



Full wwPDB EM Validation Report ⓘ

Jun 20, 2026 – 10:40 pm BST

PDB ID : 6TC3 / pdb_00006tc3
EMDB ID : EMD-10458
Title : Cryo-EM structure of an Escherichia coli ribosome-SpeFL complex stalled in response to L-ornithine (Replicate 1)
Authors : Innis, C.A.; Herrero del Valle, A.
Deposited on : 2019-11-05
Resolution : 2.70 Å(reported)
Based on initial model : 4YBB

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

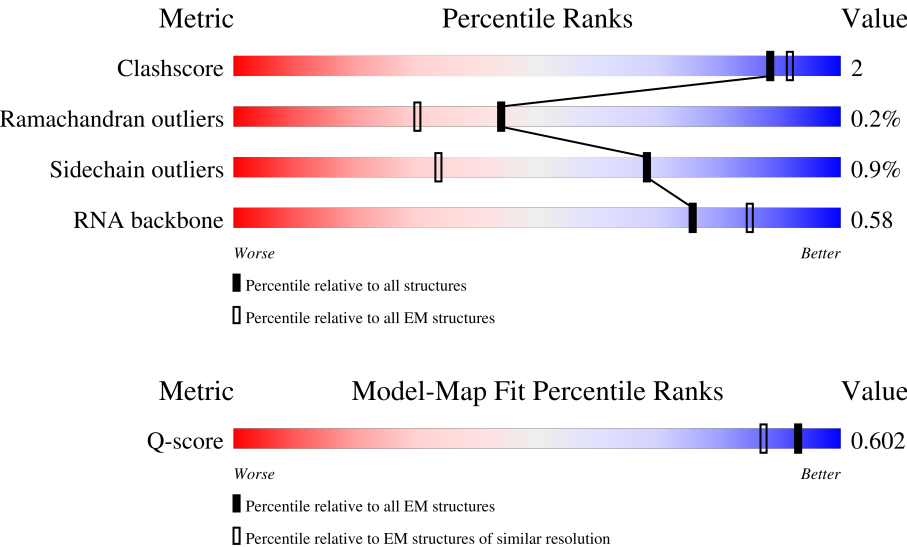
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	16S1	1534	7% 88% 12%
2	S021	241	28% 90% 7%
3	S031	233	10% 88% 12%

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Mol	Chain	Length	Quality of chain
4	S041	206	
5	S051	167	
6	S061	135	
7	S071	179	
8	S081	130	
9	S091	130	
10	S101	103	
11	S111	129	
12	S121	124	
13	S131	118	
14	S141	102	
15	S151	89	
16	S161	82	
17	S171	84	
18	S181	75	
19	S191	92	
20	S201	87	
21	S211	71	
22	23S1	2897	
23	05S1	120	
24	L021	273	
25	L031	209	
26	L041	201	
27	L051	179	
28	L061	177	

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Mol	Chain	Length	Quality of chain
29	L091	149	
30	L311	70	
31	L131	142	
32	L141	123	
33	L151	144	
34	L161	136	
35	L171	127	
36	L181	117	
37	L191	115	
38	L201	118	
39	L211	103	
40	L221	110	
41	L231	100	
42	L241	104	
43	L251	94	
44	L271	85	
45	L281	78	
46	L291	63	
47	L301	59	
48	L321	57	
49	L331	55	
50	L341	46	
51	L351	65	
52	L361	38	
53	SPE1	34	

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Mol	Chain	Length	Quality of chain
54	MRN1	7	14% 43% 57%
55	PTR1	76	78% 16% 7%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 146672 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	16S1	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S021	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S031	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S041	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S051	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S061	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S071	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S081	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S091	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S101	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S111	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S121	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S131	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S141	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S141	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S151	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S161	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S171	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S181	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S191	82	Total	C	N	O	S	0	0
			656	419	125	110	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S201	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S211	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	23S1	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	05S1	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L021	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L031	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L041	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L051	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L061	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L091	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L311	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L131	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L141	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L151	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L161	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L171	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L181	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L191	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L201	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L211	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L221	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	L231	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L241	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	L251	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L271	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L281	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L291	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L301	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L321	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L331	51	Total	C	N	O		0	0
			414	266	76	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L341	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	L351	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	L361	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called SpeFL.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SPE1	34	Total	C	N	O	S	0	0
			300	187	62	48	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SPE1	5	SER	ASN	conflict	UNP A0A4S4NWS2
SPE1	7	THR	LEU	conflict	UNP A0A4S4NWS2

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	MRN1	7	Total	C	N	O	P	0	0
			146	65	23	51	7		

- Molecule 55 is a RNA chain called P-site Arg-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	PTR1	76	Total	C	N	O	P	S	0	0
			1627	727	294	528	76	2		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	16S1	87	Total	Mg	0
			87	87	
56	23S1	249	Total	Mg	0
			249	249	
56	L231	1	Total	Mg	0
			1	1	
56	SPE1	1	Total	Mg	0
			1	1	
56	PTR1	1	Total	Mg	0
			1	1	

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	16S1	39	Total	K	0
			39	39	
57	23S1	106	Total	K	0
			106	106	
57	05S1	1	Total	K	0
			1	1	
57	L031	1	Total	K	0
			1	1	

- Molecule 58 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
58	16S1	145	Total	X	0
			145	145	
58	S021	1	Total	X	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
58	S031	1	Total 1	X 1	0
58	S081	1	Total 1	X 1	0
58	S091	1	Total 1	X 1	0
58	S111	2	Total 2	X 2	0
58	S131	1	Total 1	X 1	0
58	S171	1	Total 1	X 1	0
58	23S1	908	Total 908	X 908	0
58	05S1	9	Total 9	X 9	0
58	L021	26	Total 26	X 26	0
58	L031	17	Total 17	X 17	0
58	L041	11	Total 11	X 11	0
58	L131	6	Total 6	X 6	0
58	L141	6	Total 6	X 6	0
58	L151	5	Total 5	X 5	0
58	L161	5	Total 5	X 5	0
58	L171	5	Total 5	X 5	0
58	L181	1	Total 1	X 1	0
58	L191	4	Total 4	X 4	0
58	L201	3	Total 3	X 3	0
58	L211	1	Total 1	X 1	0
58	L221	8	Total 8	X 8	0

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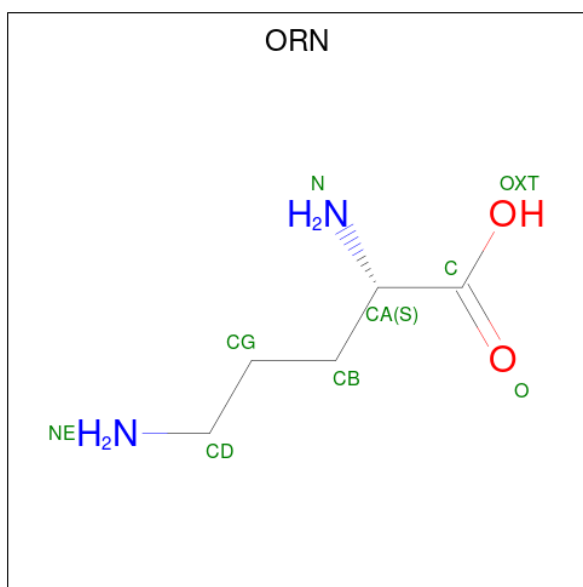
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Mol	Chain	Residues	Atoms		AltConf
58	L231	1	Total 1	X 1	0
58	L241	2	Total 2	X 2	0
58	L251	1	Total 1	X 1	0
58	L271	3	Total 3	X 3	0
58	L281	2	Total 2	X 2	0
58	L321	3	Total 3	X 3	0
58	L331	1	Total 1	X 1	0
58	L341	8	Total 8	X 8	0
58	L351	3	Total 3	X 3	0
58	SPE1	6	Total 6	X 6	0
58	MRN1	1	Total 1	X 1	0
58	PTR1	2	Total 2	X 2	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	S021	1	Total 1	Zn 1	0
59	L311	1	Total 1	Zn 1	0
59	L361	1	Total 1	Zn 1	0

- Molecule 60 is L-ornithine (CCD ID: ORN) (formula: C₅H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				AltConf
60	23S1	1	Total	C	N	O	0
			9	5	2	2	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	16S1	167	Total	O	0
			167	167	
61	S111	1	Total	O	0
			1	1	
61	S131	2	Total	O	0
			2	2	
61	S141	1	Total	O	0
			1	1	
61	S171	1	Total	O	0
			1	1	
61	23S1	619	Total	O	0
			619	619	
61	L021	3	Total	O	0
			3	3	
61	L031	2	Total	O	0
			2	2	
61	L151	2	Total	O	0
			2	2	
61	L171	2	Total	O	0
			2	2	

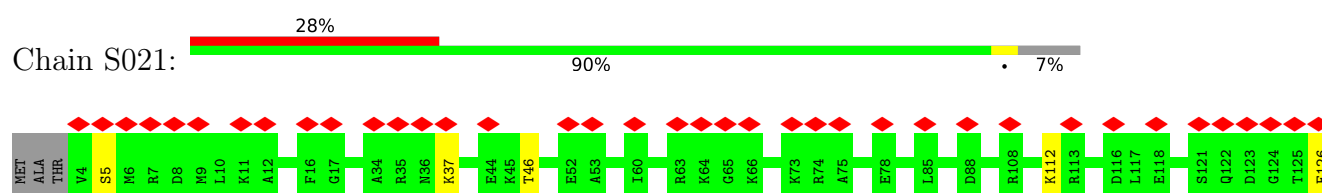
3 Residue-property plots

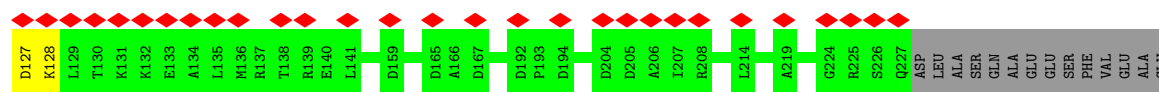
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

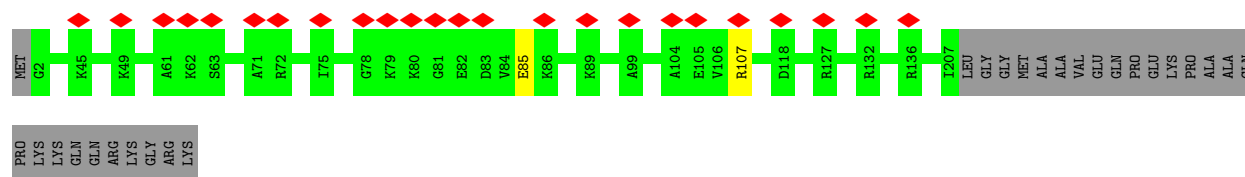
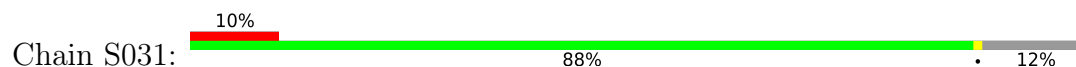


• Molecule 2: 30S ribosomal protein S2

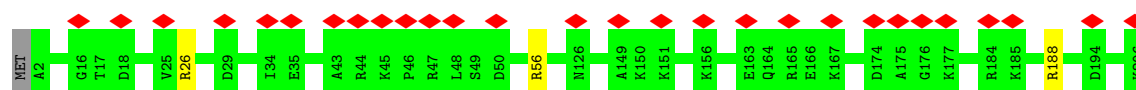




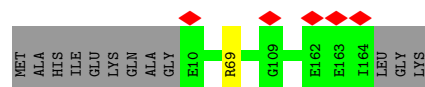
- Molecule 3: 30S ribosomal protein S3



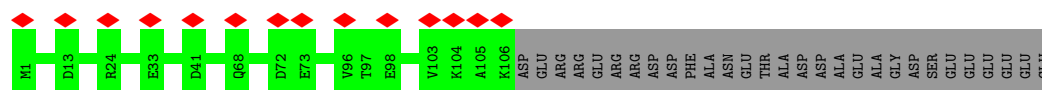
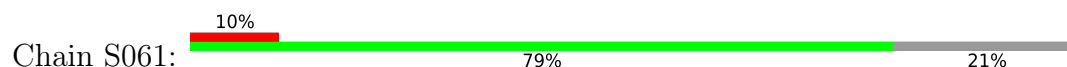
- Molecule 4: 30S ribosomal protein S4



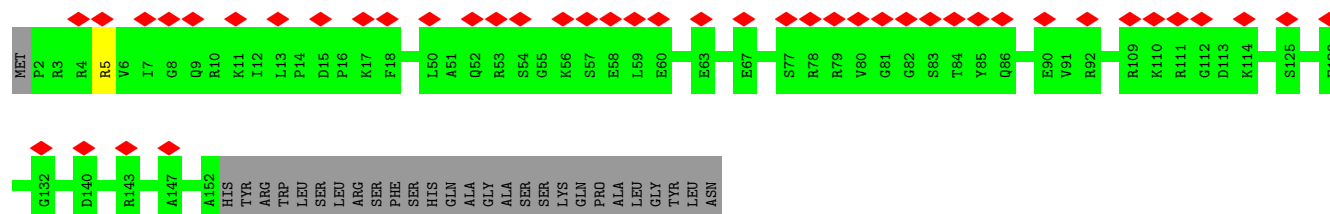
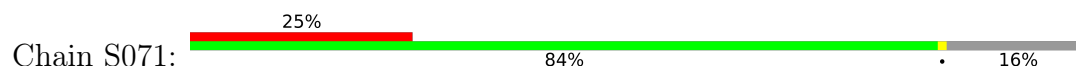
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

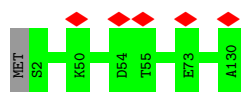


- Molecule 7: 30S ribosomal protein S7



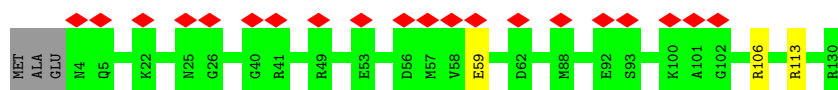
- Molecule 8: 30S ribosomal protein S8

Chain S081:  99%



- Molecule 9: 30S ribosomal protein S9

Chain S091:  95%



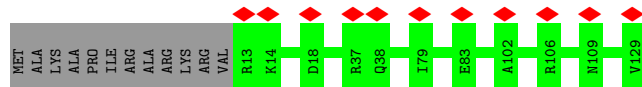
- Molecule 10: 30S ribosomal protein S10

Chain S101:  91%



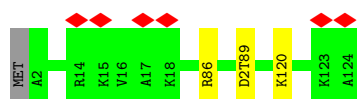
- Molecule 11: 30S ribosomal protein S11

Chain S111:  91%



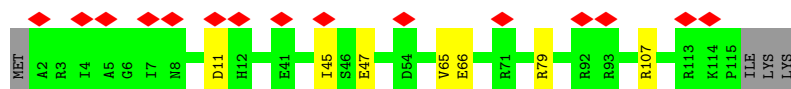
- Molecule 12: 30S ribosomal protein S12

Chain S121:  97%



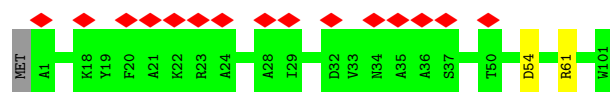
- Molecule 13: 30S ribosomal protein S13

Chain S131:  91%

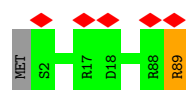


- Molecule 14: 30S ribosomal protein S14

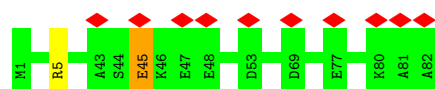
Chain S141:  97%



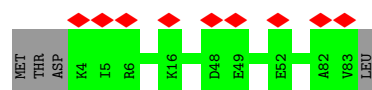
- Molecule 15: 30S ribosomal protein S15



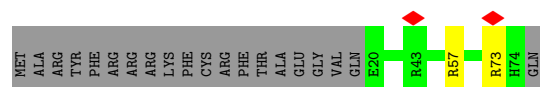
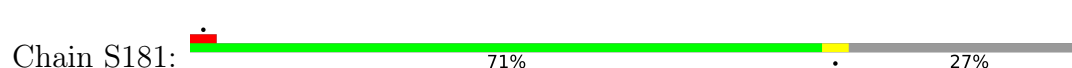
- Molecule 16: 30S ribosomal protein S16



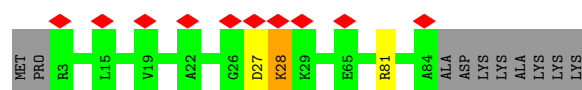
- Molecule 17: 30S ribosomal protein S17



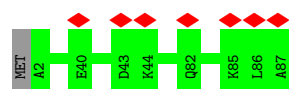
- Molecule 18: 30S ribosomal protein S18



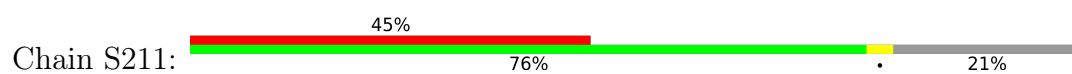
- Molecule 19: 30S ribosomal protein S19



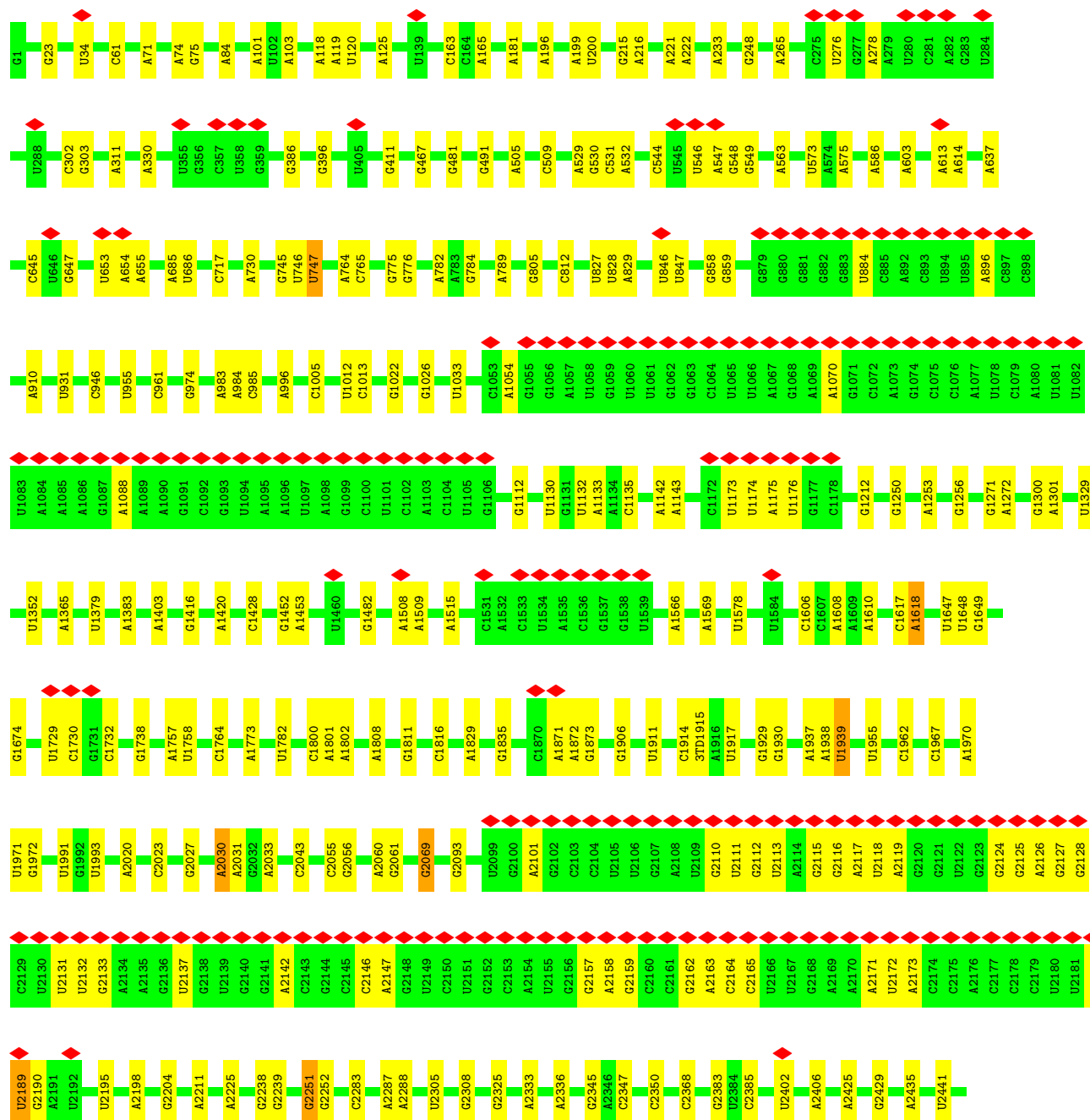
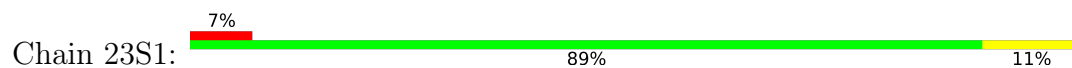
- Molecule 20: 30S ribosomal protein S20

