Full wwPDB EM Validation Report

Mar 10, 2025 – 02:26 PM EDT

PDB ID	:	9N2C
EMDB ID	:	EMD-48831
Title	:	Impacts of ribosomal RNA sequence variation on gene expression and phenotype: Cryo-EM structure of the rrsH ribosome (HBB-70S)
Authors	:	Welfer, G.A.; Brady, R.A.; Natchiar, S.K.; Watson, Z.L.; Rundlet, E.J.; Alejo, J.L.; Singh, A.P.; Mishra, N.K.; Altman, R.B.; Blanchard, S.C.
Deposited on	:	2025-01-28
Resolution	:	2.40 Å(reported)
Based on initial model	:	7N1P

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 (i) 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 (1)) were used in the production of this report:

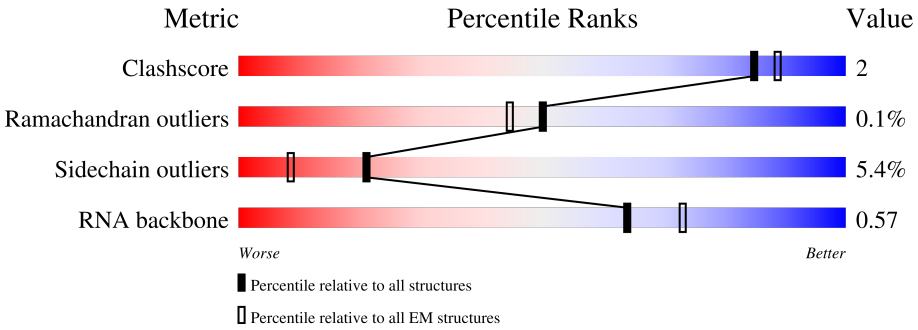
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	16	1542	74% 23%
2	SB	241	6% 82% 12% 5%
3	SC	233	77% 12% 9%
4	SD	206	88% 10%
5	SE	167	85% 10% 5%
6	SF	135	70% 7% 21%
7	SG	179	6% 70% 17% 13%

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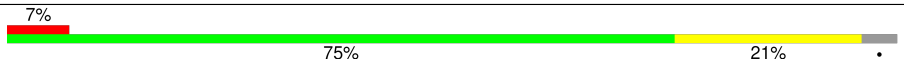
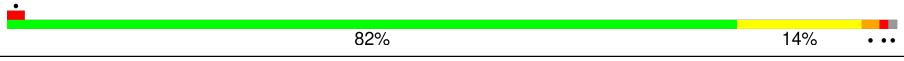
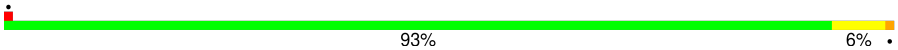
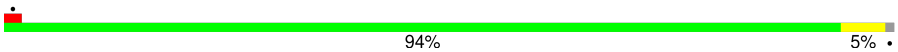
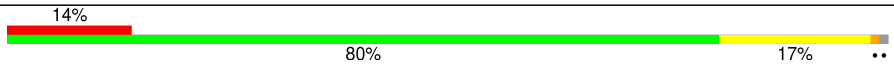
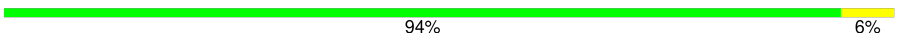
Mol	Chain	Length	Quality of chain
8	SH	130	
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120	
25	LB	273	
26	LC	209	
27	LD	201	
28	LE	179	
29	LF	177	
30	LI	149	
31	LM	142	
32	LN	123	

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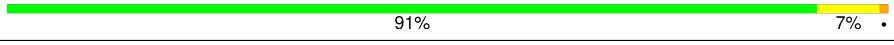
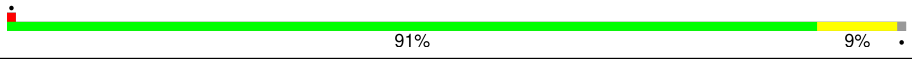
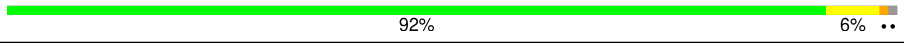
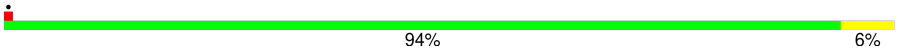
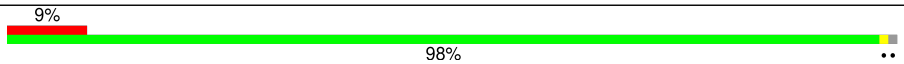
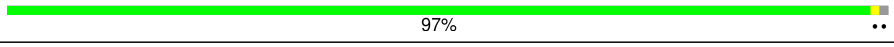
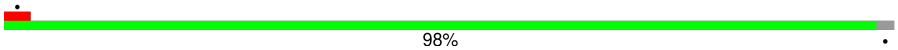
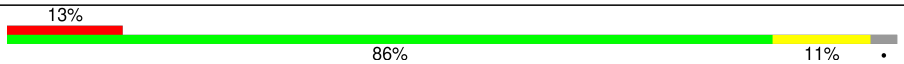
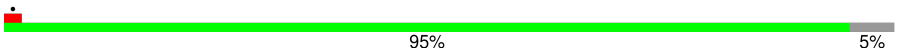
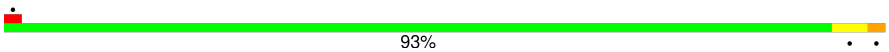
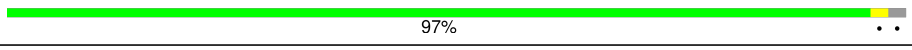
Mol	Chain	Length	Quality of chain
33	LO	144	
34	LP	136	
35	LQ	127	
36	LR	117	
37	LS	115	
38	LT	118	
39	LU	103	
40	LV	110	
41	LW	100	
42	LX	104	
43	LY	94	
44	La	85	
45	Lb	78	
46	Lc	63	
47	Ld	59	
48	Le	70	
49	Lf	57	
50	Lg	55	
51	Lh	46	
52	Li	65	
53	Lj	38	
54	Pt	77	

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 142570 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 ribosomal RNA (rRNA) from the rrnH operon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	16	1542	33087	14765	6058	10722	1542	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	229	1787	1129	320	330	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SC	212	1658	1049	311	294	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SE	158	1166	725	220	215	6	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SG	156	Total	C	N	O	S	1	0
			1244	778	241	221	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	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	SI	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	SJ	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SK	118	Total	C	N	O	S	1	0
			895	551	178	163	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SK	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SL	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	SM	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SO	88	Total	C	N	O	S	0	0
			713	439	144	129	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SP	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	SQ	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	SR	67	Total	C	N	O	S	0	0
			555	351	106	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SS	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ST	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 22 is a RNA chain called Synthetic messenger RNA (mRNA) 60 bp in length.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	mR	18	Total	C	N	O	P	0	0
			390	174	74	124	18		

- Molecule 23 is a RNA chain called 23S ribosomal RNA (rRNA) from the rrnB operon.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	23	2768	Total	C	N	O	P	0	0
			59447	26525	10946	19208	2768		

- Molecule 24 is a RNA chain called 5S large subunit ribosomal RNA of the H operon.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5	120	Total	C	N	O	P	0	0
			2572	1145	470	837	120		

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LC	209	Total	C	N	O	S	0	0
			1564	979	288	293	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LE	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LF	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LI	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LM	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	LN	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LO	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	LP	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LQ	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LS	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	LT	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	LU	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 40 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LV	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	LW	95	Total	C	N	O	S	0	0
			757	479	141	135	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LY	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	La	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lb	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	Lc	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Le	68	Total	C	N	O	S	0	0
			533	330	101	96	6		

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	Lg	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

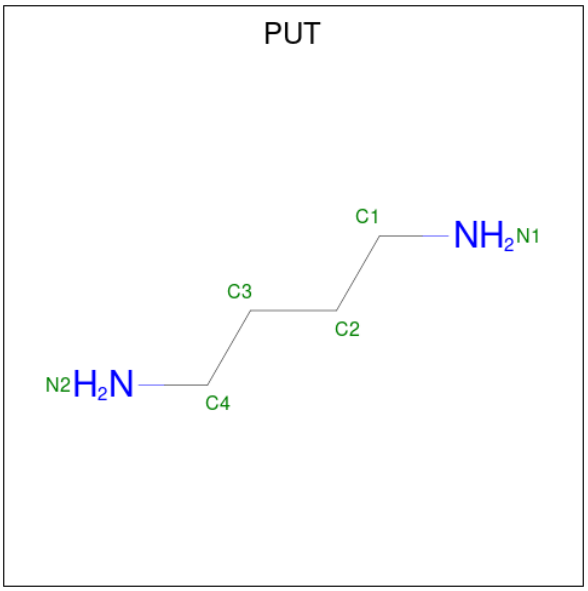
- Molecule 53 is a protein called 50S ribosomal protein L36.

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

- Molecule 54 is a RNA chain called N-formyl-methionine initiator tRNA (fMet-tRNAfMet).

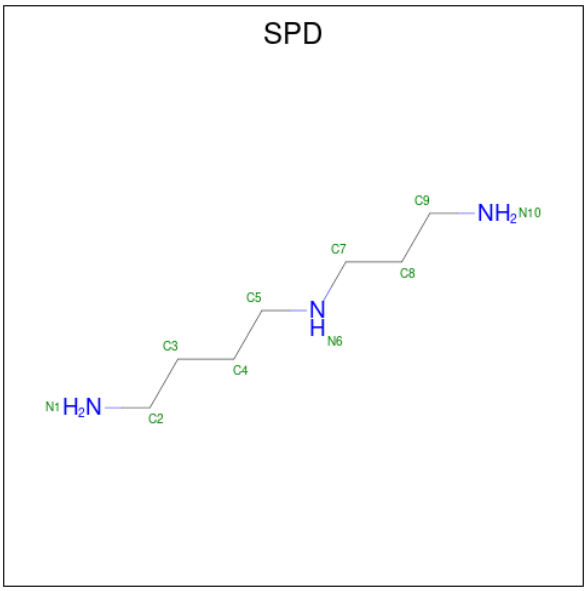
Mol	Chain	Residues	Atoms						AltConf	Trace
54	Pt	77	Total	C	N	O	P	S	0	0
			1646	734	298	536	77	1		

- Molecule 55 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms	AltConf
55	16	1	Total C N 6 4 2	0
55	23	1	Total C N 6 4 2	0
55	23	1	Total C N 6 4 2	0
55	23	1	Total C N 6 4 2	0
55	23	1	Total C N 6 4 2	0
55	23	1	Total C N 6 4 2	0
55	23	1	Total C N 6 4 2	0
55	23	1	Total C N 6 4 2	0
55	23	1	Total C N 6 4 2	0
55	23	1	Total C N 6 4 2	0

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



Mol	Chain	Residues	Atoms	AltConf
56	16	1	Total C N 10 7 3	0
56	23	1	Total C N 10 7 3	0
56	23	1	Total C N 10 7 3	0
56	23	1	Total C N 10 7 3	0
56	23	1	Total C N 10 7 3	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
57	16	74	Total Mg 74 74	0
57	mR	2	Total Mg 2 2	0
57	23	194	Total Mg 194 194	0
57	5	4	Total Mg 4 4	0
57	LB	3	Total Mg 3 3	0
57	LD	1	Total Mg 1 1	0
57	LE	1	Total Mg 1 1	0

Continued on next page...

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Mol	Chain	Residues	Atoms	AltConf
57	LO	1	Total Mg 1 1	0
57	LT	1	Total Mg 1 1	0
57	Lf	1	Total Mg 1 1	0
57	Pt	1	Total Mg 1 1	0

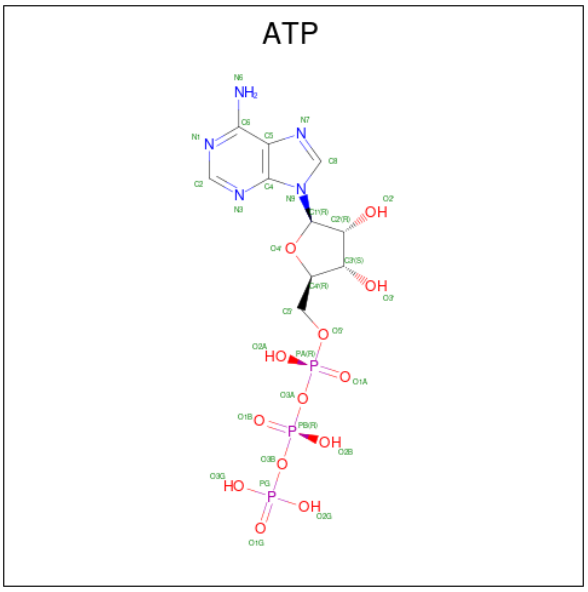
- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
58	16	9	Total K 9 9	0
58	23	39	Total K 39 39	0
58	LB	1	Total K 1 1	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

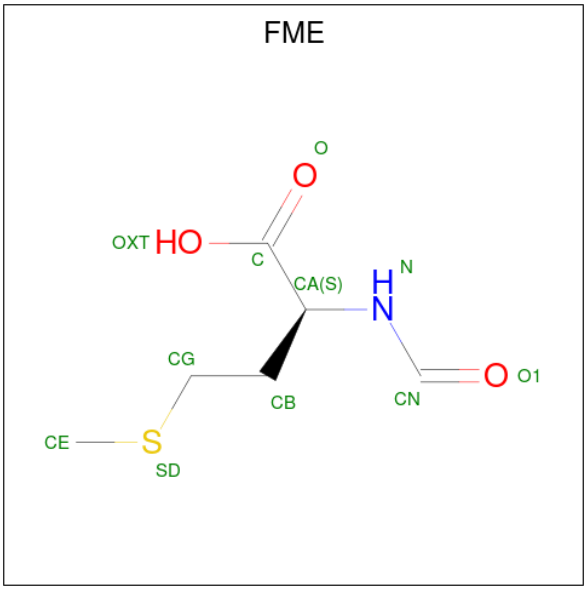
Mol	Chain	Residues	Atoms	AltConf
59	SB	1	Total Zn 1 1	0
59	Le	1	Total Zn 1 1	0
59	Lj	1	Total Zn 1 1	0

- Molecule 60 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
60	23	1	Total	C	N	O	P	0
			31	10	5	13	3	
60	23	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 61 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



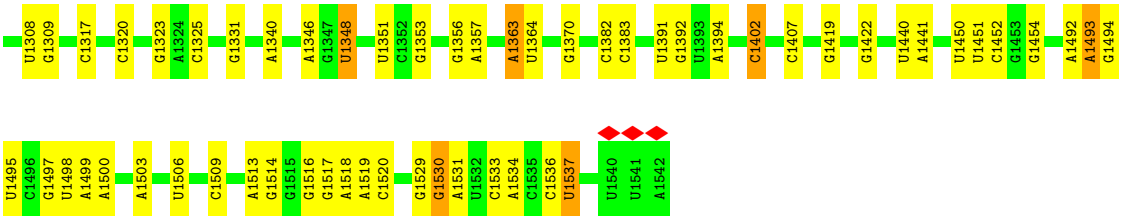
Mol	Chain	Residues	Atoms					AltConf
61	Pt	1	Total	C	N	O	S	0
			10	6	1	2	1	

3 Residue-property plots (i)

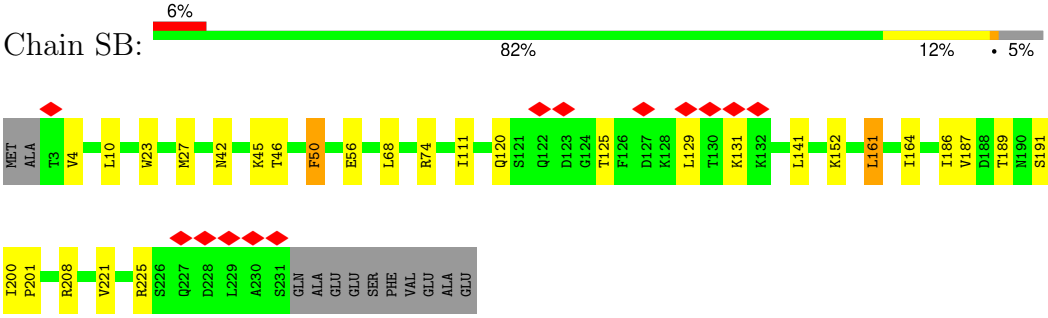
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 16S ribosomal RNA (rRNA) from the rrnH operon

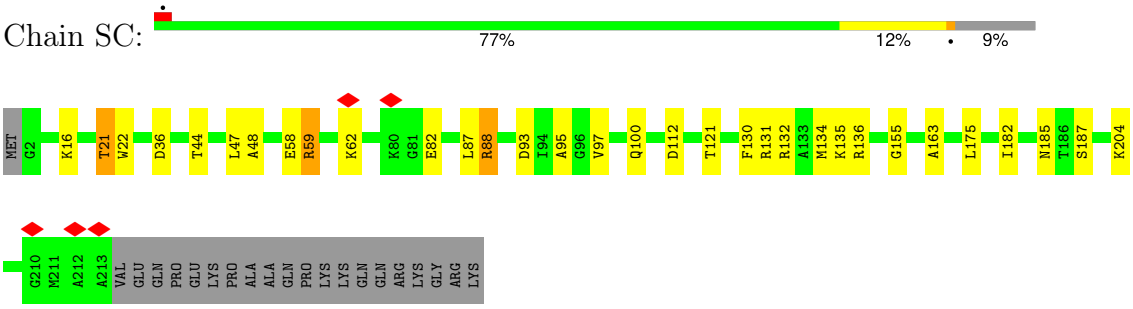
Chain 16:



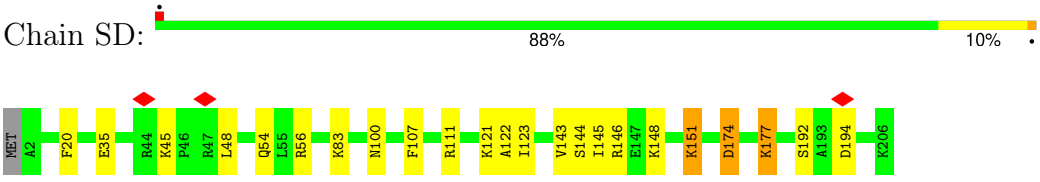
• Molecule 2: 30S ribosomal protein S2



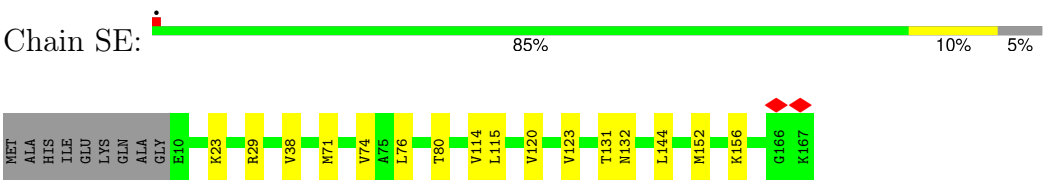
• Molecule 3: 30S ribosomal protein S3



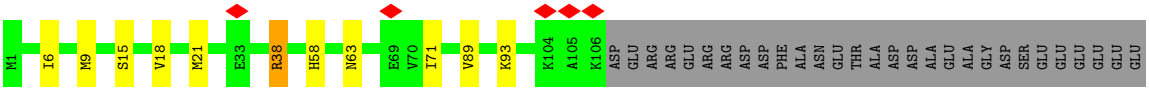
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

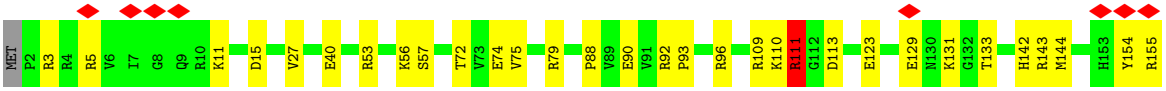


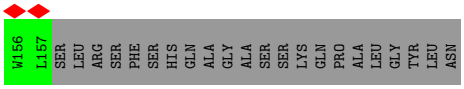
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

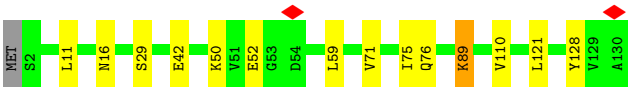
Chain SG:





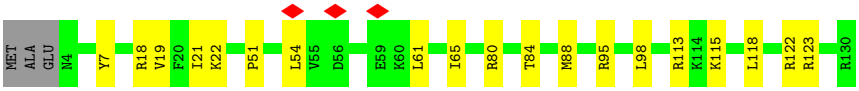
• Molecule 8: 30S ribosomal protein S8

Chain SH:



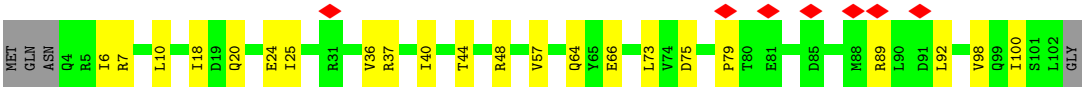
• Molecule 9: 30S ribosomal protein S9

Chain SI:



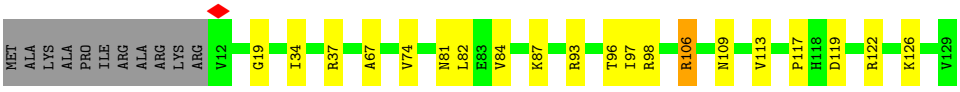
• Molecule 10: 30S ribosomal protein S10

Chain SJ:



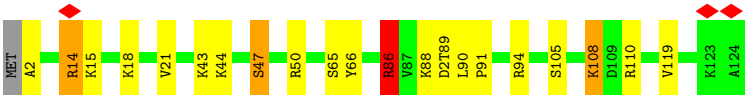
• Molecule 11: Small ribosomal subunit protein uS11

Chain SK:



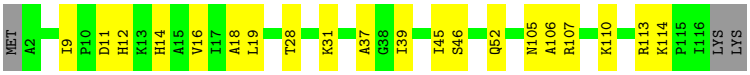
• Molecule 12: Small ribosomal subunit protein uS12

Chain SL:



• Molecule 13: 30S ribosomal protein S13

Chain SM:

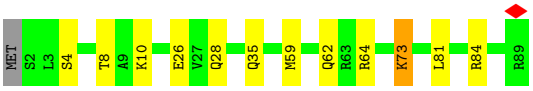


• Molecule 14: 30S ribosomal protein S14

Chain SN:

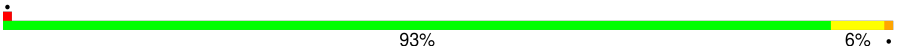
• Molecule 15: 30S ribosomal protein S15

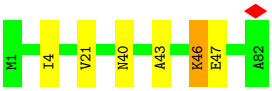
Chain SO:



• Molecule 16: 30S ribosomal protein S16

Chain SP:



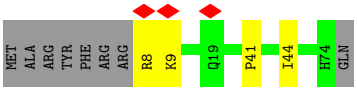


• Molecule 17: 30S ribosomal protein S17

Chain SQ:

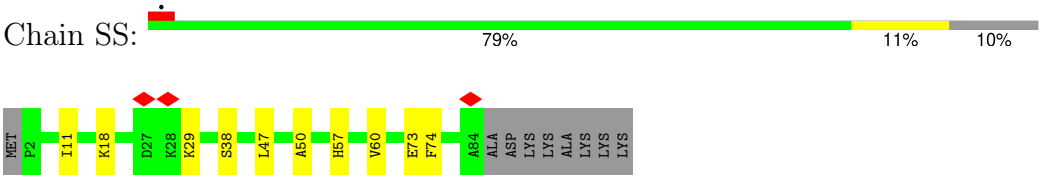
• Molecule 18: 30S ribosomal protein S18

Chain SR:



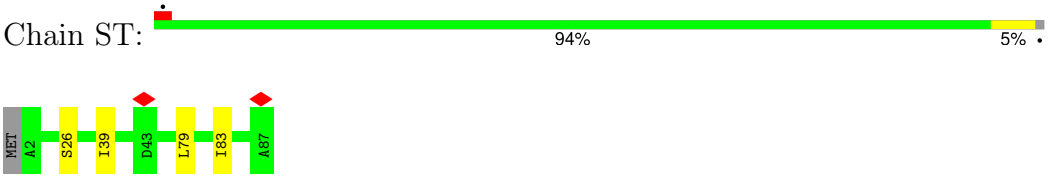
• Molecule 19: 30S ribosomal protein S19

Chain SS:



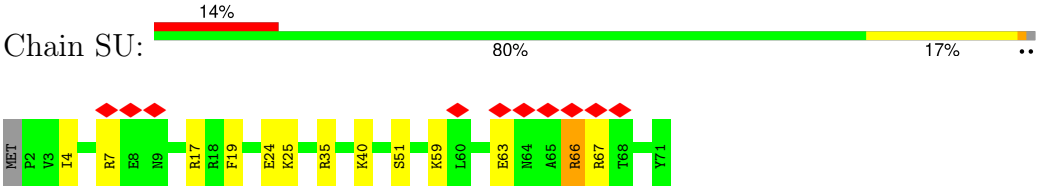
• Molecule 20: 30S ribosomal protein S20

Chain ST:



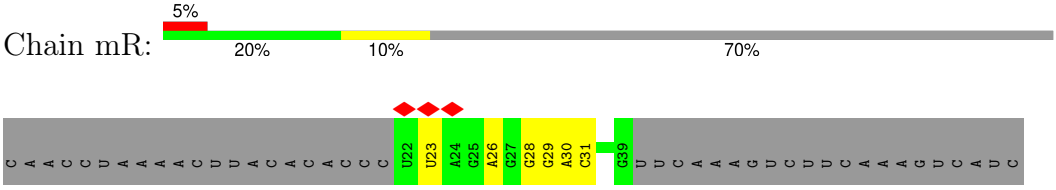
• Molecule 21: 30S ribosomal protein S21

Chain SU:



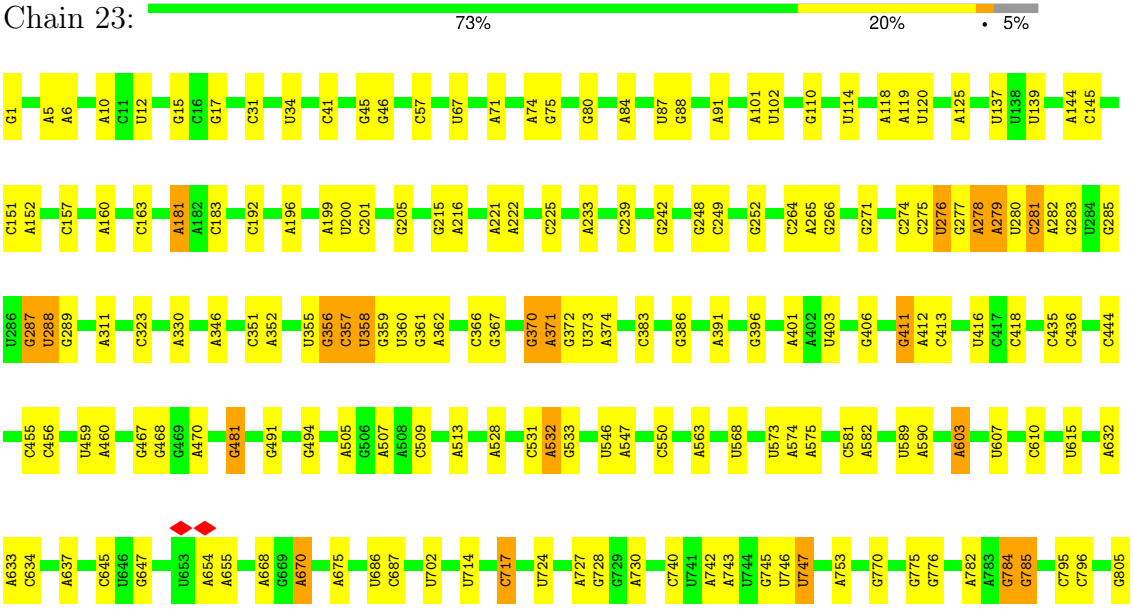
• Molecule 22: Synthetic messenger RNA (mRNA) 60 bp in length

