



## Full wwPDB EM Validation Report ⓘ

Jun 29, 2026 – 11:29 am BST

PDB ID : 9T5X / pdb\_00009t5x  
EMDB ID : EMD-55598  
Title : Structure of a stalled E. coli 70S RNC-NuoK-70 in complex with the membrane protein insertase SecYEG-YidC  
Authors : Rosales-Hernandez, C.; Busch, M.; Kamel, M.; Beckmann, R.; Kedrov, A.  
Deposited on : 2025-11-06  
Resolution : 2.85 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](mailto: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:

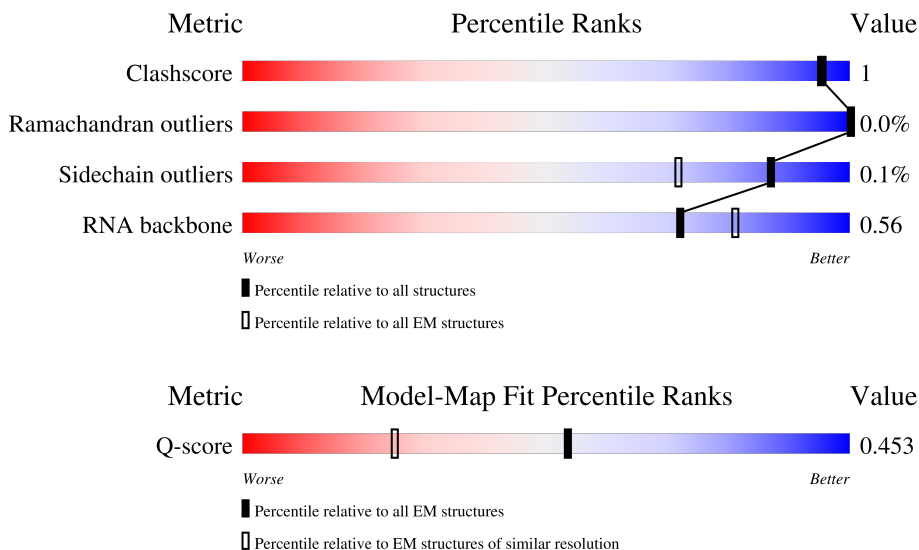
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 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 2.85 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	11965 ( 2.35 - 3.35 )

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  $\geq 3$ , 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	55	
2	1	46	
3	2	65	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	38	100%
5	4	70	77% 80% 6% 14%
6	5	2	50% 50%
7	6	443	7% 84% 11% 5%
8	7	127	14% 79% 11% 10%
9	8	110	18% 40% 10% 49%
10	9	548	22% 81% 15%
11	A	1542	81% 16% ..
12	B	241	90% 7%
13	C	233	85% 12%
14	D	206	28% 91% 8%
15	E	167	90% 7%
16	F	135	72% 24%
17	G	179	82% 15%
18	H	130	94% 5% .
19	I	130	85% 12% .
20	J	103	86% 9% 5%
21	K	129	88% 9%
22	L	124	7% 87% 12% .
23	M	118	94% . .
24	N	101	91% 8% .
25	O	89	97% ..
26	P	82	5% 88% 11% .
27	Q	84	83% 11% 6%
28	R	75	8% 87% 12%

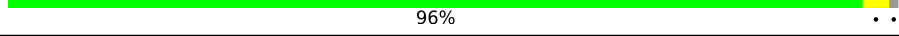
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	S	92	11% 82% 10% 9%
30	T	87	7% 90% 9%
31	U	71	55% 99%
32	V	103	37% 72% 25%
33	X	9	89% 11%
34	Y	77	83% 17%
35	Z	77	82% 17%
36	a	2904	83% 11% 5%
37	b	120	89% 10%
38	c	273	99%
39	d	209	98%
40	e	201	100%
41	f	179	94%
42	g	177	97%
43	h	149	25% 72%
44	i	142	98%
45	j	123	96%
46	k	144	98%
47	l	136	97%
48	m	127	93% 7%
49	n	117	99%
50	o	115	96%
51	p	118	98%
52	q	103	100%
53	r	110	98%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
54	s	100	 91% . 7%
55	t	104	 98% .
56	u	94	 98% .
57	v	85	 88% . 8%
58	w	78	 96% . .
59	x	63	 98% .
60	y	59	 93% 5% .
61	z	57	 95% . .

## 2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 150800 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 Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	51	417	269	76	72	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	46	377	228	90	57	2	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	64	504	323	105	74	2	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	38	302	185	65	48	4	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	60	480	299	90	85	6	0	0

- Molecule 6 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	5	2	42	19	8	13	2	0	0

- Molecule 7 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	421	3260	2158	535	550	17	0	0

- Molecule 8 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	114	874	579	149	143	3	0	0

- Molecule 9 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	56	431	287	68	72	4	0	0

- Molecule 10 is a protein called Membrane protein insertase YidC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	467	3716	2419	606	670	21	0	0

- Molecule 11 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	A	1519	32612	14552	5986	10555	1519	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	B	224	1753	1109	315	321	8	0	0

- Molecule 13 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	C	206	1624	1028	305	288	3	0	0

- Molecule 14 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	D	205	1643	1026	315	298	4	0	0

- Molecule 15 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	E	156	1152	717	217	212	6	0	0

- Molecule 16 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	F	103	839	530	151	151	7	0	0

- Molecule 17 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	G	153	1203	750	231	218	4	0	0

- Molecule 18 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	H	129	979	616	173	184	6	0	0

- Molecule 19 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	I	127	1022	634	206	179	3	0	0

- Molecule 20 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	J	98	786	493	150	142	1	0	0

- Molecule 21 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 22 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 23 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 24 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 25 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 26 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 27 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 28 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	R	66	544	345	102	96	1	0	0

- Molecule 29 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	S	84	668	427	127	112	2	0	0

- Molecule 30 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	T	86	670	414	138	115	3	0	0

- Molecule 31 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	U	70	589	366	125	97	1	0	0

- Molecule 32 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	V	77	605	403	98	101	3	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	1	MET	-	initiating methionine	UNP A7ZP93
V	2	SER	-	expression tag	UNP A7ZP93
V	3	THR	-	expression tag	UNP A7ZP93
V	73	GLY	-	expression tag	UNP A7ZP93
V	74	TYR	-	expression tag	UNP A7ZP93
V	75	PRO	-	expression tag	UNP A7ZP93
V	76	TYR	-	expression tag	UNP A7ZP93
V	77	ASP	-	expression tag	UNP A7ZP93
V	78	VAL	-	expression tag	UNP A7ZP93
V	79	PRO	-	expression tag	UNP A7ZP93
V	80	ASP	-	expression tag	UNP A7ZP93
V	81	TYR	-	expression tag	UNP A7ZP93

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
V	82	ALA	-	expression tag	UNP A7ZP93
V	83	GLY	-	expression tag	UNP A7ZP93
V	84	GLY	-	expression tag	UNP A7ZP93
V	85	SER	-	expression tag	UNP A7ZP93
V	86	GLY	-	expression tag	UNP A7ZP93
V	87	PHE	-	expression tag	UNP A7ZP93
V	88	SER	-	expression tag	UNP A7ZP93
V	89	THR	-	expression tag	UNP A7ZP93
V	90	PRO	-	expression tag	UNP A7ZP93
V	91	VAL	-	expression tag	UNP A7ZP93
V	92	TRP	-	expression tag	UNP A7ZP93
V	93	ILE	-	expression tag	UNP A7ZP93
V	94	TRP	-	expression tag	UNP A7ZP93
V	95	TRP	-	expression tag	UNP A7ZP93
V	96	TRP	-	expression tag	UNP A7ZP93
V	97	PRO	-	expression tag	UNP A7ZP93
V	98	ARG	-	expression tag	UNP A7ZP93
V	99	ILE	-	expression tag	UNP A7ZP93
V	100	ARG	-	expression tag	UNP A7ZP93
V	101	GLY	-	expression tag	UNP A7ZP93
V	102	PRO	-	expression tag	UNP A7ZP93
V	103	PRO	-	expression tag	UNP A7ZP93

- Molecule 33 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O	P		
33	X	9	189	84	31	65	9	0	0

- Molecule 34 is a RNA chain called A-site tRNA-Pro.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O	P		
34	Y	77	1646	734	297	539	76	0	0

- Molecule 35 is a RNA chain called P-site tRNA-Pro.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O	P		
35	Z	77	1644	733	295	540	76	0	0

- Molecule 36 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
36	a	2753	59127	26381	10897	19096	2753	0	0

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	b	119	2549	1135	466	829	119	0	0

- Molecule 38 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	c	271	2082	1288	423	364	7	0	0

- Molecule 39 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	d	209	1566	980	288	294	4	0	0

- Molecule 40 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	e	201	1552	974	283	290	5	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	f	177	1410	899	249	256	6	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	g	176	1323	832	243	246	2	0	0

- Molecule 43 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 44 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 45 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 46 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 47 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	l	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 48 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 49 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	n	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 50 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 51 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	p	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 52 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 53 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 54 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 55 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 56 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 57 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 58 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 59 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 60 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 61 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	3	1	Total	Zn	0
			1	1	
62	4	1	Total	Zn	0
			1	1	

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

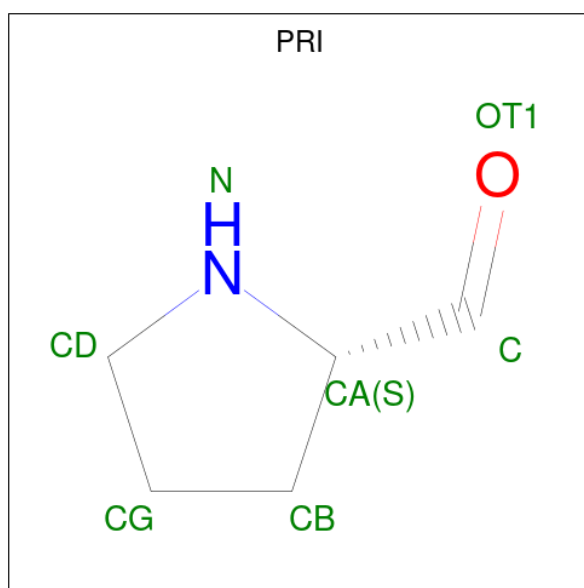
Mol	Chain	Residues	Atoms		AltConf
63	A	91	Total	Mg	0
			91	91	
63	N	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

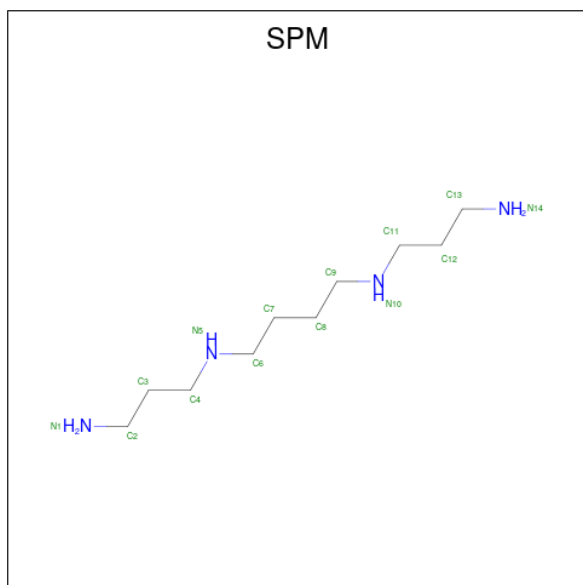
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
63	Q	1	1	1	0
63	a	207	207	207	0
63	b	5	5	5	0
63	c	1	1	1	0
63	d	1	1	1	0
63	p	1	1	1	0
63	z	1	1	1	0

- Molecule 64 is PYRROLIDINE-2-CARBALDEHYDE (CCD ID: PRI) (formula: C<sub>5</sub>H<sub>9</sub>NO).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
64	Y	1	7	5	1	1	0

- Molecule 65 is SPERMINE (CCD ID: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).



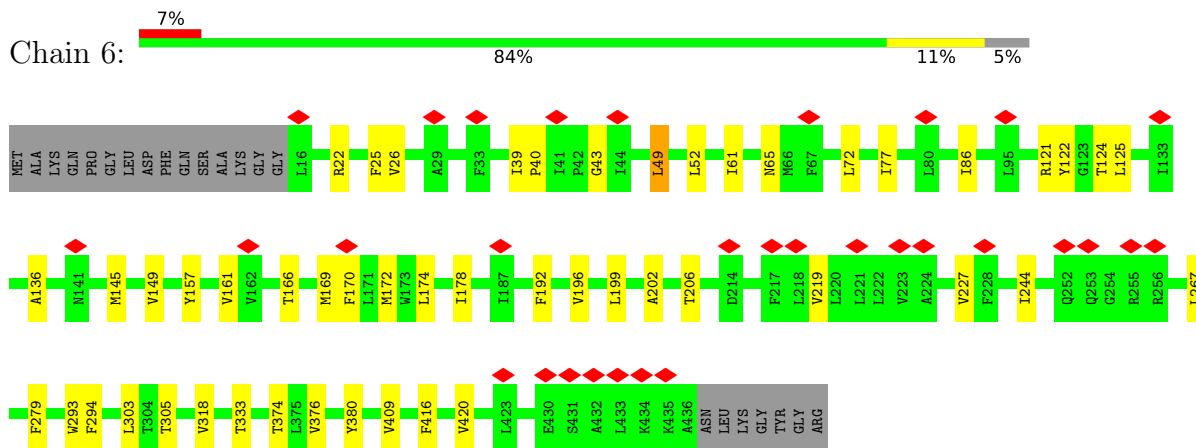
Mol	Chain	Residues	Atoms			AltConf
65	a	1	Total	C	N	0
			14	10	4	



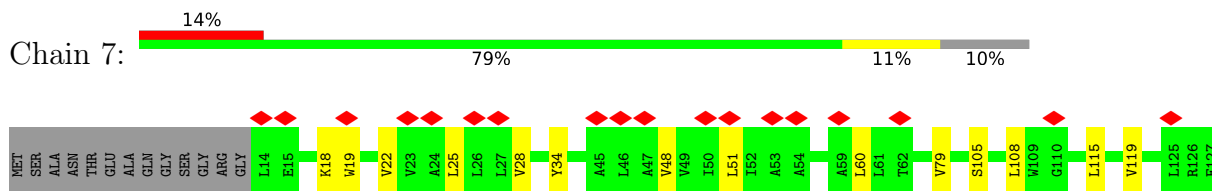
• Molecule 6: E-site tRNA



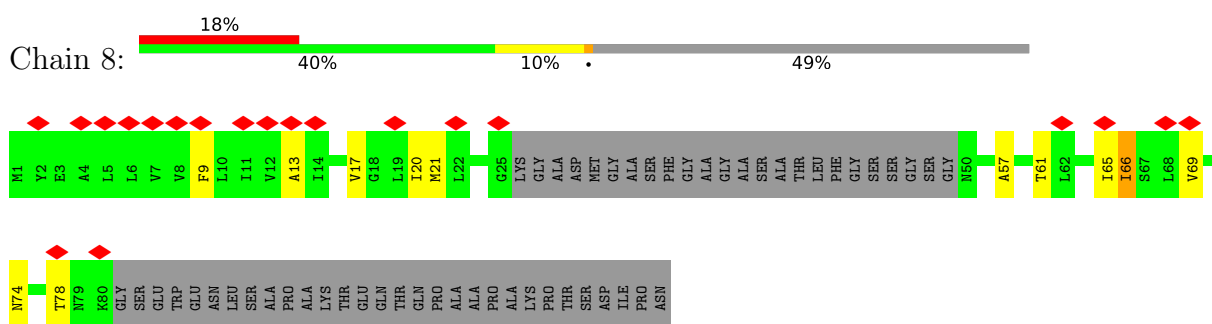
• Molecule 7: Protein translocase subunit SecY



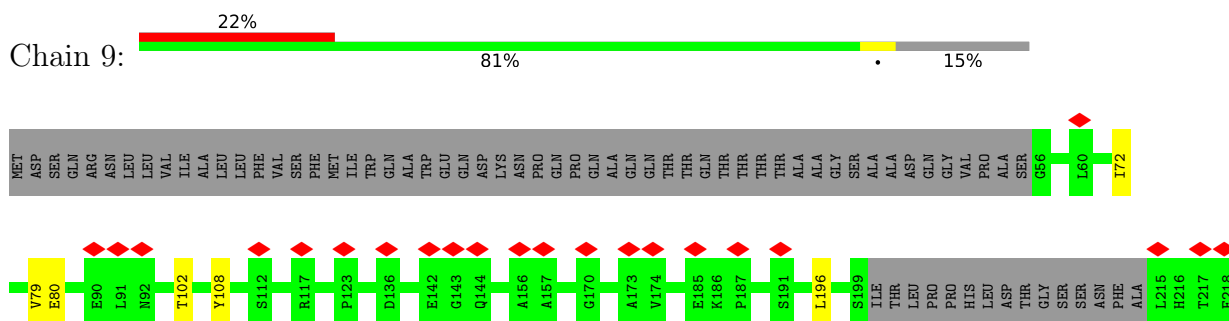
• Molecule 8: Protein translocase subunit SecE



• Molecule 9: Protein-export membrane protein SecG



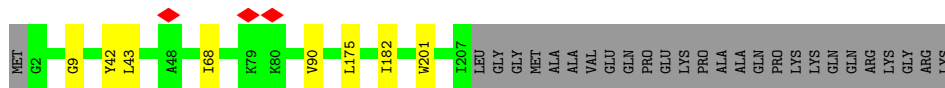
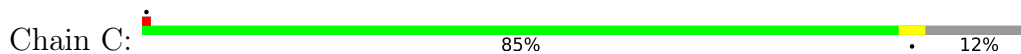
• Molecule 10: Membrane protein insertase YidC