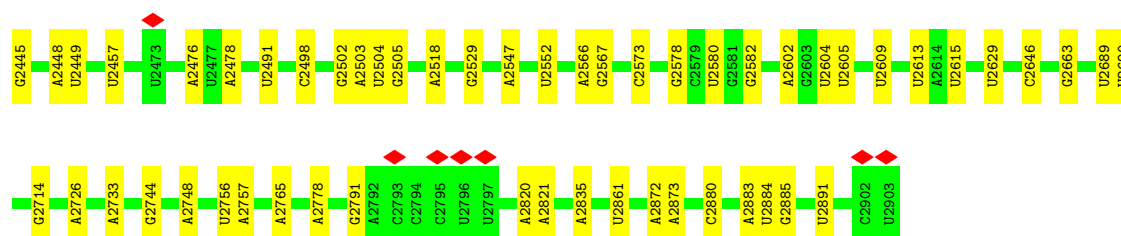


- Molecule 21: 30S ribosomal protein S21

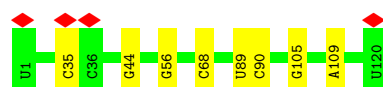


• Molecule 22: 23S rRNA

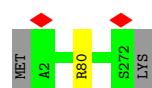




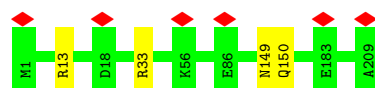
• Molecule 23: 5S rRNA



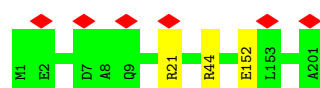
• Molecule 24: 50S ribosomal protein L2



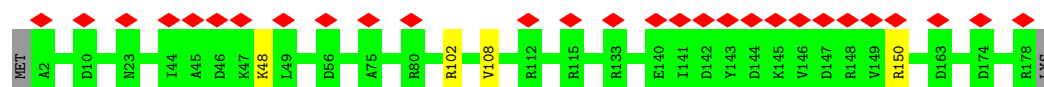
• Molecule 25: 50S ribosomal protein L3



• Molecule 26: 50S ribosomal protein L4

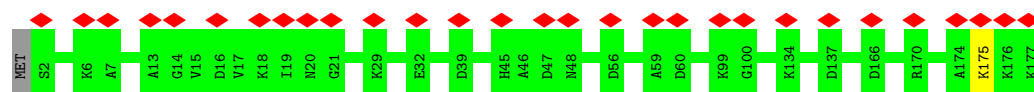


• Molecule 27: 50S ribosomal protein L5

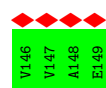
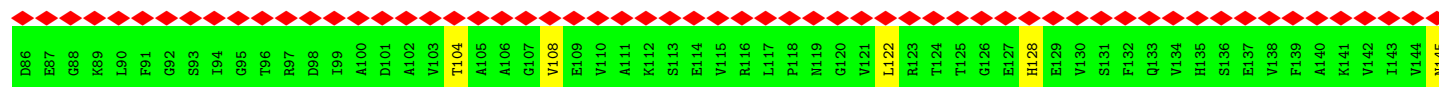
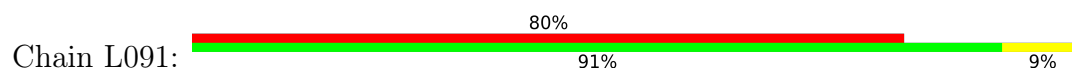


• Molecule 28: 50S ribosomal protein L6

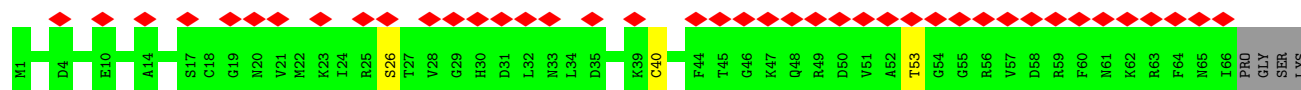




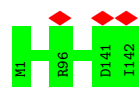
- Molecule 29: 50S ribosomal protein L9



- Molecule 30: 50S ribosomal protein L31



- Molecule 31: 50S ribosomal protein L13



- Molecule 32: 50S ribosomal protein L14



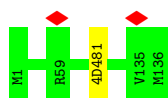
There are no outlier residues recorded for this chain.

- Molecule 33: 50S ribosomal protein L15

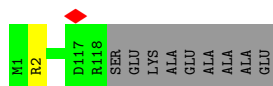


- Molecule 34: 50S ribosomal protein L16

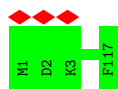




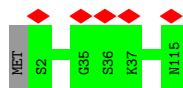
- Molecule 35: 50S ribosomal protein L17



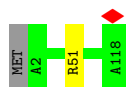
- Molecule 36: 50S ribosomal protein L18



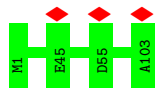
- Molecule 37: 50S ribosomal protein L19



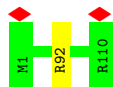
- Molecule 38: 50S ribosomal protein L20



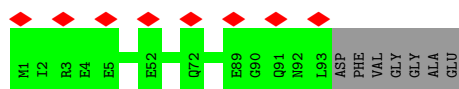
- Molecule 39: 50S ribosomal protein L21



- Molecule 40: 50S ribosomal protein L22



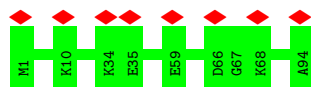
- Molecule 41: 50S ribosomal protein L23



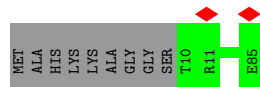
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25



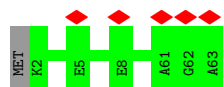
- Molecule 44: 50S ribosomal protein L27



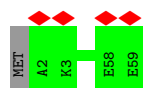
- Molecule 45: 50S ribosomal protein L28



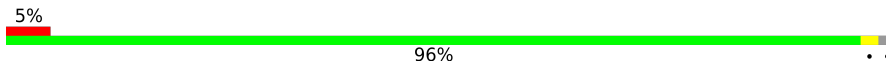
- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30

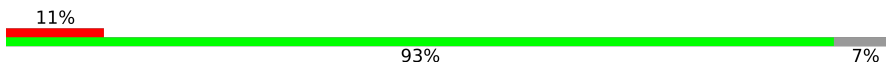


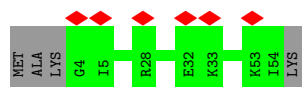
- Molecule 48: 50S ribosomal protein L32

Chain L321:  5% 96% ..

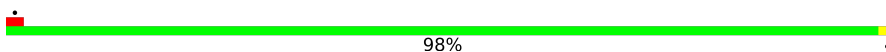


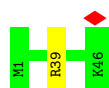
- Molecule 49: 50S ribosomal protein L33

Chain L331:  11% 93% 7%

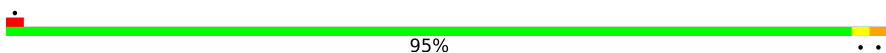


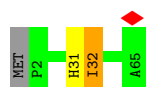
- Molecule 50: 50S ribosomal protein L34

Chain L341:  98% .

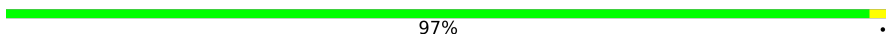


- Molecule 51: 50S ribosomal protein L35

Chain L351:  95% ...



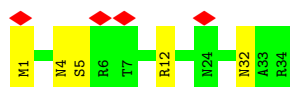
- Molecule 52: 50S ribosomal protein L36

Chain L361:  97% .



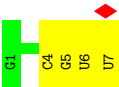
- Molecule 53: SpeFL

Chain SPE1:  12% 85% 15%

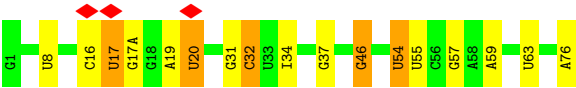
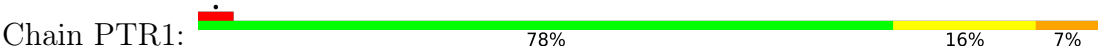


- Molecule 54: mRNA

Chain MRN1:  14% 43% 57%



• Molecule 55: P-site Arg-tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-1600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	28.760	Depositor
Minimum map value	-10.716	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	384.12003, 384.12003, 384.12003	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5335, 0.5335, 0.5335	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, OMG, RSP, MEQ, FME, 2MA, ZN, UR3, PSU, MA6, 3TD, K, OMU, G7M, 1MG, 4SU, 6MZ, UNX, MG, D2T, 2MG, 5MU, 5MC, OMC, 4D4, ORN

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	16S1	0.62	0/36593	0.74	0/57081
2	S021	0.67	0/1784	0.80	4/2403 (0.2%)
3	S031	0.80	0/1651	0.67	0/2225
4	S041	0.81	0/1665	0.60	0/2227
5	S051	0.72	0/1157	0.72	0/1557
6	S061	0.70	0/881	0.63	0/1189
7	S071	0.87	0/1195	0.75	0/1602
8	S081	0.68	0/989	0.54	0/1326
9	S091	0.97	0/1034	0.84	0/1375
10	S101	0.95	0/805	1.00	2/1089 (0.2%)
11	S111	0.82	0/893	0.58	0/1205
12	S121	0.88	0/960	0.73	0/1286
13	S131	0.93	0/892	0.95	2/1193 (0.2%)
14	S141	0.94	0/811	0.82	0/1081
15	S151	0.88	0/722	0.62	1/964 (0.1%)
16	S161	0.87	0/659	0.74	2/884 (0.2%)
17	S171	0.75	0/657	0.58	0/881
18	S181	0.87	0/462	0.53	0/621
19	S191	0.81	0/672	0.84	1/904 (0.1%)
20	S201	0.74	0/676	0.65	0/895
21	S211	1.02	0/472	0.75	1/627 (0.2%)
22	23S1	0.66	1/69120 (0.0%)	0.76	3/107824 (0.0%)
23	05S1	0.56	0/2872	0.66	0/4478
24	L021	0.84	0/2121	0.58	0/2852
25	L031	0.68	0/1576	0.52	0/2119
26	L041	0.70	0/1571	0.60	0/2113
27	L051	0.77	1/1434 (0.1%)	0.74	0/1926
28	L061	0.67	0/1343	0.67	0/1816
29	L091	0.72	0/1121	1.16	7/1515 (0.5%)
30	L311	0.81	0/531	1.09	2/709 (0.3%)
31	L131	0.73	0/1152	0.52	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	L141	0.83	0/955	0.59	0/1279
33	L151	0.82	0/1062	0.62	0/1413
34	L161	0.80	0/1081	0.55	0/1443
35	L171	0.96	0/958	0.67	0/1281
36	L181	0.83	0/910	0.59	0/1219
37	L191	0.84	0/929	0.57	0/1242
38	L201	0.91	0/960	0.54	0/1278
39	L211	0.72	0/829	0.63	0/1107
40	L221	0.80	0/864	0.51	0/1156
41	L231	0.76	0/744	0.62	0/994
42	L241	0.66	0/787	0.57	0/1051
43	L251	0.65	0/766	0.50	0/1025
44	L271	0.85	0/587	0.51	0/776
45	L281	0.92	0/635	0.55	0/848
46	L291	0.76	0/502	0.49	0/667
47	L301	0.82	0/453	0.53	0/605
48	L321	0.90	0/450	0.62	0/599
49	L331	0.62	0/421	0.61	0/561
50	L341	1.16	0/380	0.68	0/498
51	L351	0.80	0/513	0.76	1/676 (0.1%)
52	L361	0.92	0/303	0.56	0/397
53	SPE1	0.94	0/299	0.81	1/399 (0.3%)
54	MRN1	0.38	0/161	0.68	0/248
55	PTR1	0.79	5/1672 (0.3%)	0.72	0/2598
All	All	0.70	7/155692 (0.0%)	0.73	27/232878 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S021	0	2
3	S031	0	1
10	S101	0	5
13	S131	0	3
19	S191	0	3
26	L041	0	1
29	L091	0	5
30	L311	0	1
33	L151	0	1
51	L351	0	1
All	All	0	23

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	20	U	C5-C6	10.48	1.55	1.34
55	PTR1	17	U	C5-C6	10.04	1.54	1.34
22	23S1	2449	U	C5-C6	9.48	1.53	1.34
55	PTR1	34	I	N3-C4	7.61	1.51	1.35
55	PTR1	34	I	C5-C6	7.05	1.53	1.39
27	L051	108	VAL	C-N	5.66	1.39	1.33
55	PTR1	34	I	C2-N3	5.35	1.46	1.35

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	S101	27	GLU	CB-CA-C	-7.74	97.53	110.68
30	L311	26	SER	N-CA-C	7.65	118.79	108.23
13	S131	47	GLU	CB-CA-C	-7.36	102.54	109.83
10	S101	27	GLU	CA-CB-CG	6.32	126.75	114.10
19	S191	28	LYS	CA-CB-CG	5.80	125.69	114.10
13	S131	79	ARG	NE-CZ-NH2	5.79	124.41	119.20
29	L091	70	GLU	CA-C-N	5.72	135.85	126.86
29	L091	70	GLU	C-N-CA	5.72	135.85	126.86
29	L091	68	ARG	NE-CZ-NH2	-5.71	114.06	119.20
29	L091	122	LEU	CA-CB-CG	5.67	136.13	116.30
2	S021	126	PHE	CA-C-N	5.62	132.28	121.54
2	S021	126	PHE	C-N-CA	5.62	132.28	121.54
16	S161	45	GLU	CA-C-N	5.51	128.65	120.17
16	S161	45	GLU	C-N-CA	5.51	128.65	120.17
22	23S1	2872	A	N1-C6-N6	-5.33	102.61	118.60
2	S021	46	THR	CA-C-N	5.26	124.54	120.33
2	S021	46	THR	C-N-CA	5.26	124.54	120.33
30	L311	40	CYS	CB-CA-C	-5.21	102.17	110.04
22	23S1	2189	U	C2'-C3'-O3'	5.17	121.45	113.70
15	S151	89	ARG	N-CA-C	5.14	125.38	111.00
51	L351	32	ILE	N-CA-C	5.12	119.99	109.34
53	SPE1	5	SER	N-CA-C	5.09	117.72	110.24
29	L091	128	HIS	CA-C-N	-5.06	115.65	123.14
29	L091	128	HIS	C-N-CA	-5.06	115.65	123.14
21	S211	16	LEU	CA-CB-CG	5.04	133.96	116.30
29	L091	83	LYS	CA-CB-CG	5.04	124.18	114.10
22	23S1	2872	A	C5-C6-N6	5.04	138.82	123.70