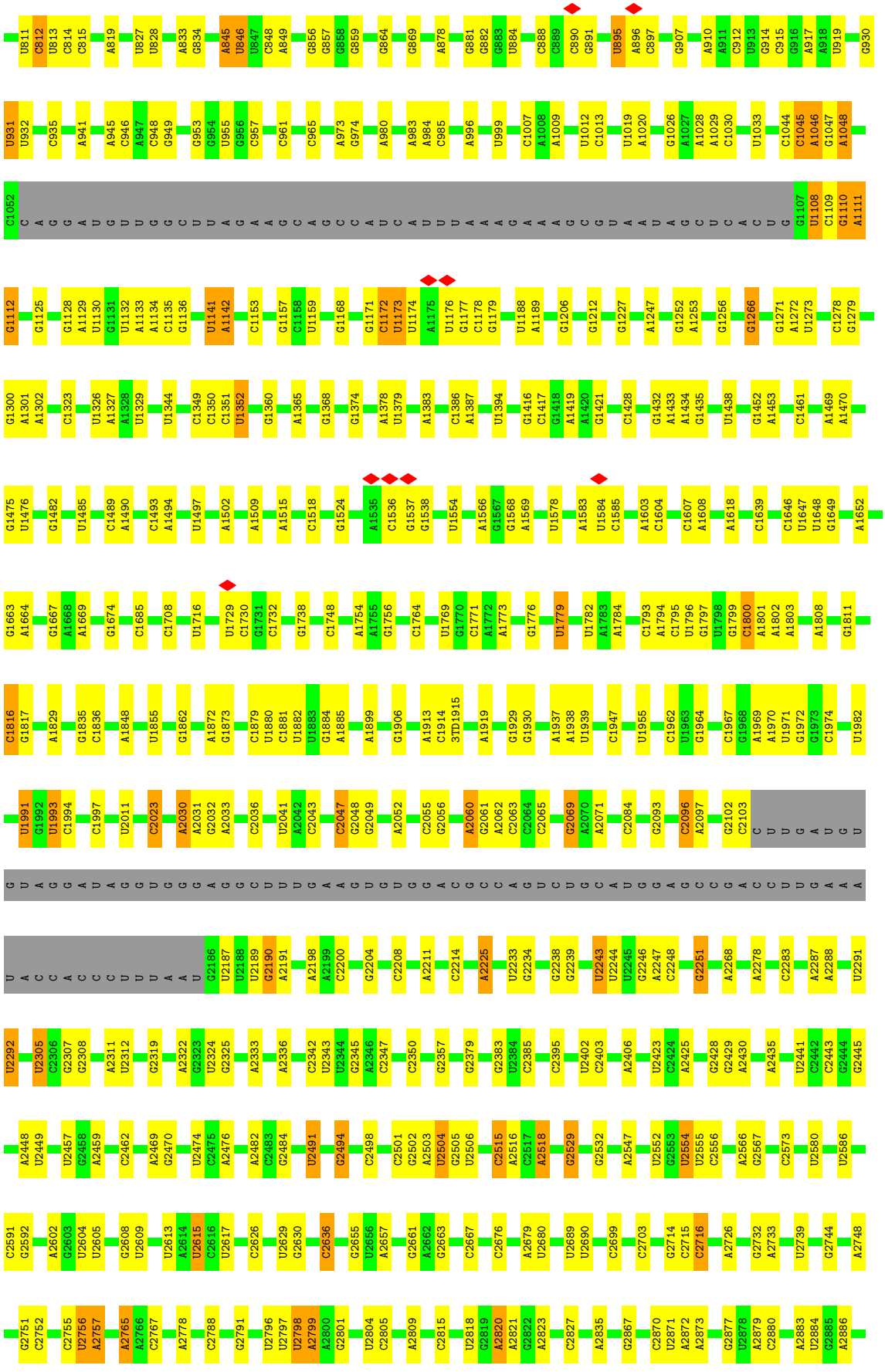
Chain mR:

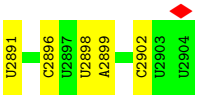


• Molecule 23: 23S ribosomal RNA (rRNA) from the rrnB operon

Chain 23:

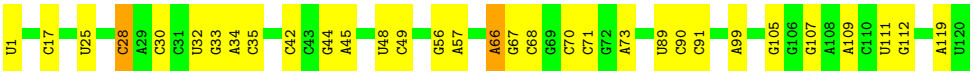






• Molecule 24: 5S large subunit ribosomal RNA of the H operon

Chain 5:

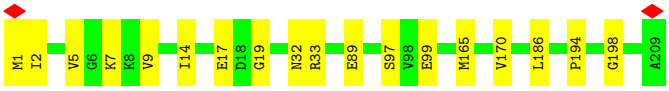


• Molecule 25: 50S ribosomal protein L2

Chain LB:

• Molecule 26: 50S ribosomal protein L3

Chain LC:

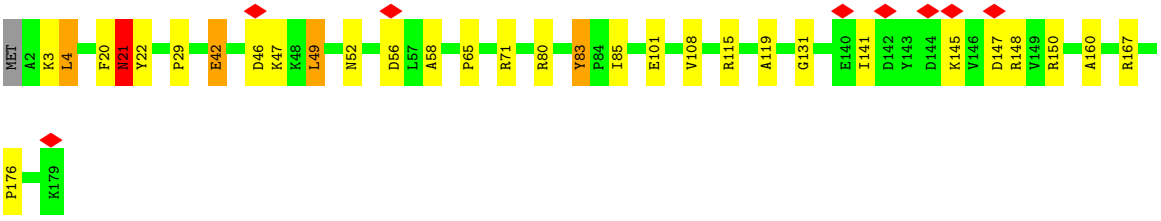


• Molecule 27: Large ribosomal subunit protein uL4

Chain LD:

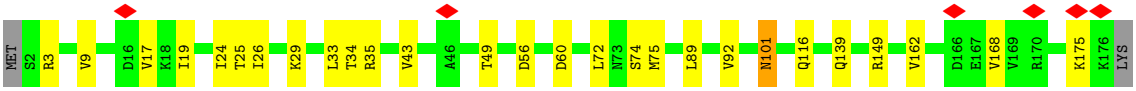
• Molecule 28: 50S ribosomal protein L5

Chain LE:



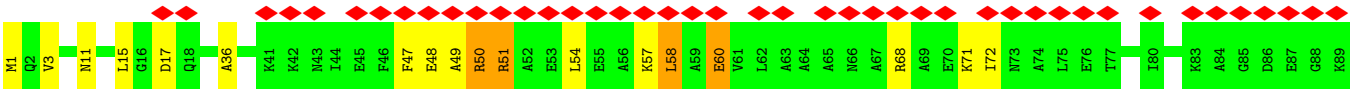
• Molecule 29: 50S ribosomal protein L6

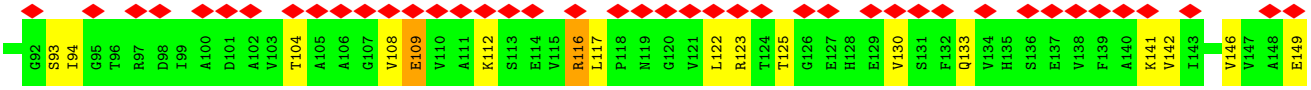
Chain LF:



• Molecule 30: 50S ribosomal protein L9

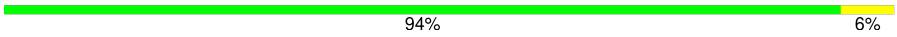
Chain LI:

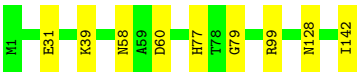




• Molecule 31: 50S ribosomal protein L13

Chain LM:



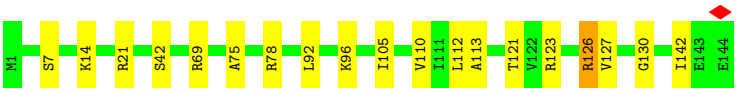


• Molecule 32: 50S ribosomal protein L14

Chain LN:

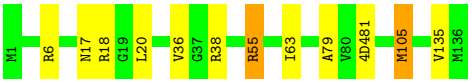
• Molecule 33: 50S ribosomal protein L15

Chain LO:



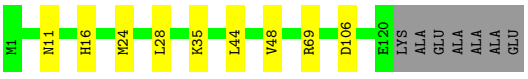
• Molecule 34: 50S ribosomal protein L16

Chain LP:



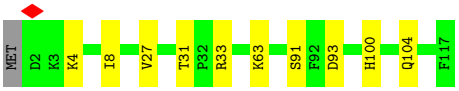
• Molecule 35: 50S ribosomal protein L17

Chain LQ:



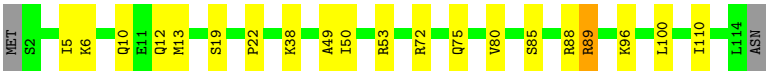
• Molecule 36: 50S ribosomal protein L18

Chain LR:



• Molecule 37: 50S ribosomal protein L19

Chain LS:

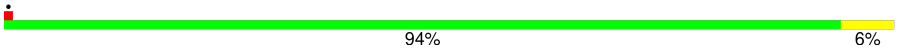


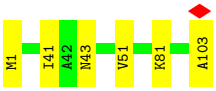
• Molecule 38: 50S ribosomal protein L20

Chain LT:

• Molecule 39: 50S ribosomal protein L21

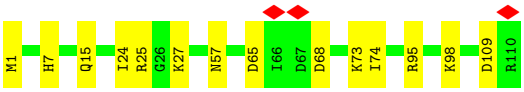
Chain LU:





• Molecule 40: Large ribosomal subunit protein uL22

Chain LV:

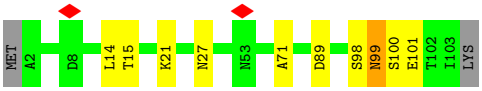


• Molecule 41: 50S ribosomal protein L23

Chain LW:

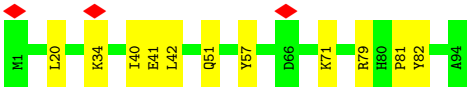
• Molecule 42: 50S ribosomal protein L24

Chain LX:



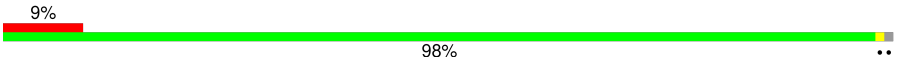
• Molecule 43: 50S ribosomal protein L25

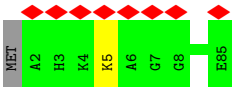
Chain LY:



• Molecule 44: 50S ribosomal protein L27

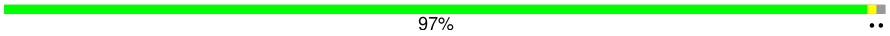
Chain La:





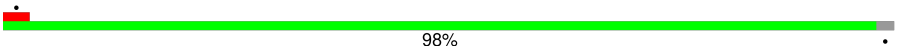
• Molecule 45: 50S ribosomal protein L28

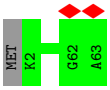
Chain Lb:



• Molecule 46: 50S ribosomal protein L29

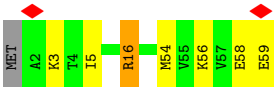
Chain Lc:





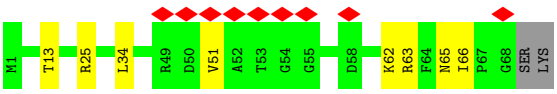
• Molecule 47: Large ribosomal subunit protein uL30

Chain Ld:



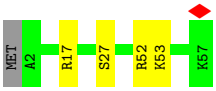
• Molecule 48: 50S ribosomal protein L31

Chain Le:



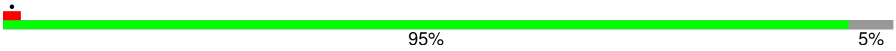
• Molecule 49: 50S ribosomal protein L32

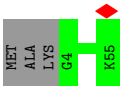
Chain Lf:



• Molecule 50: 50S ribosomal protein L33

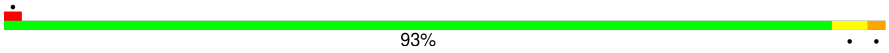
Chain Lg:

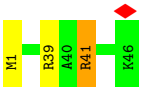




• Molecule 51: 50S ribosomal protein L34

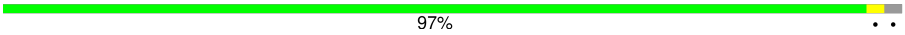
Chain Lh:





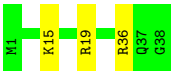
• Molecule 52: 50S ribosomal protein L35

Chain Li:



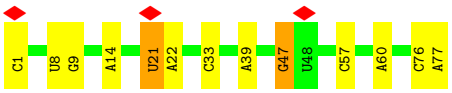
• Molecule 53: 50S ribosomal protein L36

Chain Lj:



• Molecule 54: N-formyl-methionine initiator tRNA (fMet-tRNAfMet)

Chain Pt:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	417599	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PUT, 2MG, 5MC, 4SU, G7M, OMG, 2MA, OMC, PSU, H2U, 3TD, FME, UR3, 4OC, 1MG, OMU, 4D4, ATP, K, MA6, ZN, IAS, 5MU, SPD, MG, 6MZ, D2T

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	16	0.55	0/36765	1.11	82/57346 (0.1%)
2	SB	0.39	1/1818 (0.1%)	0.65	0/2450
3	SC	0.37	0/1685	0.63	0/2270
4	SD	0.33	0/1665	0.65	0/2227
5	SE	0.38	0/1179	0.65	0/1584
6	SF	0.36	0/881	0.67	0/1189
7	SG	0.32	0/1265	0.62	0/1697
8	SH	0.32	0/989	0.61	0/1326
9	SI	0.37	0/1034	0.68	0/1375
10	SJ	0.40	0/805	0.77	0/1089
11	SK	0.39	0/902	0.68	0/1215
12	SL	0.34	0/960	0.65	0/1286
13	SM	0.32	0/900	0.73	1/1204 (0.1%)
14	SN	0.31	0/817	0.61	0/1088
15	SO	0.31	0/721	0.57	0/964
16	SP	0.34	0/659	0.66	0/884
17	SQ	0.35	0/657	0.64	0/881
18	SR	0.31	0/564	0.65	0/756
19	SS	0.30	0/680	0.62	0/915
20	ST	0.40	0/675	0.57	0/895
21	SU	0.32	0/598	0.73	0/792
22	mR	0.52	0/437	1.01	0/680
23	23	0.58	1/66049 (0.0%)	1.13	149/103033 (0.1%)
24	5	0.58	1/2876 (0.0%)	1.14	10/4483 (0.2%)
25	LB	0.36	0/2121	0.66	0/2852
26	LC	0.37	0/1585	0.65	0/2134
27	LD	0.33	0/1571	0.60	0/2113
28	LE	0.41	0/1444	0.70	1/1937 (0.1%)
29	LF	0.37	0/1333	0.60	0/1805
30	LI	0.42	0/1122	0.65	0/1515
31	LM	0.33	0/1152	0.59	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LN	0.36	0/956	0.71	0/1279
33	LO	0.33	0/1062	0.65	0/1413
34	LP	0.36	0/1091	0.67	0/1457
35	LQ	0.34	0/973	0.69	0/1301
36	LR	0.35	0/902	0.69	0/1209
37	LS	0.46	2/920 (0.2%)	0.65	0/1231
38	LT	0.35	0/960	0.65	1/1278 (0.1%)
39	LU	0.33	0/829	0.67	0/1107
40	LV	0.31	0/864	0.62	0/1156
41	LW	0.34	0/764	0.64	1/1021 (0.1%)
42	LX	0.33	0/787	0.65	0/1051
43	LY	0.37	0/766	0.61	0/1025
44	La	0.35	0/642	0.68	0/848
45	Lb	0.34	0/635	0.69	0/848
46	Lc	0.32	0/502	0.58	0/667
47	Ld	0.42	0/453	0.68	0/605
48	Le	0.40	0/543	0.64	0/726
49	Lf	0.32	0/450	0.66	0/599
50	Lg	0.31	0/433	0.61	0/576
51	Lh	0.38	0/380	0.70	0/498
52	Li	0.34	0/513	0.66	0/676
53	Lj	0.41	0/303	0.67	0/397
54	Pt	0.54	1/1744 (0.1%)	1.08	2/2716 (0.1%)
All	All	0.52	6/153381 (0.0%)	1.02	247/229220 (0.1%)

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
3	SC	0	3
5	SE	0	1
6	SF	0	1
7	SG	0	1
10	SJ	0	1
11	SK	0	2
12	SL	0	2
30	LI	0	2
32	LN	0	1
33	LO	0	1
34	LP	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	LR	0	1
37	LS	0	2
38	LT	0	1
47	Ld	0	1
48	Le	0	1
49	Lf	0	1
51	Lh	0	2
53	Lj	0	1
All	All	0	26

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	1	U	OP3-P	-7.64	1.51	1.61
23	23	1	G	OP3-P	-7.55	1.52	1.61
54	Pt	1	C	OP3-P	-7.43	1.52	1.61
37	LS	89	ARG	C-N	6.71	1.45	1.33
37	LS	88	ARG	C-N	5.70	1.47	1.34
2	SB	221	VAL	CB-CG1	-5.28	1.41	1.52

