%)	81 (100%)	0	100	100
17	Q	92/97 (95%)	92 (100%)	0	100	100
18	R	107/111 (96%)	107 (100%)	0	100	100
19	S	90/91 (99%)	90 (100%)	0	100	100
20	T	95/103 (92%)	94 (99%)	1 (1%)	70	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	U	104/105 (99%)	104 (100%)	0	100 100
22	V	80/82 (98%)	80 (100%)	0	100 100
23	W	67/71 (94%)	67 (100%)	0	100 100
24	X	68/69 (99%)	66 (97%)	2 (3%)	37 64
25	Y	45/46 (98%)	45 (100%)	0	100 100
26	Z	45/116 (39%)	45 (100%)	0	100 100
27	b	87/91 (96%)	87 (100%)	0	100 100
28	c	71/72 (99%)	71 (100%)	0	100 100
29	d	20/23 (87%)	20 (100%)	0	100 100
33	j	189/196 (96%)	189 (100%)	0	100 100
34	k	320/323 (99%)	318 (99%)	2 (1%)	84 94
35	l	288/289 (100%)	288 (100%)	0	100 100
36	m	241/245 (98%)	241 (100%)	0	100 100
37	n	139/155 (90%)	138 (99%)	1 (1%)	81 93
38	o	186/205 (91%)	186 (100%)	0	100 100
39	p	187/208 (90%)	187 (100%)	0	100 100
40	q	168/171 (98%)	168 (100%)	0	100 100
41	r	185/187 (99%)	183 (99%)	2 (1%)	70 87
42	s	145/150 (97%)	142 (98%)	3 (2%)	48 74
43	t	154/159 (97%)	154 (100%)	0	100 100
44	u	107/109 (98%)	107 (100%)	0	100 100
45	a	679/949 (72%)	674 (99%)	5 (1%)	81 93
46	e	1150/1451 (79%)	1091 (95%)	59 (5%)	20 40
47	g	180/211 (85%)	180 (100%)	0	100 100
48	v	119/132 (90%)	118 (99%)	1 (1%)	79 91
49	w	197/198 (100%)	196 (100%)	1 (0%)	86 95
51	z	1/136 (1%)	1 (100%)	0	100 100
52	0	105/254 (41%)	95 (90%)	10 (10%)	7 14
All	All	7566/8826 (86%)	7474 (99%)	92 (1%)	66 86

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	128	ARG
4	D	12	ARG
7	G	83	ARG
10	J	61	LYS
15	O	33	LYS
20	T	106	LYS
24	X	9	LYS
24	X	63	LYS
34	k	332	ARG
34	k	369	ARG
37	n	8	LYS
41	r	112	GLN
41	r	144	ASN
42	s	29	ARG
42	s	55	ARG
42	s	60	ARG
45	a	98	ASP
45	a	136	ARG
45	a	893	LYS
45	a	1017	THR
45	a	1018	ILE
46	e	8	THR
46	e	105	VAL
46	e	125	ILE
46	e	169	LEU
46	e	205	GLU
46	e	254	ASN
46	e	271	LEU
46	e	277	MET
46	e	299	THR
46	e	309	VAL
46	e	319	THR
46	e	327	THR
46	e	364	SER
46	e	394	SER
46	e	400	GLU
46	e	707	LYS
46	e	710	LYS
46	e	731	LEU
46	e	733	HIS
46	e	754	ILE
46	e	770	ILE
46	e	780	ILE

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Mol	Chain	Res	Type
46	e	797	LEU
46	e	799	THR
46	e	807	LYS
46	e	826	LEU
46	e	867	PHE
46	e	904	VAL
46	e	910	SER
46	e	924	VAL
46	e	933	LEU
46	e	978	THR
46	e	989	GLU
46	e	1032	LEU
46	e	1059	LEU
46	e	1102	CYS
46	e	1149	THR
46	e	1164	LEU
46	e	1175	PHE
46	e	1179	LEU
46	e	1189	ASN
46	e	1239	LYS
46	e	1269	LEU
46	e	1286	MET
46	e	1300	ILE
46	e	1303	MET
46	e	1341	LYS
46	e	1342	GLU
46	e	1367	THR
46	e	1379	LEU
46	e	1384	GLU
46	e	1400	PHE
46	e	1407	MET
46	e	1421	LEU
46	e	1428	VAL
46	e	1454	ILE
46	e	1464	ILE
46	e	1490	SER
46	e	1555	ARG
48	v	54	HIS
49	w	92	LYS
52	0	5	ARG
52	0	30	VAL
52	0	51	VAL

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Mol	Chain	Res	Type
52	0	52	LEU
52	0	67	LEU
52	0	76	LEU
52	0	80	VAL
52	0	93	LEU
52	0	95	GLU
52	0	189	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
45	a	121	ASN
46	e	160	ASN
46	e	189	ASN
46	e	226	ASN
46	e	233	ASN
46	e	251	ASN
46	e	805	ASN
46	e	902	ASN
46	e	1141	GLN
46	e	1288	GLN
46	e	1455	GLN
46	e	1457	ASN
46	e	1477	GLN
46	e	1499	HIS
46	e	1501	GLN
47	g	9	ASN
48	v	52	HIS
52	0	36	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	f	3211/3395 (94%)	591 (18%)	0
31	h	120/121 (99%)	12 (10%)	0
32	i	157/158 (99%)	32 (20%)	0
50	x	72/76 (94%)	19 (26%)	0
50	y	71/76 (93%)	20 (28%)	0
All	All	3631/3826 (94%)	674 (18%)	0

All (674) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	f	6	A
30	f	13	A
30	f	14	U
30	f	26	A
30	f	40	A
30	f	43	A
30	f	49	A
30	f	59	G
30	f	60	A
30	f	65	A
30	f	66	A
30	f	92	G
30	f	99	A
30	f	109	A
30	f	110	G
30	f	111	C
30	f	116	A
30	f	120	G
30	f	121	A
30	f	122	A
30	f	133	U
30	f	134	U
30	f	135	C
30	f	136	G
30	f	156	G
30	f	157	A
30	f	165	A
30	f	166	C
30	f	172	G
30	f	173	G
30	f	187	A
30	f	190	U
30	f	191	U
30	f	200	C
30	f	206	G
30	f	210	U
30	f	211	A
30	f	213	A
30	f	218	G
30	f	219	A
30	f	234	G
30	f	240	U

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Mol	Chain	Res	Type
30	f	241	G
30	f	242	C
30	f	243	G
30	f	245	U
30	f	249	U
30	f	252	U
30	f	269	G
30	f	283	G
30	f	286	U
30	f	295	A
30	f	305	U
30	f	323	A
30	f	329	U
30	f	339	C
30	f	350	C
30	f	374	A
30	f	376	G
30	f	398	A
30	f	399	A
30	f	401	U
30	f	402	A
30	f	403	C
30	f	421	G
30	f	422	A
30	f	439	C
30	f	440	A
30	f	441	U
30	f	442	G
30	f	443	G
30	f	445	G
30	f	446	U
30	f	447	U
30	f	448	U
30	f	450	G
30	f	487	U
30	f	488	U
30	f	489	U
30	f	490	C
30	f	494	G
30	f	518	G
30	f	520	U
30	f	521	A

