



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 03:02 pm BST

PDB ID : 9GHA / pdb_00009gha
EMDB ID : EMD-51350
Title : Fusidic acid-locked Escherichia coli 70S ribosome with Staphylococcus aureus EF-G and a tRNA in pe/E chimeric state (CHI)
Authors : Gonzalez-Lopez, A.; Selmer, M.
Deposited on : 2024-08-15
Resolution : 2.24 Å (reported)
Based on initial models : 7N2C, 9GHE, 8P2H

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

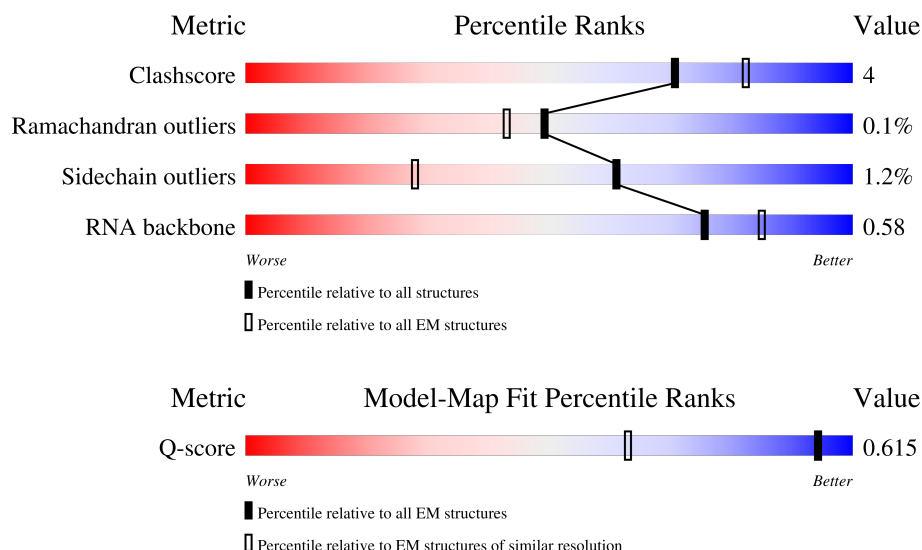
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

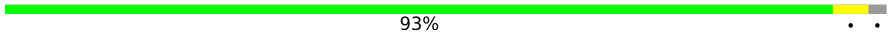
The reported resolution of this entry is 2.24 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3381 (1.75 - 2.74)

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

Mol	Chain	Length	Quality of chain
1	0	55	 80% 9% 9%
2	1	46	 93%
3	2	65	 86% 12%

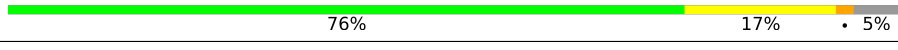
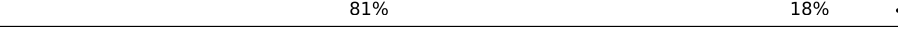
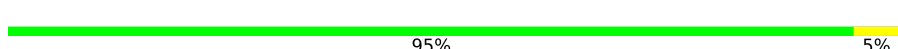
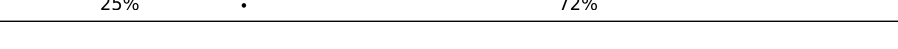
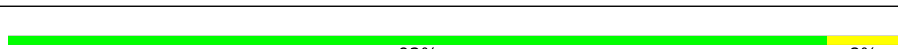
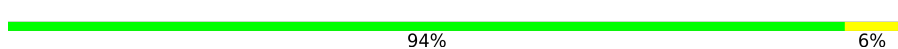
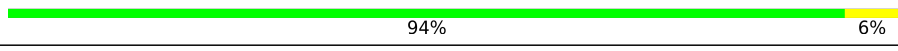
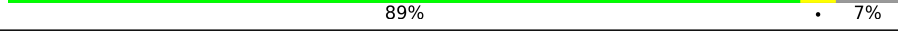
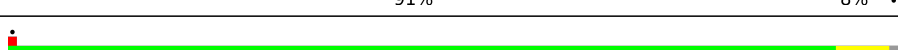
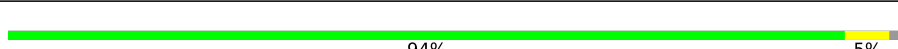
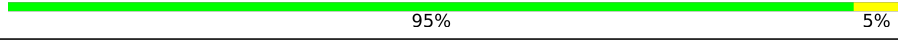
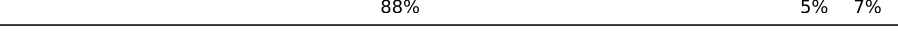
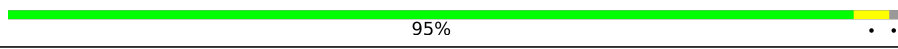
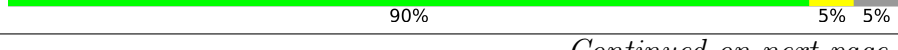
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	8	77	
7	9	24	
8	A	1554	
9	B	241	
10	C	233	
11	D	206	
12	E	167	
13	F	135	
14	G	179	
15	H	130	
16	I	130	
17	J	103	
18	K	129	
19	L	124	
20	M	118	
21	N	101	
22	O	89	
23	P	82	
24	Q	84	
25	R	75	
26	S	92	
27	T	87	
28	U	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	W	693	
30	a	2930	
31	b	119	
32	c	273	
33	d	209	
34	e	201	
35	f	179	
36	g	177	
37	h	149	
38	i	142	
39	j	123	
40	k	144	
41	l	136	
42	m	127	
43	n	117	
44	o	115	
45	p	118	
46	q	103	
47	r	110	
48	s	100	
49	t	104	
50	u	94	
51	v	85	
52	w	78	
53	x	63	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	y	59	95%
55	z	57	93% 5%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 145564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	50	Total	C	N	O	0	0
			413	267	75	71		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	48	Total	C	N	O	S	0	0
			373	232	66	69	6		

- Molecule 6 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	5	Total	C	N	O	P	0	0
			110	49	22	34	5		

- Molecule 8 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	1526	Total	C	N	O	P	0	0
			32757	14617	6009	10605	1526		

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	222	Total	C	N	O	S	0	0
			1737	1099	312	318	8		

- Molecule 10 is a protein called 30S ribosomal protein S3.