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2041	U	N3-C2-O2	-6.00	118.00	122.20
24	5	25	U	N1-C2-O2	5.99	127.00	122.80
1	16	36	C	C6-N1-C2	-5.98	117.91	120.30
23	23	999	U	N3-C2-O2	-5.98	118.02	122.20
23	23	1669	A	C2-N3-C4	5.97	113.59	110.60
1	16	1071	C	C6-N1-C2	-5.97	117.91	120.30
13	SM	19	LEU	CA-CB-CG	5.96	129.00	115.30
23	23	2815	C	C6-N1-C2	-5.95	117.92	120.30
23	23	2515	C	C6-N1-C2	-5.93	117.93	120.30
1	16	943	U	N3-C2-O2	-5.93	118.05	122.20
23	23	2292	U	C5-C6-N1	5.92	125.66	122.70
23	23	323	C	C2-N1-C1'	5.90	125.30	118.80
1	16	796	C	C6-N1-C2	-5.90	117.94	120.30
23	23	2047	C	C6-N1-C2	-5.90	117.94	120.30
23	23	2880	C	C6-N1-C2	-5.90	117.94	120.30
1	16	1119	C	C6-N1-C2	-5.90	117.94	120.30
23	23	724	U	N1-C2-O2	5.89	126.93	122.80
23	23	1800	C	C5-C6-N1	5.89	123.95	121.00
1	16	598	U	N3-C2-O2	-5.89	118.08	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2065	C	C6-N1-C2	-5.89	117.94	120.30
23	23	87	U	C5-C6-N1	5.88	125.64	122.70
24	5	25	U	N3-C2-O2	-5.88	118.09	122.20
23	23	157	C	C6-N1-C2	-5.87	117.95	120.30
24	5	70	C	C6-N1-C2	-5.86	117.95	120.30
54	Pt	57	C	C6-N1-C2	-5.86	117.95	120.30
23	23	935	C	C6-N1-C2	-5.86	117.96	120.30
23	23	845	A	C2-N3-C4	5.84	113.52	110.60
23	23	2474	U	N1-C2-O2	5.84	126.89	122.80
23	23	919	U	N1-C2-O2	5.83	126.88	122.80
23	23	383	C	N1-C2-O2	5.83	122.39	118.90
23	23	999	U	N1-C2-O2	5.82	126.87	122.80
28	LE	4	LEU	CB-CG-CD2	5.82	120.89	111.00
1	16	916	U	C5-C6-N1	5.81	125.61	122.70
23	23	192	C	C5-C6-N1	5.81	123.91	121.00
23	23	2395	C	C6-N1-C2	-5.80	117.98	120.30
1	16	1520	C	C2-N1-C1'	5.80	125.18	118.80
23	23	1323	C	N3-C2-O2	-5.80	117.84	121.90
23	23	2765	A	C2-N3-C4	5.79	113.50	110.60
1	16	643	C	C6-N1-C2	-5.78	117.99	120.30
23	23	702	U	N3-C2-O2	-5.78	118.16	122.20
24	5	17	C	C6-N1-C2	-5.78	117.99	120.30
23	23	1323	C	N1-C2-O2	5.77	122.36	118.90
23	23	201	C	N3-C2-O2	-5.73	117.89	121.90
1	16	284	C	C6-N1-C2	-5.73	118.01	120.30
1	16	17	U	N3-C2-O2	-5.72	118.19	122.20
23	23	1716	U	N1-C2-O2	5.70	126.79	122.80
23	23	1836	C	C6-N1-C2	-5.70	118.02	120.30
1	16	54	C	N1-C2-O2	5.69	122.31	118.90
1	16	1202	U	N3-C2-O2	-5.68	118.23	122.20
1	16	95	C	C2-N1-C1'	5.67	125.04	118.80
23	23	137	U	N3-C2-O2	-5.67	118.23	122.20
24	5	68	C	C6-N1-C2	-5.67	118.03	120.30
1	16	1325	C	C6-N1-C2	-5.67	118.03	120.30
23	23	1568	G	N3-C4-C5	-5.66	125.77	128.60
1	16	993	G	N3-C4-N9	5.65	129.39	126.00
23	23	607	U	N3-C2-O2	-5.64	118.25	122.20
23	23	965	C	C6-N1-C2	-5.64	118.04	120.30
1	16	316	C	C6-N1-C2	-5.64	118.05	120.30
1	16	73	C	C2-N1-C1'	5.63	124.99	118.80
23	23	1157	G	N3-C4-N9	5.63	129.38	126.00
23	23	2518	A	C2-N3-C4	5.62	113.41	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	724	U	N3-C2-O2	-5.61	118.28	122.20
23	23	919	U	N3-C2-O2	-5.60	118.28	122.20
1	16	737	C	C6-N1-C2	-5.60	118.06	120.30
24	5	91	C	C6-N1-C2	-5.59	118.06	120.30
1	16	1060	U	N3-C2-O2	-5.59	118.29	122.20
1	16	106	C	C6-N1-C2	-5.59	118.06	120.30
23	23	1855	U	N3-C2-O2	-5.58	118.29	122.20
1	16	1520	C	C6-N1-C2	-5.57	118.07	120.30
23	23	1438	U	N1-C2-O2	5.56	126.69	122.80
23	23	1716	U	N3-C2-O2	-5.56	118.31	122.20
1	16	1382	C	C6-N1-C2	-5.54	118.08	120.30
24	5	71	C	C6-N1-C2	-5.54	118.08	120.30
23	23	2248	C	C6-N1-C2	-5.54	118.08	120.30
23	23	418	C	C6-N1-C2	-5.53	118.09	120.30
23	23	2902	C	C6-N1-C2	-5.53	118.09	120.30
23	23	2052	A	N1-C2-N3	-5.52	126.54	129.30
1	16	899	C	C6-N1-C2	-5.51	118.09	120.30
23	23	114	U	C2-N1-C1'	5.50	124.30	117.70
23	23	2214	C	N1-C2-O2	5.50	122.20	118.90
23	23	200	U	N3-C2-O2	-5.49	118.35	122.20
23	23	2214	C	C6-N1-C2	-5.49	118.11	120.30
1	16	219	U	N3-C2-O2	-5.49	118.36	122.20
23	23	2036	C	C6-N1-C2	-5.49	118.11	120.30
23	23	2615	U	N3-C2-O2	-5.49	118.36	122.20
1	16	1228	C	C6-N1-C2	-5.48	118.11	120.30
24	5	42	C	N1-C2-O2	5.48	122.19	118.90
1	16	36	C	C5-C6-N1	5.48	123.74	121.00
23	23	383	C	N3-C2-O2	-5.48	118.07	121.90
38	LT	97	ASP	CB-CG-OD1	5.47	123.22	118.30
23	23	264	C	N1-C2-O2	5.47	122.18	118.90
1	16	153	C	C6-N1-C2	-5.46	118.11	120.30
1	16	221	C	C6-N1-C2	-5.45	118.12	120.30
1	16	178	C	N3-C2-O2	-5.45	118.09	121.90
23	23	814	C	C6-N1-C2	-5.45	118.12	120.30
23	23	815	C	C6-N1-C2	-5.44	118.12	120.30
23	23	2715	C	C5-C6-N1	5.44	123.72	121.00
1	16	993	G	C4-N9-C1'	5.44	133.57	126.50
41	LW	24	MET	CB-CG-SD	5.44	128.71	112.40
23	23	183	C	C6-N1-C2	-5.43	118.13	120.30
23	23	1604	C	C6-N1-C2	-5.43	118.13	120.30
1	16	611	C	N1-C2-O2	5.43	122.16	118.90
1	16	932	C	C6-N1-C2	-5.43	118.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2041	U	N1-C2-O2	5.42	126.59	122.80
24	5	28	C	C6-N1-C2	-5.42	118.13	120.30
23	23	912	C	C2-N1-C1'	5.41	124.75	118.80
1	16	140	U	C2-N1-C1'	5.41	124.19	117.70
1	16	963	G	N1-C6-O6	-5.40	116.66	119.90
23	23	2636	C	N1-C2-O2	5.40	122.14	118.90
23	23	1047	G	OP2-P-O3'	5.40	117.07	105.20
1	16	1509	C	C6-N1-C2	-5.39	118.14	120.30
23	23	1518	C	C6-N1-C2	-5.39	118.14	120.30
23	23	2699	C	C5-C6-N1	5.38	123.69	121.00
1	16	271	C	C6-N1-C2	-5.38	118.15	120.30
1	16	1348	U	N3-C2-O2	-5.38	118.43	122.20
1	16	271	C	C5-C6-N1	5.38	123.69	121.00
1	16	6	G	C4-N9-C1'	5.38	133.49	126.50
23	23	1502	A	O4'-C1'-N9	5.38	112.50	108.20
23	23	2667	C	C6-N1-C2	-5.37	118.15	120.30
1	16	1	A	C2-N3-C4	5.37	113.28	110.60
23	23	2403	C	C6-N1-C2	-5.37	118.15	120.30
23	23	1816	C	N1-C2-O2	5.36	122.12	118.90
23	23	2200	C	C6-N1-C2	-5.36	118.16	120.30
1	16	440	C	C6-N1-C2	-5.36	118.16	120.30
23	23	795	C	C6-N1-C2	-5.36	118.16	120.30
23	23	1352	U	N3-C2-O2	-5.36	118.45	122.20
23	23	2243	U	N3-C2-O2	-5.36	118.45	122.20
23	23	2902	C	C2-N1-C1'	5.36	124.69	118.80
23	23	456	C	OP1-P-O3'	5.35	116.97	105.20
23	23	2501	C	OP1-P-O3'	5.35	116.97	105.20
1	16	23	C	C6-N1-C2	-5.34	118.16	120.30
1	16	853	C	C6-N1-C2	-5.34	118.16	120.30
1	16	961	U	N3-C2-O2	-5.33	118.47	122.20
23	23	2474	U	N3-C2-O2	-5.33	118.47	122.20
1	16	536	C	C6-N1-C2	-5.32	118.17	120.30
23	23	915	C	C6-N1-C2	-5.32	118.17	120.30
23	23	31	C	C5-C6-N1	5.31	123.66	121.00
23	23	1748	C	C6-N1-C2	-5.31	118.18	120.30
1	16	961	U	N1-C2-O2	5.31	126.52	122.80
1	16	1348	U	N1-C2-O2	5.31	126.51	122.80
23	23	1708	C	C6-N1-C2	-5.30	118.18	120.30
1	16	73	C	C6-N1-C2	-5.30	118.18	120.30
1	16	980	C	N1-C2-O2	5.29	122.08	118.90
1	16	699	C	C6-N1-C2	-5.29	118.19	120.30
23	23	413	C	C6-N1-C2	-5.29	118.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	550	C	N1-C2-O2	5.29	122.07	118.90
23	23	610	C	C6-N1-C2	-5.29	118.19	120.30
23	23	1352	U	N1-C2-O2	5.29	126.50	122.80
23	23	2699	C	C6-N1-C2	-5.29	118.19	120.30
1	16	290	C	C6-N1-C2	-5.28	118.19	120.30
1	16	469	C	N1-C2-O2	5.28	122.07	118.90
1	16	611	C	C6-N1-C2	-5.28	118.19	120.30
23	23	1685	C	C6-N1-C2	-5.27	118.19	120.30
23	23	2462	C	C5-C6-N1	5.27	123.64	121.00
23	23	784	G	OP1-P-O3'	5.27	116.79	105.20
1	16	1493	A	OP2-P-O3'	5.27	116.79	105.20
1	16	932	C	C5-C6-N1	5.26	123.63	121.00
23	23	366	C	C6-N1-C2	-5.26	118.19	120.30
23	23	444	C	C6-N1-C2	-5.26	118.19	120.30
23	23	2342	C	C6-N1-C2	-5.26	118.19	120.30
23	23	702	U	N1-C2-O2	5.26	126.48	122.80
1	16	488	C	C6-N1-C2	-5.25	118.20	120.30
1	16	932	C	C2-N1-C1'	5.25	124.58	118.80
23	23	1879	C	C6-N1-C2	-5.25	118.20	120.30
1	16	1450	U	N1-C2-O2	5.25	126.47	122.80
23	23	1793	C	C6-N1-C2	-5.24	118.20	120.30
23	23	2060	A	OP1-P-O3'	5.24	116.73	105.20
23	23	1646	C	OP1-P-O3'	5.24	116.73	105.20
23	23	1476	U	N3-C2-O2	-5.24	118.53	122.20
23	23	2827	C	C6-N1-C2	-5.23	118.21	120.30
23	23	846	U	OP1-P-O3'	5.22	116.69	105.20
23	23	2896	C	C5-C6-N1	5.22	123.61	121.00
23	23	747	5MU	OP1-P-O3'	5.22	116.69	105.20
23	23	2667	C	N1-C2-O2	5.22	122.03	118.90
1	16	916	U	C2-N1-C1'	5.22	123.96	117.70
23	23	2626	C	C6-N1-C2	-5.22	118.21	120.30
23	23	2715	C	C6-N1-C2	-5.21	118.22	120.30
23	23	812	C	C6-N1-C2	-5.21	118.22	120.30
23	23	436	C	C6-N1-C2	-5.20	118.22	120.30
23	23	67	U	N3-C2-O2	-5.20	118.56	122.20
23	23	1349	C	C6-N1-C2	-5.20	118.22	120.30
23	23	416	U	N3-C2-O2	-5.19	118.56	122.20
1	16	216	U	N3-C2-O2	-5.19	118.57	122.20
23	23	370	G	O4'-C1'-N9	-5.19	104.05	108.20
1	16	132	C	C6-N1-C2	-5.19	118.22	120.30
23	23	2084	C	C6-N1-C2	-5.18	118.23	120.30
23	23	201	C	C6-N1-C2	-5.17	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16	73	C	N1-C2-O2	5.16	122.00	118.90
1	16	1450	U	N3-C2-O2	-5.16	118.59	122.20
23	23	2071	A	OP2-P-O3'	5.16	116.55	105.20
23	23	41	C	C6-N1-C2	-5.15	118.24	120.30
23	23	2676	C	C6-N1-C2	-5.15	118.24	120.30
1	16	686	U	O4'-C1'-N1	5.15	112.32	108.20
23	23	2755	C	OP2-P-O3'	5.15	116.53	105.20
23	23	1030	C	C6-N1-C2	-5.14	118.24	120.30
23	23	532	A	C2-N3-C4	5.14	113.17	110.60
23	23	1771	C	C6-N1-C2	-5.14	118.24	120.30
23	23	2870	C	C6-N1-C2	-5.14	118.24	120.30
24	5	17	C	C5-C6-N1	5.14	123.57	121.00
1	16	178	C	N1-C2-O2	5.14	121.98	118.90
23	23	1159	U	N3-C2-O2	-5.14	118.60	122.20
23	23	2474	U	C2-N1-C1'	5.14	123.87	117.70
23	23	57	C	C6-N1-C2	-5.12	118.25	120.30
23	23	550	C	C6-N1-C2	-5.12	118.25	120.30
1	16	1202	U	N1-C2-O2	5.12	126.38	122.80
1	16	1495	U	N3-C2-O2	-5.12	118.62	122.20
23	23	1947	C	C6-N1-C2	-5.12	118.25	120.30
1	16	339	C	C6-N1-C2	-5.12	118.25	120.30
1	16	385	C	C6-N1-C2	-5.11	118.25	120.30
1	16	722	G	N3-C4-C5	-5.11	126.04	128.60
23	23	1779	U	N1-C2-O2	5.10	126.37	122.80
1	16	1303	C	N3-C2-O2	-5.10	118.33	121.90
23	23	2703	C	C6-N1-C2	-5.10	118.26	120.30
1	16	1331	G	O4'-C1'-N9	5.09	112.28	108.20
23	23	1769	U	N3-C2-O2	-5.09	118.64	122.20
23	23	1044	C	OP2-P-O3'	5.09	116.40	105.20
23	23	1485	U	C2-N1-C1'	5.09	123.81	117.70
1	16	823	C	C6-N1-C2	-5.08	118.27	120.30
23	23	1350	C	C6-N1-C2	-5.08	118.27	120.30
1	16	496	A	O4'-C1'-N9	5.08	112.27	108.20
23	23	1351	C	O4'-C1'-N1	5.08	112.26	108.20
23	23	2225	A	OP1-P-O3'	5.08	116.38	105.20
23	23	796	C	C6-N1-C2	-5.08	118.27	120.30
23	23	371	A	OP1-P-O3'	5.06	116.33	105.20
23	23	2586	U	N3-C2-O2	-5.06	118.66	122.20
23	23	1994	C	C6-N1-C2	-5.05	118.28	120.30
1	16	397	A	C2-N3-C4	5.05	113.12	110.60
23	23	1993	U	N3-C2-O2	-5.05	118.66	122.20
1	16	1363	A	C2-N3-C4	5.05	113.12	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	Pt	76	C	C6-N1-C2	-5.04	118.28	120.30
1	16	308	C	C6-N1-C2	-5.04	118.28	120.30
23	23	1817	G	C2-N3-C4	5.04	114.42	111.90
23	23	2011	U	N3-C2-O2	-5.04	118.67	122.20
23	23	931	U	OP2-P-O3'	5.03	116.27	105.20
23	23	1974	C	C6-N1-C2	-5.03	118.29	120.30
23	23	813	U	N3-C2-O2	-5.03	118.68	122.20
1	16	943	U	N1-C2-O2	5.03	126.32	122.80
23	23	2190	G	OP2-P-O3'	5.02	116.25	105.20
23	23	2767	C	C6-N1-C2	-5.02	118.29	120.30
23	23	1899	A	C8-N9-C4	-5.02	103.79	105.80
1	16	99	C	C6-N1-C2	-5.02	118.29	120.30
23	23	687	C	C6-N1-C2	-5.02	118.29	120.30
1	16	214	C	N1-C2-O2	5.02	121.91	118.90
23	23	356	G	OP2-P-O3'	5.01	116.23	105.20
23	23	157	C	C5-C6-N1	5.01	123.51	121.00
1	16	854	U	N3-C2-O2	-5.01	118.69	122.20
23	23	2752	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	LI	116	ARG	Sidechain
30	LI	51	ARG	Sidechain
32	LN	17	ARG	Sidechain
33	LO	69	ARG	Sidechain
34	LP	55	ARG	Sidechain
36	LR	33	ARG	Sidechain
37	LS	53	ARG	Sidechain
37	LS	89	ARG	Sidechain
38	LT	51	ARG	Sidechain
47	Ld	16	ARG	Sidechain
48	Le	63	ARG	Sidechain
49	Lf	17	ARG	Sidechain
51	Lh	39	ARG	Sidechain
51	Lh	41	ARG	Sidechain
53	Lj	19	ARG	Sidechain
3	SC	132	ARG	Sidechain
3	SC	136	ARG	Sidechain
3	SC	88	ARG	Sidechain
5	SE	29	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	SF	38	ARG	Sidechain
7	SG	111	ARG	Sidechain
10	SJ	48	ARG	Sidechain
11	SK	106	ARG	Sidechain
11	SK	122	ARG	Sidechain
12	SL	86	ARG	Sidechain
12	SL	94	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16	33087	0	16672	77	0
2	SB	1787	0	1812	14	0
3	SC	1658	0	1732	13	0
4	SD	1643	0	1707	14	0
5	SE	1166	0	1212	7	0
6	SF	862	0	864	5	0
7	SG	1244	0	1301	11	0
8	SH	979	0	1031	7	0
9	SI	1022	0	1070	9	0
10	SJ	795	0	836	9	0
11	SK	895	0	905	6	0
12	SL	957	0	1017	12	0
13	SM	891	0	952	11	0
14	SN	805	0	844	7	0
15	SO	713	0	734	5	0
16	SP	649	0	666	3	0
17	SQ	648	0	691	5	0
18	SR	555	0	578	3	0
19	SS	663	0	688	5	0
20	ST	669	0	719	2	0
21	SU	590	0	629	5	0
22	mR	390	0	195	0	0
23	23	59447	0	29919	124	0
24	5	2572	0	1301	5	0
25	LB	2082	0	2153	7	0
26	LC	1564	0	1616	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	LD	1552	0	1619	11	0
28	LE	1420	0	1457	16	0
29	LF	1313	0	1358	12	0
30	LI	1111	0	1148	14	0
31	LM	1129	0	1162	6	0
32	LN	947	0	1023	3	0
33	LO	1053	0	1128	8	0
34	LP	1085	0	1166	8	0
35	LQ	960	0	1000	5	0
36	LR	892	0	923	4	0
37	LS	908	0	956	9	0
38	LT	947	0	1019	3	0
39	LU	816	0	839	2	0
40	LV	857	0	922	6	0
41	LW	757	0	820	5	0
42	LX	779	0	831	3	0
43	LY	753	0	780	7	0
44	La	634	0	653	0	0
45	Lb	625	0	652	0	0
46	Lc	501	0	531	0	0
47	Ld	449	0	488	0	0
48	Le	533	0	530	0	0
49	Lf	444	0	458	0	0
50	Lg	426	0	464	0	0
51	Lh	377	0	418	0	0
52	Li	504	0	572	0	0
53	Lj	302	0	340	0	0
54	Pt	1646	0	843	0	0
55	16	6	0	12	1	0
55	23	54	0	108	2	0
56	16	10	0	19	0	0
56	23	40	0	76	2	0
57	16	74	0	0	0	0
57	23	194	0	0	0	0
57	5	4	0	0	0	0
57	LB	3	0	0	0	0
57	LD	1	0	0	0	0
57	LE	1	0	0	0	0
57	LO	1	0	0	0	0
57	LT	1	0	0	0	0
57	Lf	1	0	0	0	0
57	Pt	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	mR	2	0	0	0	0
58	16	9	0	0	0	0
58	23	39	0	0	0	0
58	LB	1	0	0	0	0
59	Le	1	0	0	0	0
59	Lj	1	0	0	0	0
59	SB	1	0	0	0	0
60	23	62	0	24	0	0
61	Pt	10	0	10	0	0
All	All	142570	0	96193	448	0

