



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:29 AM UTC

PDB ID : 7MSC / pdb_00007msc
EMDB ID : EMD-23961
Title : Mtb 70SIC in complex with MtbEttA at Pre_R0 state
Authors : Cui, Z.; Zhang, J.
Deposited on : 2021-05-11
Resolution : 2.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

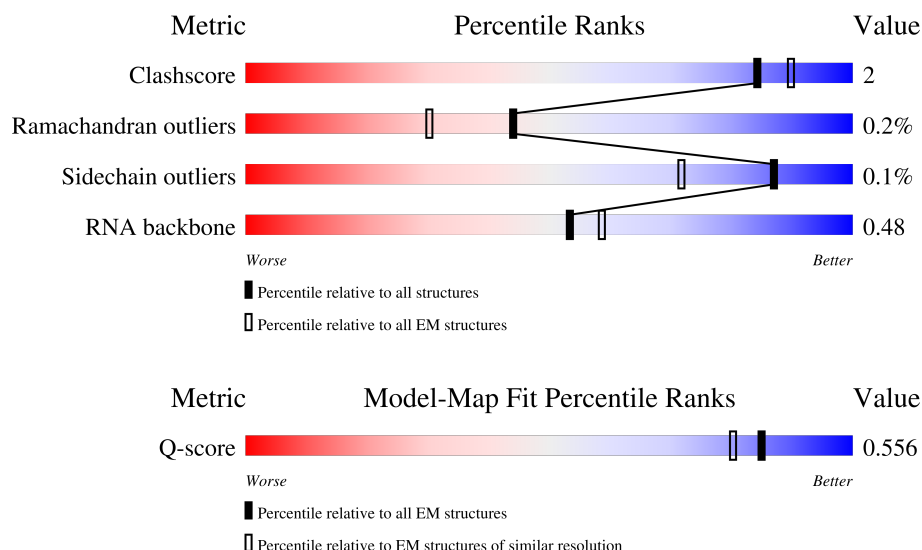
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



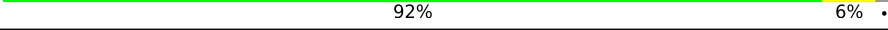
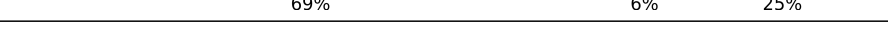
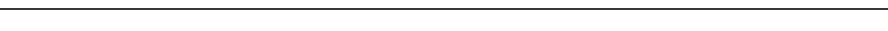
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13205 (2.47 - 3.47)

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

Mol	Chain	Length	Quality of chain
1	0	57	 95% 5%
2	1	55	 80% 9% 11%
3	2	47	 91% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	64	
5	4	37	
6	6	80	
7	7	24	
8	8	235	
9	A	3138	
10	B	115	
11	C	280	
12	D	217	
13	E	223	
14	F	187	
15	G	179	
16	H	152	
17	J	195	
18	K	122	
19	L	146	
20	M	138	
21	N	180	
22	O	122	
23	P	113	
24	Q	129	
25	R	104	
26	S	197	
27	T	100	
28	U	105	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	V	215	
30	W	86	
31	X	64	
32	Y	77	
33	Z	65	
34	a	1537	
35	c	274	
36	d	201	
37	e	220	
38	f	96	
39	g	156	
40	h	132	
41	i	151	
42	j	101	
43	k	139	
44	l	124	
45	m	124	
46	n	61	
47	o	89	
48	p	162	
49	q	135	
50	r	84	
51	s	93	
52	t	86	
53	x	558	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	y	77	5% 61% 36%
55	z	26	12% 12% 73%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 152447 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 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	54	Total	C	N	O	0	0
			429	266	94	69		

- Molecule 2 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	49	Total	C	N	O	S	0	0
			411	251	88	68	4		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	44	Total	C	N	O	S	0	0
			374	222	97	54	1		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	62	Total	C	N	O	0	0
			494	298	112	84		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			299	182	66	47	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	VAL	MET	conflict	UNP P9WH89

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	60	Total	C	N	O	S	0	0
			470	291	89	85	5		

- Molecule 7 is a protein called 50S ribosomal protein L37.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	7	22	Total	C	N	O	0	0
			186	111	47	28		

- Molecule 8 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	230	Total	C	N	O	S	0	0
			1704	1068	310	323	3		

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	3118	Total	C	N	O	P	0	0
			66958	29847	12340	21653	3118		

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	115	Total	C	N	O	P	0	0
			2458	1097	456	790	115		

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	272	Total	C	N	O	S	0	0
			2088	1277	437	369	5		

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	213	Total	C	N	O	S	0	0
			1590	985	307	292	6		

- Molecule 13 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	207	Total	C	N	O	S	0	0
			1552	958	303	289	2		

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	178	Total	C	N	O	S	0	0
			1408	885	267	251	5		

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	174	Total	C	N	O	S	0	0
			1330	836	249	244	1		

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	47	Total	C	N	O	S	0	0
			350	220	64	65	1		

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	146	Total	C	N	O	S	0	0
			1143	724	217	199	3		

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	122	Total	C	N	O	S	0	0
			941	590	180	169	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	VAL	MET	conflict	UNP A0A045HTP7

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	144	Total	C	N	O	S	0	0
			1075	666	217	190	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	134	Total	C	N	O	S	0	0
			1072	679	215	177	1		

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	116	Total	C	N	O	S	0	0
			908	574	175	158	1		

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	119	Total	C	N	O		0	0
			905	552	191	162			

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	112	Total	C	N	O	S	0	0
			907	573	174	159	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	124	Total	C	N	O		0	0
			993	616	207	170			

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	100	Total	C	N	O		0	0
			757	482	138	137			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	insertion	UNP P9WHC3

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	S	113	Total	C	N	O	0	0
			860	533	178	149		

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	T	95	Total	C	N	O	0	0
			741	469	138	134		

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	90	Total	C	N	O	S	0	0
			699	430	138	129	2		

- Molecule 29 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	V	177	Total	C	N	O	0	0
			1319	822	243	254		

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	W	76	Total	C	N	O	0	0
			560	343	116	101		

- Molecule 31 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	62	Total	C	N	O	S	0	0
			468	284	100	80	4		

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	68	Total	C	N	O	S	0	0
			560	343	109	107	1		

- Molecule 33 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	59	Total	C	N	O		0	0
			476	293	101	82			

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1519	Total	C	N	O	P	0	0
			32620	14535	5961	10605	1519		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	207	Total	C	N	O	S	0	0
			1654	1030	322	298	4		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	200	Total	C	N	O	S	0	0
			1650	1036	316	296	2		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	169	Total	C	N	O	S	0	0
			1222	770	231	218	3		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	95	Total	C	N	O	S	0	0
			757	480	133	141	3		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	155	Total	C	N	O	S	0	0
			1230	768	241	219	2		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	131	Total	C	N	O	S	0	0
			1006	631	188	186	1		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	127	Total	C	N	O	S	0	0
			992	628	195	169			

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	99	Total	C	N	O	S	0	0
			789	496	146	144	3		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	117	Total	C	N	O	S	0	0
			873	540	175	158			

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	122	Total	C	N	O	S	0	0
			959	594	197	166	2		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	116	Total	C	N	O	S	0	0
			945	578	196	168	3		

- Molecule 46 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	60	Total	C	N	O	S	0	0
			468	294	96	73	5		

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	87	Total	C	N	O		0	0
			718	449	144	125			

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	113	Total	C	N	O		0	0
			884	564	166	154			

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	95	Total	C	N	O	S	0	0
			770	482	152	133	3		

- Molecule 50 is a protein called 30S ribosomal protein S18 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	64	Total	C	N	O	S	0	0
			506	315	98	90	3		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	83	Total	C	N	O	S	0	0
			672	432	125	114	1		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	85	Total	C	N	O		0	0
			652	394	141	117			

- Molecule 53 is a protein called Energy-dependent translational throttle protein EttA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	547	Total	C	N	O	S	0	0
			4279	2693	748	826	12		

- Molecule 54 is a RNA chain called initiator tRNA (Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	77	Total	C	N	O	P	0	0
			1644	732	297	538	77		

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	7	Total	C	N	O	P	0	0
			149	67	27	48	7		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	1	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	
56	6	1	Total	Zn	0
			1	1	
56	X	1	Total	Zn	0
			1	1	
56	n	1	Total	Zn	0
			1	1	
56	r	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

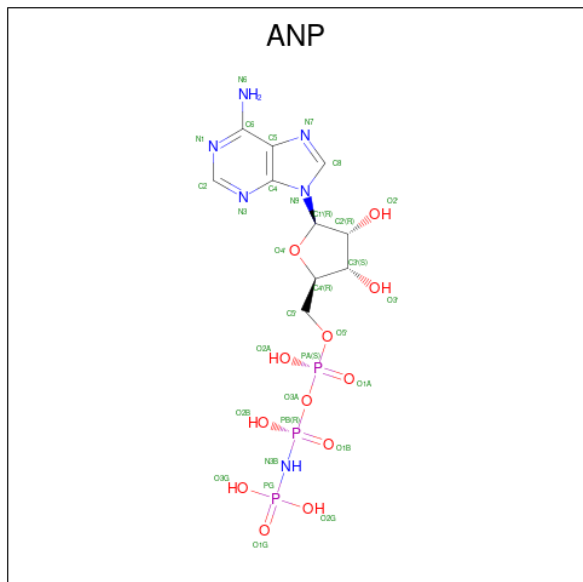
Mol	Chain	Residues	Atoms		AltConf
57	A	301	Total	Mg	0
			301	301	
57	B	5	Total	Mg	0
			5	5	
57	C	2	Total	Mg	0
			2	2	
57	D	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

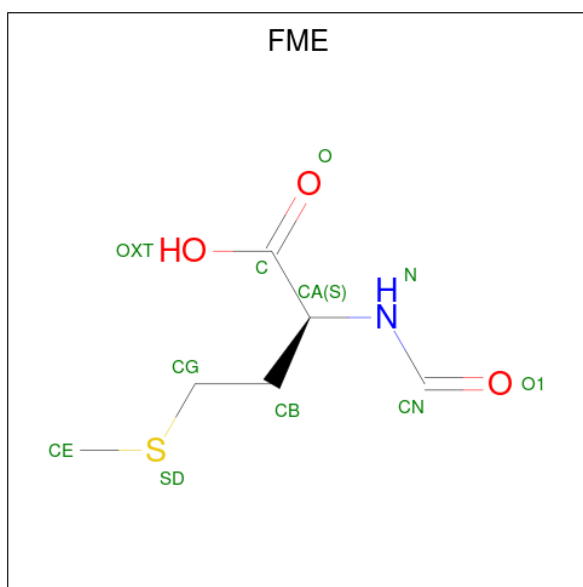
Mol	Chain	Residues	Atoms		AltConf
57	L	1	Total	Mg	0
			1	1	
57	a	130	Total	Mg	0
			130	130	
57	r	1	Total	Mg	0
			1	1	
57	x	2	Total	Mg	0
			2	2	
57	y	2	Total	Mg	0
			2	2	

- Molecule 58 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
58	x	1	Total	C	N	O	P	0
			31	10	6	12	3	
58	x	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).

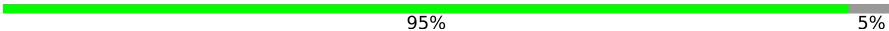


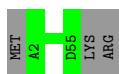
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
59	y	1	10	6	1	2	1	0

3 Residue-property plots

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

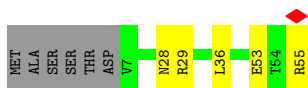
- Molecule 1: 50S ribosomal protein L32

Chain 0: 



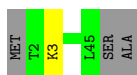
- Molecule 2: 50S ribosomal protein L33 2

Chain 1: 



- Molecule 3: 50S ribosomal protein L34

Chain 2: 



- Molecule 4: 50S ribosomal protein L35

Chain 3: 

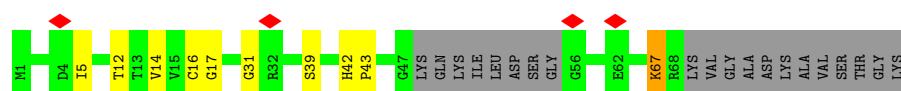


- Molecule 5: 50S ribosomal protein L36

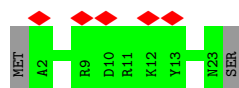
Chain 4: 



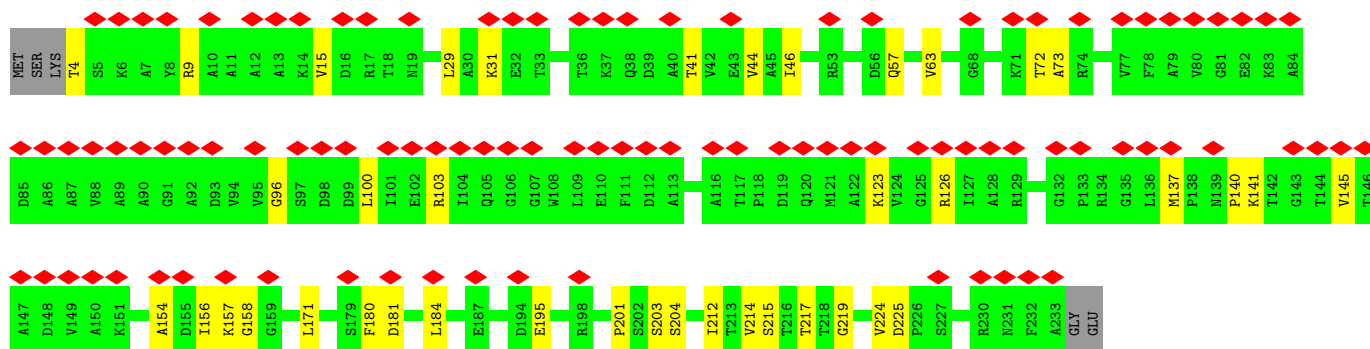
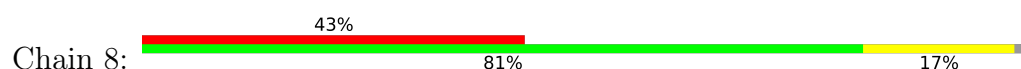
- Molecule 6: 50S ribosomal protein L31



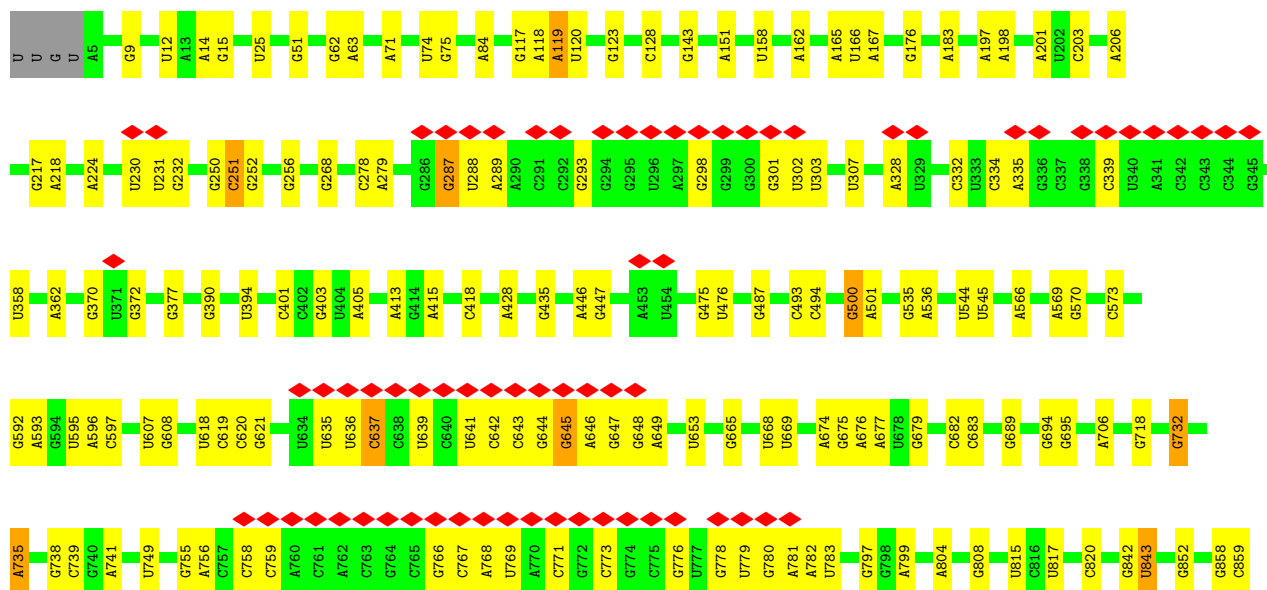
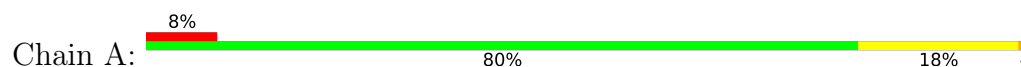
• Molecule 7: 50S ribosomal protein L37



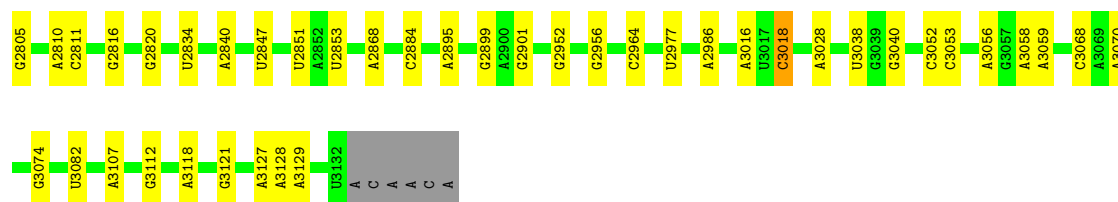
• Molecule 8: 50S ribosomal protein L1



• Molecule 9: 23S rRNA







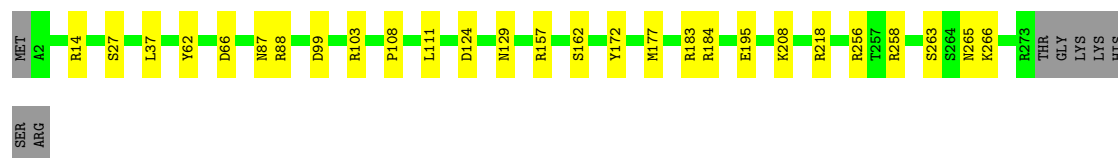
• Molecule 10: 5S rRNA

Chain B: 79% 19%



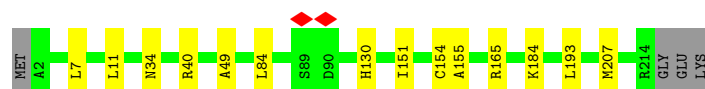
• Molecule 11: 50S ribosomal protein L2

Chain C: 88% 10%



• Molecule 12: 50S ribosomal protein L3

Chain D: 92% 6%



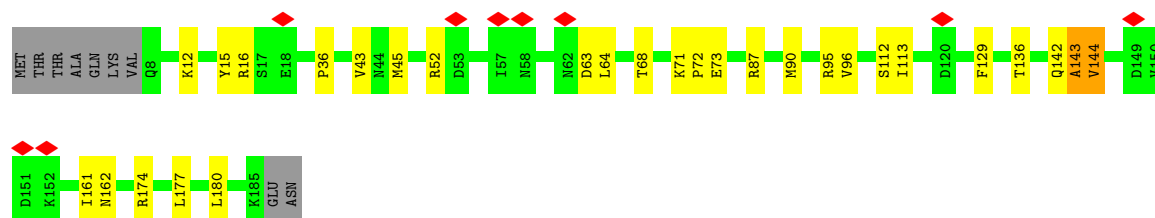
• Molecule 13: 50S ribosomal protein L4

Chain E: 89% 7%

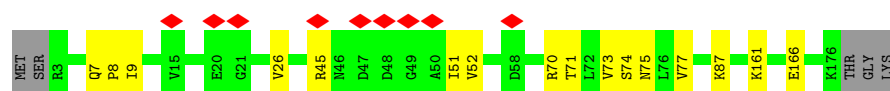
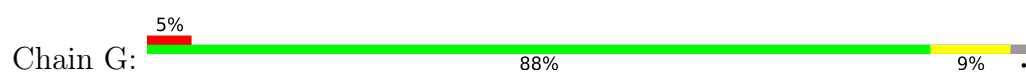