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

- Molecule 11 is a protein called 30S ribosomal protein S4.

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

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	154	Total	C	N	O	S	0	0
			1135	706	215	208	6		

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	150	Total	C	N	O	S	0	0
			1176	732	226	214	4		

- Molecule 15 is a protein called 30S ribosomal protein S8.

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

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	125	Total	C	N	O	S	0	0
			1001	622	200	176	3		

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	96	Total	C	N	O	S	0	0
			775	487	148	139	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 20 is a protein called 30S ribosomal protein S13.

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

- Molecule 21 is a protein called 30S ribosomal protein S14.

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

- Molecule 22 is a protein called 30S ribosomal protein S15.

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

- Molecule 23 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 24 is a protein called 30S ribosomal protein S17.

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

- Molecule 25 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	64	Total	C	N	O	S	0	0
			524	330	99	94	1		

- Molecule 26 is a protein called 30S ribosomal protein S19.

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

- Molecule 27 is a protein called 30S ribosomal protein S20.

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

- Molecule 28 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 29 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	666	Total	C	N	O	S	0	0
			5154	3232	865	1028	29		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2782	Total	C	N	O	P	0	0
			59756	26665	11017	19292	2782		

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

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

- Molecule 32 is a protein called 50S ribosomal protein L2.

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

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	207	Total	C	N	O	S	0	0
			1552	972	286	291	3		

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

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

- Molecule 36 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	170	Total	C	N	O	S	0	0
			1273	803	232	236	2		

- Molecule 37 is a protein called 50S ribosomal protein L9.

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

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	141	Total	C	N	O	S	0	0
			1121	709	211	198	3		

- Molecule 39 is a protein called 50S ribosomal protein L14.

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

- Molecule 40 is a protein called 50S ribosomal protein L15.

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

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	modified residue	UNP P0ADY7

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 48 is a protein called 50S ribosomal protein L23.

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

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	93	Total	C	N	O	S	0	0
			717	452	135	130			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 54 is a protein called 50S ribosomal protein L30.

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

- Molecule 55 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

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

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
57	A	14	Total	K	0
			14	14	
57	F	1	Total	K	0
			1	1	
57	a	74	Total	K	0
			74	74	
57	c	3	Total	K	0
			3	3	
57	e	1	Total	K	0
			1	1	
57	t	1	Total	K	0
			1	1	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

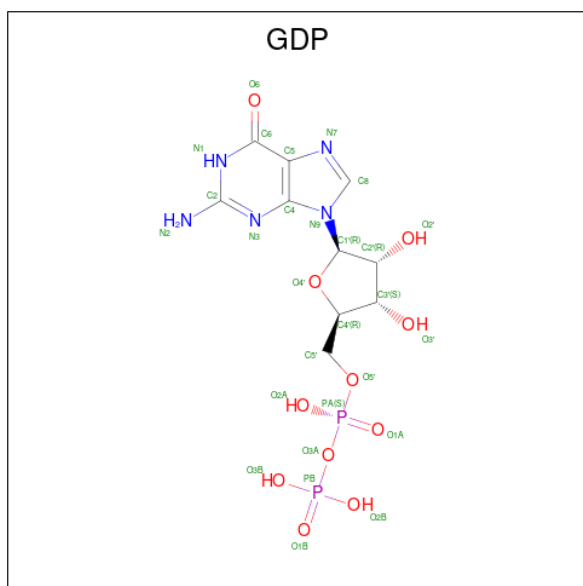
Mol	Chain	Residues	Atoms		AltConf
58	A	27	Total	Mg	0
			27	27	
58	W	1	Total	Mg	0
			1	1	
58	a	233	Total	Mg	0
			233	233	

Continued on next page...

Continued from previous page...

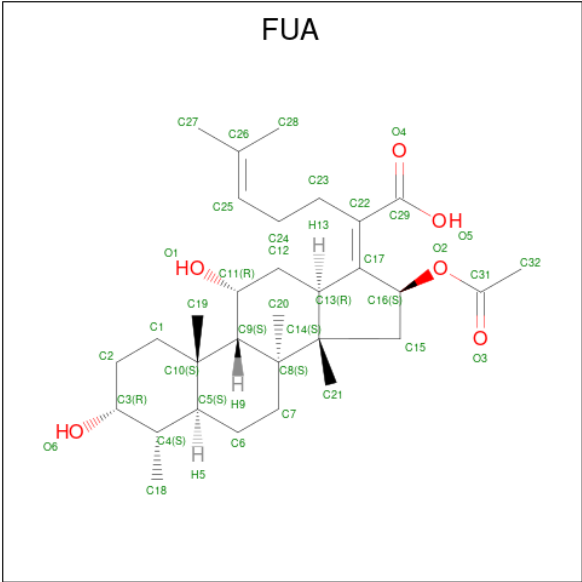
Mol	Chain	Residues	Atoms		AltConf
58	b	3	Total	Mg	0
			3	3	
58	c	3	Total	Mg	0
			3	3	
58	d	2	Total	Mg	0
			2	2	
58	k	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
59	W	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 60 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
60	W	1	Total	C	O	0
			37	31	6	

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: 50S ribosomal protein L33

Chain 0:  80% 9% 9%



- Molecule 2: 50S ribosomal protein L34

Chain 1:  93% . .