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

All (448) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:881:G:H1	23:23:895:U:H3	0.92	0.91
23:23:17:G:H4'	38:LT:25:TYR:HE1	1.44	0.82
23:23:2494:G:O2'	34:LP:79:ALA:HA	1.81	0.81
12:SL:50:ARG:HB3	12:SL:66:TYR:HE1	1.52	0.75
1:16:1402:4OC:H5	1:16:1500:A:H61	1.52	0.74
1:16:664:G:H22	1:16:741:G:H1	1.33	0.73
26:LC:5:VAL:H	26:LC:32:ASN:HD21	1.36	0.73
23:23:355:U:H2'	23:23:356:G:H8	1.55	0.71
23:23:17:G:H4'	38:LT:25:TYR:CE1	2.25	0.71
29:LF:149:ARG:HA	29:LF:162:VAL:HG13	1.73	0.70
25:LB:230:HIS:HD2	25:LB:232:HIS:H	1.37	0.70
23:23:2798:U:H4'	23:23:2799:A:H5'	1.75	0.68
1:16:526:C:OP2	12:SL:88:LYS:HE3	1.94	0.67
23:23:2102:G:H1	23:23:2187:U:H3	1.39	0.67
26:LC:19:GLY:HA3	37:LS:80:VAL:CG2	2.25	0.66
9:SI:113:ARG:HH22	10:SJ:64:GLN:HE22	1.42	0.65
3:SC:131:ARG:HG3	3:SC:135:LYS:HE3	1.79	0.64
34:LP:135:VAL:HG13	43:LY:57:TYR:CD2	2.32	0.64
7:SG:110:LYS:HD2	7:SG:133:THR:HG21	1.80	0.63
26:LC:19:GLY:HA3	37:LS:80:VAL:HG23	1.79	0.63
29:LF:24:ILE:HD11	29:LF:72:LEU:HD21	1.81	0.63
1:16:1086:U:H3	1:16:1099:G:H22	1.45	0.62
7:SG:74:GLU:O	7:SG:88:PRO:HA	1.99	0.62
28:LE:4:LEU:HD12	28:LE:101:GLU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LF:19:ILE:HA	29:LF:24:ILE:HG22	1.80	0.62
42:LX:99:ASN:O	42:LX:101:GLU:N	2.29	0.62
1:16:8:A:H61	4:SD:54:GLN:HE22	1.48	0.62
1:16:843:U:H1'	1:16:846:G:C8	2.34	0.61
2:SB:42:ASN:HD21	2:SB:45:LYS:HE2	1.63	0.61
23:23:1141:U:H4'	23:23:1142:A:O4'	1.98	0.61
19:SS:60:VAL:HG11	19:SS:74:PHE:HB2	1.83	0.61
1:16:996:A:H2'	1:16:997:U:C6	2.36	0.61
37:LS:10:GLN:HA	37:LS:13:MET:HG3	1.83	0.61
43:LY:40:ILE:HD12	43:LY:42:LEU:HD21	1.83	0.60
4:SD:107:PHE:HB3	4:SD:145:ILE:HD11	1.83	0.60
4:SD:100:ASN:HD22	4:SD:111:ARG:HE	1.49	0.60
23:23:281:C:H2'	23:23:282:A:C8	2.36	0.60
41:LW:56:GLU:HG2	41:LW:88:LYS:HG2	1.82	0.60
23:23:355:U:H2'	23:23:356:G:C8	2.37	0.59
6:SF:18:VAL:HA	6:SF:21:MET:HG3	1.84	0.59
1:16:1043:G:HO2'	1:16:1044:A:H8	1.49	0.59
23:23:2023:C:H5'	23:23:2617:U:H4'	1.85	0.58
1:16:82:G:H3'	1:16:83:C:H6	1.68	0.58
23:23:1266:G:H5"	40:LV:15:GLN:HE22	1.69	0.58
23:23:1652:A:H62	35:LQ:11:ASN:HD21	1.50	0.58
10:SJ:10:LEU:HB3	10:SJ:18:ILE:HD11	1.85	0.58
29:LF:149:ARG:HA	29:LF:162:VAL:CG1	2.34	0.58
23:23:1028:A:N6	23:23:1125:G:H2'	2.17	0.58
28:LE:20:PHE:O	28:LE:21:ASN:C	2.41	0.57
16:SP:4:ILE:HG12	16:SP:21:VAL:HG22	1.86	0.57
23:23:288:U:H2'	23:23:289:G:C8	2.40	0.57
9:SI:115:LYS:HB2	9:SI:118:LEU:HD12	1.87	0.57
7:SG:75:VAL:HG11	7:SG:144:MET:HG2	1.86	0.57
23:23:274:C:H2'	23:23:275:C:O4'	2.04	0.57
23:23:1028:A:H61	23:23:1125:G:H2'	1.70	0.57
1:16:325:A:N7	55:16:1601:PUT:N1	2.51	0.57
23:23:1045:C:H4'	23:23:1046:A:H5"	1.86	0.56
1:16:677:U:H3	1:16:713:G:H22	1.52	0.56
9:SI:7:TYR:HE1	9:SI:18:ARG:HB3	1.70	0.56
3:SC:131:ARG:CG	3:SC:135:LYS:HE3	2.36	0.56
28:LE:46:ASP:O	28:LE:49:LEU:HG	2.06	0.56
40:LV:25:ARG:NH1	40:LV:74:ILE:O	2.38	0.56
5:SE:74:VAL:HG23	5:SE:144:LEU:O	2.06	0.56
29:LF:33:LEU:HD13	29:LF:75:MET:HG2	1.86	0.56
2:SB:120:GLN:HG3	2:SB:125:THR:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SC:22:TRP:HB3	3:SC:59:ARG:HG2	1.89	0.55
28:LE:119:ALA:O	28:LE:167:ARG:NH1	2.38	0.55
23:23:568:U:H1'	23:23:2030:6MZ:H9C1	1.88	0.55
23:23:848:C:H2'	23:23:849:A:H8	1.70	0.55
8:SH:29:SER:HB3	8:SH:59:LEU:HB2	1.90	0.54
41:LW:3:ARG:NH1	41:LW:5:GLU:OE2	2.41	0.54
23:23:856:G:H2'	23:23:857:G:C8	2.43	0.54
1:16:993:G:O2'	1:16:994:A:N7	2.40	0.54
7:SG:56:LYS:NZ	7:SG:57:SER:OG	2.41	0.54
23:23:12:U:H2'	23:23:12:U:O2	2.07	0.54
25:LB:144:VAL:HB	25:LB:154:LEU:HB2	1.88	0.54
3:SC:21:THR:HG23	3:SC:58:GLU:HG2	1.89	0.54
19:SS:50:ALA:HB1	19:SS:57:HIS:HB3	1.90	0.54
27:LD:191:ASP:HA	27:LD:194:LYS:HE2	1.90	0.53
28:LE:108:VAL:HG11	28:LE:176:PRO:HG2	1.90	0.53
1:16:999:C:H2'	1:16:1000:A:C8	2.43	0.53
23:23:2189:U:H2'	23:23:2190:G:H8	1.74	0.53
40:LV:68:ASP:OD1	40:LV:68:ASP:N	2.41	0.53
24:5:48:U:H2'	24:5:49:C:C6	2.44	0.53
23:23:632:A:H2'	23:23:633:A:C8	2.43	0.53
32:LN:17:ARG:HB2	32:LN:45:GLU:HG2	1.91	0.53
1:16:999:C:H2'	1:16:1000:A:H8	1.73	0.53
26:LC:97:SER:OG	26:LC:99:GLU:OE2	2.24	0.53
1:16:82:G:H3'	1:16:83:C:C6	2.44	0.53
23:23:568:U:O4	39:LU:81:LYS:NZ	2.42	0.52
30:LI:93:SER:OG	30:LI:123:ARG:NH1	2.42	0.52
23:23:1188:U:H2'	23:23:1189:A:H8	1.74	0.52
7:SG:27:VAL:HG21	7:SG:40:GLU:HG3	1.90	0.52
12:SL:110:ARG:HB2	12:SL:119:VAL:HG21	1.92	0.52
23:23:864:G:OP2	55:23:3007:PUT:N1	2.41	0.52
33:LO:127:VAL:HG21	33:LO:142:ILE:HG12	1.92	0.52
5:SE:38:VAL:HG11	5:SE:114:VAL:HG22	1.91	0.52
14:SN:79:LEU:HB2	14:SN:84:VAL:HG23	1.92	0.52
23:23:288:U:H2'	23:23:289:G:H8	1.74	0.52
10:SJ:66:GLU:HB2	14:SN:99:ALA:HB2	1.91	0.52
35:LQ:24:MET:HG2	35:LQ:44:LEU:HD13	1.92	0.52
35:LQ:106:ASP:OD1	35:LQ:106:ASP:N	2.43	0.52
2:SB:46:THR:HB	2:SB:201:PRO:HG2	1.92	0.52
4:SD:123:ILE:HD13	4:SD:145:ILE:HG12	1.92	0.52
6:SF:38:ARG:HB3	6:SF:63:ASN:HB2	1.91	0.52
13:SM:28:THR:HA	13:SM:31:LYS:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:840:C:H2'	1:16:841:C:C6	2.44	0.51
5:SE:74:VAL:HG21	5:SE:144:LEU:HB3	1.92	0.51
10:SJ:6:ILE:HG12	10:SJ:79:PRO:HB3	1.92	0.51
29:LF:101:ASN:OD1	29:LF:116:GLN:NE2	2.44	0.51
23:23:281:C:H2'	23:23:282:A:H8	1.75	0.51
31:LM:60:ASP:OD1	31:LM:60:ASP:N	2.35	0.51
3:SC:44:THR:O	3:SC:48:ALA:HB2	2.11	0.50
39:LU:41:ILE:HD13	39:LU:103:ALA:HA	1.93	0.50
3:SC:95:ALA:O	3:SC:97:VAL:HG23	2.11	0.50
16:SP:46:LYS:HE3	16:SP:47:GLU:HB3	1.93	0.50
28:LE:58:ALA:HB2	28:LE:65:PRO:HD3	1.93	0.50
1:16:127:G:O3'	17:SQ:6:ARG:NH2	2.44	0.50
23:23:953:G:OP1	34:LP:18[A]:ARG:NH2	2.35	0.50
34:LP:36:VAL:HG12	43:LY:82:TYR:HB2	1.94	0.50
1:16:86:G:H2'	1:16:87:C:O4'	2.11	0.50
2:SB:4:VAL:HG11	2:SB:50:PHE:CD2	2.47	0.50
29:LF:89:LEU:HD12	29:LF:162:VAL:HG23	1.94	0.50
4:SD:192:SER:OG	4:SD:194:ASP:OD1	2.29	0.49
23:23:668:A:H2'	23:23:670:A:H62	1.75	0.49
1:16:94:G:H4'	1:16:95:C:H5'	1.94	0.49
29:LF:17:VAL:HG23	29:LF:26:ILE:HG12	1.94	0.49
4:SD:107:PHE:CG	4:SD:145:ILE:HD11	2.46	0.49
23:23:603:A:H5"	23:23:655:A:H61	1.77	0.49
28:LE:147:ASP:N	28:LE:147:ASP:OD1	2.44	0.49
1:16:1029:U:O2	1:16:1032:G:O6	2.30	0.49
17:SQ:76:VAL:HG12	17:SQ:77:ARG:HG2	1.95	0.49
1:16:949:A:N7	13:SM:105:ASN:ND2	2.61	0.49
4:SD:123:ILE:CD1	4:SD:145:ILE:HG12	2.43	0.49
23:23:2820:A:H2'	23:23:2820:A:N3	2.27	0.49
30:LI:71:LYS:HD3	30:LI:72:ILE:HD12	1.94	0.49
38:LT:72:ASN:HB3	38:LT:110:VAL:HG11	1.94	0.49
5:SE:76:LEU:HD22	5:SE:120:VAL:HG22	1.95	0.49
1:16:673:A:H2'	1:16:674:G:C8	2.47	0.49
27:LD:18:THR:HA	27:LD:106:LYS:HG2	1.94	0.49
23:23:144:A:H2'	23:23:145:C:C6	2.47	0.49
23:23:785:G:H4'	23:23:1779:U:H4'	1.95	0.49
30:LI:49:ALA:HB3	30:LI:50:ARG:HH11	1.77	0.49
36:LR:100:HIS:O	36:LR:104:GLN:NE2	2.45	0.49
13:SM:18:ALA:HB3	13:SM:45:ILE:HD12	1.95	0.49
3:SC:47:LEU:HD11	3:SC:87:LEU:HD21	1.95	0.48
4:SD:122:ALA:O	4:SD:145:ILE:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:83:C:H4'	1:16:84:U:C5	2.47	0.48
24:5:66:A:H61	24:5:107:G:H2'	1.78	0.48
1:16:946:A:H2'	1:16:947:G:C8	2.48	0.48
23:23:1173:U:H2'	23:23:1174:U:C6	2.49	0.48
27:LD:97:ASN:HB2	27:LD:100:MET:HG3	1.94	0.48
5:SE:80:THR:HA	5:SE:120:VAL:HG13	1.94	0.48
40:LV:24:ILE:HA	40:LV:27:LYS:HD2	1.95	0.48
6:SF:6:ILE:HD12	6:SF:89:VAL:HG22	1.96	0.48
3:SC:155:GLY:HA2	3:SC:163:ALA:HB1	1.95	0.48
5:SE:115:LEU:HD13	5:SE:123:VAL:HG11	1.96	0.48
40:LV:65:ASP:N	40:LV:65:ASP:OD1	2.47	0.48
1:16:826:C:O2	8:SH:16:ASN:ND2	2.47	0.48
8:SH:76:GLN:HG2	8:SH:128:TYR:HB2	1.96	0.48
3:SC:131:ARG:O	3:SC:135:LYS:HG3	2.14	0.48
11:SK:87:LYS:HB2	11:SK:113:VAL:HG23	1.96	0.48
14:SN:49:GLN:NE2	19:SS:11:ILE:O	2.46	0.48
23:23:881:G:N2	23:23:895:U:O2	2.37	0.48
23:23:2680:U:H5'	26:LC:194:PRO:HA	1.95	0.48
31:LM:58:ASN:HD21	31:LM:128:ASN:HD22	1.62	0.48
6:SF:9:MET:HA	6:SF:58:HIS:O	2.14	0.47
28:LE:52:ASN:ND2	28:LE:147:ASP:OD2	2.47	0.47
1:16:1071:C:H2'	1:16:1072:G:H8	1.79	0.47
2:SB:199:VAL:HG12	2:SB:201:PRO:HD3	1.96	0.47
35:LQ:28:LEU:HD23	35:LQ:48:VAL:HG21	1.94	0.47
1:16:1356:G:H2'	1:16:1357:A:C8	2.50	0.47
1:16:81:A:H3'	1:16:82:G:H8	1.79	0.47
23:23:2243:U:H2'	23:23:2244:U:C6	2.49	0.47
25:LB:232:HIS:HA	25:LB:242:LYS:HD2	1.95	0.47
23:23:468:G:H5"	27:LD:55:SER:HB3	1.95	0.47
23:23:1386:C:H2'	23:23:1387:A:C8	2.49	0.47
13:SM:18:ALA:CB	13:SM:45:ILE:HD12	2.44	0.47
23:23:1802:A:H2'	23:23:1803:A:C8	2.49	0.47
1:16:88:U:H2'	1:16:89:U:C6	2.50	0.47
1:16:477:C:H2'	1:16:478:A:C8	2.49	0.47
1:16:769:G:H4'	1:16:1513:A:H4'	1.95	0.47
30:LI:125:THR:OG1	30:LI:146:VAL:O	2.30	0.47
23:23:357:C:H2'	23:23:358:U:C6	2.50	0.47
1:16:524:G:H2'	1:16:525:C:C6	2.50	0.47
1:16:844:G:H22	18:SR:8:ARG:HA	1.79	0.47
12:SL:110:ARG:HD2	12:SL:110:ARG:HA	1.76	0.47
23:23:373:U:H2'	23:23:374:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1108:U:H2'	23:23:1109:C:O4'	2.15	0.46
30:LI:71:LYS:NZ	30:LI:108:VAL:O	2.39	0.46
33:LO:78:ARG:HG2	33:LO:113:ALA:HB3	1.96	0.46
2:SB:111:ILE:HD12	2:SB:152:LYS:HA	1.97	0.46
4:SD:107:PHE:CB	4:SD:145:ILE:HD11	2.45	0.46
23:23:727:A:OP2	55:23:3003:PUT:N1	2.47	0.46
23:23:2591:C:H2'	23:23:2592:G:C8	2.51	0.46
23:23:2756:U:H1'	23:23:2757:A:H5"	1.97	0.46
25:LB:180:GLU:OE2	25:LB:267:ILE:HG23	2.15	0.46
27:LD:63:LYS:HB3	27:LD:63:LYS:HE3	1.78	0.46
30:LI:104:THR:HG22	30:LI:109:GLU:HA	1.97	0.46
11:SK:67:ALA:HB2	11:SK:96:THR:HG23	1.97	0.46
15:SO:26:GLU:HG3	15:SO:81:LEU:HD22	1.98	0.46
23:23:1019:U:H2'	23:23:1020:A:C8	2.50	0.46
24:5:28:C:H5"	36:LR:31:THR:HG21	1.97	0.46
4:SD:174:ASP:OD1	4:SD:177:LYS:HG3	2.14	0.46
23:23:2898:U:H2'	23:23:2899:A:C8	2.50	0.46
1:16:315:A:O2'	1:16:330:C:H4'	2.16	0.46
23:23:2096:C:H2'	23:23:2097:A:C8	2.51	0.46
17:SQ:19:LYS:HB2	17:SQ:19:LYS:HE3	1.68	0.46
1:16:87:C:H2'	1:16:88:U:C6	2.51	0.46
28:LE:20:PHE:O	28:LE:22:TYR:N	2.49	0.46
41:LW:93:LEU:HD12	41:LW:93:LEU:HA	1.76	0.46
20:ST:39:ILE:HD11	20:ST:83:ILE:HG13	1.97	0.46
23:23:160:A:N3	23:23:2208:C:O2'	2.48	0.46
23:23:2804:U:H2'	23:23:2805:C:C6	2.51	0.46
32:LN:77:ILE:HG12	37:LS:72:ARG:HG2	1.98	0.46
42:LX:89:ASP:N	42:LX:89:ASP:OD1	2.47	0.46
8:SH:11:LEU:HD22	8:SH:75:ILE:HD11	1.98	0.46
10:SJ:40:ILE:HD13	10:SJ:73:LEU:HD23	1.97	0.46
23:23:833:A:H2'	23:23:834:G:C8	2.51	0.46
23:23:1129:A:N6	23:23:2491:U:OP1	2.47	0.46
23:23:1434:A:H2'	23:23:1435:G:C8	2.51	0.46
23:23:1469:A:H2'	23:23:1470:A:C8	2.51	0.46
23:23:278:A:N3	23:23:278:A:H2'	2.30	0.45
24:5:30:C:H1'	24:5:57:A:H61	1.80	0.45
1:16:439:U:H5"	4:SD:121:LYS:HD2	1.98	0.45
1:16:553:A:H5"	12:SL:21:VAL:HG21	1.98	0.45
12:SL:15:LYS:H	12:SL:15:LYS:HG2	1.57	0.45
18:SR:9:LYS:NZ	18:SR:44:ILE:O	2.46	0.45
23:23:280:U:H2'	23:23:281:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2679:A:H4'	26:LC:170:VAL:HG11	1.97	0.45
28:LE:80:ARG:H	28:LE:83:TYR:HD2	1.63	0.45
30:LI:3:VAL:CG1	30:LI:36:ALA:HB1	2.46	0.45
1:16:556:C:OP1	12:SL:14:ARG:NH2	2.46	0.45
23:23:494:G:H21	40:LV:57:ASN:HD21	1.63	0.45
43:LY:20:LEU:HD11	43:LY:41:GLU:HG2	1.99	0.45
4:SD:48:LEU:HD21	4:SD:56:ARG:HG3	1.97	0.45
23:23:675:A:N3	23:23:2443:C:O2'	2.43	0.45
26:LC:19:GLY:CA	37:LS:80:VAL:HG23	2.46	0.45
13:SM:11:ASP:HB2	13:SM:46:SER:HB3	1.99	0.45
23:23:1796:U:H2'	23:23:1797:G:C8	2.52	0.45
23:23:2554:U:H2'	23:23:2555:U:C6	2.51	0.45
1:16:568:G:O6	12:SL:2:ALA:N	2.50	0.45
23:23:151:C:H2'	23:23:152:A:H8	1.81	0.45
23:23:1110:G:H1'	23:23:1111:A:C8	2.51	0.45
23:23:276:U:H2'	23:23:277:G:C2	2.52	0.45
27:LD:10:SER:OG	27:LD:11:ALA:N	2.48	0.45
30:LI:94:ILE:HB	30:LI:122:LEU:HB2	1.99	0.45
1:16:1218:C:H2'	1:16:1219:A:C8	2.52	0.44
7:SG:111:ARG:HE	7:SG:123:GLU:HG2	1.82	0.44
10:SJ:10:LEU:HD11	10:SJ:25:ILE:HD12	1.99	0.44
11:SK:84:VAL:HG11	11:SK:97:ILE:HG12	1.99	0.44
33:LO:92:LEU:O	33:LO:96:LYS:HG3	2.16	0.44
34:LP:17:ASN:O	34:LP:38:ARG:NH1	2.50	0.44
6:SF:71:ILE:HD13	6:SF:71:ILE:HA	1.88	0.44
16:SP:40:ASN:HB3	16:SP:43:ALA:HB2	1.99	0.44
32:LN:24:VAL:HG13	32:LN:33:ALA:HB2	2.00	0.44
1:16:996:A:H2'	1:16:997:U:H6	1.80	0.44
1:16:1255:G:O2'	1:16:1258:G:N3	2.47	0.44
2:SB:27:MET:HG3	2:SB:189:THR:HA	1.99	0.44
27:LD:149:ILE:HB	27:LD:188:MET:HG3	1.99	0.44
1:16:330:C:H2'	1:16:331:G:H8	1.82	0.44
23:23:945:A:H1'	56:23:3012:SPD:H91	1.98	0.44
33:LO:126:ARG:H	33:LO:126:ARG:HG2	1.62	0.44
1:16:337:G:H2'	1:16:338:A:C8	2.52	0.44
1:16:674:G:H2'	1:16:675:A:H8	1.82	0.44
23:23:2871:U:OP1	35:LQ:69:ARG:NH2	2.51	0.44
28:LE:29:PRO:HB3	28:LE:160:ALA:HB2	2.00	0.44
23:23:181:A:H1'	23:23:435:C:H5'	1.99	0.44
23:23:459:U:H2'	23:23:460:A:H8	1.83	0.44
13:SM:106:ALA:HB3	13:SM:110:LYS:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1174:U:H1'	23:23:1177:G:C5	2.52	0.44
29:LF:25:THR:HB	29:LF:34:THR:HG23	1.99	0.44
33:LO:112:LEU:HD12	33:LO:130:GLY:HA3	2.00	0.44
13:SM:37:ALA:HB1	13:SM:39:ILE:HD12	2.00	0.44
15:SO:4:SER:O	15:SO:8:THR:OG1	2.33	0.44
15:SO:73:LYS:HD3	15:SO:73:LYS:HA	1.88	0.44
31:LM:99:ARG:HD2	31:LM:99:ARG:HA	1.82	0.44
1:16:1308:U:H2'	1:16:1309:G:H8	1.81	0.44
1:16:1348:U:H4'	9:SI:122:ARG:HD2	2.00	0.44
1:16:1391:U:H2'	1:16:1392:G:C8	2.52	0.44
23:23:1794:A:H2'	23:23:1795:C:C6	2.53	0.44
3:SC:22:TRP:CB	3:SC:59:ARG:HG2	2.47	0.43
14:SN:64:CYS:HB2	14:SN:80:SER:HB3	1.99	0.43
27:LD:3:LEU:HD13	27:LD:120:VAL:HG21	2.00	0.43
2:SB:131:LYS:HD2	2:SB:131:LYS:HA	1.72	0.43
21:SU:4:ILE:HG12	21:SU:19:PHE:HB2	1.99	0.43
23:23:1754:A:N1	23:23:2716:C:O2'	2.49	0.43
23:23:2788:C:O2'	23:23:2809:A:N3	2.48	0.43
30:LI:57:LYS:HA	30:LI:60:GLU:HG2	2.00	0.43
37:LS:22:PRO:HD3	37:LS:50:ILE:HD12	2.00	0.43
7:SG:93:PRO:HA	7:SG:96:ARG:HB2	2.00	0.43
11:SK:19:GLY:O	11:SK:82:LEU:HA	2.18	0.43
14:SN:83:LYS:HA	14:SN:83:LYS:HD3	1.81	0.43
23:23:287:G:H3'	23:23:288:U:H6	1.83	0.43
23:23:742:A:H2'	23:23:743:A:C8	2.53	0.43
23:23:1028:A:H2'	23:23:1029:A:C8	2.53	0.43
1:16:559:A:H4'	1:16:560:A:H3'	2.00	0.43
8:SH:89:LYS:HB3	8:SH:89:LYS:HE3	1.65	0.43
10:SJ:10:LEU:HD21	10:SJ:98:VAL:HG13	1.99	0.43
23:23:1796:U:H2'	23:23:1797:G:H8	1.82	0.43
2:SB:4:VAL:HG11	2:SB:50:PHE:HD2	1.83	0.43
23:23:1009:A:N3	23:23:1153:C:O2'	2.45	0.43
23:23:2532:G:O2'	23:23:2657:A:N1	2.50	0.43
56:23:3015:SPD:HN11	56:23:3015:SPD:H42	1.70	0.43
30:LI:58:LEU:HD12	30:LI:58:LEU:HA	1.76	0.43
36:LR:27:VAL:HA	36:LR:93:ASP:HB3	2.01	0.43
1:16:714:G:H2'	1:16:715:A:C8	2.54	0.43
1:16:928:G:O2'	1:16:1533:C:OP1	2.36	0.43
23:23:589:U:H2'	23:23:590:A:C8	2.54	0.43
23:23:1048:A:OP2	23:23:1110:G:N2	2.48	0.43
23:23:2529:G:H4'	29:LF:175:LYS:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:LP:20:LEU:HD13	43:LY:81:PRO:HG3	2.01	0.43
1:16:933:G:O6	7:SG:3:ARG:NH2	2.49	0.43
11:SK:34:ILE:HB	11:SK:74:VAL:HG21	2.00	0.43
23:23:351:C:H2'	23:23:352:A:C8	2.54	0.43
1:16:86:G:H2'	1:16:87:C:C4'	2.48	0.43
1:16:1530:G:H2'	1:16:1531:A:C8	2.54	0.43
23:23:1019:U:H2'	23:23:1020:A:H8	1.83	0.43
1:16:1536:C:H2'	1:16:1537:U:C6	2.54	0.43
3:SC:175:LEU:HD23	3:SC:182:ILE:HD13	2.00	0.43
15:SO:35:GLN:HG2	15:SO:59:MET:SD	2.59	0.43
1:16:254:G:O2'	17:SQ:18:GLU:O	2.37	0.43
1:16:656:G:O2'	15:SO:28:GLN:NE2	2.45	0.43
9:SI:19:VAL:HG22	9:SI:65:ILE:HG12	2.00	0.43
23:23:811:U:H2'	33:LO:21:ARG:HA	2.00	0.43
23:23:1326:U:H2'	23:23:1327:A:H8	1.84	0.43
37:LS:100:LEU:HD11	37:LS:110:ILE:HD11	2.00	0.43
1:16:757:U:H2'	1:16:758:C:O4'	2.19	0.42
11:SK:117:PRO:HD2	21:SU:35:ARG:HD3	2.01	0.42
12:SL:90:LEU:HA	12:SL:91:PRO:HD3	1.94	0.42
42:LX:14:LEU:HD11	42:LX:71:ALA:HB2	2.00	0.42
2:SB:74:ARG:HA	2:SB:74:ARG:HD3	1.76	0.42
9:SI:51:PRO:HG3	9:SI:80:ARG:HG3	2.00	0.42
12:SL:108:LYS:HB2	12:SL:108:LYS:HE2	1.73	0.42
23:23:2515:C:H2'	23:23:2516:A:H8	1.84	0.42
31:LM:31:GLU:HG2	31:LM:142:ILE:HD12	1.99	0.42
1:16:85:U:H4'	1:16:86:G:C4	2.54	0.42
1:16:580:C:H2'	1:16:581:G:O4'	2.20	0.42
12:SL:86:ARG:HE	12:SL:86:ARG:HB3	1.44	0.42
23:23:459:U:H2'	23:23:460:A:C8	2.54	0.42
30:LI:15:LEU:HD11	30:LI:47:PHE:HE1	1.84	0.42
7:SG:72:THR:H	7:SG:142:HIS:HE1	1.68	0.42
13:SM:114:LYS:HE2	13:SM:114:LYS:HB2	1.79	0.42
19:SS:60:VAL:HG11	19:SS:74:PHE:CB	2.48	0.42
23:23:1007:C:OP1	31:LM:39:LYS:NZ	2.53	0.42
23:23:1881:C:H2'	23:23:1882:U:O4'	2.20	0.42
1:16:519:C:OP2	12:SL:47:SER:OG	2.37	0.42
2:SB:129:LEU:HG	2:SB:131:LYS:H	1.84	0.42
3:SC:130:PHE:O	3:SC:134:MET:HG3	2.20	0.42
9:SI:84:THR:HG23	9:SI:98:LEU:HD13	2.01	0.42
23:23:1779:U:OP2	23:23:1784:A:N6	2.40	0.42
21:SU:63:GLU:OE1	21:SU:66:ARG:NH2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LB:145:GLU:HB2	25:LB:188:CYS:HB3	2.01	0.42
20:ST:79:LEU:HD23	20:ST:79:LEU:HA	1.88	0.42
23:23:581:C:H2'	23:23:582:A:C8	2.55	0.42
23:23:1434:A:H2'	23:23:1435:G:H8	1.83	0.42
13:SM:39:ILE:HD11	13:SM:52:GLN:HB3	2.02	0.42
21:SU:25:LYS:HD3	21:SU:25:LYS:HA	1.82	0.42
23:23:2096:C:H2'	23:23:2097:A:H8	1.84	0.42
23:23:2291:U:H2'	23:23:2292:U:C6	2.55	0.42
25:LB:211:ALA:O	25:LB:216:VAL:HG13	2.20	0.42
30:LI:11:ASN:OD1	30:LI:11:ASN:N	2.53	0.42
23:23:1111:A:N3	23:23:1112:G:H1'	2.35	0.42
24:5:111:U:H2'	24:5:112:G:H8	1.84	0.42
26:LC:14:ILE:HA	37:LS:12:GLN:HE22	1.83	0.42
23:23:714:U:H1'	23:23:717:C:H5	1.83	0.41
23:23:1432:G:H2'	23:23:1433:A:C8	2.55	0.41
23:23:2246:G:H2'	23:23:2247:A:C8	2.55	0.41
1:16:269:C:H2'	1:16:270:A:C8	2.56	0.41
1:16:672:U:H2'	1:16:673:A:C8	2.55	0.41
23:23:287:G:H3'	23:23:288:U:C6	2.55	0.41
23:23:1394:U:H4'	23:23:1603:A:H4'	2.01	0.41
26:LC:7:LYS:HE3	26:LC:198:GLY:HA2	2.01	0.41
27:LD:106:LYS:HG3	27:LD:200:LEU:HD13	2.02	0.41
33:LO:75:ALA:HB2	33:LO:105:ILE:HD12	2.01	0.41
34:LP:135:VAL:HG13	43:LY:57:TYR:CE2	2.55	0.41
1:16:80:A:H2'	1:16:81:A:C8	2.55	0.41
1:16:713:G:H2'	1:16:714:G:C8	2.55	0.41
9:SI:21:ILE:CG2	9:SI:61:LEU:HD22	2.50	0.41
1:16:458:U:H2'	1:16:459:A:C8	2.55	0.41
1:16:458:U:H2'	1:16:459:A:H8	1.84	0.41
1:16:677:U:O2	1:16:777:A:O2'	2.33	0.41
23:23:2246:G:H2'	23:23:2247:A:H8	1.85	0.41
25:LB:243:HIS:HA	25:LB:244:PRO:HD3	1.91	0.41
41:LW:34:VAL:HG21	41:LW:43:ILE:HD11	2.02	0.41
1:16:464:U:O2'	1:16:466:A:N7	2.47	0.41
23:23:275:C:H2'	23:23:276:U:O4'	2.19	0.41
23:23:2047:C:H2'	23:23:2048:G:H8	1.84	0.41
23:23:2251:OMG:HM23	23:23:2251:OMG:H1'	1.81	0.41
23:23:2796:U:H3	23:23:2799:A:H61	1.67	0.41
30:LI:130:VAL:HG23	30:LI:142:VAL:HB	2.02	0.41
2:SB:187:VAL:HG13	2:SB:191:SER:HB2	2.03	0.41
4:SD:151:LYS:HD2	4:SD:151:LYS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:391:A:H1'	23:23:411:G:O4'	2.21	0.41
23:23:2312:U:H5'	28:LE:85:ILE:HD11	2.03	0.41
23:23:2751:G:C4	29:LF:3:ARG:HD2	2.56	0.41
28:LE:42:GLU:H	28:LE:42:GLU:HG2	1.56	0.41
37:LS:49:ALA:HB1	37:LS:96:LYS:HE3	2.02	0.41
1:16:674:G:H2'	1:16:675:A:C8	2.56	0.41
1:16:1253:G:H2'	1:16:1254:A:H8	1.85	0.41
4:SD:121:LYS:O	4:SD:146:ARG:NH1	2.53	0.41
1:16:51:A:N7	1:16:114:U:O2'	2.52	0.41
1:16:1151:A:H5"	10:SJ:44:THR:HG23	2.02	0.41
1:16:1187:G:H5'	9:SI:115:LYS:HE2	2.03	0.41
2:SB:186:ILE:HD13	2:SB:200:ILE:HB	2.03	0.41
10:SJ:37:ARG:HB2	10:SJ:75:ASP:HB2	2.02	0.41
13:SM:18:ALA:HB3	13:SM:45:ILE:CD1	2.50	0.41
13:SM:31:LYS:HE3	13:SM:31:LYS:HB2	1.96	0.41
23:23:151:C:H2'	23:23:152:A:C8	2.56	0.41
23:23:279:A:H3'	23:23:280:U:C6	2.56	0.41
23:23:2305:U:H5"	28:LE:131:GLY:HA3	2.03	0.41
27:LD:119:ILE:O	27:LD:187:VAL:HA	2.21	0.41
28:LE:56:ASP:OD2	28:LE:150:ARG:NH2	2.46	0.41
30:LI:68:ARG:NH1	30:LI:109:GLU:O	2.53	0.41
33:LO:110:VAL:HB	33:LO:127:VAL:HG13	2.02	0.41
43:LY:51:GLN:HE22	43:LY:79:ARG:HH12	1.68	0.41
21:SU:40:LYS:HB3	21:SU:40:LYS:HE2	1.89	0.41
23:23:481:G:O2'	23:23:507:A:N1	2.44	0.41
36:LR:4:LYS:O	36:LR:8:ILE:HG12	2.21	0.41
8:SH:50:LYS:NZ	8:SH:52:GLU:OE2	2.44	0.40
17:SQ:81:LYS:HE2	17:SQ:81:LYS:HB3	1.92	0.40
23:23:5:A:H2'	23:23:6:A:C8	2.56	0.40
23:23:1880:U:H2'	23:23:1881:C:C6	2.56	0.40
27:LD:153:LEU:HD12	27:LD:153:LEU:HA	1.93	0.40
28:LE:141:ILE:H	28:LE:141:ILE:HG13	1.74	0.40
5:SE:156:LYS:HG2	8:SH:71:VAL:HG13	2.01	0.40
7:SG:129:GLU:O	7:SG:131:LYS:NZ	2.54	0.40
19:SS:18:LYS:HB2	19:SS:18:LYS:HE2	1.86	0.40
23:23:1172:C:H2'	23:23:1173:U:O4'	2.21	0.40
23:23:1667:G:O2'	23:23:1991:U:O4	2.38	0.40
34:LP:63:ILE:HG12	34:LP:105:MET:HG3	2.03	0.40
41:LW:51:PHE:CD2	41:LW:93:LEU:HD21	2.56	0.40
1:16:1144:G:N2	1:16:1146:A:H62	2.20	0.40
18:SR:41:PRO:HG2	18:SR:44:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LF:29:LYS:H	29:LF:29:LYS:HG2	1.64	0.40
1:16:1179:A:H2'	1:16:1180:A:O4'	2.21	0.40
2:SB:68:LEU:HD23	2:SB:161:LEU:HD11	2.03	0.40
3:SC:36:ASP:OD1	3:SC:59:ARG:NH1	2.55	0.40
7:SG:53:ARG:HE	7:SG:53:ARG:HB2	1.57	0.40
14:SN:62:ASN:HD22	14:SN:62:ASN:HA	1.69	0.40
23:23:848:C:H2'	23:23:849:A:C8	2.54	0.40
23:23:948:C:H2'	23:23:949:G:H8	1.85	0.40
23:23:2233:U:H2'	23:23:2234:G:C8	2.56	0.40
23:23:2898:U:H2'	23:23:2899:A:H8	1.85	0.40
31:LM:77:HIS:CD2	31:LM:79:GLY:H	2.39	0.40
1:16:1513:A:H2'	1:16:1514:G:C8	2.56	0.40
14:SN:10:GLU:HG3	14:SN:63:ARG:HD2	2.03	0.40
23:23:1278:C:H2'	23:23:1279:G:H8	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	SB	227/241 (94%)	216 (95%)	10 (4%)	1 (0%)	30 44
3	SC	210/233 (90%)	205 (98%)	5 (2%)	0	100 100
4	SD	203/206 (98%)	203 (100%)	0	0	100 100
5	SE	156/167 (93%)	154 (99%)	2 (1%)	0	100 100
6	SF	104/135 (77%)	102 (98%)	2 (2%)	0	100 100
7	SG	155/179 (87%)	152 (98%)	3 (2%)	0	100 100
8	SH	127/130 (98%)	121 (95%)	6 (5%)	0	100 100
9	SI	125/130 (96%)	121 (97%)	4 (3%)	0	100 100
10	SJ	97/103 (94%)	92 (95%)	4 (4%)	1 (1%)	13 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	SK	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
12	SL	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
13	SM	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	SN	98/101 (97%)	98 (100%)	0	0	100	100
15	SO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	SP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	SQ	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
18	SR	65/75 (87%)	61 (94%)	4 (6%)	0	100	100
19	SS	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
20	ST	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	SU	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
25	LB	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
26	LC	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
27	LD	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
28	LE	176/179 (98%)	168 (96%)	7 (4%)	1 (1%)	22	33
29	LF	173/177 (98%)	165 (95%)	8 (5%)	0	100	100
30	LI	147/149 (99%)	134 (91%)	13 (9%)	0	100	100
31	LM	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
32	LN	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	LO	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
34	LP	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
35	LQ	118/127 (93%)	116 (98%)	2 (2%)	0	100	100
36	LR	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
37	LS	111/115 (96%)	109 (98%)	2 (2%)	0	100	100
38	LT	115/118 (98%)	115 (100%)	0	0	100	100
39	LU	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
40	LV	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
41	LW	93/100 (93%)	92 (99%)	0	1 (1%)	12	18
42	LX	100/104 (96%)	92 (92%)	6 (6%)	2 (2%)	6	8
43	LY	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
44	La	82/85 (96%)	79 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	Lb	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
46	Lc	60/63 (95%)	60 (100%)	0	0	100	100
47	Ld	56/59 (95%)	56 (100%)	0	0	100	100
48	Le	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
49	Lf	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
50	Lg	50/55 (91%)	48 (96%)	2 (4%)	0	100	100
51	Lh	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	Li	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
53	Lj	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	5637/5913 (95%)	5473 (97%)	158 (3%)	6 (0%)	50	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	SB	164	ILE
28	LE	21	ASN
42	LX	98	SER
42	LX	100	SER
10	SJ	57	VAL
41	LW	2	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SB	190/199 (96%)	181 (95%)	9 (5%)	22	38
3	SC	172/190 (90%)	159 (92%)	13 (8%)	11	18
4	SD	172/173 (99%)	162 (94%)	10 (6%)	17	29
5	SE	120/126 (95%)	115 (96%)	5 (4%)	25	43
6	SF	92/116 (79%)	90 (98%)	2 (2%)	47	67
7	SG	130/147 (88%)	118 (91%)	12 (9%)	7	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	SH	104/105 (99%)	100 (96%)	4 (4%)	28 47
9	SI	105/107 (98%)	100 (95%)	5 (5%)	21 37
10	SJ	87/90 (97%)	80 (92%)	7 (8%)	10 16
11	SK	91/98 (93%)	84 (92%)	7 (8%)	10 17
12	SL	102/103 (99%)	93 (91%)	9 (9%)	8 13
13	SM	93/96 (97%)	87 (94%)	6 (6%)	14 24
14	SN	83/84 (99%)	81 (98%)	2 (2%)	44 64
15	SO	76/77 (99%)	71 (93%)	5 (7%)	14 23
16	SP	65/65 (100%)	64 (98%)	1 (2%)	60 77
17	SQ	74/78 (95%)	66 (89%)	8 (11%)	5 7
18	SR	58/65 (89%)	58 (100%)	0	100 100
19	SS	72/79 (91%)	68 (94%)	4 (6%)	17 30
20	ST	65/66 (98%)	64 (98%)	1 (2%)	60 77
21	SU	60/61 (98%)	53 (88%)	7 (12%)	4 6
25	LB	216/218 (99%)	207 (96%)	9 (4%)	25 43
26	LC	164/164 (100%)	156 (95%)	8 (5%)	21 36
27	LD	165/165 (100%)	160 (97%)	5 (3%)	36 57
28	LE	149/150 (99%)	139 (93%)	10 (7%)	13 23
29	LF	136/138 (99%)	125 (92%)	11 (8%)	9 15
30	LI	114/114 (100%)	99 (87%)	15 (13%)	3 4
31	LM	116/116 (100%)	116 (100%)	0	100 100
32	LN	104/104 (100%)	96 (92%)	8 (8%)	10 17
33	LO	103/103 (100%)	97 (94%)	6 (6%)	17 29
34	LP	109/108 (101%)	106 (97%)	3 (3%)	38 59
35	LQ	100/103 (97%)	98 (98%)	2 (2%)	50 70
36	LR	86/87 (99%)	84 (98%)	2 (2%)	45 66
37	LS	98/100 (98%)	92 (94%)	6 (6%)	15 27
38	LT	89/90 (99%)	85 (96%)	4 (4%)	23 40
39	LU	84/84 (100%)	81 (96%)	3 (4%)	30 49
40	LV	93/93 (100%)	87 (94%)	6 (6%)	14 24
41	LW	82/84 (98%)	75 (92%)	7 (8%)	8 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	LX	83/85 (98%)	79 (95%)	4 (5%)	21 37
43	LY	78/78 (100%)	76 (97%)	2 (3%)	41 62
44	La	62/63 (98%)	61 (98%)	1 (2%)	58 76
45	Lb	67/68 (98%)	66 (98%)	1 (2%)	60 77
46	Lc	54/55 (98%)	54 (100%)	0	100 100
47	Ld	48/49 (98%)	41 (85%)	7 (15%)	2 3
48	Le	60/62 (97%)	53 (88%)	7 (12%)	4 6
49	Lf	47/48 (98%)	44 (94%)	3 (6%)	14 24
50	Lg	47/49 (96%)	47 (100%)	0	100 100
51	Lh	38/38 (100%)	36 (95%)	2 (5%)	19 33
52	Li	51/52 (98%)	50 (98%)	1 (2%)	50 70
53	Lj	34/34 (100%)	32 (94%)	2 (6%)	16 28
All	All	4688/4827 (97%)	4436 (95%)	252 (5%)	21 32