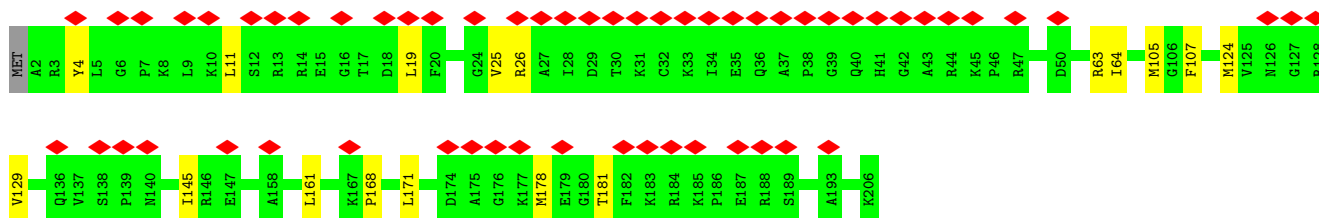
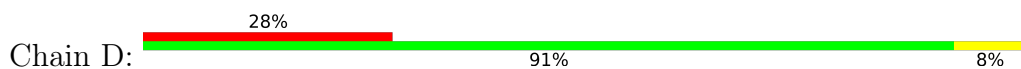




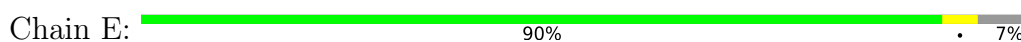
- Molecule 13: Small ribosomal subunit protein uS3



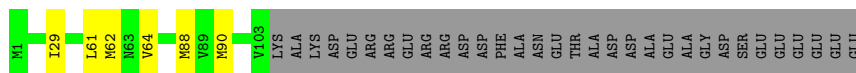
- Molecule 14: Small ribosomal subunit protein uS4



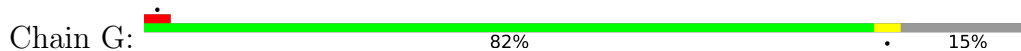
- Molecule 15: Small ribosomal subunit protein uS5



- Molecule 16: Small ribosomal subunit protein bS6, fully modified isoform




- Molecule 17: Small ribosomal subunit protein uS7



- Molecule 18: Small ribosomal subunit protein uS8




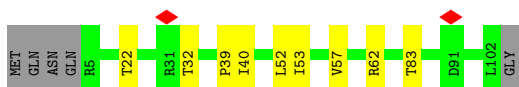
- Molecule 19: Small ribosomal subunit protein uS9

Chain I:  85% 12%




- Molecule 20: Small ribosomal subunit protein uS10

Chain J:  86% 9% 5%




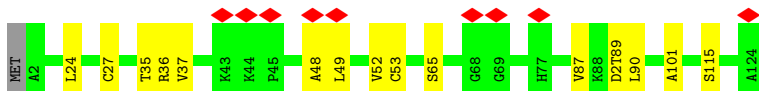
- Molecule 21: Small ribosomal subunit protein uS11

Chain K:  88% 9%



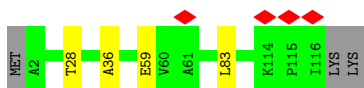
- Molecule 22: Small ribosomal subunit protein uS12

Chain L:  7% 87% 12%



- Molecule 23: Small ribosomal subunit protein uS13

Chain M:  94%



- Molecule 24: Small ribosomal subunit protein uS14

Chain N:  91% 8%

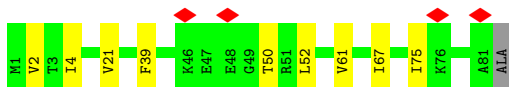
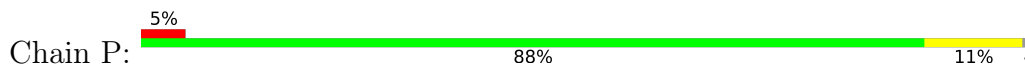


- Molecule 25: Small ribosomal subunit protein uS15

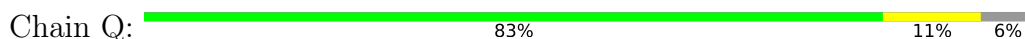
Chain O:  97%



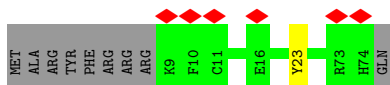
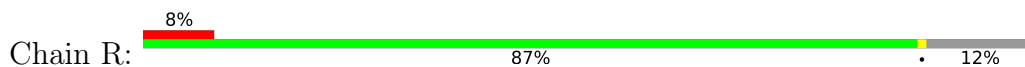
- Molecule 26: Small ribosomal subunit protein bS16



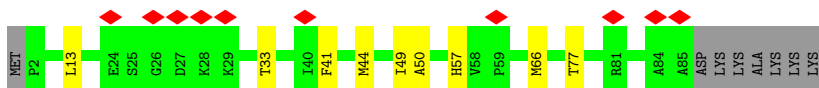
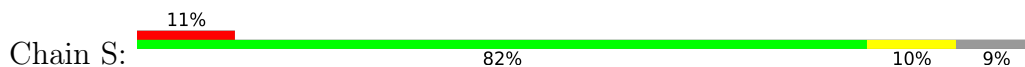
- Molecule 27: Small ribosomal subunit protein uS17



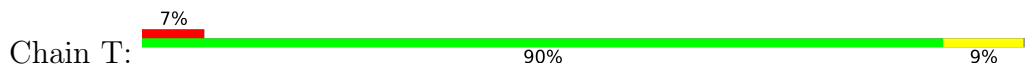
- Molecule 28: Small ribosomal subunit protein bS18



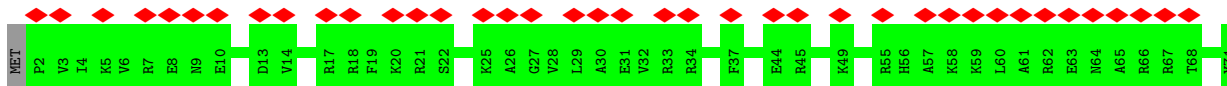
- Molecule 29: Small ribosomal subunit protein uS19



- Molecule 30: Small ribosomal subunit protein bS20

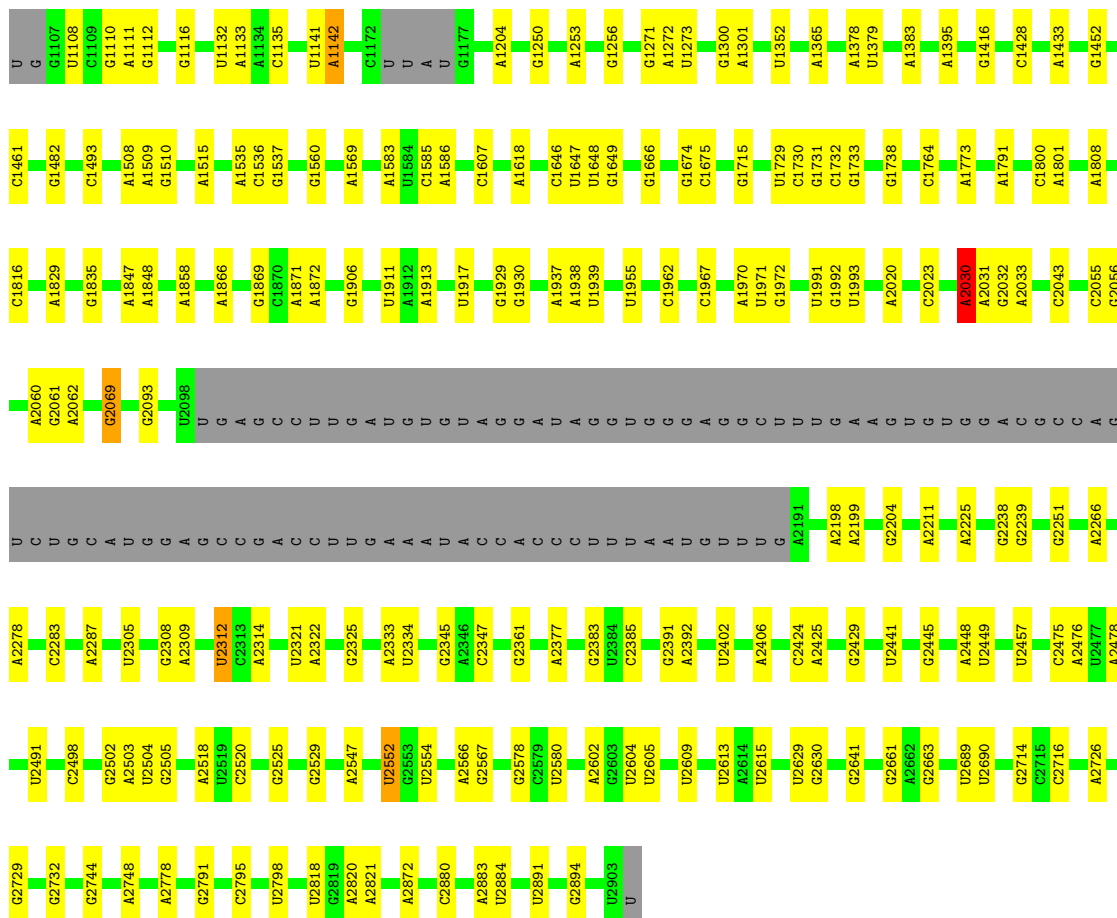


- Molecule 31: Small ribosomal subunit protein bS21

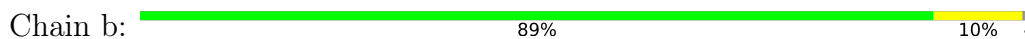


- Molecule 32: NADH-quinone oxidoreductase subunit K





• Molecule 37: 5S rRNA



• Molecule 38: Large ribosomal subunit protein uL2



• Molecule 39: Large ribosomal subunit protein uL3



• Molecule 40: Large ribosomal subunit protein uL4

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 41: Large ribosomal subunit protein uL5

Chain f:  94%



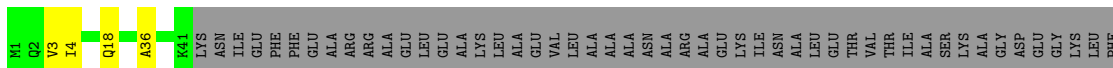
- Molecule 42: Large ribosomal subunit protein uL6

Chain g:  97%



- Molecule 43: Large ribosomal subunit protein bL9

Chain h:  25% 72%



- Molecule 44: Large ribosomal subunit protein uL13

Chain i:  98%



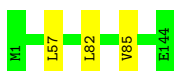
- Molecule 45: Large ribosomal subunit protein uL14

Chain j:  96%



- Molecule 46: Large ribosomal subunit protein uL15

Chain k:  98%



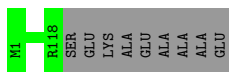
- Molecule 47: 50S ribosomal protein L16

Chain l:  97%



- Molecule 48: Large ribosomal subunit protein bL17

Chain m:  93% 7%



- Molecule 49: Large ribosomal subunit protein uL18

Chain n:  99%



- Molecule 50: Large ribosomal subunit protein bL19

Chain o:  96%



- Molecule 51: Large ribosomal subunit protein bL20

Chain p:  98%



- Molecule 52: Large ribosomal subunit protein bL21

Chain q:  100%

There are no outlier residues recorded for this chain.

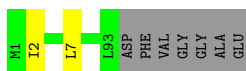
- Molecule 53: Large ribosomal subunit protein uL22

Chain r:  98%



- Molecule 54: Large ribosomal subunit protein uL23

Chain s:  91% 7%



- Molecule 55: Large ribosomal subunit protein uL24

Chain t: 98% .



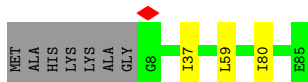
- Molecule 56: Large ribosomal subunit protein bL25

Chain u: 98% .



- Molecule 57: Large ribosomal subunit protein bL27

Chain v: 88% . 8%



- Molecule 58: Large ribosomal subunit protein bL28

Chain w: 96% . .



- Molecule 59: Large ribosomal subunit protein uL29

Chain x: 98% .



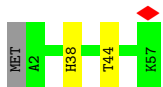
- Molecule 60: Large ribosomal subunit protein uL30

Chain y: 93% . 5%



- Molecule 61: Large ribosomal subunit protein bL32

Chain z: 95% . .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58063	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.417	Depositor
Minimum map value	-0.436	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.13	Depositor
Map size ( $\text{\AA}$ )	494.36, 494.36, 494.36	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.727, 0.727, 0.727	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MEQ, 6MZ, G7M, 4OC, SPM, PRI, OMC, ZN, OMU, H2U, 1MG, PSU, 2MA, MA6, OMG, UR3, MG, 2MG, D2T, 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	0.17	0/424	0.29	0/565
2	1	0.34	0/380	0.28	0/498
3	2	0.29	0/513	0.31	0/676
4	3	0.26	0/303	0.33	0/397
5	4	0.14	0/488	0.28	0/649
6	5	0.09	0/46	0.18	0/69
7	6	0.20	0/3335	0.41	0/4526
8	7	0.17	0/887	0.40	0/1209
9	8	0.24	0/434	0.52	0/584
10	9	0.15	0/3813	0.33	0/5179
11	A	0.19	1/36236 (0.0%)	0.29	0/56520
12	B	0.14	0/1784	0.31	0/2403
13	C	0.13	0/1651	0.28	0/2225
14	D	0.14	0/1665	0.31	0/2227
15	E	0.17	0/1165	0.31	0/1568
16	F	0.17	0/858	0.30	0/1160
17	G	0.14	0/1219	0.31	0/1635
18	H	0.16	0/989	0.31	0/1326
19	I	0.12	0/1034	0.30	0/1375
20	J	0.13	0/796	0.30	0/1077
21	K	0.13	0/893	0.29	0/1205
22	L	0.17	0/960	0.38	0/1286
23	M	0.13	0/900	0.31	0/1204
24	N	0.12	0/817	0.27	0/1088
25	O	0.15	0/722	0.30	0/964
26	P	0.16	0/653	0.33	0/877
27	Q	0.16	0/650	0.36	0/871
28	R	0.14	0/553	0.26	0/742
29	S	0.13	0/685	0.29	0/922
30	T	0.18	0/676	0.33	0/895
31	U	0.13	0/597	0.30	0/792

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	V	0.21	0/627	0.42	0/859
33	X	0.15	0/209	0.21	0/323
34	Y	0.15	0/1840	0.26	0/2869
35	Z	0.15	0/1837	0.24	0/2864
36	a	0.36	0/65718	0.31	0/102519
37	b	0.25	0/2850	0.26	0/4444
38	c	0.29	0/2121	0.32	0/2852
39	d	0.31	0/1576	0.31	0/2119
40	e	0.30	0/1571	0.31	0/2113
41	f	0.17	0/1434	0.37	0/1926
42	g	0.16	0/1343	0.31	0/1816
43	h	0.21	0/306	0.32	0/413
44	i	0.32	0/1152	0.30	0/1551
45	j	0.30	0/955	0.31	0/1279
46	k	0.30	0/1062	0.31	0/1413
47	l	0.29	0/1093	0.30	0/1460
48	m	0.33	0/958	0.35	0/1281
49	n	0.19	0/902	0.31	0/1209
50	o	0.29	0/929	0.30	0/1242
51	p	0.36	0/960	0.34	0/1278
52	q	0.30	0/829	0.28	0/1107
53	r	0.32	0/864	0.35	0/1156
54	s	0.28	0/744	0.30	0/994
55	t	0.26	0/787	0.32	0/1051
56	u	0.25	0/766	0.32	0/1025
57	v	0.29	0/599	0.29	0/792
58	w	0.28	0/635	0.30	0/848
59	x	0.23	0/502	0.31	0/667
60	y	0.29	0/453	0.34	0/605
61	z	0.31	0/450	0.30	0/599
All	All	0.28	1/162198 (0.0%)	0.31	0/241388

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	527	G7M	O3'-P	5.12	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	417	0	451	0	0
2	1	377	0	418	0	0
3	2	504	0	572	1	0
4	3	302	0	341	0	0
5	4	480	0	479	3	0
6	5	42	0	23	0	0
7	6	3260	0	3416	37	0
8	7	874	0	966	13	0
9	8	431	0	475	9	0
10	9	3716	0	3720	13	0
11	A	32612	0	16429	30	0
12	B	1753	0	1780	3	0
13	C	1624	0	1696	5	0
14	D	1643	0	1707	14	0
15	E	1152	0	1196	3	0
16	F	839	0	833	6	0
17	G	1203	0	1254	4	0
18	H	979	0	1031	5	0
19	I	1022	0	1070	13	0
20	J	786	0	828	7	0
21	K	877	0	887	2	0
22	L	957	0	1017	12	0
23	M	891	0	952	3	0
24	N	805	0	844	8	0
25	O	714	0	734	1	0
26	P	643	0	661	7	0
27	Q	641	0	682	6	0
28	R	544	0	565	1	0
29	S	668	0	693	7	0
30	T	670	0	719	4	0
31	U	589	0	629	0	0
32	V	605	0	588	2	0
33	X	189	0	98	0	0
34	Y	1646	0	832	0	0
35	Z	1644	0	832	2	0
36	a	59127	0	29762	19	0
37	b	2549	0	1291	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	c	2082	0	2154	1	0
39	d	1566	0	1618	2	0
40	e	1552	0	1619	0	0
41	f	1410	0	1444	7	0
42	g	1323	0	1371	2	0
43	h	303	0	327	2	0
44	i	1129	0	1162	2	0
45	j	946	0	1023	3	0
46	k	1053	0	1129	2	0
47	l	1074	0	1157	4	0
48	m	945	0	989	0	0
49	n	892	0	923	0	0
50	o	917	0	962	2	0
51	p	947	0	1019	1	0
52	q	816	0	839	0	0
53	r	857	0	922	1	0
54	s	738	0	807	1	0
55	t	779	0	831	0	0
56	u	753	0	780	2	0
57	v	592	0	607	2	0
58	w	625	0	652	1	0
59	x	501	0	531	0	0
60	y	449	0	488	2	0
61	z	444	0	458	1	0
62	3	1	0	0	0	0
62	4	1	0	0	0	0
63	A	91	0	0	0	0
63	N	1	0	0	0	0
63	Q	1	0	0	0	0
63	a	207	0	0	0	0
63	b	5	0	0	0	0
63	c	1	0	0	0	0
63	d	1	0	0	0	0
63	p	1	0	0	0	0
63	z	1	0	0	0	0
64	Y	7	0	8	0	0
65	a	14	0	26	0	0
All	All	150800	0	104317	243	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 1.