- Molecule 3: 50S ribosomal protein L35

Chain 2:  86% 12% .



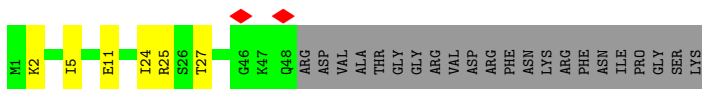
- Molecule 4: 50S ribosomal protein L36

Chain 3:  87% 13%



- Molecule 5: 50S ribosomal protein L31

Chain 4:  60% 9% 31%



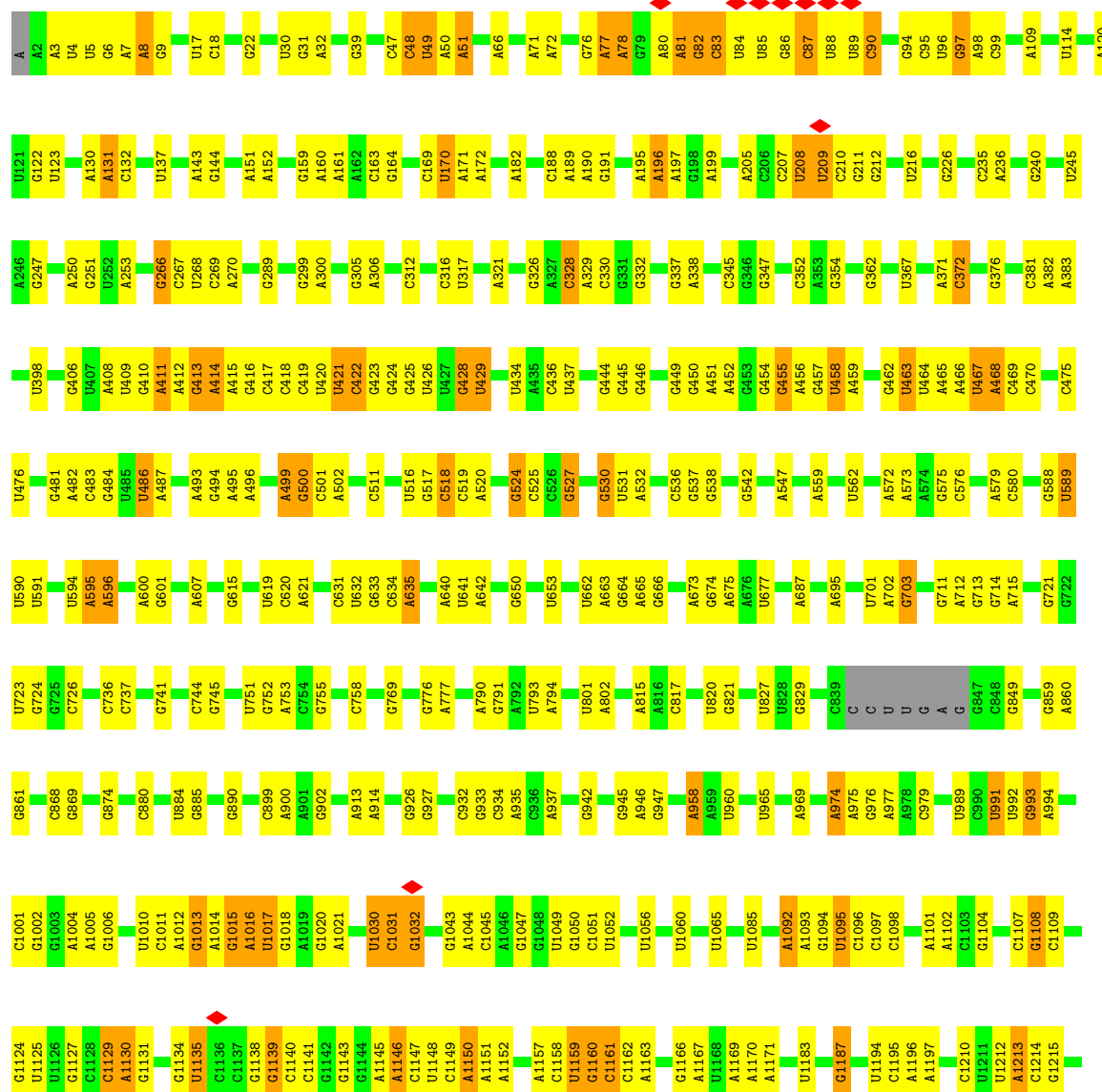
- Molecule 6: tRNA

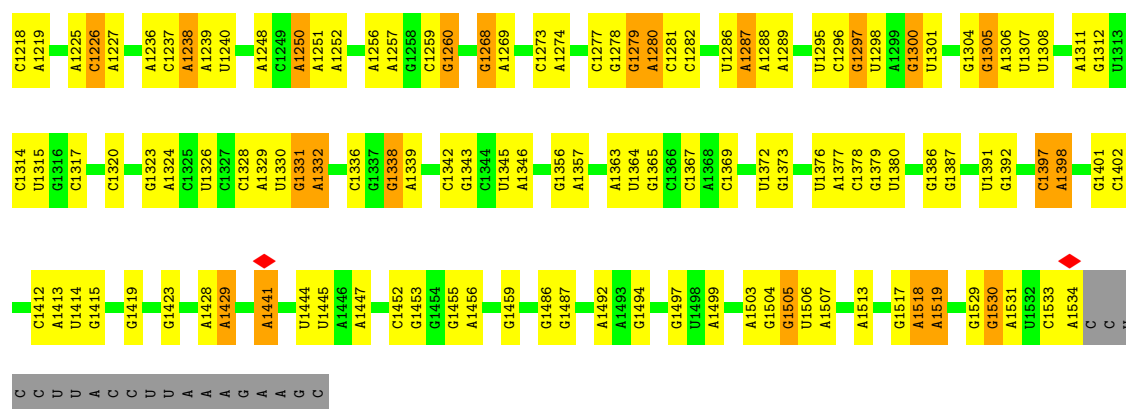


Chain 9: 12% 8% 79%

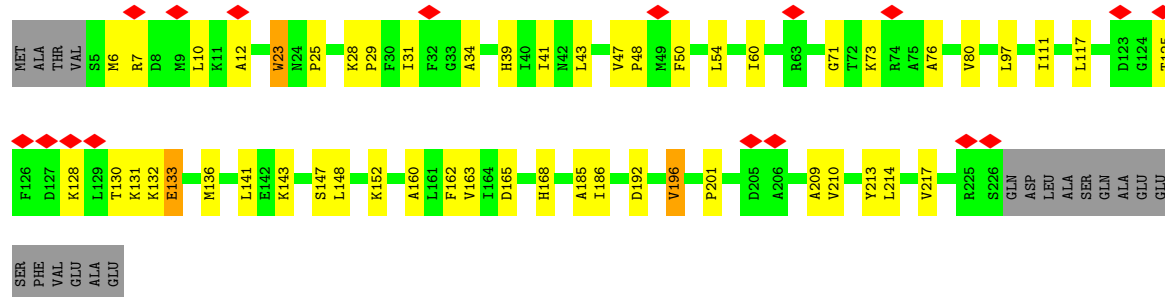


Chain A: 64% 29% 6%

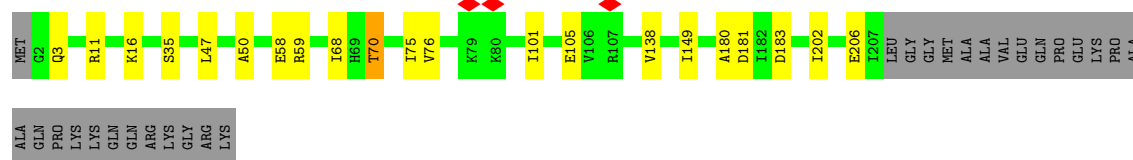
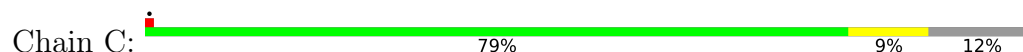




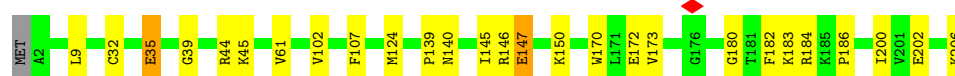