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	L041	152	GLU	Peptide
29	L091	104	THR	Peptide
29	L091	108	VAL	Peptide
29	L091	145	ASN	Peptide
29	L091	41	LYS	Peptide
29	L091	66	ASN	Peptide
33	L151	35	HIS	Peptide
30	L311	53	THR	Peptide
51	L351	31	HIS	Peptide
2	S021	128	LYS	Peptide
2	S021	5	SER	Peptide
3	S031	85	GLU	Peptide
10	S101	27	GLU	Peptide
10	S101	56	HIS	Peptide
10	S101	57	VAL	Mainchain
10	S101	82	LYS	Peptide
10	S101	92	LEU	Peptide
13	S131	11	ASP	Peptide
13	S131	45	ILE	Peptide
13	S131	65	VAL	Peptide
19	S191	27	ASP	Peptide
19	S191	28	LYS	Peptide
19	S191	81	ARG	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16S1	32930	0	0	0	0
2	S021	1753	0	0	0	0
3	S031	1624	0	0	0	0
4	S041	1643	0	0	0	0
5	S051	1144	0	0	0	0
6	S061	862	0	0	0	0
7	S071	1181	0	0	0	0
8	S081	979	0	0	0	0
9	S091	1022	0	0	0	0
10	S101	795	0	0	0	0
11	S111	877	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	S121	957	0	0	0	0
13	S131	883	0	0	0	0
14	S141	799	0	0	0	0
15	S151	714	0	0	0	0
16	S161	649	0	0	0	0
17	S171	648	0	0	0	0
18	S181	455	0	0	0	0
19	S191	656	0	0	0	0
20	S201	670	0	0	0	0
21	S211	465	0	0	0	0
22	23S1	62209	0	0	0	0
23	05S1	2569	0	0	0	0
24	L021	2082	0	0	0	0
25	L031	1566	0	0	0	0
26	L041	1552	0	0	0	0
27	L051	1410	0	0	0	0
28	L061	1323	0	0	0	0
29	L091	1110	0	0	0	0
30	L311	522	0	0	0	0
31	L131	1129	0	0	0	0
32	L141	946	0	0	0	0
33	L151	1053	0	0	0	0
34	L161	1075	0	0	0	0
35	L171	945	0	0	0	0
36	L181	900	0	0	0	0
37	L191	917	0	0	0	0
38	L201	947	0	0	0	0
39	L211	816	0	0	0	0
40	L221	857	0	0	0	0
41	L231	738	0	0	0	0
42	L241	779	0	0	0	0
43	L251	753	0	0	0	0
44	L271	580	0	0	0	0
45	L281	625	0	0	0	0
46	L291	501	0	0	0	0
47	L301	449	0	0	0	0
48	L321	444	0	0	0	0
49	L331	414	0	0	0	0
50	L341	377	0	0	0	0
51	L351	504	0	0	0	0
52	L361	302	0	0	0	0
53	SPE1	300	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	MRN1	146	0	0	0	0
55	PTR1	1627	0	0	0	0
56	16S1	87	0	0	0	0
56	23S1	249	0	0	0	0
56	L231	1	0	0	0	0
56	PTR1	1	0	0	0	0
56	SPE1	1	0	0	0	0
57	05S1	1	0	0	0	0
57	16S1	39	0	0	0	0
57	23S1	106	0	0	0	0
57	L031	1	0	0	0	0
58	05S1	9	0	0	0	0
58	16S1	145	0	0	0	0
58	23S1	908	0	0	0	0
58	L021	26	0	0	0	0
58	L031	17	0	0	0	0
58	L041	11	0	0	0	0
58	L131	6	0	0	0	0
58	L141	6	0	0	0	0
58	L151	5	0	0	0	0
58	L161	5	0	0	0	0
58	L171	5	0	0	0	0
58	L181	1	0	0	0	0
58	L191	4	0	0	0	0
58	L201	3	0	0	0	0
58	L211	1	0	0	0	0
58	L221	8	0	0	0	0
58	L231	1	0	0	0	0
58	L241	2	0	0	0	0
58	L251	1	0	0	0	0
58	L271	3	0	0	0	0
58	L281	2	0	0	0	0
58	L321	3	0	0	0	0
58	L331	1	0	0	0	0
58	L341	8	0	0	0	0
58	L351	3	0	0	0	0
58	MRN1	1	0	0	0	0
58	PTR1	2	0	0	0	0
58	S021	1	0	0	0	0
58	S031	1	0	0	0	0
58	S081	1	0	0	0	0
58	S091	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	S111	2	0	0	0	0
58	S131	1	0	0	0	0
58	S171	1	0	0	0	0
58	SPE1	6	0	0	0	0
59	L311	1	0	0	0	0
59	L361	1	0	0	0	0
59	S021	1	0	0	0	0
60	23S1	9	0	0	0	0
61	16S1	167	0	0	0	0
61	23S1	619	0	0	0	0
61	L021	3	0	0	0	0
61	L031	2	0	0	0	0
61	L151	2	0	0	0	0
61	L171	2	0	0	0	0
61	S111	1	0	0	0	0
61	S131	2	0	0	0	0
61	S141	1	0	0	0	0
61	S171	1	0	0	0	0
All	All	146672	0	0	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S021	222/241 (92%)	208 (94%)	13 (6%)	1 (0%)	24	48
3	S031	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
4	S041	203/206 (98%)	200 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S051	153/167 (92%)	144 (94%)	9 (6%)	0	100	100
6	S061	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	S071	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
8	S081	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
9	S091	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
10	S101	97/103 (94%)	91 (94%)	5 (5%)	1 (1%)	12	32
11	S111	115/129 (89%)	106 (92%)	9 (8%)	0	100	100
12	S121	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
13	S131	112/118 (95%)	105 (94%)	6 (5%)	1 (1%)	14	35
14	S141	99/102 (97%)	85 (86%)	13 (13%)	1 (1%)	12	32
15	S151	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	S161	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	9	25
17	S171	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
18	S181	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
19	S191	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
20	S201	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
21	S211	54/71 (76%)	54 (100%)	0	0	100	100
24	L021	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
25	L031	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	48
26	L041	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
27	L051	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
28	L061	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
29	L091	147/149 (99%)	129 (88%)	17 (12%)	1 (1%)	18	41
30	L311	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
31	L131	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
32	L141	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	L151	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	18	41
34	L161	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
35	L171	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
36	L181	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
37	L191	112/115 (97%)	109 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	L201	115/118 (98%)	115 (100%)	0	0	100	100
39	L211	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
40	L221	108/110 (98%)	108 (100%)	0	0	100	100
41	L231	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
42	L241	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
43	L251	92/94 (98%)	92 (100%)	0	0	100	100
44	L271	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
45	L281	75/78 (96%)	75 (100%)	0	0	100	100
46	L291	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	L301	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	L321	54/57 (95%)	54 (100%)	0	0	100	100
49	L331	49/55 (89%)	49 (100%)	0	0	100	100
50	L341	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	L351	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	20
52	L361	36/38 (95%)	36 (100%)	0	0	100	100
53	SPE1	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5607/5948 (94%)	5389 (96%)	209 (4%)	9 (0%)	44	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	S101	57	VAL
25	L031	149	ASN
51	L351	32	ILE
13	S131	66	GLU
14	S141	54	ASP
16	S161	45	GLU
29	L091	45	GLU
33	L151	36	LYS
2	S021	127	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S021	186/199 (94%)	184 (99%)	2 (1%)	65	85
3	S031	170/190 (90%)	169 (99%)	1 (1%)	78	91
4	S041	172/173 (99%)	169 (98%)	3 (2%)	53	79
5	S051	118/126 (94%)	117 (99%)	1 (1%)	73	88
6	S061	92/116 (79%)	92 (100%)	0	100	100
7	S071	124/147 (84%)	123 (99%)	1 (1%)	73	88
8	S081	104/105 (99%)	104 (100%)	0	100	100
9	S091	105/107 (98%)	102 (97%)	3 (3%)	37	67
10	S101	87/90 (97%)	87 (100%)	0	100	100
11	S111	90/99 (91%)	90 (100%)	0	100	100
12	S121	102/103 (99%)	100 (98%)	2 (2%)	48	76
13	S131	92/96 (96%)	91 (99%)	1 (1%)	65	85
14	S141	79/84 (94%)	78 (99%)	1 (1%)	61	83
15	S151	76/77 (99%)	75 (99%)	1 (1%)	61	83
16	S161	65/65 (100%)	64 (98%)	1 (2%)	57	81
17	S171	74/78 (95%)	74 (100%)	0	100	100
18	S181	48/65 (74%)	46 (96%)	2 (4%)	26	55
19	S191	71/79 (90%)	71 (100%)	0	100	100
20	S201	65/66 (98%)	65 (100%)	0	100	100
21	S211	48/61 (79%)	47 (98%)	1 (2%)	47	75
24	L021	216/218 (99%)	215 (100%)	1 (0%)	81	92
25	L031	163/163 (100%)	161 (99%)	2 (1%)	63	84
26	L041	165/165 (100%)	163 (99%)	2 (1%)	63	84
27	L051	148/150 (99%)	145 (98%)	3 (2%)	48	76
28	L061	137/138 (99%)	136 (99%)	1 (1%)	76	90
29	L091	114/114 (100%)	112 (98%)	2 (2%)	51	78
30	L311	59/62 (95%)	59 (100%)	0	100	100
31	L131	116/116 (100%)	116 (100%)	0	100	100
32	L141	104/104 (100%)	104 (100%)	0	100	100
33	L151	103/103 (100%)	102 (99%)	1 (1%)	68	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	L161	108/108 (100%)	108 (100%)	0	100	100
35	L171	98/103 (95%)	97 (99%)	1 (1%)	68	86
36	L181	87/87 (100%)	87 (100%)	0	100	100
37	L191	99/100 (99%)	99 (100%)	0	100	100
38	L201	89/90 (99%)	88 (99%)	1 (1%)	65	85
39	L211	84/84 (100%)	84 (100%)	0	100	100
40	L221	93/93 (100%)	92 (99%)	1 (1%)	65	85
41	L231	80/84 (95%)	80 (100%)	0	100	100
42	L241	83/85 (98%)	83 (100%)	0	100	100
43	L251	78/78 (100%)	78 (100%)	0	100	100
44	L271	57/63 (90%)	57 (100%)	0	100	100
45	L281	67/68 (98%)	65 (97%)	2 (3%)	36	66
46	L291	54/55 (98%)	54 (100%)	0	100	100
47	L301	48/49 (98%)	48 (100%)	0	100	100
48	L321	47/48 (98%)	46 (98%)	1 (2%)	47	75
49	L331	45/49 (92%)	45 (100%)	0	100	100
50	L341	38/38 (100%)	37 (97%)	1 (3%)	40	70
51	L351	51/52 (98%)	51 (100%)	0	100	100
52	L361	34/34 (100%)	33 (97%)	1 (3%)	37	67
53	SPE1	31/31 (100%)	28 (90%)	3 (10%)	8	20
All	All	4664/4858 (96%)	4621 (99%)	43 (1%)	68	87

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S021	37	LYS
2	S021	112	LYS
3	S031	107	ARG
4	S041	26	ARG
4	S041	56	ARG
4	S041	188	ARG
5	S051	69	ARG
7	S071	5	ARG
9	S091	59	GLU
9	S091	106	ARG

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Mol	Chain	Res	Type
9	S091	113	ARG
12	S121	86	ARG
12	S121	120	LYS
13	S131	107	ARG
14	S141	61	ARG
15	S151	89	ARG
16	S161	5	ARG
18	S181	57	ARG
18	S181	73	ARG
21	S211	7	ARG
24	L021	80	ARG
25	L031	13	ARG
25	L031	33	ARG
26	L041	21	ARG
26	L041	44	ARG
27	L051	48	LYS
27	L051	102	ARG
27	L051	150	ARG
28	L061	175	LYS
29	L091	57	LYS
29	L091	71	LYS
33	L151	78	ARG
35	L171	2	ARG
38	L201	51	ARG
40	L221	92	ARG
45	L281	27	ARG
45	L281	72	ARG
48	L321	40	ARG
50	L341	39	ARG
52	L361	12	ARG
53	SPE1	4	ASN
53	SPE1	12	ARG
53	SPE1	32	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16S1	1533/1534 (99%)	176 (11%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	23S1	2894/2897 (99%)	298 (10%)	18 (0%)
23	05S1	119/120 (99%)	8 (6%)	0
54	MRN1	6/7 (85%)	3 (50%)	1 (16%)
55	PTR1	72/76 (94%)	13 (18%)	1 (1%)
All	All	4624/4634 (99%)	498 (10%)	21 (0%)

All (498) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16S1	4	U
1	16S1	7	A
1	16S1	9	G
1	16S1	32	A
1	16S1	39	G
1	16S1	47	C
1	16S1	48	C
1	16S1	50	A
1	16S1	51	A
1	16S1	71	A
1	16S1	72	A
1	16S1	75	G
1	16S1	76	G
1	16S1	78	A
1	16S1	79	G
1	16S1	83	C
1	16S1	84	U
1	16S1	85	U
1	16S1	86	G
1	16S1	87	C
1	16S1	88	U
1	16S1	89	U
1	16S1	95	C
1	16S1	98	A
1	16S1	116	A
1	16S1	130	A
1	16S1	131	A
1	16S1	164	G
1	16S1	181	A
1	16S1	197	A
1	16S1	210	C
1	16S1	226	G
1	16S1	245	U

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Mol	Chain	Res	Type
1	16S1	247	G
1	16S1	251	G
1	16S1	266	G
1	16S1	267	C
1	16S1	289	G
1	16S1	306	A
1	16S1	321	A
1	16S1	328	C
1	16S1	352	C
1	16S1	354	G
1	16S1	367	U
1	16S1	372	C
1	16S1	373	A
1	16S1	384	G
1	16S1	392	C
1	16S1	397	A
1	16S1	406	G
1	16S1	413	G
1	16S1	414	A
1	16S1	429	U
1	16S1	435	A
1	16S1	439	U
1	16S1	467	U
1	16S1	468	A
1	16S1	478	A
1	16S1	479	U
1	16S1	481	G
1	16S1	484	G
1	16S1	486	U
1	16S1	497	G
1	16S1	509	A
1	16S1	511	C
1	16S1	513	C
1	16S1	516	PSU
1	16S1	518	C
1	16S1	527	G7M
1	16S1	528	C
1	16S1	532	A
1	16S1	547	A
1	16S1	559	A
1	16S1	572	A
1	16S1	573	A

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Mol	Chain	Res	Type
1	16S1	576	C
1	16S1	577	G
1	16S1	579	A
1	16S1	633	G
1	16S1	650	G
1	16S1	653	U
1	16S1	665	A
1	16S1	718	A
1	16S1	721	G
1	16S1	722	G
1	16S1	734	G
1	16S1	748	G
1	16S1	755	G
1	16S1	777	A
1	16S1	793	U
1	16S1	794	A
1	16S1	815	A
1	16S1	817	C
1	16S1	821	G
1	16S1	828	U
1	16S1	832	G
1	16S1	841	C
1	16S1	842	U
1	16S1	843	U
1	16S1	846	G
1	16S1	926	G
1	16S1	934	C
1	16S1	942	G
1	16S1	960	U
1	16S1	966	2MG
1	16S1	969	A
1	16S1	975	A
1	16S1	976	G
1	16S1	977	A
1	16S1	993	G
1	16S1	1004	A
1	16S1	1005	A
1	16S1	1019	A
1	16S1	1020	G
1	16S1	1026	G
1	16S1	1028	C
1	16S1	1029	U

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Mol	Chain	Res	Type
1	16S1	1030	U
1	16S1	1032	G
1	16S1	1045	C
1	16S1	1053	G
1	16S1	1065	U
1	16S1	1094	G
1	16S1	1095	U
1	16S1	1101	A
1	16S1	1132	C
1	16S1	1139	G
1	16S1	1140	C
1	16S1	1141	C
1	16S1	1157	A
1	16S1	1158	C
1	16S1	1159	U
1	16S1	1169	A
1	16S1	1184	G
1	16S1	1196	A
1	16S1	1197	A
1	16S1	1212	U
1	16S1	1213	A
1	16S1	1225	A
1	16S1	1226	C
1	16S1	1227	A
1	16S1	1238	A
1	16S1	1256	A
1	16S1	1257	A
1	16S1	1258	G
1	16S1	1260	G
1	16S1	1280	A
1	16S1	1285	A
1	16S1	1299	A
1	16S1	1300	G
1	16S1	1302	C
1	16S1	1317	C
1	16S1	1318	A
1	16S1	1320	C
1	16S1	1340	A
1	16S1	1346	A
1	16S1	1353	G
1	16S1	1363	A
1	16S1	1364	U

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Mol	Chain	Res	Type
1	16S1	1370	G
1	16S1	1419	G
1	16S1	1429	A
1	16S1	1432	G
1	16S1	1441	A
1	16S1	1487	G
1	16S1	1492	A
1	16S1	1493	A
1	16S1	1497	G
1	16S1	1499	A
1	16S1	1502	A
1	16S1	1503	A
1	16S1	1506	U
1	16S1	1517	G
1	16S1	1519	MA6
1	16S1	1529	G
1	16S1	1530	G
22	23S1	23	G
22	23S1	34	U
22	23S1	61	C
22	23S1	71	A
22	23S1	74	A
22	23S1	75	G
22	23S1	84	A
22	23S1	101	A
22	23S1	103	A
22	23S1	118	A
22	23S1	119	A
22	23S1	120	U
22	23S1	163	C
22	23S1	165	A
22	23S1	181	A
22	23S1	196	A
22	23S1	199	A
22	23S1	200	U
22	23S1	215	G
22	23S1	216	A
22	23S1	221	A
22	23S1	222	A
22	23S1	233	A
22	23S1	248	G
22	23S1	265	A

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Mol	Chain	Res	Type
22	23S1	276	U
22	23S1	278	A
22	23S1	302	C
22	23S1	303	G
22	23S1	311	A
22	23S1	330	A
22	23S1	386	G
22	23S1	396	G
22	23S1	411	G
22	23S1	467	G
22	23S1	481	G
22	23S1	491	G
22	23S1	505	A
22	23S1	509	C
22	23S1	529	A
22	23S1	530	G
22	23S1	531	C
22	23S1	532	A
22	23S1	544	C
22	23S1	546	U
22	23S1	547	A
22	23S1	548	G
22	23S1	549	G
22	23S1	563	A
22	23S1	573	U
22	23S1	575	A
22	23S1	586	A
22	23S1	603	A
22	23S1	613	A
22	23S1	614	A
22	23S1	637	A
22	23S1	645	C
22	23S1	647	G
22	23S1	653	U
22	23S1	654	A
22	23S1	655	A
22	23S1	686	U
22	23S1	717	C
22	23S1	730	A
22	23S1	747	5MU
22	23S1	765	C
22	23S1	775	G

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Mol	Chain	Res	Type
22	23S1	776	G
22	23S1	782	A
22	23S1	784	G
22	23S1	789	A
22	23S1	805	G
22	23S1	812	C
22	23S1	827	U
22	23S1	828	U
22	23S1	829	A
22	23S1	846	U
22	23S1	847	U
22	23S1	858	G
22	23S1	859	G
22	23S1	884	U
22	23S1	896	A
22	23S1	910	A
22	23S1	931	U
22	23S1	946	C
22	23S1	961	C
22	23S1	974	G
22	23S1	983	A
22	23S1	984	A
22	23S1	985	C
22	23S1	996	A
22	23S1	1005	C
22	23S1	1012	U
22	23S1	1013	C
22	23S1	1022	G
22	23S1	1026	G
22	23S1	1033	U
22	23S1	1054	A
22	23S1	1070	A
22	23S1	1088	A
22	23S1	1112	G
22	23S1	1130	U
22	23S1	1132	U
22	23S1	1133	A
22	23S1	1135	C
22	23S1	1142	A
22	23S1	1143	A
22	23S1	1173	U
22	23S1	1174	U

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Mol	Chain	Res	Type
22	23S1	1175	A
22	23S1	1176	U
22	23S1	1212	G
22	23S1	1250	G
22	23S1	1253	A
22	23S1	1256	G
22	23S1	1271	G
22	23S1	1272	A
22	23S1	1300	G
22	23S1	1301	A
22	23S1	1329	U
22	23S1	1352	U
22	23S1	1365	A
22	23S1	1379	U
22	23S1	1383	A
22	23S1	1403	A
22	23S1	1416	G
22	23S1	1420	A
22	23S1	1428	C
22	23S1	1452	G
22	23S1	1453	A
22	23S1	1482	G
22	23S1	1508	A
22	23S1	1509	A
22	23S1	1515	A
22	23S1	1566	A
22	23S1	1569	A
22	23S1	1578	U
22	23S1	1606	C
22	23S1	1608	A
22	23S1	1610	A
22	23S1	1617	C
22	23S1	1618	6MZ
22	23S1	1647	U
22	23S1	1648	U
22	23S1	1649	G
22	23S1	1674	G
22	23S1	1729	U
22	23S1	1730	C
22	23S1	1732	C
22	23S1	1738	G
22	23S1	1757	A

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Mol	Chain	Res	Type
22	23S1	1758	U
22	23S1	1764	C
22	23S1	1773	A
22	23S1	1782	U
22	23S1	1800	C
22	23S1	1801	A
22	23S1	1802	A
22	23S1	1808	A
22	23S1	1811	G
22	23S1	1816	C
22	23S1	1829	A
22	23S1	1871	A
22	23S1	1872	A
22	23S1	1873	G
22	23S1	1906	G
22	23S1	1914	C
22	23S1	1929	G
22	23S1	1930	G
22	23S1	1937	A
22	23S1	1938	A
22	23S1	1939	5MU
22	23S1	1955	U
22	23S1	1967	C
22	23S1	1970	A
22	23S1	1971	U
22	23S1	1972	G
22	23S1	1991	U
22	23S1	1993	U
22	23S1	2020	A
22	23S1	2023	C
22	23S1	2027	G
22	23S1	2030	6MZ
22	23S1	2031	A
22	23S1	2033	A
22	23S1	2043	C
22	23S1	2055	C
22	23S1	2056	G
22	23S1	2060	A
22	23S1	2061	G
22	23S1	2069	G7M
22	23S1	2093	G
22	23S1	2101	A

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Mol	Chain	Res	Type
22	23S1	2110	G
22	23S1	2111	U
22	23S1	2112	G
22	23S1	2113	U
22	23S1	2115	G
22	23S1	2116	G
22	23S1	2117	A
22	23S1	2118	U
22	23S1	2119	A
22	23S1	2124	G
22	23S1	2125	G
22	23S1	2126	A
22	23S1	2127	G
22	23S1	2128	G
22	23S1	2131	U
22	23S1	2132	U
22	23S1	2133	G
22	23S1	2137	U
22	23S1	2142	A
22	23S1	2146	C
22	23S1	2147	A
22	23S1	2157	G
22	23S1	2158	A
22	23S1	2159	G
22	23S1	2163	A
22	23S1	2164	C
22	23S1	2165	C
22	23S1	2171	A
22	23S1	2172	U
22	23S1	2173	A
22	23S1	2182	U
22	23S1	2183	A
22	23S1	2188	U
22	23S1	2189	U
22	23S1	2190	G
22	23S1	2195	U
22	23S1	2198	A
22	23S1	2204	G
22	23S1	2211	A
22	23S1	2225	A
22	23S1	2238	G
22	23S1	2239	G