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	10	LEU
2	SB	23	TRP
2	SB	50	PHE
2	SB	56	GLU
2	SB	141	LEU
2	SB	161	LEU
2	SB	197	ASP
2	SB	208	ARG
2	SB	225	ARG
3	SC	16	LYS
3	SC	21	THR
3	SC	59	ARG
3	SC	62	LYS
3	SC	82	GLU
3	SC	88	ARG
3	SC	93	ASP
3	SC	100	GLN
3	SC	112	ASP
3	SC	121	THR
3	SC	185	ASN
3	SC	187	SER

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Mol	Chain	Res	Type
3	SC	204	LYS
4	SD	20	PHE
4	SD	35	GLU
4	SD	45	LYS
4	SD	83	LYS
4	SD	143	VAL
4	SD	144	SER
4	SD	148	LYS
4	SD	151	LYS
4	SD	174	ASP
4	SD	177	LYS
5	SE	23	LYS
5	SE	71	MET
5	SE	131	THR
5	SE	132	ASN
5	SE	152	MET
6	SF	15	SER
6	SF	93	LYS
7	SG	5	ARG
7	SG	11	LYS
7	SG	15	ASP
7	SG	79	ARG
7	SG	90	GLU
7	SG	92	ARG
7	SG	109	ARG
7	SG	111	ARG
7	SG	113	ASP
7	SG	143	ARG
7	SG	154	TYR
7	SG	155	ARG
8	SH	42	GLU
8	SH	89	LYS
8	SH	110	VAL
8	SH	121	LEU
9	SI	22	LYS
9	SI	54	LEU
9	SI	88	MET
9	SI	95	ARG
9	SI	123	ARG
10	SJ	7	ARG
10	SJ	20	GLN
10	SJ	24	GLU

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Mol	Chain	Res	Type
10	SJ	36	VAL
10	SJ	89	ARG
10	SJ	92	LEU
10	SJ	100	ILE
11	SK	37	ARG
11	SK	81	ASN
11	SK	93	ARG
11	SK	98	ARG
11	SK	106	ARG
11	SK	109	ASN
11	SK	126	LYS
12	SL	14	ARG
12	SL	18	LYS
12	SL	43	LYS
12	SL	44	LYS
12	SL	47	SER
12	SL	65	SER
12	SL	86	ARG
12	SL	105	SER
12	SL	108	LYS
13	SM	9	ILE
13	SM	12	HIS
13	SM	14	HIS
13	SM	16	VAL
13	SM	107	ARG
13	SM	113	ARG
14	SN	26	GLU
14	SN	54	ASP
15	SO	10	LYS
15	SO	62	GLN
15	SO	64	ARG
15	SO	73	LYS
15	SO	84	ARG
16	SP	46	LYS
17	SQ	19	LYS
17	SQ	28	PHE
17	SQ	40	ARG
17	SQ	50	ASN
17	SQ	57	ASP
17	SQ	59	VAL
17	SQ	72	SER
17	SQ	77	ARG

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Mol	Chain	Res	Type
19	SS	29	LYS
19	SS	38	SER
19	SS	47	LEU
19	SS	73	GLU
20	ST	26	SER
21	SU	7	ARG
21	SU	17	ARG
21	SU	24	GLU
21	SU	51	SER
21	SU	59	LYS
21	SU	66	ARG
21	SU	67	ARG
25	LB	13	ARG
25	LB	97	LYS
25	LB	163	GLN
25	LB	183	LYS
25	LB	214	ARG
25	LB	216	VAL
25	LB	242	LYS
25	LB	251	GLN
25	LB	265	LYS
26	LC	1	MET
26	LC	2	ILE
26	LC	9	VAL
26	LC	17	GLU
26	LC	33	ARG
26	LC	89	GLU
26	LC	165	MET
26	LC	186	LEU
27	LD	1	MET
27	LD	6	LYS
27	LD	22	ASP
27	LD	88	ARG
27	LD	184	ASP
28	LE	3	LYS
28	LE	21	ASN
28	LE	42	GLU
28	LE	47	LYS
28	LE	49	LEU
28	LE	71	ARG
28	LE	83	TYR
28	LE	115	ARG

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Mol	Chain	Res	Type
28	LE	145	LYS
28	LE	148	ARG
29	LF	9	VAL
29	LF	35	ARG
29	LF	43	VAL
29	LF	49	THR
29	LF	56	ASP
29	LF	60	ASP
29	LF	74	SER
29	LF	92	VAL
29	LF	101	ASN
29	LF	139	GLN
29	LF	168	VAL
30	LI	1	MET
30	LI	17	ASP
30	LI	48	GLU
30	LI	50	ARG
30	LI	51	ARG
30	LI	54	LEU
30	LI	58	LEU
30	LI	60	GLU
30	LI	109	GLU
30	LI	112	LYS
30	LI	116	ARG
30	LI	117	LEU
30	LI	133	GLN
30	LI	141	LYS
30	LI	149	GLU
32	LN	17	ARG
32	LN	49	ARG
32	LN	58	LEU
32	LN	80	ASP
32	LN	89	ASN
32	LN	108	ARG
32	LN	113	MET
32	LN	114	LYS
33	LO	7	SER
33	LO	14	LYS
33	LO	42	SER
33	LO	121	THR
33	LO	123	ARG
33	LO	126	ARG

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Mol	Chain	Res	Type
34	LP	6	ARG
34	LP	55	ARG
34	LP	105	MET
35	LQ	16	HIS
35	LQ	35	LYS
36	LR	63	LYS
36	LR	91	SER
37	LS	5	ILE
37	LS	6	LYS
37	LS	19	SER
37	LS	38	LYS
37	LS	75	GLN
37	LS	85	SER
38	LT	14	HIS
38	LT	28	ARG
38	LT	51	ARG
38	LT	112	LYS
39	LU	1	MET
39	LU	43	ASN
39	LU	51	VAL
40	LV	1	MET
40	LV	7	HIS
40	LV	73	LYS
40	LV	95	ARG
40	LV	98	LYS
40	LV	109	ASP
41	LW	24	MET
41	LW	49	LYS
41	LW	59	ASN
41	LW	64	LYS
41	LW	93	LEU
41	LW	94	ASP
41	LW	95	PHE
42	LX	15	THR
42	LX	21	LYS
42	LX	27	ASN
42	LX	99	ASN
43	LY	34	LYS
43	LY	71	LYS
44	La	5	LYS
45	Lb	77	LYS
47	Ld	3	LYS

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Mol	Chain	Res	Type
47	Ld	5	ILE
47	Ld	16	ARG
47	Ld	54	MET
47	Ld	56	LYS
47	Ld	58	GLU
47	Ld	59	GLU
48	Le	13	THR
48	Le	25	ARG
48	Le	34	LEU
48	Le	51	VAL
48	Le	62	LYS
48	Le	65	ASN
48	Le	66	ILE
49	Lf	27	SER
49	Lf	52	ARG
49	Lf	53	LYS
51	Lh	1	MET
51	Lh	41	ARG
52	Li	31	HIS
53	Lj	15	LYS
53	Lj	36	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	51	ASN
2	SB	203	ASN
4	SD	54	GLN
4	SD	59	GLN
4	SD	71	GLN
4	SD	89	ASN
4	SD	100	ASN
4	SD	126	ASN
4	SD	136	GLN
5	SE	12	GLN
5	SE	19	ASN
5	SE	132	ASN
6	SF	14	GLN
6	SF	17	GLN
6	SF	63	ASN
7	SG	122	ASN
7	SG	142	HIS

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Mol	Chain	Res	Type
8	SH	18	GLN
8	SH	67	GLN
9	SI	31	ASN
10	SJ	4	GLN
10	SJ	64	GLN
10	SJ	99	GLN
11	SK	40	ASN
11	SK	81	ASN
11	SK	109	ASN
12	SL	112	GLN
14	SN	60	GLN
14	SN	62	ASN
15	SO	28	GLN
15	SO	40	GLN
16	SP	26	ASN
16	SP	63	GLN
16	SP	79	ASN
18	SR	31	ASN
18	SR	74	HIS
19	SS	69	HIS
20	ST	52	ASN
20	ST	55	GLN
25	LB	153	GLN
25	LB	230	HIS
26	LC	32	ASN
26	LC	150	GLN
26	LC	173	GLN
27	LD	41	GLN
27	LD	90	GLN
27	LD	97	ASN
27	LD	195	GLN
28	LE	127	ASN
29	LF	38	ASN
29	LF	101	ASN
29	LF	116	GLN
30	LI	28	ASN
31	LM	77	HIS
31	LM	128	ASN
32	LN	82	ASN
33	LO	93	ASN
34	LP	3	GLN
34	LP	17	ASN

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Mol	Chain	Res	Type
34	LP	97	GLN
35	LQ	11	ASN
35	LQ	81	ASN
35	LQ	107	ASN
37	LS	12	GLN
37	LS	75	GLN
38	LT	14	HIS
40	LV	15	GLN
40	LV	31	GLN
40	LV	40	ASN
40	LV	57	ASN
41	LW	59	ASN
42	LX	53	ASN
42	LX	99	ASN
43	LY	75	GLN
43	LY	78	GLN
45	Lb	23	ASN
46	Lc	20	ASN
46	Lc	25	GLN
46	Lc	39	GLN
48	Le	61	ASN
49	Lf	5	GLN
49	Lf	6	ASN
50	Lg	46	HIS
52	Li	31	HIS
53	Lj	37	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1538/1542 (99%)	246 (15%)	6 (0%)
22	mR	17/60 (28%)	6 (35%)	0
23	23	2761/2904 (95%)	385 (13%)	20 (0%)
24	5	119/120 (99%)	16 (13%)	1 (0%)
54	Pt	76/77 (98%)	8 (10%)	0
All	All	4511/4703 (95%)	661 (14%)	27 (0%)

All (661) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	2	A

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Mol	Chain	Res	Type
1	16	5	U
1	16	6	G
1	16	9	G
1	16	16	A
1	16	22	G
1	16	32	A
1	16	39	G
1	16	47	C
1	16	48	C
1	16	50	A
1	16	51	A
1	16	60	A
1	16	69	G
1	16	71	A
1	16	75	G
1	16	76	G
1	16	77	A
1	16	79	G
1	16	81	A
1	16	82	G
1	16	83	C
1	16	84	U
1	16	85	U
1	16	86	G
1	16	87	C
1	16	88	U
1	16	92	U
1	16	94	G
1	16	95	C
1	16	97	G
1	16	98	A
1	16	121	U
1	16	122	G
1	16	130	A
1	16	131	A
1	16	137	U
1	16	138	G
1	16	140	U
1	16	141	G
1	16	151	A
1	16	159	G
1	16	163	C

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Mol	Chain	Res	Type
1	16	164	G
1	16	177	G
1	16	182	A
1	16	191	G
1	16	197	A
1	16	198	G
1	16	201	G
1	16	206	C
1	16	209	U
1	16	210	C
1	16	217	C
1	16	226	G
1	16	240	G
1	16	245	U
1	16	247	G
1	16	251	G
1	16	266	G
1	16	267	C
1	16	289	G
1	16	301	G
1	16	306	A
1	16	321	A
1	16	328	C
1	16	329	A
1	16	330	C
1	16	332	G
1	16	352	C
1	16	354	G
1	16	367	U
1	16	372	C
1	16	384	G
1	16	388	G
1	16	398	U
1	16	406	G
1	16	413	G
1	16	414	A
1	16	421	U
1	16	422	C
1	16	424	G
1	16	429	U
1	16	436	C
1	16	453	G

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Mol	Chain	Res	Type
1	16	467	U
1	16	468	A
1	16	479	U
1	16	484	G
1	16	486	U
1	16	495	A
1	16	496	A
1	16	497	G
1	16	509	A
1	16	511	C
1	16	518	C
1	16	521	G
1	16	524	G
1	16	527	G7M
1	16	533	A
1	16	545	C
1	16	547	A
1	16	548	G
1	16	559	A
1	16	562	U
1	16	564	C
1	16	572	A
1	16	573	A
1	16	576	C
1	16	577	G
1	16	579	A
1	16	596	A
1	16	633	G
1	16	650	G
1	16	653	U
1	16	665	A
1	16	686	U
1	16	687	A
1	16	704	A
1	16	721	G
1	16	723	U
1	16	724	G
1	16	733	G
1	16	755	G
1	16	777	A
1	16	792	A
1	16	793	U

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Mol	Chain	Res	Type
1	16	794	A
1	16	815	A
1	16	817	C
1	16	828	U
1	16	832	G
1	16	836	G
1	16	840	C
1	16	841	C
1	16	842	U
1	16	843	U
1	16	844	G
1	16	845	A
1	16	846	G
1	16	856	C
1	16	914	A
1	16	922	G
1	16	926	G
1	16	931	C
1	16	934	C
1	16	935	A
1	16	937	A
1	16	945	G
1	16	960	U
1	16	969	A
1	16	975	A
1	16	976	G
1	16	977	A
1	16	978	A
1	16	989	U
1	16	992	U
1	16	993	G
1	16	1004	A
1	16	1006	C
1	16	1016	A
1	16	1017	U
1	16	1020	A
1	16	1025	U
1	16	1030	U
1	16	1031	C
1	16	1032	G
1	16	1033	G
1	16	1042	A

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Mol	Chain	Res	Type
1	16	1043	G
1	16	1044	A
1	16	1066	C
1	16	1070	U
1	16	1085	U
1	16	1094	G
1	16	1095	U
1	16	1101	A
1	16	1124	G
1	16	1133	G
1	16	1135	U
1	16	1136	C
1	16	1137	C
1	16	1138	G
1	16	1139	G
1	16	1140	C
1	16	1141	C
1	16	1143	G
1	16	1151	A
1	16	1158	C
1	16	1159	U
1	16	1167	A
1	16	1184	G
1	16	1196	A
1	16	1197	A
1	16	1212	U
1	16	1213	A
1	16	1226	C
1	16	1227	A
1	16	1228	C
1	16	1238	A
1	16	1239	A
1	16	1243	C
1	16	1250	A
1	16	1256	A
1	16	1257	A
1	16	1258	G
1	16	1260	G
1	16	1261	A
1	16	1270	G
1	16	1280	A
1	16	1285	A

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Mol	Chain	Res	Type
1	16	1287	A
1	16	1290	G
1	16	1300	G
1	16	1305	G
1	16	1317	C
1	16	1320	C
1	16	1323	G
1	16	1340	A
1	16	1346	A
1	16	1351	U
1	16	1353	G
1	16	1363	A
1	16	1364	U
1	16	1370	G
1	16	1383	C
1	16	1394	A
1	16	1419	G
1	16	1422	G
1	16	1440	U
1	16	1441	A
1	16	1451	U
1	16	1452	C
1	16	1454	G
1	16	1492	A
1	16	1493	A
1	16	1494	G
1	16	1497	G
1	16	1499	A
1	16	1503	A
1	16	1506	U
1	16	1517	G
1	16	1529	G
1	16	1530	G
1	16	1534	A
1	16	1537	U
22	mR	23	U
22	mR	26	A
22	mR	28	G
22	mR	29	G
22	mR	30	A
22	mR	31	C
23	23	10	A

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Mol	Chain	Res	Type
23	23	15	G
23	23	34	U
23	23	45	G
23	23	46	G
23	23	71	A
23	23	74	A
23	23	75	G
23	23	80	G
23	23	84	A
23	23	88	G
23	23	91	A
23	23	101	A
23	23	102	U
23	23	110	G
23	23	118	A
23	23	119	A
23	23	120	U
23	23	125	A
23	23	139	U
23	23	163	C
23	23	181	A
23	23	196	A
23	23	199	A
23	23	205	G
23	23	215	G
23	23	216	A
23	23	221	A
23	23	222	A
23	23	225	C
23	23	233	A
23	23	239	C
23	23	242	G
23	23	248	G
23	23	252	G
23	23	265	A
23	23	266	G
23	23	271	G
23	23	276	U
23	23	278	A
23	23	279	A
23	23	281	C
23	23	283	G

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Mol	Chain	Res	Type
23	23	285	G
23	23	287	G
23	23	288	U
23	23	311	A
23	23	330	A
23	23	346	A
23	23	357	C
23	23	358	U
23	23	359	G
23	23	360	U
23	23	361	G
23	23	362	A
23	23	367	G
23	23	370	G
23	23	371	A
23	23	372	G
23	23	386	G
23	23	396	G
23	23	401	A
23	23	403	U
23	23	406	G
23	23	412	A
23	23	455	C
23	23	467	G
23	23	470	A
23	23	481	G
23	23	491	G
23	23	505	A
23	23	509	C
23	23	513	A
23	23	528	A
23	23	531	C
23	23	532	A
23	23	533	G
23	23	546	U
23	23	547	A
23	23	563	A
23	23	573	U
23	23	574	A
23	23	575	A
23	23	603	A
23	23	615	U

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Mol	Chain	Res	Type
23	23	634	C
23	23	637	A
23	23	645	C
23	23	647	G
23	23	654	A
23	23	670	A
23	23	686	U
23	23	717	C
23	23	728	G
23	23	730	A
23	23	740	C
23	23	747	5MU
23	23	753	A
23	23	770	G
23	23	775	G
23	23	776	G
23	23	782	A
23	23	784	G
23	23	785	G
23	23	805	G
23	23	812	C
23	23	819	A
23	23	827	U
23	23	828	U
23	23	845	A
23	23	846	U
23	23	859	G
23	23	869	G
23	23	878	A
23	23	882	G
23	23	884	U
23	23	888	C
23	23	890	C
23	23	891	G
23	23	895	U
23	23	896	A
23	23	897	C
23	23	907	G
23	23	910	A
23	23	914	G
23	23	917	A
23	23	930	G

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Mol	Chain	Res	Type
23	23	931	U
23	23	932	U
23	23	941	A
23	23	946	C
23	23	957	C
23	23	961	C
23	23	974	G
23	23	980	A
23	23	983	A
23	23	984	A
23	23	985	C
23	23	996	A
23	23	1012	U
23	23	1013	C
23	23	1026	G
23	23	1033	U
23	23	1045	C
23	23	1046	A
23	23	1048	A
23	23	1108	U
23	23	1110	G
23	23	1111	A
23	23	1112	G
23	23	1128	G
23	23	1130	U
23	23	1132	U
23	23	1133	A
23	23	1134	A
23	23	1135	C
23	23	1136	G
23	23	1142	A
23	23	1168	G
23	23	1171	G
23	23	1172	C
23	23	1173	U
23	23	1176	U
23	23	1178	C
23	23	1179	G
23	23	1206	G
23	23	1212	G
23	23	1227	G
23	23	1247	A

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Mol	Chain	Res	Type
23	23	1252	G
23	23	1253	A
23	23	1256	G
23	23	1266	G
23	23	1271	G
23	23	1272	A
23	23	1273	U
23	23	1300	G
23	23	1301	A
23	23	1302	A
23	23	1329	U
23	23	1344	U
23	23	1352	U
23	23	1360	G
23	23	1365	A
23	23	1368	G
23	23	1374	G
23	23	1378	A
23	23	1379	U
23	23	1383	A
23	23	1416	G
23	23	1417	C
23	23	1419	A
23	23	1421	G
23	23	1428	C
23	23	1452	G
23	23	1453	A
23	23	1461	C
23	23	1475	G
23	23	1482	G
23	23	1489	C
23	23	1490	A
23	23	1493	C
23	23	1494	A
23	23	1497	U
23	23	1509	A
23	23	1515	A
23	23	1524	G
23	23	1536	C
23	23	1537	G
23	23	1538	G
23	23	1554	U

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Mol	Chain	Res	Type
23	23	1566	A
23	23	1569	A
23	23	1578	U
23	23	1583	A
23	23	1584	U
23	23	1585	C
23	23	1607	C
23	23	1608	A
23	23	1639	C
23	23	1647	U
23	23	1648	U
23	23	1649	G
23	23	1663	G
23	23	1664	A
23	23	1674	G
23	23	1729	U
23	23	1730	C
23	23	1732	C
23	23	1738	G
23	23	1756	G
23	23	1764	C
23	23	1773	A
23	23	1776	G
23	23	1782	U
23	23	1799	G
23	23	1800	C
23	23	1801	A
23	23	1808	A
23	23	1811	G
23	23	1816	C
23	23	1829	A
23	23	1848	A
23	23	1862	G
23	23	1872	A
23	23	1873	G
23	23	1884	G
23	23	1885	A
23	23	1906	G
23	23	1913	A
23	23	1914	C
23	23	1919	A
23	23	1929	G

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Mol	Chain	Res	Type
23	23	1930	G
23	23	1937	A
23	23	1938	A
23	23	1955	U
23	23	1964	G
23	23	1967	C
23	23	1969	A
23	23	1970	A
23	23	1971	U
23	23	1972	G
23	23	1982	U
23	23	1991	U
23	23	1993	U
23	23	1997	C
23	23	2023	C
23	23	2031	A
23	23	2032	G
23	23	2033	A
23	23	2043	C
23	23	2049	G
23	23	2055	C
23	23	2056	G
23	23	2060	A
23	23	2061	G
23	23	2062	A
23	23	2063	C
23	23	2069	G7M
23	23	2093	G
23	23	2096	C
23	23	2103	C
23	23	2191	A
23	23	2198	A
23	23	2204	G
23	23	2211	A
23	23	2225	A
23	23	2238	G
23	23	2239	G
23	23	2268	A
23	23	2278	A
23	23	2283	C
23	23	2287	A
23	23	2288	A

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Mol	Chain	Res	Type
23	23	2305	U
23	23	2307	G
23	23	2308	G
23	23	2311	A
23	23	2319	G
23	23	2322	A
23	23	2325	G
23	23	2333	A
23	23	2336	A
23	23	2343	U
23	23	2345	G
23	23	2347	C
23	23	2350	C
23	23	2357	G
23	23	2379	G
23	23	2383	G
23	23	2385	C
23	23	2402	U
23	23	2406	A
23	23	2423	U
23	23	2425	A
23	23	2428	G
23	23	2429	G
23	23	2430	A
23	23	2435	A
23	23	2441	U
23	23	2448	A
23	23	2459	A
23	23	2469	A
23	23	2470	G
23	23	2476	A
23	23	2482	A
23	23	2484	G
23	23	2491	U
23	23	2494	G
23	23	2502	G
23	23	2504	PSU
23	23	2505	G
23	23	2506	U
23	23	2518	A
23	23	2529	G
23	23	2547	A

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Mol	Chain	Res	Type
23	23	2554	U
23	23	2556	C
23	23	2566	A
23	23	2567	G
23	23	2573	C
23	23	2602	A
23	23	2608	G
23	23	2609	U
23	23	2613	U
23	23	2615	U
23	23	2629	U
23	23	2630	G
23	23	2636	C
23	23	2655	G
23	23	2661	G
23	23	2663	G
23	23	2689	U
23	23	2690	U
23	23	2714	G
23	23	2716	C
23	23	2726	A
23	23	2732	G
23	23	2733	A
23	23	2739	U
23	23	2744	G
23	23	2748	A
23	23	2757	A
23	23	2765	A
23	23	2778	A
23	23	2791	G
23	23	2797	U
23	23	2798	U
23	23	2799	A
23	23	2801	G
23	23	2818	U
23	23	2820	A
23	23	2821	A
23	23	2823	A
23	23	2835	A
23	23	2867	G
23	23	2872	A
23	23	2873	A

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Mol	Chain	Res	Type
23	23	2877	G
23	23	2879	A
23	23	2883	A
23	23	2884	U
23	23	2886	A
23	23	2891	U
24	5	32	U
24	5	33	G
24	5	34	A
24	5	35	C
24	5	44	G
24	5	45	A
24	5	56	G
24	5	66	A
24	5	67	G
24	5	73	A
24	5	89	U
24	5	90	C
24	5	99	A
24	5	105	G
24	5	109	A
24	5	119	A
54	Pt	9	G
54	Pt	14	A
54	Pt	21	H2U
54	Pt	22	A
54	Pt	39	A
54	Pt	47	G7M
54	Pt	60	A
54	Pt	77	A

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16	80	A
1	16	83	C
1	16	438	U
1	16	843	U
1	16	1043	G
1	16	1136	C
23	23	242	G
23	23	249	C

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Mol	Chain	Res	Type
23	23	278	A
23	23	411	G
23	23	573	U
23	23	784	G
23	23	827	U
23	23	973	A
23	23	984	A
23	23	1110	G
23	23	1111	A
23	23	1141	U
23	23	1489	C
23	23	1490	A
23	23	2062	A
23	23	2324	U
23	23	2430	A
23	23	2756	U
23	23	2798	U
23	23	2873	A
24	5	34	A