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Mol	Chain	Res	Type
30	f	523	A
30	f	535	G
30	f	536	U
30	f	543	C
30	f	544	C
30	f	546	C
30	f	547	G
30	f	548	G
30	f	551	A
30	f	552	G
30	f	555	U
30	f	557	A
30	f	559	A
30	f	578	A
30	f	579	G
30	f	589	A
30	f	597	G
30	f	604	G
30	f	608	A
30	f	609	G
30	f	611	A
30	f	620	U
30	f	621	A
30	f	622	A
30	f	637	C
30	f	638	C
30	f	649	A
30	f	660	A
30	f	677	A
30	f	681	U
30	f	684	G
30	f	690	A
30	f	691	A
30	f	705	A
30	f	712	G
30	f	715	A
30	f	716	A
30	f	719	U
30	f	720	A
30	f	758	C
30	f	763	G
30	f	764	U

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Mol	Chain	Res	Type
30	f	765	C
30	f	766	U
30	f	767	U
30	f	776	U
30	f	777	U
30	f	780	A
30	f	781	G
30	f	785	G
30	f	786	A
30	f	806	A
30	f	817	A
30	f	830	A
30	f	846	A
30	f	849	C
30	f	850	U
30	f	861	C
30	f	874	U
30	f	879	U
30	f	896	A
30	f	907	G
30	f	908	G
30	f	914	A
30	f	916	G
30	f	917	A
30	f	920	A
30	f	921	A
30	f	924	G
30	f	925	A
30	f	937	G
30	f	944	C
30	f	959	C
30	f	960	U
30	f	981	U
30	f	982	C
30	f	991	G
30	f	994	G
30	f	1001	G
30	f	1002	A
30	f	1010	G
30	f	1015	U
30	f	1016	C
30	f	1017	C

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Mol	Chain	Res	Type
30	f	1018	G
30	f	1021	G
30	f	1024	G
30	f	1025	A
30	f	1028	U
30	f	1036	A
30	f	1041	U
30	f	1047	A
30	f	1049	C
30	f	1063	G
30	f	1064	A
30	f	1065	A
30	f	1072	G
30	f	1081	U
30	f	1087	G
30	f	1093	A
30	f	1094	U
30	f	1095	U
30	f	1097	G
30	f	1098	A
30	f	1103	A
30	f	1104	G
30	f	1117	G
30	f	1131	G
30	f	1144	U
30	f	1153	A
30	f	1159	A
30	f	1160	C
30	f	1177	G
30	f	1180	A
30	f	1181	U
30	f	1192	C
30	f	1193	A
30	f	1196	C
30	f	1197	A
30	f	1201	C
30	f	1202	A
30	f	1208	U
30	f	1217	A
30	f	1218	U
30	f	1219	C
30	f	1222	G

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Mol	Chain	Res	Type
30	f	1225	A
30	f	1227	C
30	f	1235	U
30	f	1236	G
30	f	1238	C
30	f	1241	U
30	f	1242	G
30	f	1244	A
30	f	1245	A
30	f	1251	A
30	f	1252	A
30	f	1254	C
30	f	1258	U
30	f	1259	A
30	f	1263	A
30	f	1264	G
30	f	1265	U
30	f	1269	U
30	f	1272	C
30	f	1277	C
30	f	1278	A
30	f	1279	C
30	f	1282	G
30	f	1285	G
30	f	1286	A
30	f	1287	A
30	f	1295	G
30	f	1307	G
30	f	1308	A
30	f	1309	U
30	f	1313	G
30	f	1330	A
30	f	1348	U
30	f	1349	G
30	f	1351	U
30	f	1352	A
30	f	1354	G
30	f	1355	A
30	f	1356	U
30	f	1357	G
30	f	1386	A
30	f	1392	G

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Mol	Chain	Res	Type
30	f	1399	A
30	f	1400	G
30	f	1419	A
30	f	1434	G
30	f	1437	C
30	f	1446	A
30	f	1450	G
30	f	1481	A
30	f	1482	A
30	f	1483	G
30	f	1487	G
30	f	1488	G
30	f	1502	C
30	f	1508	C
30	f	1536	G
30	f	1539	A
30	f	1555	U
30	f	1556	C
30	f	1557	A
30	f	1560	G
30	f	1562	C
30	f	1563	C
30	f	1566	A
30	f	1568	U
30	f	1569	U
30	f	1572	U
30	f	1573	G
30	f	1575	A
30	f	1576	G
30	f	1580	A
30	f	1581	C
30	f	1582	C
30	f	1583	A
30	f	1589	A
30	f	1590	G
30	f	1605	A
30	f	1607	U
30	f	1620	U
30	f	1629	U
30	f	1639	C
30	f	1642	A
30	f	1643	A

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Mol	Chain	Res	Type
30	f	1645	U
30	f	1657	C
30	f	1683	A
30	f	1716	U
30	f	1717	U
30	f	1724	U
30	f	1725	C
30	f	1736	G
30	f	1741	A
30	f	1750	A
30	f	1751	G
30	f	1760	A
30	f	1761	C
30	f	1764	U
30	f	1765	U
30	f	1766	G
30	f	1770	G
30	f	1775	G
30	f	1780	G
30	f	1797	A
30	f	1814	A
30	f	1816	A
30	f	1819	U
30	f	1820	U
30	f	1821	U
30	f	1835	A
30	f	1839	A
30	f	1840	U
30	f	1841	A
30	f	1842	A
30	f	1846	C
30	f	1849	C
30	f	1850	A
30	f	1866	C
30	f	1867	A
30	f	1880	U
30	f	1881	A
30	f	1893	A
30	f	1906	G
30	f	1943	C
30	f	1952	G
30	f	1953	G

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Mol	Chain	Res	Type
30	f	1954	G
30	f	2094	C
30	f	2101	C
30	f	2102	U
30	f	2111	G
30	f	2112	U
30	f	2113	A
30	f	2114	C
30	f	2121	G
30	f	2122	G
30	f	2131	A
30	f	2134	G
30	f	2140	U
30	f	2144	A
30	f	2158	A
30	f	2160	G
30	f	2169	G
30	f	2176	U
30	f	2201	G
30	f	2206	G
30	f	2207	A
30	f	2208	A
30	f	2209	U
30	f	2222	A
30	f	2223	A
30	f	2225	U
30	f	2228	A
30	f	2249	G
30	f	2270	A
30	f	2272	G
30	f	2273	G
30	f	2274	U
30	f	2281	A
30	f	2282	U
30	f	2288	G
30	f	2307	G
30	f	2308	C
30	f	2310	U
30	f	2313	A
30	f	2314	U
30	f	2315	G
30	f	2334	U