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Mol	Chain	Res	Type
22	23S1	2252	G
22	23S1	2283	C
22	23S1	2287	A
22	23S1	2288	A
22	23S1	2305	U
22	23S1	2308	G
22	23S1	2325	G
22	23S1	2333	A
22	23S1	2336	A
22	23S1	2345	G
22	23S1	2347	C
22	23S1	2350	C
22	23S1	2368	C
22	23S1	2383	G
22	23S1	2385	C
22	23S1	2402	U
22	23S1	2406	A
22	23S1	2425	A
22	23S1	2429	G
22	23S1	2435	A
22	23S1	2441	U
22	23S1	2448	A
22	23S1	2476	A
22	23S1	2478	A
22	23S1	2491	U
22	23S1	2502	G
22	23S1	2505	G
22	23S1	2518	A
22	23S1	2529	G
22	23S1	2547	A
22	23S1	2566	A
22	23S1	2567	G
22	23S1	2573	C
22	23S1	2578	G
22	23S1	2582	G
22	23S1	2602	A
22	23S1	2609	U
22	23S1	2613	U
22	23S1	2615	U
22	23S1	2629	U
22	23S1	2646	C
22	23S1	2663	G

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Mol	Chain	Res	Type
22	23S1	2689	U
22	23S1	2690	U
22	23S1	2714	G
22	23S1	2726	A
22	23S1	2733	A
22	23S1	2744	G
22	23S1	2748	A
22	23S1	2757	A
22	23S1	2765	A
22	23S1	2778	A
22	23S1	2791	G
22	23S1	2820	A
22	23S1	2821	A
22	23S1	2835	A
22	23S1	2861	U
22	23S1	2873	A
22	23S1	2880	C
22	23S1	2883	A
22	23S1	2884	U
22	23S1	2885	G
22	23S1	2891	U
23	05S1	35	C
23	05S1	44	G
23	05S1	56	G
23	05S1	68	C
23	05S1	89	U
23	05S1	90	C
23	05S1	105	G
23	05S1	109	A
54	MRN1	4	C
54	MRN1	6	U
54	MRN1	7	U
55	PTR1	16	C
55	PTR1	17	U
55	PTR1	17(A)	G
55	PTR1	19	A
55	PTR1	20	U
55	PTR1	31	G
55	PTR1	32	RSP
55	PTR1	46	G7M
55	PTR1	54	5MU
55	PTR1	57	G

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Mol	Chain	Res	Type
55	PTR1	59	A
55	PTR1	63	U
55	PTR1	76	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16S1	1225	A
22	23S1	125	A
22	23S1	199	A
22	23S1	685	A
22	23S1	764	A
22	23S1	784	G
22	23S1	984	A
22	23S1	1142	A
22	23S1	1508	A
22	23S1	1608	A
22	23S1	1970	A
22	23S1	2146	C
22	23S1	2162	G
22	23S1	2188	U
22	23S1	2189	U
22	23S1	2251	OMG
22	23S1	2518	A
22	23S1	2756	U
22	23S1	2873	A
54	MRN1	5	G
55	PTR1	19	A

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

44 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
22	PSU	23S1	2604	22	18,21,22	3.98	7 (38%)	22,30,33	1.75	4 (18%)
1	G7M	16S1	527	57,1	23,26,27	2.57	8 (34%)	35,39,42	2.19	11 (31%)
22	PSU	23S1	746	22,56	18,21,22	3.99	7 (38%)	22,30,33	1.96	5 (22%)
22	PSU	23S1	2605	22	18,21,22	4.03	7 (38%)	22,30,33	1.70	4 (18%)
55	4SU	PTR1	8	55	18,21,22	3.48	8 (44%)	26,30,33	1.80	5 (19%)
22	G7M	23S1	2069	22,57	23,26,27	2.51	8 (34%)	35,39,42	2.16	13 (37%)
22	OMC	23S1	2498	22,56	19,22,23	2.77	8 (42%)	26,31,34	1.00	1 (3%)
22	2MG	23S1	2445	22	23,26,27	2.63	8 (34%)	32,38,41	2.34	13 (40%)
1	2MG	16S1	1516	1	23,26,27	2.64	8 (34%)	32,38,41	2.27	13 (40%)
22	PSU	23S1	2457	22	18,21,22	4.03	7 (38%)	22,30,33	2.05	6 (27%)
1	PSU	16S1	516	56,1	18,21,22	4.03	8 (44%)	22,30,33	1.74	6 (27%)
22	PSU	23S1	1911	22	18,21,22	4.13	7 (38%)	22,30,33	1.94	5 (22%)
22	2MG	23S1	1835	22	23,26,27	2.59	9 (39%)	32,38,41	2.26	13 (40%)
55	PSU	PTR1	55	55	18,21,22	4.22	7 (38%)	22,30,33	1.92	5 (22%)
22	5MU	23S1	1939	22,57	19,22,23	0.70	0	28,32,35	1.27	4 (14%)
1	MA6	16S1	1518	1	23,26,27	1.85	5 (21%)	34,38,41	3.16	12 (35%)
53	FME	SPE1	1	53	8,9,10	1.00	1 (12%)	7,9,11	0.98	0
1	5MC	16S1	967	1	18,22,23	3.35	7 (38%)	26,32,35	1.13	2 (7%)
22	PSU	23S1	955	22	18,21,22	3.99	7 (38%)	22,30,33	1.92	4 (18%)
22	PSU	23S1	2504	22,57	18,21,22	4.06	7 (38%)	22,30,33	1.76	4 (18%)
22	1MG	23S1	745	22	22,26,27	2.55	7 (31%)	33,39,42	1.79	7 (21%)
1	4OC	16S1	1402	56,1	20,23,24	2.94	8 (40%)	26,32,35	1.11	2 (7%)
1	UR3	16S1	1498	1	19,22,23	2.98	8 (42%)	26,32,35	1.43	2 (7%)
1	2MG	16S1	1207	57,1	23,26,27	2.67	9 (39%)	32,38,41	2.09	10 (31%)
22	6MZ	23S1	2030	22	22,25,26	3.89	7 (31%)	30,36,39	2.61	10 (33%)
22	PSU	23S1	2580	22,57	18,21,22	4.03	7 (38%)	22,30,33	2.14	6 (27%)
22	OMG	23S1	2251	55,22,57	23,26,27	2.32	8 (34%)	33,38,41	2.05	12 (36%)
1	2MG	16S1	966	1	23,26,27	2.79	9 (39%)	32,38,41	2.23	10 (31%)
34	4D4	L161	81	34	9,11,12	2.51	4 (44%)	8,13,15	1.14	1 (12%)
55	2MG	PTR1	37	55	23,26,27	2.69	9 (39%)	32,38,41	2.20	11 (34%)
55	RSP	PTR1	32	55	17,21,22	3.96	6 (35%)	22,30,33	1.23	2 (9%)
1	5MC	16S1	1407	1	18,22,23	3.30	7 (38%)	26,32,35	0.99	3 (11%)
22	PSU	23S1	1917	22	18,21,22	4.09	7 (38%)	22,30,33	1.62	4 (18%)
22	5MU	23S1	747	22	19,22,23	0.92	2 (10%)	28,32,35	1.31	3 (10%)
22	OMU	23S1	2552	22,56	19,22,23	2.77	7 (36%)	26,31,34	1.84	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	6MZ	23S1	1618	22	22,25,26	3.95	6 (27%)	30,36,39	2.51	10 (33%)
55	5MU	PTR1	54	55	19,22,23	0.98	2 (10%)	28,32,35	1.21	4 (14%)
22	3TD	23S1	1915	22	18,22,23	3.99	8 (44%)	22,32,35	1.56	2 (9%)
1	MA6	16S1	1519	1	23,26,27	1.80	4 (17%)	34,38,41	3.17	11 (32%)
25	MEQ	L031	150	25	8,9,10	1.58	2 (25%)	5,10,12	1.80	1 (20%)
22	2MA	23S1	2503	22,56,57	22,25,26	3.64	8 (36%)	33,37,40	2.23	8 (24%)
22	5MC	23S1	1962	22,57	18,22,23	3.26	7 (38%)	26,32,35	1.00	2 (7%)
55	G7M	PTR1	46	55	23,26,27	2.64	8 (34%)	35,39,42	2.25	12 (34%)
12	D2T	S121	89	12	7,9,10	1.03	0	6,11,13	2.27	3 (50%)

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
22	PSU	23S1	2604	22	-	0/7/25/26	0/2/2/2
1	G7M	16S1	527	57,1	-	2/7/25/26	0/3/3/3
22	PSU	23S1	746	22,56	-	1/7/25/26	0/2/2/2
22	PSU	23S1	2605	22	-	0/7/25/26	0/2/2/2
55	4SU	PTR1	8	55	-	1/7/25/26	0/2/2/2
22	G7M	23S1	2069	22,57	-	2/7/25/26	0/3/3/3
22	OMC	23S1	2498	22,56	-	0/9/27/28	0/2/2/2
22	2MG	23S1	2445	22	-	1/9/27/28	0/3/3/3
1	2MG	16S1	1516	1	-	0/9/27/28	0/3/3/3
22	PSU	23S1	2457	22	-	0/7/25/26	0/2/2/2
1	PSU	16S1	516	56,1	-	0/7/25/26	0/2/2/2
22	PSU	23S1	1911	22	-	0/7/25/26	0/2/2/2
22	2MG	23S1	1835	22	-	0/9/27/28	0/3/3/3
55	PSU	PTR1	55	55	-	0/7/25/26	0/2/2/2
22	5MU	23S1	1939	22,57	-	2/7/25/26	0/2/2/2
1	MA6	16S1	1518	1	-	0/11/29/30	0/3/3/3
53	FME	SPE1	1	53	-	4/7/9/11	-
1	5MC	16S1	967	1	-	0/7/25/26	0/2/2/2
22	PSU	23S1	955	22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2504	22,57	-	2/7/25/26	0/2/2/2
22	1MG	23S1	745	22	-	0/7/25/26	0/3/3/3
1	4OC	16S1	1402	56,1	-	1/9/29/30	0/2/2/2
1	UR3	16S1	1498	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	16S1	1207	57,1	-	0/9/27/28	0/3/3/3
22	6MZ	23S1	2030	22	-	2/9/27/28	0/3/3/3
22	PSU	23S1	2580	22,57	-	1/7/25/26	0/2/2/2
22	OMG	23S1	2251	55,22,57	-	1/9/27/28	0/3/3/3
1	2MG	16S1	966	1	-	2/9/27/28	0/3/3/3
34	4D4	L161	81	34	-	3/11/12/14	-
55	2MG	PTR1	37	55	-	0/9/27/28	0/3/3/3
55	RSP	PTR1	32	55	-	2/7/25/26	0/2/2/2
1	5MC	16S1	1407	1	-	0/7/25/26	0/2/2/2
22	PSU	23S1	1917	22	-	0/7/25/26	0/2/2/2
22	5MU	23S1	747	22	-	0/7/25/26	0/2/2/2
22	OMU	23S1	2552	22,56	-	0/9/27/28	0/2/2/2
22	6MZ	23S1	1618	22	-	0/9/27/28	0/3/3/3
55	5MU	PTR1	54	55	-	2/7/25/26	0/2/2/2
22	3TD	23S1	1915	22	-	0/7/25/26	0/2/2/2
1	MA6	16S1	1519	1	-	3/11/29/30	0/3/3/3
25	MEQ	L031	150	25	-	2/8/9/11	-
22	2MA	23S1	2503	22,56,57	-	2/7/25/26	0/3/3/3
22	5MC	23S1	1962	22,57	-	0/7/25/26	0/2/2/2
55	G7M	PTR1	46	55	-	1/7/25/26	0/3/3/3
12	D2T	S121	89	12	-	1/7/12/14	-