• Molecule 14: 50S ribosomal protein L5

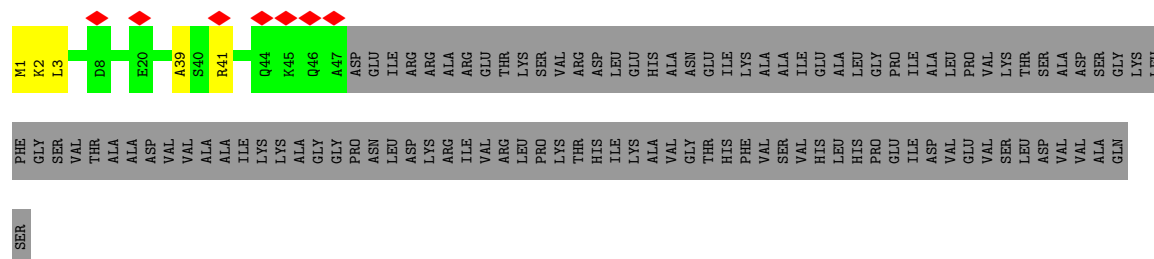
Chain F: 80% 14% 5%



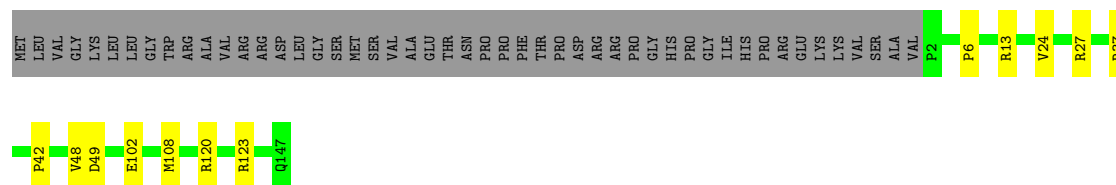
• Molecule 15: 50S ribosomal protein L6



- Molecule 16: 50S ribosomal protein L9



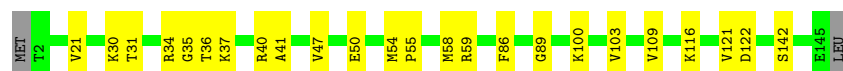
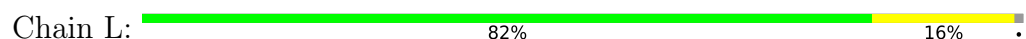
- Molecule 17: 50S ribosomal protein L13



- Molecule 18: 50S ribosomal protein L14



- Molecule 19: 50S ribosomal protein L15

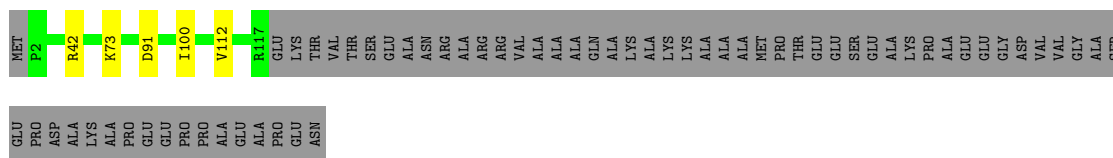


- Molecule 20: 50S ribosomal protein L16



- Molecule 21: 50S ribosomal protein L17

Chain N:  62% 36%



- Molecule 22: 50S ribosomal protein L18

Chain O:  84% 14%



- Molecule 23: 50S ribosomal protein L19

Chain P:  90% 9%



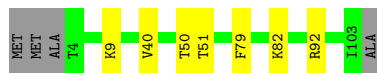
- Molecule 24: 50S ribosomal protein L20

Chain Q:  86% 10%



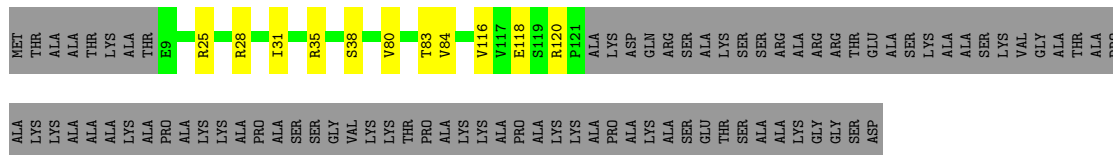
- Molecule 25: 50S ribosomal protein L21

Chain R:  89% 7%



- Molecule 26: 50S ribosomal protein L22

Chain S:  52% 6% 43%

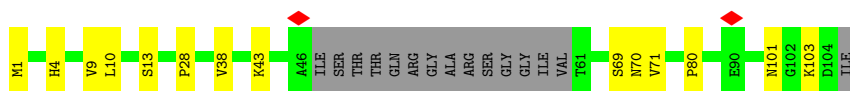


- Molecule 27: 50S ribosomal protein L23

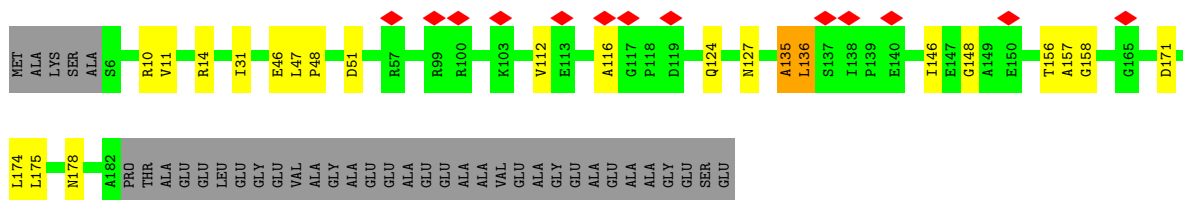
Chain T:  88% 7% 5%



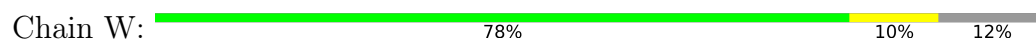
- Molecule 28: 50S ribosomal protein L24



- Molecule 29: 50S ribosomal protein L25



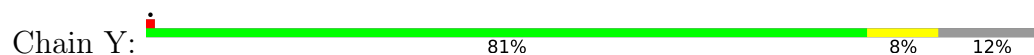
- Molecule 30: 50S ribosomal protein L27



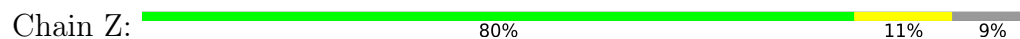
- Molecule 31: 50S ribosomal protein L28



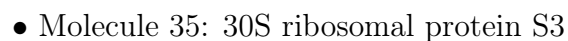
- Molecule 32: 50S ribosomal protein L29



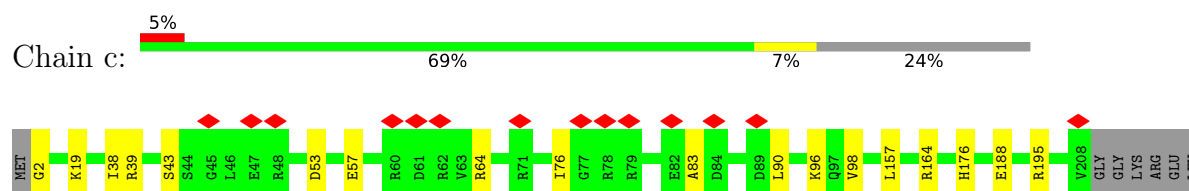
- Molecule 33: 50S ribosomal protein L30



Chain a:

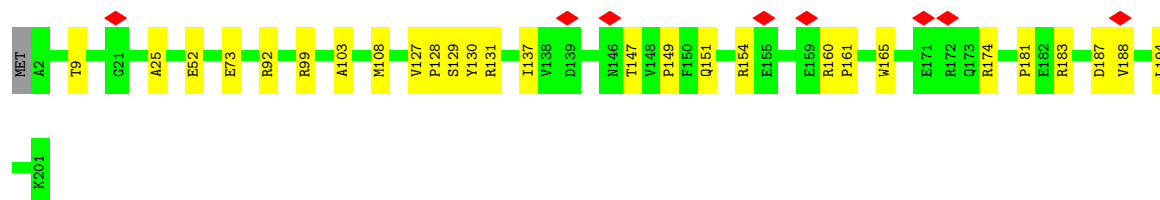


Chain c:



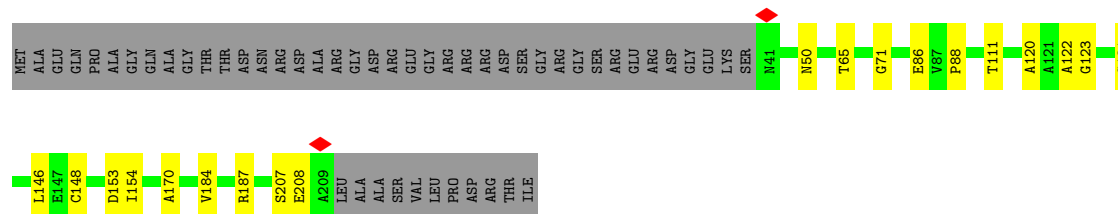
- Molecule 36: 30S ribosomal protein S4

Chain d:



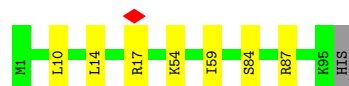
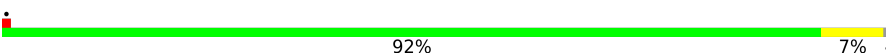
- Molecule 37: 30S ribosomal protein S5

Chain e:



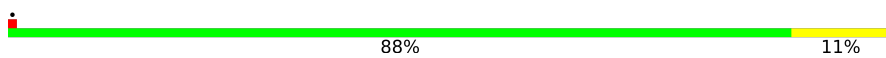
- Molecule 38: 30S ribosomal protein S6

Chain f:



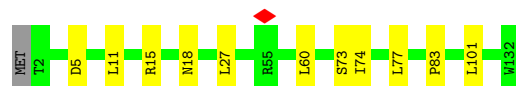
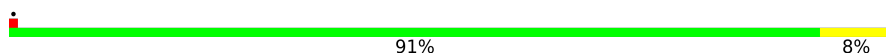
- Molecule 39: 30S ribosomal protein S7

Chain g:



- Molecule 40: 30S ribosomal protein S8

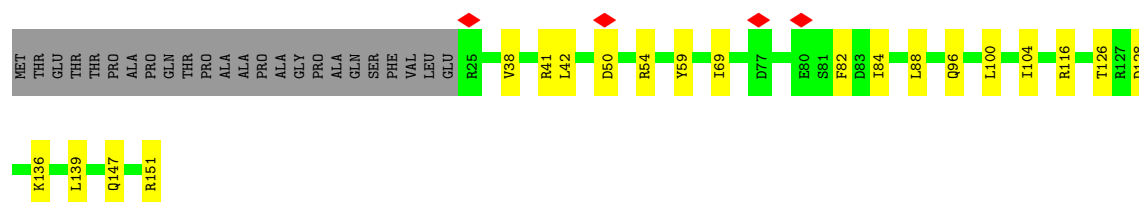
Chain h:



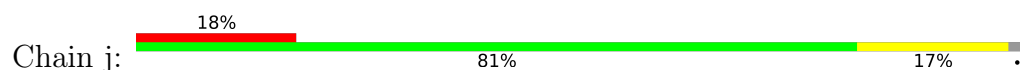
- Molecule 41: 30S ribosomal protein S9

Chain i:





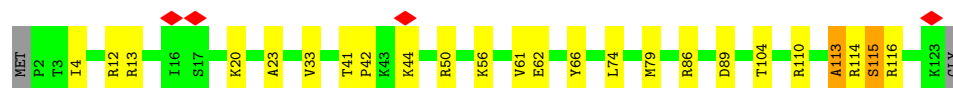
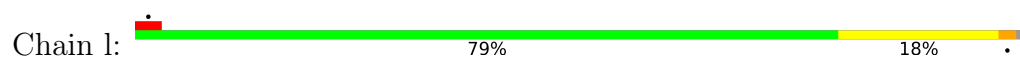
- Molecule 42: 30S ribosomal protein S10



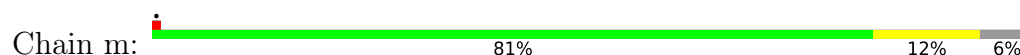
- Molecule 43: 30S ribosomal protein S11



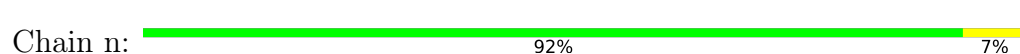
- Molecule 44: 30S ribosomal protein S12



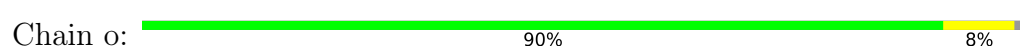
- Molecule 45: 30S ribosomal protein S13

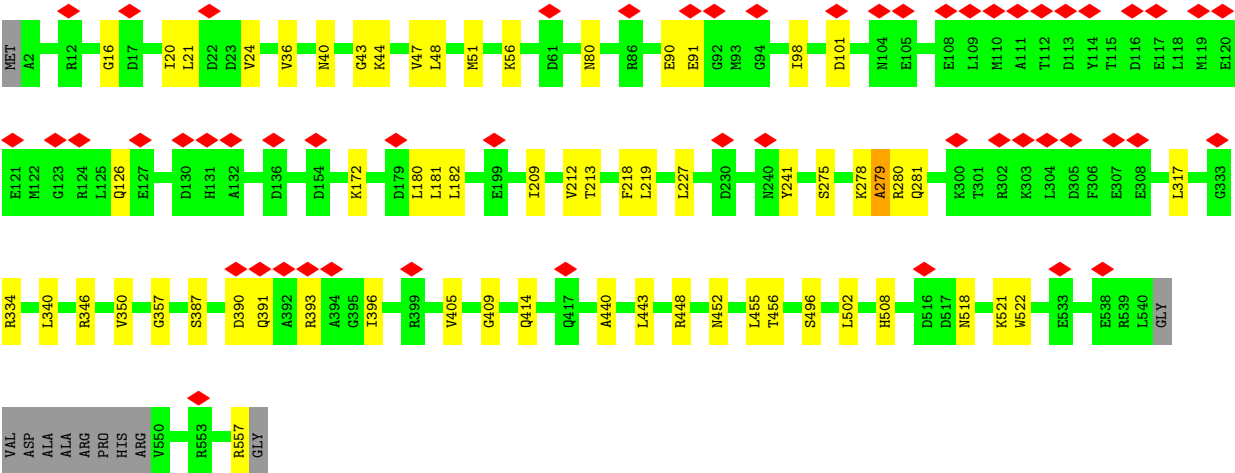


- Molecule 46: 30S ribosomal protein S14 type Z

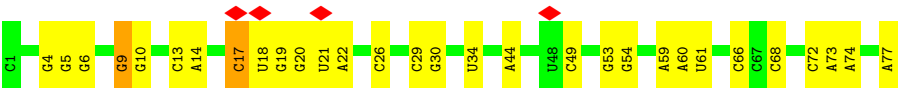


- Molecule 47: 30S ribosomal protein S15

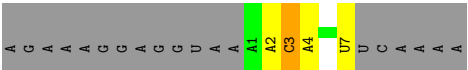




• Molecule 54: initiator tRNA (Met)



• Molecule 55: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126715	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.423	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, ZN, ANP, 4OC, 2MG, 5MU, UR3, FME, OMG, MG, G7M, 5MC

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	0	0.51	0/435	0.60	0/581
2	1	0.42	0/418	0.54	0/557
3	2	0.56	0/377	0.64	0/494
4	3	0.47	0/499	0.56	0/664
5	4	0.42	0/303	0.62	0/402
6	6	0.34	0/479	0.69	0/641
7	7	0.26	0/188	0.55	0/243
8	8	0.21	0/1728	0.43	0/2339
9	A	0.50	0/74925	0.40	1/116904 (0.0%)
10	B	0.38	0/2748	0.33	0/4280
11	C	0.53	0/2129	0.63	0/2861
12	D	0.48	0/1613	0.57	0/2174
13	E	0.48	0/1575	0.58	0/2129
14	F	0.33	0/1429	0.61	3/1921 (0.2%)
15	G	0.27	0/1351	0.51	0/1824
16	H	0.27	0/353	0.58	0/474
17	J	0.49	0/1170	0.50	0/1584
18	K	0.48	0/951	0.63	1/1278 (0.1%)
19	L	0.50	0/1088	0.56	0/1453
20	M	0.41	0/1098	0.57	0/1481
21	N	0.50	0/925	0.56	0/1242
22	O	0.40	0/914	0.59	0/1228
23	P	0.46	0/922	0.57	0/1236
24	Q	0.56	0/1006	0.63	2/1349 (0.1%)
25	R	0.45	0/766	0.59	0/1030
26	S	0.49	0/874	0.58	0/1186
27	T	0.43	0/751	0.55	0/1012
28	U	0.39	0/705	0.74	2/941 (0.2%)
29	V	0.30	0/1336	0.57	0/1820
30	W	0.45	0/565	0.62	0/752
31	X	0.51	0/476	0.59	0/638
32	Y	0.40	0/564	0.57	0/756

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.46	0/480	0.58	0/645
34	a	0.43	0/36331	0.36	0/56686
35	c	0.34	0/1678	0.53	0/2254
36	d	0.32	0/1683	0.56	0/2269
37	e	0.36	0/1238	0.51	0/1673
38	f	0.31	0/767	0.50	0/1036
39	g	0.34	0/1250	0.56	0/1686
40	h	0.41	0/1021	0.52	0/1379
41	i	0.33	0/1010	0.57	0/1356
42	j	0.36	0/803	0.63	0/1086
43	k	0.32	0/891	0.50	0/1204
44	l	0.41	0/970	0.77	0/1295
45	m	0.36	0/953	0.61	0/1274
46	n	0.41	0/477	0.60	0/634
47	o	0.39	0/727	0.59	0/973
48	p	0.35	0/901	0.63	0/1217
49	q	0.35	0/782	0.64	0/1045
50	r	0.34	0/511	0.59	0/685
51	s	0.31	0/690	0.53	0/928
52	t	0.35	0/654	0.47	0/867
53	x	0.27	0/4357	0.49	0/5897
54	y	0.35	0/1836	0.38	0/2859
55	z	0.46	0/166	0.60	0/256
All	All	0.45	0/164837	0.44	9/246678 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	8	0	1
20	M	0	1
25	R	0	1
28	U	0	1
29	V	0	2
44	l	0	2
47	o	0	1
53	x	0	1
All	All	0	10

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2488	G	C2'-C3'-O3'	5.92	118.39	109.50
14	F	143	ALA	CA-C-N	5.77	132.35	121.97
14	F	143	ALA	C-N-CA	5.77	132.35	121.97
24	Q	72	ASN	CA-C-N	5.45	131.94	121.54
24	Q	72	ASN	C-N-CA	5.45	131.94	121.54
18	K	110	ARG	CA-CB-CG	5.16	124.43	114.10
14	F	144	VAL	N-CA-CB	-5.13	102.77	111.23
28	U	38	VAL	CA-C-N	5.02	131.13	121.54
28	U	38	VAL	C-N-CA	5.02	131.13	121.54

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	8	225	ASP	Mainchain
20	M	78	PRO	Peptide
25	R	50	THR	Peptide
28	U	101	ASN	Peptide
29	V	135	ALA	Peptide
29	V	136	LEU	Peptide
44	l	113	ALA	Peptide
44	l	115	SER	Peptide
47	o	44	LYS	Peptide
53	x	279	ALA	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	0	429	0	465	0	0
2	1	411	0	422	4	0
3	2	374	0	410	1	0
4	3	494	0	533	8	0
5	4	299	0	323	3	0
6	6	470	0	460	6	0
7	7	186	0	202	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	8	1704	0	1767	21	0
9	A	66958	0	33723	150	0
10	B	2458	0	1254	5	0
11	C	2088	0	2123	19	0
12	D	1590	0	1632	9	0
13	E	1552	0	1593	5	0
14	F	1408	0	1449	16	0
15	G	1330	0	1390	9	0
16	H	350	0	367	3	0
17	J	1143	0	1173	8	0
18	K	941	0	1005	8	0
19	L	1075	0	1136	16	0
20	M	1072	0	1115	5	0
21	N	908	0	956	4	0
22	O	905	0	943	9	0
23	P	907	0	947	8	0
24	Q	993	0	1040	9	0
25	R	757	0	817	4	0
26	S	860	0	903	6	0
27	T	741	0	792	5	0
28	U	699	0	738	7	0
29	V	1319	0	1365	11	0
30	W	560	0	581	8	0
31	X	468	0	480	2	0
32	Y	560	0	570	3	0
33	Z	476	0	509	5	0
34	a	32620	0	16427	88	0
35	c	1654	0	1694	12	0
36	d	1650	0	1671	14	0
37	e	1222	0	1291	12	0
38	f	757	0	796	6	0
39	g	1230	0	1288	10	0
40	h	1006	0	1041	8	0
41	i	992	0	1052	13	0
42	j	789	0	821	13	0
43	k	873	0	887	10	0
44	l	959	0	1045	19	0
45	m	945	0	992	8	0
46	n	468	0	492	3	0
47	o	718	0	760	4	0
48	p	884	0	933	4	0
49	q	770	0	833	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	r	506	0	527	2	0
51	s	672	0	690	3	0
52	t	652	0	703	5	0
53	x	4279	0	4246	37	0
54	y	1644	0	835	9	0
55	z	149	0	76	1	0
56	1	1	0	0	0	0
56	4	1	0	0	0	0
56	6	1	0	0	0	0
56	X	1	0	0	0	0
56	n	1	0	0	0	0
56	r	1	0	0	0	0
57	A	301	0	0	0	0
57	B	5	0	0	0	0
57	C	2	0	0	0	0
57	D	1	0	0	0	0
57	L	1	0	0	0	0
57	a	130	0	0	0	0
57	r	1	0	0	0	0
57	x	2	0	0	0	0
57	y	2	0	0	0	0
58	x	62	0	26	3	0
59	y	10	0	10	1	0
All	All	152447	0	102319	538	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 2.