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Mol	Chain	Res	Type
30	f	2335	G
30	f	2336	U
30	f	2373	A
30	f	2374	C
30	f	2375	G
30	f	2385	G
30	f	2388	U
30	f	2393	G
30	f	2397	A
30	f	2402	A
30	f	2403	G
30	f	2404	A
30	f	2411	U
30	f	2419	A
30	f	2437	G
30	f	2446	U
30	f	2447	A
30	f	2450	G
30	f	2461	A
30	f	2463	G
30	f	2464	U
30	f	2468	A
30	f	2469	G
30	f	2470	C
30	f	2471	U
30	f	2472	U
30	f	2474	G
30	f	2479	C
30	f	2480	A
30	f	2484	A
30	f	2486	A
30	f	2487	U
30	f	2488	A
30	f	2494	A
30	f	2495	C
30	f	2496	C
30	f	2499	U
30	f	2501	U
30	f	2502	A
30	f	2503	G
30	f	2505	U
30	f	2514	U

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Mol	Chain	Res	Type
30	f	2515	A
30	f	2522	G
30	f	2526	C
30	f	2531	C
30	f	2537	U
30	f	2538	U
30	f	2539	C
30	f	2540	A
30	f	2541	U
30	f	2542	U
30	f	2544	U
30	f	2547	A
30	f	2548	C
30	f	2549	G
30	f	2552	C
30	f	2554	A
30	f	2555	G
30	f	2561	A
30	f	2569	A
30	f	2570	U
30	f	2571	U
30	f	2572	C
30	f	2573	G
30	f	2581	U
30	f	2585	G
30	f	2593	A
30	f	2594	C
30	f	2606	G
30	f	2607	G
30	f	2614	G
30	f	2648	G
30	f	2651	G
30	f	2652	U
30	f	2656	A
30	f	2674	A
30	f	2677	G
30	f	2678	A
30	f	2689	A
30	f	2691	A
30	f	2694	A
30	f	2696	A
30	f	2704	A

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Mol	Chain	Res	Type
30	f	2714	G
30	f	2719	U
30	f	2728	G
30	f	2729	U
30	f	2740	A
30	f	2752	U
30	f	2753	G
30	f	2755	C
30	f	2772	C
30	f	2773	C
30	f	2777	G
30	f	2778	G
30	f	2788	C
30	f	2796	G
30	f	2800	G
30	f	2801	A
30	f	2803	A
30	f	2810	C
30	f	2814	G
30	f	2817	A
30	f	2818	U
30	f	2821	C
30	f	2834	G
30	f	2842	U
30	f	2844	C
30	f	2845	A
30	f	2849	C
30	f	2860	U
30	f	2867	C
30	f	2871	G
30	f	2872	A
30	f	2876	C
30	f	2887	A
30	f	2898	G
30	f	2899	C
30	f	2911	A
30	f	2914	G
30	f	2923	U
30	f	2935	U
30	f	2936	A
30	f	2941	A
30	f	2942	C

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Mol	Chain	Res	Type
30	f	2947	G
30	f	2971	A
30	f	2983	C
30	f	2990	G
30	f	2992	U
30	f	2996	U
30	f	2997	G
30	f	3006	A
30	f	3012	A
30	f	3056	U
30	f	3059	G
30	f	3078	U
30	f	3079	U
30	f	3080	G
30	f	3086	A
30	f	3092	C
30	f	3104	U
30	f	3113	A
30	f	3122	A
30	f	3130	A
30	f	3131	U
30	f	3142	A
30	f	3143	C
30	f	3151	U
30	f	3154	C
30	f	3155	U
30	f	3156	U
30	f	3157	U
30	f	3165	A
30	f	3170	A
30	f	3173	G
30	f	3174	A
30	f	3175	U
30	f	3176	G
30	f	3179	U
30	f	3181	C
30	f	3186	A
30	f	3187	A
30	f	3196	U
30	f	3207	U
30	f	3209	A
30	f	3217	C

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Mol	Chain	Res	Type
30	f	3218	A
30	f	3219	G
30	f	3228	C
30	f	3229	G
30	f	3243	A
30	f	3245	A
30	f	3247	G
30	f	3259	U
30	f	3263	G
30	f	3269	U
30	f	3270	U
30	f	3273	A
30	f	3276	G
30	f	3281	U
30	f	3287	U
30	f	3288	G
30	f	3289	G
30	f	3294	A
30	f	3295	A
30	f	3303	G
30	f	3304	U
30	f	3307	A
30	f	3313	U
30	f	3316	A
30	f	3317	U
30	f	3318	G
30	f	3319	U
30	f	3320	A
30	f	3341	U
30	f	3342	A
30	f	3345	G
30	f	3351	U
30	f	3352	U
30	f	3353	G
30	f	3354	U
30	f	3355	U
30	f	3369	G
30	f	3375	A
30	f	3378	C
30	f	3382	U
30	f	3383	G
30	f	3386	G

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Mol	Chain	Res	Type
30	f	3389	U
30	f	3390	G
30	f	3396	U
31	h	7	G
31	h	29	C
31	h	53	U
31	h	54	U
31	h	55	A
31	h	65	G
31	h	73	C
31	h	74	C
31	h	95	A
31	h	102	A
31	h	112	G
31	h	121	U
32	i	23	U
32	i	34	U
32	i	35	C
32	i	39	G
32	i	48	A
32	i	52	A
32	i	53	A
32	i	59	A
32	i	62	C
32	i	63	G
32	i	80	A
32	i	81	U
32	i	82	U
32	i	83	C
32	i	84	C
32	i	85	G
32	i	86	U
32	i	87	G
32	i	90	U
32	i	95	G
32	i	104	A
32	i	105	A
32	i	106	C
32	i	111	A
32	i	113	U
32	i	125	U
32	i	126	A

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Mol	Chain	Res	Type
32	i	138	A
32	i	151	C
32	i	152	G
32	i	157	U
32	i	158	U
50	x	5	G
50	x	9	G
50	x	15	G
50	x	16	U
50	x	17	C
50	x	18	G
50	x	22	G
50	x	28	U
50	x	35	G
50	x	37	A
50	x	38	U
50	x	39	G
50	x	46	G
50	x	48	C
50	x	56	C
50	x	57	G
50	x	58	A
50	x	60	U
50	x	74	C
50	y	7	G
50	y	9	G
50	y	13	U
50	y	17	C
50	y	23	C
50	y	26	G
50	y	34	I
50	y	35	G
50	y	36	C
50	y	38	U
50	y	43	G
50	y	45	G
50	y	46	G
50	y	47	U
50	y	48	C
50	y	56	C
50	y	58	A
50	y	61	C