All (284) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1618	6MZ	C6-N6	17.10	1.52	1.34
22	23S1	2030	6MZ	C6-N6	16.67	1.52	1.34
55	PTR1	32	RSP	C2-N3	12.27	1.49	1.36
22	23S1	1915	3TD	C6-C5	11.53	1.48	1.35
22	23S1	2504	PSU	C6-C5	11.20	1.48	1.35
55	PTR1	55	PSU	C6-C5	11.19	1.48	1.35
22	23S1	1911	PSU	C6-C5	11.08	1.48	1.35
22	23S1	1917	PSU	C6-C5	11.08	1.48	1.35
22	23S1	2503	2MA	C4-N3	11.08	1.48	1.34
22	23S1	2457	PSU	C6-C5	10.98	1.48	1.35
22	23S1	2605	PSU	C6-C5	10.91	1.48	1.35
22	23S1	955	PSU	C6-C5	10.83	1.47	1.35
22	23S1	2580	PSU	C6-C5	10.77	1.47	1.35
22	23S1	2604	PSU	C6-C5	10.71	1.47	1.35
1	16S1	516	PSU	C6-C5	10.68	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	746	PSU	C6-C5	10.65	1.47	1.35
22	23S1	1911	PSU	C2-N1	9.38	1.49	1.36
55	PTR1	55	PSU	C2-N1	9.36	1.49	1.36
22	23S1	1917	PSU	C2-N1	9.13	1.49	1.36
22	23S1	2605	PSU	C2-N1	9.11	1.49	1.36
1	16S1	516	PSU	C2-N1	9.09	1.49	1.36
22	23S1	2604	PSU	C2-N1	8.98	1.48	1.36
22	23S1	2457	PSU	C2-N1	8.90	1.48	1.36
22	23S1	746	PSU	C2-N1	8.83	1.48	1.36
1	16S1	1407	5MC	C6-C5	8.73	1.48	1.34
22	23S1	2504	PSU	C2-N1	8.72	1.48	1.36
22	23S1	2580	PSU	C2-N1	8.68	1.48	1.36
22	23S1	955	PSU	C2-N1	8.58	1.48	1.36
1	16S1	967	5MC	C6-C5	8.53	1.48	1.34
22	23S1	1962	5MC	C6-C5	8.44	1.48	1.34
22	23S1	1915	3TD	C2-N1	8.24	1.47	1.37
1	16S1	1498	UR3	C2-N1	8.05	1.50	1.38
55	PTR1	55	PSU	C2-N3	7.20	1.49	1.37
1	16S1	966	2MG	C2-N3	7.03	1.45	1.31
22	23S1	2503	2MA	C2-N3	7.03	1.46	1.34
55	PTR1	8	4SU	C4-N3	7.02	1.45	1.37
55	PTR1	37	2MG	C2-N3	6.90	1.45	1.31
22	23S1	2580	PSU	C2-N3	6.78	1.49	1.37
22	23S1	2504	PSU	C2-N3	6.74	1.49	1.37
22	23S1	1911	PSU	C2-N3	6.74	1.49	1.37
22	23S1	955	PSU	C2-N3	6.70	1.49	1.37
1	16S1	1516	2MG	C2-N3	6.69	1.44	1.31
1	16S1	1207	2MG	C2-N3	6.65	1.44	1.31
22	23S1	1917	PSU	C2-N3	6.60	1.48	1.37
55	PTR1	8	4SU	C2-N1	6.58	1.49	1.38
22	23S1	746	PSU	C2-N3	6.56	1.48	1.37
22	23S1	2605	PSU	C2-N3	6.50	1.48	1.37
1	16S1	516	PSU	C2-N3	6.49	1.48	1.37
22	23S1	2457	PSU	C2-N3	6.45	1.48	1.37
22	23S1	2445	2MG	C2-N3	6.42	1.44	1.31
55	PTR1	8	4SU	C2-N3	6.41	1.49	1.38
22	23S1	745	1MG	C4-N3	6.38	1.49	1.34
22	23S1	1835	2MG	C2-N3	6.31	1.44	1.31
55	PTR1	46	G7M	C4-N3	6.30	1.49	1.34
22	23S1	2604	PSU	C2-N3	6.29	1.48	1.37
22	23S1	2552	OMU	C2-N1	6.28	1.48	1.38
22	23S1	745	1MG	C2-N3	6.25	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	966	2MG	C4-N3	6.23	1.49	1.34
1	16S1	527	G7M	C4-N3	6.19	1.49	1.34
1	16S1	1402	4OC	C4-N3	6.16	1.43	1.32
1	16S1	967	5MC	C4-N3	6.15	1.44	1.34
1	16S1	1402	4OC	C6-C5	6.00	1.49	1.35
22	23S1	2251	OMG	C4-N3	5.99	1.48	1.34
1	16S1	1207	2MG	C4-N3	5.90	1.48	1.34
22	23S1	2503	2MA	C2-N1	5.90	1.44	1.34
22	23S1	2552	OMU	C2-N3	5.90	1.48	1.38
22	23S1	1962	5MC	C4-N3	5.87	1.44	1.34
22	23S1	2069	G7M	C4-N3	5.85	1.48	1.34
55	PTR1	32	RSP	C6-C5	5.80	1.48	1.35
55	PTR1	37	2MG	C4-N3	5.79	1.48	1.34
34	L161	81	4D4	CZ-NE	5.77	1.44	1.33
1	16S1	1516	2MG	C4-N3	5.72	1.47	1.34
1	16S1	967	5MC	C2-N3	5.66	1.47	1.36
22	23S1	2498	OMC	C6-C5	5.65	1.48	1.35
1	16S1	1498	UR3	C6-C5	5.63	1.48	1.35
22	23S1	1962	5MC	C2-N3	5.60	1.47	1.36
22	23S1	2445	2MG	C4-N3	5.59	1.47	1.34
1	16S1	1518	MA6	C6-N6	5.54	1.53	1.36
1	16S1	1402	4OC	C2-N3	5.52	1.47	1.36
22	23S1	1835	2MG	C4-N3	5.51	1.47	1.34
55	PTR1	8	4SU	C6-C5	5.50	1.47	1.35
22	23S1	2498	OMC	C2-N3	5.50	1.47	1.36
55	PTR1	46	G7M	C2-N3	5.49	1.46	1.33
1	16S1	1407	5MC	C2-N3	5.45	1.47	1.36
1	16S1	527	G7M	C2-N3	5.43	1.46	1.33
1	16S1	1519	MA6	C6-N6	5.40	1.52	1.36
1	16S1	1407	5MC	C4-N3	5.38	1.43	1.34
22	23S1	2069	G7M	C5-N7	-5.38	1.32	1.39
1	16S1	966	2MG	C2-N2	5.26	1.45	1.33
22	23S1	2503	2MA	C6-N1	5.25	1.42	1.35
1	16S1	527	G7M	C5-N7	-5.22	1.33	1.39
22	23S1	2552	OMU	C6-C5	5.16	1.47	1.35
55	PTR1	32	RSP	C4-N4	5.11	1.46	1.33
55	PTR1	32	RSP	C4-N3	5.10	1.44	1.34
55	PTR1	37	2MG	C2-N2	5.03	1.44	1.33
22	23S1	1915	3TD	C6-N1	4.97	1.44	1.36
1	16S1	1207	2MG	C2-N2	4.94	1.44	1.33
22	23S1	2251	OMG	C2-N3	4.90	1.45	1.33
55	PTR1	55	PSU	C6-N1	4.87	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	46	G7M	C5-N7	-4.80	1.33	1.39
1	16S1	1516	2MG	C2-N2	4.78	1.44	1.33
22	23S1	2445	2MG	C2-N2	4.76	1.43	1.33
22	23S1	2069	G7M	C2-N3	4.75	1.44	1.33
1	16S1	516	PSU	C6-N1	4.75	1.44	1.36
22	23S1	1917	PSU	C6-N1	4.68	1.44	1.36
1	16S1	966	2MG	C2-N1	4.67	1.44	1.36
1	16S1	1498	UR3	C2-N3	4.64	1.48	1.39
22	23S1	1911	PSU	C6-N1	4.62	1.43	1.36
22	23S1	1915	3TD	C1'-C5	-4.59	1.39	1.50
22	23S1	1835	2MG	C2-N2	4.58	1.43	1.33
22	23S1	746	PSU	C6-N1	4.56	1.43	1.36
55	PTR1	8	4SU	C4-S4	-4.50	1.59	1.68
22	23S1	2503	2MA	C5-C6	4.49	1.53	1.41
1	16S1	1407	5MC	C6-N1	4.49	1.45	1.38
55	PTR1	37	2MG	C2-N1	4.49	1.43	1.36
1	16S1	1207	2MG	C2-N1	4.45	1.43	1.36
22	23S1	2604	PSU	C6-N1	4.44	1.43	1.36
22	23S1	2498	OMC	C2-N1	4.44	1.49	1.40
22	23S1	2457	PSU	C6-N1	4.44	1.43	1.36
22	23S1	2498	OMC	C4-N4	4.42	1.44	1.33
22	23S1	745	1MG	C2-N2	4.41	1.42	1.34
22	23S1	2605	PSU	C6-N1	4.41	1.43	1.36
22	23S1	955	PSU	C6-N1	4.34	1.43	1.36
22	23S1	2504	PSU	C6-N1	4.34	1.43	1.36
22	23S1	2498	OMC	C4-N3	4.33	1.43	1.34
1	16S1	1498	UR3	O4-C4	-4.33	1.14	1.23
22	23S1	2251	OMG	C2-N2	4.31	1.44	1.34
22	23S1	2580	PSU	C6-N1	4.29	1.43	1.36
55	PTR1	8	4SU	C5-C4	4.28	1.48	1.42
22	23S1	1915	3TD	C2-N3	4.20	1.47	1.38
1	16S1	1516	2MG	C2-N1	4.11	1.43	1.36
1	16S1	967	5MC	C4-N4	4.10	1.44	1.34
1	16S1	1402	4OC	C4-N4	4.06	1.44	1.35
55	PTR1	46	G7M	C5-C6	4.03	1.54	1.43
22	23S1	1835	2MG	C2-N1	4.02	1.43	1.36
1	16S1	967	5MC	C6-N1	3.98	1.44	1.38
55	PTR1	46	G7M	C2-N2	3.92	1.43	1.34
22	23S1	2445	2MG	C2-N1	3.90	1.43	1.36
1	16S1	967	5MC	C2-N1	3.90	1.48	1.40
1	16S1	1407	5MC	C4-N4	3.90	1.44	1.34
1	16S1	1402	4OC	C2-N1	3.88	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1962	5MC	C4-N4	3.88	1.44	1.34
1	16S1	527	G7M	C5-C6	3.84	1.54	1.43
22	23S1	1962	5MC	C6-N1	3.83	1.44	1.38
55	PTR1	55	PSU	C4-N3	3.77	1.45	1.38
22	23S1	2069	G7M	C2-N2	3.73	1.43	1.34
1	16S1	527	G7M	C2-N2	3.71	1.43	1.34
22	23S1	2503	2MA	C6-N6	-3.71	1.24	1.34
22	23S1	2445	2MG	C5-N7	-3.69	1.31	1.39
22	23S1	1835	2MG	C5-N7	-3.68	1.31	1.39
22	23S1	2069	G7M	C5-C6	3.63	1.53	1.43
22	23S1	2552	OMU	O4-C4	-3.62	1.17	1.24
1	16S1	1402	4OC	O2-C2	-3.59	1.17	1.23
1	16S1	1402	4OC	C5-C4	3.57	1.48	1.40
22	23S1	1962	5MC	C2-N1	3.56	1.47	1.40
1	16S1	1516	2MG	C5-N7	-3.51	1.32	1.39
1	16S1	1407	5MC	C2-N1	3.48	1.47	1.40
55	PTR1	32	RSP	C6-N1	3.47	1.46	1.38
22	23S1	745	1MG	C5-N7	-3.47	1.32	1.39
22	23S1	2069	G7M	C4-N9	-3.47	1.29	1.38
22	23S1	1911	PSU	C4-N3	3.45	1.45	1.38
22	23S1	955	PSU	C4-N3	3.44	1.45	1.38
22	23S1	2552	OMU	C4-N3	3.43	1.44	1.38
22	23S1	1917	PSU	C4-N3	3.41	1.45	1.38
1	16S1	966	2MG	C5-N7	-3.40	1.32	1.39
22	23S1	2504	PSU	C4-N3	3.39	1.45	1.38
55	PTR1	37	2MG	C5-N7	-3.37	1.32	1.39
1	16S1	516	PSU	C4-N3	3.37	1.45	1.38
1	16S1	1518	MA6	C5-C4	-3.36	1.32	1.39
22	23S1	2030	6MZ	C5-N7	-3.34	1.32	1.39
22	23S1	2251	OMG	C5-N7	-3.31	1.32	1.39
1	16S1	1519	MA6	C5-C4	-3.30	1.32	1.39
55	PTR1	46	G7M	C6-N1	3.30	1.45	1.38
22	23S1	2580	PSU	C4-N3	3.29	1.44	1.38
22	23S1	2445	2MG	O6-C6	-3.28	1.17	1.23
22	23S1	2604	PSU	C4-N3	3.28	1.44	1.38
22	23S1	745	1MG	C5-C6	3.26	1.53	1.45
22	23S1	1618	6MZ	C5-N7	-3.25	1.32	1.39
22	23S1	2030	6MZ	C8-N9	-3.21	1.31	1.37
25	L031	150	MEQ	OE1-CD	-3.20	1.16	1.23
1	16S1	1407	5MC	O2-C2	-3.20	1.17	1.23
22	23S1	2503	2MA	C8-N7	3.18	1.37	1.31
1	16S1	1207	2MG	C5-N7	-3.17	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2605	PSU	C4-N3	3.16	1.44	1.38
55	PTR1	32	RSP	C2-S2	-3.15	1.59	1.67
34	L161	81	4D4	CZ-NH2	3.15	1.44	1.32
22	23S1	1618	6MZ	C8-N9	-3.14	1.31	1.37
22	23S1	1962	5MC	O2-C2	-3.13	1.17	1.23
22	23S1	2498	OMC	O2-C2	-3.13	1.17	1.23
22	23S1	746	PSU	C4-N3	3.08	1.44	1.38
22	23S1	1835	2MG	O6-C6	-3.06	1.17	1.23
1	16S1	527	G7M	C6-N1	3.06	1.44	1.38
22	23S1	2069	G7M	C6-N1	3.05	1.44	1.38
55	PTR1	46	G7M	C4-N9	-3.04	1.30	1.38
22	23S1	2457	PSU	C4-N3	3.02	1.44	1.38
22	23S1	2251	OMG	O6-C6	-3.01	1.17	1.23
1	16S1	1498	UR3	O2-C2	-3.00	1.17	1.22
1	16S1	1498	UR3	C5-C4	3.00	1.51	1.43
1	16S1	1518	MA6	C8-N9	-2.98	1.32	1.37
22	23S1	2552	OMU	O2-C2	-2.97	1.17	1.23
1	16S1	1402	4OC	C6-N1	2.97	1.45	1.38
1	16S1	527	G7M	C4-N9	-2.94	1.30	1.38
1	16S1	1519	MA6	C5-N7	-2.93	1.33	1.39
1	16S1	967	5MC	O2-C2	-2.92	1.18	1.23
1	16S1	1516	2MG	O6-C6	-2.91	1.18	1.23
1	16S1	1518	MA6	C5-N7	-2.88	1.33	1.39
1	16S1	966	2MG	O6-C6	-2.87	1.18	1.23
55	PTR1	8	4SU	C6-N1	2.86	1.44	1.38
22	23S1	2580	PSU	O4-C4	-2.85	1.18	1.23
22	23S1	2498	OMC	C6-N1	2.83	1.44	1.38
22	23S1	2030	6MZ	C5-C4	-2.81	1.33	1.39
22	23S1	1835	2MG	C4-N9	-2.78	1.30	1.38
55	PTR1	54	5MU	C2-N1	2.77	1.42	1.38
1	16S1	1207	2MG	O6-C6	-2.76	1.18	1.23
22	23S1	2457	PSU	O4-C4	-2.74	1.18	1.23
22	23S1	2445	2MG	C4-N9	-2.73	1.31	1.38
55	PTR1	37	2MG	O6-C6	-2.72	1.18	1.23
1	16S1	1519	MA6	C8-N9	-2.71	1.32	1.37
22	23S1	2503	2MA	C5-N7	-2.70	1.33	1.39
22	23S1	745	1MG	O6-C6	-2.69	1.17	1.23
22	23S1	2580	PSU	O4'-C1'	-2.69	1.40	1.43
22	23S1	1618	6MZ	C5-C4	-2.68	1.34	1.39
1	16S1	1207	2MG	C4-N9	-2.67	1.31	1.38
1	16S1	1516	2MG	C4-N9	-2.63	1.31	1.38
22	23S1	1915	3TD	O2-C2	-2.62	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1618	6MZ	C9-N6	2.58	1.49	1.45
22	23S1	2604	PSU	O4-C4	-2.58	1.18	1.23
55	PTR1	46	G7M	C2-N1	2.57	1.44	1.37
22	23S1	955	PSU	O4-C4	-2.55	1.18	1.23
22	23S1	746	PSU	O4-C4	-2.53	1.18	1.23
1	16S1	527	G7M	C2-N1	2.53	1.43	1.37
22	23S1	2605	PSU	O4-C4	-2.53	1.18	1.23
22	23S1	2030	6MZ	C6-N1	-2.51	1.31	1.35
55	PTR1	37	2MG	C4-N9	-2.46	1.31	1.38
34	L161	81	4D4	CZ-NH1	-2.43	1.24	1.34
22	23S1	2251	OMG	C4-N9	-2.43	1.31	1.38
22	23S1	2504	PSU	O4-C4	-2.42	1.19	1.23
1	16S1	1207	2MG	C5-C6	2.40	1.53	1.44
55	PTR1	8	4SU	O2-C2	-2.38	1.18	1.23
22	23S1	2552	OMU	C6-N1	2.38	1.43	1.38
1	16S1	1498	UR3	C6-N1	2.37	1.43	1.38
55	PTR1	37	2MG	C5-C6	2.36	1.53	1.44
22	23S1	747	5MU	C5M-C5	-2.36	1.44	1.50
22	23S1	2030	6MZ	C9-N6	2.35	1.49	1.45
22	23S1	1915	3TD	C4-N3	2.33	1.45	1.40
22	23S1	746	PSU	O4'-C1'	-2.33	1.40	1.43
1	16S1	516	PSU	O4-C4	-2.32	1.19	1.23
1	16S1	966	2MG	C4-N9	-2.31	1.32	1.38
22	23S1	1911	PSU	O4-C4	-2.30	1.19	1.23
22	23S1	1917	PSU	O4-C4	-2.29	1.19	1.23
22	23S1	2069	G7M	C2-N1	2.29	1.43	1.37
22	23S1	1917	PSU	C1'-C5	2.29	1.55	1.50
1	16S1	1516	2MG	C5-C6	2.29	1.52	1.44
22	23S1	2445	2MG	C5-C6	2.28	1.52	1.44
1	16S1	516	PSU	O4'-C1'	-2.27	1.40	1.43
1	16S1	966	2MG	C6-N1	2.26	1.43	1.38
1	16S1	1207	2MG	C6-N1	2.25	1.43	1.38
22	23S1	2605	PSU	C1'-C5	2.23	1.55	1.50
25	L031	150	MEQ	CD-NE2	2.23	1.44	1.34
22	23S1	2251	OMG	C5-C6	2.21	1.52	1.44
22	23S1	2504	PSU	C1'-C5	2.20	1.55	1.50
55	PTR1	55	PSU	C1'-C5	2.18	1.55	1.50
22	23S1	2251	OMG	C2-N1	2.17	1.43	1.37
1	16S1	966	2MG	C5-C6	2.17	1.52	1.44
22	23S1	2030	6MZ	C8-N7	2.16	1.35	1.31
55	PTR1	55	PSU	O4-C4	-2.14	1.19	1.23
22	23S1	2498	OMC	C5-C4	2.13	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2604	PSU	C1'-C5	2.12	1.55	1.50
1	16S1	1498	UR3	C3U-N3	-2.11	1.43	1.47
22	23S1	747	5MU	C2-N1	2.10	1.41	1.38
1	16S1	1518	MA6	C6-N1	-2.10	1.30	1.34
22	23S1	1618	6MZ	C8-N7	2.08	1.35	1.31
22	23S1	1835	2MG	C5-C6	2.08	1.52	1.44
22	23S1	2457	PSU	O4'-C1'	-2.08	1.41	1.43
22	23S1	1915	3TD	O4-C4	-2.08	1.18	1.23
22	23S1	1835	2MG	C6-N1	2.07	1.42	1.38
22	23S1	955	PSU	C1'-C5	2.06	1.54	1.50
22	23S1	1911	PSU	C1'-C5	2.05	1.54	1.50
1	16S1	516	PSU	C1'-C5	2.04	1.54	1.50
55	PTR1	37	2MG	C6-N1	2.04	1.42	1.38
22	23S1	745	1MG	C4-N9	-2.04	1.32	1.38
55	PTR1	54	5MU	C2-N3	2.04	1.41	1.38
53	SPE1	1	FME	CA-N	-2.02	1.43	1.46
34	L161	81	4D4	OB-CB	-2.01	1.39	1.43