All (243) 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)
19:I:88:MET:HE3	19:I:98:LEU:HD12	1.51	0.92
8:7:28:VAL:HG11	8:7:48:VAL:HG11	1.60	0.84
11:A:992:U:O2	11:A:1044:A:N7	2.16	0.79
11:A:157:U:O2	11:A:164:G:O6	2.10	0.69
5:4:42:PRO:O	5:4:45:THR:O	2.10	0.69
19:I:52:LEU:HD13	19:I:58:VAL:HG23	1.75	0.69
7:6:26:VAL:HA	7:6:178:ILE:HD11	1.75	0.68
22:L:35:THR:HG22	22:L:36:ARG:H	1.59	0.68
35:Z:10:G:O6	35:Z:46:G:N2	2.24	0.68
14:D:145:ILE:HD13	14:D:178:MET:HB3	1.75	0.67
7:6:157:TYR:O	7:6:161:VAL:HG23	1.94	0.67
7:6:202:ALA:O	7:6:206:THR:HG23	1.95	0.66
36:a:1433:A:N1	36:a:1560:G:O6	2.28	0.66
38:c:29:PRO:HG2	38:c:34:LEU:HD11	1.79	0.65
7:6:61:ILE:HD11	7:6:72:LEU:HD13	1.79	0.65
21:K:55:SER:O	21:K:59:THR:HG23	1.95	0.65
7:6:124:THR:HG21	7:6:172:MET:HE2	1.80	0.64
10:9:72:ILE:HG22	10:9:79:VAL:HG22	1.78	0.64
36:a:568:U:H1'	36:a:2030:6MZ:H9C1	1.79	0.64
20:J:32:THR:CG2	20:J:83:THR:HG22	2.28	0.63
9:8:74:ASN:O	9:8:78:THR:HG23	1.99	0.62
8:7:25:LEU:HD21	8:7:51:LEU:HD23	1.80	0.62
11:A:992:U:C2	11:A:1044:A:N7	2.68	0.61
7:6:52:LEU:HD11	7:6:145:MET:HE1	1.82	0.61
26:P:39:PHE:CD1	26:P:50:THR:HG22	2.35	0.61
24:N:46:LEU:HD22	29:S:13:LEU:HD23	1.81	0.61
7:6:196:VAL:HG13	8:7:108:LEU:HD21	1.83	0.61
14:D:168:PRO:HG3	14:D:171:LEU:HD12	1.83	0.61
5:4:42:PRO:O	5:4:45:THR:C	2.44	0.60
27:Q:60:GLU:C	27:Q:61:ILE:HD12	2.26	0.60
7:6:166:THR:HG23	9:8:17:VAL:CG1	2.31	0.60
11:A:1441:A:H62	11:A:1461:G:H21	1.48	0.60
9:8:57:ALA:O	9:8:61:THR:HG23	2.02	0.60
11:A:180:U:O4	11:A:195:A:N7	2.34	0.59
11:A:35:G:H21	22:L:115:SER:HB2	1.67	0.59
14:D:4:TYR:CZ	14:D:11:LEU:HD22	2.37	0.59
14:D:107:PHE:CG	14:D:145:ILE:HD11	2.38	0.59
19:I:84:THR:HG23	19:I:98:LEU:HD13	1.85	0.59
14:D:168:PRO:CG	14:D:171:LEU:HD12	2.33	0.58
11:A:1321:U:O2	29:S:77:THR:HG21	2.04	0.58
11:A:1518:MA6:N6	11:A:1519:MA6:H93	2.18	0.57
30:T:28:MET:HE1	30:T:67:ILE:HD13	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:136:ALA:HB2	7:6:161:VAL:HG21	1.87	0.57
36:a:745:1MG:O2'	36:a:746:PSU:H5''	2.04	0.57
20:J:32:THR:HG23	20:J:83:THR:HG22	1.87	0.57
19:I:88:MET:HE3	19:I:98:LEU:CD1	2.30	0.57
11:A:589:U:O2	11:A:650:G:O6	2.23	0.56
12:B:104:TRP:HA	12:B:107:VAL:HG22	1.87	0.56
12:B:114:LEU:HD13	12:B:144:LEU:HB3	1.86	0.56
24:N:66:GLN:HG3	24:N:79:LEU:HD22	1.87	0.56
22:L:37:VAL:HG13	22:L:53:CYS:SG	2.45	0.56
11:A:1088:G:H21	11:A:1167:A:H61	1.52	0.56
16:F:88:MET:HG3	16:F:90:MET:HE2	1.88	0.55
14:D:25:VAL:HB	14:D:161:LEU:HD21	1.89	0.55
11:A:34:C:O2'	22:L:101:ALA:HB2	2.07	0.54
11:A:823:C:HO2'	18:H:2:SER:N	2.05	0.54
42:g:24:ILE:HD13	42:g:72:LEU:HD11	1.88	0.54
14:D:105:MET:HG3	14:D:171:LEU:HD13	1.89	0.54
7:6:121:ARG:O	7:6:124:THR:HG22	2.08	0.54
22:L:87:VAL:CG2	22:L:90:LEU:HD23	2.38	0.54
30:T:31:PHE:O	30:T:35:VAL:HG23	2.08	0.54
19:I:46:MET:HE3	19:I:46:MET:O	2.08	0.54
8:7:115:LEU:O	8:7:119:VAL:HG23	2.08	0.53
7:6:122:TYR:HA	7:6:125:LEU:HD12	1.90	0.53
3:2:54:ASP:HB3	46:k:57:LEU:HD22	1.91	0.53
7:6:293:TRP:CD1	7:6:303:LEU:HD21	2.42	0.52
26:P:61:VAL:CG2	26:P:67:ILE:HD11	2.39	0.52
17:G:30:LEU:HD13	17:G:30:LEU:O	2.09	0.52
19:I:46:MET:HE1	19:I:53:GLU:OE1	2.10	0.52
29:S:33:THR:HG21	29:S:49:ILE:HD11	1.91	0.52
8:7:25:LEU:O	8:7:28:VAL:HG12	2.09	0.52
11:A:1088:G:H21	11:A:1167:A:N6	2.07	0.52
11:A:1328:C:OP1	23:M:28:THR:HG21	2.10	0.52
47:l:53:MET:HG3	47:l:120:ALA:HB2	1.90	0.52
7:6:25:PHE:CE2	7:6:178:ILE:HD12	2.44	0.52
27:Q:21:ILE:HD12	27:Q:21:ILE:O	2.10	0.52
19:I:60:LYS:C	19:I:61:LEU:HD22	2.35	0.52
27:Q:59:VAL:HG23	27:Q:61:ILE:HD11	1.91	0.52
13:C:9:GLY:HA3	24:N:89:MET:HE3	1.91	0.52
7:6:376:VAL:HG21	8:7:79:VAL:CG1	2.39	0.51
16:F:90:MET:HE1	28:R:23:TYR:OH	2.10	0.51
26:P:39:PHE:CE1	26:P:50:THR:HG22	2.45	0.51
11:A:1441:A:N6	11:A:1461:G:H21	2.08	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:2552:OMU:H6	36:a:2552:OMU:O5'	2.10	0.51
9:8:65:ILE:O	9:8:69:VAL:HG23	2.10	0.51
7:6:86:ILE:HD11	7:6:279:PHE:CD1	2.46	0.51
10:9:108:TYR:CE1	10:9:196:LEU:HD11	2.46	0.51
13:C:175:LEU:HD23	13:C:182:ILE:HD13	1.92	0.50
30:T:4:ILE:HG22	30:T:6:SER:H	1.77	0.50
20:J:52:LEU:HD21	20:J:62:ARG:HH21	1.76	0.50
10:9:471:MET:HE1	10:9:506:PHE:CE1	2.46	0.50
41:f:58:ALA:HB2	41:f:65:PRO:HD3	1.94	0.50
10:9:316:LYS:O	10:9:320:VAL:HG22	2.12	0.50
36:a:2314:A:H1'	41:f:155:THR:HG21	1.94	0.49
10:9:438:TYR:HD1	10:9:441:MET:HE2	1.77	0.49
12:B:57:LEU:HD23	12:B:217:VAL:HG23	1.94	0.49
19:I:118:LEU:HD22	19:I:124:ARG:HG2	1.93	0.49
60:y:47:MET:O	60:y:51:VAL:HG22	2.12	0.49
14:D:11:LEU:HD23	14:D:63:ARG:HG2	1.94	0.49
13:C:175:LEU:HD21	13:C:201:TRP:CD1	2.47	0.49
11:A:1441:A:H62	11:A:1461:G:N2	2.11	0.49
14:D:105:MET:HE3	14:D:171:LEU:HD22	1.95	0.49
20:J:53:ILE:HG22	24:N:85:ARG:CD	2.43	0.48
9:8:9:PHE:CD1	9:8:66:ILE:HG23	2.48	0.48
7:6:124:THR:CG2	7:6:172:MET:HE2	2.43	0.48
22:L:24:LEU:HD12	22:L:27:CYS:O	2.13	0.48
19:I:88:MET:HE1	19:I:94:LEU:C	2.37	0.48
22:L:87:VAL:HG21	22:L:90:LEU:HD23	1.96	0.48
18:H:12:THR:HG22	18:H:16:ASN:ND2	2.29	0.47
27:Q:11:ARG:C	27:Q:23:VAL:HG23	2.39	0.47
10:9:471:MET:HE2	10:9:517:TYR:HB2	1.95	0.47
27:Q:64:CYS:SG	27:Q:74:THR:HG23	2.55	0.47
44:i:114:LEU:HG	44:i:118:MET:HE3	1.96	0.47
11:A:112:G:H21	11:A:354:G:C4'	2.27	0.47
14:D:25:VAL:HG22	14:D:26:ARG:HG3	1.96	0.47
36:a:876:C:H42	36:a:901:C:N4	2.13	0.47
10:9:313:ILE:HD12	10:9:316:LYS:HG3	1.98	0.46
16:F:61:LEU:HD12	16:F:62:MET:N	2.30	0.46
11:A:1144:G:H21	11:A:1146:A:H62	1.62	0.46
26:P:52:LEU:HD21	26:P:75:ILE:HG13	1.97	0.46
11:A:448:A:N7	11:A:486:U:O4	2.49	0.46
20:J:22:THR:HG21	20:J:39:PRO:HB3	1.98	0.46
43:h:4:ILE:HG22	43:h:18:GLN:HG2	1.96	0.46
24:N:6:MET:HE3	24:N:63:ARG:NH2	2.30	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:50:LEU:HD22	17:G:124:LEU:HB3	1.97	0.46
36:a:2641:G:OP1	44:i:78:THR:HG22	2.15	0.46
7:6:170:PHE:CZ	7:6:174:LEU:HD11	2.51	0.46
14:D:124:MET:HE1	14:D:129:VAL:HG13	1.98	0.46
11:A:352:C:HO2'	11:A:354:G:P	2.39	0.45
14:D:19:LEU:HD22	14:D:64:ILE:HG13	1.97	0.45
19:I:35:LEU:HD11	19:I:48:VAL:HG11	1.99	0.45
23:M:36:ALA:HB3	23:M:59:GLU:OE1	2.16	0.45
47:l:53:MET:CG	47:l:120:ALA:HB2	2.46	0.45
29:S:50:ALA:HB1	29:S:57:HIS:HB3	1.98	0.45
7:6:196:VAL:CG1	8:7:108:LEU:HD21	2.45	0.45
14:D:25:VAL:HB	14:D:161:LEU:HD11	1.98	0.45
11:A:1088:G:N2	11:A:1167:A:H61	2.13	0.45
45:j:38:ILE:HD11	45:j:112:PHE:HZ	1.81	0.45
36:a:571:U:C5	36:a:2030:6MZ:H9	2.51	0.45
10:9:409:MET:HE1	32:V:52:GLY:CA	2.47	0.45
7:6:199:LEU:HD11	8:7:105:SER:HB2	1.98	0.45
11:A:35:G:H21	22:L:115:SER:CB	2.30	0.45
26:P:4:ILE:HD12	26:P:21:VAL:HG22	1.98	0.45
11:A:1125:U:O4'	20:J:40:ILE:HD13	2.16	0.44
23:M:83:LEU:HD11	29:S:66:MET:HE2	1.98	0.44
7:6:166:THR:HG23	9:8:17:VAL:HG13	1.98	0.44
7:6:244:ILE:HD12	7:6:267:LEU:HD11	1.99	0.44
7:6:65:ASN:HB2	7:6:72:LEU:HD11	2.00	0.44
10:9:408:MET:HE3	32:V:47:ALA:HB1	2.00	0.44
17:G:66:LEU:HD11	17:G:101:MET:HG3	2.00	0.44
53:r:4:ILE:HG22	53:r:106:VAL:HG22	1.99	0.44
36:a:930:G:H1'	60:y:25:LEU:HD11	2.00	0.44
7:6:305:THR:HG23	8:7:34:TYR:CZ	2.53	0.44
18:H:12:THR:HG22	18:H:16:ASN:HD21	1.83	0.44
22:L:52:VAL:HG13	22:L:65:SER:O	2.18	0.44
25:O:43:PHE:CE2	25:O:56:LEU:HD22	2.53	0.44
26:P:4:ILE:CD1	26:P:21:VAL:HG22	2.48	0.44
7:6:43:GLY:O	7:6:149:VAL:HG22	2.18	0.43
47:l:20:LEU:HD13	56:u:81:PRO:HG2	2.00	0.43
17:G:29:ILE:HD12	17:G:101:MET:HE2	2.00	0.43
36:a:2392:A:N6	36:a:2424:C:O2	2.51	0.43
36:a:2032:G:C5	39:d:150:MEQ:HE3	2.53	0.43
21:K:31:ILE:HG12	21:K:46:THR:HG22	1.99	0.43
11:A:713:G:H2'	11:A:714:G:C8	2.53	0.43
47:l:135:VAL:HG11	56:u:57:TYR:CD2	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:53:ILE:HG22	24:N:85:ARG:HD2	1.99	0.43
24:N:78:GLY:O	24:N:79:LEU:HD23	2.18	0.43
57:v:37:ILE:HG21	57:v:80:ILE:HG21	2.00	0.43
45:j:19:VAL:HB	45:j:41:ILE:HD13	1.99	0.43
10:9:527:GLN:OE1	10:9:530:LEU:HD23	2.18	0.43
7:6:125:LEU:HD11	9:8:21:MET:SD	2.58	0.43
7:6:416:PHE:O	7:6:420:VAL:HG22	2.19	0.43
13:C:42:TYR:CZ	13:C:90:VAL:HG11	2.54	0.43
15:E:115:LEU:HD13	15:E:123:VAL:HG11	2.01	0.43
19:I:19:VAL:HG21	19:I:82:GLY:HA3	2.01	0.43
7:6:294:PHE:HB3	7:6:303:LEU:HD23	2.01	0.43
19:I:88:MET:HA	19:I:88:MET:HE2	2.01	0.43
7:6:136:ALA:CB	7:6:161:VAL:HG21	2.48	0.42
10:9:313:ILE:HD12	10:9:316:LYS:CG	2.49	0.42
11:A:673:A:H2'	11:A:674:G:C8	2.54	0.42
50:o:110:ILE:HG22	50:o:111:LYS:O	2.18	0.42
7:6:22:ARG:O	7:6:26:VAL:HG23	2.19	0.42
7:6:192:PHE:CD1	7:6:409:VAL:HG12	2.53	0.42
22:L:48:ALA:O	22:L:49:LEU:HD12	2.18	0.42
15:E:38:VAL:HG11	15:E:114:VAL:HG22	2.01	0.42
16:F:29:ILE:HD12	16:F:64:VAL:HG11	2.00	0.42
36:a:1141:U:H4'	36:a:1142:A:O4'	2.19	0.42
50:o:22:PRO:HD3	50:o:50:ILE:HD12	2.00	0.42
8:7:18:LYS:O	8:7:22:VAL:HG13	2.20	0.42
10:9:511:SER:O	10:9:514:VAL:HG12	2.20	0.42
16:F:61:LEU:HD12	16:F:62:MET:H	1.84	0.42
22:L:48:ALA:C	22:L:49:LEU:HD12	2.44	0.42
43:h:3:VAL:HG22	43:h:36:ALA:HB1	2.01	0.42
7:6:39:ILE:HD12	7:6:40:PRO:O	2.19	0.42
7:6:49:LEU:H	7:6:49:LEU:HD22	1.84	0.42
11:A:71:A:H61	11:A:99:C:H1'	1.84	0.42
11:A:1149:C:N4	11:A:1150:A:H62	2.18	0.42
30:T:44:LYS:HG3	30:T:86:LEU:HD22	2.02	0.42
58:w:6:GLN:O	58:w:71:LEU:HD11	2.20	0.42
36:a:876:C:H42	36:a:901:C:H41	1.67	0.42
9:8:20:ILE:HG13	9:8:21:MET:HE2	2.02	0.42
41:f:25:VAL:O	41:f:28:VAL:HG12	2.20	0.42
14:D:105:MET:HE2	14:D:181:THR:N	2.34	0.42
24:N:46:LEU:HD22	29:S:13:LEU:CD2	2.47	0.42
36:a:75:G:H22	36:a:111:A:H2	1.68	0.42
42:g:76:VAL:HA	42:g:79:VAL:HG22	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Q:47:HIS:HB3	27:Q:74:THR:HG22	2.01	0.41
8:7:25:LEU:CD2	8:7:51:LEU:HD23	2.49	0.41
11:A:1518:MA6:O5'	11:A:1518:MA6:H8	2.20	0.41
15:E:149:SER:O	15:E:153:VAL:HG23	2.20	0.41
7:6:376:VAL:HG21	8:7:79:VAL:HG13	2.02	0.41
11:A:793:U:C4	11:A:1518:MA6:H91	2.56	0.41
35:Z:33:U:H3	35:Z:39:A:H61	1.67	0.41
9:8:13:ALA:O	9:8:17:VAL:HG13	2.20	0.41
19:I:52:LEU:HD12	19:I:53:GLU:N	2.35	0.41
7:6:219:VAL:O	7:6:219:VAL:HG13	2.21	0.41
8:7:19:TRP:CE2	8:7:60:LEU:HD23	2.56	0.41
16:F:88:MET:CG	16:F:90:MET:HE2	2.49	0.41
7:6:333:THR:HG21	7:6:374:THR:CG2	2.51	0.41
11:A:515:G:H2'	11:A:516:PSU:H6	1.84	0.41
36:a:820:A:H4'	36:a:836:G:H22	1.85	0.41
36:a:1433:A:C6	36:a:1560:G:O6	2.73	0.41
22:L:35:THR:HG22	22:L:36:ARG:N	2.33	0.41
41:f:12:VAL:HG13	41:f:172:ALA:CB	2.51	0.41
7:6:124:THR:HG23	7:6:169:MET:HE1	2.03	0.41
10:9:80:GLU:CG	10:9:102:THR:HG23	2.51	0.41
18:H:105:SER:HB2	18:H:126:ILE:HD11	2.02	0.41
26:P:39:PHE:HD1	26:P:50:THR:HG22	1.81	0.41
29:S:41:PHE:H	29:S:44:MET:HE3	1.86	0.41
39:d:25:THR:HG21	39:d:193:VAL:HG22	2.02	0.41
13:C:43:LEU:HD22	13:C:68:ILE:HD11	2.03	0.41
46:k:82:LEU:O	46:k:85:VAL:HG12	2.21	0.41
61:z:38:HIS:HB3	61:z:44:THR:HG22	2.03	0.40
18:H:11:LEU:HD22	18:H:75:ILE:HD11	2.02	0.40
36:a:2312:U:H5'	41:f:85:ILE:HD11	2.02	0.40
41:f:12:VAL:HG13	41:f:172:ALA:HB1	2.03	0.40
54:s:2:ILE:HB	54:s:7:LEU:HD21	2.04	0.40
5:4:18:CYS:SG	5:4:40:CYS:CB	3.04	0.40
7:6:39:ILE:HD11	7:6:77:ILE:HB	2.02	0.40
36:a:580:U:O3'	51:p:31:VAL:HG13	2.22	0.40
36:a:1666:G:H4'	45:j:6:THR:HG23	2.03	0.40
41:f:85:ILE:HD12	41:f:85:ILE:C	2.46	0.40
57:v:59:LEU:HD12	57:v:80:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
5	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
7	6	419/443 (95%)	408 (97%)	11 (3%)	0	100	100
8	7	112/127 (88%)	101 (90%)	11 (10%)	0	100	100
9	8	52/110 (47%)	51 (98%)	1 (2%)	0	100	100
10	9	461/548 (84%)	428 (93%)	33 (7%)	0	100	100
12	B	222/241 (92%)	218 (98%)	4 (2%)	0	100	100
13	C	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
14	D	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
15	E	154/167 (92%)	145 (94%)	9 (6%)	0	100	100
16	F	101/135 (75%)	98 (97%)	3 (3%)	0	100	100
17	G	151/179 (84%)	144 (95%)	7 (5%)	0	100	100
18	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
19	I	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
20	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	25
21	K	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
22	L	120/124 (97%)	107 (89%)	13 (11%)	0	100	100
23	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
24	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
25	O	86/89 (97%)	86 (100%)	0	0	100	100
26	P	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
27	Q	77/84 (92%)	68 (88%)	9 (12%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	R	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
29	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
30	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
31	U	68/71 (96%)	68 (100%)	0	0	100	100
32	V	75/103 (73%)	66 (88%)	8 (11%)	1 (1%)	9	21
38	c	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
39	d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24	42
40	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
41	f	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
42	g	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
43	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
44	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
45	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
46	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
47	l	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
48	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
49	n	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
50	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
51	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
52	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
53	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
54	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
55	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
56	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
57	v	76/85 (89%)	72 (95%)	4 (5%)	0	100	100
58	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
59	x	60/63 (95%)	60 (100%)	0	0	100	100
60	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
61	z	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
All	All	6604/7244 (91%)	6322 (96%)	279 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	d	149	ASN
20	J	57	VAL
32	V	28	ARG