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Mol	Chain	Res	Type
50	y	75	C
50	y	76	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
48	5CT	v	51	48	13,14,15	0.76	0	9,15,17	1.29	1 (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
48	5CT	v	51	48	-	9/13/14/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	v	51	5CT	C4-C3-C2	-2.20	108.84	113.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	v	51	5CT	NZ-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
48	v	51	5CT	O1-C2-C3-C4
48	v	51	5CT	C2-C3-C4-N1
48	v	51	5CT	C-CA-CB-CG
48	v	51	5CT	N-CA-CB-CG
48	v	51	5CT	NZ-C1-C2-O1
48	v	51	5CT	C1-C2-C3-C4
48	v	51	5CT	CE-CD-CG-CB
48	v	51	5CT	C2-C1-NZ-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 20 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	SPD	f	3401	-	9,9,9	0.32	0	8,8,8	0.86	0

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
56	SPD	f	3401	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	f	3401	SPD	C3-C4-C5-N6
56	f	3401	SPD	N6-C7-C8-C9
56	f	3401	SPD	C2-C3-C4-C5
56	f	3401	SPD	C8-C7-N6-C5
56	f	3401	SPD	C4-C5-N6-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

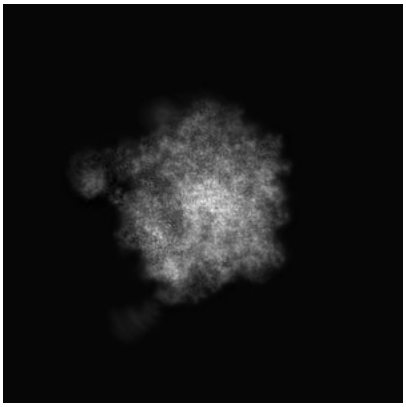
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15296. These allow visual inspection of the internal detail of the map and identification of artifacts.

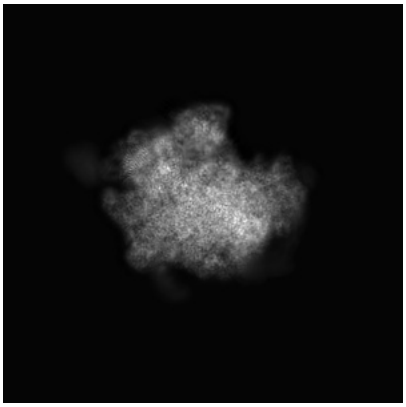
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

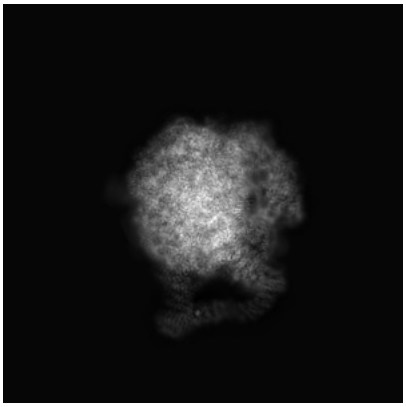
6.1.1 Primary map



X



Y

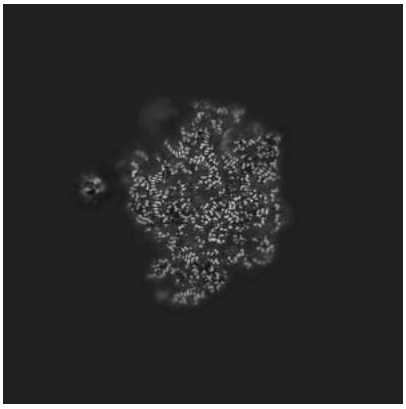


Z

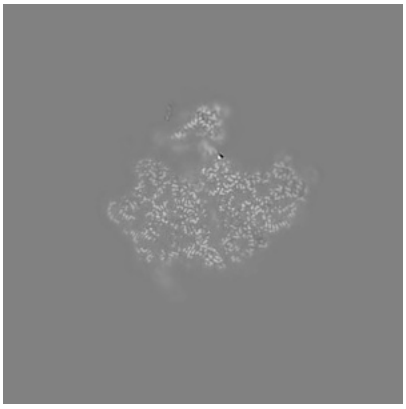
The images above show the map projected in three orthogonal directions.

6.2 Central slices

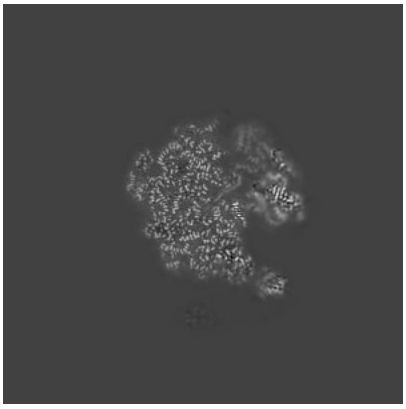
6.2.1 Primary map



X Index: 225



Y Index: 225

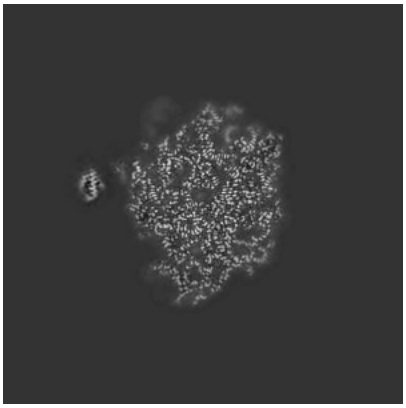


Z Index: 225

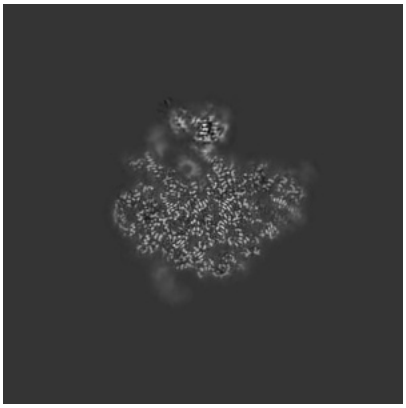
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

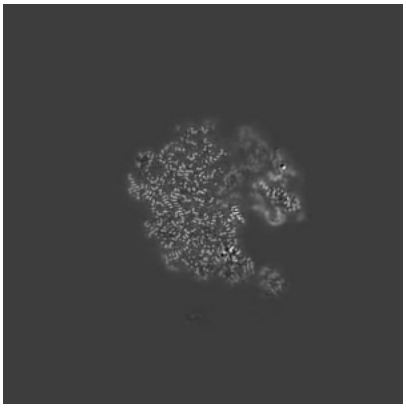
6.3.1 Primary map



X Index: 219



Y Index: 237

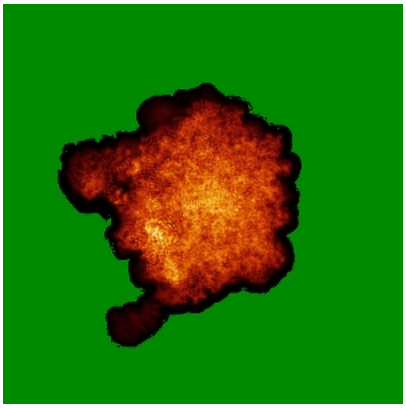


Z Index: 222

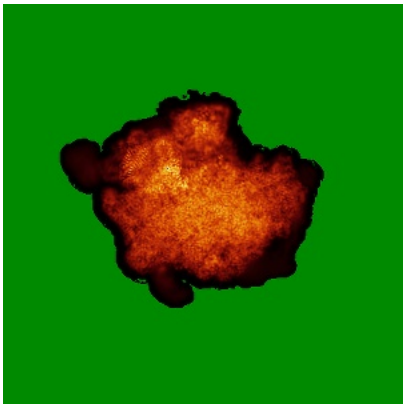
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