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

40 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	$\#\|Z\| > 2$
1	5MC	16	967	1	19,22,23	1.50	3 (15%)	26,32,35	1.10	2 (7%)
12	D2T	SL	89	12	8,9,10	7.08	2 (25%)	6,11,13	2.60	3 (50%)
1	G7M	16	527	1	20,26,27	1.16	3 (15%)	16,39,42	0.42	0
23	5MU	23	747	23	19,22,23	1.42	6 (31%)	27,32,35	2.05	10 (37%)
23	1MG	23	745	23	19,26,27	0.87	1 (5%)	18,39,42	1.28	3 (16%)
54	H2U	Pt	21	54	18,21,22	0.93	2 (11%)	19,30,33	0.94	0
1	5MC	16	1407	1	19,22,23	1.38	2 (10%)	26,32,35	1.41	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MG	16	1516	1	18,26,27	0.89	1 (5%)	16,38,41	1.43	4 (25%)
34	4D4	LP	81	34	9,11,12	2.03	2 (22%)	7,13,15	1.78	3 (42%)
23	6MZ	23	1618	23	17,25,26	0.92	1 (5%)	15,36,39	2.11	4 (26%)
23	2MG	23	1835	23	18,26,27	0.87	1 (5%)	16,38,41	1.46	4 (25%)
11	IAS	SK	119	11	6,7,8	1.33	1 (16%)	3,8,10	0.65	0
23	PSU	23	2457	23	18,21,22	1.42	3 (16%)	21,30,33	2.05	5 (23%)
23	G7M	23	2069	23	20,26,27	1.17	3 (15%)	16,39,42	0.53	0
23	PSU	23	2605	23	18,21,22	1.47	3 (16%)	21,30,33	2.07	5 (23%)
54	G7M	Pt	47	54	20,26,27	2.58	4 (20%)	16,39,42	1.12	2 (12%)
23	3TD	23	1915	23	19,22,23	1.26	2 (10%)	23,32,35	2.02	3 (13%)
1	UR3	16	1498	1	19,22,23	0.89	0	26,32,35	1.81	4 (15%)
23	PSU	23	955	23	18,21,22	1.38	4 (22%)	21,30,33	2.07	3 (14%)
23	H2U	23	2449	23	18,21,22	1.10	2 (11%)	19,30,33	1.07	1 (5%)
23	5MU	23	1939	58,23	19,22,23	1.37	5 (26%)	27,32,35	2.31	6 (22%)
1	2MG	16	966	1	18,26,27	0.91	1 (5%)	16,38,41	1.11	2 (12%)
54	OMC	Pt	33	54	19,22,23	0.85	0	25,31,34	1.29	3 (12%)
23	6MZ	23	2030	23	17,25,26	0.84	0	15,36,39	2.89	4 (26%)
23	OMC	23	2498	57,23	19,22,23	0.84	0	25,31,34	1.13	2 (8%)
23	2MA	23	2503	58,57,23	18,25,26	0.90	0	20,37,40	1.66	5 (25%)
23	PSU	23	2604	23	18,21,22	1.43	3 (16%)	21,30,33	2.13	3 (14%)
1	4OC	16	1402	1,57	20,23,24	0.78	0	25,32,35	2.15	7 (28%)
1	PSU	16	516	1,57	18,21,22	1.43	4 (22%)	21,30,33	2.04	4 (19%)
1	MA6	16	1518	1	19,26,27	1.12	2 (10%)	18,38,41	2.28	4 (22%)
1	MA6	16	1519	1	19,26,27	1.04	1 (5%)	18,38,41	2.16	3 (16%)
23	2MG	23	2445	23	18,26,27	0.92	1 (5%)	16,38,41	1.20	2 (12%)
23	PSU	23	746	57,23	18,21,22	1.45	3 (16%)	21,30,33	2.16	5 (23%)
23	PSU	23	2580	23	18,21,22	1.40	3 (16%)	21,30,33	2.28	4 (19%)
23	PSU	23	2504	58,23	18,21,22	0.91	1 (5%)	21,30,33	0.74	0
23	OMU	23	2552	23	19,22,23	1.17	3 (15%)	25,31,34	1.88	6 (24%)
23	5MC	23	1962	58,23	19,22,23	1.54	3 (15%)	26,32,35	0.98	2 (7%)
23	OMG	23	2251	54,23	19,26,27	0.95	1 (5%)	21,38,41	1.05	2 (9%)
54	4SU	Pt	8	54	18,21,22	1.86	4 (22%)	25,30,33	2.32	5 (20%)
1	2MG	16	1207	1	18,26,27	0.93	1 (5%)	16,38,41	1.20	2 (12%)

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
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	4/7/12/14	-
1	G7M	16	527	1	-	2/3/25/26	0/3/3/3
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
23	1MG	23	745	23	-	0/3/25/26	0/3/3/3
54	H2U	Pt	21	54	-	2/7/38/39	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3
34	4D4	LP	81	34	-	2/11/12/14	-
23	6MZ	23	1618	23	-	4/5/27/28	0/3/3/3
23	2MG	23	1835	23	-	0/5/27/28	0/3/3/3
11	IAS	SK	119	11	-	0/7/7/8	-
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
23	G7M	23	2069	23	-	0/3/25/26	0/3/3/3
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
54	G7M	Pt	47	54	-	2/3/25/26	0/3/3/3
23	3TD	23	1915	23	-	0/7/25/26	0/2/2/2
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
23	5MU	23	1939	58,23	-	0/7/25/26	0/2/2/2
1	2MG	16	966	1	-	0/5/27/28	0/3/3/3
54	OMC	Pt	33	54	-	0/9/27/28	0/2/2/2
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
23	OMC	23	2498	57,23	-	0/9/27/28	0/2/2/2
23	2MA	23	2503	58,57,23	-	1/3/25/26	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
1	4OC	16	1402	1,57	-	2/9/29/30	0/2/2/2
1	PSU	16	516	1,57	-	0/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	16	1519	1	-	3/7/29/30	0/3/3/3
23	2MG	23	2445	23	-	1/5/27/28	0/3/3/3
23	PSU	23	746	57,23	-	1/7/25/26	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
23	PSU	23	2504	58,23	-	0/7/25/26	0/2/2/2
23	OMU	23	2552	23	-	0/9/27/28	0/2/2/2
23	5MC	23	1962	58,23	-	0/7/25/26	0/2/2/2
23	OMG	23	2251	54,23	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4SU	Pt	8	54	-	0/7/25/26	0/2/2/2
1	2MG	16	1207	1	-	0/5/27/28	0/3/3/3

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	SL	89	D2T	CB-CA	-19.05	1.48	1.54
54	Pt	47	G7M	C8-N9	7.20	1.46	1.33
54	Pt	47	G7M	C8-N7	7.02	1.45	1.33
23	23	1962	5MC	C5-C4	5.55	1.48	1.44
1	16	967	5MC	C5-C4	5.36	1.48	1.44
54	Pt	8	4SU	C4-S4	-5.13	1.59	1.68
12	SL	89	D2T	CB-SB	-5.10	1.77	1.82
34	LP	81	4D4	CZ-NE	5.01	1.42	1.33
1	16	1407	5MC	C5-C4	4.49	1.47	1.44
54	Pt	47	G7M	C5-C4	3.95	1.47	1.39
23	23	2605	PSU	C6-C5	3.76	1.39	1.35
23	23	2504	PSU	C6-C5	3.48	1.39	1.35
23	23	2604	PSU	C6-C5	3.46	1.39	1.35
23	23	746	PSU	C6-C5	3.37	1.39	1.35
1	16	527	G7M	C8-N9	3.35	1.39	1.33
23	23	2069	G7M	C8-N9	3.34	1.39	1.33
54	Pt	8	4SU	C4-N3	-3.26	1.34	1.37
23	23	2580	PSU	C6-C5	3.20	1.38	1.35
1	16	1518	MA6	C6-C5	3.17	1.49	1.44
23	23	1915	3TD	C6-C5	3.16	1.38	1.35
1	16	1519	MA6	C6-C5	3.04	1.49	1.44
23	23	746	PSU	C4-N3	-3.01	1.33	1.38
54	Pt	8	4SU	C5-C4	-3.00	1.38	1.42
23	23	747	5MU	C4-N3	-3.00	1.33	1.38
23	23	2457	PSU	C4-N3	-3.00	1.33	1.38
23	23	2605	PSU	C4-N3	-2.98	1.33	1.38
23	23	2457	PSU	C6-C5	2.98	1.38	1.35
1	16	516	PSU	C6-C5	2.97	1.38	1.35
23	23	955	PSU	C6-C5	2.93	1.38	1.35
23	23	2251	OMG	C6-N1	-2.89	1.33	1.37
1	16	516	PSU	C4-N3	-2.88	1.33	1.38
23	23	1939	5MU	C4-N3	-2.87	1.33	1.38
23	23	2449	H2U	C2-N3	-2.84	1.33	1.38
23	23	955	PSU	C4-N3	-2.81	1.33	1.38
23	23	2552	OMU	C4-N3	-2.79	1.33	1.38
1	16	1407	5MC	C6-C5	2.78	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	LP	81	4D4	CZ-NH1	2.75	1.44	1.34
23	23	1939	5MU	C6-C5	2.74	1.39	1.34
23	23	1962	5MC	C6-C5	2.72	1.39	1.34
23	23	2604	PSU	C4-N3	-2.71	1.33	1.38
23	23	1915	3TD	C2-N1	-2.68	1.33	1.37
1	16	966	2MG	C6-N1	-2.67	1.33	1.37
1	16	1207	2MG	C6-N1	-2.61	1.33	1.37
11	SK	119	IAS	CB-CG	2.61	1.56	1.50
54	Pt	47	G7M	C6-N1	-2.55	1.33	1.37
23	23	745	1MG	C2-N1	2.52	1.41	1.37
23	23	1939	5MU	C6-N1	-2.52	1.33	1.38
23	23	747	5MU	C6-C5	2.49	1.38	1.34
23	23	2445	2MG	C6-N1	-2.49	1.34	1.37
23	23	2449	H2U	C4-N3	-2.44	1.33	1.37
23	23	747	5MU	C2-N1	2.43	1.42	1.38
1	16	967	5MC	C6-N1	-2.43	1.33	1.38
23	23	2580	PSU	C4-N3	-2.42	1.34	1.38
1	16	967	5MC	C6-C5	2.41	1.38	1.34
54	Pt	21	H2U	C2-N3	-2.39	1.33	1.38
23	23	1835	2MG	C6-N1	-2.38	1.34	1.37
23	23	2605	PSU	C2-N3	-2.38	1.33	1.37
23	23	747	5MU	C6-N1	-2.38	1.34	1.38
23	23	746	PSU	C2-N3	-2.36	1.33	1.37
23	23	2069	G7M	C5-C6	-2.35	1.39	1.45
23	23	1618	6MZ	C6-C5	2.34	1.48	1.44
1	16	1516	2MG	C6-N1	-2.34	1.34	1.37
1	16	527	G7M	C8-N7	2.29	1.37	1.33
23	23	2457	PSU	C2-N3	-2.29	1.33	1.37
1	16	527	G7M	C5-C6	-2.29	1.39	1.45
1	16	516	PSU	C2-N3	-2.26	1.33	1.37
54	Pt	21	H2U	C4-N3	-2.24	1.33	1.37
23	23	747	5MU	C2-N3	-2.23	1.34	1.38
54	Pt	8	4SU	C2-N3	-2.23	1.34	1.38
23	23	2552	OMU	C5-C4	-2.22	1.38	1.43
23	23	2069	G7M	C8-N7	2.19	1.37	1.33
23	23	1939	5MU	C2-N3	-2.19	1.34	1.38
23	23	2552	OMU	C2-N3	-2.17	1.34	1.38
23	23	1962	5MC	C6-N1	-2.14	1.34	1.38
23	23	955	PSU	C2-N3	-2.13	1.34	1.37
23	23	747	5MU	C4-C5	2.13	1.48	1.44
23	23	2580	PSU	O4'-C1'	-2.12	1.40	1.43
23	23	2604	PSU	C2-N3	-2.11	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	516	PSU	C2-N1	-2.09	1.33	1.36
23	23	1939	5MU	C4-C5	2.06	1.48	1.44
23	23	955	PSU	C2-N1	-2.05	1.34	1.36
1	16	1518	MA6	C6-N1	2.03	1.35	1.32

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2030	6MZ	C2-N1-C6	7.74	122.61	116.60
23	23	746	PSU	N1-C2-N3	7.04	122.60	115.17
23	23	1915	3TD	N1-C2-N3	7.02	121.23	116.13
1	16	1518	MA6	C2-N1-C6	7.01	123.72	116.84
23	23	2580	PSU	N1-C2-N3	6.88	122.43	115.17
1	16	1498	UR3	C4-N3-C2	-6.84	119.08	124.58
54	Pt	8	4SU	C4-N3-C2	-6.80	120.80	127.31
23	23	2604	PSU	N1-C2-N3	6.62	122.15	115.17
23	23	2605	PSU	N1-C2-N3	6.56	122.08	115.17
1	16	1519	MA6	C2-N1-C6	6.45	123.17	116.84
23	23	2457	PSU	N1-C2-N3	6.45	121.97	115.17
1	16	1402	4OC	O2-C2-N3	-6.43	112.19	122.33
23	23	955	PSU	N1-C2-N3	6.36	121.88	115.17
1	16	516	PSU	N1-C2-N3	6.34	121.86	115.17
54	Pt	8	4SU	C5-C4-N3	6.12	120.44	114.75
23	23	1618	6MZ	C2-N1-C6	6.08	121.32	116.60
23	23	2030	6MZ	C9-N6-C6	-5.81	117.46	122.85
23	23	1939	5MU	C4-N3-C2	-5.77	119.78	127.34
23	23	1939	5MU	N3-C2-N1	5.71	122.32	114.89
23	23	747	5MU	N3-C2-N1	5.49	122.03	114.89
23	23	1915	3TD	C4-N3-C2	-5.04	119.27	124.61
23	23	2552	OMU	N3-C2-N1	4.79	121.13	114.89
23	23	747	5MU	C4-N3-C2	-4.69	121.19	127.34
1	16	1402	4OC	C1'-N1-C2	4.67	128.75	118.44
23	23	1939	5MU	C5-C4-N3	4.60	119.32	115.32
23	23	2580	PSU	O2-C2-N1	-4.53	118.12	122.79
23	23	2580	PSU	C4-N3-C2	-4.50	120.17	126.37
23	23	1939	5MU	O4-C4-C5	-4.48	119.79	124.92
23	23	2503	2MA	C5-C6-N6	4.47	127.11	120.31
54	Pt	8	4SU	C5-C4-S4	-4.46	119.22	124.31
1	16	1407	5MC	O2-C2-N3	-4.44	115.33	122.33
23	23	746	PSU	C4-N3-C2	-4.38	120.33	126.37
1	16	1518	MA6	C4-C5-N7	-4.33	104.76	109.34
23	23	955	PSU	C4-N3-C2	-4.26	120.50	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2604	PSU	C4-N3-C2	-4.24	120.53	126.37
12	SL	89	D2T	CB1-SB-CB	4.23	109.97	102.36
23	23	2552	OMU	C4-N3-C2	-4.18	121.43	126.61
23	23	2457	PSU	C4-N3-C2	-4.14	120.66	126.37
1	16	1519	MA6	C4-C5-N7	-4.14	104.96	109.34
1	16	1518	MA6	N3-C2-N1	-4.10	123.11	128.67
54	Pt	8	4SU	N3-C2-N1	4.04	120.15	114.89
23	23	2605	PSU	C4-N3-C2	-4.03	120.82	126.37
23	23	1939	5MU	C5-C6-N1	-4.03	118.94	123.31
23	23	2030	6MZ	N3-C2-N1	-3.97	123.29	128.67
1	16	516	PSU	C4-N3-C2	-3.95	120.94	126.37
23	23	1618	6MZ	N3-C2-N1	-3.94	123.33	128.67
1	16	1519	MA6	N3-C2-N1	-3.88	123.40	128.67
23	23	2604	PSU	O2-C2-N1	-3.80	118.87	122.79
54	Pt	33	OMC	O2-C2-N3	-3.78	116.37	122.33
1	16	1402	4OC	O2-C2-N1	3.76	126.27	118.90
23	23	1939	5MU	O2-C2-N1	-3.59	118.12	122.80
1	16	516	PSU	O2-C2-N1	-3.55	119.13	122.79
23	23	955	PSU	O2-C2-N1	-3.55	119.13	122.79
1	16	1498	UR3	C5-C4-N3	3.49	119.63	115.04
34	LP	81	4D4	NE-CZ-NH2	3.48	126.66	120.67
23	23	2552	OMU	C5-C4-N3	3.46	119.65	114.80
23	23	747	5MU	C5-C4-N3	3.42	118.29	115.32
12	SL	89	D2T	OD2-CG-CB	3.39	120.48	113.15
23	23	2457	PSU	O2-C2-N1	-3.35	119.33	122.79
23	23	746	PSU	O2-C2-N1	-3.34	119.34	122.79
23	23	2498	OMC	O2-C2-N3	-3.31	117.11	122.33
23	23	2030	6MZ	C4-C5-N7	-3.26	105.89	109.34
23	23	1962	5MC	C5-C6-N1	-3.19	119.84	123.31
23	23	2503	2MA	C5-C6-N1	-3.16	117.10	120.84
1	16	967	5MC	C5-C6-N1	-3.16	119.89	123.31
1	16	1516	2MG	C8-N7-C5	3.08	107.79	102.55
23	23	2251	OMG	C8-N7-C5	3.06	107.75	102.55
23	23	2445	2MG	C8-N7-C5	3.02	107.68	102.55
23	23	745	1MG	C8-N7-C5	3.00	107.66	102.55
1	16	1407	5MC	C5-C4-N3	-3.00	118.68	121.75
23	23	1835	2MG	N1-C2-N2	2.95	119.57	116.56
23	23	1835	2MG	C8-N7-C5	2.93	107.53	102.55
1	16	1207	2MG	C8-N7-C5	2.91	107.51	102.55
23	23	747	5MU	O4-C4-C5	-2.91	121.59	124.92
1	16	966	2MG	C8-N7-C5	2.91	107.50	102.55
23	23	2605	PSU	O2-C2-N1	-2.91	119.79	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2552	OMU	O2-C2-N1	-2.89	119.04	122.80
23	23	2552	OMU	O4-C4-C5	-2.88	120.20	125.16
23	23	2552	OMU	C6-N1-C2	-2.80	117.59	121.00
23	23	2449	H2U	C5-C4-N3	2.78	119.65	116.69
1	16	1516	2MG	N1-C2-N2	2.77	119.39	116.56
23	23	747	5MU	C1'-N1-C2	2.77	122.56	117.59
1	16	967	5MC	C5-C4-N3	-2.73	118.95	121.75
54	Pt	33	OMC	C1'-N1-C2	2.72	124.45	118.44
23	23	747	5MU	C5-C6-N1	-2.68	120.41	123.31
54	Pt	47	G7M	CN7-N7-C8	-2.67	112.57	125.43
1	16	1402	4OC	C1'-N1-C6	-2.62	115.18	120.78
23	23	2503	2MA	N3-C2-N1	-2.61	121.19	125.77
1	16	1402	4OC	C6-N1-C2	-2.60	116.06	120.46
23	23	745	1MG	C5-C6-N1	2.55	117.65	113.96
23	23	746	PSU	C5-C6-N1	-2.55	118.61	122.14
23	23	1618	6MZ	C4-C5-N7	-2.54	106.66	109.34
1	16	1498	UR3	C1'-N1-C2	2.52	121.17	117.04
23	23	2580	PSU	O4'-C1'-C2'	2.52	108.64	105.15
23	23	2503	2MA	C2-N1-C6	2.51	121.96	118.10
54	Pt	47	G7M	O4'-C1'-N9	2.51	112.07	108.75
23	23	1962	5MC	C5-C4-N3	-2.51	119.19	121.75
1	16	1402	4OC	C5-C4-N3	-2.50	118.69	122.60
23	23	2503	2MA	CM2-C2-N1	2.43	120.77	117.13
54	Pt	33	OMC	O2-C2-N1	2.37	123.54	118.90
23	23	1915	3TD	C3'-C2'-C1'	2.36	104.47	101.69
23	23	745	1MG	O6-C6-C5	-2.35	120.32	124.18
23	23	747	5MU	O2-C2-N3	-2.33	117.19	121.49
1	16	516	PSU	O4'-C1'-C2'	2.30	108.33	105.15
23	23	1835	2MG	C5-C6-N1	2.29	118.44	114.07
1	16	1402	4OC	C6-C5-C4	2.29	119.75	117.00
23	23	1618	6MZ	C9-N6-C6	-2.24	120.77	122.85
23	23	2251	OMG	C5-C6-N1	2.22	118.31	114.07
12	SL	89	D2T	OD1-CG-CB	-2.19	117.85	122.44
23	23	2445	2MG	C5-C6-N1	2.19	118.25	114.07
23	23	747	5MU	C6-N1-C2	-2.19	119.12	121.30
1	16	1407	5MC	O2-C2-N1	2.18	123.17	118.90
23	23	746	PSU	O2-C2-N3	-2.14	118.06	121.86
1	16	1207	2MG	C5-C6-N1	2.14	118.14	114.07
23	23	2457	PSU	C5-C6-N1	-2.12	119.20	122.14
34	LP	81	4D4	O-C-CA	-2.12	119.33	124.77
1	16	1516	2MG	N2-C2-N3	-2.11	117.82	120.51
23	23	2605	PSU	O2-C2-N3	-2.10	118.12	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16	966	2MG	C5-C6-N1	2.08	118.04	114.07
34	LP	81	4D4	NH1-CZ-NE	-2.06	114.58	119.27
1	16	1516	2MG	C5-C6-N1	2.06	118.00	114.07
1	16	1518	MA6	C9-N6-C6	2.05	125.06	119.40
54	Pt	8	4SU	C1'-N1-C2	2.04	121.26	117.59
23	23	2605	PSU	C5-C6-N1	-2.04	119.31	122.14
23	23	1835	2MG	O6-C6-C5	-2.04	120.28	124.32
23	23	2498	OMC	O2-C2-N1	2.04	122.89	118.90
23	23	747	5MU	C5M-C5-C4	2.04	120.96	118.78
23	23	747	5MU	C5M-C5-C6	-2.03	120.10	122.85
1	16	1498	UR3	C3U-N3-C2	2.02	120.86	117.33
23	23	2457	PSU	O4'-C1'-C2'	2.01	107.93	105.15

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	1402	4OC	O4'-C1'-N1-C2
1	16	1402	4OC	O4'-C1'-N1-C6
1	16	1519	MA6	C5-C6-N6-C9
12	SL	89	D2T	CA-CB-CG-OD1
12	SL	89	D2T	CA-CB-CG-OD2
23	23	1618	6MZ	O4'-C4'-C5'-O5'
23	23	2251	OMG	C1'-C2'-O2'-CM2
1	16	527	G7M	C3'-C4'-C5'-O5'
1	16	1519	MA6	O4'-C4'-C5'-O5'
54	Pt	47	G7M	O4'-C4'-C5'-O5'
54	Pt	47	G7M	C3'-C4'-C5'-O5'
23	23	2030	6MZ	O4'-C4'-C5'-O5'
23	23	1618	6MZ	C3'-C4'-C5'-O5'
23	23	2030	6MZ	C3'-C4'-C5'-O5'
1	16	1519	MA6	C3'-C4'-C5'-O5'
54	Pt	21	H2U	O4'-C4'-C5'-O5'
1	16	527	G7M	O4'-C4'-C5'-O5'
23	23	2445	2MG	C3'-C4'-C5'-O5'
34	LP	81	4D4	OB-CB-CG-CD
12	SL	89	D2T	CG-CB-SB-CB1
34	LP	81	4D4	CA-CB-CG-CD
12	SL	89	D2T	SB-CB-CG-OD2
54	Pt	21	H2U	C3'-C4'-C5'-O5'
23	23	746	PSU	O4'-C1'-C5-C6
23	23	2503	2MA	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
23	23	1618	6MZ	N1-C6-N6-C9
23	23	1618	6MZ	C5-C6-N6-C9

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	23	2030	6MZ	1	0
1	16	1402	4OC	1	0
23	23	2251	OMG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 353 ligands modelled in this entry, 335 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	SPD	23	3014	-	9,9,9	0.15	0	8,8,8	0.21	0
60	ATP	23	3002	-	28,33,33	0.61	0	34,52,52	0.84	2 (5%)
56	SPD	23	3012	-	9,9,9	0.30	0	8,8,8	0.47	0
55	PUT	23	3007	-	5,5,5	0.13	0	4,4,4	0.14	0
55	PUT	16	1601	-	5,5,5	0.11	0	4,4,4	0.21	0
55	PUT	23	3010	-	5,5,5	0.12	0	4,4,4	0.19	0
61	FME	Pt	101	54	8,9,10	0.61	0	8,9,11	1.14	1 (12%)
55	PUT	23	3006	-	5,5,5	0.09	0	4,4,4	0.25	0
55	PUT	23	3009	-	5,5,5	0.10	0	4,4,4	0.23	0
56	SPD	23	3013	-	9,9,9	0.15	0	8,8,8	0.18	0
55	PUT	23	3008	-	5,5,5	0.15	0	4,4,4	0.19	0
56	SPD	23	3015	-	9,9,9	0.32	0	8,8,8	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
60	ATP	23	3001	-	28,33,33	0.64	0	34,52,52	0.64	1 (2%)
55	PUT	23	3005	-	5,5,5	0.12	0	4,4,4	0.19	0
56	SPD	16	1602	-	9,9,9	0.30	0	8,8,8	0.46	0
55	PUT	23	3004	-	5,5,5	0.08	0	4,4,4	0.32	0
55	PUT	23	3011	-	5,5,5	0.14	0	4,4,4	0.16	0
55	PUT	23	3003	-	5,5,5	0.12	0	4,4,4	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SPD	23	3014	-	-	2/7/7/7	-
60	ATP	23	3002	-	-	2/18/38/38	0/3/3/3
56	SPD	23	3012	-	-	4/7/7/7	-
55	PUT	23	3007	-	-	2/3/3/3	-
55	PUT	16	1601	-	-	0/3/3/3	-
55	PUT	23	3010	-	-	0/3/3/3	-
61	FME	Pt	101	54	-	5/7/9/11	-
55	PUT	23	3006	-	-	1/3/3/3	-
55	PUT	23	3009	-	-	0/3/3/3	-
56	SPD	23	3013	-	-	6/7/7/7	-
55	PUT	23	3008	-	-	1/3/3/3	-
56	SPD	23	3015	-	-	4/7/7/7	-
60	ATP	23	3001	-	-	3/18/38/38	0/3/3/3
55	PUT	23	3005	-	-	1/3/3/3	-
56	SPD	16	1602	-	-	5/7/7/7	-
55	PUT	23	3004	-	-	1/3/3/3	-
55	PUT	23	3011	-	-	0/3/3/3	-
55	PUT	23	3003	-	-	1/3/3/3	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	23	3002	ATP	C4'-O4'-C1'	-3.44	106.77	109.92
61	Pt	101	FME	O-C-CA	-2.85	117.43	124.77
60	23	3002	ATP	C5-C6-N6	2.31	123.83	120.31
60	23	3001	ATP	C5-C6-N6	2.30	123.82	120.31