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	55 (100%)	0	100	100
7	6	344/359 (96%)	340 (99%)	4 (1%)	63	80
8	7	91/99 (92%)	91 (100%)	0	100	100
9	8	48/84 (57%)	47 (98%)	1 (2%)	47	70
10	9	400/469 (85%)	398 (100%)	2 (0%)	81	90
12	B	186/199 (94%)	186 (100%)	0	100	100
13	C	170/190 (90%)	170 (100%)	0	100	100
14	D	172/173 (99%)	172 (100%)	0	100	100
15	E	119/126 (94%)	119 (100%)	0	100	100
16	F	90/116 (78%)	90 (100%)	0	100	100
17	G	126/147 (86%)	126 (100%)	0	100	100
18	H	104/105 (99%)	104 (100%)	0	100	100
19	I	105/107 (98%)	105 (100%)	0	100	100
20	J	86/90 (96%)	86 (100%)	0	100	100
21	K	90/99 (91%)	90 (100%)	0	100	100
22	L	102/103 (99%)	102 (100%)	0	100	100
23	M	93/96 (97%)	93 (100%)	0	100	100
24	N	83/84 (99%)	83 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	O	76/77 (99%)	76 (100%)	0	100	100
26	P	65/65 (100%)	64 (98%)	1 (2%)	57	77
27	Q	73/78 (94%)	73 (100%)	0	100	100
28	R	57/65 (88%)	57 (100%)	0	100	100
29	S	72/79 (91%)	72 (100%)	0	100	100
30	T	65/66 (98%)	65 (100%)	0	100	100
31	U	60/61 (98%)	60 (100%)	0	100	100
32	V	59/81 (73%)	59 (100%)	0	100	100
38	c	216/218 (99%)	216 (100%)	0	100	100
39	d	163/163 (100%)	163 (100%)	0	100	100
40	e	165/165 (100%)	165 (100%)	0	100	100
41	f	148/150 (99%)	148 (100%)	0	100	100
42	g	137/138 (99%)	137 (100%)	0	100	100
43	h	32/114 (28%)	32 (100%)	0	100	100
44	i	116/116 (100%)	116 (100%)	0	100	100
45	j	104/104 (100%)	104 (100%)	0	100	100
46	k	103/103 (100%)	103 (100%)	0	100	100
47	l	109/109 (100%)	109 (100%)	0	100	100
48	m	98/103 (95%)	98 (100%)	0	100	100
49	n	86/87 (99%)	86 (100%)	0	100	100
50	o	99/100 (99%)	99 (100%)	0	100	100
51	p	89/90 (99%)	89 (100%)	0	100	100
52	q	84/84 (100%)	84 (100%)	0	100	100
53	r	93/93 (100%)	93 (100%)	0	100	100
54	s	80/84 (95%)	80 (100%)	0	100	100
55	t	83/85 (98%)	83 (100%)	0	100	100
56	u	78/78 (100%)	78 (100%)	0	100	100
57	v	59/63 (94%)	59 (100%)	0	100	100
58	w	67/68 (98%)	67 (100%)	0	100	100
59	x	54/55 (98%)	54 (100%)	0	100	100
60	y	48/49 (98%)	48 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	z	47/48 (98%)	47 (100%)	0	100	100
All	All	5518/5920 (93%)	5510 (100%)	8 (0%)	87	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	6	49	LEU
7	6	227	VAL
7	6	318	VAL
7	6	380	TYR
9	8	66	ILE
10	9	334	TRP
10	9	444	VAL
26	P	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	19	HIS
5	4	65	ASN
7	6	314	GLN
8	7	33	ASN
9	8	72	ASN
10	9	95	GLN
10	9	175	ASN
10	9	268	ASN
10	9	304	ASN
13	C	41	GLN
14	D	198	HIS
15	E	97	GLN
15	E	148	ASN
20	J	70	HIS
20	J	99	GLN
26	P	29	ASN
26	P	59	HIS
32	V	57	GLN
41	f	5	HIS
45	j	93	GLN
48	m	31	HIS
49	n	29	HIS
50	o	66	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
51	p	44	GLN
52	q	82	HIS
53	r	9	HIS
56	u	12	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1516/1542 (98%)	236 (15%)	3 (0%)
33	X	8/9 (88%)	1 (12%)	0
34	Y	76/77 (98%)	12 (15%)	2 (2%)
35	Z	76/77 (98%)	11 (14%)	0
36	a	2749/2904 (94%)	302 (10%)	0
37	b	118/120 (98%)	12 (10%)	0
6	5	1/2 (50%)	1 (100%)	0
All	All	4544/4731 (96%)	575 (12%)	5 (0%)

All (575) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	76	A
11	A	5	U
11	A	7	A
11	A	9	G
11	A	22	G
11	A	31	G
11	A	32	A
11	A	39	G
11	A	47	C
11	A	48	C
11	A	51	A
11	A	58	C
11	A	71	A
11	A	80	A
11	A	83	C
11	A	84	U
11	A	85	U
11	A	86	G
11	A	87	C
11	A	95	C
11	A	121	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	A	122	G
11	A	131	A
11	A	134	G
11	A	136	C
11	A	143	A
11	A	144	G
11	A	163	C
11	A	164	G
11	A	173	U
11	A	182	A
11	A	183	C
11	A	191	G
11	A	197	A
11	A	226	G
11	A	240	G
11	A	245	U
11	A	247	G
11	A	251	G
11	A	253	A
11	A	262	A
11	A	266	G
11	A	267	C
11	A	289	G
11	A	306	A
11	A	321	A
11	A	328	C
11	A	332	G
11	A	344	A
11	A	347	G
11	A	351	G
11	A	352	C
11	A	353	A
11	A	354	G
11	A	355	C
11	A	356	A
11	A	360	G
11	A	361	G
11	A	367	U
11	A	369	G
11	A	372	C
11	A	373	A
11	A	388	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	A	389	A
11	A	392	C
11	A	398	U
11	A	406	G
11	A	411	A
11	A	412	A
11	A	413	G
11	A	414	A
11	A	415	A
11	A	421	U
11	A	422	C
11	A	423	G
11	A	424	G
11	A	429	U
11	A	438	U
11	A	448	A
11	A	453	G
11	A	456	A
11	A	457	G
11	A	458	U
11	A	465	A
11	A	467	U
11	A	468	A
11	A	478	A
11	A	479	U
11	A	481	G
11	A	484	G
11	A	486	U
11	A	495	A
11	A	497	G
11	A	499	A
11	A	500	G
11	A	504	C
11	A	505	G
11	A	509	A
11	A	510	A
11	A	511	C
11	A	518	C
11	A	521	G
11	A	527	G7M
11	A	531	U
11	A	532	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	A	535	A
11	A	547	A
11	A	564	C
11	A	572	A
11	A	573	A
11	A	576	C
11	A	577	G
11	A	618	C
11	A	619	U
11	A	620	C
11	A	633	G
11	A	639	G
11	A	642	A
11	A	650	G
11	A	665	A
11	A	687	A
11	A	702	A
11	A	703	G
11	A	723	U
11	A	724	G
11	A	734	G
11	A	747	A
11	A	755	G
11	A	777	A
11	A	793	U
11	A	794	A
11	A	799	G
11	A	815	A
11	A	817	C
11	A	828	U
11	A	832	G
11	A	890	G
11	A	902	G
11	A	914	A
11	A	934	C
11	A	935	A
11	A	958	A
11	A	960	U
11	A	966	2MG
11	A	969	A
11	A	971	G
11	A	975	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	A	976	G
11	A	977	A
11	A	983	A
11	A	989	U
11	A	992	U
11	A	994	A
11	A	996	A
11	A	1003	G
11	A	1004	A
11	A	1006	G
11	A	1009	U
11	A	1028	C
11	A	1029	U
11	A	1030	U
11	A	1031	C
11	A	1032	G
11	A	1036	A
11	A	1039	G
11	A	1042	A
11	A	1044	A
11	A	1050	G
11	A	1056	U
11	A	1063	C
11	A	1065	U
11	A	1066	C
11	A	1085	U
11	A	1088	G
11	A	1094	G
11	A	1095	U
11	A	1101	A
11	A	1132	C
11	A	1133	G
11	A	1135	U
11	A	1136	C
11	A	1137	C
11	A	1139	G
11	A	1140	C
11	A	1152	A
11	A	1159	U
11	A	1167	A
11	A	1184	G
11	A	1193	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	A	1196	A
11	A	1197	A
11	A	1213	A
11	A	1215	G
11	A	1225	A
11	A	1227	A
11	A	1236	A
11	A	1238	A
11	A	1241	G
11	A	1248	A
11	A	1257	A
11	A	1260	G
11	A	1275	A
11	A	1278	G
11	A	1280	A
11	A	1286	U
11	A	1287	A
11	A	1300	G
11	A	1305	G
11	A	1317	C
11	A	1319	A
11	A	1320	C
11	A	1322	C
11	A	1336	C
11	A	1346	A
11	A	1363	A
11	A	1364	U
11	A	1370	G
11	A	1378	C
11	A	1379	G
11	A	1381	U
11	A	1419	G
11	A	1429	A
11	A	1441	A
11	A	1445	U
11	A	1448	C
11	A	1450	U
11	A	1451	U
11	A	1487	G
11	A	1492	A
11	A	1494	G
11	A	1497	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	A	1503	A
11	A	1506	U
11	A	1517	G
11	A	1529	G
11	A	1530	G
11	A	1534	A
33	X	7	C
34	Y	9	G
34	Y	14	A
34	Y	20	G
34	Y	21	U
34	Y	22	A
34	Y	46	G
34	Y	48	U
34	Y	49	C
34	Y	73	G
34	Y	74	A
34	Y	75	C
34	Y	76	C
35	Z	17	U
35	Z	19	G
35	Z	20	G
35	Z	21	U
35	Z	22	A
35	Z	46	G
35	Z	47	G
35	Z	48	U
35	Z	50	G
35	Z	76	C
35	Z	77	A
36	a	10	A
36	a	15	G
36	a	34	U
36	a	45	G
36	a	63	A
36	a	71	A
36	a	74	A
36	a	75	G
36	a	88	G
36	a	96	C
36	a	101	A
36	a	102	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	a	118	A
36	a	120	U
36	a	125	A
36	a	139	U
36	a	142	A
36	a	149	A
36	a	163	C
36	a	181	A
36	a	196	A
36	a	199	A
36	a	215	G
36	a	216	A
36	a	222	A
36	a	248	G
36	a	250	G
36	a	272	A
36	a	275	C
36	a	277	G
36	a	278	A
36	a	281	C
36	a	285	G
36	a	288	U
36	a	311	A
36	a	329	G
36	a	330	A
36	a	345	A
36	a	362	A
36	a	386	G
36	a	396	G
36	a	405	U
36	a	411	G
36	a	412	A
36	a	435	C
36	a	443	A
36	a	481	G
36	a	491	G
36	a	505	A
36	a	509	C
36	a	510	C
36	a	531	C
36	a	532	A
36	a	533	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	a	543	G
36	a	544	C
36	a	545	U
36	a	546	U
36	a	547	A
36	a	549	G
36	a	556	A
36	a	563	A
36	a	573	U
36	a	575	A
36	a	588	U
36	a	603	A
36	a	615	U
36	a	627	A
36	a	637	A
36	a	645	C
36	a	646	U
36	a	647	G
36	a	654	A
36	a	655	A
36	a	686	U
36	a	717	C
36	a	729	G
36	a	730	A
36	a	738	G
36	a	747	U
36	a	764	A
36	a	775	G
36	a	776	G
36	a	782	A
36	a	784	G
36	a	785	G
36	a	789	A
36	a	805	G
36	a	812	C
36	a	827	U
36	a	828	U
36	a	846	U
36	a	847	U
36	a	857	G
36	a	859	G
36	a	869	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	a	879	G
36	a	883	G
36	a	888	C
36	a	890	C
36	a	891	G
36	a	892	A
36	a	893	C
36	a	895	U
36	a	896	A
36	a	899	A
36	a	907	G
36	a	910	A
36	a	914	G
36	a	931	U
36	a	932	U
36	a	946	C
36	a	961	C
36	a	973	A
36	a	974	G
36	a	983	A
36	a	996	A
36	a	1005	C
36	a	1012	U
36	a	1013	C
36	a	1026	G
36	a	1027	A
36	a	1033	U
36	a	1045	C
36	a	1046	A
36	a	1047	G
36	a	1108	U
36	a	1110	G
36	a	1111	A
36	a	1112	G
36	a	1116	G
36	a	1132	U
36	a	1133	A
36	a	1135	C
36	a	1142	A
36	a	1204	A
36	a	1250	G
36	a	1253	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	a	1256	G
36	a	1271	G
36	a	1272	A
36	a	1273	U
36	a	1300	G
36	a	1301	A
36	a	1352	U
36	a	1365	A
36	a	1378	A
36	a	1379	U
36	a	1383	A
36	a	1395	A
36	a	1416	G
36	a	1428	C
36	a	1452	G
36	a	1461	C
36	a	1482	G
36	a	1493	C
36	a	1508	A
36	a	1509	A
36	a	1510	G
36	a	1515	A
36	a	1535	A
36	a	1536	C
36	a	1537	G
36	a	1569	A
36	a	1583	A
36	a	1585	C
36	a	1586	A
36	a	1607	C
36	a	1646	C
36	a	1647	U
36	a	1648	U
36	a	1649	G
36	a	1674	G
36	a	1675	C
36	a	1715	G
36	a	1729	U
36	a	1730	C
36	a	1731	G
36	a	1732	C
36	a	1733	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	a	1738	G
36	a	1764	C
36	a	1773	A
36	a	1791	A
36	a	1800	C
36	a	1801	A
36	a	1808	A
36	a	1816	C
36	a	1829	A
36	a	1847	A
36	a	1848	A
36	a	1858	A
36	a	1866	A
36	a	1869	G
36	a	1871	A
36	a	1872	A
36	a	1906	G
36	a	1913	A
36	a	1929	G
36	a	1930	G
36	a	1937	A
36	a	1938	A
36	a	1939	U
36	a	1955	U
36	a	1967	C
36	a	1970	A
36	a	1971	U
36	a	1972	G
36	a	1991	U
36	a	1992	G
36	a	1993	U
36	a	2020	A
36	a	2023	C
36	a	2030	6MZ
36	a	2031	A
36	a	2033	A
36	a	2043	C
36	a	2055	C
36	a	2056	G
36	a	2060	A
36	a	2061	G
36	a	2062	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	a	2069	G7M
36	a	2093	G
36	a	2198	A
36	a	2199	A
36	a	2204	G
36	a	2211	A
36	a	2225	A
36	a	2238	G
36	a	2239	G
36	a	2266	A
36	a	2278	A
36	a	2283	C
36	a	2287	A
36	a	2305	U
36	a	2308	G
36	a	2309	A
36	a	2312	U
36	a	2321	U
36	a	2322	A
36	a	2325	G
36	a	2333	A
36	a	2334	U
36	a	2345	G
36	a	2347	C
36	a	2361	G
36	a	2377	A
36	a	2383	G
36	a	2385	C
36	a	2391	G
36	a	2402	U
36	a	2406	A
36	a	2425	A
36	a	2429	G
36	a	2441	U
36	a	2448	A
36	a	2475	C
36	a	2476	A
36	a	2478	A
36	a	2491	U
36	a	2502	G
36	a	2505	G
36	a	2518	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	a	2520	C
36	a	2525	G
36	a	2529	G
36	a	2547	A
36	a	2554	U
36	a	2566	A
36	a	2567	G
36	a	2578	G
36	a	2602	A
36	a	2609	U
36	a	2613	U
36	a	2615	U
36	a	2629	U
36	a	2630	G
36	a	2661	G
36	a	2663	G
36	a	2689	U
36	a	2690	U
36	a	2714	G
36	a	2716	C
36	a	2726	A
36	a	2729	G
36	a	2732	G
36	a	2744	G
36	a	2748	A
36	a	2778	A
36	a	2791	G
36	a	2795	C
36	a	2798	U
36	a	2818	U
36	a	2820	A
36	a	2821	A
36	a	2872	A
36	a	2880	C
36	a	2883	A
36	a	2884	U
36	a	2891	U
36	a	2894	G
37	b	9	G
37	b	11	C
37	b	13	G
37	b	16	G