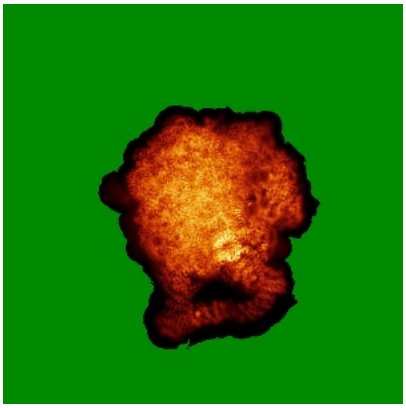
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

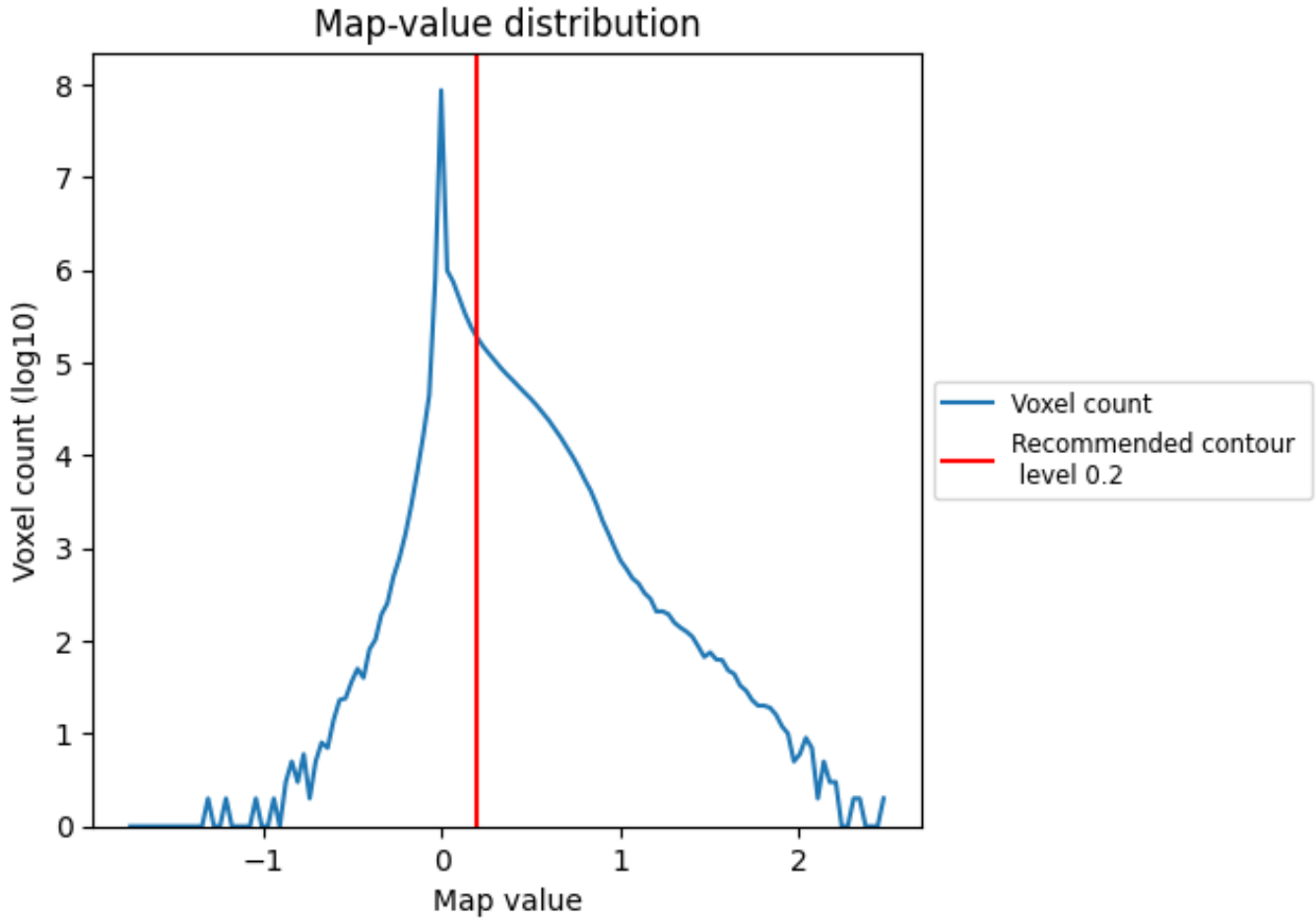
6.6 Mask visualisation (i)