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	Pt	101	FME	O1-CN-N-CA
61	Pt	101	FME	N-CA-CB-CG
60	23	3001	ATP	C3'-C4'-C5'-O5'
61	Pt	101	FME	CA-CB-CG-SD
60	23	3001	ATP	O4'-C4'-C5'-O5'
56	23	3015	SPD	N6-C7-C8-C9
56	23	3013	SPD	N6-C7-C8-C9
56	23	3013	SPD	C4-C5-N6-C7
56	23	3012	SPD	C2-C3-C4-C5
56	23	3015	SPD	C3-C4-C5-N6
56	16	1602	SPD	N6-C7-C8-C9
56	23	3013	SPD	C8-C7-N6-C5
56	23	3013	SPD	C7-C8-C9-N10
56	23	3015	SPD	N1-C2-C3-C4
56	23	3012	SPD	C3-C4-C5-N6
56	23	3014	SPD	N6-C7-C8-C9
56	16	1602	SPD	N1-C2-C3-C4
56	16	1602	SPD	C2-C3-C4-C5
56	23	3012	SPD	C7-C8-C9-N10
61	Pt	101	FME	C-CA-CB-CG
55	23	3004	PUT	C2-C3-C4-N2
55	23	3007	PUT	C1-C2-C3-C4
56	23	3014	SPD	C7-C8-C9-N10
60	23	3002	ATP	PG-O3B-PB-O1B
55	23	3003	PUT	N1-C1-C2-C3
55	23	3006	PUT	C2-C3-C4-N2
55	23	3008	PUT	N1-C1-C2-C3
56	23	3013	SPD	N1-C2-C3-C4
56	23	3012	SPD	C4-C5-N6-C7
61	Pt	101	FME	CB-CG-SD-CE
56	23	3015	SPD	C2-C3-C4-C5
56	23	3013	SPD	C3-C4-C5-N6
55	23	3005	PUT	N1-C1-C2-C3
55	23	3007	PUT	N1-C1-C2-C3
56	16	1602	SPD	C4-C5-N6-C7
56	16	1602	SPD	C7-C8-C9-N10
60	23	3001	ATP	PG-O3B-PB-O2B
60	23	3002	ATP	PG-O3B-PB-O2B

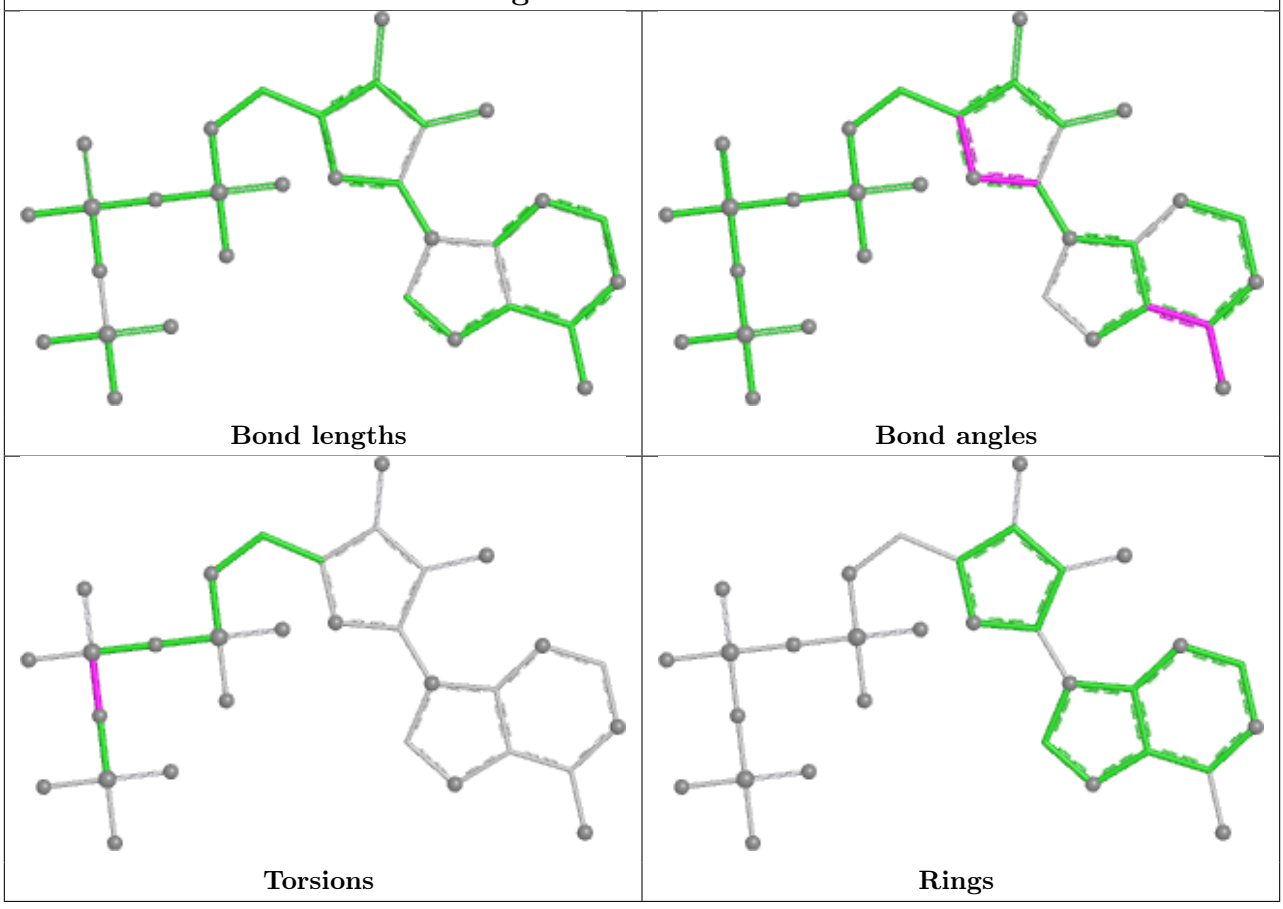
There are no ring outliers.

5 monomers are involved in 5 short contacts:

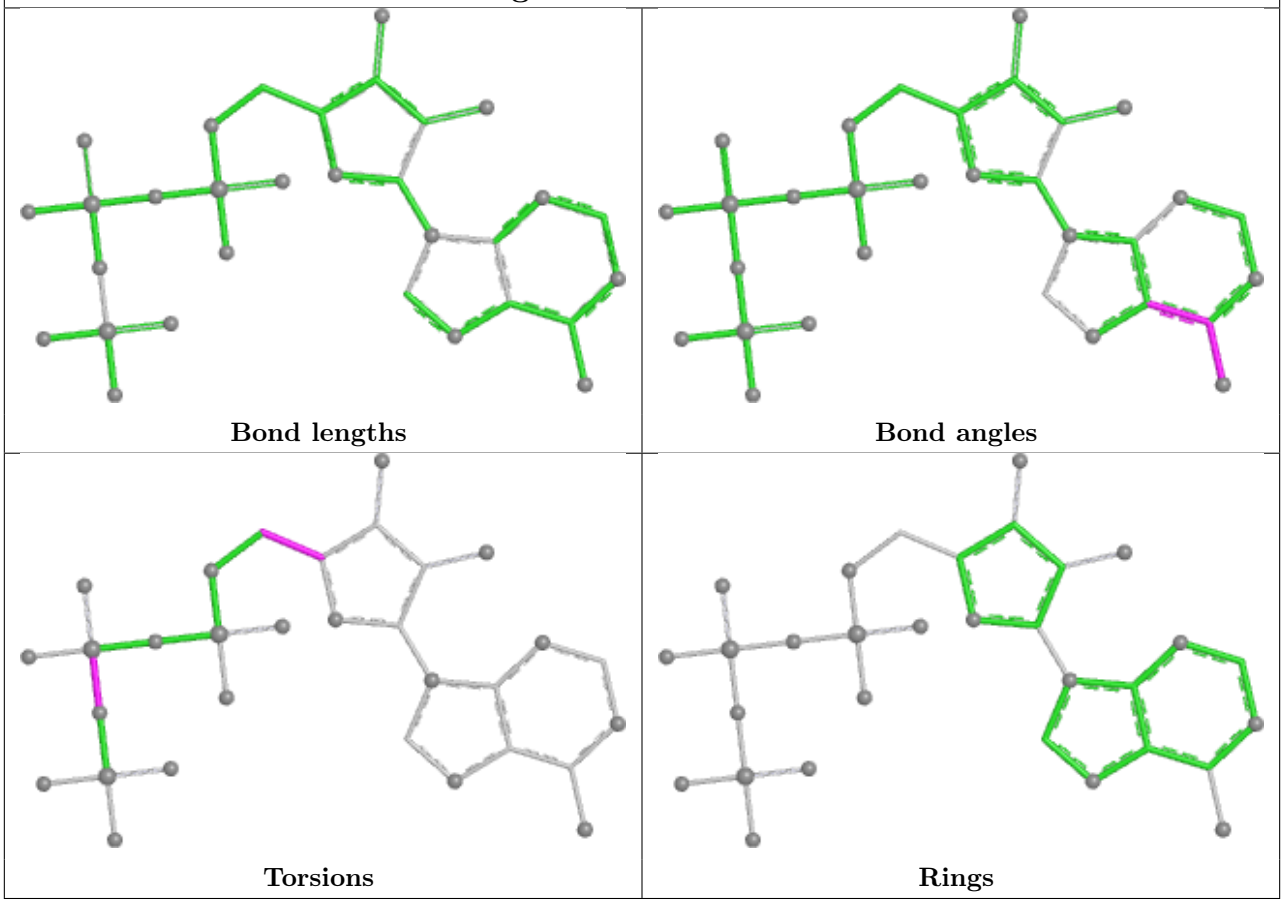
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	23	3012	SPD	1	0
55	23	3007	PUT	1	0
55	16	1601	PUT	1	0
56	23	3015	SPD	1	0
55	23	3003	PUT	1	0

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

Ligand ATP 23 3002



Ligand ATP 23 3001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

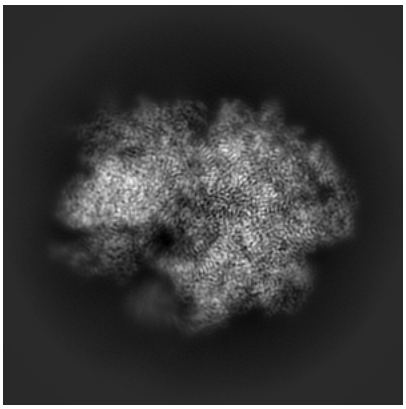
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48831. These allow visual inspection of the internal detail of the map and identification of artifacts.

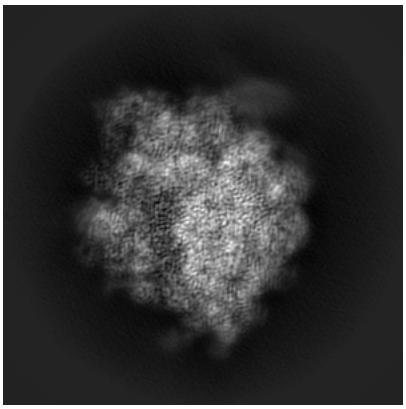
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

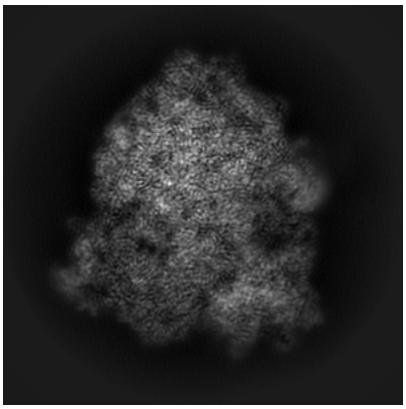
6.1.1 Primary map



X

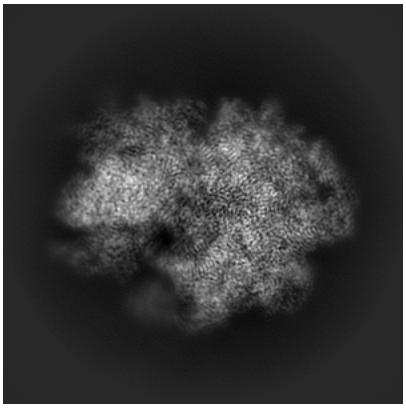


Y

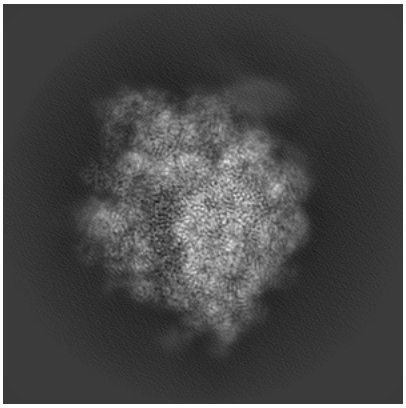


Z

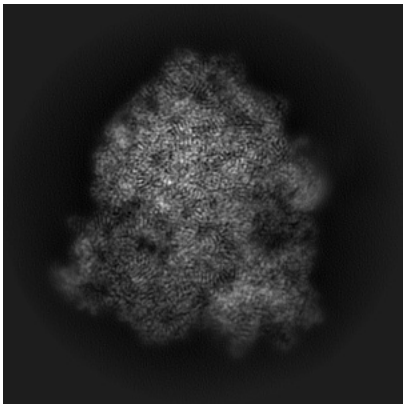
6.1.2 Raw map



X



Y

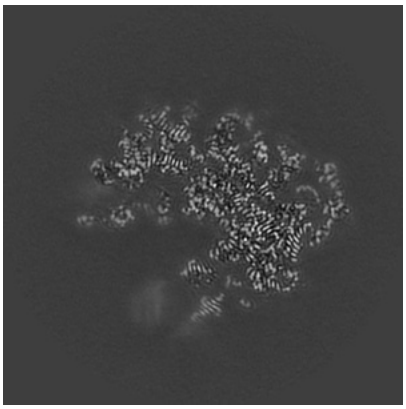


Z

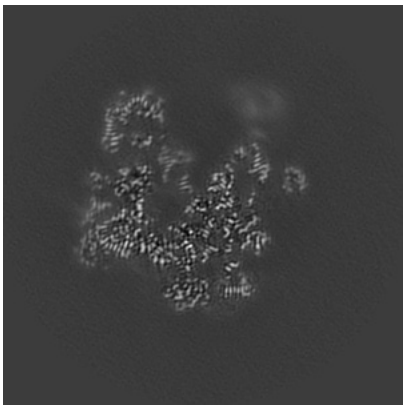
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

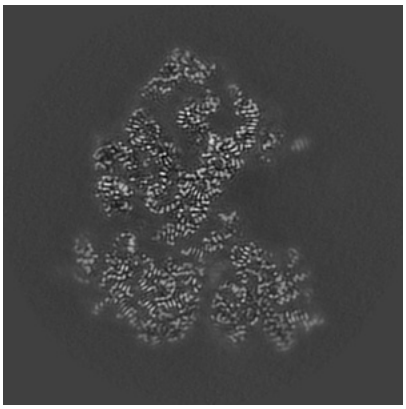
6.2.1 Primary map



X Index: 160

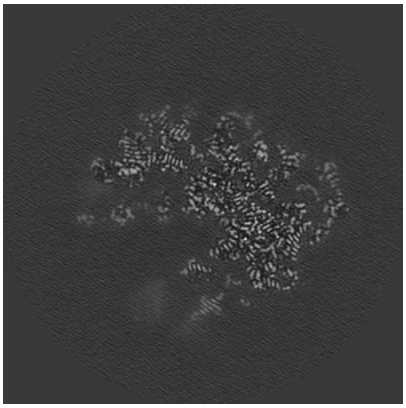


Y Index: 160

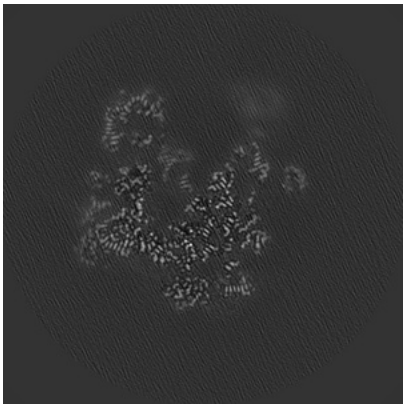


Z Index: 160

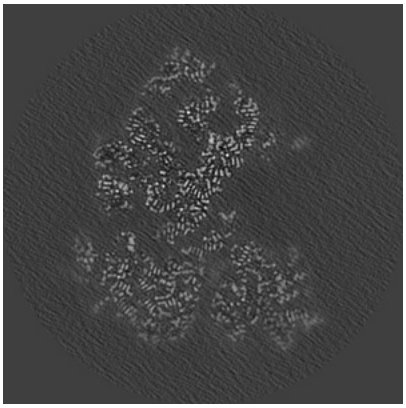
6.2.2 Raw map



X Index: 160



Y Index: 160

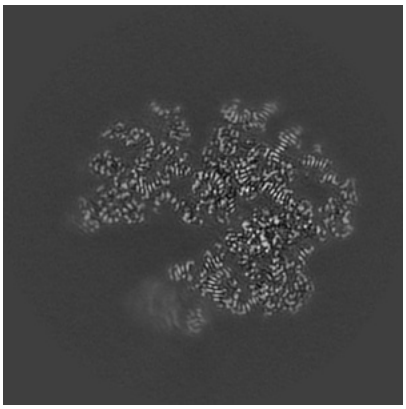


Z Index: 160

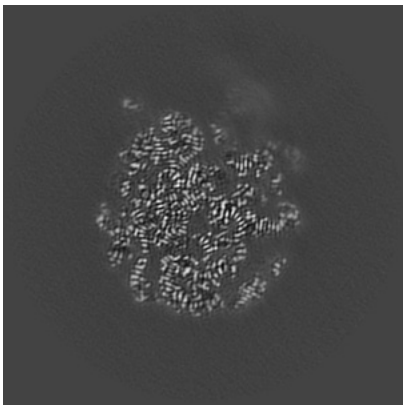
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

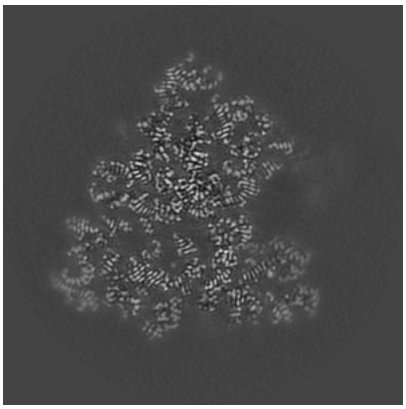
6.3.1 Primary map



X Index: 149

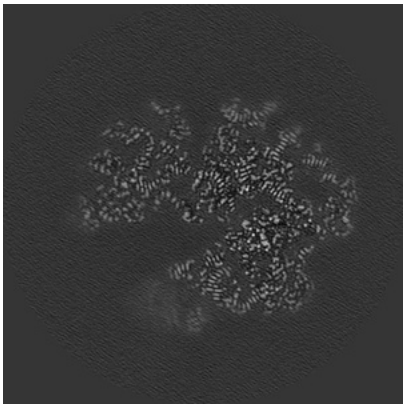


Y Index: 196

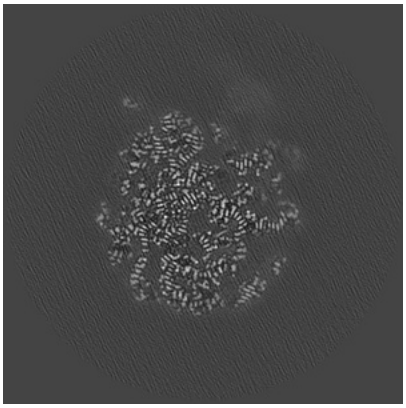


Z Index: 179

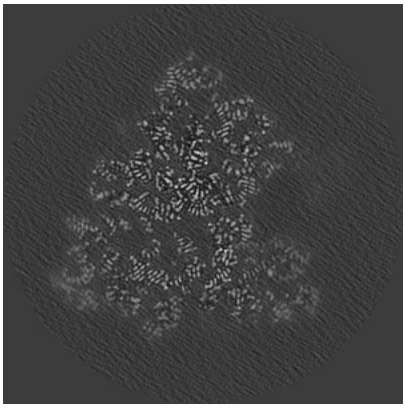
6.3.2 Raw map



X Index: 149



Y Index: 196

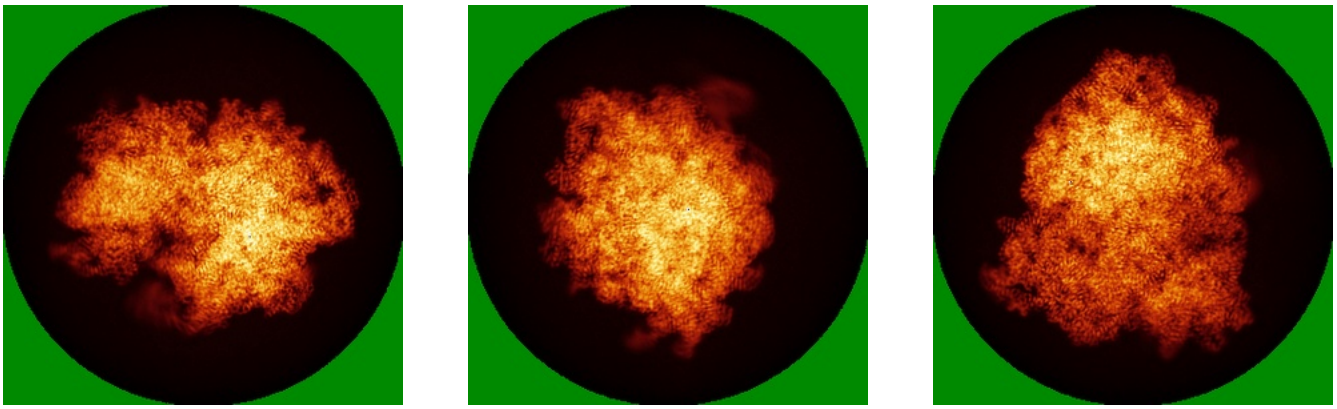


Z Index: 179

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

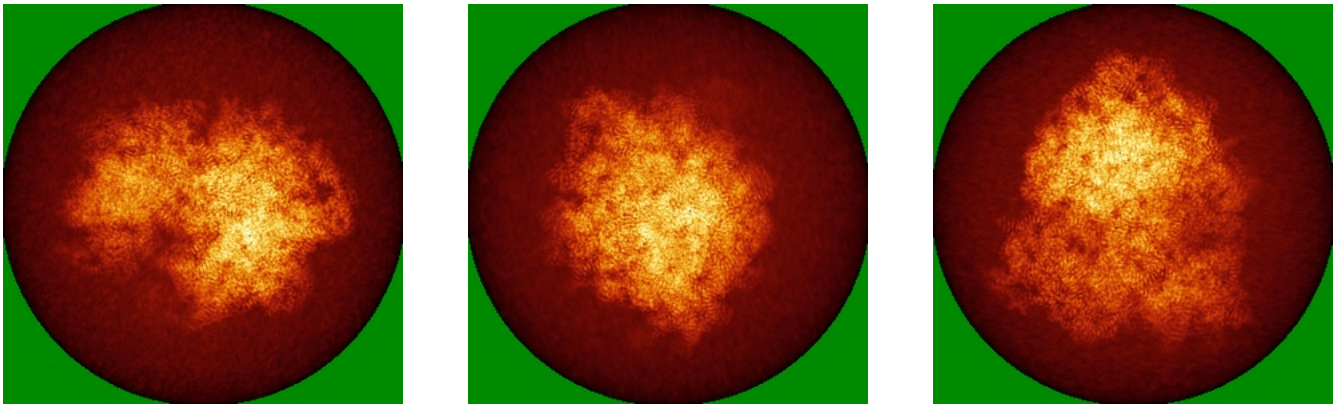
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

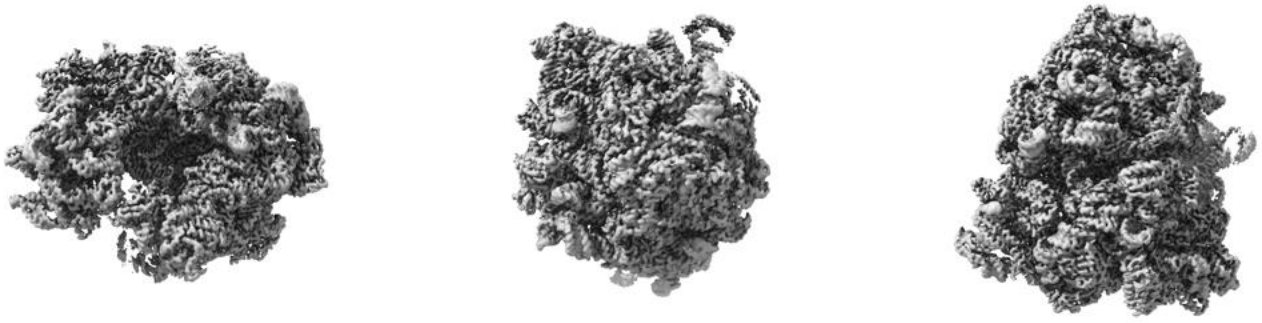


X Y Z

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)

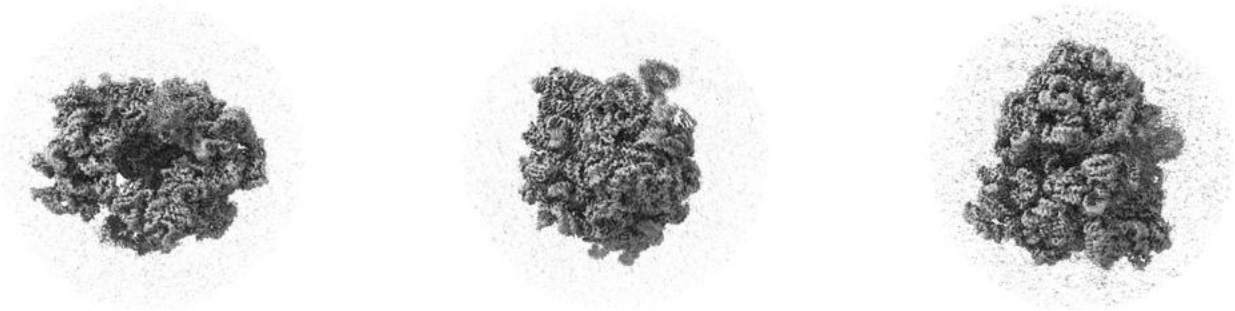
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

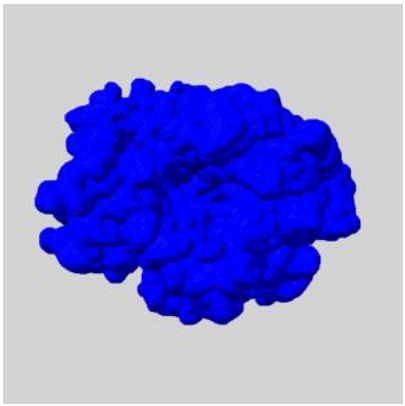
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