• Molecule 9: 30S ribosomal protein S2



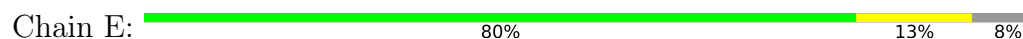
• Molecule 10: 30S ribosomal protein S3



• Molecule 11: 30S ribosomal protein S4

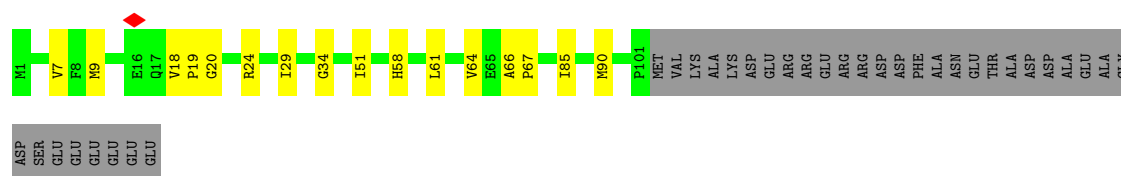


• Molecule 12: 30S ribosomal protein S5



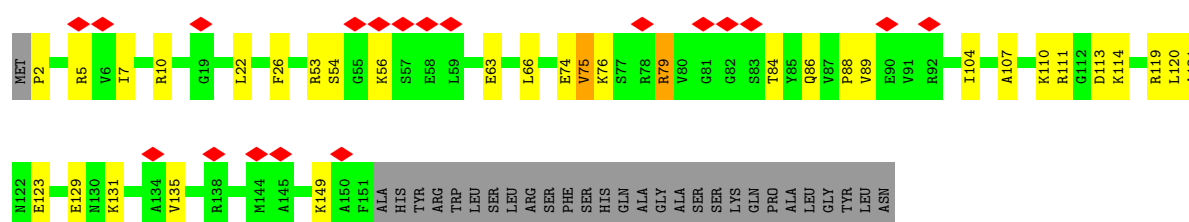
- Molecule 13: 30S ribosomal protein S6

Chain F:  63% 12% 25%



- Molecule 14: 30S ribosomal protein S7

Chain G:  11% 65% 17% 16%



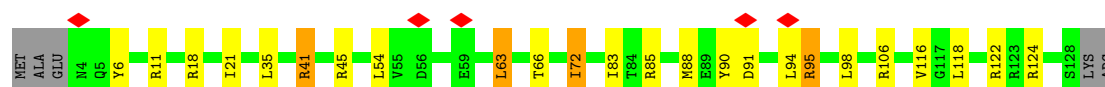
- Molecule 15: 30S ribosomal protein S8

Chain H:  86% 12% ..