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
37	b	24	G
37	b	35	C
37	b	42	C
37	b	67	G
37	b	89	U
37	b	90	C
37	b	99	A
37	b	109	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	428	G
11	A	1035	A
11	A	1304	G
34	Y	13	C
34	Y	48	U

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

34 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
36	1MG	a	745	36	22,26,27	2.61	7 (31%)	33,39,42	1.79	9 (27%)
36	OMU	a	2552	36	19,22,23	3.07	8 (42%)	26,31,34	1.80	5 (19%)
11	2MG	A	966	11	23,26,27	2.87	9 (39%)	32,38,41	2.47	11 (34%)
36	2MA	a	2503	36,63	22,25,26	1.56	4 (18%)	33,37,40	4.38	12 (36%)
36	PSU	a	746	36,63	18,21,22	1.09	1 (5%)	22,30,33	1.61	4 (18%)
36	PSU	a	1911	36	18,21,22	1.06	1 (5%)	22,30,33	1.83	4 (18%)
11	UR3	A	1498	11,63	19,22,23	2.77	7 (36%)	26,32,35	1.33	2 (7%)
36	OMC	a	2498	36,63	19,22,23	2.81	8 (42%)	26,31,34	0.68	0
11	MA6	A	1519	11	23,26,27	1.57	4 (17%)	34,38,41	3.74	11 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	2MG	A	1516	11	23,26,27	2.75	9 (39%)	32,38,41	2.49	13 (40%)
39	MEQ	d	150	39	8,9,10	0.85	0	5,10,12	0.77	0
36	H2U	a	2449	36	18,21,22	2.61	5 (27%)	21,30,33	2.22	5 (23%)
36	6MZ	a	2030	36	22,25,26	2.47	5 (22%)	30,36,39	2.84	12 (40%)
36	PSU	a	955	36	18,21,22	1.07	2 (11%)	22,30,33	1.81	4 (18%)
11	5MC	A	967	11	18,22,23	3.65	8 (44%)	26,32,35	1.03	2 (7%)
36	2MG	a	2445	36	23,26,27	2.61	9 (39%)	32,38,41	2.26	13 (40%)
36	6MZ	a	1618	36	22,25,26	2.45	5 (22%)	30,36,39	2.59	11 (36%)
36	PSU	a	2504	36	18,21,22	1.09	2 (11%)	22,30,33	1.87	5 (22%)
11	2MG	A	1207	11	23,26,27	2.86	9 (39%)	32,38,41	2.46	11 (34%)
36	OMG	a	2251	35,36	23,26,27	2.33	8 (34%)	33,38,41	1.90	9 (27%)
36	2MG	a	1835	36	23,26,27	2.72	8 (34%)	32,38,41	2.34	11 (34%)
11	G7M	A	527	11	23,26,27	2.88	10 (43%)	35,39,42	2.14	10 (28%)
36	5MC	a	1962	36	18,22,23	3.46	8 (44%)	26,32,35	1.03	2 (7%)
36	PSU	a	2580	36	18,21,22	1.08	3 (16%)	22,30,33	1.94	6 (27%)
11	PSU	A	516	11	18,21,22	1.00	1 (5%)	22,30,33	1.97	6 (27%)
11	4OC	A	1402	11	20,23,24	3.46	8 (40%)	26,32,35	0.87	1 (3%)
36	G7M	a	2069	36	23,26,27	2.88	9 (39%)	35,39,42	2.17	10 (28%)
36	PSU	a	2604	36	18,21,22	1.05	2 (11%)	22,30,33	1.90	5 (22%)
36	PSU	a	2605	36	18,21,22	1.04	2 (11%)	22,30,33	1.87	5 (22%)
36	PSU	a	2457	36	18,21,22	1.06	3 (16%)	22,30,33	1.97	6 (27%)
11	5MC	A	1407	11	18,22,23	3.59	8 (44%)	26,32,35	0.99	2 (7%)
22	D2T	L	89	22	7,9,10	1.21	0	6,11,13	1.66	1 (16%)
36	PSU	a	1917	36	18,21,22	1.10	1 (5%)	22,30,33	1.74	4 (18%)
11	MA6	A	1518	11	23,26,27	1.55	4 (17%)	34,38,41	3.63	11 (32%)

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
36	1MG	a	745	36	-	0/7/25/26	0/3/3/3
36	OMU	a	2552	36	-	0/9/27/28	0/2/2/2
11	2MG	A	966	11	-	2/9/27/28	0/3/3/3
36	2MA	a	2503	36,63	-	1/7/25/26	0/3/3/3
36	PSU	a	746	36,63	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PSU	a	1911	36	-	0/7/25/26	0/2/2/2
11	UR3	A	1498	11,63	-	0/7/25/26	0/2/2/2
36	OMC	a	2498	36,63	-	0/9/27/28	0/2/2/2
11	MA6	A	1519	11	-	3/11/29/30	0/3/3/3
11	2MG	A	1516	11	-	0/9/27/28	0/3/3/3
39	MEQ	d	150	39	-	2/8/9/11	-
36	H2U	a	2449	36	-	0/7/38/39	0/2/2/2
36	6MZ	a	2030	36	-	2/9/27/28	0/3/3/3
36	PSU	a	955	36	-	0/7/25/26	0/2/2/2
11	5MC	A	967	11	-	0/7/25/26	0/2/2/2
36	2MG	a	2445	36	-	0/9/27/28	0/3/3/3
36	6MZ	a	1618	36	-	0/9/27/28	0/3/3/3
36	PSU	a	2504	36	-	0/7/25/26	0/2/2/2
11	2MG	A	1207	11	-	0/9/27/28	0/3/3/3
36	OMG	a	2251	35,36	-	0/9/27/28	0/3/3/3
36	2MG	a	1835	36	-	0/9/27/28	0/3/3/3
11	G7M	A	527	11	-	3/7/25/26	0/3/3/3
36	5MC	a	1962	36	-	0/7/25/26	0/2/2/2
36	PSU	a	2580	36	-	2/7/25/26	0/2/2/2
11	PSU	A	516	11	-	2/7/25/26	0/2/2/2
11	4OC	A	1402	11	-	1/9/29/30	0/2/2/2
36	G7M	a	2069	36	-	1/7/25/26	0/3/3/3
36	PSU	a	2604	36	-	0/7/25/26	0/2/2/2
36	PSU	a	2605	36	-	0/7/25/26	0/2/2/2
36	PSU	a	2457	36	-	0/7/25/26	0/2/2/2
11	5MC	A	1407	11	-	0/7/25/26	0/2/2/2
22	D2T	L	89	22	-	0/7/12/14	-
36	PSU	a	1917	36	-	1/7/25/26	0/2/2/2
11	MA6	A	1518	11	-	3/11/29/30	0/3/3/3

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	1618	6MZ	C6-N6	9.55	1.44	1.34
36	a	2030	6MZ	C6-N6	9.48	1.44	1.34
11	A	967	5MC	C6-C5	9.04	1.49	1.34
11	A	1407	5MC	C6-C5	8.73	1.48	1.34
36	a	1962	5MC	C6-C5	8.31	1.48	1.34
11	A	1207	2MG	C2-N3	7.61	1.46	1.31
11	A	966	2MG	C2-N3	7.58	1.46	1.31
36	a	2449	H2U	C2-N1	7.53	1.46	1.35

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1498	UR3	C2-N1	7.41	1.49	1.38
36	a	2069	G7M	C5-N7	-7.40	1.30	1.39
11	A	1402	4OC	C4-N3	7.22	1.45	1.32
36	a	2552	OMU	C2-N3	7.05	1.50	1.38
36	a	1835	2MG	C2-N3	7.03	1.45	1.31
11	A	1402	4OC	C4-N4	6.87	1.50	1.35
36	a	2552	OMU	C2-N1	6.87	1.49	1.38
11	A	1516	2MG	C2-N3	6.81	1.44	1.31
11	A	967	5MC	C4-N3	6.72	1.45	1.34
11	A	527	G7M	C5-N7	-6.70	1.31	1.39
11	A	1407	5MC	C4-N3	6.68	1.45	1.34
11	A	527	G7M	C4-N3	6.55	1.49	1.34
36	a	1962	5MC	C4-N3	6.48	1.45	1.34
11	A	1402	4OC	C2-N3	6.42	1.49	1.36
11	A	1402	4OC	C6-C5	6.41	1.50	1.35
11	A	1407	5MC	C2-N3	6.40	1.49	1.36
11	A	967	5MC	C2-N3	6.40	1.49	1.36
11	A	966	2MG	C4-N3	6.36	1.49	1.34
11	A	1207	2MG	C4-N3	6.33	1.49	1.34
36	a	745	1MG	C2-N3	6.30	1.45	1.34
36	a	2445	2MG	C2-N3	6.25	1.43	1.31
11	A	1498	UR3	C6-C5	6.21	1.49	1.35
36	a	1962	5MC	C2-N3	6.19	1.48	1.36
36	a	2069	G7M	C4-N3	6.15	1.48	1.34
36	a	2552	OMU	C6-C5	6.07	1.49	1.35
36	a	745	1MG	C4-N3	6.05	1.48	1.34
36	a	1835	2MG	C4-N3	5.97	1.48	1.34
36	a	745	1MG	C2-N2	5.93	1.44	1.34
36	a	2251	OMG	C4-N3	5.88	1.48	1.34
36	a	2498	OMC	C2-N3	5.79	1.48	1.36
36	a	2498	OMC	C6-C5	5.76	1.48	1.35
11	A	1516	2MG	C4-N3	5.61	1.47	1.34
11	A	966	2MG	C2-N2	5.56	1.45	1.33
11	A	1207	2MG	C2-N2	5.51	1.45	1.33
36	a	2445	2MG	C4-N3	5.43	1.47	1.34
36	a	2449	H2U	C2-N3	5.36	1.47	1.38
11	A	527	G7M	C2-N3	5.36	1.46	1.33
36	a	2251	OMG	C2-N3	5.29	1.45	1.33
11	A	1516	2MG	C2-N2	5.29	1.45	1.33
36	a	1835	2MG	C2-N2	5.19	1.44	1.33
11	A	1516	2MG	C2-N1	5.08	1.44	1.36
36	a	2069	G7M	C2-N3	4.92	1.45	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1207	2MG	C2-N1	4.91	1.44	1.36
11	A	966	2MG	C2-N1	4.87	1.44	1.36
11	A	967	5MC	C6-N1	4.86	1.46	1.38
36	a	2498	OMC	C4-N4	4.74	1.45	1.33
11	A	1407	5MC	C6-N1	4.73	1.46	1.38
11	A	1518	MA6	C6-N6	4.67	1.50	1.36
36	a	2445	2MG	C2-N2	4.63	1.43	1.33
36	a	1962	5MC	C6-N1	4.62	1.45	1.38
11	A	1519	MA6	C6-N6	4.56	1.50	1.36
36	a	2498	OMC	C4-N3	4.54	1.43	1.34
36	a	2445	2MG	C2-N1	4.42	1.43	1.36
11	A	527	G7M	C2-N2	4.41	1.44	1.34
11	A	1498	UR3	C2-N3	4.40	1.47	1.39
11	A	967	5MC	C2-N1	4.36	1.49	1.40
11	A	967	5MC	C4-N4	4.34	1.45	1.34
36	a	1835	2MG	C2-N1	4.27	1.43	1.36
11	A	1407	5MC	C4-N4	4.24	1.45	1.34
11	A	1402	4OC	C5-C4	4.22	1.49	1.40
11	A	1407	5MC	C2-N1	4.19	1.49	1.40
36	a	2251	OMG	C2-N2	4.18	1.44	1.34
11	A	1402	4OC	C2-N1	4.17	1.49	1.40
36	a	1962	5MC	C4-N4	4.15	1.44	1.34
36	a	2449	H2U	C4-N3	4.13	1.44	1.37
36	a	2069	G7M	C2-N2	4.06	1.43	1.34
36	a	2552	OMU	C4-N3	4.03	1.45	1.38
36	a	1962	5MC	C2-N1	4.02	1.48	1.40
36	a	2503	2MA	C6-N6	3.96	1.44	1.34
36	a	2498	OMC	C2-N1	3.79	1.48	1.40
11	A	527	G7M	C5-C6	3.55	1.53	1.43
36	a	1835	2MG	C5-N7	-3.53	1.32	1.39
36	a	2069	G7M	O6-C6	-3.52	1.16	1.23
36	a	1917	PSU	C6-C5	3.46	1.39	1.35
36	a	745	1MG	C5-N7	-3.45	1.32	1.39
36	a	2503	2MA	C5-C4	-3.44	1.32	1.39
36	a	2251	OMG	C5-N7	-3.44	1.32	1.39
36	a	2030	6MZ	C5-N7	-3.44	1.32	1.39
36	a	2445	2MG	C5-N7	-3.43	1.32	1.39
11	A	1402	4OC	C6-N1	3.39	1.46	1.38
11	A	527	G7M	C2-N1	3.35	1.46	1.37
36	a	1911	PSU	C6-C5	3.34	1.39	1.35
36	a	2030	6MZ	C5-C4	-3.33	1.32	1.39
11	A	1498	UR3	O2-C2	-3.32	1.16	1.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1207	2MG	C5-N7	-3.24	1.32	1.39
36	a	746	PSU	C6-C5	3.23	1.39	1.35
11	A	527	G7M	O6-C6	-3.22	1.17	1.23
36	a	1618	6MZ	C5-C4	-3.21	1.33	1.39
36	a	2069	G7M	C5-C6	3.18	1.52	1.43
11	A	966	2MG	C5-N7	-3.14	1.33	1.39
36	a	2498	OMC	O2-C2	-3.13	1.17	1.23
36	a	2445	2MG	C4-N9	-3.13	1.29	1.38
11	A	1516	2MG	C5-N7	-3.10	1.33	1.39
11	A	516	PSU	C6-C5	3.10	1.38	1.35
36	a	2069	G7M	C2-N1	3.09	1.45	1.37
36	a	2069	G7M	CN7-N7	-3.00	1.41	1.46
36	a	1618	6MZ	C5-N7	-2.99	1.33	1.39
36	a	2449	H2U	O2-C2	-2.95	1.17	1.23
36	a	2251	OMG	O6-C6	-2.92	1.18	1.23
11	A	1519	MA6	C5-C4	-2.91	1.33	1.39
36	a	2604	PSU	C6-C5	2.91	1.38	1.35
36	a	955	PSU	C6-C5	2.84	1.38	1.35
36	a	2445	2MG	O6-C6	-2.82	1.18	1.23
36	a	745	1MG	C5-C6	2.80	1.52	1.45
36	a	2504	PSU	C6-C5	2.78	1.38	1.35
36	a	1835	2MG	O6-C6	-2.78	1.18	1.23
11	A	1498	UR3	O4-C4	-2.78	1.17	1.23
36	a	2498	OMC	C6-N1	2.76	1.44	1.38
11	A	1402	4OC	O2-C2	-2.73	1.18	1.23
11	A	1516	2MG	C4-N9	-2.72	1.31	1.38
36	a	2605	PSU	C6-C5	2.72	1.38	1.35
11	A	1518	MA6	C5-C4	-2.72	1.33	1.39
36	a	2552	OMU	O4-C4	-2.71	1.19	1.24
36	a	2069	G7M	C4-N9	-2.69	1.31	1.38
11	A	527	G7M	CN7-N7	-2.68	1.42	1.46
36	a	2030	6MZ	C8-N9	-2.66	1.32	1.37
36	a	2457	PSU	C6-C5	2.65	1.38	1.35
36	a	2580	PSU	C6-C5	2.63	1.38	1.35
36	a	2552	OMU	C6-N1	2.62	1.44	1.38
11	A	1519	MA6	C5-N7	-2.62	1.34	1.39
11	A	1516	2MG	C6-N1	2.60	1.43	1.38
11	A	966	2MG	O6-C6	-2.57	1.18	1.23
11	A	1516	2MG	O6-C6	-2.57	1.18	1.23
36	a	1835	2MG	C4-N9	-2.53	1.31	1.38
11	A	1207	2MG	C5-C6	2.52	1.53	1.44
11	A	1207	2MG	O6-C6	-2.51	1.18	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	2449	H2U	O4-C4	-2.50	1.18	1.23
36	a	2552	OMU	O2-C2	-2.49	1.18	1.23
11	A	1518	MA6	C5-N7	-2.47	1.34	1.39
11	A	966	2MG	C5-C6	2.47	1.53	1.44
11	A	1516	2MG	C5-C6	2.46	1.53	1.44
36	a	2552	OMU	C5-C4	2.46	1.49	1.43
11	A	966	2MG	C6-N1	2.46	1.43	1.38
36	a	1962	5MC	O2-C2	-2.44	1.19	1.23
36	a	2030	6MZ	C6-N1	-2.42	1.31	1.35
36	a	1618	6MZ	C8-N9	-2.41	1.33	1.37
11	A	1519	MA6	C8-N9	-2.38	1.33	1.37
11	A	1207	2MG	C6-N1	2.35	1.43	1.38
11	A	1518	MA6	C8-N9	-2.32	1.33	1.37
36	a	2503	2MA	C8-N9	-2.32	1.33	1.37
36	a	745	1MG	O6-C6	-2.31	1.18	1.23
11	A	1407	5MC	O2-C2	-2.29	1.19	1.23
36	a	2251	OMG	C5-C6	2.27	1.52	1.44
11	A	967	5MC	O2-C2	-2.25	1.19	1.23
36	a	2580	PSU	O4'-C1'	-2.25	1.40	1.43
36	a	2498	OMC	C5-C4	2.22	1.48	1.42
11	A	527	G7M	C6-N1	2.21	1.42	1.38
36	a	1618	6MZ	C6-N1	-2.19	1.31	1.35
36	a	2251	OMG	C2-N1	2.18	1.43	1.37
36	a	2445	2MG	C5-C6	2.17	1.52	1.44
36	a	955	PSU	C4-C5	-2.15	1.38	1.44
36	a	745	1MG	C4-N9	-2.15	1.32	1.38
36	a	2580	PSU	C4-C5	-2.14	1.38	1.44
11	A	1498	UR3	C6-N1	2.14	1.43	1.38
36	a	2251	OMG	C4-N9	-2.12	1.32	1.38
36	a	1835	2MG	C5-C6	2.11	1.52	1.44
36	a	2503	2MA	C5-N7	-2.10	1.35	1.39
36	a	2605	PSU	C4-C5	-2.09	1.38	1.44
11	A	1498	UR3	C5-C4	2.09	1.49	1.43
36	a	2504	PSU	C4-C5	-2.08	1.38	1.44
11	A	527	G7M	C4-N9	-2.06	1.32	1.38
11	A	967	5MC	CM5-C5	2.06	1.55	1.50
36	a	2457	PSU	O4'-C1'	-2.05	1.41	1.43
36	a	2457	PSU	C4-C5	-2.03	1.38	1.44
36	a	2445	2MG	C6-N1	2.02	1.42	1.38
11	A	1207	2MG	C4-N9	-2.01	1.32	1.38
36	a	2604	PSU	C4-C5	-2.01	1.38	1.44
11	A	966	2MG	C4-N9	-2.01	1.32	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	1962	5MC	CM5-C5	2.00	1.55	1.50
11	A	1407	5MC	CM5-C5	2.00	1.55	1.50