All (538) 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)
9:A:1574:C:H42	9:A:1630:G:H1	1.40	0.69
24:Q:44:ASN:HD21	25:R:79:PHE:HB3	1.57	0.67
34:a:999:C:H42	34:a:1016:G:H1	1.41	0.67
9:A:2390:G:N2	9:A:2391:G:N7	2.43	0.67
34:a:1224:U:H5''	41:i:147:GLN:HB2	1.79	0.65
26:S:28:ARG:HA	26:S:31:ILE:HG12	1.78	0.65
42:j:11:LYS:HG2	42:j:71:LYS:HG2	1.78	0.64
9:A:1692:U:O4	21:N:73:LYS:NZ	2.30	0.64
34:a:308:G:OP1	48:p:28:ARG:NH2	2.32	0.63
29:V:112:VAL:HG13	29:V:146:ILE:HD13	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:910:A:OP1	11:C:218:ARG:NH2	2.32	0.63
44:l:74:LEU:HD21	44:l:104:THR:HG22	1.81	0.63
9:A:843:U:OP2	47:o:88:ARG:NH2	2.32	0.63
34:a:402:C:H5''	36:d:128:PRO:HD2	1.81	0.63
34:a:655:G:H22	34:a:732:G:H1	1.47	0.63
19:L:103:VAL:HG21	19:L:109:VAL:HG12	1.82	0.62
18:K:76:TYR:HB2	23:P:72:THR:HB	1.82	0.62
26:S:35:ARG:NH1	26:S:84:VAL:O	2.33	0.61
37:e:86:GLU:HG3	37:e:88:PRO:HD2	1.81	0.61
9:A:1057:G:H4'	33:Z:37:ARG:HH22	1.66	0.61
22:O:32:ARG:NH1	22:O:49:ASP:OD2	2.33	0.61
11:C:66:ASP:OD2	11:C:103:ARG:NH1	2.34	0.60
41:i:126:THR:HG22	41:i:128:ASP:H	1.65	0.60
34:a:517:C:O2'	34:a:518:G7M:O4'	2.19	0.60
34:a:871:C:H5'	40:h:83:PRO:HG2	1.83	0.60
34:a:1209:C:OP1	46:n:9:LYS:NZ	2.34	0.60
9:A:2751:G:OP1	12:D:165:ARG:NH1	2.34	0.60
34:a:1144:G:OP1	42:j:72:ARG:NH2	2.35	0.60
9:A:1201:C:N4	9:A:1227:A:OP2	2.34	0.60
34:a:1181:U:OP1	42:j:53:ARG:NH2	2.35	0.60
12:D:7:LEU:H	12:D:34:ASN:HD21	1.50	0.59
18:K:63:VAL:HG12	18:K:106:LEU:HD11	1.84	0.59
23:P:38:ARG:NH2	34:a:345:G:OP1	2.35	0.59
35:c:38:ILE:HG12	35:c:90:LEU:HD11	1.83	0.59
54:y:6:G:H1	54:y:68:C:H42	1.51	0.59
9:A:1517:C:H5	9:A:1532:G:H1	1.50	0.59
17:J:42:PRO:HB3	24:Q:68:ALA:HB2	1.84	0.59
26:S:38:SER:HA	26:S:80:VAL:HA	1.85	0.59
34:a:124:U:H5'	49:q:57:ARG:HH12	1.66	0.59
15:G:7:GLN:OE1	15:G:70:ARG:NH2	2.35	0.59
34:a:241:U:OP1	44:l:13:ARG:NH1	2.36	0.59
53:x:36:VAL:HG22	53:x:227:LEU:HB3	1.84	0.59
5:4:8:LYS:NZ	9:A:2705:C:OP1	2.35	0.59
8:8:137:MET:SD	53:x:126:GLN:NE2	2.76	0.58
9:A:1576:C:O2	38:f:17:ARG:NH2	2.36	0.58
15:G:51:ILE:HG21	15:G:73:VAL:HG11	1.84	0.58
9:A:2025:A:N6	9:A:2062:G:O2'	2.34	0.58
10:B:29:C:OP1	22:O:9:ARG:NH1	2.33	0.58
9:A:1354:G:OP2	25:R:92:ARG:NH1	2.36	0.58
34:a:919:G:N2	55:z:3:C:O2'	2.34	0.58
36:d:147:THR:HG22	36:d:149:PRO:HD2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:42:HIS:ND1	6:6:43:PRO:O	2.36	0.58
9:A:2364:G:H2'	9:A:2365:A:H8	1.69	0.58
9:A:2707:A:N6	9:A:2719:G:O2'	2.37	0.58
34:a:1121:A:H4'	41:i:41:ARG:HE	1.69	0.58
41:i:42:LEU:HD11	41:i:82:PHE:HB3	1.85	0.58
34:a:1350:U:H3	34:a:1356:A:H62	1.52	0.58
36:d:151:GLN:OE1	36:d:154:ARG:NH2	2.37	0.57
9:A:645:G:N2	9:A:647:G:O6	2.37	0.57
9:A:732:G:H1	9:A:739:C:H5	1.52	0.57
18:K:4:GLN:OE1	18:K:23:ARG:NH2	2.37	0.57
49:q:60:ARG:NH1	49:q:78:GLU:O	2.38	0.57
35:c:57:GLU:OE2	35:c:64:ARG:NH1	2.36	0.57
9:A:2187:G:HO2'	34:a:1412:G:HO2'	1.51	0.57
9:A:1647:U:H2'	9:A:1648:A:H8	1.70	0.57
34:a:1091:C:N4	34:a:1094:C:OP1	2.38	0.57
18:K:107:ARG:HG3	18:K:112:MET:HE1	1.86	0.57
32:Y:14:THR:O	32:Y:64:ARG:NH1	2.37	0.57
34:a:211:G:O2'	34:a:216:A:N6	2.38	0.57
44:l:23:ALA:HB1	44:l:61:VAL:HG21	1.87	0.57
8:8:57:GLN:NE2	8:8:203:SER:O	2.38	0.56
32:Y:36:MET:HG3	32:Y:47:LEU:HD11	1.86	0.56
15:G:87:LYS:HB3	15:G:166:GLU:HG2	1.86	0.56
34:a:674:G:N2	43:k:49:GLY:O	2.38	0.56
36:d:137:ILE:HG21	36:d:174:ARG:HH21	1.70	0.56
47:o:25:PRO:HB2	47:o:70:ILE:HD12	1.86	0.56
9:A:2597:C:O2	19:L:59:ARG:NH1	2.38	0.56
22:O:31:PRO:HB2	22:O:46:LEU:HD22	1.86	0.56
40:h:18:ASN:ND2	40:h:74:ILE:O	2.38	0.56
17:J:13:ARG:NH2	17:J:49:ASP:O	2.39	0.56
42:j:46:LYS:NZ	42:j:66:GLU:OE1	2.38	0.56
53:x:396:ILE:HD12	53:x:440:ALA:HB1	1.87	0.56
36:d:103:ALA:HB1	36:d:108:MET:HG3	1.87	0.56
34:a:259:G:OP1	52:t:75:LYS:NZ	2.38	0.56
42:j:66:GLU:OE2	42:j:68:ARG:NH1	2.39	0.56
18:K:115:ILE:HG23	18:K:121:VAL:HG21	1.87	0.56
34:a:1308:G:N1	34:a:1311:A:OP2	2.38	0.56
15:G:9:ILE:HD12	15:G:74:SER:HB3	1.88	0.55
5:4:27:CYS:SG	5:4:28:SER:N	2.79	0.55
8:8:96:GLY:HA3	8:8:100:LEU:HD22	1.88	0.55
9:A:2174:A:H2	9:A:2181:U:H3	1.55	0.55
36:d:73:GLU:OE2	36:d:131:ARG:NH1	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:177:MET:HE2	11:C:183:ARG:HB2	1.88	0.55
35:c:188:GLU:HG2	35:c:195:ARG:HD2	1.89	0.55
26:S:118:GLU:OE2	26:S:120:ARG:NH1	2.40	0.55
34:a:1432:G:OP2	52:t:33:ARG:NH2	2.40	0.55
53:x:390:ASP:HB2	53:x:393:ARG:HG2	1.89	0.55
9:A:674:A:OP2	25:R:82:LYS:NZ	2.40	0.55
9:A:1928:U:O2	11:C:14:ARG:NH1	2.41	0.55
14:F:63:ASP:OD2	14:F:142:GLN:NE2	2.39	0.54
53:x:357:GLY:H	58:x:601:ANP:HNB1	1.55	0.54
37:e:187:ARG:NH1	40:h:73:SER:O	2.41	0.54
39:g:75:VAL:HG21	39:g:144:MET:HG3	1.89	0.54
45:m:7:VAL:HG11	45:m:22:ILE:HG12	1.90	0.54
49:q:110:ARG:NH1	49:q:132:GLU:OE2	2.39	0.54
9:A:872:A:O2'	9:A:1894:U:OP1	2.22	0.54
9:A:1988:C:H5	23:P:93:ARG:HH21	1.55	0.54
41:i:151:ARG:NH2	54:y:34:U:OP2	2.34	0.54
34:a:459:G:H21	34:a:464:C:H42	1.55	0.54
9:A:1471:U:OP1	27:T:19:LYS:NZ	2.39	0.54
53:x:80:ASN:ND2	53:x:90:GLU:OE2	2.37	0.54
9:A:1772:G:O2'	9:A:1775:G:N1	2.39	0.54
30:W:56:ASP:OD1	30:W:58:THR:OG1	2.25	0.54
37:e:120:ALA:HB3	37:e:123:GLY:H	1.72	0.54
6:6:16:CYS:SG	6:6:17:GLY:N	2.81	0.53
8:8:15:VAL:HG22	8:8:29:LEU:HD13	1.90	0.53
29:V:14:ARG:HG2	29:V:46:GLU:HG3	1.90	0.53
34:a:1314:C:OP1	51:s:78:ARG:NH2	2.41	0.53
53:x:391:GLN:OE1	53:x:452:ASN:ND2	2.41	0.53
8:8:201:PRO:HG2	8:8:204:SER:HB2	1.90	0.53
9:A:1201:C:N4	9:A:1226:U:OP2	2.41	0.53
4:3:12:LYS:NZ	9:A:251:C:O2	2.40	0.53
9:A:2352:G:H2'	9:A:2354:A:H62	1.74	0.53
42:j:59:LYS:HE2	42:j:62:ARG:HH22	1.73	0.53
9:A:842:G:OP2	47:o:88:ARG:NH1	2.41	0.53
58:x:602:ANP:O1B	58:x:602:ANP:O2A	2.26	0.53
25:R:9:LYS:NZ	25:R:40:VAL:O	2.42	0.53
34:a:191:C:N4	49:q:55:GLY:O	2.41	0.53
12:D:11:LEU:HD22	23:P:3:ARG:HD3	1.90	0.53
22:O:115:ALA:HB1	22:O:120:LEU:HD12	1.90	0.53
53:x:44:LYS:HB3	53:x:212:VAL:HG11	1.91	0.53
39:g:22:LEU:HD21	39:g:66:LEU:HD12	1.90	0.53
9:A:1718:G:H1	9:A:1750:C:H42	1.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1570:U:O2'	9:A:1633:A:N6	2.42	0.53
36:d:52:GLU:HG2	36:d:194:LEU:HB2	1.90	0.52
34:a:1486:A:OP1	44:l:44:LYS:NZ	2.41	0.52
9:A:2207:A:O2'	9:A:2210:G:N3	2.37	0.52
9:A:2707:A:OP1	20:M:120:ARG:NH1	2.41	0.52
11:C:124:ASP:O	11:C:129:ASN:ND2	2.41	0.52
14:F:87:ARG:NH2	53:x:409:GLY:O	2.41	0.52
34:a:1055:G:O2'	34:a:1182:G:N2	2.43	0.52
9:A:2105:G:N2	9:A:2109:G:O6	2.39	0.52
35:c:76:ILE:HA	35:c:83:ALA:HB2	1.91	0.52
4:3:47:ARG:NH1	9:A:735:A:OP1	2.39	0.52
43:k:29:GLY:HA2	43:k:47:PRO:HD3	1.91	0.52
9:A:569:A:OP2	28:U:43:LYS:NZ	2.40	0.52
9:A:1569:C:N4	9:A:1633:A:OP2	2.43	0.52
24:Q:73:ASP:OD1	24:Q:114:ARG:NH2	2.43	0.52
13:E:47:GLN:HE22	13:E:190:ASN:HB2	1.75	0.52
19:L:89:GLY:HA2	19:L:121:VAL:HG12	1.92	0.51
53:x:98:ILE:HA	53:x:101:ASP:HB2	1.92	0.51
4:3:5:LYS:NZ	9:A:256:G:N7	2.58	0.51
9:A:418:C:O2	28:U:69:SER:OG	2.28	0.51
9:A:500:G:OP2	9:A:2644:A:O2'	2.25	0.51
9:A:768:A:O2'	9:A:771:C:N4	2.43	0.51
9:A:1832:G:OP2	27:T:43:LYS:NZ	2.39	0.51
9:A:3074:G:N2	21:N:91:ASP:O	2.40	0.51
36:d:127:VAL:HG23	36:d:130:TYR:HB2	1.93	0.51
22:O:88:LYS:HD2	22:O:119:GLY:HA3	1.91	0.51
34:a:962:A:OP1	42:j:57:LYS:NZ	2.42	0.51
36:d:183:ARG:HH22	36:d:188:VAL:HG22	1.76	0.51
8:8:46:ILE:HB	8:8:171:LEU:HB2	1.91	0.51
9:A:2051:G:OP1	11:C:88:ARG:NH2	2.41	0.51
9:A:1745:C:H5''	9:A:1746:U:H5	1.76	0.51
53:x:443:LEU:O	53:x:448:ARG:NH1	2.44	0.51
4:3:28:ASN:O	4:3:36:LYS:NZ	2.39	0.51
9:A:1471:U:OP2	27:T:62:ARG:NH2	2.44	0.51
28:U:1:MET:HE3	28:U:28:PRO:HA	1.93	0.51
34:a:964:G:N2	34:a:1356:A:OP2	2.42	0.51
47:o:26:GLU:HG3	47:o:81:LEU:HD22	1.93	0.51
34:a:413:A:OP2	34:a:427:G:N2	2.42	0.51
45:m:65:LYS:HG3	45:m:70:LEU:HB2	1.93	0.51
9:A:1567:U:O2'	9:A:1569:C:N4	2.44	0.51
42:j:63:GLU:HG3	46:n:45:ARG:HE	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:k:45:THR:HG22	43:k:51:VAL:HA	1.93	0.51
45:m:87:TYR:OH	45:m:91:ARG:NH2	2.39	0.51
2:l:55:ARG:HG2	53:x:56:LYS:HB2	1.93	0.50
33:Z:50:VAL:HG22	33:Z:53:LEU:HB2	1.93	0.50
36:d:9:THR:HG21	36:d:25:ALA:HB3	1.92	0.50
8:8:154:ALA:O	8:8:158:GLY:N	2.44	0.50
9:A:2270:G:OP1	9:A:2692:G:O2'	2.28	0.50
34:a:254:G:OP1	49:q:123:LYS:NZ	2.42	0.50
4:3:57:ARG:NH1	19:L:50:GLU:OE2	2.44	0.50
29:V:175:LEU:HD21	29:V:178:ASN:HB2	1.94	0.50
16:H:2:LYS:HG3	16:H:39:ALA:HB3	1.93	0.50
34:a:969:G:OP2	34:a:1350:U:O2'	2.29	0.50
9:A:1098:G:N2	9:A:1114:C:OP1	2.32	0.50
9:A:1516:A:O2'	9:A:1527:U:O2	2.29	0.50
19:L:34:ARG:NH1	19:L:40:ARG:O	2.41	0.50
9:A:307:U:O2'	16:H:41:ARG:NH1	2.44	0.50
9:A:1136:C:OP1	17:J:37:ARG:NH1	2.42	0.50
11:C:172:TYR:HB3	11:C:184:ARG:HG2	1.94	0.50
43:k:33:ILE:HG12	43:k:42:VAL:HG22	1.94	0.50
9:A:1071:U:OP2	19:L:36:THR:OG1	2.30	0.50
9:A:2244:C:O2'	9:A:3058:A:N3	2.45	0.50
38:f:10:LEU:HB2	38:f:59:ILE:HB	1.94	0.50
9:A:1170:C:H2'	9:A:1171:G:H8	1.77	0.50
34:a:1001:C:H42	34:a:1014:G:H1	1.60	0.50
9:A:873:G:H1	9:A:882:C:H5	1.59	0.49
14:F:52:ARG:HB3	53:x:414:GLN:HG2	1.94	0.49
39:g:69:VAL:HG23	39:g:100:ALA:HB1	1.93	0.49
9:A:1457:C:HO2'	9:A:2248:G:HO2'	1.59	0.49
9:A:2368:G:O2'	9:A:2393:G:N2	2.46	0.49
41:i:136:LYS:HB2	41:i:139:LEU:HD12	1.94	0.49
8:8:72:THR:O	8:8:157:LYS:NZ	2.45	0.49
30:W:11:ARG:O	30:W:14:ARG:NH1	2.44	0.49
9:A:820:C:OP1	11:C:218:ARG:NH1	2.45	0.49
17:J:24:VAL:HG23	17:J:27:ARG:H	1.77	0.49
9:A:2740:G:H5''	9:A:2741:A:H5''	1.95	0.49
14:F:15:TYR:OH	14:F:36:PRO:O	2.29	0.49
41:i:69:ILE:HD12	41:i:100:LEU:HD23	1.94	0.49
53:x:279:ALA:O	53:x:281:GLN:N	2.46	0.49
8:8:181:ASP:HB2	8:8:184:LEU:HD13	1.94	0.49
20:M:35:GLN:HE21	20:M:100:GLY:HA2	1.77	0.49
51:s:2:PRO:HD2	51:s:7:LYS:HG3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1824:C:H2'	9:A:1825:A:H8	1.78	0.49
14:F:12:LYS:HE2	14:F:16:ARG:HH22	1.78	0.49
19:L:122:ASP:OD1	19:L:142:SER:OG	2.30	0.49
2:1:28:ASN:ND2	9:A:2523:C:OP2	2.46	0.49
8:8:4:THR:OG1	8:8:9:ARG:NH2	2.46	0.49
15:G:71:THR:O	15:G:75:ASN:ND2	2.46	0.49
41:i:50:ASP:OD1	41:i:50:ASP:N	2.43	0.49
9:A:668:U:H5''	19:L:30:LYS:HE2	1.94	0.48
34:a:1386:U:HO2'	34:a:1494:C:HO2'	1.50	0.48
43:k:43:THR:HA	43:k:54:TRP:HA	1.94	0.48
9:A:1189:U:H4'	9:A:1190:U:H5'	1.94	0.48
34:a:555:C:OP1	44:l:12:ARG:NH1	2.46	0.48
9:A:776:G:OP1	19:L:116:LYS:NZ	2.46	0.48
9:A:1554:G:H1	9:A:1651:C:H42	1.62	0.48
34:a:1182:G:H5'	35:c:176:HIS:HE1	1.77	0.48
34:a:653:C:O2'	34:a:827:G:OP1	2.31	0.48
37:e:71:GLY:HA3	37:e:148:CYS:HB3	1.96	0.48
6:6:14:VAL:HG21	14:F:113:ILE:HG21	1.95	0.48
9:A:2741:A:O2'	9:A:2743:G:OP2	2.30	0.48
35:c:57:GLU:HG2	35:c:64:ARG:HB3	1.95	0.48
44:l:33:VAL:HG12	44:l:56:LYS:HB3	1.94	0.48
8:8:100:LEU:HA	8:8:103:ARG:HE	1.78	0.48
9:A:1656:G:O2'	9:A:1816:A:N6	2.46	0.48
9:A:2309:C:H5	9:A:2675:G:H1	1.60	0.48
27:T:7:PRO:HG3	27:T:48:LYS:HD2	1.95	0.48
34:a:458:G:H1	34:a:465:U:H3	1.61	0.48
37:e:207:SER:OG	37:e:208:GLU:OE1	2.31	0.48
34:a:857:A:H5'	37:e:122:ALA:HB2	1.94	0.48
34:a:1171:A:OP2	41:i:116:ARG:NH2	2.47	0.48
35:c:157:LEU:HD12	35:c:164:ARG:HG2	1.96	0.48
53:x:405:VAL:HG12	53:x:455:LEU:HD21	1.94	0.48
9:A:117:G:OP2	9:A:119:A:O2'	2.31	0.48
9:A:946:C:H5	9:A:1322:G:H1	1.62	0.48
34:a:554:A:O2'	34:a:557:G:O2'	2.30	0.48
35:c:90:LEU:HD23	35:c:98:VAL:HG11	1.96	0.48
40:h:11:LEU:HD22	40:h:77:LEU:HD22	1.96	0.48
53:x:40:ASN:OD1	58:x:602:ANP:O2G	2.32	0.48
9:A:166:U:H3	31:X:41:ARG:HH12	1.60	0.48
34:a:546:C:OP2	44:l:20:LYS:NZ	2.47	0.48
34:a:1355:A:H5'	34:a:1356:A:H5''	1.96	0.48
8:8:73:ALA:HB1	8:8:156:ILE:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:10:ARG:NH1	29:V:11:VAL:O	2.47	0.47
42:j:53:ARG:HE	42:j:63:GLU:HG2	1.78	0.47
53:x:350:VAL:HG22	53:x:508:HIS:HB2	1.95	0.47
6:6:39:SER:HB2	14:F:112:SER:HA	1.95	0.47
8:8:215:SER:OG	8:8:219:GLY:O	2.32	0.47
9:A:3052:C:OP1	21:N:42:ARG:NH2	2.46	0.47
14:F:68:THR:HG21	14:F:96:VAL:HG11	1.96	0.47
9:A:2572:C:H42	30:W:75:ARG:HE	1.61	0.47
42:j:9:ARG:HB2	42:j:99:ASN:HB2	1.95	0.47
11:C:62:TYR:HA	11:C:87:ASN:HD21	1.79	0.47
11:C:162:SER:HB3	11:C:195:GLU:HG3	1.96	0.47
11:C:258:ARG:NH1	11:C:265:ASN:OD1	2.45	0.47
37:e:184:VAL:HG11	40:h:101:LEU:HD22	1.96	0.47
9:A:1901:G:HO2'	18:K:6:SER:HG	1.54	0.47
9:A:2956:G:O2'	9:A:3082:U:OP1	2.32	0.47
11:C:108:PRO:HD2	11:C:111:LEU:HD22	1.97	0.47
14:F:87:ARG:HG2	14:F:90:MET:HE3	1.97	0.47
36:d:165:TRP:CD1	36:d:181:PRO:HB3	2.49	0.47
49:q:52:LYS:HD2	49:q:53:PRO:HD2	1.96	0.47
4:3:57:ARG:NH2	19:L:47:VAL:O	2.48	0.47
9:A:2106:C:H42	9:A:2109:G:H1'	1.80	0.47
21:N:100:ILE:HG13	21:N:112:VAL:HG13	1.97	0.47
37:e:50:ASN:OD1	37:e:65:THR:OG1	2.33	0.47
14:F:73:GLU:OE1	14:F:95:ARG:NH2	2.47	0.47
37:e:120:ALA:HB2	37:e:170:ALA:HB2	1.97	0.47
38:f:14:LEU:HD11	38:f:84:SER:HB3	1.97	0.47
50:r:50:ALA:HB1	50:r:52:ARG:HH11	1.77	0.47
23:P:105:LYS:NZ	34:a:1426:A:OP1	2.41	0.47
29:V:31:ILE:HG22	29:V:47:LEU:HB2	1.96	0.47
34:a:38:G:N3	44:l:115:SER:OG	2.48	0.47
53:x:387:SER:OG	53:x:456:THR:O	2.31	0.47
14:F:43:VAL:HG22	14:F:161:ILE:HG12	1.96	0.47
34:a:697:A:H2	43:k:51:VAL:HG21	1.80	0.47
8:8:123:LYS:HG2	8:8:126:ARG:HH11	1.81	0.46
9:A:1525:U:H4'	9:A:1838:A:H4'	1.95	0.46
34:a:494:C:OP1	44:l:116:ARG:NH2	2.41	0.46
34:a:1371:C:O2	39:g:76:ARG:NH1	2.46	0.46
9:A:1953:G:H1	9:A:1976:G:H1	1.63	0.46
11:C:37:LEU:HG	11:C:62:TYR:HB2	1.96	0.46
22:O:72:LYS:HB3	22:O:107:ARG:HD3	1.98	0.46
34:a:65:U:O2'	34:a:378:C:O2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:p:5:ILE:HG12	48:p:22:VAL:HG22	1.97	0.46
9:A:2677:A:H4'	9:A:2678:C:H5''	1.96	0.46
53:x:21:LEU:HD21	53:x:47:VAL:HG22	1.97	0.46
4:3:19:THR:HG23	9:A:755:G:H5''	1.98	0.46
9:A:2551:C:H2'	9:A:2552:A:H8	1.79	0.46
34:a:1210:C:H2'	34:a:1211:A:C8	2.50	0.46
53:x:219:LEU:HD22	53:x:241:TYR:HB2	1.97	0.46
9:A:2202:G:O2'	9:A:2205:C:OP1	2.33	0.46
53:x:20:ILE:HG23	53:x:43:GLY:HA3	1.97	0.46
9:A:1382:A:OP2	24:Q:6:ARG:NH1	2.48	0.46
20:M:51:ARG:HD3	20:M:66:ILE:HD11	1.97	0.46
29:V:157:ALA:N	29:V:174:LEU:O	2.48	0.46
31:X:56:ILE:HG12	31:X:61:ILE:HD11	1.97	0.46
45:m:4:LEU:HD21	45:m:56:LEU:HG	1.97	0.46
53:x:340:LEU:HD13	53:x:522:TRP:HB2	1.96	0.46
9:A:682:C:H5''	24:Q:34:LYS:HE2	1.97	0.46
9:A:986:A:H5'	30:W:69:PHE:CD2	2.51	0.46
53:x:21:LEU:HD12	53:x:24:VAL:HG11	1.96	0.46
9:A:858:G:C6	11:C:208:LYS:HB2	2.50	0.46
18:K:122:LEU:HD22	23:P:69:VAL:HG11	1.98	0.46
39:g:75:VAL:HG22	39:g:86:GLN:HB3	1.97	0.46
8:8:41:THR:H	8:8:217:THR:HG23	1.80	0.46
9:A:403:G:N2	13:E:177:ASN:O	2.49	0.46
9:A:1057:G:O2'	33:Z:25:THR:O	2.33	0.46
9:A:1267:G:H21	17:J:108:MET:HE2	1.80	0.46
23:P:99:LEU:HD21	23:P:109:ILE:HD11	1.97	0.46
53:x:317:LEU:HD23	53:x:346:ARG:HG3	1.98	0.46
9:A:487:G:OP1	9:A:2327:A:O2'	2.34	0.46
9:A:1712:G:H21	9:A:1756:A:H62	1.63	0.46
34:a:446:G:H21	34:a:478:A:H62	1.62	0.46
53:x:20:ILE:HG22	53:x:21:LEU:HD22	1.97	0.46
16:H:1:MET:HE2	16:H:3:LEU:HD21	1.99	0.45
53:x:334:ARG:NH2	53:x:357:GLY:O	2.49	0.45
34:a:446:G:O6	34:a:476:G:O2'	2.32	0.45
35:c:39:ARG:O	35:c:43:SER:OG	2.33	0.45
41:i:88:LEU:HD12	41:i:96:GLN:HB3	1.98	0.45
33:Z:2:SER:OG	33:Z:3:GLN:N	2.48	0.45
45:m:29:ARG:NH1	45:m:32:GLU:OE2	2.41	0.45
53:x:48:LEU:HG	53:x:182:LEU:HD22	1.98	0.45
9:A:2052:U:OP2	11:C:157:ARG:NE	2.49	0.45
9:A:2396:G:H4'	9:A:2397:U:H5'	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:g:18:TYR:OH	39:g:48:GLU:OE2	2.32	0.45