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

7 Map analysis

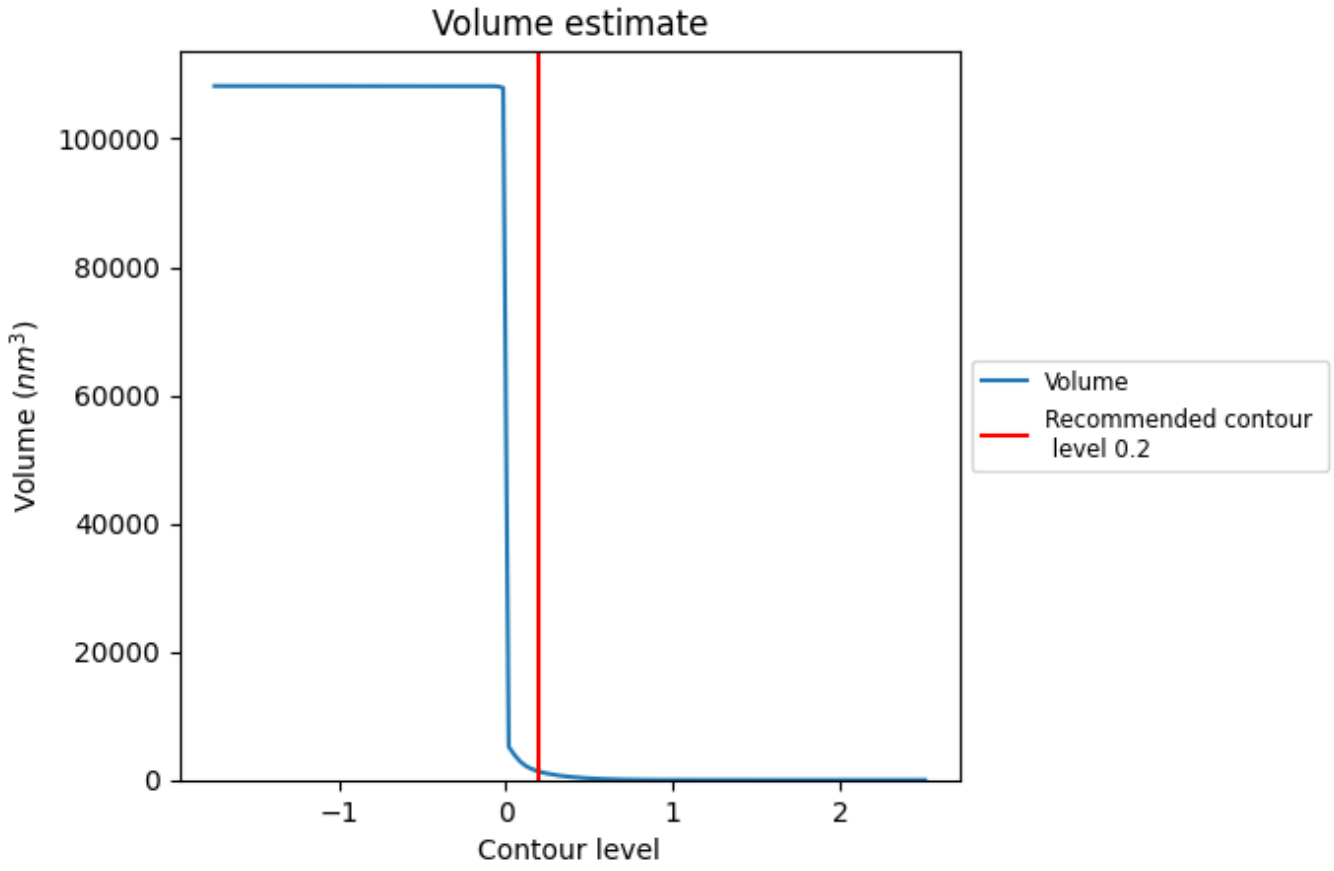
This section contains the results of statistical analysis of the map.

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.

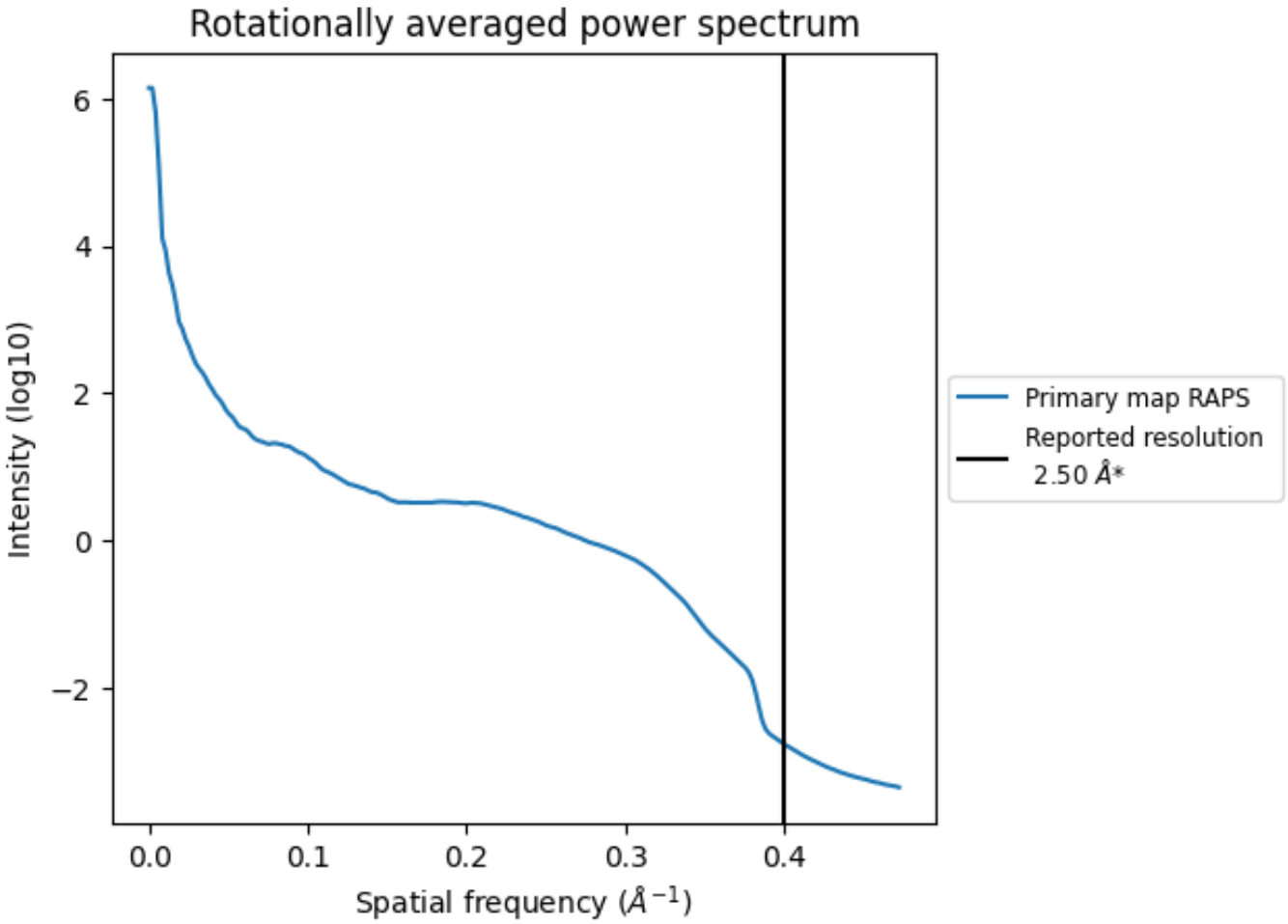
7.2 Volume estimate



The volume at the recommended contour level is 1316 nm^3; this corresponds to an approximate mass of 1189 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)