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	2503	2MA	CM2-C2-N3	17.13	143.90	117.15
11	A	1519	MA6	N1-C6-N6	-15.58	100.04	117.08
11	A	1518	MA6	N1-C6-N6	-15.12	100.55	117.08
36	a	2503	2MA	CM2-C2-N1	-13.30	96.38	117.15
11	A	1519	MA6	C5-C6-N6	8.46	140.03	125.30
11	A	1518	MA6	C5-C6-N6	8.20	139.59	125.30
36	a	2449	H2U	C4-N3-C2	-7.32	119.72	125.79
11	A	1516	2MG	C2-N3-C4	6.69	120.34	112.04
11	A	966	2MG	C2-N3-C4	6.51	120.11	112.04
11	A	1207	2MG	C2-N3-C4	6.46	120.05	112.04
36	a	2030	6MZ	C5-C4-N3	-6.44	118.35	126.75
36	a	2030	6MZ	C9-N6-C6	-6.40	117.36	122.87
36	a	1835	2MG	C2-N3-C4	6.07	119.57	112.04
36	a	2503	2MA	N9-C8-N7	-5.71	106.11	113.91
36	a	1618	6MZ	C5-C4-N3	-5.69	119.33	126.75
36	a	2552	OMU	C4-N3-C2	-5.64	119.14	126.58
36	a	2445	2MG	C2-N3-C4	5.63	119.03	112.04
11	A	1207	2MG	C1'-N9-C8	-5.50	111.03	126.70
11	A	1518	MA6	N1-C2-N3	-5.50	120.01	128.60
11	A	1516	2MG	C1'-N9-C8	-5.49	111.07	126.70
11	A	1519	MA6	N1-C2-N3	-5.48	120.03	128.60
11	A	966	2MG	C1'-N9-C8	-5.48	111.09	126.70
36	a	2503	2MA	C5-C4-N3	-5.46	121.05	127.19
36	a	745	1MG	C5-C4-N3	-5.46	119.61	128.46
36	a	1618	6MZ	N1-C2-N3	-5.44	120.09	128.60
36	a	2251	OMG	C5-C4-N3	-5.43	119.65	128.46
36	a	1835	2MG	C1'-N9-C8	-5.39	111.35	126.70
11	A	527	G7M	CN7-N7-C5	5.32	133.38	126.77
36	a	2030	6MZ	C4-C5-C6	5.29	120.91	116.81
11	A	1518	MA6	C5-C4-N3	-5.20	119.96	126.75
11	A	1519	MA6	C5-C4-N3	-5.18	119.99	126.75
36	a	2030	6MZ	N1-C2-N3	-5.13	120.58	128.60
36	a	1618	6MZ	C9-N6-C6	-5.09	118.49	122.87
11	A	1207	2MG	C5-C4-N3	-5.06	120.25	128.46
11	A	1207	2MG	C1'-N9-C4	5.03	141.45	126.50
11	A	1498	UR3	C4-N3-C2	-5.01	119.85	124.56

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	966	2MG	C5-C4-N3	-4.96	120.41	128.46
36	a	2457	PSU	C4-N3-C2	-4.94	119.22	126.34
36	a	2504	PSU	C4-N3-C2	-4.90	119.28	126.34
11	A	966	2MG	C1'-N9-C4	4.89	141.04	126.50
36	a	2604	PSU	C4-N3-C2	-4.88	119.30	126.34
36	a	2605	PSU	C4-N3-C2	-4.88	119.30	126.34
11	A	516	PSU	N1-C2-N3	4.88	120.66	115.13
36	a	2445	2MG	C1'-N9-C8	-4.87	112.82	126.70
11	A	516	PSU	C4-N3-C2	-4.87	119.32	126.34
36	a	2457	PSU	N1-C2-N3	4.86	120.64	115.13
36	a	2069	G7M	CN7-N7-C5	4.83	132.77	126.77
11	A	1516	2MG	C1'-N9-C4	4.82	140.82	126.50
36	a	2580	PSU	C4-N3-C2	-4.78	119.45	126.34
36	a	1835	2MG	C1'-N9-C4	4.77	140.69	126.50
36	a	2504	PSU	N1-C2-N3	4.75	120.51	115.13
36	a	2604	PSU	N1-C2-N3	4.75	120.51	115.13
36	a	955	PSU	C4-N3-C2	-4.74	119.51	126.34
36	a	2605	PSU	N1-C2-N3	4.74	120.50	115.13
36	a	2580	PSU	N1-C2-N3	4.74	120.50	115.13
36	a	1911	PSU	C4-N3-C2	-4.72	119.53	126.34
36	a	2503	2MA	N6-C6-N1	-4.64	110.47	117.03
11	A	1519	MA6	N9-C8-N7	-4.62	107.60	113.91
36	a	1911	PSU	N1-C2-N3	4.59	120.33	115.13
36	a	746	PSU	C4-N3-C2	-4.53	119.81	126.34
36	a	2069	G7M	C1'-N9-C4	-4.51	113.10	126.50
36	a	955	PSU	N1-C2-N3	4.51	120.23	115.13
36	a	1917	PSU	C4-N3-C2	-4.49	119.87	126.34
36	a	1618	6MZ	C4-C5-C6	4.42	120.23	116.81
36	a	1917	PSU	N1-C2-N3	4.40	120.12	115.13
36	a	2445	2MG	C2-N1-C6	-4.36	119.46	124.48
11	A	527	G7M	C2-N3-C4	4.36	120.06	112.30
36	a	1835	2MG	C5-C4-N3	-4.32	121.45	128.46
11	A	527	G7M	C5-C4-N3	-4.31	119.88	128.15
11	A	1516	2MG	C2-N1-C6	-4.28	119.56	124.48
36	a	2251	OMG	C2-N3-C4	4.27	119.91	112.30
11	A	1516	2MG	C5-C4-N3	-4.23	121.60	128.46
11	A	1518	MA6	N9-C8-N7	-4.22	108.14	113.91
36	a	2030	6MZ	N9-C8-N7	-4.22	108.15	113.91
36	a	2069	G7M	C2-N3-C4	4.20	119.78	112.30
36	a	746	PSU	N1-C2-N3	4.16	119.84	115.13
36	a	2445	2MG	C1'-N9-C4	4.15	138.83	126.50
11	A	966	2MG	C2-N1-C6	-4.11	119.75	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1207	2MG	C2-N1-C6	-4.10	119.76	124.48
36	a	2069	G7M	C5-C4-N3	-4.07	120.35	128.15
36	a	2552	OMU	N3-C2-N1	4.05	120.27	114.89
36	a	2449	H2U	N3-C2-N1	4.03	120.92	116.65
36	a	2030	6MZ	N3-C4-N9	4.00	133.67	127.08
11	A	527	G7M	CN7-N7-C8	-3.96	118.73	124.84
36	a	2069	G7M	C5-C6-N1	3.96	120.05	111.79
36	a	1618	6MZ	N9-C8-N7	-3.92	108.55	113.91
36	a	2449	H2U	O2-C2-N1	-3.90	118.21	123.11
11	A	527	G7M	C5-C6-N1	3.90	119.94	111.79
11	A	516	PSU	O2-C2-N1	-3.88	118.52	122.79
11	A	1519	MA6	C4-C5-C6	3.85	120.19	115.88
36	a	2445	2MG	C5-C4-N3	-3.85	122.22	128.46
36	a	2503	2MA	C4-N9-C8	3.81	109.86	105.73
36	a	1618	6MZ	C4-N9-C1'	-3.78	117.60	126.59
36	a	2030	6MZ	C2-N3-C4	3.77	120.65	111.75
11	A	1518	MA6	C4-C5-C6	3.75	120.08	115.88
36	a	2069	G7M	O6-C6-C5	-3.71	119.69	128.06
11	A	527	G7M	C1'-N9-C4	-3.69	115.54	126.50
36	a	1618	6MZ	C2-N3-C4	3.66	120.40	111.75
36	a	2069	G7M	CN7-N7-C8	-3.64	119.22	124.84
36	a	2503	2MA	C5-N7-C8	3.63	108.67	103.51
36	a	2030	6MZ	C4-N9-C1'	-3.62	117.97	126.59
36	a	1835	2MG	C2-N1-C6	-3.59	120.34	124.48
36	a	745	1MG	C2-N3-C4	3.59	120.04	111.98
11	A	1518	MA6	C2-N1-C6	3.55	120.15	111.75
36	a	2445	2MG	N9-C8-N7	-3.55	106.71	113.39
36	a	2030	6MZ	C5-N7-C8	3.52	108.51	103.51
36	a	2552	OMU	C5-C4-N3	3.50	120.08	114.84
11	A	1519	MA6	C2-N1-C6	3.49	120.01	111.75
11	A	1518	MA6	C2-N3-C4	3.47	119.94	111.75
11	A	527	G7M	O6-C6-C5	-3.45	120.28	128.06
36	a	1618	6MZ	N3-C4-N9	3.44	132.75	127.08
11	A	1519	MA6	C2-N3-C4	3.44	119.87	111.75
36	a	2069	G7M	C1'-N9-C8	3.40	138.23	126.74
11	A	1519	MA6	N3-C4-N9	3.37	132.63	127.08
36	a	1618	6MZ	C1'-N9-C8	3.36	134.72	127.14
36	a	745	1MG	N9-C4-N3	3.33	132.62	125.94
11	A	967	5MC	C5-C6-N1	-3.31	119.93	123.34
36	a	2030	6MZ	C1'-N9-C8	3.29	134.56	127.14
11	A	527	G7M	N9-C4-N3	3.28	132.53	125.94
11	A	1518	MA6	N3-C4-N9	3.27	132.48	127.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	2503	2MA	N3-C2-N1	-3.26	119.72	125.72
11	A	1516	2MG	N9-C8-N7	-3.24	107.28	113.39
36	a	2251	OMG	N9-C4-N3	3.23	132.43	125.94
11	A	966	2MG	N9-C8-N7	-3.22	107.32	113.39
36	a	1835	2MG	N9-C8-N7	-3.20	107.36	113.39
11	A	1519	MA6	C5-N7-C8	3.19	108.05	103.51
36	a	2251	OMG	C2-N1-C6	-3.18	119.29	125.10
36	a	2580	PSU	O2-C2-N1	-3.10	119.38	122.79
36	a	2503	2MA	N3-C4-N9	3.08	131.27	126.99
36	a	2069	G7M	C2-N1-C6	-3.07	119.51	125.10
36	a	2069	G7M	N9-C4-N3	3.06	132.08	125.94
11	A	1207	2MG	N9-C8-N7	-3.03	107.69	113.39
36	a	2552	OMU	O4-C4-C5	-3.02	119.85	125.16
36	a	2457	PSU	C6-C5-C4	2.97	120.28	118.20
36	a	2251	OMG	C1 <sup>?</sup> -N9-C4	-2.92	117.82	126.50
22	L	89	D2T	OD1-CG-CB	-2.92	116.33	122.44
11	A	1518	MA6	C5-N7-C8	2.89	107.61	103.51
11	A	527	G7M	C2-N1-C6	-2.89	119.83	125.10
36	a	1835	2MG	N1-C2-N3	-2.88	119.50	123.95
11	A	527	G7M	C1 <sup>?</sup> -N9-C8	2.87	136.43	126.74
11	A	1516	2MG	N1-C2-N3	-2.85	119.55	123.95
36	a	2457	PSU	O2-C2-N1	-2.84	119.66	122.79
36	a	1911	PSU	O2-C2-N1	-2.81	119.70	122.79
36	a	745	1MG	N9-C8-N7	-2.80	108.11	113.39
36	a	2449	H2U	C5-C4-N3	2.79	119.79	116.65
36	a	2504	PSU	O2-C2-N1	-2.78	119.73	122.79
36	a	1618	6MZ	C5-N7-C8	2.77	107.44	103.51
36	a	955	PSU	O2-C2-N1	-2.76	119.75	122.79
36	a	2251	OMG	C1 <sup>?</sup> -N9-C8	2.72	134.44	126.70
36	a	745	1MG	C5-C6-N1	2.70	120.12	114.91
11	A	966	2MG	N1-C2-N3	-2.68	119.81	123.95
36	a	2604	PSU	O2-C2-N1	-2.68	119.84	122.79
36	a	2605	PSU	O2-C2-N1	-2.67	119.85	122.79
11	A	1519	MA6	C4-N9-C8	2.67	108.62	105.73
11	A	966	2MG	C5-C6-N1	2.66	119.95	113.19
11	A	1516	2MG	C5-C6-N1	2.66	119.94	113.19
36	a	1835	2MG	C5-C6-N1	2.61	119.83	113.19
11	A	1207	2MG	C5-C6-N1	2.59	119.78	113.19
36	a	2251	OMG	C5-C6-N1	2.59	119.76	113.19
11	A	1207	2MG	N9-C4-N3	2.59	131.13	125.94
11	A	1516	2MG	O6-C6-C5	-2.58	119.75	126.60
11	A	1207	2MG	N1-C2-N3	-2.58	119.97	123.95