39:g:26:LEU:HD13	39:g:101:LEU:HD22	1.98	0.45
9:A:1235:G:H2'	9:A:1236:G:H8	1.81	0.45
15:G:45:ARG:HH21	15:G:51:ILE:HG13	1.81	0.45
34:a:136:C:H5'	49:q:43:GLY:HA3	1.98	0.45
9:A:2895:A:O2'	15:G:161:LYS:NZ	2.49	0.45
18:K:64:ARG:NH2	18:K:81:GLU:OE2	2.43	0.45
9:A:2391:G:N1	9:A:2393:G:OP1	2.49	0.45
14:F:129:PHE:HE2	14:F:174:ARG:HB2	1.81	0.45
29:V:171:ASP:HB2	29:V:174:LEU:HG	1.99	0.45
34:a:706:A:H2'	34:a:707:A:C8	2.52	0.45
49:q:68:LYS:H	49:q:68:LYS:HD2	1.82	0.45
17:J:6:PRO:HG2	17:J:48:VAL:HG21	1.98	0.45
19:L:36:THR:HG22	19:L:37:LYS:H	1.82	0.45
28:U:13:SER:OG	28:U:70:ASN:OD1	2.35	0.45
8:8:212:ILE:HG23	8:8:224:VAL:HB	1.98	0.45
34:a:837:U:O2'	34:a:838:U:O2	2.35	0.45
34:a:1136:G:H21	34:a:1138:A:H62	1.64	0.45
34:a:1294:U:H3	45:m:14:ARG:HH21	1.65	0.45
45:m:54:ILE:HA	45:m:57:ARG:HG2	1.98	0.45
51:s:2:PRO:HB2	51:s:7:LYS:HD2	1.99	0.45
9:A:1194:U:H2'	9:A:1195:U:H4'	1.98	0.44
9:A:2289:A:H4'	12:D:151:ILE:HG12	1.98	0.44
29:V:124:GLN:HE22	29:V:127:ASN:HD21	1.65	0.44
34:a:554:A:H3'	44:l:12:ARG:HH12	1.82	0.44
41:i:84:ILE:HD13	41:i:104:ILE:HD11	1.99	0.44
6:6:12:THR:HG23	6:6:31:GLY:HA2	1.99	0.44
10:B:13:C:OP2	10:B:69:C:O2'	2.34	0.44
9:A:804:A:O2'	13:E:74:GLN:OE1	2.25	0.44
12:D:154:CYS:SG	12:D:155:ALA:N	2.84	0.44
14:F:177:LEU:HD23	14:F:180:LEU:HD12	2.00	0.44
34:a:496:G:H1	34:a:517:C:H42	1.64	0.44
34:a:967:A:OP1	46:n:29:ARG:NH2	2.51	0.44
6:6:67:LYS:H	6:6:67:LYS:HG2	1.56	0.44
20:M:52:ILE:HD12	20:M:56:ARG:HH22	1.81	0.44
19:L:31:THR:HB	19:L:35:GLY:H	1.82	0.44
34:a:381:A:H2'	34:a:382:A:C8	2.53	0.44
34:a:516:C:OP1	44:l:86:ARG:NH1	2.50	0.44
9:A:1172:C:H2'	9:A:1173:A:H8	1.83	0.44
22:O:42:ILE:HD12	22:O:111:LEU:HD12	1.98	0.44
34:a:355:A:N3	34:a:367:U:O2'	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:g:150:ALA:HB1	43:k:69:THR:HG21	2.00	0.44
44:l:50:ARG:NH2	44:l:89:ASP:OD2	2.45	0.44
44:l:113:ALA:O	44:l:115:SER:N	2.38	0.44
9:A:986:A:H5'	30:W:69:PHE:HD2	1.82	0.44
26:S:83:THR:HB	26:S:116:VAL:HB	1.99	0.44
30:W:38:VAL:HB	30:W:59:LEU:HD12	2.00	0.44
32:Y:50:VAL:HA	32:Y:53:GLU:HG2	1.99	0.44
9:A:883:U:O2'	9:A:1403:A:N1	2.51	0.43
10:B:3:A:N1	10:B:21:G:O2'	2.40	0.43
12:D:40:ARG:HB2	12:D:49:ALA:H	1.83	0.43
22:O:99:ARG:NH1	22:O:102:TYR:O	2.44	0.43
34:a:1051:U:OP2	35:c:2:GLY:N	2.51	0.43
37:e:111:THR:HB	37:e:153:ASP:HB2	2.00	0.43
9:A:637:C:H42	9:A:646:A:H61	1.66	0.43
34:a:1120:C:H42	34:a:1135:G:H1	1.65	0.43
38:f:87:ARG:NH1	50:r:73:GLU:O	2.51	0.43
34:a:748:U:OP1	34:a:813:G:O2'	2.32	0.43
9:A:1685:C:H2'	9:A:1686:A:C8	2.53	0.43
8:8:44:VAL:HG22	8:8:214:VAL:HG22	2.00	0.43
9:A:2013:U:OP2	9:A:2018:A:N6	2.45	0.43
9:A:2426:U:H2'	9:A:2427:G:H8	1.83	0.43
12:D:84:LEU:HD13	12:D:207:MET:HE2	2.00	0.43
15:G:26:VAL:HG21	15:G:77:VAL:HG12	2.00	0.43
19:L:55:PRO:HD2	19:L:58:MET:HE3	1.99	0.43
42:j:18:ILE:HG23	42:j:72:ARG:HH12	1.84	0.43
9:A:683:C:H5'	24:Q:31:LEU:HD22	2.00	0.43
43:k:111:GLN:HE21	43:k:117:VAL:HG21	1.83	0.43
4:3:33:LEU:HD23	4:3:36:LYS:HD2	2.00	0.43
8:8:31:LYS:NZ	8:8:180:PHE:O	2.35	0.43
9:A:2566:A:H2'	9:A:2567:A:C8	2.54	0.43
19:L:86:PHE:HE1	19:L:100:LYS:HE3	1.83	0.43
34:a:9:G:O6	37:e:131:SER:N	2.52	0.43
54:y:9:G:O2'	54:y:10:G:N7	2.52	0.43
9:A:668:U:O2'	9:A:938:G:OP2	2.33	0.43
9:A:2052:U:H2'	11:C:157:ARG:HG2	2.00	0.43
9:A:2513:C:O2'	20:M:84:GLY:O	2.36	0.43
9:A:2516:A:N7	30:W:12:ASN:ND2	2.65	0.43
2:1:36:LEU:H	2:1:53:GLU:HG3	1.83	0.43
12:D:184:LYS:HB3	12:D:193:LEU:HD12	2.01	0.43
34:a:968:A:H4'	34:a:969:G:H5''	2.00	0.43
34:a:759:A:N3	34:a:1505:U:O2'	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:3:LYS:HD3	9:A:882:C:H5''	2.02	0.42
14:F:136:THR:OG1	14:F:162:ASN:ND2	2.52	0.42
35:c:19:LYS:HE3	35:c:53:ASP:HB2	2.00	0.42
53:x:518:ASN:HD22	53:x:521:LYS:HD3	1.84	0.42
54:y:17:C:OP1	54:y:61:U:O2'	2.31	0.42
10:B:14:A:H3'	10:B:15:G:H8	1.84	0.42
36:d:160:ARG:HA	36:d:161:PRO:HD3	1.91	0.42
45:m:77:ASP:OD1	45:m:80:ARG:NH1	2.48	0.42
34:a:701:G:OP1	38:f:54:LYS:NZ	2.37	0.42
34:a:802:C:O2'	34:a:894:A:N1	2.53	0.42
44:l:41:THR:HA	44:l:42:PRO:HD3	1.84	0.42
24:Q:64:ARG:HD3	24:Q:100:ILE:HD11	2.02	0.42
37:e:146:LEU:HD13	37:e:154:ILE:HG21	2.00	0.42
40:h:27:LEU:HD11	40:h:60:LEU:HD23	2.00	0.42
49:q:102:ASP:OD1	49:q:102:ASP:N	2.50	0.42
52:t:28:LEU:HD22	52:t:58:LEU:HD23	2.01	0.42
53:x:278:LYS:HG2	54:y:73:A:H5'	1.99	0.42
14:F:71:LYS:HA	14:F:72:PRO:HD3	1.90	0.42
22:O:34:VAL:HA	22:O:98:ASP:HB3	2.01	0.42
24:Q:117:LEU:HD12	24:Q:118:PRO:HD2	2.01	0.42
29:V:48:PRO:HB2	29:V:51:ASP:HB2	2.01	0.42
30:W:14:ARG:H	30:W:14:ARG:HD3	1.84	0.42
9:A:1166:C:H42	9:A:1247:G:H1	1.68	0.42
9:A:2367:U:H6	9:A:2396:G:H1	1.66	0.42
34:a:492:C:H2'	34:a:493:A:C8	2.55	0.42
9:A:1576:C:O2'	38:f:17:ARG:NH1	2.53	0.42
9:A:2373:A:H4'	9:A:2374:C:H5'	2.01	0.42
9:A:3018:C:N4	17:J:102:GLU:OE2	2.53	0.42
34:a:389:U:O3'	48:p:29:ARG:NH2	2.53	0.42
41:i:54:ARG:HH11	41:i:59:TYR:HD1	1.67	0.42
53:x:275:SER:O	54:y:72:C:O2'	2.37	0.42
54:y:29:C:H2'	54:y:30:G:H8	1.85	0.42
12:D:130:HIS:CD2	12:D:165:ARG:HB3	2.54	0.42
15:G:8:PRO:HB3	15:G:52:VAL:HG22	2.01	0.42
23:P:51:GLY:HA2	23:P:56:GLU:HG3	2.01	0.42
28:U:9:VAL:HB	28:U:71:VAL:HB	2.02	0.42
34:a:64:G:N7	52:t:6:SER:OG	2.36	0.42
41:i:38:VAL:HG12	41:i:88:LEU:HD13	2.01	0.42
42:j:7:ARG:HB3	42:j:101:GLN:HB2	2.02	0.42
43:k:97:LYS:HB3	43:k:123:VAL:HG23	2.01	0.42
9:A:2356:A:H61	9:A:2405:G:H21	1.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:939:A:H2'	34:a:940:G:C8	2.55	0.41
34:a:1384:U:H2'	34:a:1385:G:C8	2.54	0.41
54:y:29:C:H2'	54:y:30:G:C8	2.54	0.41
8:8:140:PRO:HB3	8:8:145:VAL:HB	2.02	0.41
9:A:1560:U:H5	9:A:1643:G:H21	1.68	0.41
28:U:10:LEU:HD23	28:U:80:PRO:HG3	2.02	0.41
35:c:96:LYS:HE3	35:c:96:LYS:HB2	1.92	0.41
13:E:130:ILE:HD13	13:E:200:VAL:HB	2.01	0.41
14:F:45:MET:HG2	14:F:64:LEU:HD11	2.02	0.41
9:A:648:G:H2'	9:A:649:A:H8	1.86	0.41
9:A:2078:U:H5''	11:C:256:ARG:HG2	2.02	0.41
34:a:70:C:H2'	34:a:71:G:C8	2.56	0.41
53:x:91:GLU:HB3	53:x:172:LYS:HB3	2.03	0.41
54:y:59:A:O2'	54:y:61:U:OP2	2.35	0.41
2:1:29:ARG:HH12	53:x:16:GLY:HA3	1.86	0.41
44:l:33:VAL:HG23	44:l:79:MET:HE1	2.02	0.41
44:l:110:ARG:HH21	44:l:113:ALA:HB3	1.85	0.41
42:j:43:PRO:O	42:j:71:LYS:NZ	2.53	0.41
48:p:28:ARG:H	48:p:28:ARG:HG2	1.66	0.41
9:A:1280:C:O2'	24:Q:121:VAL:O	2.31	0.41
11:C:263:SER:O	11:C:266:LYS:NZ	2.54	0.41
19:L:34:ARG:HD3	19:L:41:ALA:HA	2.03	0.41
34:a:513:C:OP2	44:l:66:TYR:OH	2.30	0.41
40:h:5:ASP:HB2	40:h:83:PRO:HG3	2.03	0.41
9:A:535:G:H4'	9:A:536:A:H5'	2.03	0.41
9:A:768:A:H1'	9:A:771:C:H41	1.85	0.41
9:A:278:C:H2'	9:A:279:A:H8	1.84	0.41
9:A:679:G:O2'	9:A:1385:A:OP1	2.38	0.41
9:A:1116:C:O2'	9:A:1129:A:N3	2.48	0.41
9:A:2406:A:C6	53:x:557:ARG:HD2	2.55	0.41
10:B:61:U:H2'	10:B:62:G:C8	2.56	0.41
17:J:120:ARG:O	17:J:123:ARG:NH1	2.53	0.41
19:L:54:MET:HA	19:L:55:PRO:HD3	1.96	0.41
33:Z:23:LEU:HG	33:Z:50:VAL:HG21	2.02	0.41
34:a:707:A:N3	43:k:130:GLY:HA2	2.36	0.41
34:a:945:U:H4'	34:a:957:A:N1	2.36	0.41
36:d:92:ARG:HH21	36:d:129:SER:HB3	1.85	0.41
39:g:113:GLU:HB2	39:g:119:ARG:HG2	2.03	0.41
53:x:51:MET:HE2	53:x:180:LEU:HD21	2.01	0.41
53:x:496:SER:HB3	53:x:502:LEU:HD11	2.03	0.41
5:4:1:VAL:N	9:A:2764:G:O2'	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:287:G:N2	9:A:288:U:O4	2.42	0.41
9:A:2312:U:HO2'	9:A:2834:U:H3	1.63	0.41
27:T:68:ARG:HD2	27:T:73:TYR:HE1	1.86	0.41
29:V:156:THR:HG22	29:V:158:GLY:H	1.86	0.41
36:d:99:ARG:HH22	36:d:187:ASP:HB3	1.86	0.41
9:A:1219:U:N3	9:A:1231:C:O2	2.54	0.40
9:A:1397:G:O5'	26:S:25:ARG:NH2	2.52	0.40
9:A:2412:C:H2'	9:A:2413:A:C8	2.55	0.40
9:A:3028:A:N6	9:A:3127:A:OP2	2.46	0.40
8:8:141:LYS:HE2	8:8:141:LYS:HB2	1.94	0.40
9:A:162:A:N3	9:A:2445:C:O2'	2.54	0.40
9:A:1737:G:N2	11:C:99:ASP:O	2.41	0.40
9:A:2093:A:H2	9:A:2121:G:H21	1.69	0.40
9:A:2301:C:O2'	59:y:101:FME:O	2.37	0.40
9:A:2371:A:H61	9:A:2391:G:H22	1.69	0.40
34:a:1002:G:N2	34:a:1013:G:O6	2.41	0.40
34:a:1431:A:OP2	52:t:29:ARG:NH1	2.54	0.40
44:l:12:ARG:HA	44:l:12:ARG:HD3	1.93	0.40
53:x:181:LEU:HD12	53:x:209:ILE:HG12	2.04	0.40
8:8:63:VAL:HG23	8:8:195:GLU:HG3	2.04	0.40
9:A:636:U:O2'	9:A:637:C:O5'	2.38	0.40
9:A:2006:G:H1	9:A:2217:C:H5	1.69	0.40
13:E:30:LEU:HD12	13:E:118:ARG:HD3	2.03	0.40
34:a:815:U:H2'	34:a:816:A:C8	2.56	0.40
34:a:997:G:O5'	34:a:1018:U:N3	2.55	0.40
9:A:607:U:H2'	9:A:608:G:H8	1.86	0.40
9:A:1222:G:H21	9:A:1227:A:H62	1.68	0.40
29:V:116:ALA:HA	29:V:148:GLY:HA2	2.04	0.40
34:a:49:G:O2'	34:a:364:U:O2	2.38	0.40
44:l:56:LYS:NZ	44:l:62:GLU:OE1	2.43	0.40
53:x:213:THR:HG21	53:x:218:PHE:HD2	1.87	0.40
9:A:84:A:OP1	28:U:4:HIS:NE2	2.55	0.40
9:A:334:C:H2'	9:A:335:A:H8	1.86	0.40
34:a:869:A:H4'	40:h:15:ARG:HH22	1.86	0.40
34:a:971:A:O2'	34:a:1314:C:N3	2.53	0.40
39:g:78:ARG:HD2	39:g:156:TRP:HE1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	52/57 (91%)	52 (100%)	0	0	100	100
2	1	47/55 (86%)	47 (100%)	0	0	100	100
3	2	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
4	3	60/64 (94%)	57 (95%)	3 (5%)	0	100	100
5	4	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
6	6	56/80 (70%)	51 (91%)	5 (9%)	0	100	100
7	7	20/24 (83%)	19 (95%)	1 (5%)	0	100	100
8	8	228/235 (97%)	214 (94%)	14 (6%)	0	100	100
11	C	270/280 (96%)	256 (95%)	13 (5%)	1 (0%)	30	62
12	D	211/217 (97%)	195 (92%)	16 (8%)	0	100	100
13	E	205/223 (92%)	200 (98%)	5 (2%)	0	100	100
14	F	176/187 (94%)	156 (89%)	18 (10%)	2 (1%)	11	40
15	G	172/179 (96%)	157 (91%)	15 (9%)	0	100	100
16	H	45/152 (30%)	41 (91%)	4 (9%)	0	100	100
17	J	144/195 (74%)	141 (98%)	3 (2%)	0	100	100
18	K	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
19	L	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
20	M	132/138 (96%)	124 (94%)	8 (6%)	0	100	100
21	N	114/180 (63%)	111 (97%)	3 (3%)	0	100	100
22	O	117/122 (96%)	113 (97%)	4 (3%)	0	100	100
23	P	110/113 (97%)	98 (89%)	12 (11%)	0	100	100
24	Q	122/129 (95%)	121 (99%)	1 (1%)	0	100	100
25	R	98/104 (94%)	90 (92%)	7 (7%)	1 (1%)	12	42
26	S	111/197 (56%)	110 (99%)	1 (1%)	0	100	100
27	T	93/100 (93%)	88 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	U	86/105 (82%)	77 (90%)	9 (10%)	0	100	100
29	V	175/215 (81%)	153 (87%)	20 (11%)	2 (1%)	11	40
30	W	74/86 (86%)	67 (90%)	7 (10%)	0	100	100
31	X	60/64 (94%)	59 (98%)	1 (2%)	0	100	100
32	Y	66/77 (86%)	63 (96%)	3 (4%)	0	100	100
33	Z	57/65 (88%)	55 (96%)	2 (4%)	0	100	100
35	c	205/274 (75%)	182 (89%)	23 (11%)	0	100	100
36	d	198/201 (98%)	182 (92%)	16 (8%)	0	100	100
37	e	167/220 (76%)	155 (93%)	12 (7%)	0	100	100
38	f	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
39	g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
40	h	129/132 (98%)	121 (94%)	8 (6%)	0	100	100
41	i	125/151 (83%)	115 (92%)	10 (8%)	0	100	100
42	j	97/101 (96%)	87 (90%)	10 (10%)	0	100	100
43	k	115/139 (83%)	103 (90%)	12 (10%)	0	100	100
44	l	120/124 (97%)	95 (79%)	23 (19%)	2 (2%)	7	30
45	m	114/124 (92%)	103 (90%)	11 (10%)	0	100	100
46	n	58/61 (95%)	56 (97%)	1 (2%)	1 (2%)	7	30
47	o	85/89 (96%)	79 (93%)	5 (6%)	1 (1%)	10	38
48	p	111/162 (68%)	95 (86%)	15 (14%)	1 (1%)	14	45
49	q	93/135 (69%)	79 (85%)	14 (15%)	0	100	100
50	r	62/84 (74%)	58 (94%)	4 (6%)	0	100	100
51	s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
52	t	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
53	x	543/558 (97%)	500 (92%)	42 (8%)	1 (0%)	43	73
All	All	6072/6981 (87%)	5641 (93%)	419 (7%)	12 (0%)	44	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	F	143	ALA
14	F	144	VAL
25	R	51	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	l	114	ARG
46	n	17	ALA
48	p	46	PRO
29	V	136	LEU
53	x	280	ARG
47	o	19	GLU
11	C	27	SER
29	V	135	ALA
44	l	4	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	44/47 (94%)	44 (100%)	0	100	100
2	1	46/51 (90%)	46 (100%)	0	100	100
3	2	38/40 (95%)	38 (100%)	0	100	100
4	3	53/54 (98%)	53 (100%)	0	100	100
5	4	35/35 (100%)	34 (97%)	1 (3%)	37	68
6	6	51/66 (77%)	49 (96%)	2 (4%)	28	60
7	7	18/20 (90%)	18 (100%)	0	100	100
8	8	175/179 (98%)	175 (100%)	0	100	100
11	C	212/219 (97%)	212 (100%)	0	100	100
12	D	163/166 (98%)	163 (100%)	0	100	100
13	E	159/172 (92%)	159 (100%)	0	100	100
14	F	147/155 (95%)	147 (100%)	0	100	100
15	G	143/147 (97%)	143 (100%)	0	100	100
16	H	36/121 (30%)	36 (100%)	0	100	100
17	J	120/161 (74%)	120 (100%)	0	100	100
18	K	101/101 (100%)	101 (100%)	0	100	100
19	L	108/110 (98%)	107 (99%)	1 (1%)	70	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	M	110/114 (96%)	109 (99%)	1 (1%)	70	85
21	N	94/139 (68%)	94 (100%)	0	100	100
22	O	91/93 (98%)	91 (100%)	0	100	100
23	P	98/99 (99%)	98 (100%)	0	100	100
24	Q	97/99 (98%)	97 (100%)	0	100	100
25	R	81/83 (98%)	81 (100%)	0	100	100
26	S	87/140 (62%)	87 (100%)	0	100	100
27	T	81/83 (98%)	81 (100%)	0	100	100
28	U	77/88 (88%)	76 (99%)	1 (1%)	61	81
29	V	142/164 (87%)	142 (100%)	0	100	100
30	W	55/62 (89%)	55 (100%)	0	100	100
31	X	51/52 (98%)	51 (100%)	0	100	100
32	Y	60/66 (91%)	60 (100%)	0	100	100
33	Z	51/55 (93%)	51 (100%)	0	100	100
35	c	170/210 (81%)	170 (100%)	0	100	100
36	d	176/177 (99%)	176 (100%)	0	100	100
37	e	121/159 (76%)	121 (100%)	0	100	100
38	f	84/85 (99%)	84 (100%)	0	100	100
39	g	130/131 (99%)	130 (100%)	0	100	100
40	h	107/108 (99%)	107 (100%)	0	100	100
41	i	102/120 (85%)	102 (100%)	0	100	100
42	j	89/90 (99%)	89 (100%)	0	100	100
43	k	90/107 (84%)	90 (100%)	0	100	100
44	l	104/105 (99%)	104 (100%)	0	100	100
45	m	99/104 (95%)	99 (100%)	0	100	100
46	n	46/47 (98%)	46 (100%)	0	100	100
47	o	77/79 (98%)	77 (100%)	0	100	100
48	p	90/125 (72%)	90 (100%)	0	100	100
49	q	85/105 (81%)	85 (100%)	0	100	100
50	r	54/72 (75%)	54 (100%)	0	100	100
51	s	75/85 (88%)	75 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	t	64/65 (98%)	64 (100%)	0	100	100
53	x	453/460 (98%)	453 (100%)	0	100	100
All	All	5040/5615 (90%)	5034 (100%)	6 (0%)	87	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	4	8	LYS
6	6	5	ILE
6	6	67	LYS
19	L	21	VAL
20	M	94	VAL
28	U	103	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	49	GLN
4	3	63	ASN
8	8	231	ASN
11	C	81	HIS
11	C	87	ASN
11	C	203	ASN
12	D	15	GLN
12	D	130	HIS
13	E	47	GLN
14	F	34	GLN
14	F	142	GLN
16	H	11	HIS
16	H	28	ASN
16	H	44	GLN
19	L	126	HIS
20	M	28	ASN
21	N	62	ASN
23	P	82	HIS
24	Q	27	GLN
24	Q	39	GLN
24	Q	44	ASN
24	Q	77	ASN
24	Q	122	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	S	51	GLN
27	T	41	GLN
29	V	91	GLN
29	V	124	GLN
29	V	154	GLN
30	W	12	ASN
35	c	122	GLN
35	c	176	HIS
36	d	115	HIS
36	d	173	GLN
37	e	163	ASN
40	h	117	GLN
41	i	65	HIS
41	i	67	GLN
43	k	111	GLN
43	k	126	GLN
44	l	75	GLN
44	l	77	HIS
45	m	101	GLN
47	o	50	HIS
48	p	15	ASN
51	s	57	HIS
51	s	69	HIS
52	t	7	GLN
53	x	15	HIS
53	x	126	GLN
53	x	214	HIS
53	x	255	GLN
53	x	310	GLN
53	x	391	GLN
53	x	452	ASN
53	x	518	ASN
53	x	552	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	114/115 (99%)	17 (14%)	0
34	a	1518/1537 (98%)	253 (16%)	0
54	y	76/77 (98%)	20 (26%)	0
55	z	6/26 (23%)	4 (66%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	A	3116/3138 (99%)	440 (14%)	3 (0%)
All	All	4830/4893 (98%)	734 (15%)	3 (0%)