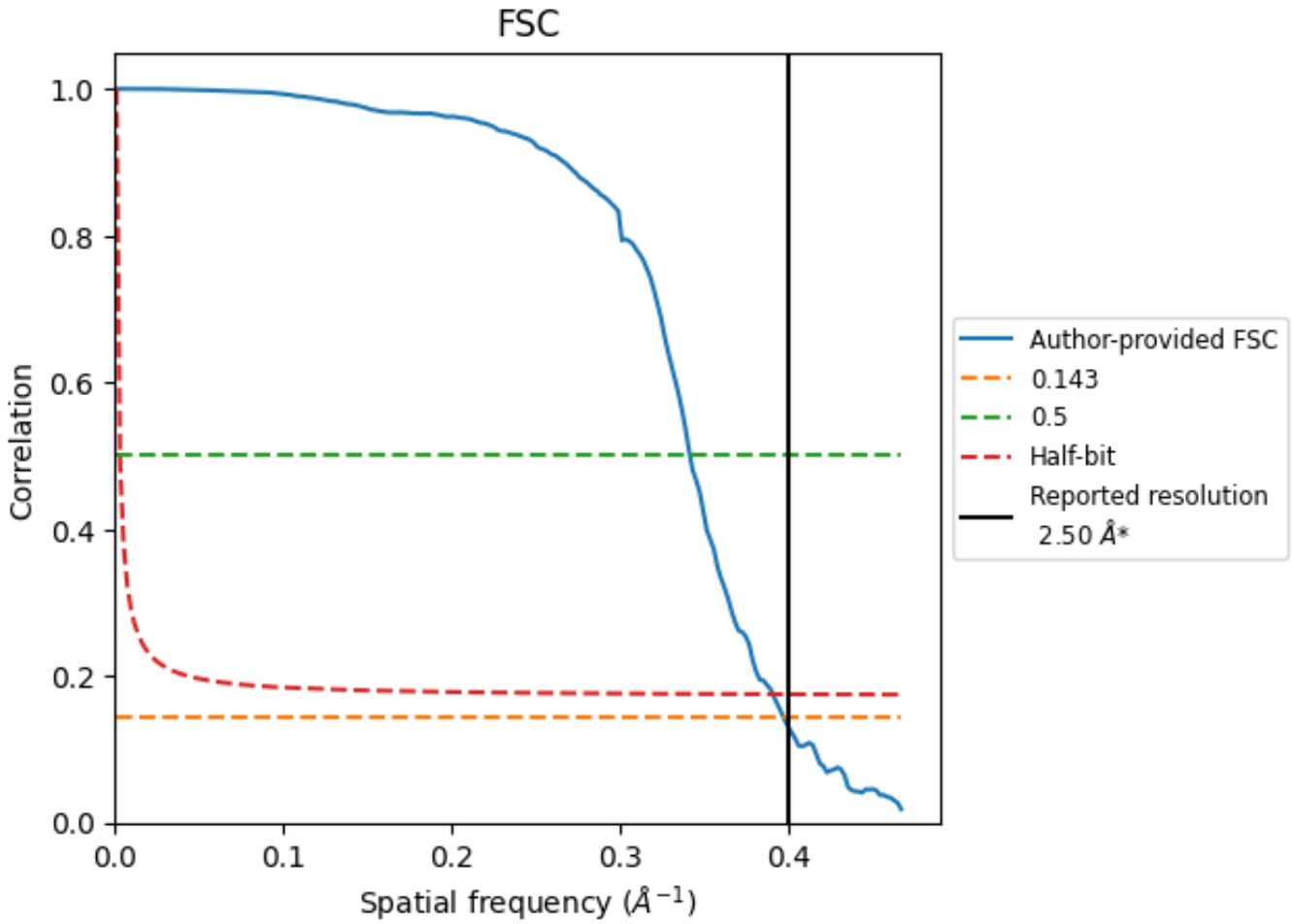


*Reported resolution corresponds to spatial frequency of 0.400 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

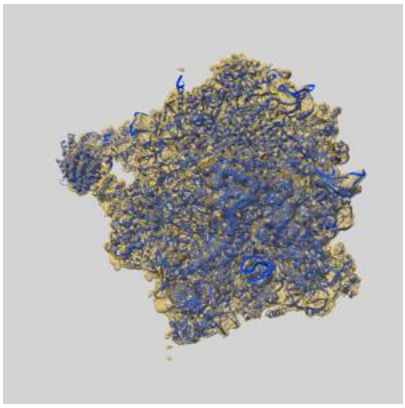
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.52	2.93	2.56
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

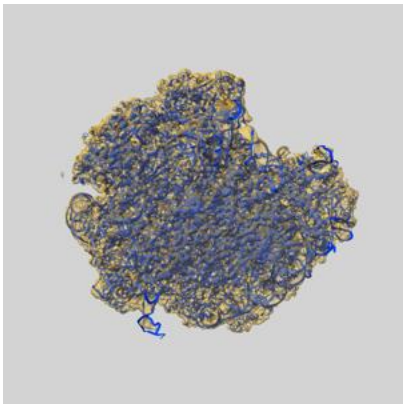
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15296 and PDB model 8AAF. Per-residue inclusion information can be found in section 3 on page 15.

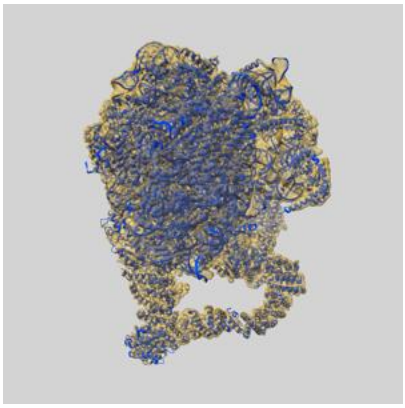
9.1 Map-model overlay



X



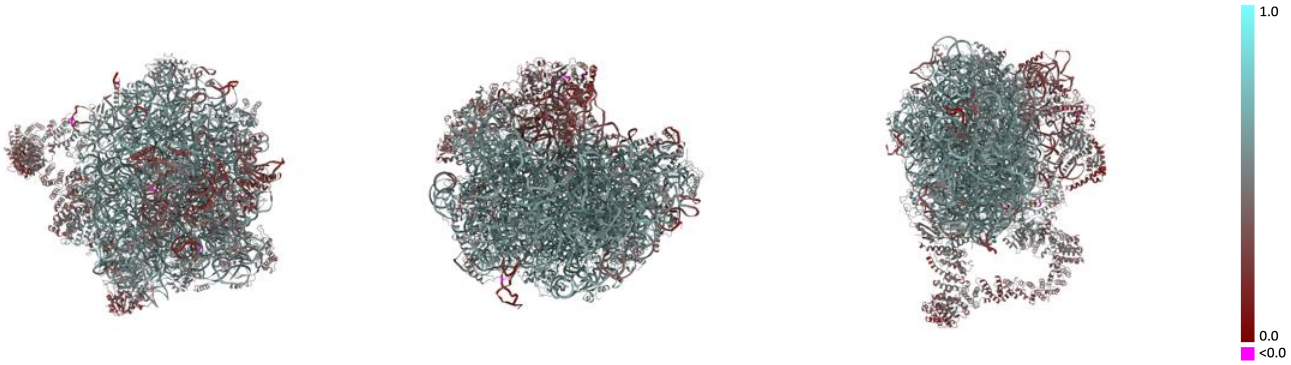
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