All (271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1519	MA6	N1-C6-N6	-11.92	104.06	117.08
1	16S1	1518	MA6	N1-C6-N6	-11.76	104.23	117.08
22	23S1	2030	6MZ	C9-N6-C6	-7.60	116.33	122.87
22	23S1	2503	2MA	C5-C4-N3	-7.00	119.31	127.19
22	23S1	2445	2MG	C2-N3-C4	6.92	120.62	112.04
1	16S1	1518	MA6	C5-C6-N6	6.49	136.60	125.30
1	16S1	1516	2MG	C2-N3-C4	6.47	120.06	112.04
22	23S1	1835	2MG	C2-N3-C4	6.41	119.98	112.04
1	16S1	966	2MG	C2-N3-C4	6.39	119.97	112.04
1	16S1	1519	MA6	C5-C6-N6	6.36	136.38	125.30
55	PTR1	46	G7M	C1'-N9-C8	-6.29	105.51	126.74
1	16S1	1519	MA6	N1-C2-N3	-6.28	118.78	128.60
1	16S1	1207	2MG	C2-N3-C4	6.18	119.70	112.04
55	PTR1	37	2MG	C2-N3-C4	6.13	119.64	112.04
1	16S1	1518	MA6	N1-C2-N3	-6.03	119.17	128.60
22	23S1	1618	6MZ	N1-C2-N3	-6.01	119.19	128.60
55	PTR1	46	G7M	C1'-N9-C4	5.92	144.08	126.50
22	23S1	2552	OMU	C4-N3-C2	-5.86	118.85	126.58
22	23S1	2030	6MZ	N1-C2-N3	-5.81	119.51	128.60
1	16S1	527	G7M	C1'-N9-C8	-5.71	107.45	126.74
55	PTR1	8	4SU	C4-N3-C2	-5.62	121.88	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1618	6MZ	C5-C4-N3	-5.53	119.54	126.75
1	16S1	527	G7M	C1'-N9-C4	5.49	142.81	126.50
22	23S1	745	1MG	C5-C4-N3	-5.31	119.85	128.46
1	16S1	1498	UR3	C4-N3-C2	-5.30	119.57	124.56
22	23S1	2069	G7M	C1'-N9-C8	-5.09	109.56	126.74
22	23S1	2580	PSU	C4-N3-C2	-5.09	119.01	126.34
22	23S1	1915	3TD	N1-C2-N3	5.09	120.15	116.14
22	23S1	2457	PSU	N1-C2-N3	5.07	120.88	115.13
22	23S1	2580	PSU	N1-C2-N3	5.01	120.81	115.13
22	23S1	2445	2MG	C2-N1-C6	-5.01	118.72	124.48
22	23S1	746	PSU	C4-N3-C2	-5.00	119.14	126.34
22	23S1	1911	PSU	C4-N3-C2	-4.98	119.17	126.34
22	23S1	2445	2MG	C5-C4-N3	-4.93	120.46	128.46
1	16S1	1516	2MG	C2-N1-C6	-4.93	118.80	124.48
22	23S1	2503	2MA	N9-C8-N7	-4.88	107.24	113.91
1	16S1	1516	2MG	C5-C4-N3	-4.86	120.58	128.46
55	PTR1	37	2MG	C5-C4-N3	-4.84	120.60	128.46
22	23S1	1835	2MG	C2-N1-C6	-4.82	118.93	124.48
22	23S1	2503	2MA	N3-C4-N9	4.82	133.67	126.99
22	23S1	2030	6MZ	N9-C8-N7	-4.79	107.36	113.91
22	23S1	2457	PSU	C4-N3-C2	-4.79	119.44	126.34
55	PTR1	55	PSU	C4-N3-C2	-4.78	119.45	126.34
1	16S1	966	2MG	C5-C4-N3	-4.78	120.71	128.46
22	23S1	955	PSU	C4-N3-C2	-4.78	119.46	126.34
22	23S1	746	PSU	N1-C2-N3	4.77	120.54	115.13
22	23S1	1835	2MG	C5-C4-N3	-4.76	120.74	128.46
22	23S1	2069	G7M	C1'-N9-C4	4.75	140.61	126.50
1	16S1	1518	MA6	N9-C8-N7	-4.74	107.44	113.91
22	23S1	2251	OMG	C5-C4-N3	-4.69	120.86	128.46
22	23S1	1618	6MZ	N9-C8-N7	-4.68	107.51	113.91
22	23S1	955	PSU	N1-C2-N3	4.66	120.41	115.13
1	16S1	1519	MA6	C5-C4-N3	-4.63	120.71	126.75
22	23S1	1911	PSU	N1-C2-N3	4.63	120.38	115.13
22	23S1	1618	6MZ	C9-N6-C6	-4.57	118.94	122.87
55	PTR1	8	4SU	C5-C4-N3	4.57	118.93	114.69
1	16S1	1518	MA6	C5-C4-N3	-4.56	120.80	126.75
55	PTR1	37	2MG	C2-N1-C6	-4.55	119.24	124.48
22	23S1	2030	6MZ	C5-C4-N3	-4.53	120.84	126.75
1	16S1	1519	MA6	N9-C8-N7	-4.48	107.78	113.91
22	23S1	2605	PSU	C4-N3-C2	-4.46	119.91	126.34
22	23S1	2604	PSU	C4-N3-C2	-4.43	119.96	126.34
55	PTR1	55	PSU	N1-C2-N3	4.32	120.03	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1207	2MG	C5-C4-N3	-4.28	121.52	128.46
1	16S1	516	PSU	C4-N3-C2	-4.26	120.19	126.34
22	23S1	2504	PSU	N1-C2-N3	4.26	119.96	115.13
22	23S1	2504	PSU	C4-N3-C2	-4.24	120.22	126.34
22	23S1	2251	OMG	C2-N3-C4	4.23	119.84	112.30
1	16S1	966	2MG	C2-N1-C6	-4.20	119.65	124.48
22	23S1	2069	G7M	C2-N3-C4	4.18	119.75	112.30
1	16S1	1207	2MG	C2-N1-C6	-4.16	119.69	124.48
22	23S1	2604	PSU	N1-C2-N3	4.15	119.83	115.13
22	23S1	2552	OMU	N3-C2-N1	4.08	120.30	114.89
1	16S1	527	G7M	C2-N3-C4	4.00	119.42	112.30
22	23S1	2069	G7M	C5-C6-N1	3.99	120.11	111.79
1	16S1	527	G7M	C5-C6-N1	3.97	120.09	111.79
55	PTR1	46	G7M	C2-N3-C4	3.97	119.38	112.30
55	PTR1	46	G7M	C5-C6-N1	3.97	120.08	111.79
22	23S1	1618	6MZ	C2-N3-C4	3.96	121.10	111.75
1	16S1	1519	MA6	C2-N1-C6	3.94	121.05	111.75
22	23S1	1917	PSU	C4-N3-C2	-3.91	120.70	126.34
1	16S1	1518	MA6	C2-N1-C6	3.90	120.97	111.75
22	23S1	2605	PSU	N1-C2-N3	3.87	119.52	115.13
22	23S1	1618	6MZ	N3-C4-N9	3.85	133.43	127.08
1	16S1	516	PSU	N1-C2-N3	3.82	119.46	115.13
1	16S1	966	2MG	C1'-N9-C8	-3.82	115.83	126.70
22	23S1	1915	3TD	C4-N3-C2	-3.76	120.53	124.61
22	23S1	2552	OMU	C5-C4-N3	3.76	120.46	114.84
22	23S1	745	1MG	C2-N3-C4	3.73	120.37	111.98
1	16S1	1519	MA6	C2-N3-C4	3.68	120.44	111.75
22	23S1	2251	OMG	O3'-C3'-C2'	3.67	121.58	111.17
22	23S1	747	5MU	C6-C5-C4	3.65	121.08	118.03
22	23S1	745	1MG	N9-C4-N3	3.65	133.27	125.94
22	23S1	1917	PSU	N1-C2-N3	3.64	119.25	115.13
12	S121	89	D2T	CB1-SB-CB	3.63	109.00	102.44
1	16S1	1518	MA6	C4-C5-C6	3.55	119.85	115.88
22	23S1	2457	PSU	C6-N1-C2	-3.54	119.06	122.68
22	23S1	2503	2MA	C5-N7-C8	3.53	108.52	103.51
1	16S1	1518	MA6	C2-N3-C4	3.51	120.05	111.75
55	PTR1	37	2MG	C1'-N9-C8	-3.50	116.73	126.70
25	L031	150	MEQ	CG-CD-NE2	3.49	121.13	116.29
22	23S1	1962	5MC	C5-C6-N1	-3.41	119.83	123.34
22	23S1	955	PSU	C6-N1-C2	-3.40	119.21	122.68
22	23S1	2030	6MZ	C2-N3-C4	3.35	119.66	111.75
22	23S1	1618	6MZ	C4-C5-C6	3.35	119.40	116.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2504	PSU	C6-N1-C2	-3.34	119.27	122.68
1	16S1	1518	MA6	C5-N7-C8	3.33	108.24	103.51
22	23S1	2580	PSU	C6-C5-C4	3.33	120.53	118.20
22	23S1	2069	G7M	CN7-N7-C5	3.27	130.84	126.77
22	23S1	745	1MG	N9-C8-N7	-3.27	107.23	113.39
22	23S1	2580	PSU	C6-N1-C2	-3.26	119.35	122.68
22	23S1	1618	6MZ	C5-N7-C8	3.23	108.10	103.51
1	16S1	1519	MA6	C4-C5-C6	3.22	119.48	115.88
55	PTR1	54	5MU	C4-N3-C2	-3.20	123.20	127.35
22	23S1	2069	G7M	O6-C6-C5	-3.19	120.87	128.06
22	23S1	746	PSU	C6-N1-C2	-3.18	119.43	122.68
22	23S1	2251	OMG	N9-C8-N7	-3.18	107.39	113.39
1	16S1	527	G7M	C5-C4-N3	-3.16	122.09	128.15
1	16S1	966	2MG	C1'-N9-C4	3.16	135.88	126.50
22	23S1	1835	2MG	C1'-N9-C8	-3.16	117.71	126.70
55	PTR1	55	PSU	O2-C2-N1	-3.15	119.32	122.79
22	23S1	1917	PSU	C6-N1-C2	-3.14	119.48	122.68
22	23S1	2457	PSU	C6-C5-C4	3.13	120.39	118.20
22	23S1	2580	PSU	O2-C2-N1	-3.13	119.35	122.79
22	23S1	2030	6MZ	C4-N9-C8	3.13	109.12	105.73
55	PTR1	32	RSP	S2-C2-N3	-3.11	116.09	121.49
12	S121	89	D2T	OD2-CG-CB	3.10	119.85	113.15
22	23S1	1939	5MU	C4-N3-C2	-3.08	123.37	127.35
22	23S1	746	PSU	C6-C5-C4	3.07	120.34	118.20
22	23S1	2445	2MG	N9-C8-N7	-3.07	107.61	113.39
1	16S1	967	5MC	C5-C6-N1	-3.07	120.18	123.34
1	16S1	1519	MA6	C5-N7-C8	3.06	107.86	103.51
1	16S1	527	G7M	O6-C6-C5	-3.04	121.20	128.06
22	23S1	747	5MU	C4-N3-C2	-3.03	123.42	127.35
55	PTR1	55	PSU	C6-C5-C4	3.03	120.32	118.20
1	16S1	1516	2MG	N9-C8-N7	-3.03	107.69	113.39
22	23S1	2030	6MZ	C5-N7-C8	3.03	107.81	103.51
22	23S1	2552	OMU	O4-C4-C5	-3.02	119.85	125.16
22	23S1	2445	2MG	C1'-N9-C8	-3.00	118.16	126.70
55	PTR1	8	4SU	N3-C2-N1	3.00	118.87	114.89
55	PTR1	37	2MG	C1'-N9-C4	2.99	135.37	126.50
1	16S1	1516	2MG	CM2-N2-C2	-2.98	117.28	123.86
1	16S1	1207	2MG	N9-C8-N7	-2.98	107.79	113.39
22	23S1	2445	2MG	C5-C6-N1	2.96	120.70	113.19
22	23S1	955	PSU	O2-C2-N1	-2.94	119.55	122.79
22	23S1	1618	6MZ	C4-N9-C8	2.94	108.91	105.73
22	23S1	1835	2MG	N9-C8-N7	-2.93	107.86	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1911	PSU	C6-C5-C4	2.93	120.25	118.20
1	16S1	1402	4OC	O2-C2-N3	-2.93	117.57	122.33
1	16S1	1516	2MG	C5-C6-N1	2.92	120.59	113.19
22	23S1	2251	OMG	C2-N1-C6	-2.90	119.81	125.10
22	23S1	2030	6MZ	N3-C4-N9	2.89	131.85	127.08
55	PTR1	8	4SU	C5-C4-S4	-2.89	120.74	124.47
55	PTR1	46	G7M	C5-C4-N3	-2.89	122.61	128.15
22	23S1	2503	2MA	C1'-N9-C8	-2.89	120.61	127.14
22	23S1	1911	PSU	C6-N1-C2	-2.89	119.73	122.68
1	16S1	1519	MA6	N3-C4-N9	2.88	131.82	127.08
1	16S1	966	2MG	N9-C4-N3	2.87	131.71	125.94
22	23S1	2445	2MG	CM2-N2-C2	-2.87	117.52	123.86
22	23S1	2069	G7M	CN7-N7-C8	-2.87	120.42	124.84
22	23S1	1835	2MG	CM2-N2-C2	-2.87	117.53	123.86
1	16S1	527	G7M	C2-N1-C6	-2.86	119.89	125.10
55	PTR1	46	G7M	O6-C6-C5	-2.86	121.62	128.06
22	23S1	1939	5MU	C6-C5-C4	2.85	120.42	118.03
1	16S1	1518	MA6	N3-C4-N9	2.85	131.78	127.08
1	16S1	516	PSU	C6-C5-C4	2.85	120.19	118.20
22	23S1	2503	2MA	C4-N9-C8	2.83	108.80	105.73
22	23S1	2498	OMC	O2-C2-N3	-2.83	117.73	122.33
1	16S1	966	2MG	N9-C8-N7	-2.83	108.06	113.39
1	16S1	1518	MA6	C4-N9-C8	2.83	108.79	105.73
22	23S1	2030	6MZ	C4-C5-C6	2.82	119.00	116.81
22	23S1	2503	2MA	N3-C2-N1	-2.82	120.53	125.72
22	23S1	2251	OMG	O3'-C3'-C4'	2.82	119.20	111.05
55	PTR1	37	2MG	N9-C8-N7	-2.81	108.09	113.39
55	PTR1	46	G7M	CN7-N7-C5	2.81	130.25	126.77
1	16S1	966	2MG	O6-C6-C5	-2.81	119.15	126.60
22	23S1	2069	G7M	N2-C2-N1	2.79	122.66	116.71
1	16S1	966	2MG	C5-C6-N1	2.76	120.21	113.19
22	23S1	2604	PSU	C6-N1-C2	-2.76	119.86	122.68
22	23S1	1835	2MG	O6-C6-C5	-2.75	119.31	126.60
1	16S1	527	G7M	CN7-N7-C5	2.73	130.16	126.77
22	23S1	2251	OMG	C5-C6-N1	2.73	120.12	113.19
22	23S1	746	PSU	O2-C2-N1	-2.73	119.79	122.79
55	PTR1	32	RSP	C1'-N1-C2	2.71	124.44	118.44
22	23S1	1835	2MG	C5-C6-N1	2.71	120.07	113.19
22	23S1	745	1MG	C5-C6-N1	2.68	120.09	114.91
1	16S1	516	PSU	C6-N1-C2	-2.68	119.95	122.68
22	23S1	1835	2MG	C1'-N9-C4	2.68	134.45	126.50
55	PTR1	46	G7M	C2-N1-C6	-2.67	120.23	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1516	2MG	C1'-N9-C8	-2.67	119.11	126.70
1	16S1	1207	2MG	C5-C6-N1	2.66	119.95	113.19
1	16S1	966	2MG	N1-C2-N3	-2.66	119.84	123.95
55	PTR1	46	G7M	N9-C8-N7	-2.64	105.68	112.21
22	23S1	2251	OMG	N9-C4-N3	2.64	131.24	125.94
55	PTR1	55	PSU	C6-N1-C2	-2.64	119.99	122.68
55	PTR1	54	5MU	C6-C5-C4	2.63	120.23	118.03
22	23S1	2457	PSU	O2-C2-N1	-2.63	119.90	122.79
22	23S1	2069	G7M	C5-C4-N3	-2.62	123.12	128.15
22	23S1	2069	G7M	C2-N1-C6	-2.60	120.36	125.10
22	23S1	2069	G7M	N9-C8-N7	-2.60	105.78	112.21
1	16S1	1207	2MG	C1'-N9-C8	-2.60	119.30	126.70
55	PTR1	46	G7M	CN7-N7-C8	-2.59	120.84	124.84
55	PTR1	37	2MG	C5-C6-N1	2.56	119.70	113.19
1	16S1	527	G7M	CN7-N7-C8	-2.56	120.89	124.84
1	16S1	967	5MC	CM5-C5-C6	-2.56	119.44	122.85
1	16S1	1516	2MG	O6-C6-C5	-2.55	119.84	126.60
55	PTR1	37	2MG	N9-C4-N3	2.53	131.03	125.94
22	23S1	2030	6MZ	C4-N9-C1'	-2.53	120.56	126.59
22	23S1	2605	PSU	C6-N1-C2	-2.53	120.09	122.68
22	23S1	2445	2MG	C1'-N9-C4	2.53	134.01	126.50
22	23S1	1939	5MU	C5-C6-N1	-2.53	120.74	123.34
1	16S1	527	G7M	N9-C8-N7	-2.52	105.97	112.21
1	16S1	1519	MA6	C4-N9-C8	2.50	108.44	105.73
1	16S1	1402	4OC	C6-C5-C4	2.49	120.01	116.96
22	23S1	2445	2MG	O6-C6-C5	-2.49	120.00	126.60
1	16S1	1407	5MC	C5-C6-N1	-2.47	120.79	123.34
1	16S1	1207	2MG	N1-C2-N3	-2.46	120.15	123.95
1	16S1	1498	UR3	C6-N1-C2	-2.45	119.59	121.79
22	23S1	2069	G7M	C6-C5-N7	2.45	135.21	132.25
22	23S1	2445	2MG	N1-C2-N3	-2.44	120.18	123.95
34	L161	81	4D4	CG-CD-NE	-2.42	104.87	111.87
22	23S1	2580	PSU	O4'-C1'-C2'	2.42	108.55	105.14
22	23S1	745	1MG	C1'-N9-C4	-2.41	119.35	126.50
1	16S1	1207	2MG	O6-C6-C5	-2.39	120.25	126.60
22	23S1	2503	2MA	C6-C5-C4	2.39	120.39	117.18
1	16S1	1207	2MG	CM2-N2-C2	-2.38	118.61	123.86
22	23S1	2251	OMG	O6-C6-C5	-2.37	120.30	126.60
22	23S1	2251	OMG	C2'-C1'-N9	-2.37	109.62	114.22
55	PTR1	37	2MG	CM2-N2-C2	-2.37	118.63	123.86
22	23S1	2445	2MG	N9-C4-N3	2.36	130.67	125.94
22	23S1	2251	OMG	C3'-C2'-C1'	-2.34	98.50	102.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	PTR1	37	2MG	O6-C6-C5	-2.32	120.44	126.60
22	23S1	745	1MG	C8-N7-C5	2.25	108.30	104.24
22	23S1	2504	PSU	O2-C2-N1	-2.24	120.32	122.79
22	23S1	1835	2MG	N9-C4-N3	2.24	130.44	125.94
22	23S1	1962	5MC	CM5-C5-C6	-2.24	119.86	122.85
22	23S1	1911	PSU	O2-C2-N1	-2.24	120.33	122.79
1	16S1	1516	2MG	N1-C2-N3	-2.24	120.50	123.95
1	16S1	1516	2MG	N9-C4-N3	2.23	130.41	125.94
22	23S1	2604	PSU	C6-C5-C4	2.23	119.75	118.20
22	23S1	1618	6MZ	C5-C6-N1	2.21	120.56	118.20
1	16S1	1516	2MG	C1'-N9-C4	2.21	133.06	126.50
22	23S1	1835	2MG	N1-C2-N3	-2.19	120.56	123.95
55	PTR1	46	G7M	C6-C5-N7	2.18	134.89	132.25
22	23S1	1939	5MU	C5-C4-N3	2.18	117.17	115.31
1	16S1	1407	5MC	C5-C4-N3	-2.18	119.33	121.67
22	23S1	2445	2MG	C8-N7-C5	2.17	108.16	104.24
22	23S1	2069	G7M	N1-C2-N3	-2.16	119.29	123.32
55	PTR1	8	4SU	C1'-N1-C2	2.15	121.46	117.57
22	23S1	2251	OMG	C8-N7-C5	2.14	108.12	104.24
1	16S1	1407	5MC	O2-C2-N3	-2.12	118.89	122.33
22	23S1	2552	OMU	O2-C2-N1	-2.11	119.98	122.79
1	16S1	527	G7M	N2-C2-N1	2.10	121.18	116.71
55	PTR1	37	2MG	N1-C2-N3	-2.09	120.72	123.95
1	16S1	1516	2MG	C8-N7-C5	2.08	108.01	104.24
1	16S1	1518	MA6	C4-C5-N7	-2.06	108.11	110.62
55	PTR1	54	5MU	C5M-C5-C6	-2.05	120.11	122.85
22	23S1	2457	PSU	O4'-C1'-C2'	2.05	108.03	105.14
22	23S1	1835	2MG	C8-N7-C5	2.04	107.93	104.24
12	S12I	89	D2T	OD2-CG-OD1	-2.04	119.46	124.09
22	23S1	1917	PSU	C6-C5-C4	2.04	119.62	118.20
55	PTR1	46	G7M	N2-C2-N1	2.04	121.05	116.71
22	23S1	2605	PSU	C6-C5-C4	2.03	119.62	118.20
1	16S1	1207	2MG	C1'-N9-C4	2.03	132.53	126.50
55	PTR1	54	5MU	C5-C4-N3	2.02	117.04	115.31
1	16S1	516	PSU	O4'-C1'-C2'	2.02	108.00	105.14
1	16S1	1516	2MG	C4-C5-N7	-2.01	107.53	110.72
22	23S1	2445	2MG	C4-C5-N7	-2.01	107.53	110.72
1	16S1	516	PSU	O2-C2-N1	-2.01	120.58	122.79
22	23S1	747	5MU	C5-C6-N1	-2.01	121.28	123.34
22	23S1	1835	2MG	C4-C5-N7	-2.00	107.55	110.72

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16S1	527	G7M	O4'-C4'-C5'-O5'
1	16S1	527	G7M	C3'-C4'-C5'-O5'
1	16S1	966	2MG	O4'-C4'-C5'-O5'
1	16S1	966	2MG	C3'-C4'-C5'-O5'
1	16S1	1519	MA6	O4'-C4'-C5'-O5'
25	L031	150	MEQ	N-CA-CB-CG
25	L031	150	MEQ	C-CA-CB-CG
53	SPE1	1	FME	C-CA-CB-CG
55	PTR1	32	RSP	C3'-C4'-C5'-O5'
55	PTR1	54	5MU	C3'-C4'-C5'-O5'
22	23S1	2030	6MZ	O4'-C4'-C5'-O5'
22	23S1	2504	PSU	O4'-C4'-C5'-O5'
1	16S1	1519	MA6	C3'-C4'-C5'-O5'
22	23S1	2030	6MZ	C3'-C4'-C5'-O5'
22	23S1	2504	PSU	C3'-C4'-C5'-O5'
55	PTR1	32	RSP	O4'-C4'-C5'-O5'
53	SPE1	1	FME	N-CA-CB-CG
55	PTR1	54	5MU	O4'-C4'-C5'-O5'
34	L161	81	4D4	OB-CB-CG-CD
22	23S1	1939	5MU	C3'-C4'-C5'-O5'
22	23S1	1939	5MU	O4'-C4'-C5'-O5'
55	PTR1	46	G7M	C4'-C5'-O5'-P
12	S121	89	D2T	CG-CB-SB-CB1
22	23S1	2445	2MG	C3'-C4'-C5'-O5'
1	16S1	1402	4OC	O4'-C4'-C5'-O5'
34	L161	81	4D4	CA-CB-CG-CD
22	23S1	2069	G7M	C4'-C5'-O5'-P
53	SPE1	1	FME	CA-CB-CG-SD
22	23S1	2069	G7M	O4'-C4'-C5'-O5'
22	23S1	2503	2MA	C4'-C5'-O5'-P
55	PTR1	8	4SU	O4'-C4'-C5'-O5'
22	23S1	2251	OMG	C1'-C2'-O2'-CM2
1	16S1	1519	MA6	C5-C6-N6-C10
22	23S1	2580	PSU	O4'-C4'-C5'-O5'
22	23S1	746	PSU	O4'-C1'-C5-C6
22	23S1	2503	2MA	O4'-C4'-C5'-O5'
34	L161	81	4D4	O-C-CA-CB
53	SPE1	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1691 ligands modelled in this entry, 489 are monoatomic and 1201 are unknown - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	ORN	23S1	3001	-	7,8,8	0.76	0	8,9,9	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	ORN	23S1	3001	-	-	2/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	23S1	3001	ORN	N-CA-CB-CG
60	23S1	3001	ORN	C-CA-CB-CG

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	23S1	2
55	PTR1	1
10	S101	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	23S1	885:C	O3'	892:A	P	13.12
1	PTR1	46:G7M	O3'	48:C	P	5.31
1	23S1	2099:U	O3'	2100:G	P	4.47
1	S101	53:ILE	C	54:SER	N	1.18

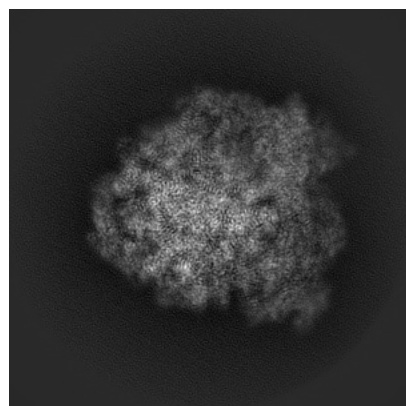
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10458. These allow visual inspection of the internal detail of the map and identification of artifacts.