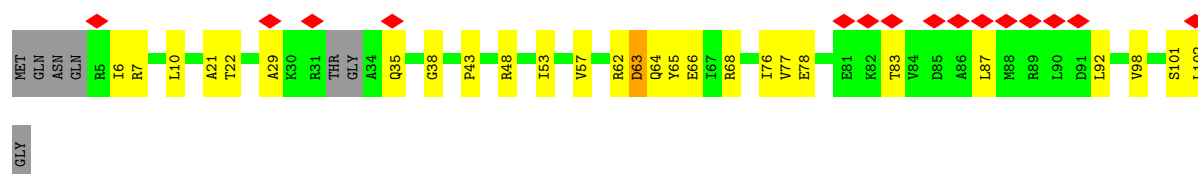
- Molecule 16: 30S ribosomal protein S9

Chain I:  78% 15% ..



- Molecule 17: 30S ribosomal protein S10

Chain J:  15% 67% 25% 7%



- Molecule 18: Small ribosomal subunit protein uS11

Chain K:  84% 7% 9%



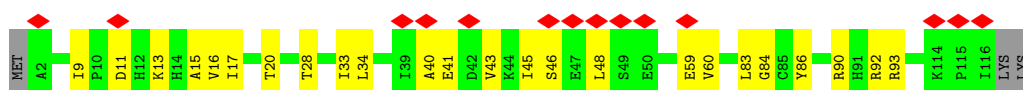
- Molecule 19: 30S ribosomal protein S12

Chain L: 84% 13% ..



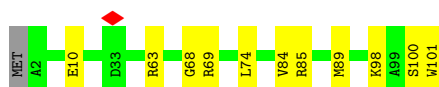
- Molecule 20: 30S ribosomal protein S13

Chain M: 12% 77% 20% .



- Molecule 21: 30S ribosomal protein S14

Chain N: 88% 11% .



- Molecule 22: 30S ribosomal protein S15

Chain O: 94% ..



- Molecule 23: 30S ribosomal protein S16

Chain P: 87% 10% .



- Molecule 24: 30S ribosomal protein S17

Chain Q: 81% 12% 6%

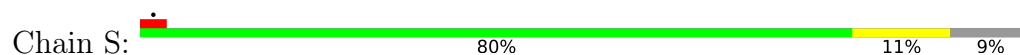


- Molecule 25: 30S ribosomal protein S18

Chain R: 75% 11% 15%



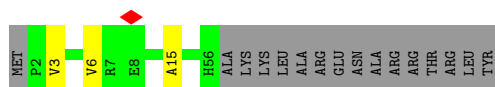
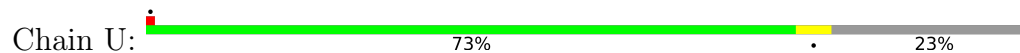
- Molecule 26: 30S ribosomal protein S19



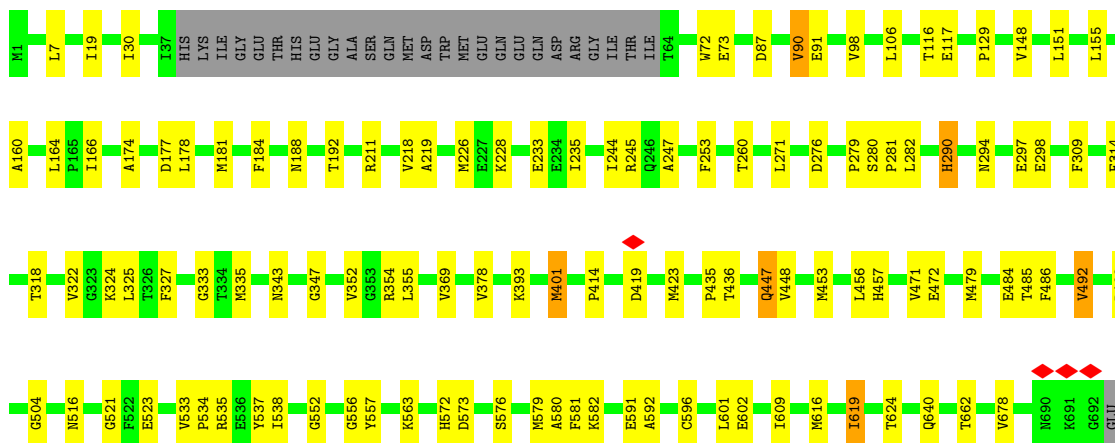
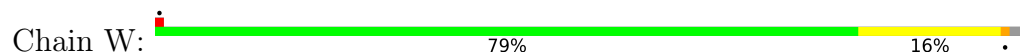
- Molecule 27: 30S ribosomal protein S20



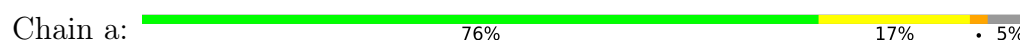
- Molecule 28: 30S ribosomal protein S21