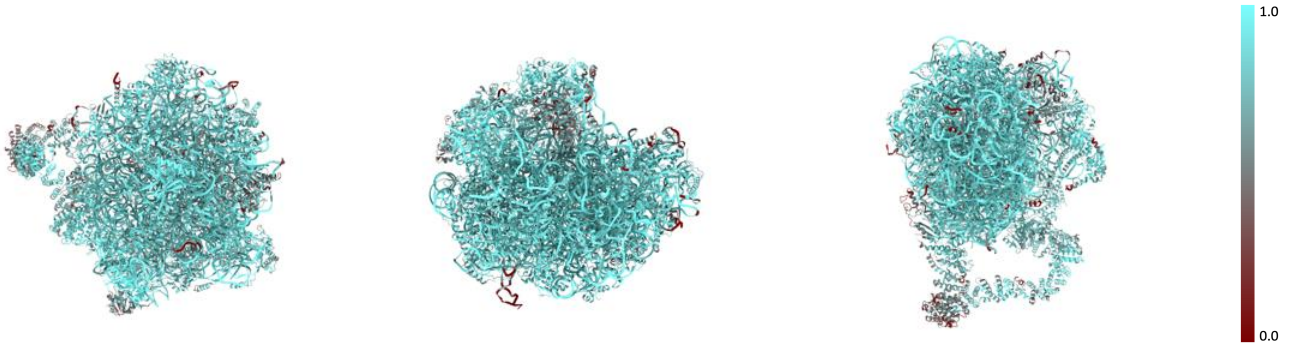
9.2 Q-score mapped to coordinate model (i)



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.

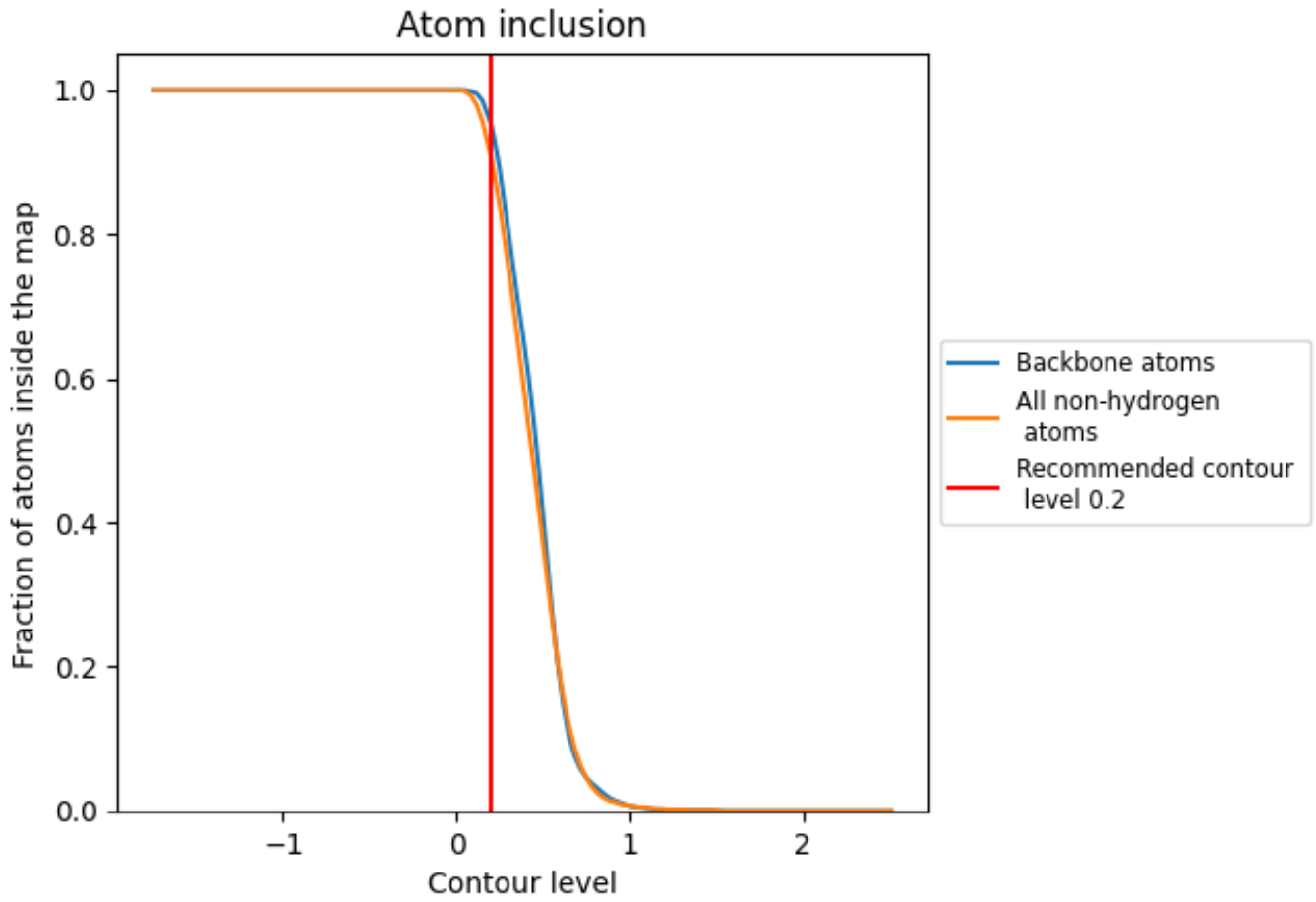
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.5360
0	0.5990	0.3310
1	0.7000	0.3950
A	0.9700	0.6130
B	0.9410	0.5890
C	0.9200	0.5910
D	0.9420	0.5890
E	0.8750	0.5540
F	0.9200	0.5820
G	0.9000	0.5640
H	0.7980	0.4780
I	0.9420	0.5450
J	0.9220	0.5820
K	0.9020	0.5750
L	0.9030	0.5720
M	0.8480	0.5270
N	0.9360	0.5970
O	0.8890	0.5430
P	0.8330	0.5210
Q	0.8570	0.5540
R	0.9350	0.6020
S	0.9670	0.6220
T	0.9090	0.5770
U	0.8930	0.5570
V	0.8650	0.5320
W	0.9900	0.6270
X	0.7830	0.5030
Y	0.9490	0.6030
Z	0.9570	0.5900
a	0.8480	0.3780
b	0.8880	0.5770
c	0.9030	0.5720
d	0.4150	0.4170
e	0.6940	0.3990
f	0.9660	0.5740

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Chain	Atom inclusion	Q-score
g	0.7960	0.4720
h	0.9920	0.5690
i	0.9820	0.5990
j	0.9460	0.6050
k	0.9370	0.5860
l	0.9190	0.5780
m	0.8340	0.4920
n	0.8520	0.5300
o	0.9180	0.5720
p	0.8460	0.5240
q	0.9240	0.5700
r	0.8820	0.5470
s	0.8060	0.4560
t	0.9040	0.5620
u	0.8960	0.5500
v	0.6300	0.4210
w	0.4840	0.2890
x	0.9730	0.3510
y	0.8980	0.2690
z	0.8840	0.4150