All (734) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	9	G
9	A	12	U
9	A	14	A
9	A	15	G
9	A	25	U
9	A	51	G
9	A	62	G
9	A	63	A
9	A	71	A
9	A	74	U
9	A	75	G
9	A	118	A
9	A	119	A
9	A	120	U
9	A	123	G
9	A	128	C
9	A	143	G
9	A	151	A
9	A	158	U
9	A	165	A
9	A	167	A
9	A	176	G
9	A	183	A
9	A	197	A
9	A	198	A
9	A	201	A
9	A	203	C
9	A	206	A
9	A	217	G
9	A	218	A
9	A	224	A
9	A	230	U
9	A	231	U
9	A	232	G
9	A	250	G
9	A	251	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	252	G
9	A	268	G
9	A	287	G
9	A	289	A
9	A	293	G
9	A	298	G
9	A	301	G
9	A	302	U
9	A	303	U
9	A	328	A
9	A	332	C
9	A	339	C
9	A	358	U
9	A	362	A
9	A	370	G
9	A	372	G
9	A	377	G
9	A	390	G
9	A	394	U
9	A	401	C
9	A	405	A
9	A	413	A
9	A	415	A
9	A	428	A
9	A	435	G
9	A	446	A
9	A	447	G
9	A	475	G
9	A	476	U
9	A	493	C
9	A	494	C
9	A	500	G
9	A	501	A
9	A	544	U
9	A	545	U
9	A	566	A
9	A	570	G
9	A	573	C
9	A	592	G
9	A	593	A
9	A	595	U
9	A	596	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	597	C
9	A	618	U
9	A	619	C
9	A	620	C
9	A	621	G
9	A	635	U
9	A	637	C
9	A	639	U
9	A	641	U
9	A	642	C
9	A	643	C
9	A	644	G
9	A	645	G
9	A	653	U
9	A	665	G
9	A	669	U
9	A	675	G
9	A	676	A
9	A	677	A
9	A	689	G
9	A	694	G
9	A	695	G
9	A	706	A
9	A	718	G
9	A	732	G
9	A	735	A
9	A	738	G
9	A	741	A
9	A	749	U
9	A	756	A
9	A	758	C
9	A	759	C
9	A	766	G
9	A	767	C
9	A	769	U
9	A	773	C
9	A	778	G
9	A	779	U
9	A	780	G
9	A	781	A
9	A	782	A
9	A	783	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	797	G
9	A	799	A
9	A	808	G
9	A	815	U
9	A	817	U
9	A	843	U
9	A	852	G
9	A	859	C
9	A	865	C
9	A	876	U
9	A	891	U
9	A	894	G
9	A	899	G
9	A	904	G
9	A	905	G
9	A	906	G
9	A	910	A
9	A	911	A
9	A	913	G
9	A	914	G
9	A	921	A
9	A	926	C
9	A	929	U
9	A	930	G
9	A	934	G
9	A	938	G
9	A	941	C
9	A	943	C
9	A	956	U
9	A	957	U
9	A	988	G
9	A	1025	A
9	A	1026	C
9	A	1039	A
9	A	1040	A
9	A	1044	C
9	A	1059	A
9	A	1069	A
9	A	1074	G
9	A	1087	A
9	A	1089	G
9	A	1096	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1102	A
9	A	1103	A
9	A	1112	A
9	A	1118	G
9	A	1125	G
9	A	1135	C
9	A	1138	A
9	A	1142	G
9	A	1151	G
9	A	1155	G
9	A	1159	G
9	A	1162	U
9	A	1176	G
9	A	1177	A
9	A	1186	A
9	A	1187	G
9	A	1189	U
9	A	1190	U
9	A	1191	G
9	A	1195	U
9	A	1196	A
9	A	1199	A
9	A	1200	G
9	A	1201	C
9	A	1202	A
9	A	1207	C
9	A	1208	C
9	A	1212	G
9	A	1216	G
9	A	1217	A
9	A	1218	G
9	A	1219	U
9	A	1221	C
9	A	1225	A
9	A	1226	U
9	A	1234	U
9	A	1237	U
9	A	1240	A
9	A	1241	G
9	A	1248	U
9	A	1259	U
9	A	1261	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1262	A
9	A	1264	C
9	A	1265	G
9	A	1271	C
9	A	1273	A
9	A	1302	C
9	A	1304	U
9	A	1305	U
9	A	1308	G
9	A	1342	C
9	A	1343	G
9	A	1368	A
9	A	1381	G
9	A	1384	A
9	A	1387	G
9	A	1390	G
9	A	1396	A
9	A	1399	A
9	A	1402	G
9	A	1403	A
9	A	1404	C
9	A	1406	A
9	A	1432	A
9	A	1437	C
9	A	1452	C
9	A	1456	C
9	A	1461	C
9	A	1483	U
9	A	1491	G
9	A	1496	A
9	A	1499	G
9	A	1501	C
9	A	1510	U
9	A	1515	A
9	A	1545	G
9	A	1567	U
9	A	1568	A
9	A	1571	A
9	A	1580	A
9	A	1581	A
9	A	1592	U
9	A	1609	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1622	G
9	A	1636	U
9	A	1646	G
9	A	1656	G
9	A	1657	A
9	A	1658	A
9	A	1665	A
9	A	1666	C
9	A	1693	G
9	A	1696	A
9	A	1697	A
9	A	1698	C
9	A	1705	G
9	A	1720	G
9	A	1722	G
9	A	1727	A
9	A	1730	C
9	A	1746	U
9	A	1754	A
9	A	1768	G
9	A	1773	U
9	A	1774	U
9	A	1775	G
9	A	1776	A
9	A	1791	U
9	A	1792	C
9	A	1803	A
9	A	1806	A
9	A	1809	A
9	A	1821	G
9	A	1832	G
9	A	1833	C
9	A	1841	C
9	A	1842	C
9	A	1843	A
9	A	1845	A
9	A	1865	A
9	A	1881	U
9	A	1883	C
9	A	1888	U
9	A	1889	A
9	A	1909	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1948	A
9	A	1949	U
9	A	1950	A
9	A	1964	U
9	A	1966	C
9	A	1967	G
9	A	1970	G
9	A	1990	G
9	A	1992	A
9	A	1998	U
9	A	2007	A
9	A	2010	G
9	A	2025	A
9	A	2034	C
9	A	2035	G
9	A	2043	A
9	A	2045	G
9	A	2050	U
9	A	2061	U
9	A	2063	A
9	A	2094	C
9	A	2105	G
9	A	2107	A
9	A	2108	A
9	A	2109	G
9	A	2132	C
9	A	2144	G
9	A	2152	C
9	A	2167	G
9	A	2168	G
9	A	2175	A
9	A	2176	A
9	A	2180	C
9	A	2193	U
9	A	2203	C
9	A	2205	C
9	A	2208	A
9	A	2209	U
9	A	2210	G
9	A	2223	C
9	A	2229	U
9	A	2231	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	2261	A
9	A	2269	A
9	A	2270	G
9	A	2281	C
9	A	2290	G
9	A	2293	C
9	A	2294	G
9	A	2297	A
9	A	2298	A
9	A	2299	G
9	A	2329	U
9	A	2330	G
9	A	2349	G
9	A	2350	U
9	A	2353	G
9	A	2354	A
9	A	2356	A
9	A	2363	A
9	A	2364	G
9	A	2370	G
9	A	2371	A
9	A	2373	A
9	A	2383	C
9	A	2384	A
9	A	2388	G
9	A	2390	G
9	A	2392	C
9	A	2396	G
9	A	2397	U
9	A	2408	A
9	A	2427	G
9	A	2435	A
9	A	2463	A
9	A	2476	G
9	A	2477	G
9	A	2489	G
9	A	2497	G
9	A	2517	G
9	A	2521	C
9	A	2525	A
9	A	2543	A
9	A	2545	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	2546	G
9	A	2558	C
9	A	2559	G
9	A	2560	A
9	A	2563	G
9	A	2565	A
9	A	2573	A
9	A	2574	A
9	A	2583	G
9	A	2585	C
9	A	2588	C
9	A	2621	G
9	A	2623	A
9	A	2629	G
9	A	2641	C
9	A	2644	A
9	A	2661	U
9	A	2663	A
9	A	2667	G
9	A	2668	A
9	A	2678	C
9	A	2679	C
9	A	2686	A
9	A	2712	C
9	A	2714	A
9	A	2716	A
9	A	2729	U
9	A	2742	U
9	A	2743	G
9	A	2751	G
9	A	2756	A
9	A	2767	G
9	A	2773	G
9	A	2781	G
9	A	2792	U
9	A	2804	A
9	A	2805	G
9	A	2810	A
9	A	2811	C
9	A	2816	G
9	A	2820	G
9	A	2840	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	2847	U
9	A	2851	U
9	A	2853	U
9	A	2868	A
9	A	2884	C
9	A	2899	G
9	A	2901	G
9	A	2952	G
9	A	2964	C
9	A	2977	U
9	A	2986	A
9	A	3016	A
9	A	3018	C
9	A	3038	U
9	A	3040	G
9	A	3053	C
9	A	3056	A
9	A	3059	A
9	A	3068	C
9	A	3070	A
9	A	3107	A
9	A	3112	G
9	A	3118	A
9	A	3121	G
9	A	3128	A
9	A	3129	A
10	B	3	A
10	B	4	C
10	B	8	G
10	B	14	A
10	B	24	A
10	B	40	U
10	B	43	G
10	B	44	A
10	B	55	U
10	B	56	A
10	B	64	C
10	B	84	C
10	B	85	U
10	B	101	G
10	B	105	A
10	B	114	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	B	115	A
34	a	12	G
34	a	25	G
34	a	35	A
34	a	42	G
34	a	50	C
34	a	51	U
34	a	53	A
34	a	54	A
34	a	61	C
34	a	78	U
34	a	86	G
34	a	89	A
34	a	90	U
34	a	91	A
34	a	92	C
34	a	93	U
34	a	116	C
34	a	117	A
34	a	125	G
34	a	127	U
34	a	142	G
34	a	167	A
34	a	169	U
34	a	178	G
34	a	179	G
34	a	180	A
34	a	185	G
34	a	186	G
34	a	189	U
34	a	192	A
34	a	194	G
34	a	203	U
34	a	204	G
34	a	206	A
34	a	213	U
34	a	214	U
34	a	215	U
34	a	216	A
34	a	217	G
34	a	219	G
34	a	244	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	246	G
34	a	247	C
34	a	250	G
34	a	265	G
34	a	266	C
34	a	270	C
34	a	278	A
34	a	280	G
34	a	288	G
34	a	320	A
34	a	326	A
34	a	328	A
34	a	329	C
34	a	346	G
34	a	351	C
34	a	353	G
34	a	355	A
34	a	366	U
34	a	371	C
34	a	372	A
34	a	387	G
34	a	389	U
34	a	391	C
34	a	397	C
34	a	403	G
34	a	405	G
34	a	410	A
34	a	411	U
34	a	412	G
34	a	420	U
34	a	421	C
34	a	422	G
34	a	428	U
34	a	434	U
34	a	438	U
34	a	440	A
34	a	451	A
34	a	452	G
34	a	453	G
34	a	455	C
34	a	457	G
34	a	459	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	460	U
34	a	461	U
34	a	463	U
34	a	465	U
34	a	466	C
34	a	467	G
34	a	470	U
34	a	473	A
34	a	475	G
34	a	476	G
34	a	485	G
34	a	488	G
34	a	502	C
34	a	503	U
34	a	504	A
34	a	509	C
34	a	512	G
34	a	517	C
34	a	518	G7M
34	a	524	A
34	a	529	U
34	a	536	C
34	a	538	A
34	a	550	A
34	a	553	U
34	a	555	C
34	a	557	G
34	a	563	A
34	a	564	A
34	a	567	A
34	a	568	G
34	a	570	U
34	a	598	A
34	a	611	U
34	a	623	U
34	a	624	G
34	a	630	G
34	a	644	A
34	a	656	G
34	a	657	G
34	a	686	A
34	a	694	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	709	A
34	a	712	G
34	a	740	A
34	a	746	G
34	a	749	G
34	a	768	A
34	a	784	U
34	a	785	A
34	a	805	A
34	a	806	A
34	a	808	C
34	a	832	C
34	a	833	U
34	a	834	U
34	a	836	C
34	a	837	U
34	a	838	U
34	a	845	C
34	a	863	U
34	a	866	A
34	a	878	G
34	a	882	A
34	a	883	G
34	a	893	A
34	a	895	G
34	a	900	A
34	a	907	A
34	a	910	G
34	a	911	A
34	a	919	G
34	a	925	C
34	a	927	C
34	a	928	A
34	a	941	C
34	a	953	U
34	a	959	2MG
34	a	962	A
34	a	964	G
34	a	968	A
34	a	969	G
34	a	970	A
34	a	985	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	986	G
34	a	990	U
34	a	994	C
34	a	995	A
34	a	997	G
34	a	998	A
34	a	1014	G
34	a	1016	G
34	a	1018	U
34	a	1019	C
34	a	1020	C
34	a	1021	C
34	a	1022	U
34	a	1023	U
34	a	1024	G
34	a	1025	U
34	a	1033	G
34	a	1056	U
34	a	1061	U
34	a	1069	U
34	a	1085	G
34	a	1086	U
34	a	1092	A
34	a	1117	U
34	a	1124	A
34	a	1126	G
34	a	1128	A
34	a	1129	A
34	a	1131	G
34	a	1149	A
34	a	1150	C
34	a	1151	U
34	a	1160	C
34	a	1163	C
34	a	1174	G
34	a	1176	G
34	a	1188	A
34	a	1189	A
34	a	1192	C
34	a	1205	A
34	a	1219	A
34	a	1230	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	1249	U
34	a	1250	G
34	a	1252	G
34	a	1270	G
34	a	1272	A
34	a	1277	U
34	a	1278	A
34	a	1279	A
34	a	1282	G
34	a	1292	G
34	a	1294	U
34	a	1310	A
34	a	1314	C
34	a	1327	U
34	a	1328	C
34	a	1330	G
34	a	1332	G
34	a	1345	G
34	a	1351	C
34	a	1355	A
34	a	1356	A
34	a	1363	G
34	a	1371	C
34	a	1372	G
34	a	1383	U
34	a	1387	A
34	a	1389	A
34	a	1390	C
34	a	1391	A
34	a	1394	G
34	a	1395	4OC
34	a	1419	A
34	a	1435	G
34	a	1439	A
34	a	1480	G
34	a	1485	A
34	a	1486	A
34	a	1492	A
34	a	1496	A
34	a	1498	G
34	a	1510	G
34	a	1512	MA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	1522	G
34	a	1523	G
54	y	4	G
54	y	5	G
54	y	9	G
54	y	13	C
54	y	14	A
54	y	17	C
54	y	18	U
54	y	19	G
54	y	20	G
54	y	21	U
54	y	22	A
54	y	26	C
54	y	44	A
54	y	49	C
54	y	53	G
54	y	54	G
54	y	60	A
54	y	66	C
54	y	74	A
54	y	77	A
55	z	2	A
55	z	3	C
55	z	4	A
55	z	7	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	913	G
9	A	2349	G
9	A	2488	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	UR3	a	1491	34	19,22,23	2.63	6 (31%)	26,32,35	1.82	4 (15%)
9	OMG	A	2791	9	23,26,27	2.30	9 (39%)	32,38,41	1.93	7 (21%)
34	MA6	a	1511	34	23,26,27	1.64	5 (21%)	33,38,41	3.17	12 (36%)
34	5MC	a	960	34	19,22,23	3.54	8 (42%)	26,32,35	0.98	1 (3%)
34	MA6	a	1512	34	23,26,27	1.55	4 (17%)	33,38,41	3.27	12 (36%)
34	G7M	a	518	34	23,26,27	3.50	11 (47%)	34,39,42	1.76	8 (23%)
34	2MG	a	959	34	23,26,27	2.77	7 (30%)	33,38,41	2.41	9 (27%)
9	5MU	A	2177	9	19,22,23	4.71	7 (36%)	27,32,35	3.72	9 (33%)
34	4OC	a	1395	34	20,23,24	3.01	8 (40%)	25,32,35	0.94	2 (8%)