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	966	2MG	N9-C4-N3	2.57	131.11	125.94
36	a	2251	OMG	N9-C8-N7	-2.57	108.55	113.39
36	a	2445	2MG	C5-C6-N1	2.54	119.65	113.19
36	a	2503	2MA	C5-C6-N6	2.52	128.92	123.43
36	a	1835	2MG	O6-C6-C5	-2.51	119.95	126.60
11	A	966	2MG	O6-C6-C5	-2.51	119.95	126.60
36	a	2445	2MG	O6-C6-C5	-2.50	119.97	126.60
36	a	2580	PSU	C6-C5-C4	2.50	119.94	118.20
36	a	2604	PSU	C6-C5-C4	2.49	119.94	118.20
36	a	1917	PSU	O2-C2-N1	-2.48	120.06	122.79
36	a	746	PSU	O2-C2-N1	-2.47	120.07	122.79
36	a	745	1MG	CM1-N1-C6	2.45	121.45	117.69
11	A	966	2MG	C8-N7-C5	2.42	108.62	104.24
36	a	2503	2MA	C4-N9-C1'	-2.41	120.84	126.59
36	a	2503	2MA	C4-C5-N7	-2.41	107.68	110.62
11	A	1516	2MG	CM2-N2-C2	-2.41	118.54	123.86
11	A	1402	4OC	C6-C5-C4	2.40	119.90	116.96
36	a	2449	H2U	C5-C6-N1	2.40	119.51	111.61
11	A	516	PSU	C6-C5-C4	2.38	119.86	118.20
11	A	1207	2MG	O6-C6-C5	-2.38	120.29	126.60
36	a	1911	PSU	C6-C5-C4	2.38	119.86	118.20
36	a	2580	PSU	O4'-C1'-C2'	2.37	108.48	105.14
36	a	1962	5MC	C5-C6-N1	-2.36	120.91	123.34
11	A	1518	MA6	C4-N9-C8	2.33	108.25	105.73
36	a	2251	OMG	O6-C6-C5	-2.33	120.42	126.60
11	A	1207	2MG	C8-N7-C5	2.32	108.44	104.24
36	a	745	1MG	C2-N1-C6	-2.30	119.08	120.95
11	A	1407	5MC	C5-C6-N1	-2.30	120.98	123.34
11	A	967	5MC	CM5-C5-C6	-2.29	119.79	122.85
36	a	2552	OMU	O2-C2-N1	-2.29	119.75	122.79
36	a	1917	PSU	C6-N1-C2	-2.27	120.36	122.68
36	a	2580	PSU	C6-N1-C2	-2.27	120.36	122.68
11	A	1407	5MC	CM5-C5-C6	-2.26	119.82	122.85
36	a	2445	2MG	C8-N7-C5	2.25	108.32	104.24
36	a	955	PSU	C6-N1-C2	-2.25	120.38	122.68
36	a	2030	6MZ	C4-C5-N7	-2.24	107.89	110.62
11	A	1516	2MG	C4-C5-N7	-2.24	107.18	110.72
36	a	2605	PSU	C6-N1-C2	-2.21	120.42	122.68
36	a	2445	2MG	N1-C2-N3	-2.20	120.55	123.95
36	a	745	1MG	C1'-N9-C4	-2.18	120.01	126.50
36	a	1962	5MC	CM5-C5-C6	-2.18	119.94	122.85
11	A	1516	2MG	C8-N7-C5	2.17	108.17	104.24

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	2445	2MG	C4-C5-N7	-2.16	107.31	110.72
11	A	516	PSU	C6-N1-C2	-2.14	120.49	122.68
36	a	2030	6MZ	C5-C6-N1	2.13	120.47	118.20
36	a	2604	PSU	C6-N1-C2	-2.12	120.52	122.68
36	a	2504	PSU	C6-C5-C4	2.11	119.68	118.20
36	a	1835	2MG	C8-N7-C5	2.09	108.02	104.24
36	a	1835	2MG	N9-C4-N3	2.08	130.11	125.94
36	a	2445	2MG	CM2-N2-C2	-2.07	119.28	123.86
36	a	746	PSU	C6-N1-C2	-2.07	120.57	122.68
36	a	745	1MG	O6-C6-C5	-2.07	119.21	124.70
11	A	1516	2MG	C5-C4-N9	2.07	109.38	105.63
11	A	1498	UR3	C3U-N3-C2	2.06	120.93	117.31
36	a	1618	6MZ	C5-C6-N1	2.06	120.40	118.20
36	a	2445	2MG	C5-C4-N9	2.06	109.37	105.63
36	a	2457	PSU	O4'-C1'-C2'	2.05	108.04	105.14
36	a	2504	PSU	C6-N1-C2	-2.05	120.59	122.68
36	a	2457	PSU	C6-N1-C2	-2.04	120.59	122.68
11	A	516	PSU	O4'-C1'-C2'	2.02	107.99	105.14
36	a	2605	PSU	C6-C5-C4	2.02	119.61	118.20

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	527	G7M	O4'-C4'-C5'-O5'
11	A	527	G7M	C3'-C4'-C5'-O5'
11	A	1518	MA6	C5-C6-N6-C10
11	A	1519	MA6	C5-C6-N6-C10
36	a	2030	6MZ	O4'-C4'-C5'-O5'
36	a	2030	6MZ	C3'-C4'-C5'-O5'
11	A	516	PSU	O4'-C4'-C5'-O5'
11	A	1518	MA6	N1-C6-N6-C10
11	A	1519	MA6	N1-C6-N6-C10
11	A	516	PSU	C3'-C4'-C5'-O5'
11	A	966	2MG	C3'-C4'-C5'-O5'
36	a	2580	PSU	O4'-C4'-C5'-O5'
11	A	1518	MA6	C5-C6-N6-C9
39	d	150	MEQ	OE1-CD-CG-CB
39	d	150	MEQ	NE2-CD-CG-CB
11	A	1402	4OC	O4'-C4'-C5'-O5'
11	A	1519	MA6	C5-C6-N6-C9
11	A	966	2MG	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	a	2069	G7M	O4'-C4'-C5'-O5'
11	A	527	G7M	C4'-C5'-O5'-P
36	a	2503	2MA	O4'-C4'-C5'-O5'
36	a	2580	PSU	C3'-C4'-C5'-O5'
36	a	1917	PSU	O4'-C4'-C5'-O5'
36	a	746	PSU	O4'-C1'-C5-C6

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	a	745	1MG	1	0
36	a	2552	OMU	1	0
36	a	746	PSU	1	0
11	A	1519	MA6	1	0
39	d	150	MEQ	1	0
36	a	2030	6MZ	2	0
11	A	516	PSU	1	0
11	A	1518	MA6	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 313 ligands modelled in this entry, 311 are monoatomic - leaving 2 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	$\# Z  > 2$
65	SPM	a	6208	-	13,13,13	0.35	0	12,12,12	0.83	0
64	PRI	Y	101	34	5,7,7	0.66	0	7,8,8	1.29	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	SPM	a	6208	-	-	3/11/11/11	-
64	PRI	Y	101	34	-	0/0/9/9	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	Y	101	PRI	OT1-C-CA	-2.40	118.50	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
65	a	6208	SPM	C11-C12-C13-N14
65	a	6208	SPM	C2-C3-C4-N5
65	a	6208	SPM	C3-C4-N5-C6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

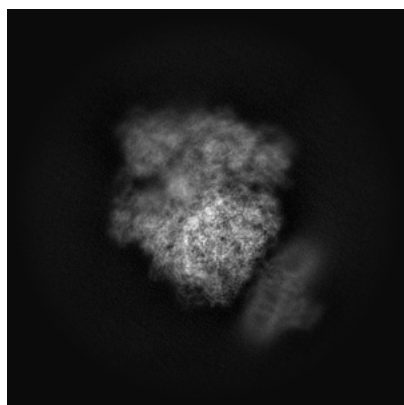
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55598. These allow visual inspection of the internal detail of the map and identification of artifacts.

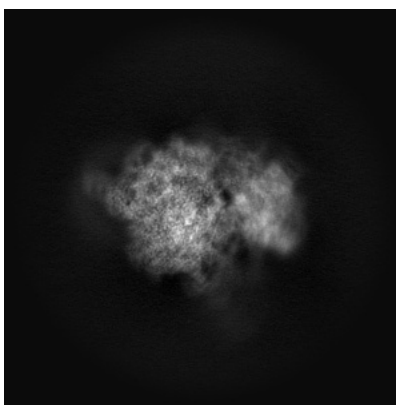
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

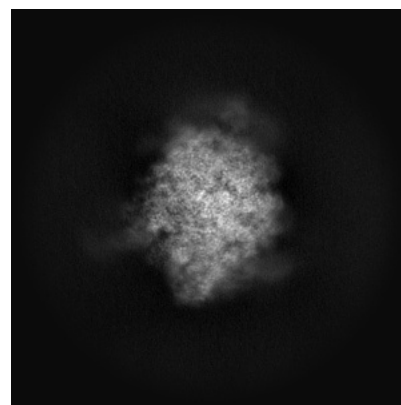
#### 6.1.1 Primary map



X



Y

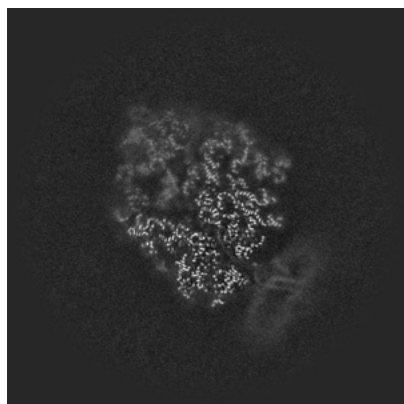


Z

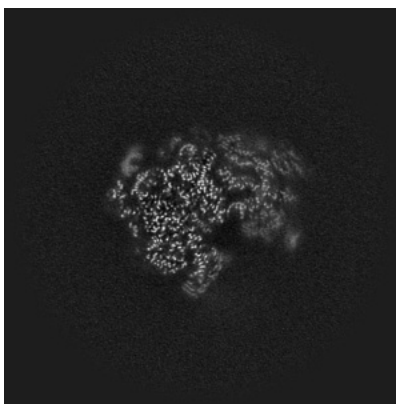
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

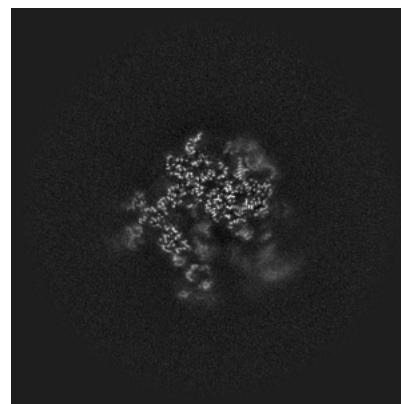
#### 6.2.1 Primary map



X Index: 340



Y Index: 340

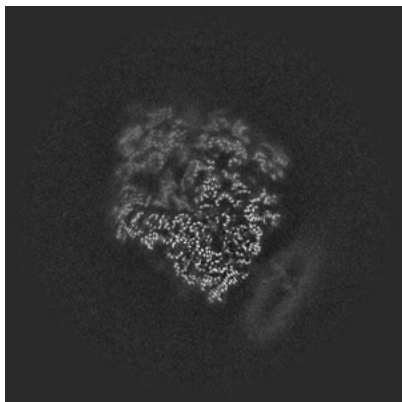


Z Index: 340

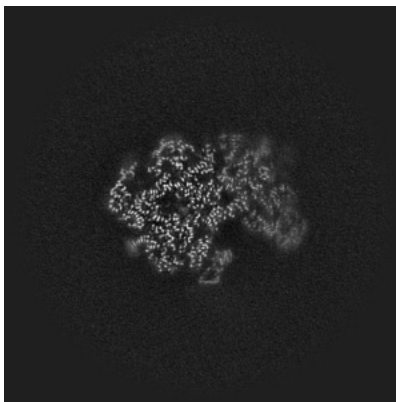
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

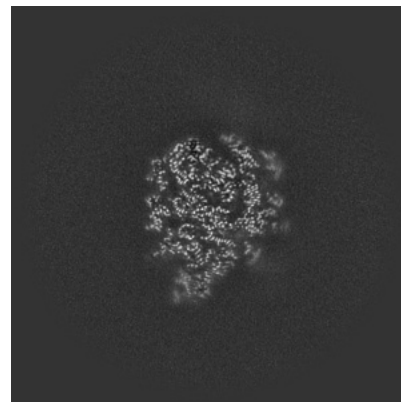
### 6.3.1 Primary map



X Index: 333



Y Index: 355



Z Index: 292

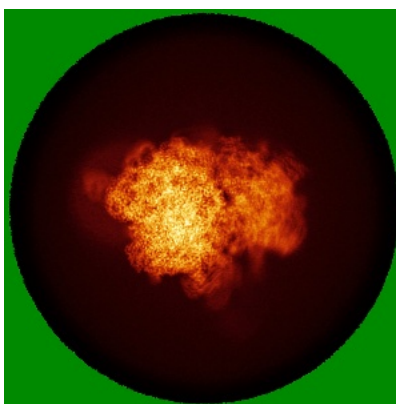
The images above show the largest variance slices of the map in three orthogonal directions.

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

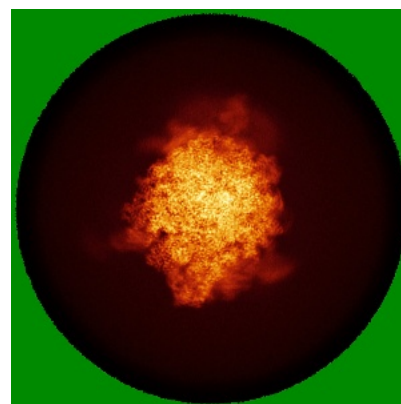
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

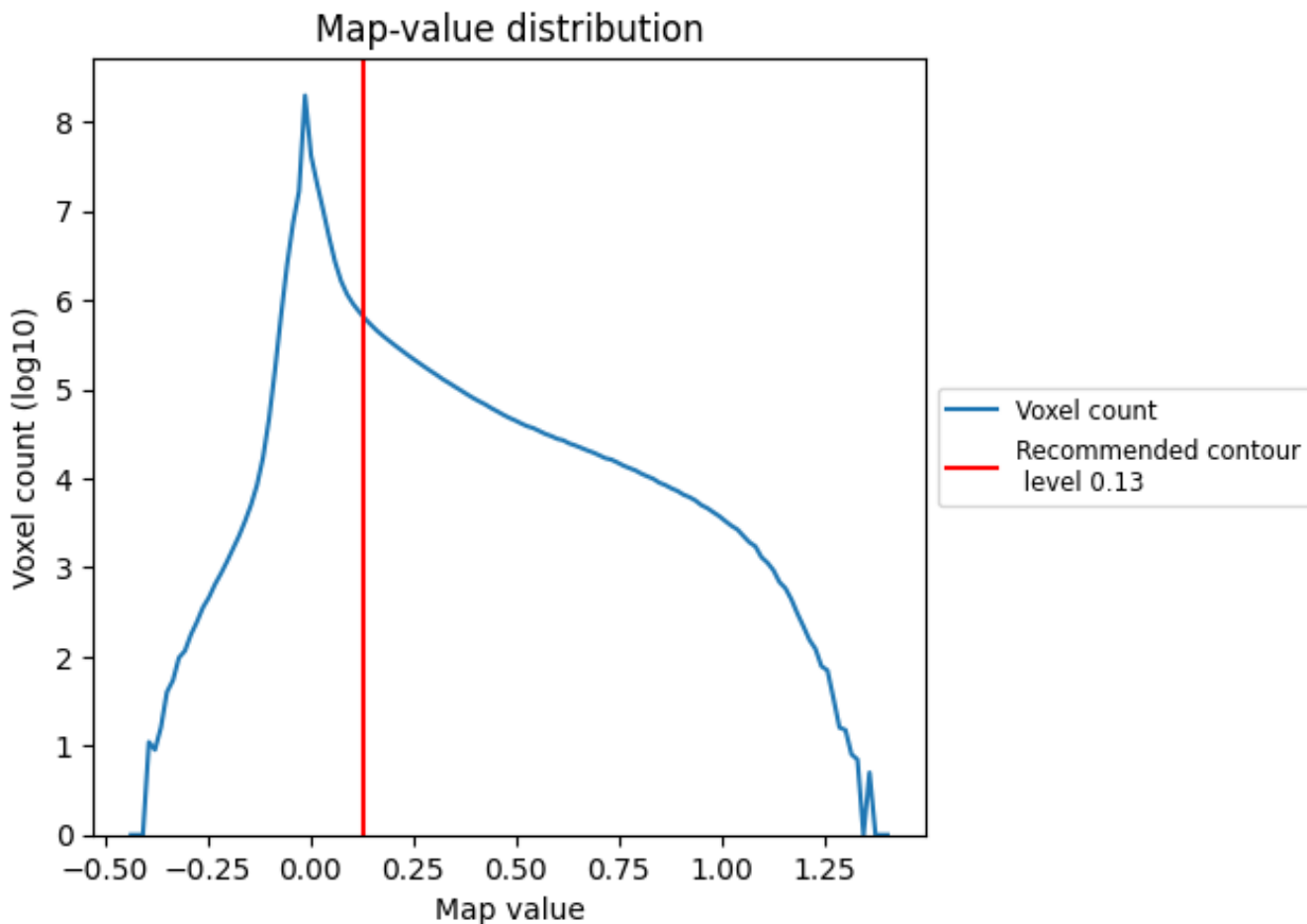
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

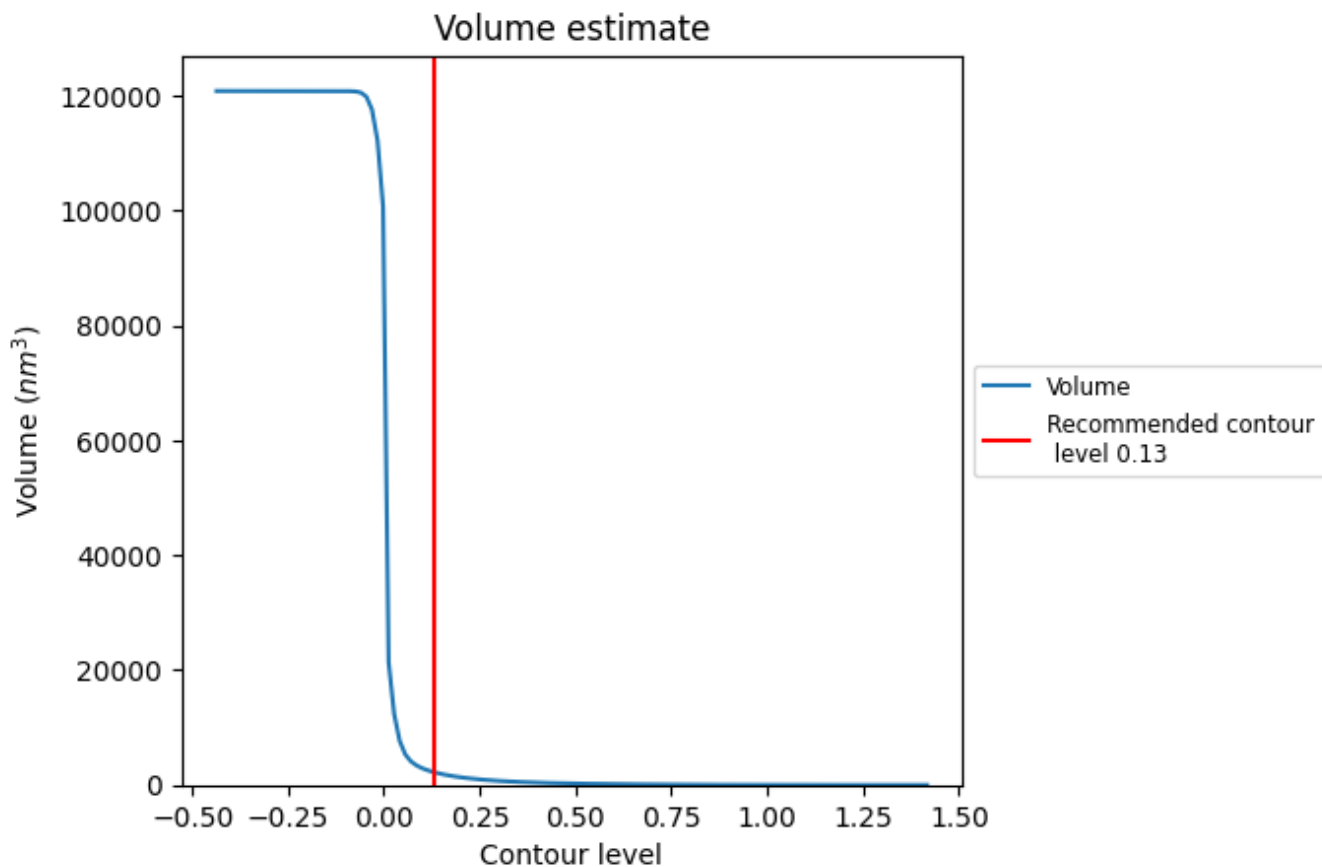
This section contains the results of statistical analysis of the map.