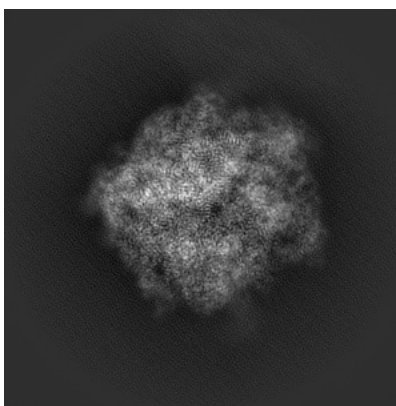
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

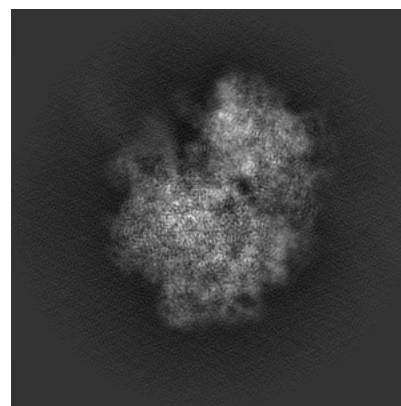
6.1.1 Primary map



X

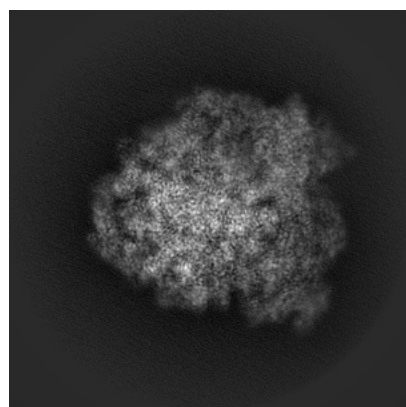


Y

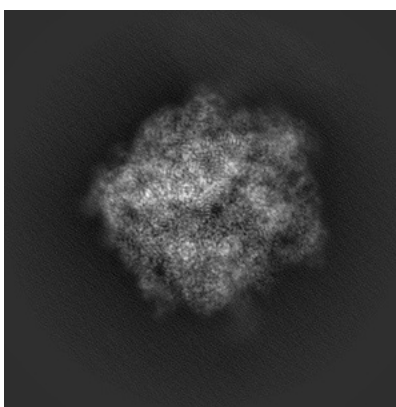


Z

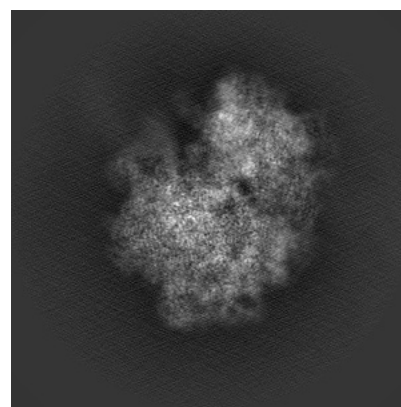
6.1.2 Raw map



X



Y

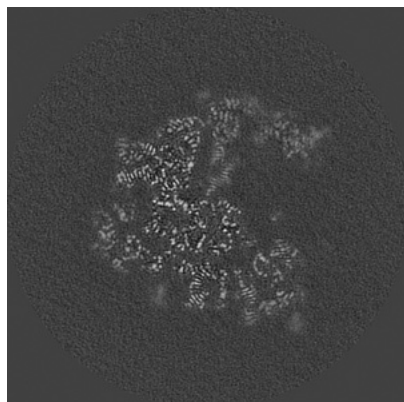


Z

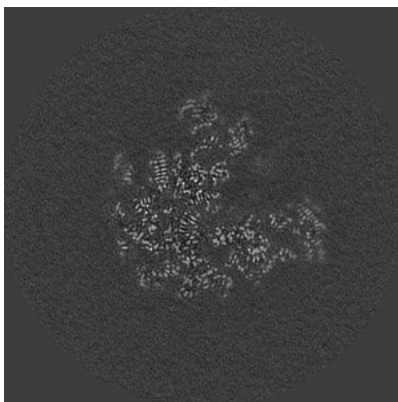
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

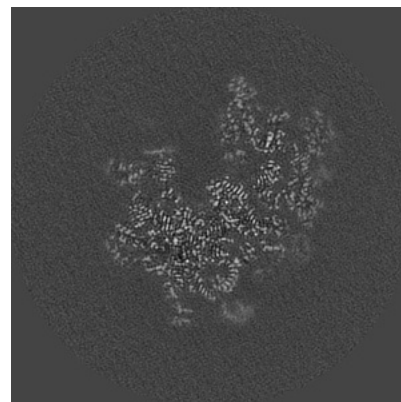
6.2.1 Primary map



X Index: 360

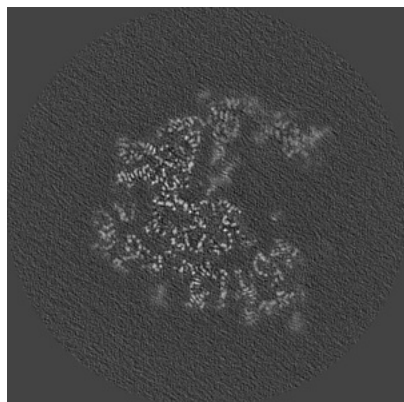


Y Index: 360

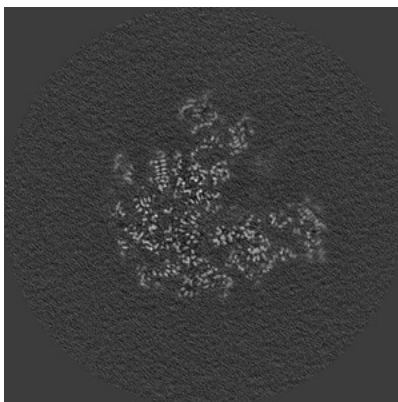


Z Index: 360

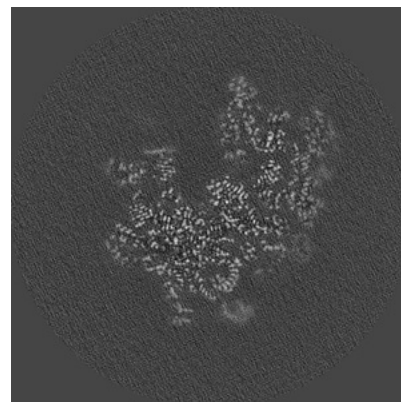
6.2.2 Raw map



X Index: 180



Y Index: 180

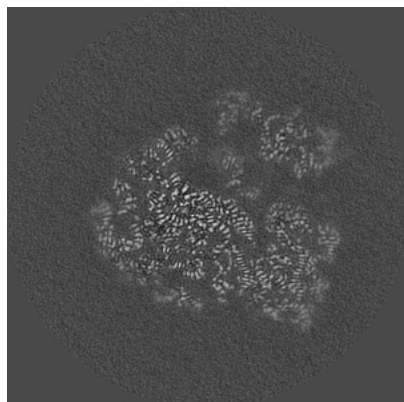


Z Index: 180

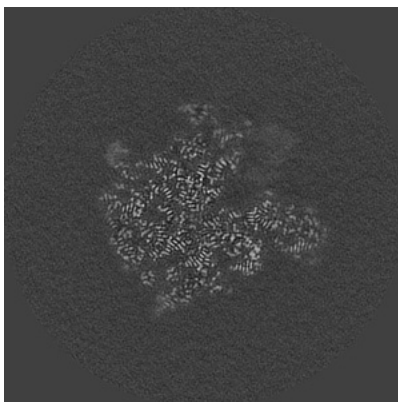
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

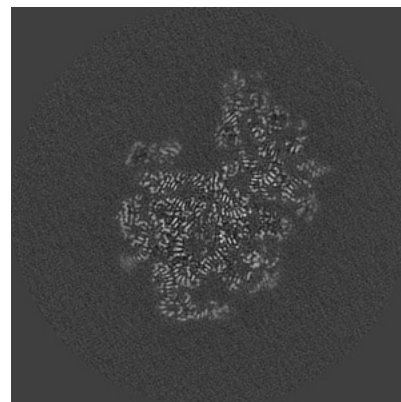
6.3.1 Primary map



X Index: 382

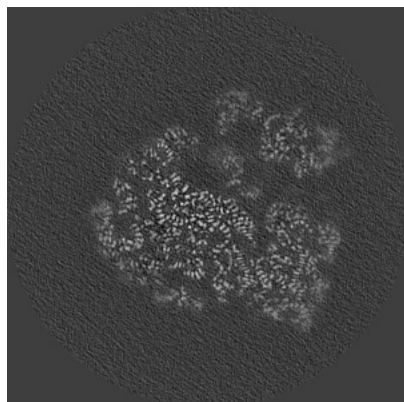


Y Index: 340

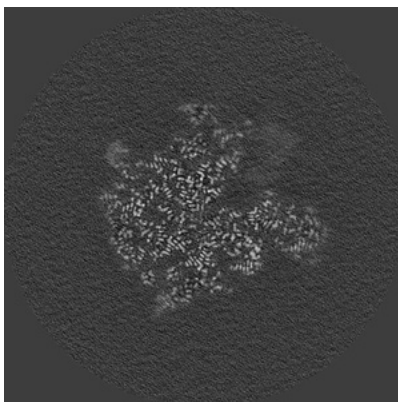


Z Index: 328

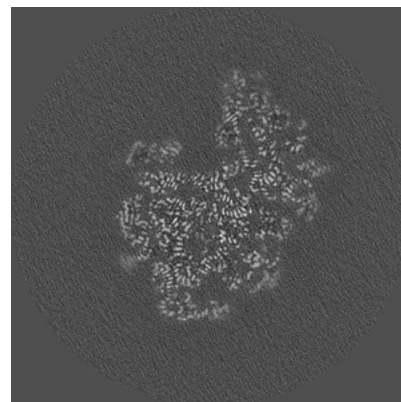
6.3.2 Raw map



X Index: 191



Y Index: 170

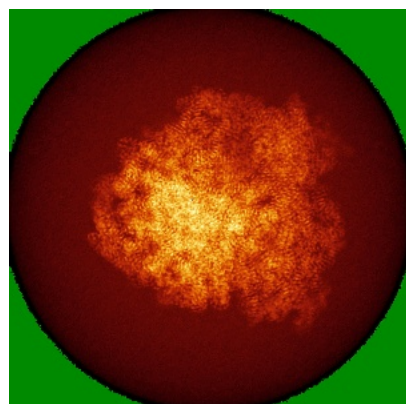


Z Index: 164

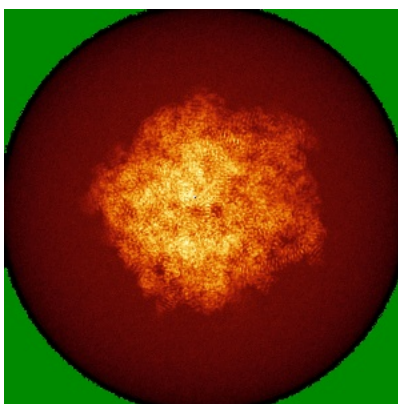
The images above show the largest variance slices of the map in three orthogonal directions.

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

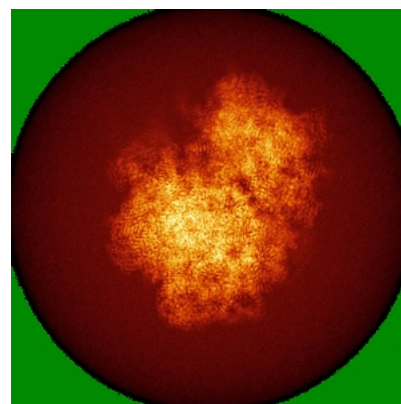
6.4.1 Primary map



X

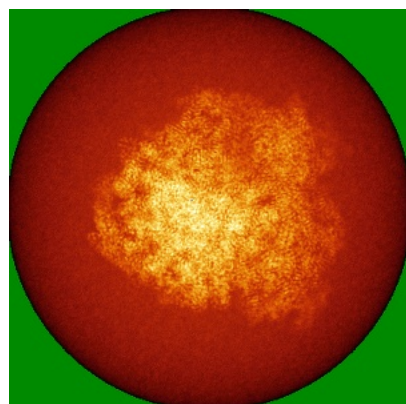


Y

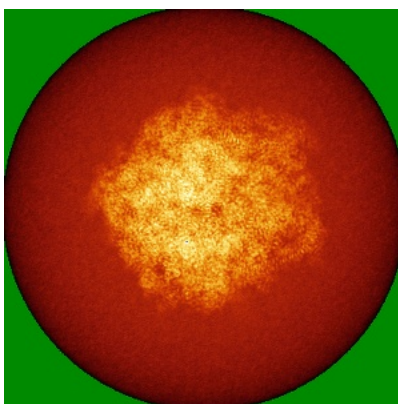


Z

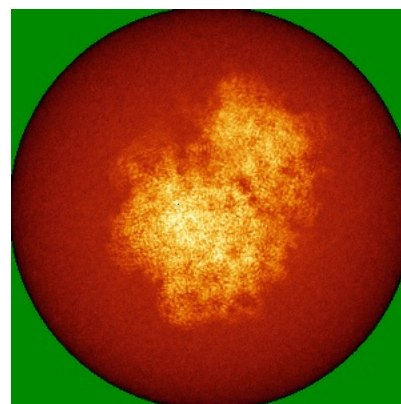
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

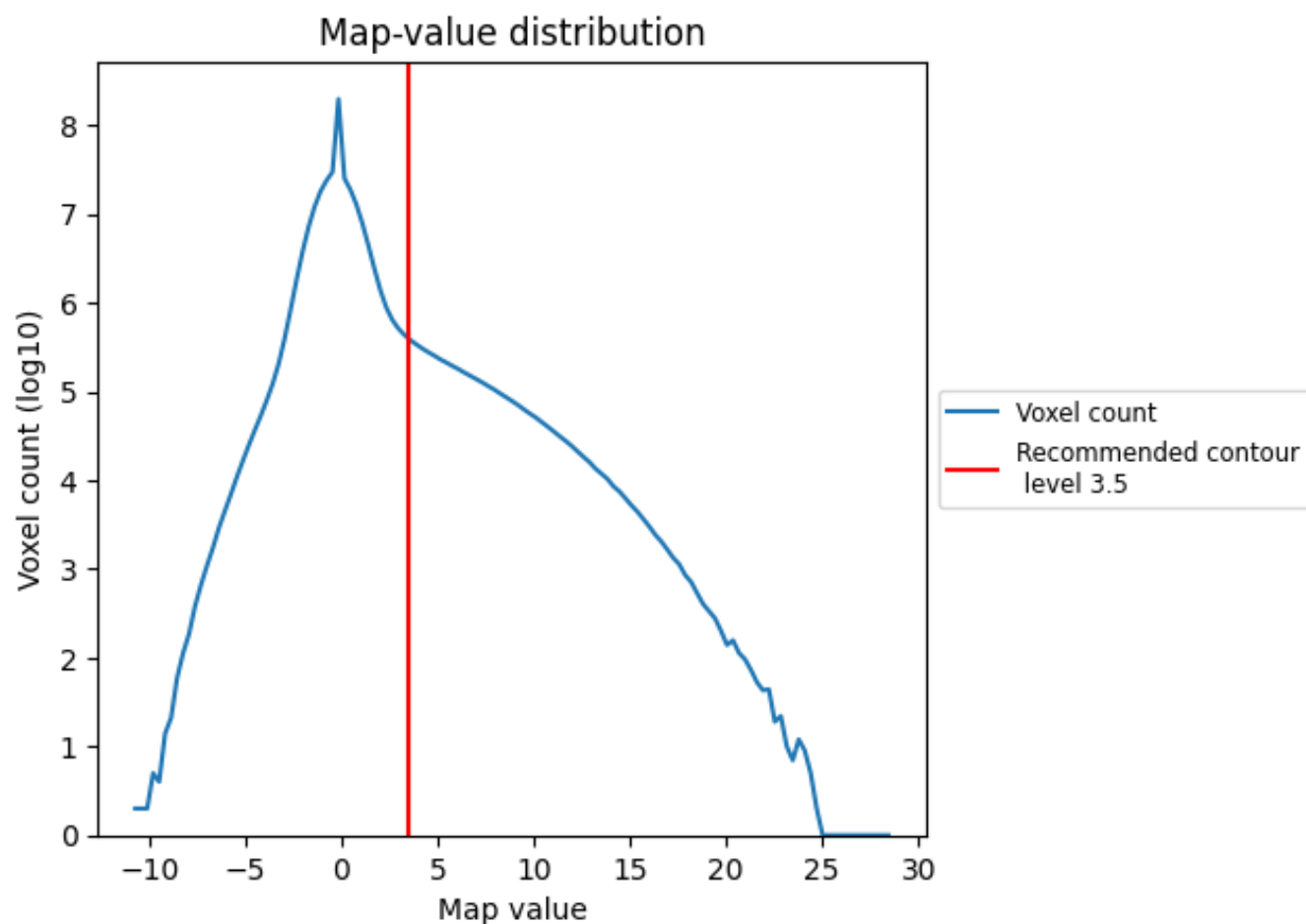
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

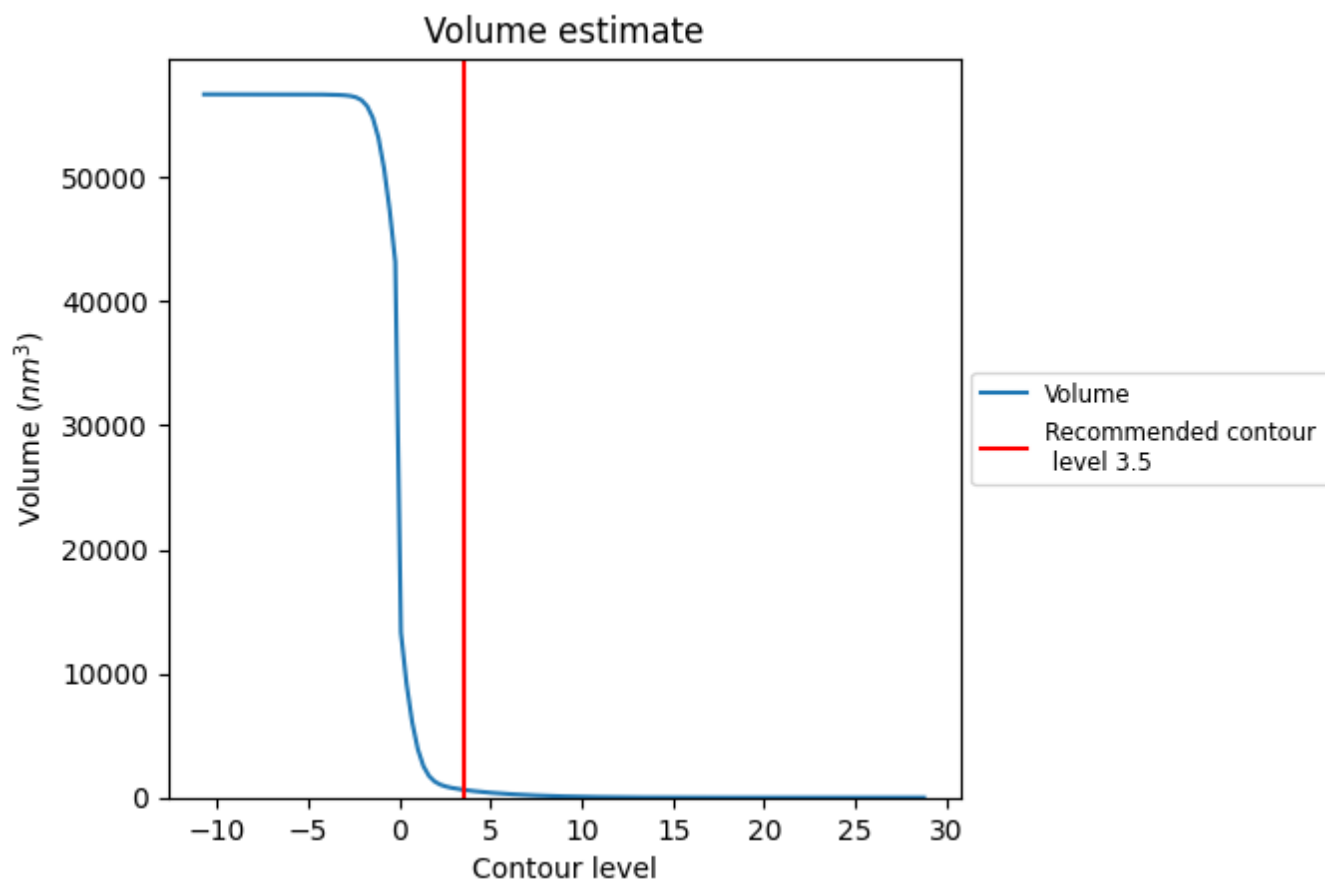
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