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
34	UR3	a	1491	34	-	1/7/25/26	0/2/2/2
9	OMG	A	2791	9	-	0/9/27/28	0/3/3/3
34	MA6	a	1511	34	-	0/11/29/30	0/3/3/3
34	5MC	a	960	34	-	0/7/25/26	0/2/2/2
34	MA6	a	1512	34	-	3/11/29/30	0/3/3/3
34	G7M	a	518	34	-	0/7/25/26	0/3/3/3
34	2MG	a	959	34	-	2/9/27/28	0/3/3/3
9	5MU	A	2177	9	-	0/7/25/26	0/2/2/2
34	4OC	a	1395	34	-	2/9/29/30	0/2/2/2

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2177	5MU	C6-N1	10.50	1.55	1.38
9	A	2177	5MU	C2-N1	10.28	1.54	1.38
34	a	518	G7M	C8-N7	10.20	1.50	1.33
9	A	2177	5MU	C4-C5	8.91	1.59	1.44
34	a	960	5MC	C6-C5	8.79	1.48	1.34
9	A	2177	5MU	C4-N3	-8.15	1.23	1.38
34	a	959	2MG	C2-N3	7.04	1.45	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1395	4OC	C4-N3	6.75	1.44	1.32
34	a	959	2MG	C4-N3	6.60	1.49	1.34
34	a	960	5MC	C4-N3	6.37	1.44	1.34
34	a	1491	UR3	C6-C5	6.28	1.49	1.35
34	a	1491	UR3	C2-N1	6.19	1.47	1.38
34	a	1395	4OC	C6-C5	6.16	1.49	1.35
9	A	2177	5MU	C6-C5	6.07	1.44	1.34
34	a	1395	4OC	C2-N3	6.02	1.48	1.36
9	A	2791	OMG	C4-N3	5.98	1.47	1.34
34	a	960	5MC	C2-N3	5.84	1.47	1.36
34	a	959	2MG	C2-N2	5.49	1.44	1.33
34	a	518	G7M	C8-N9	5.48	1.50	1.35
34	a	518	G7M	C2-N3	5.48	1.46	1.33
34	a	518	G7M	C4-N3	5.40	1.46	1.34
34	a	960	5MC	C5-C4	5.14	1.48	1.44
9	A	2791	OMG	C2-N3	5.11	1.45	1.33
34	a	1491	UR3	C2-N3	5.09	1.49	1.39
34	a	518	G7M	C2-N2	4.75	1.45	1.34
34	a	1395	4OC	C4-N4	4.49	1.45	1.36
34	a	518	G7M	C5-N7	4.46	1.44	1.39
34	a	960	5MC	C4-N4	4.23	1.44	1.34
34	a	959	2MG	C2-N1	4.18	1.43	1.36
34	a	960	5MC	C6-N1	4.09	1.45	1.38
34	a	1511	MA6	C6-N6	4.01	1.47	1.36
9	A	2791	OMG	C2-N2	3.90	1.43	1.34
34	a	1512	MA6	C6-N6	3.79	1.47	1.36
34	a	960	5MC	C2-N1	3.72	1.47	1.40
34	a	1511	MA6	C5-C4	-3.70	1.32	1.39
34	a	1395	4OC	C2-N1	3.61	1.47	1.40
34	a	1512	MA6	C5-C4	-3.60	1.32	1.39
9	A	2177	5MU	O4-C4	-3.40	1.17	1.23
34	a	959	2MG	C5-N7	-3.39	1.32	1.39
34	a	518	G7M	C2-N1	3.32	1.45	1.37
9	A	2791	OMG	C5-N7	-3.12	1.32	1.39
34	a	518	G7M	C5-C6	3.11	1.51	1.43
9	A	2177	5MU	O2-C2	-3.08	1.17	1.23
34	a	1395	4OC	C5-C4	3.07	1.47	1.41
34	a	960	5MC	O2-C2	-3.06	1.18	1.23
9	A	2791	OMG	O6-C6	-3.03	1.17	1.23
34	a	1395	4OC	C6-N1	3.02	1.45	1.38
34	a	1511	MA6	C5-N7	-3.00	1.33	1.39
34	a	1512	MA6	C5-N7	-2.93	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1395	4OC	O2-C2	-2.87	1.18	1.23
34	a	518	G7M	O6-C6	-2.83	1.18	1.23
34	a	959	2MG	O6-C6	-2.77	1.18	1.23
34	a	1511	MA6	C8-N9	-2.76	1.32	1.37
34	a	1512	MA6	C8-N9	-2.70	1.33	1.37
34	a	1491	UR3	C6-N1	2.69	1.44	1.38
34	a	518	G7M	C6-N1	2.66	1.43	1.38
34	a	1511	MA6	C4-N9	-2.46	1.32	1.37
9	A	2791	OMG	C4-N9	-2.27	1.32	1.38
34	a	1491	UR3	O2-C2	-2.27	1.18	1.22
9	A	2791	OMG	C2-N1	2.20	1.43	1.37
34	a	959	2MG	C5-C6	2.19	1.52	1.44
9	A	2791	OMG	C5-C6	2.18	1.52	1.44
9	A	2791	OMG	C6-N1	2.18	1.42	1.38
34	a	518	G7M	C4-N9	2.07	1.43	1.38
34	a	1491	UR3	O4-C4	-2.04	1.19	1.23

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2177	5MU	C5-C4-N3	12.36	126.06	115.32
34	a	1512	MA6	N1-C6-N6	-11.21	103.20	116.86
34	a	1511	MA6	N1-C6-N6	-10.93	103.54	116.86
9	A	2177	5MU	C5-C6-N1	-9.51	112.98	123.31
34	a	1511	MA6	C5-C6-N6	8.06	138.10	125.33
34	a	1512	MA6	C5-C6-N6	7.90	137.84	125.33
34	a	959	2MG	C2-N3-C4	7.72	121.65	112.00
34	a	959	2MG	C5-C4-N3	-6.39	118.22	128.39
34	a	1512	MA6	N1-C2-N3	-6.18	119.23	128.58
34	a	1511	MA6	N1-C2-N3	-5.92	119.62	128.58
34	a	1491	UR3	C4-N3-C2	-5.84	119.88	124.58
9	A	2791	OMG	C5-C4-N3	-5.24	120.06	128.39
9	A	2177	5MU	O4-C4-C5	-5.20	118.97	124.92
9	A	2177	5MU	C4-N3-C2	-4.94	120.86	127.34
34	a	1512	MA6	C5-C4-N3	-4.93	119.92	126.72
9	A	2791	OMG	C2-N3-C4	4.89	120.72	112.30
9	A	2177	5MU	N3-C2-N1	4.85	121.21	114.89
34	a	1511	MA6	N9-C8-N7	-4.83	107.08	113.94
34	a	518	G7M	C2-N3-C4	4.76	120.49	112.30
34	a	959	2MG	C2-N1-C6	-4.52	119.09	124.55
34	a	1512	MA6	N9-C8-N7	-4.28	107.86	113.94
34	a	959	2MG	N9-C4-N3	4.27	134.49	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	518	G7M	C5-C6-N1	4.17	120.45	111.84
34	a	518	G7M	C5-C4-N3	-4.14	120.33	128.15
34	a	1512	MA6	C4-C5-C6	4.09	120.14	115.91
34	a	1511	MA6	C2-N1-C6	3.96	121.49	111.83
34	a	1491	UR3	C5-C4-N3	3.89	120.17	115.04
34	a	1512	MA6	C2-N1-C6	3.77	121.04	111.83
34	a	1511	MA6	C4-C5-C6	3.69	119.73	115.91
9	A	2177	5MU	C5M-C5-C4	3.68	122.71	118.78
34	a	1512	MA6	C2-N3-C4	3.64	120.71	111.83
34	a	1511	MA6	C5-C4-N3	-3.61	121.75	126.72
9	A	2177	5MU	C5M-C5-C6	-3.59	117.99	122.85
34	a	1491	UR3	C1'-N1-C2	3.44	122.67	117.04
34	a	959	2MG	N1-C2-N2	3.40	120.03	116.56
9	A	2791	OMG	C2-N1-C6	-3.26	119.20	125.11
34	a	1512	MA6	C5-N7-C8	3.15	108.41	103.45
9	A	2177	5MU	O2-C2-N1	-3.12	118.73	122.80
34	a	960	5MC	C5-C6-N1	-3.06	119.99	123.31
34	a	1511	MA6	C5-N7-C8	3.05	108.25	103.45
9	A	2791	OMG	N9-C8-N7	-2.97	107.89	113.40
9	A	2791	OMG	N9-C4-N3	2.96	131.87	125.95
34	a	518	G7M	C2-N1-C6	-2.95	119.75	125.11
34	a	1511	MA6	C2-N3-C4	2.95	119.03	111.83
34	a	518	G7M	O6-C6-C5	-2.91	121.51	128.01
34	a	959	2MG	C5-C6-N1	2.89	120.62	113.25
34	a	1511	MA6	C4-N9-C8	2.89	108.77	105.74
34	a	1512	MA6	C4-C5-N7	-2.86	107.32	110.58
9	A	2791	OMG	C5-C6-N1	2.84	120.49	113.25
34	a	1512	MA6	C5-C4-N9	2.80	108.86	105.81
9	A	2177	5MU	O4-C4-N3	-2.75	114.95	120.11
9	A	2791	OMG	O6-C6-C5	-2.67	119.50	126.53
34	a	959	2MG	O6-C6-C5	-2.63	119.58	126.53
34	a	1511	MA6	C4-C5-N7	-2.53	107.68	110.58
34	a	959	2MG	N9-C8-N7	-2.52	108.73	113.40
34	a	1491	UR3	C6-N1-C2	-2.51	119.75	121.80
34	a	959	2MG	N1-C2-N3	-2.38	119.67	123.68
34	a	518	G7M	C5-C4-N9	2.37	110.94	105.88
34	a	1512	MA6	N3-C4-N9	2.37	131.20	127.17
34	a	1511	MA6	C5-C4-N9	2.21	108.22	105.81
34	a	518	G7M	CN7-N7-C5	2.20	129.54	126.80
34	a	518	G7M	N9-C8-N7	-2.14	107.28	112.48
34	a	1395	4OC	C6-C5-C4	2.08	119.50	117.00
34	a	1395	4OC	C5-C4-N3	-2.02	119.44	122.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	1395	4OC	O4'-C4'-C5'-O5'
34	a	1512	MA6	O4'-C4'-C5'-O5'
34	a	1512	MA6	C3'-C4'-C5'-O5'
34	a	959	2MG	C3'-C4'-C5'-O5'
34	a	1395	4OC	C3'-C4'-C5'-O5'
34	a	959	2MG	O4'-C4'-C5'-O5'
34	a	1512	MA6	C4'-C5'-O5'-P
34	a	1491	UR3	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	518	G7M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 454 ligands modelled in this entry, 451 are monoatomic - leaving 3 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	$\# Z > 2$
58	ANP	x	601	57	33,33,33	0.91	2 (6%)	45,52,52	0.70	2 (4%)
59	FME	y	101	54	8,9,10	0.94	0	8,9,11	1.35	1 (12%)
58	ANP	x	602	57	33,33,33	0.98	2 (6%)	45,52,52	0.73	1 (2%)

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
58	ANP	x	601	57	-	5/18/38/38	0/3/3/3
59	FME	y	101	54	-	3/7/9/11	-
58	ANP	x	602	57	-	7/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	x	601	ANP	PB-O3A	-2.97	1.55	1.59
58	x	602	ANP	PB-O3A	-2.88	1.55	1.59
58	x	602	ANP	PA-O3A	-2.88	1.56	1.59
58	x	601	ANP	PA-O3A	-2.01	1.57	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	y	101	FME	C-CA-N	2.76	114.83	109.50
58	x	601	ANP	O1B-PB-N3B	-2.20	108.53	111.77
58	x	601	ANP	O1G-PG-N3B	-2.04	108.76	111.77
58	x	602	ANP	O1B-PB-N3B	-2.03	108.79	111.77

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	x	601	ANP	PB-N3B-PG-O1G
58	x	601	ANP	PG-N3B-PB-O1B
58	x	601	ANP	PG-N3B-PB-O3A
58	x	601	ANP	PA-O3A-PB-O2B
58	x	601	ANP	C5'-O5'-PA-O3A
58	x	602	ANP	PB-N3B-PG-O1G
58	x	602	ANP	PG-N3B-PB-O1B
58	x	602	ANP	PA-O3A-PB-O2B
58	x	602	ANP	C5'-O5'-PA-O1A
58	x	602	ANP	O4'-C4'-C5'-O5'
58	x	602	ANP	C3'-C4'-C5'-O5'
59	y	101	FME	CA-CB-CG-SD
59	y	101	FME	CB-CG-SD-CE
59	y	101	FME	N-CA-CB-CG

Continued on next page...

Continued from previous page...