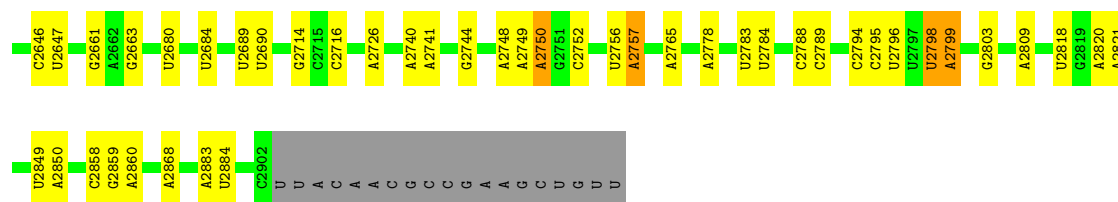
- Molecule 29: Elongation factor G



- Molecule 30: 23S rRNA

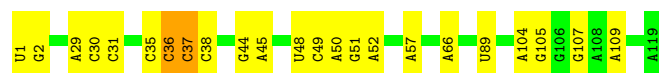


A2468	G2315	A1791	A1580	U1405	C1170	U1060	U746	A547	C351	A181
A2469	A2322	C1800	U1584	U1406	G1171	U1061	U747	G548	C352	A191
U2473	G2323	A1801	G1585	U1409	U	G1062		G549	C353	C192
U2474	U2324	U1993	A1586	U1412	U	U1065	A764	G555	A354	
A2476	A2014	C1816	C1605	U1413	U	A1069	G775	A563	G356	A196
A2477	A2015	U1829	C1606	A1413	G	A1070	G776	U358	C357	A199
U2478	A2020	A1829	C1607	G1416	G1179	U1071	A781	U359	U360	U200
U2491	A2023	C1838	A1608	G1419	U1180	C1072	A782	U361	G361	A204
G2502	C2023	C1838	A1609	A1419	U1181	A1077	A783	A574	A362	
A2503	U2026	A1847	G1619	C1428	G1182	U1078	G784	A575		C210
U2504	U2030	A1948	A1637	U1434	U1183	C1079	G785	U365	U366	
G2505	A2030	A1853	U1647	G1435	G1187	A1080	A792	A586	C366	G215
A2518	G2032	A1853	U1648	G1451	U1188	U1081		U588	G366	A216
U2522	A2033	A1858	U1649	G1452	U1198	U1082	G805	U589		A221
A2529	G2038	U1859	G1674	G1453	G1225	A1086	U811	U593	G411	A222
G2530	U2039	G1860	U1680	G1454	A1253	U1087	C812	U594	U448	A244
A2546	C2043	G1871	U1681	G1455	G1256	A1088	U813	C595	U451	G246
A2547	C2055	A1872	G1682	U1458		A1089	C814	A603		G247
U2548	G2056	A1872	U1683	U1459	G1271	A1090	U827	A609	A454	G248
G2552	U2060	U1898	U1698	U1460	A1272	G1093	U828	C610	C455	A255
G2553	G2061	C1905	G1710	A1469	A1275	U1094	G834	A614	G476	A265
U2554	A2062	G1906	G1715	A1470	U1276	U1097	U835	U615	A477	
U2555	G2069	G1907	G1721	G1482	A1287	U1101	A845	A627	A478	A272
G2556	U2071	U1911	G1721	U1490	C1295	C1102	U846		A480	G273
G2557	G2087	A1912	U1728	C1493	G1300	A1103	U849	C634	G481	C274
A2566	G2093	C1914	C1727	U1506	U1105	G1104	U850	C635	A482	C275
G2567	U2096	3TD1915	U1729	C1507	A1301	U1106	C851	G636	A483	
U2573	C2096	U1916	C1730	U1508	A1321	G1112	U852	A637	G491	A278
U2580	U2097	U1917	G1734	A1509	A1327	G1116	G858	G638	A492	A279
G2591	U2097	A1918	G1737	G1510	A1328	U1116	U861	U639	G493	U280
G2592	U2097	A1918	G1738	A1515	U1352	G1125	G862	C640	G494	C281
A2602	U2097	A1927	U1738	A1528	U1357	G1128	G869	A644	U499	G285
G2603	U2097	G1929	A1744	G1529	C1357	A1129	U870	C645	G500	U288
U2604	U2097	U1931	U1744	G1536	G1358	U1130	U871	U646	A501	G289
U2605	U2097	A1932	C1760	U1534	G1361	U1132	U872	G647	A502	G308
U2609	U2097	G1933	C1764	A1535	C1362	U1133	A878	A654	A503	A309
A2448	U2305	A1937	A1773	G1537	A1365	A1134	G	A655	A504	A310
U2449	U2306	U1939	A1778	G1538	U1378	C1135	G	U696	A505	A311
U2457	U2307	U1955	U1778	A1569	A1379	A1142	G		C509	A322
G2458	U2308	U1967	U1782	A1570	U1383	A1143	G	A716	C531	A330
A2459	U2311	C1967	A1783	A1571	A1386	A1144	G	C717	G533	A340
U2460	U2312	A1970	A1784	U1578	C1386	A1151	U	A718	U534	C341
A2461	U2313	U1971	C1790	A1579	A1387	A1169	A	G728	C544	A345
C2462	U2314						C	A730	U546	A346



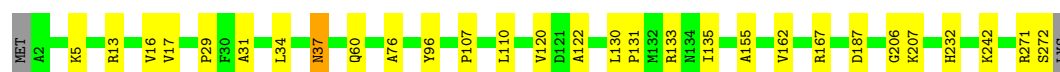
• Molecule 31: 5S rRNA

Chain b: 81% 18% .



• Molecule 32: 50S ribosomal protein L2

Chain c: 89% 10% .



• Molecule 33: 50S ribosomal protein L3

Chain d: 92% 7% .



• Molecule 34: 50S ribosomal protein L4

Chain e: 95% 5%



• Molecule 35: 50S ribosomal protein L5

Chain f: 76% 22% ..

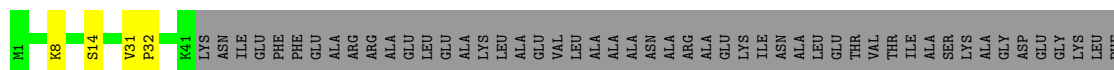


• Molecule 36: 50S ribosomal protein L6

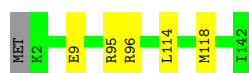
Chain g: 81% 13% . .