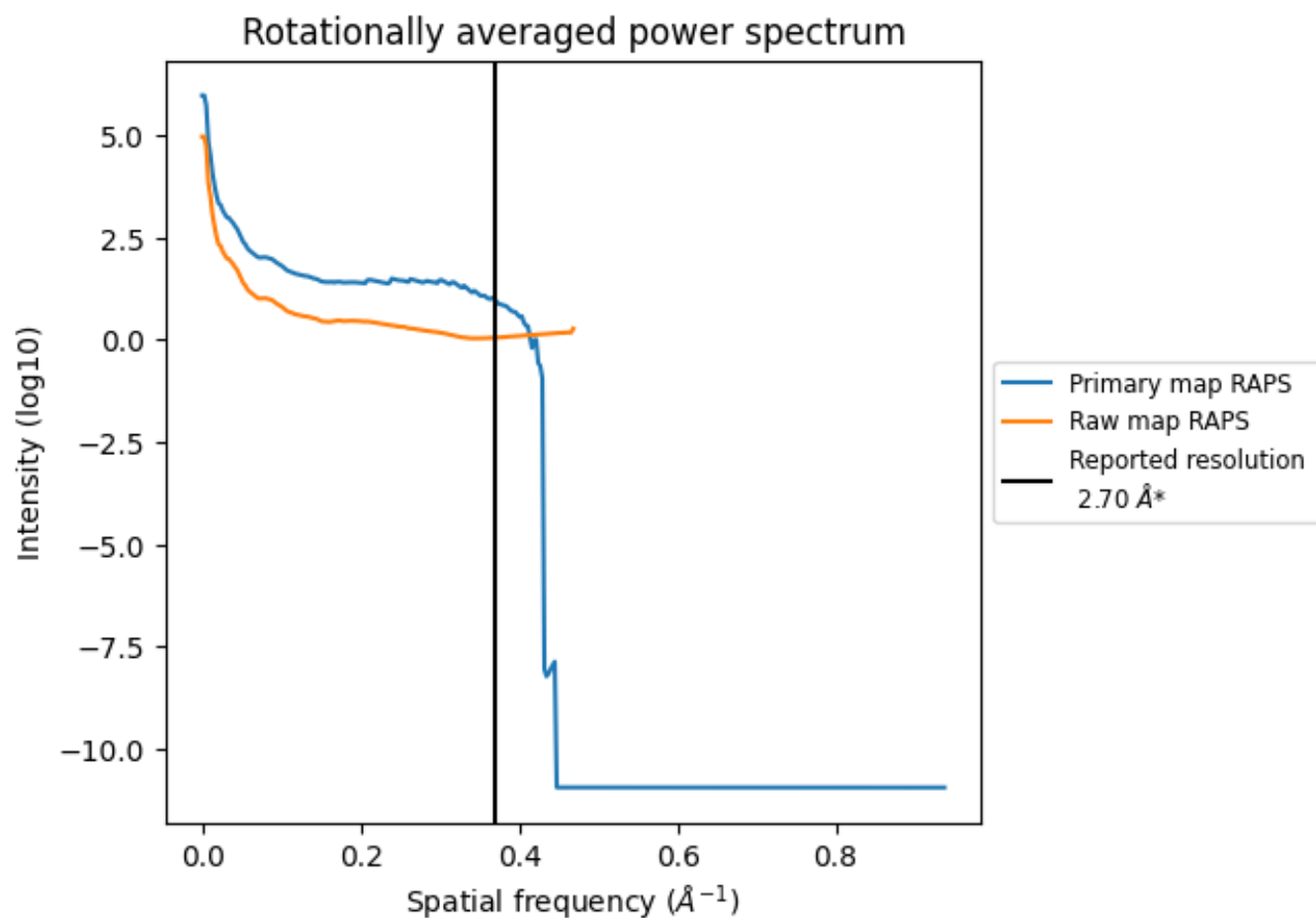
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 627 nm³; this corresponds to an approximate mass of 566 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

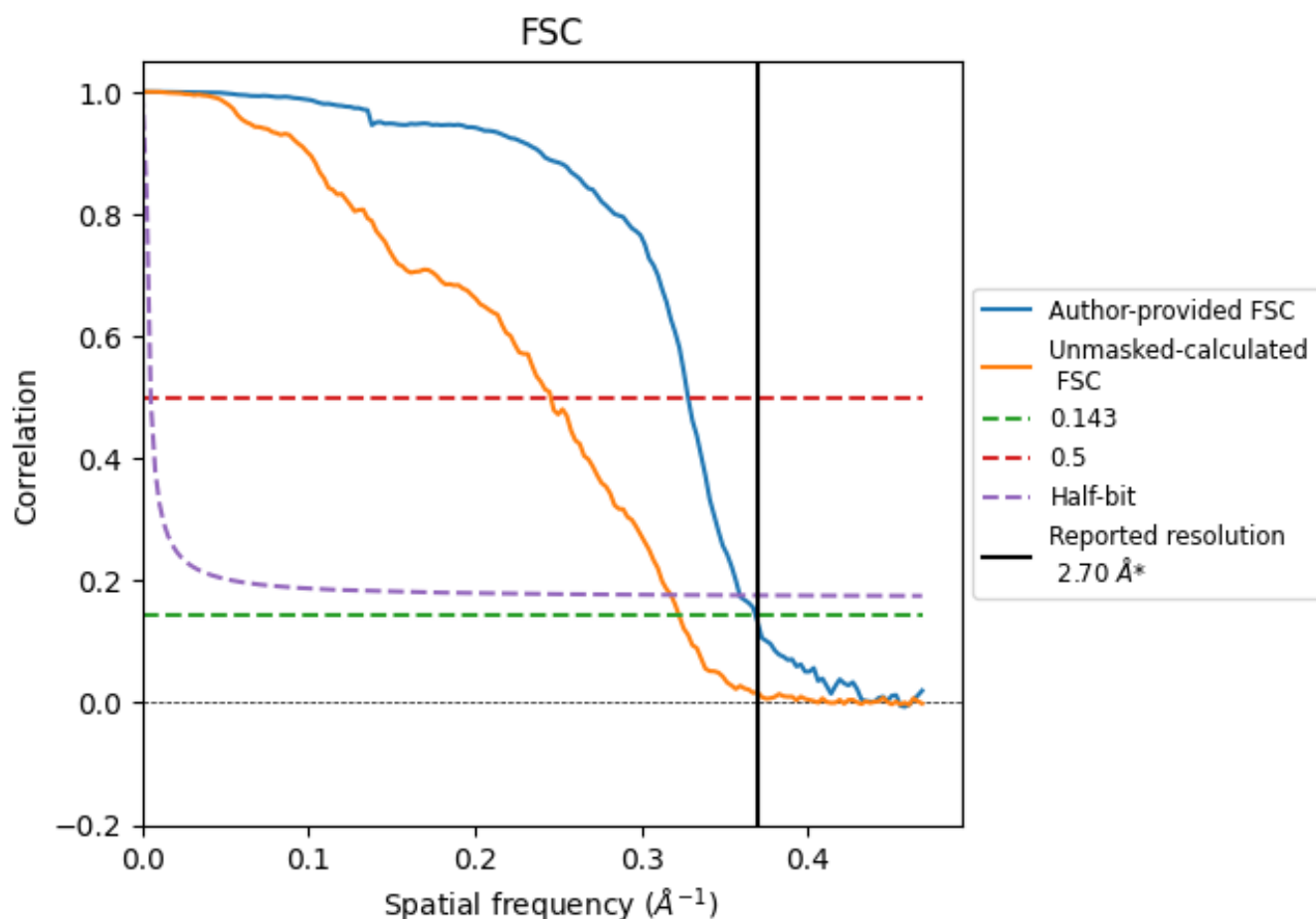


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

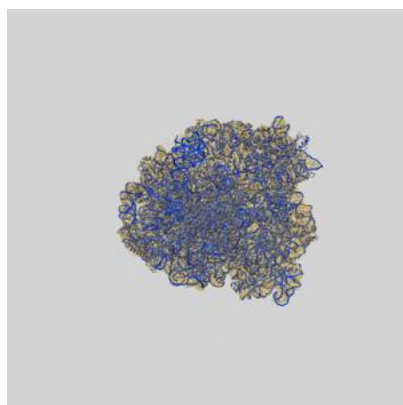
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.05	2.79
Unmasked-calculated*	3.10	4.07	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.10 differs from the reported value 2.7 by more than 10 %

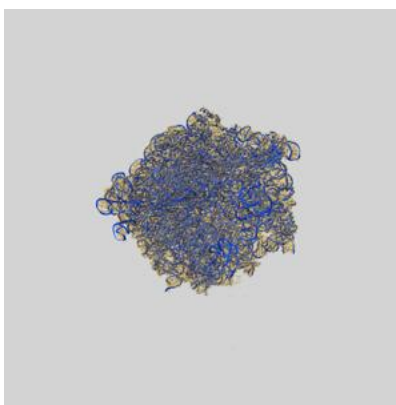
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10458 and PDB model 6TC3. Per-residue inclusion information can be found in section [3](#) on page [18](#).

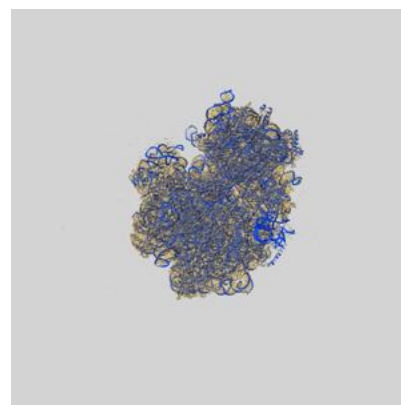
9.1 Map-model overlay [i](#)



X



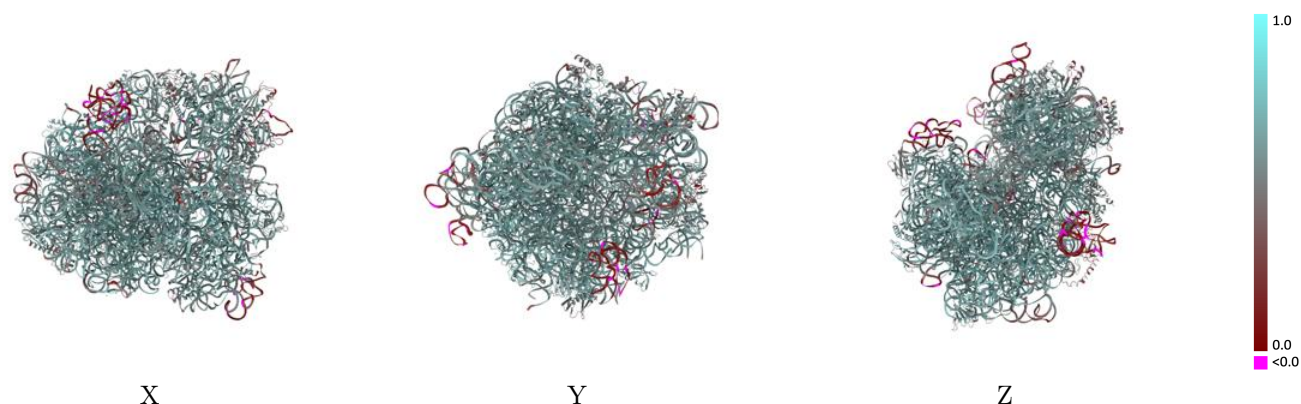
Y



Z

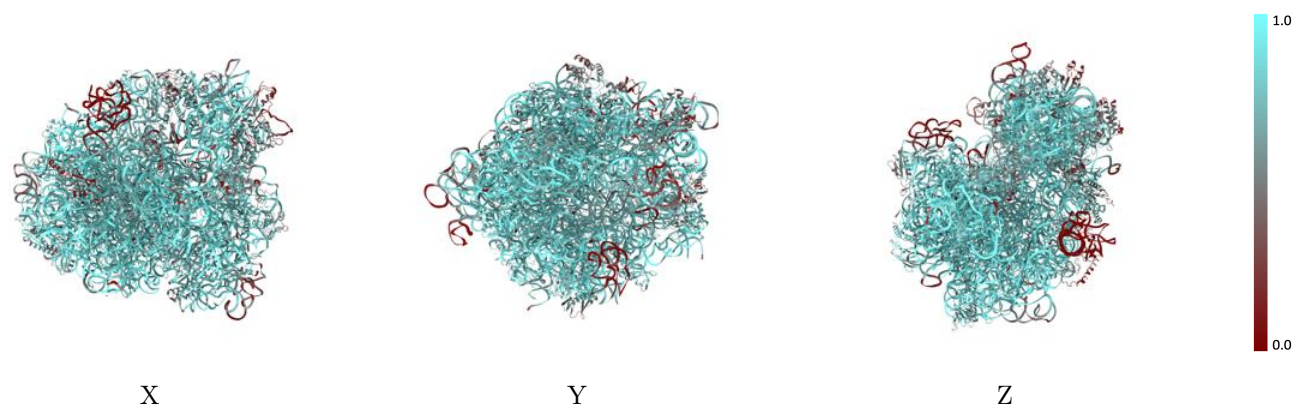
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



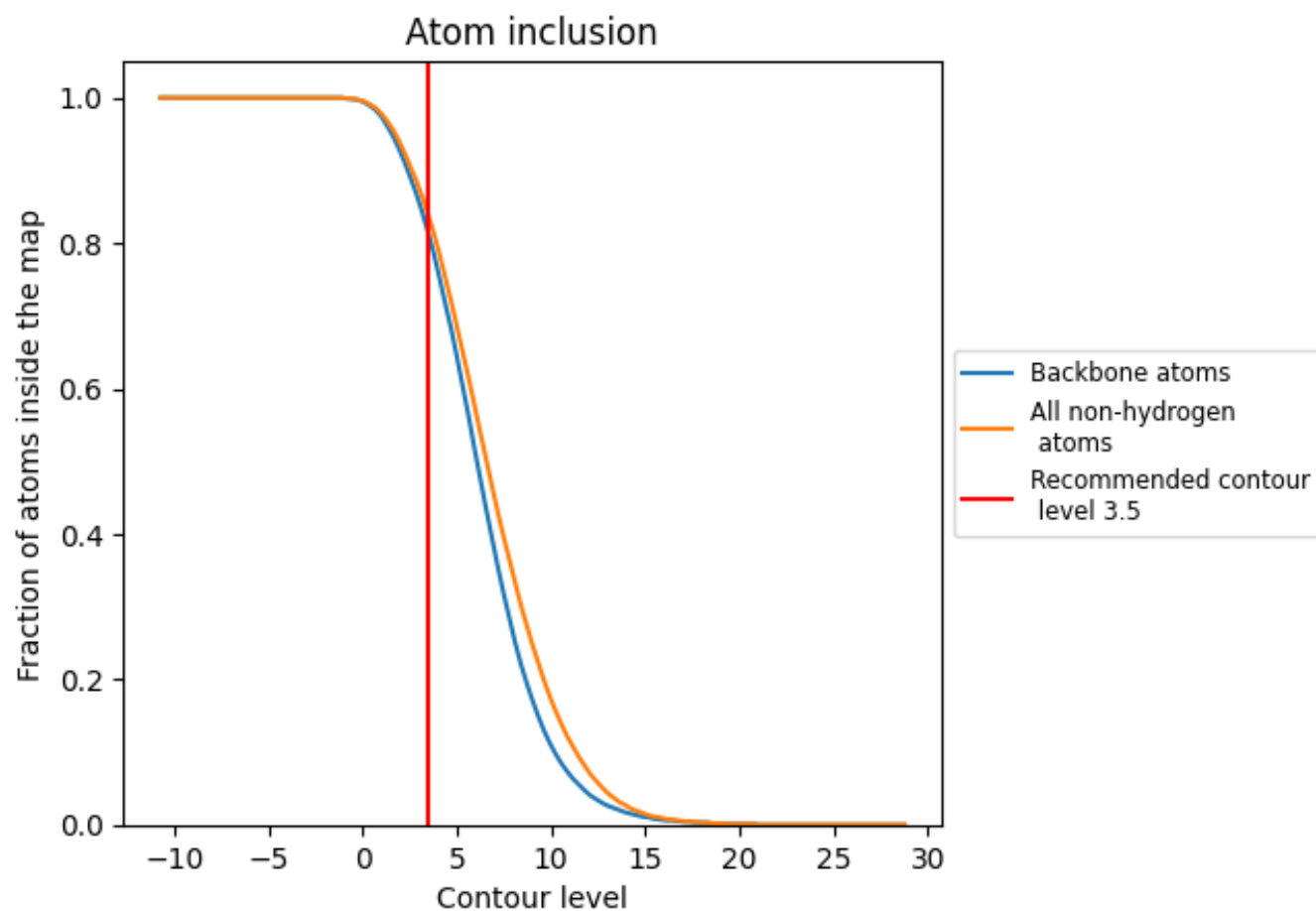
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 84% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.6020
05S1	 0.9050	 0.6180
16S1	 0.8790	 0.6030
23S1	 0.8960	 0.6160
L021	 0.9020	 0.6630
L031	 0.8800	 0.6530
L041	 0.8000	 0.6160
L051	 0.6400	 0.5350
L061	 0.6370	 0.5290
L091	 0.2050	 0.3810
L131	 0.8840	 0.6470
L141	 0.8640	 0.6510
L151	 0.8480	 0.6370
L161	 0.8590	 0.6390
L171	 0.9380	 0.6700
L181	 0.7710	 0.6020
L191	 0.8410	 0.6380
L201	 0.9220	 0.6640
L211	 0.8230	 0.6250
L221	 0.8640	 0.6440
L231	 0.7680	 0.5900
L241	 0.7300	 0.5800
L251	 0.7590	 0.5920
L271	 0.8820	 0.6430
L281	 0.8380	 0.6400
L291	 0.6890	 0.5660
L301	 0.8510	 0.6220
L311	 0.3520	 0.3840
L321	 0.8330	 0.6260
L331	 0.7490	 0.6070
L341	 0.9170	 0.6640
L351	 0.9130	 0.6680
L361	 0.8500	 0.6190
MRN1	 0.7010	 0.5430
PTR1	 0.7090	 0.5300



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Chain	Atom inclusion	Q-score
S021	 0.5180	 0.5090
S031	 0.7040	 0.5640
S041	 0.6380	 0.5630
S051	 0.7930	 0.6000
S061	 0.6250	 0.5330
S071	 0.5120	 0.4950
S081	 0.7860	 0.6080
S091	 0.6450	 0.5400
S101	 0.5050	 0.4980
S111	 0.7100	 0.5750
S121	 0.7610	 0.5930
S131	 0.6420	 0.5290
S141	 0.6770	 0.5250
S151	 0.7870	 0.5880
S161	 0.7400	 0.5820
S171	 0.6520	 0.5520
S181	 0.7940	 0.5970
S191	 0.6310	 0.5290
S201	 0.7340	 0.5800
S211	 0.4140	 0.4880
SPE1	 0.7480	 0.6620