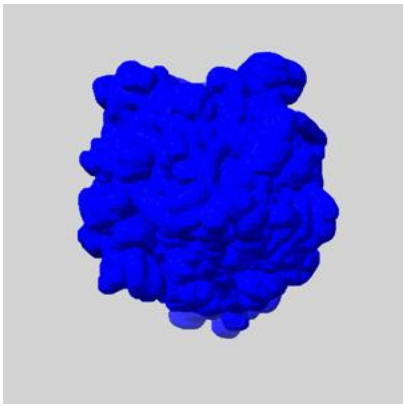
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

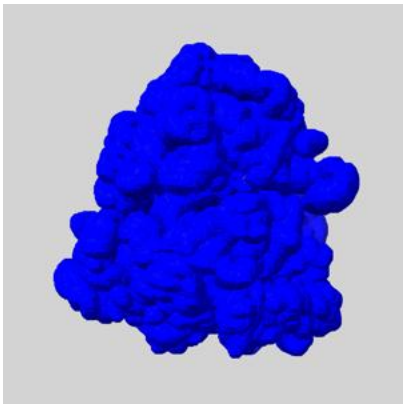
6.6.1 emd_48831_msk_1.map



X



Y

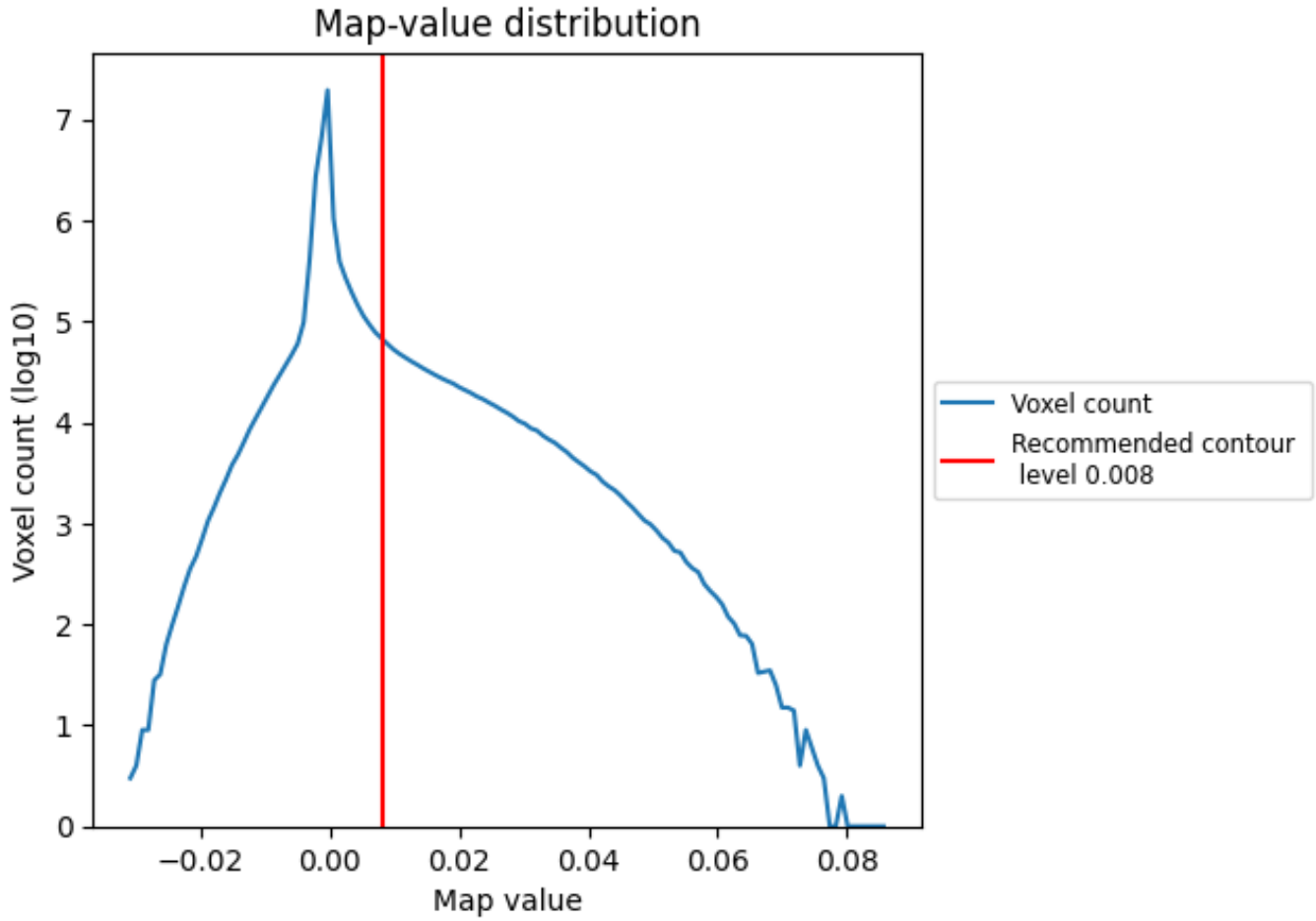


Z

7 Map analysis

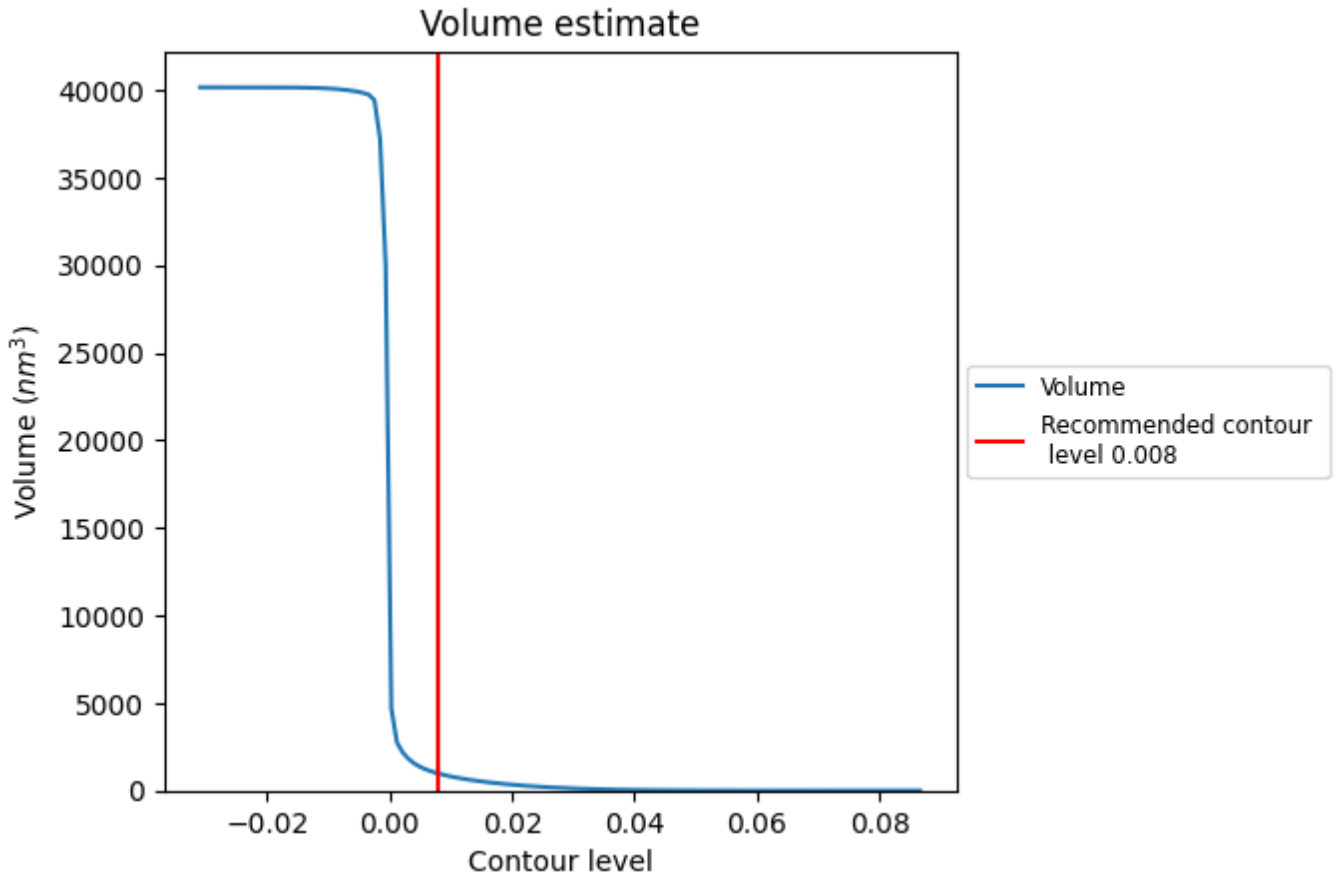
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

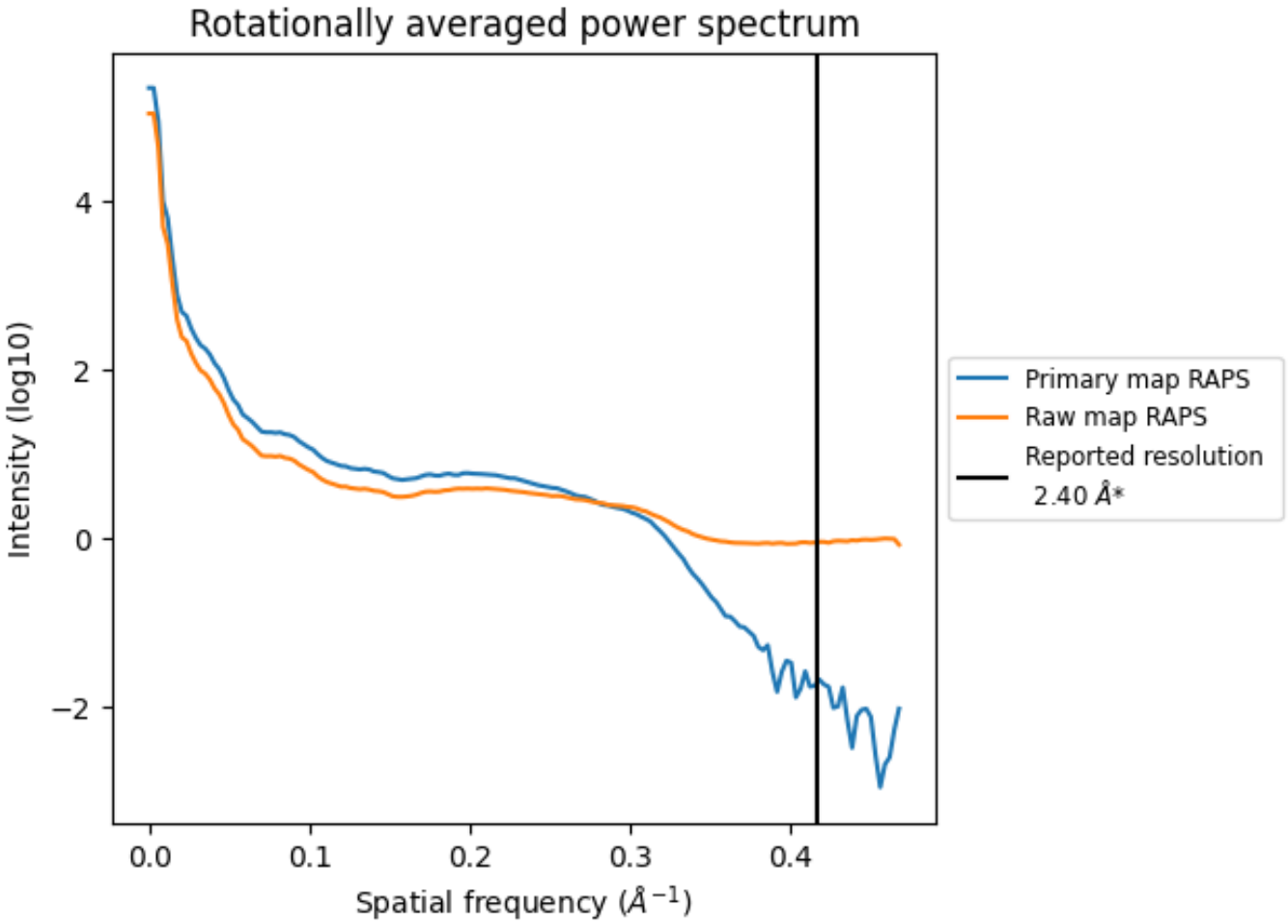
7.2 Volume estimate



The volume at the recommended contour level is 972 nm^3; this corresponds to an approximate mass of 878 kDa.

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

7.3 Rotationally averaged power spectrum (i)

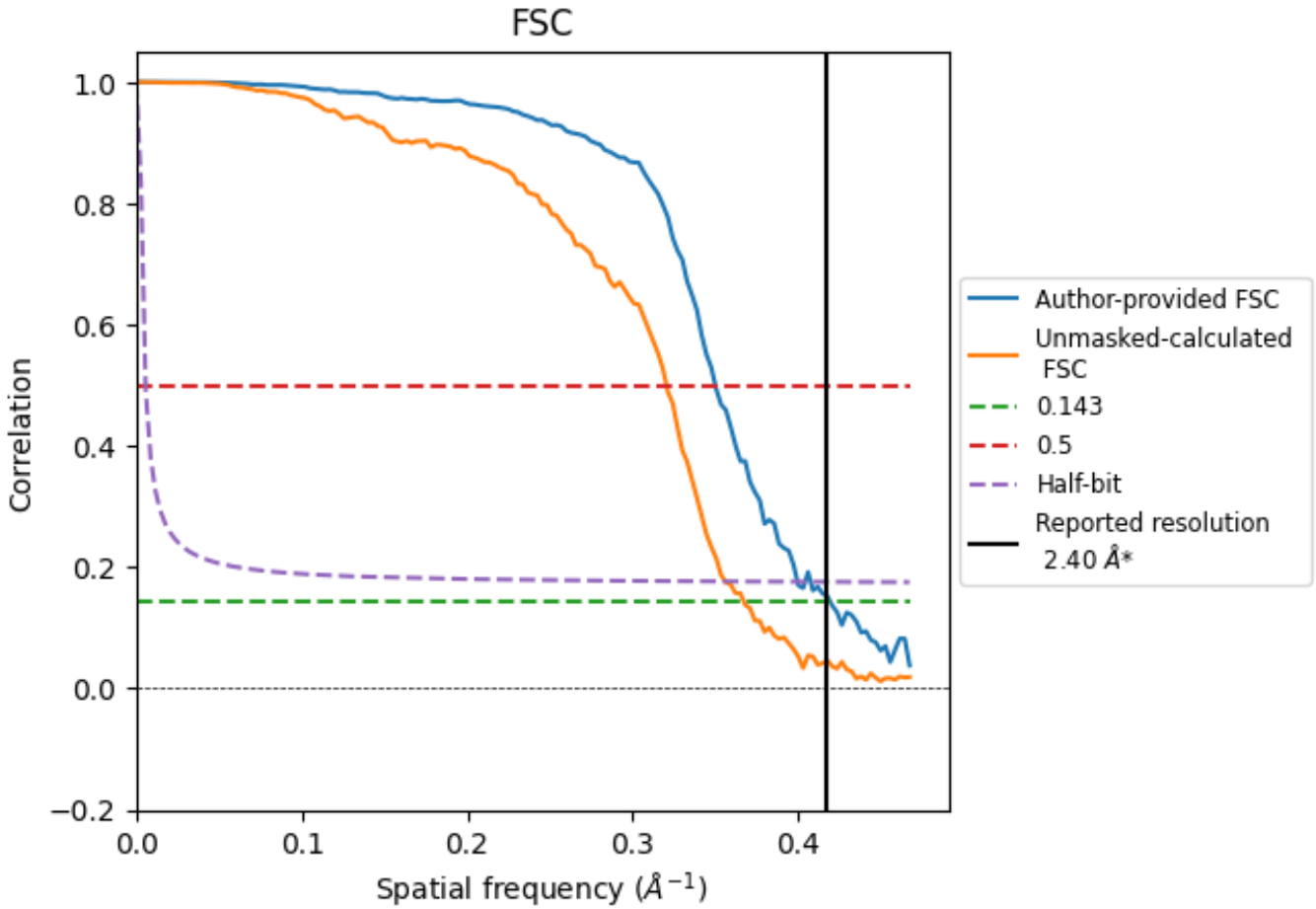


*Reported resolution corresponds to spatial frequency of 0.417 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8.2 Resolution estimates (i)

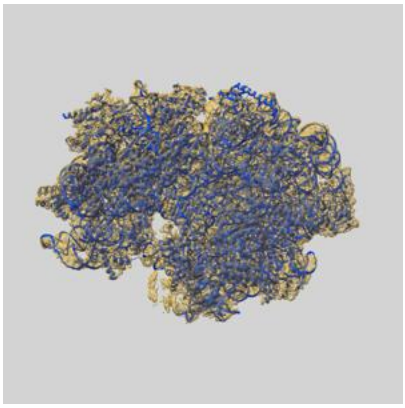
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.38	2.86	2.50
Unmasked-calculated*	2.72	3.12	2.81

*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 2.72 differs from the reported value 2.4 by more than 10 %

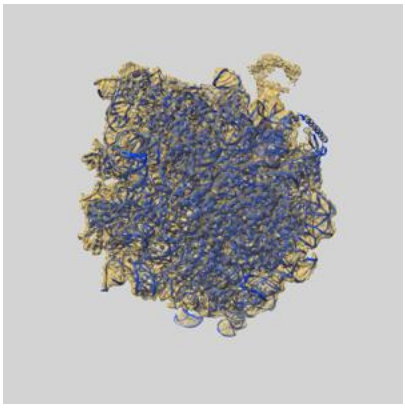
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48831 and PDB model 9N2C. Per-residue inclusion information can be found in section 3 on page 17.

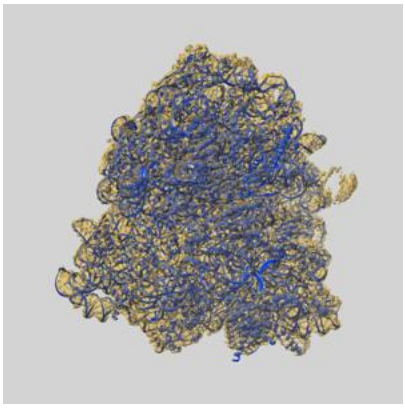
9.1 Map-model overlay



X



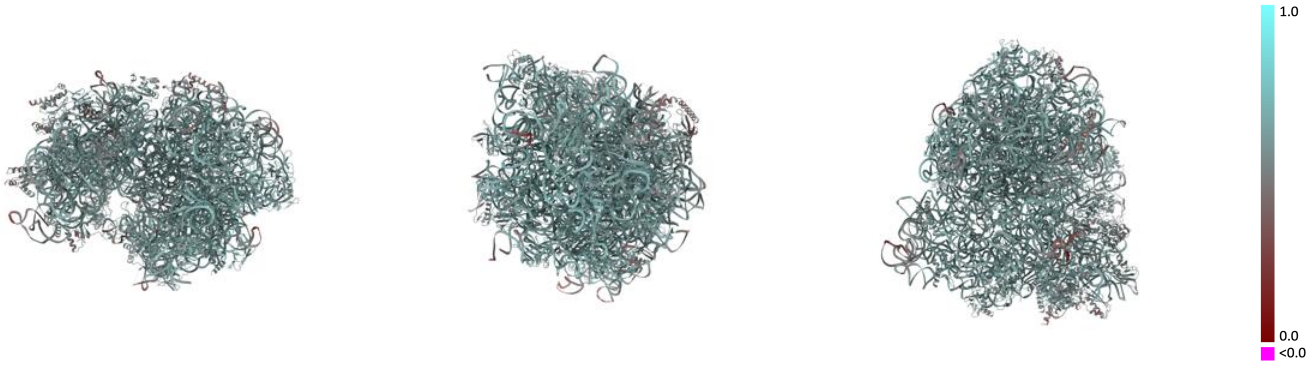
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

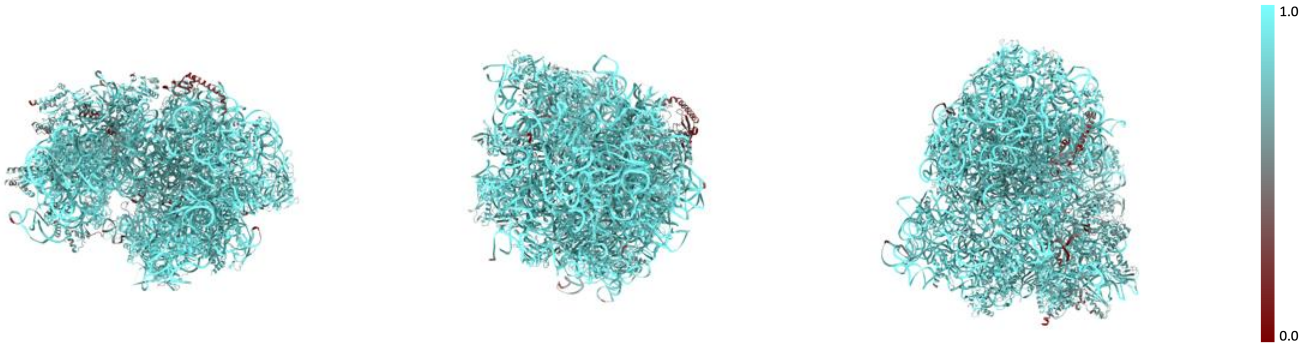
9.2 Q-score mapped to coordinate model



X Y Z

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

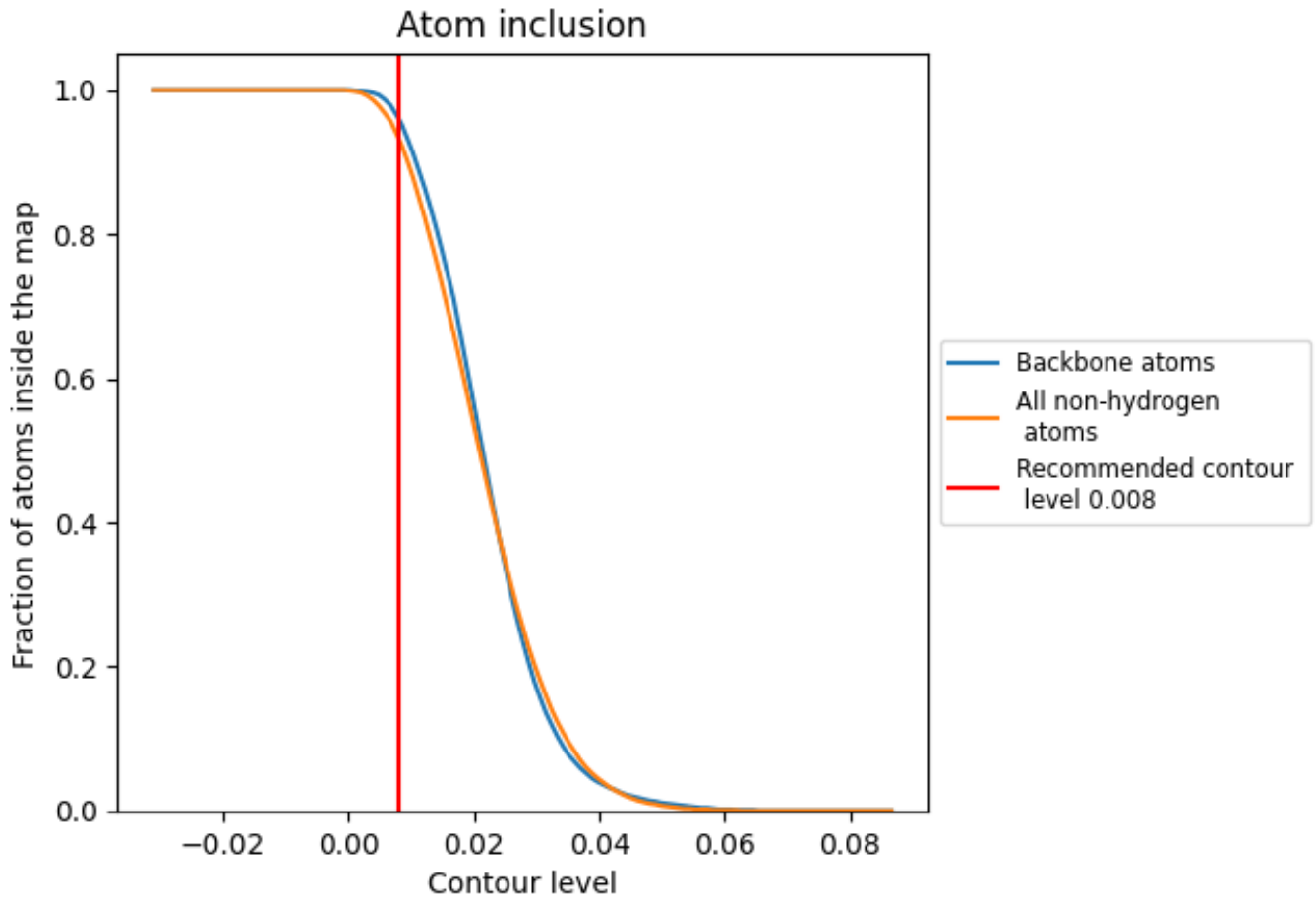
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9340	0.5990
16	0.9680	0.5900
23	0.9780	0.6150
5	0.9720	0.5990
LB	0.9350	0.6350
LC	0.9190	0.6200
LD	0.8920	0.6060
LE	0.7920	0.5550
LF	0.7850	0.5390
LI	0.3920	0.4690
LM	0.9240	0.6180
LN	0.9020	0.6220
LO	0.9090	0.6120
LP	0.9100	0.6190
LQ	0.9510	0.6310
LR	0.8750	0.5730
LS	0.8960	0.6190
LT	0.9450	0.6290
LU	0.9000	0.6080
LV	0.8990	0.6140
LW	0.8560	0.5980
LX	0.8790	0.5870
LY	0.8550	0.5870
La	0.8450	0.6150
Lb	0.9070	0.6210
Lc	0.8570	0.5690
Ld	0.8990	0.6110
Le	0.6810	0.5120
Lf	0.9040	0.6250
Lg	0.8570	0.6060
Lh	0.9490	0.6460
Li	0.9490	0.6420
Lj	0.9350	0.6220
Pt	0.8910	0.5800
SB	0.7560	0.5360

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SC	0.8380	0.5750
SD	0.8500	0.5770
SE	0.8830	0.5960
SF	0.7980	0.5510
SG	0.7110	0.5200
SH	0.8870	0.6040
SI	0.8460	0.5680
SJ	0.7640	0.5240
SK	0.8640	0.5760
SL	0.8780	0.6070
SM	0.8310	0.5640
SN	0.8610	0.5770
SO	0.8840	0.5890
SP	0.8800	0.5870
SQ	0.8170	0.5690
SR	0.8440	0.5690
SS	0.8420	0.5600
ST	0.8850	0.5820
SU	0.6980	0.5210
mR	0.6990	0.5100