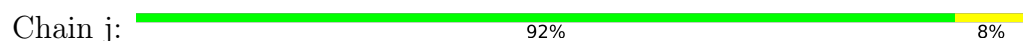
- Molecule 37: 50S ribosomal protein L9



- Molecule 38: 50S ribosomal protein L13



- Molecule 39: 50S ribosomal protein L14



- Molecule 40: 50S ribosomal protein L15



- Molecule 41: 50S ribosomal protein L16

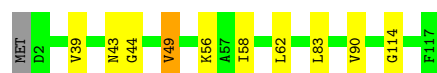


- Molecule 42: 50S ribosomal protein L17

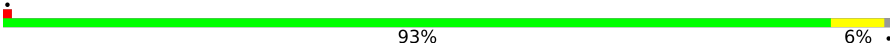


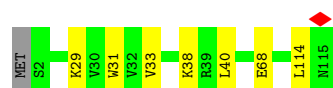
- Molecule 43: 50S ribosomal protein L18

Chain n:  91% 8% ..

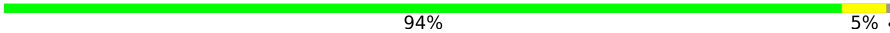


- Molecule 44: 50S ribosomal protein L19

Chain o:  93% 6% .



- Molecule 45: 50S ribosomal protein L20

Chain p:  94% 5% .

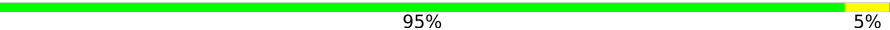


- Molecule 46: 50S ribosomal protein L21

Chain q:  89% 11%



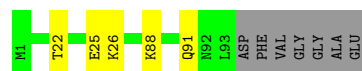
- Molecule 47: 50S ribosomal protein L22

Chain r:  95% 5% .



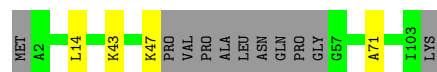
- Molecule 48: 50S ribosomal protein L23

Chain s:  88% 5% 7%

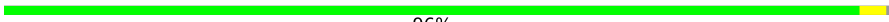


- Molecule 49: 50S ribosomal protein L24

Chain t:  86% 11%



- Molecule 50: 50S ribosomal protein L25

Chain u:  96% ..

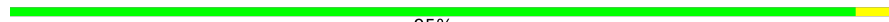


- Molecule 51: 50S ribosomal protein L27

Chain v:  82% 6% 12%



- Molecule 52: 50S ribosomal protein L28

Chain w:  95% ..

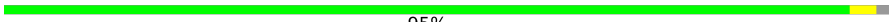


- Molecule 53: 50S ribosomal protein L29

Chain x:  90% 5% 5%



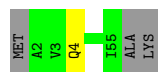
- Molecule 54: 50S ribosomal protein L30

Chain y:  95% ..