### 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.

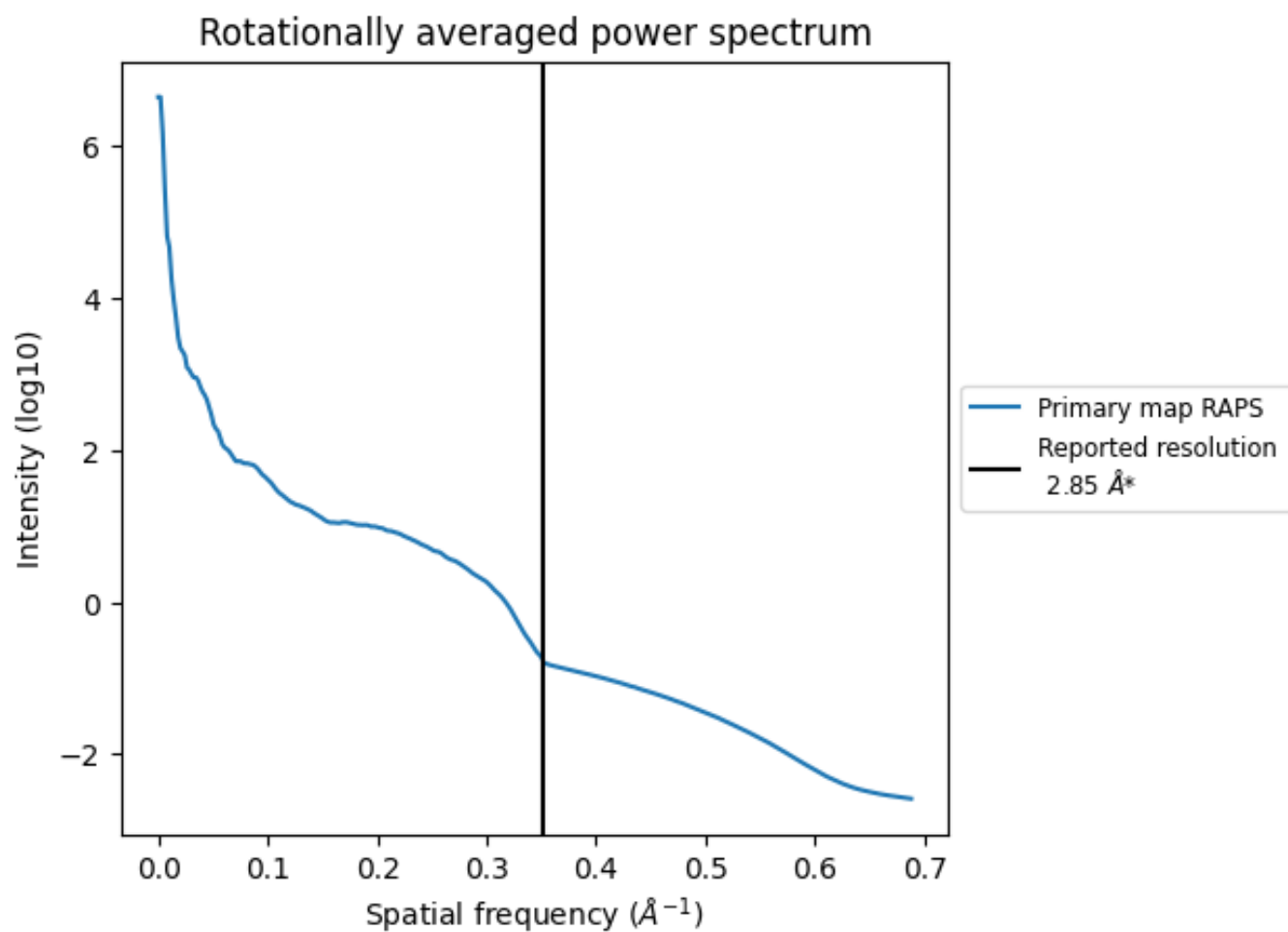
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2236 nm<sup>3</sup>; this corresponds to an approximate mass of 2020 kDa.

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

### 7.3 Rotationally averaged power spectrum i



\*Reported resolution corresponds to spatial frequency of 0.351 Å<sup>-1</sup>

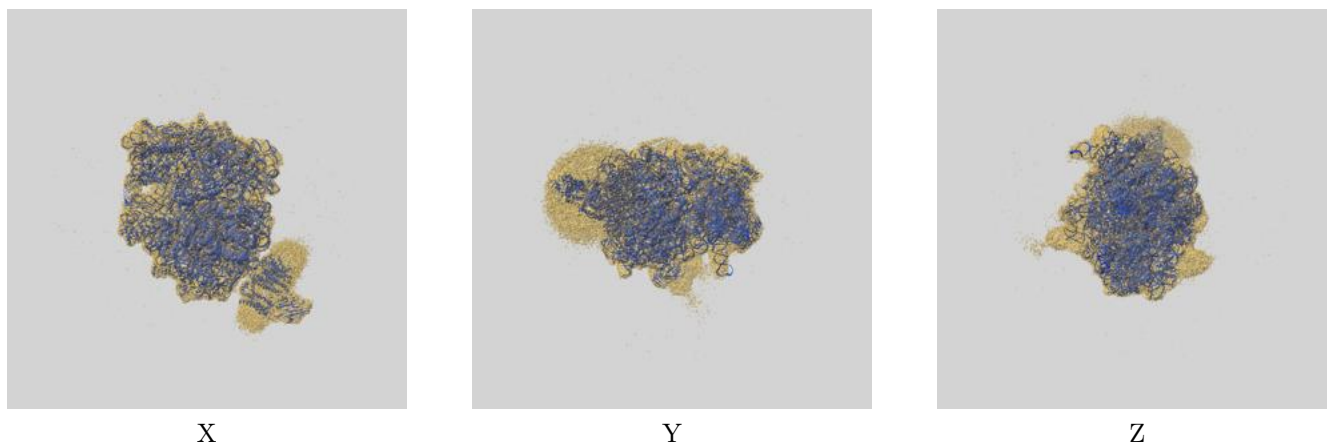
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

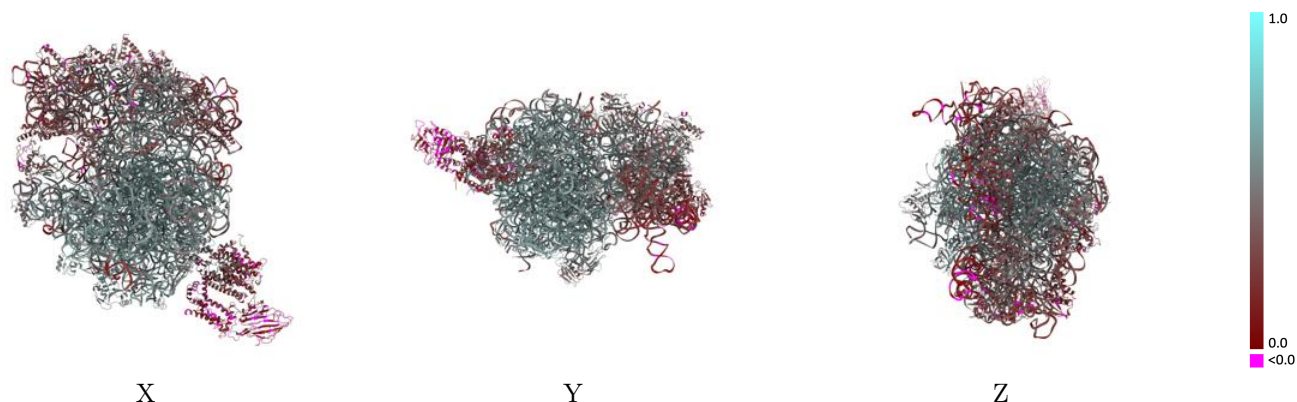
This section contains information regarding the fit between EMDB map EMD-55598 and PDB model 9T5X. Per-residue inclusion information can be found in section 3 on page 18.

### 9.1 Map-model overlay [i](#)



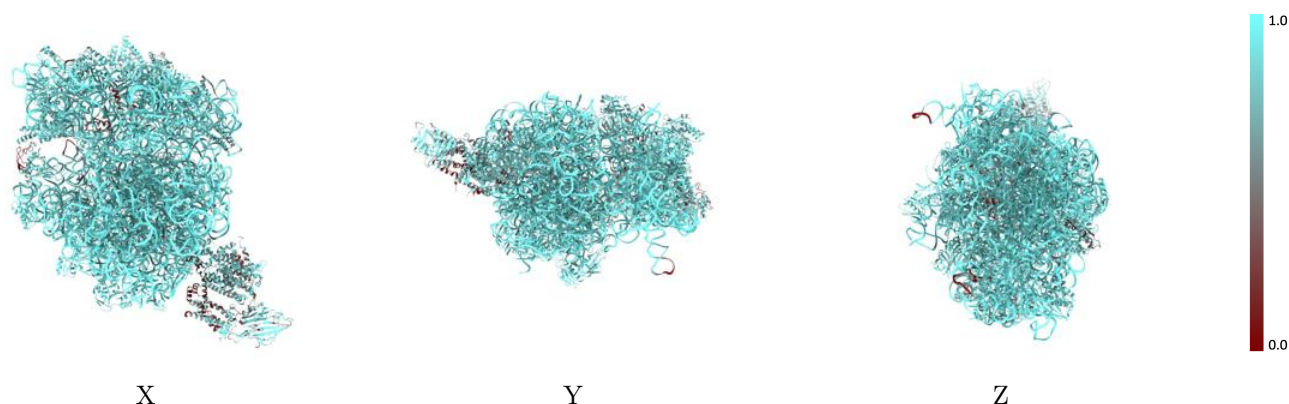
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



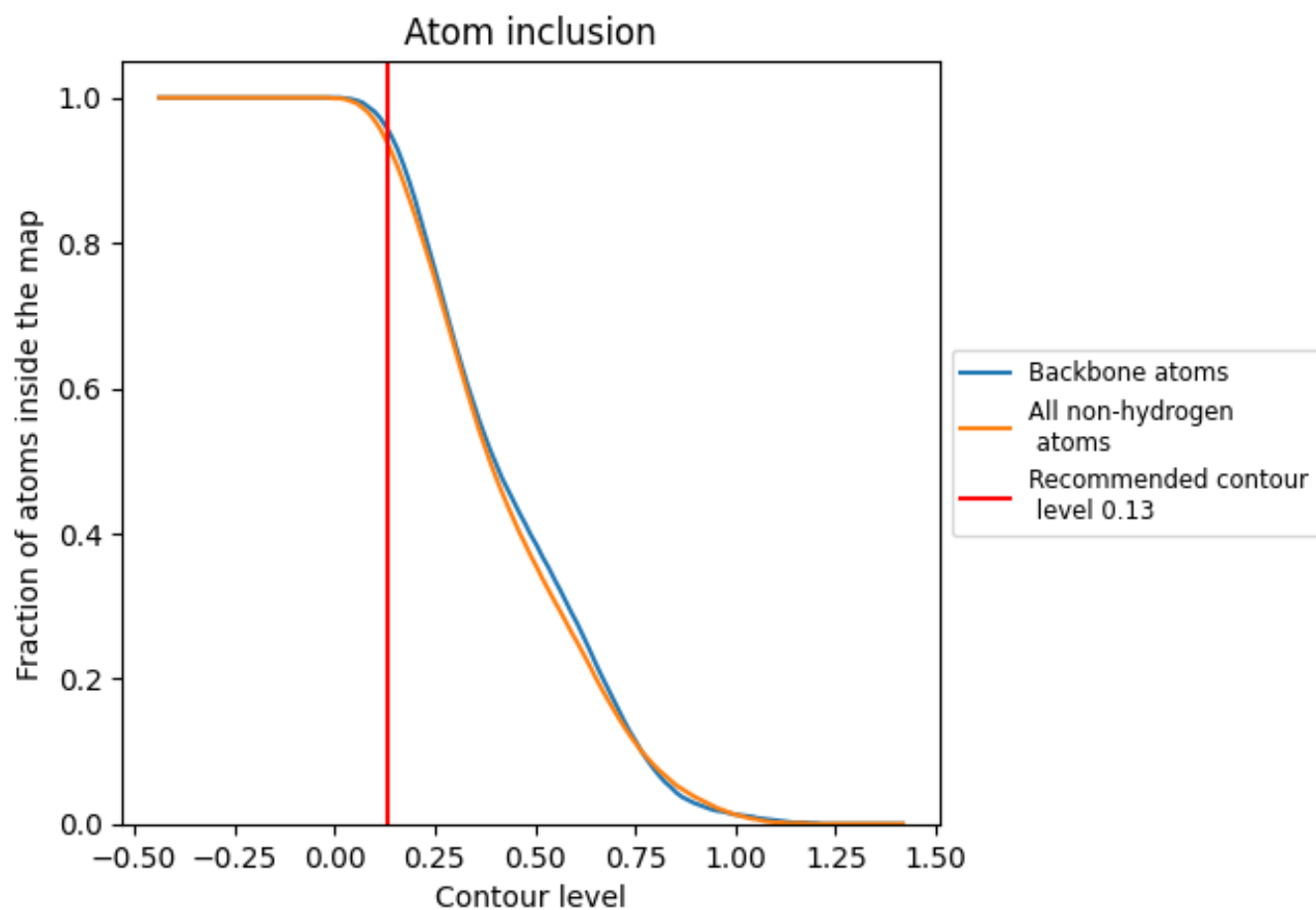
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9400	 0.4530
0	 0.8900	 0.5100
1	 0.9750	 0.5950
2	 0.9760	 0.5840
3	 0.9420	 0.5110
4	 0.1210	 0.0410
5	 0.8810	 0.4960
6	 0.7090	 0.2650
7	 0.6620	 0.2270
8	 0.5160	 0.1650
9	 0.6370	 0.0930
A	 0.9710	 0.3720
B	 0.8650	 0.3550
C	 0.8930	 0.3760
D	 0.6400	 0.1980
E	 0.9430	 0.4730
F	 0.9020	 0.4100
G	 0.8220	 0.2470
H	 0.9430	 0.4710
I	 0.9220	 0.2480
J	 0.8870	 0.3010
K	 0.8860	 0.3800
L	 0.8170	 0.2690
M	 0.8340	 0.2370
N	 0.9420	 0.3220
O	 0.9140	 0.4260
P	 0.8370	 0.2740
Q	 0.8950	 0.3640
R	 0.8180	 0.3780
S	 0.8020	 0.2580
T	 0.8200	 0.2440
U	 0.4270	 0.2580
V	 0.4430	 0.2370
X	 0.9580	 0.4400
Y	 0.9020	 0.4010



*Continued on next page...*

Continued from previous page...

Chain	Atom inclusion	Q-score
Z	 0.9540	 0.3700
a	 0.9920	 0.5490
b	 0.9930	 0.4690
c	 0.9730	 0.5810
d	 0.9710	 0.5760
e	 0.9670	 0.5570
f	 0.9020	 0.3790
g	 0.9310	 0.4500
h	 0.9600	 0.5120
i	 0.9710	 0.5700
j	 0.9690	 0.5750
k	 0.9780	 0.5670
l	 0.9650	 0.5620
m	 0.9860	 0.5880
n	 0.9580	 0.4710
o	 0.9440	 0.5600
p	 0.9870	 0.5820
q	 0.9670	 0.5690
r	 0.9650	 0.5710
s	 0.9330	 0.5510
t	 0.9560	 0.5410
u	 0.9610	 0.5320
v	 0.9600	 0.5700
w	 0.9580	 0.5200
x	 0.9280	 0.4960
y	 0.9630	 0.5640
z	 0.9600	 0.5660