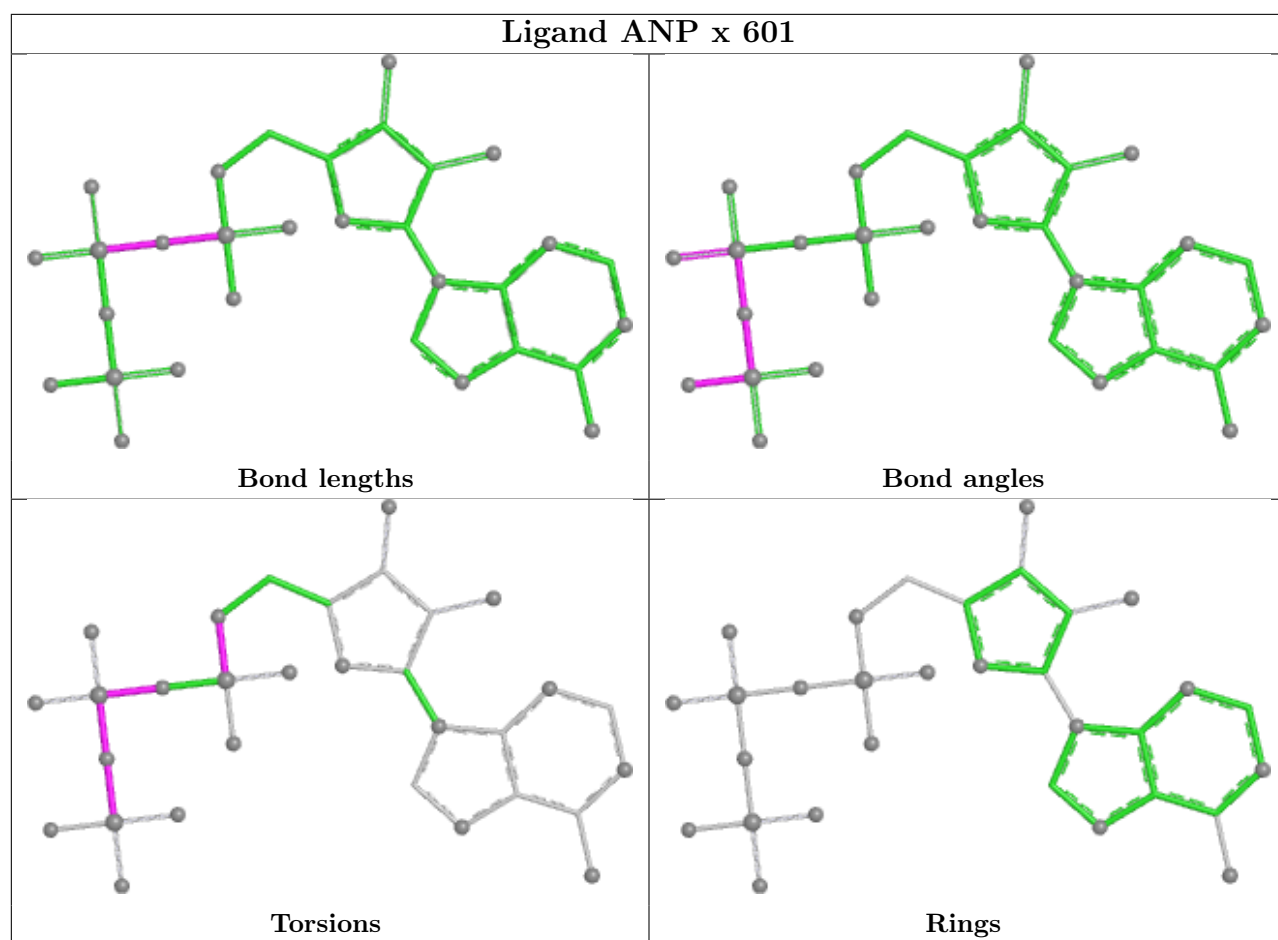
Mol	Chain	Res	Type	Atoms
58	x	602	ANP	PA-O3A-PB-O1B

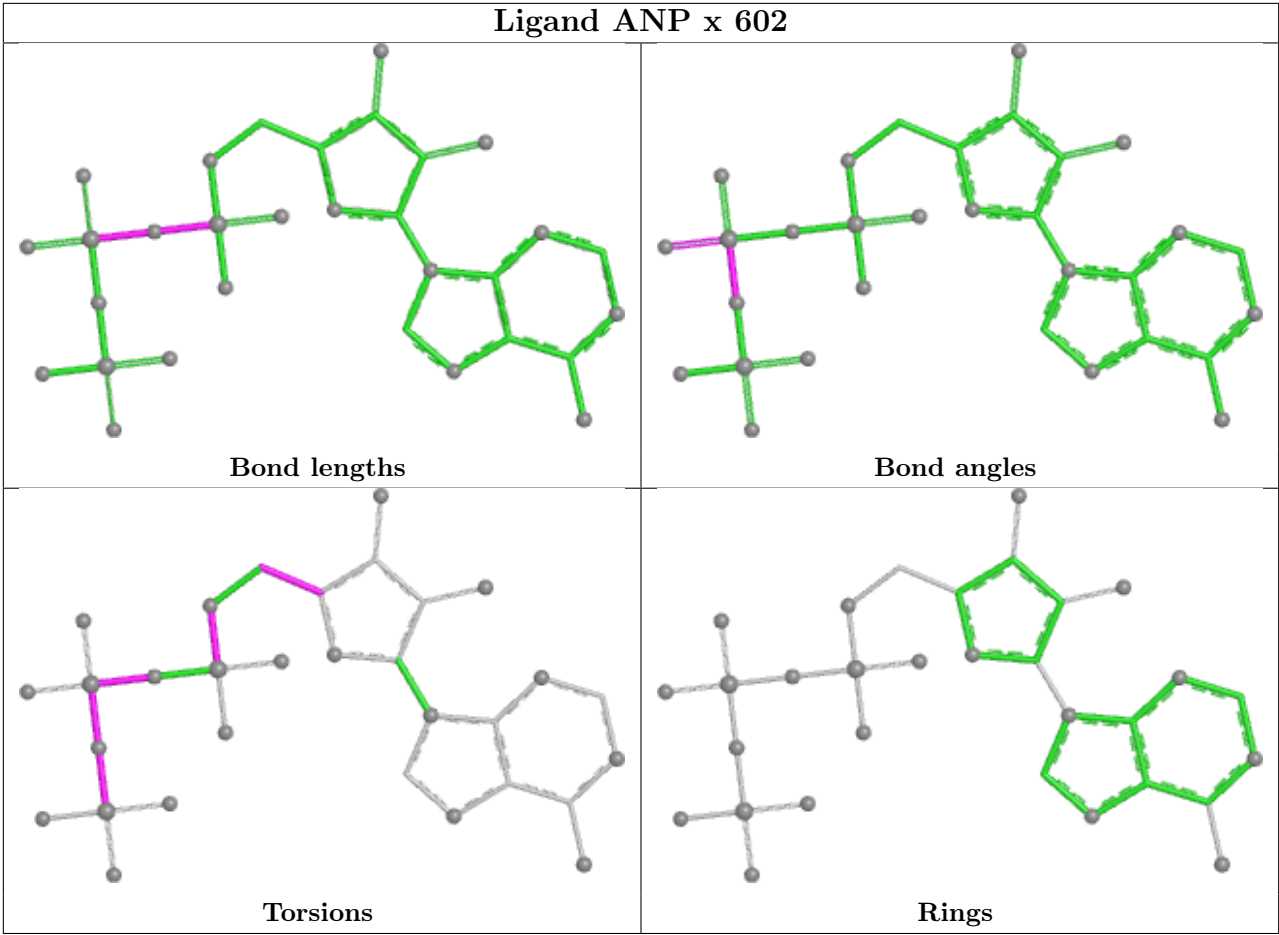
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	x	601	ANP	1	0
59	y	101	FME	1	0
58	x	602	ANP	2	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	76:U	O3'	77:A	P	3.14

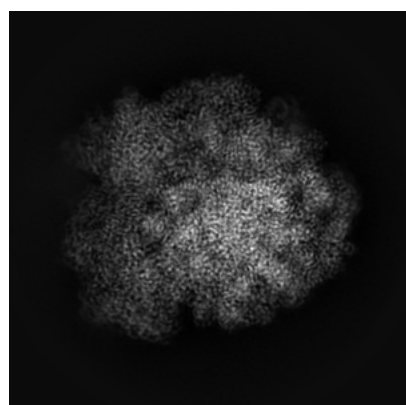
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23961. These allow visual inspection of the internal detail of the map and identification of artifacts.

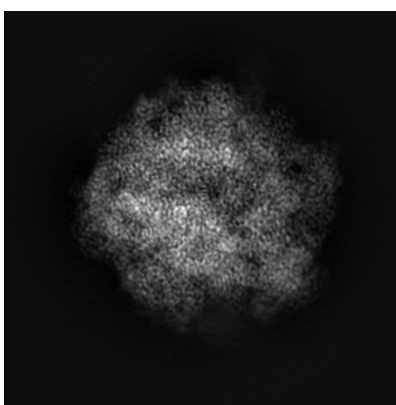
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

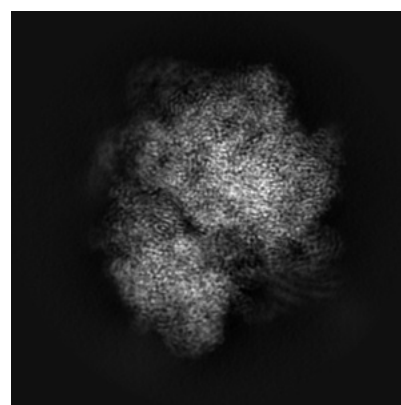
6.1.1 Primary map



X



Y

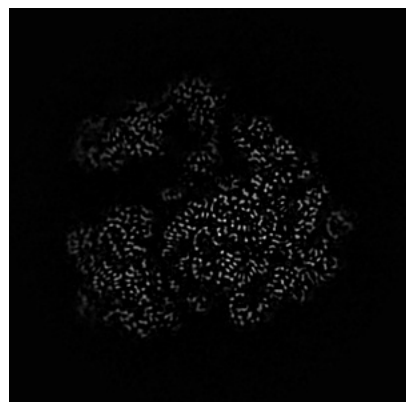


Z

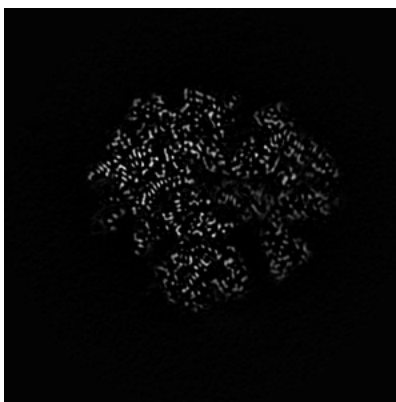
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

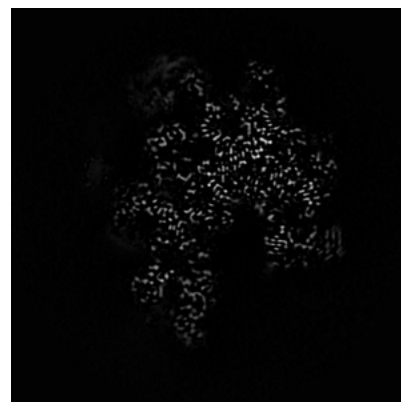
6.2.1 Primary map



X Index: 160



Y Index: 160

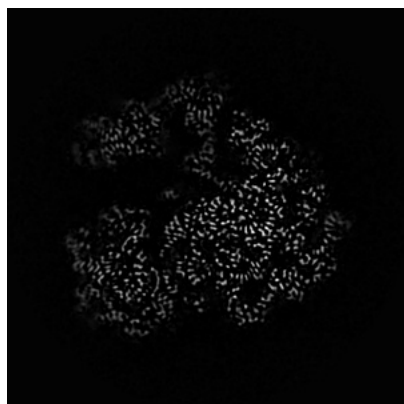


Z Index: 160

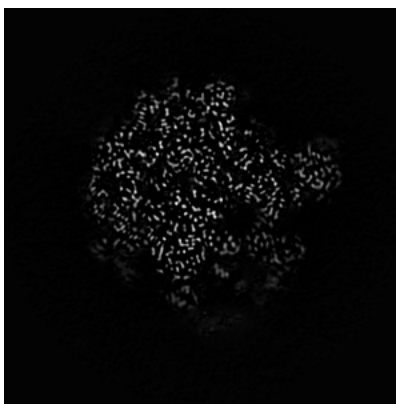
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

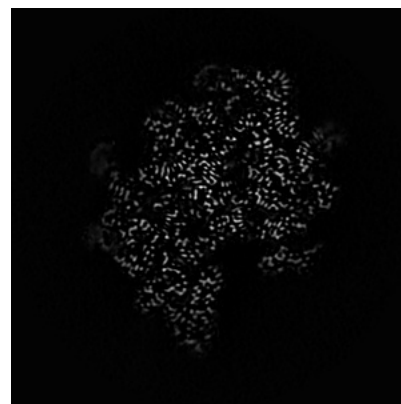
6.3.1 Primary map



X Index: 162



Y Index: 183

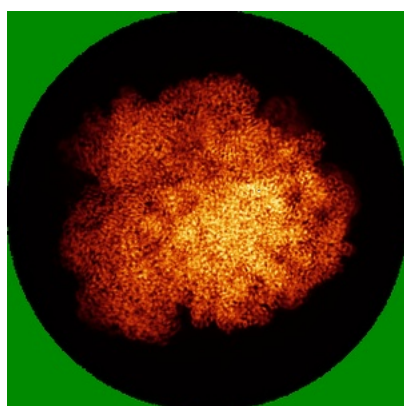


Z Index: 144

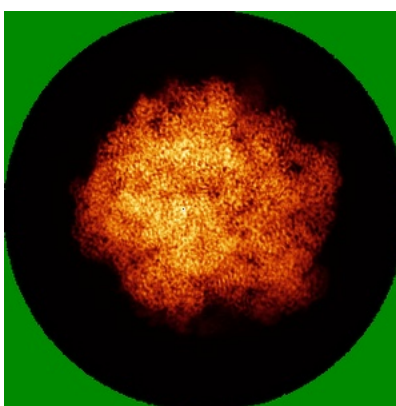
The images above show the largest variance slices of the map in three orthogonal directions.

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

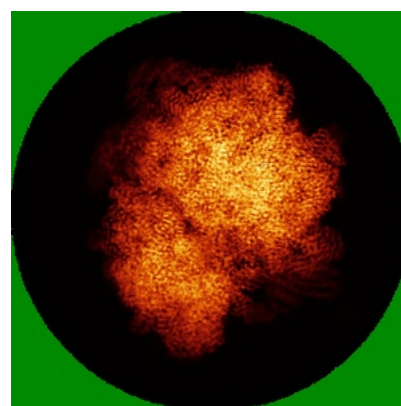
6.4.1 Primary map



X



Y

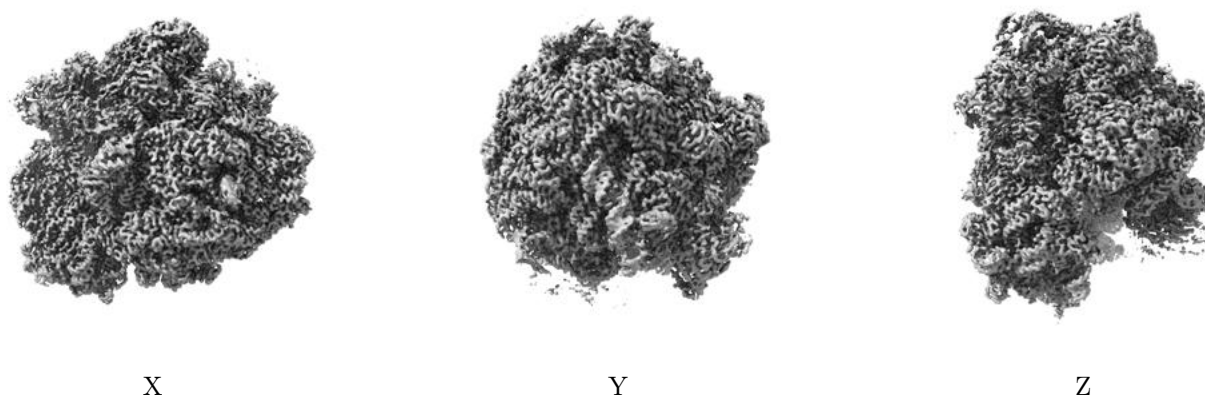


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

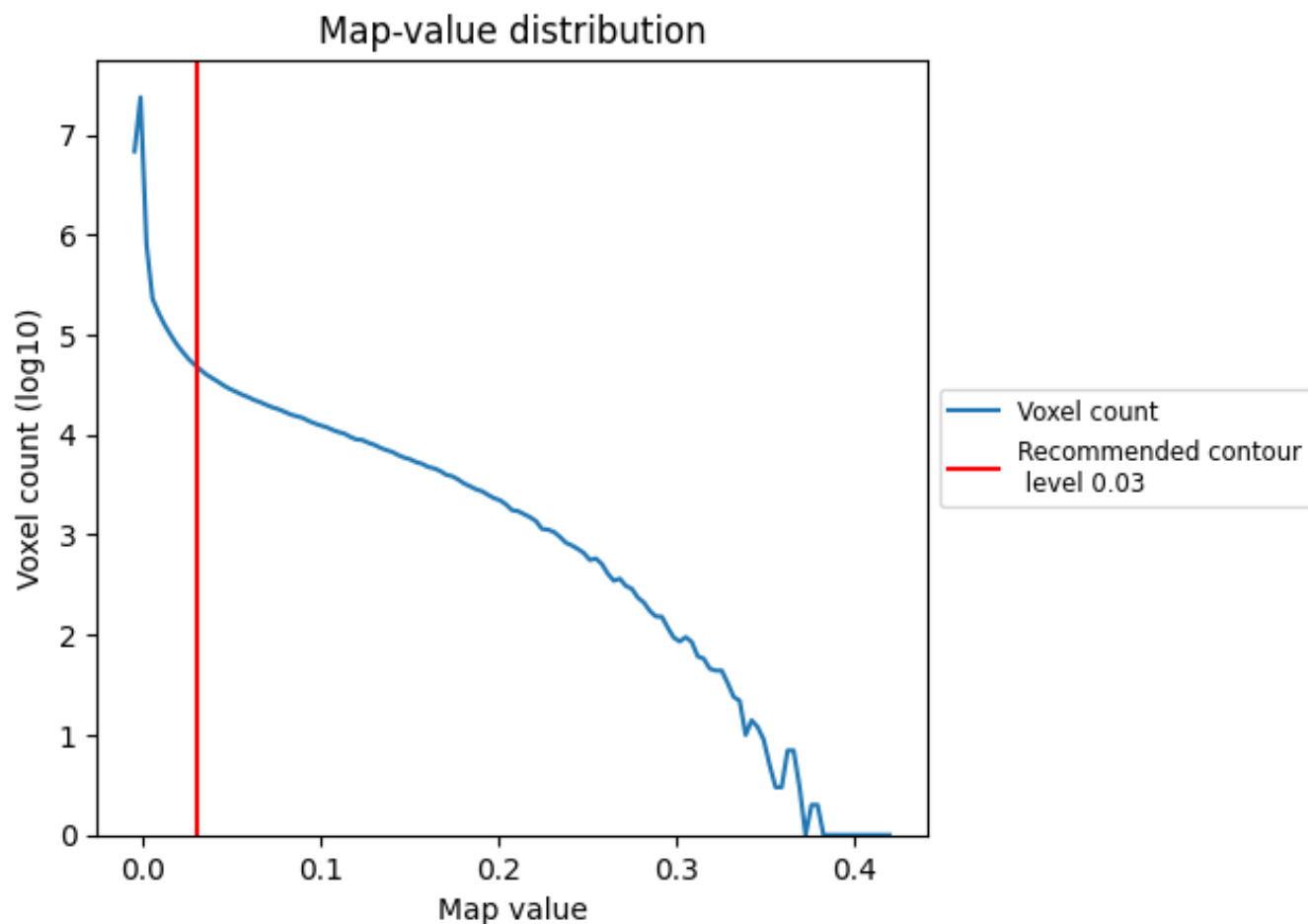
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

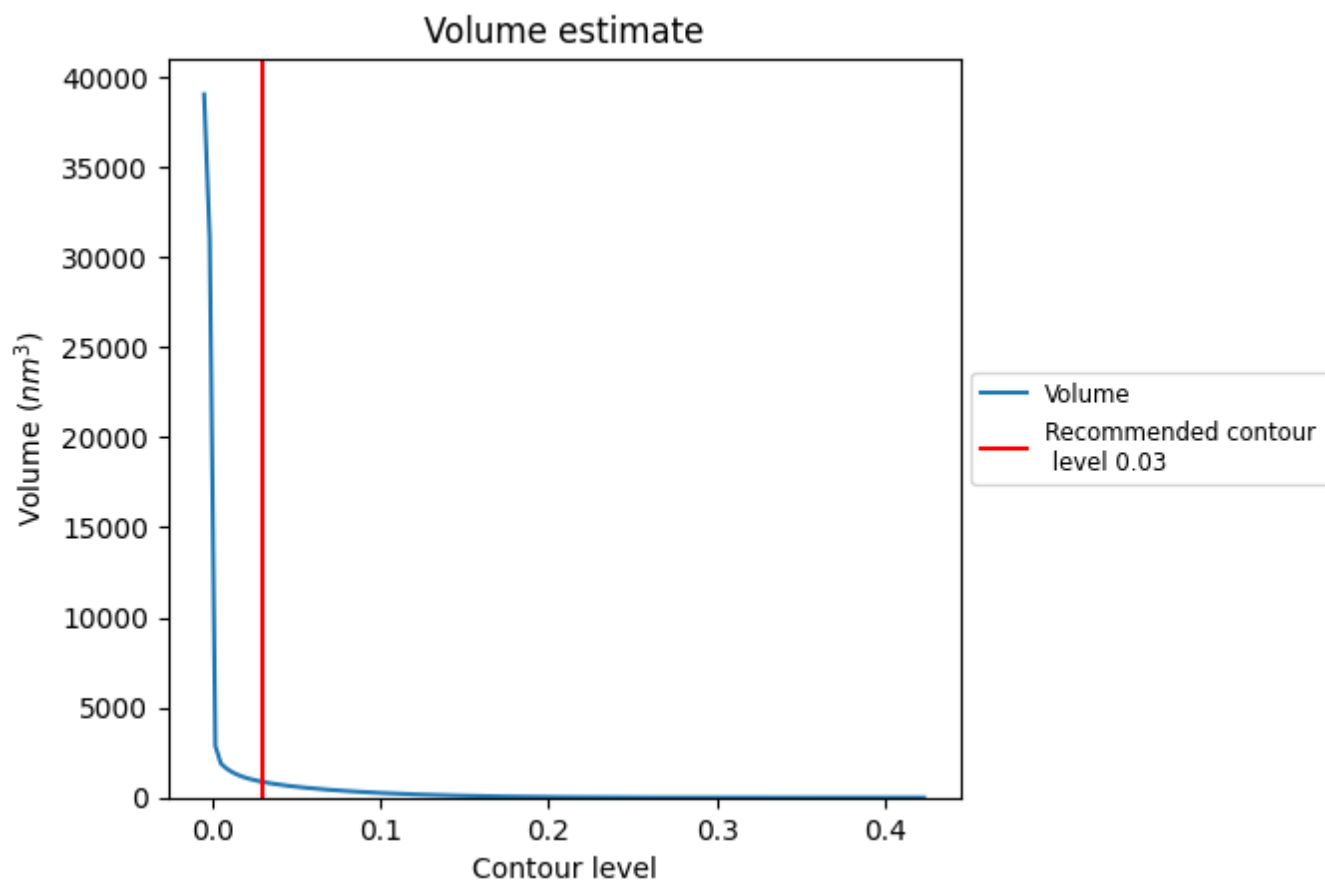
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

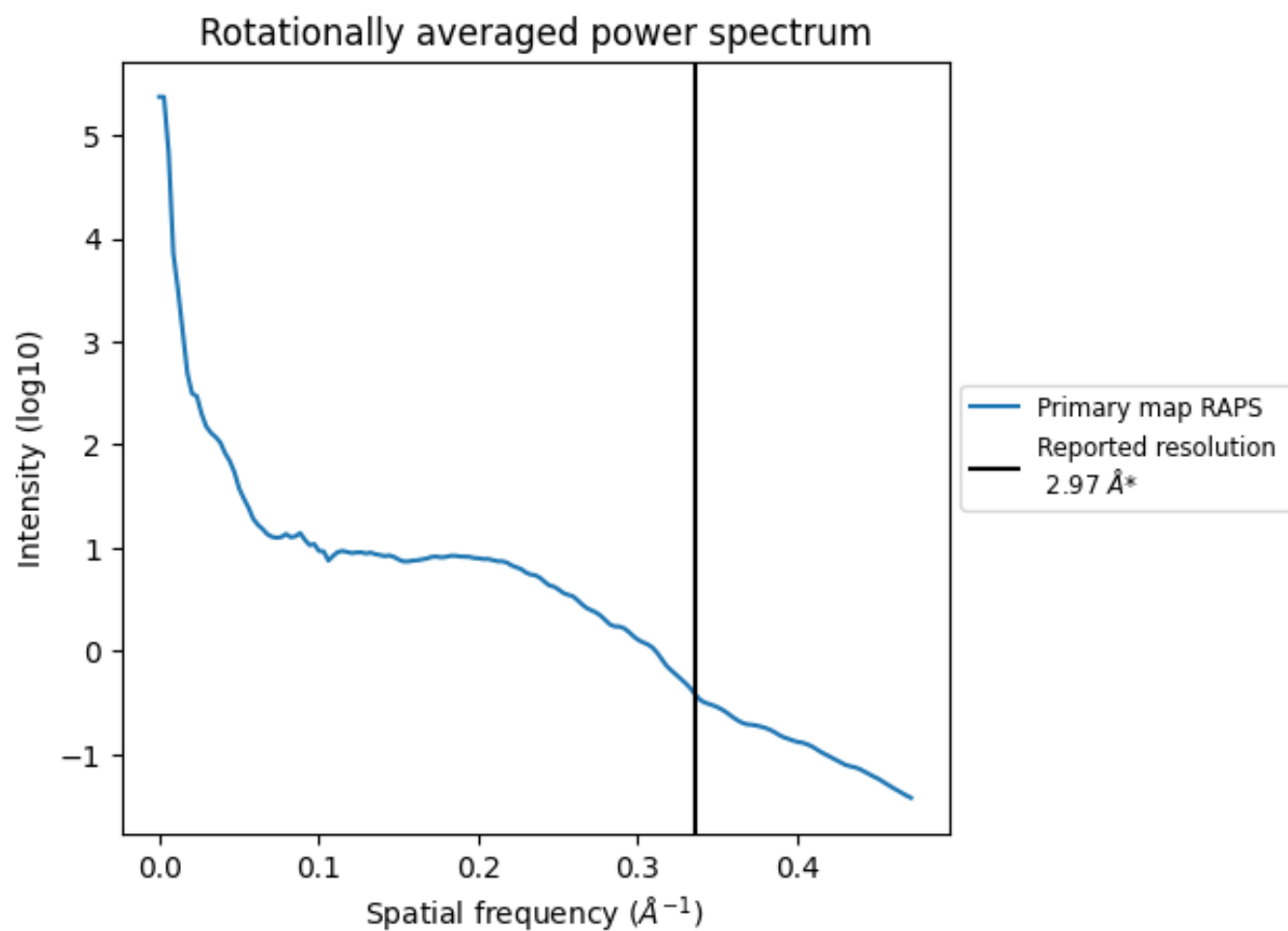
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 873 nm³; this corresponds to an approximate mass of 788 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

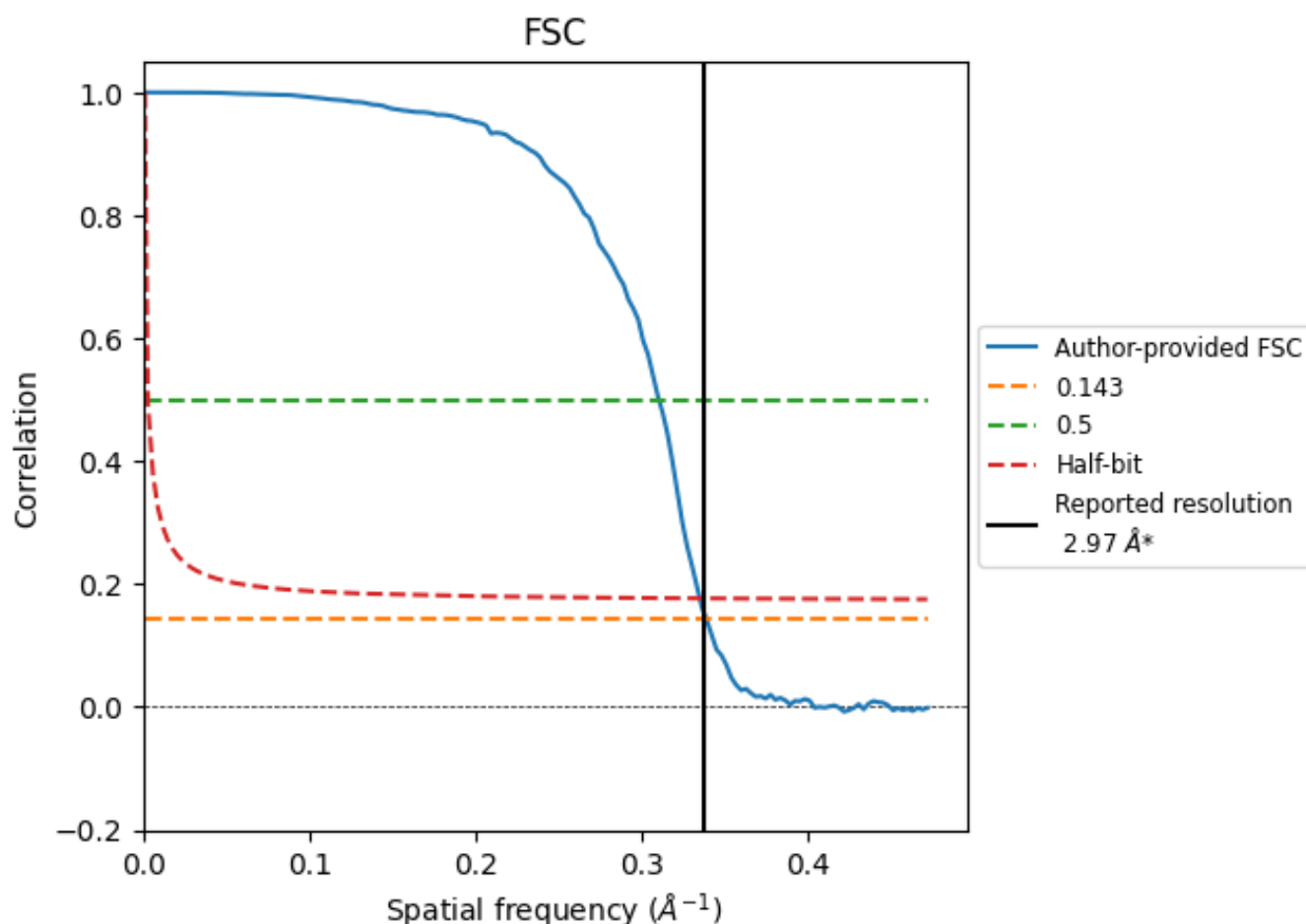


*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

8.2 Resolution estimates [i](#)

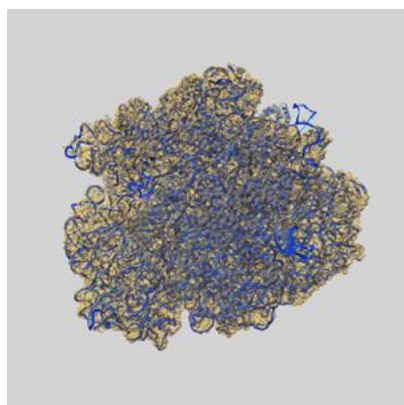
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.95	3.22	2.99
Unmasked-calculated*	-	-	-

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

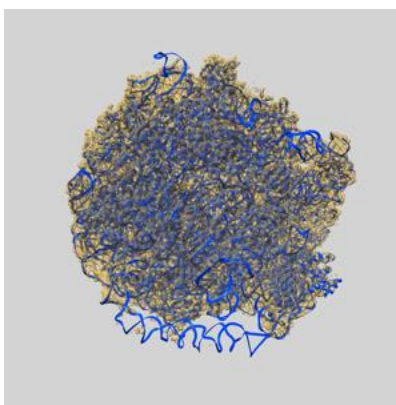
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23961 and PDB model 7MSC. Per-residue inclusion information can be found in section 3 on page 17.

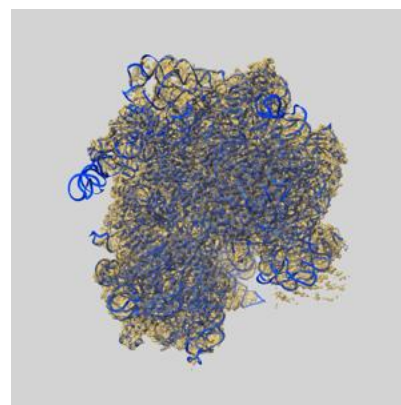
9.1 Map-model overlay [i](#)



X



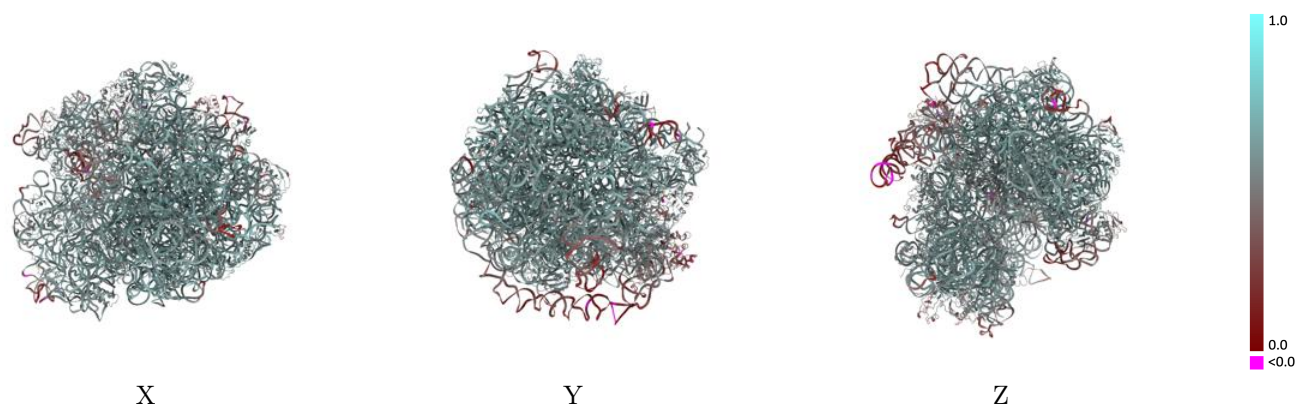
Y



Z

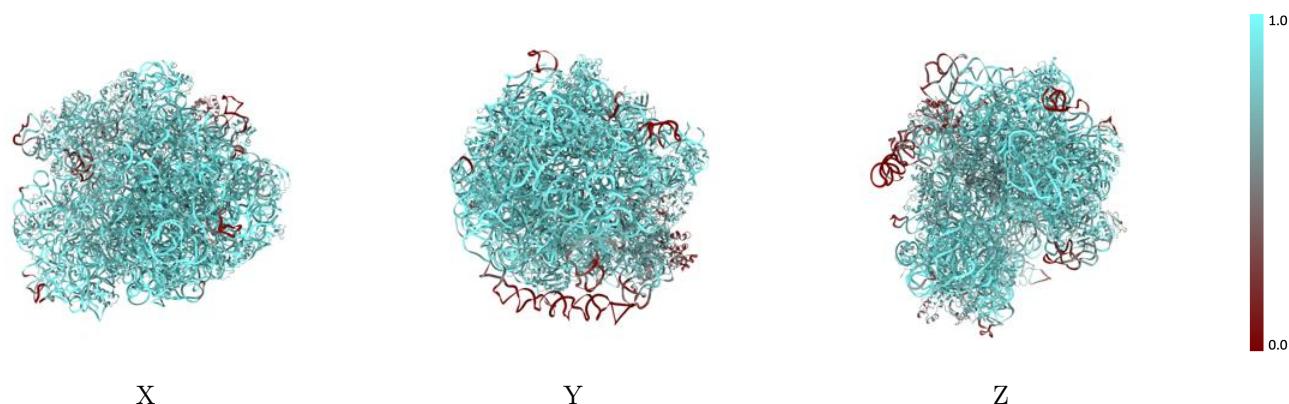
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



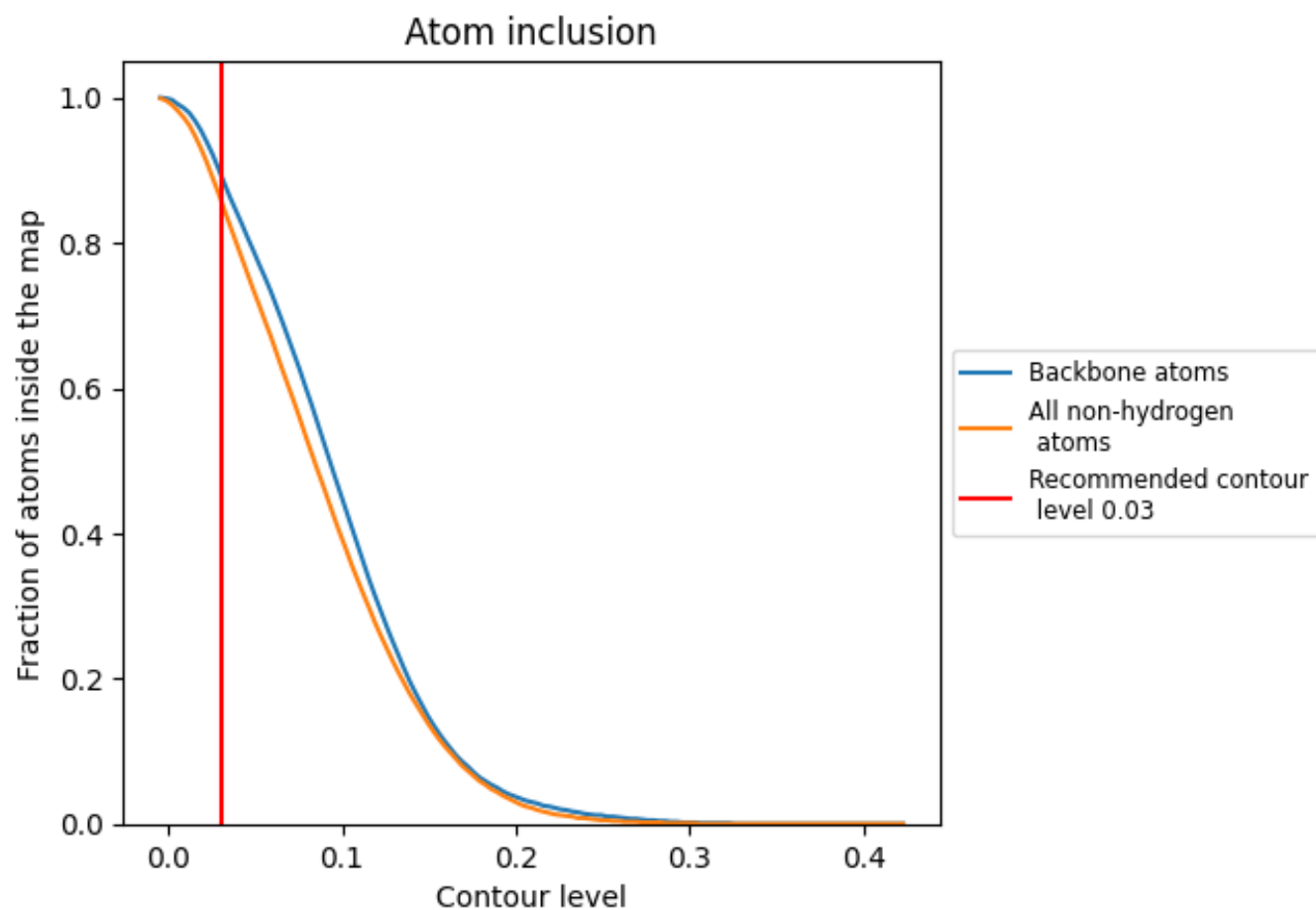
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.5560
0	 0.8880	 0.5840
1	 0.8840	 0.5680
2	 0.9190	 0.6150
3	 0.9110	 0.6080
4	 0.8890	 0.5840
6	 0.7410	 0.4880
7	 0.5890	 0.5610
8	 0.4750	 0.3770
A	 0.8780	 0.5610
B	 0.9260	 0.5720
C	 0.9000	 0.6010
D	 0.8750	 0.5830
E	 0.8840	 0.5800
F	 0.7650	 0.5070
G	 0.7340	 0.4840
H	 0.6210	 0.4740
J	 0.8840	 0.5860
K	 0.8660	 0.5770
L	 0.8780	 0.5870
M	 0.8740	 0.5780
N	 0.8890	 0.5920
O	 0.8270	 0.5540
P	 0.8620	 0.5740
Q	 0.8920	 0.5960
R	 0.8700	 0.5830
S	 0.9110	 0.5930
T	 0.8580	 0.5590
U	 0.8180	 0.5350
V	 0.7150	 0.4990
W	 0.9080	 0.5790
X	 0.9050	 0.5880
Y	 0.8120	 0.5450
Z	 0.8640	 0.5640
a	 0.9120	 0.5680



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	 0.7350	 0.5030
d	 0.7630	 0.5100
e	 0.8120	 0.5470
f	 0.7480	 0.5250
g	 0.7840	 0.5330
h	 0.8410	 0.5570
i	 0.7660	 0.5200
j	 0.6680	 0.4500
k	 0.7830	 0.5300
l	 0.8120	 0.5360
m	 0.7980	 0.5220
n	 0.8800	 0.5690
o	 0.8260	 0.5500
p	 0.7860	 0.5220
q	 0.8010	 0.5220
r	 0.7820	 0.5210
s	 0.8090	 0.5350
t	 0.7930	 0.5430
x	 0.6830	 0.5050
y	 0.8550	 0.5380
z	 0.7650	 0.4930