- Molecule 55: 50S ribosomal protein L32

Chain z:  93% • 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88568	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.714	Depositor
Minimum map value	-0.317	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	388.8, 388.8, 388.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.648, 0.648, 0.648	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D2T, K, OMC, IAS, 3TD, 6MZ, OMG, PSU, 4D4, 2MA, H2U, MEQ, MS6, GDP, 1MG, MA6, OMU, 2MG, 5MC, MG, ZN, FUA, 5MU, UR3, G7M, 4OC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.47	0/420	0.79	0/560
2	1	0.48	0/370	0.88	0/487
3	2	0.50	0/513	0.85	0/676
4	3	0.48	0/303	0.72	0/397
5	4	0.49	0/380	0.84	0/508
6	8	0.54	0/1832	0.76	0/2855
7	9	0.59	0/123	0.75	0/190
8	A	0.54	0/36398	0.75	0/56774
9	B	0.46	0/1768	0.94	0/2381
10	C	0.47	0/1651	0.82	0/2225
11	D	0.45	0/1665	0.88	0/2227
12	E	0.49	0/1148	0.83	0/1545
13	F	0.45	0/843	0.81	0/1140
14	G	0.47	0/1190	0.91	0/1595
15	H	0.48	0/989	0.83	0/1326
16	I	0.45	0/1013	0.85	0/1350
17	J	0.48	0/784	0.87	0/1059
18	K	0.52	0/884	0.83	0/1191
19	L	0.47	0/945	0.79	0/1268
20	M	0.47	0/900	0.91	0/1204
21	N	0.47	0/817	0.89	0/1088
22	O	0.43	0/722	0.91	0/964
23	P	0.46	0/639	0.81	0/859
24	Q	0.46	0/650	0.74	0/871
25	R	0.45	0/532	0.91	0/715
26	S	0.49	0/685	0.84	0/922
27	T	0.46	0/676	0.93	0/895
28	U	0.47	0/467	0.90	0/620
29	W	0.46	0/5244	0.84	0/7091
30	a	0.52	1/66355 (0.0%)	0.77	8/103511 (0.0%)
31	b	0.53	0/2850	0.76	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.49	0/2121	0.79	0/2852
33	d	0.47	0/1562	0.78	0/2102
34	e	0.46	0/1571	0.84	0/2113
35	f	0.45	0/1434	0.87	0/1926
36	g	0.49	0/1291	0.83	1/1747 (0.1%)
37	h	0.48	0/306	0.79	0/413
38	i	0.46	0/1144	0.83	0/1541
39	j	0.47	0/955	0.79	0/1279
40	k	0.48	0/1062	0.83	0/1413
41	l	0.47	0/1073	0.80	0/1433
42	m	0.46	0/958	0.85	0/1281
43	n	0.47	0/902	0.86	0/1209
44	o	0.47	0/929	0.73	0/1242
45	p	0.46	0/960	0.89	0/1278
46	q	0.46	0/829	0.73	0/1107
47	r	0.47	0/852	0.83	0/1142
48	s	0.46	0/744	0.79	0/994
49	t	0.46	0/721	0.75	0/956
50	u	0.46	0/758	0.81	0/1015
51	v	0.48	0/576	0.76	0/762
52	w	0.47	0/635	0.83	0/848
53	x	0.41	0/492	0.89	0/655
54	y	0.46	0/453	0.81	0/605
55	z	0.47	0/435	0.84	0/581
All	All	0.51	1/156519 (0.0%)	0.79	9/233432 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	2	0	1
4	3	0	1
10	C	0	1
11	D	0	1
14	G	0	1
16	I	0	2
17	J	0	2
18	K	0	1
19	L	0	1
36	g	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
38	i	0	1
45	p	0	1
52	w	0	1
53	x	0	1
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2069	G7M	O3'-P	5.17	1.61	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2546	U	O3'-P-O5'	-7.53	92.71	104.00
30	a	1905	C	O3'-P-O5'	-6.46	94.32	104.00
30	a	781	A	O3'-P-O5'	-6.03	94.96	104.00
30	a	2324	U	C2'-C3'-O3'	-5.88	104.89	113.70
30	a	1378	A	O3'-P-O5'	-5.77	95.34	104.00
30	a	1971	U	O3'-P-O5'	-5.71	95.44	104.00
36	g	155	GLU	CB-CA-C	5.64	116.98	108.86
30	a	310	A	O3'-P-O5'	-5.49	95.77	104.00
30	a	204	A	O3'-P-O5'	-5.17	96.25	104.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	13	ARG	Sidechain
4	3	36	ARG	Sidechain
10	C	11	ARG	Sidechain
11	D	184	ARG	Sidechain
14	G	79	ARG	Sidechain
16	I	41	ARG	Sidechain
16	I	95	ARG	Sidechain
17	J	38	GLY	Peptide
17	J	62	ARG	Sidechain
18	K	118	HIS	Peptide
19	L	9	ARG	Sidechain
36	g	35	ARG	Sidechain
38	i	96	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
45	p	51	ARG	Sidechain
52	w	74	ARG	Sidechain
53	x	52	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	0	413	0	448	4	0
2	1	367	0	405	2	0
3	2	504	0	572	4	0
4	3	302	0	340	3	0
5	4	373	0	370	4	0
6	8	1640	0	837	13	0
7	9	110	0	55	1	0
8	A	32757	0	16505	265	0
9	B	1737	0	1763	28	0
10	C	1624	0	1696	13	0
11	D	1643	0	1707	15	0
12	E	1135	0	1179	12	0
13	F	824	0	815	10	0
14	G	1176	0	1233	20	0
15	H	979	0	1031	9	0
16	I	1001	0	1044	14	0
17	J	775	0	817	24	0
18	K	877	0	883	4	0
19	L	942	0	999	9	0
20	M	891	0	952	16	0
21	N	805	0	844	12	0
22	O	714	0	734	3	0
23	P	629	0	643	6	0
24	Q	641	0	682	5	0
25	R	524	0	543	5	0
26	S	668	0	693	7	0
27	T	670	0	719	3	0
28	U	460	0	486	2	0
29	W	5154	0	5064	68	0
30	a	59756	0	30054	195	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	b	2549	0	1291	11	0
32	c	2082	0	2153	16	0
33	d	1552	0	1601	8	0
34	e	1552	0	1619	7	0
35	f	1410	0	1444	31	0
36	g	1273	0	1322	12	0
37	h	303	0	327	2	0
38	i	1121	0	1150	1	0
39	j	946	0	1023	8	0
40	k	1053	0	1129	4	0
41	l	1075	0	1145	4	0
42	m	945	0	989	3	0
43	n	892	0	923	4	0
44	o	917	0	962	5	0
45	p	947	0	1019	4	0
46	q	816	0	839	6	0
47	r	845	0	909	4	0
48	s	738	0	807	3	0
49	t	717	0	766	3	0
50	u	745	0	768	2	0
51	v	569	0	581	3	0
52	w	625	0	652	1	0
53	x	491	0	523	1	0
54	y	449	0	488	1	0
55	z	429	0	440	1	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	14	0	0	0	0
57	F	1	0	0	0	0
57	a	74	0	0	0	0
57	c	3	0	0	0	0
57	e	1	0	0	0	0
57	t	1	0	0	0	0
58	A	27	0	0	0	0
58	W	1	0	0	0	0
58	a	233	0	0	0	0
58	b	3	0	0	0	0
58	c	3	0	0	0	0
58	d	2	0	0	0	0
58	k	1	0	0	0	0
58	z	1	0	0	0	0
59	W	28	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	W	37	0	47	5	0
All	All	145564	0	99042	845	0

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

All (845) 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)
14:G:79:ARG:HA	14:G:84:THR:HA	1.23	1.10
8:A:1016:A:H1'	8:A:1017:U:H4'	1.45	0.96
17:J:48:ARG:HG2	17:J:66:GLU:HG3	1.50	0.91
8:A:424:G:O2'	8:A:425:G:H5'	1.77	0.84
8:A:411:A:N3	8:A:413:G:H5''	1.95	0.81
29:W:322:VAL:HG21	29:W:325:LEU:HD21	1.64	0.78
30:a:483:A:H5''	49:t:47:LYS:HD2	1.64	0.78
4:3:11:CYS:SG	4:3:14:CYS:N	2.57	0.77
8:A:1330:U:H2'	8:A:1331:G:O4'	1.85	0.76
8:A:1107:C:H3'	8:A:1108:G:H5''	1.68	0.76
29:W:322:VAL:CG2	29:W:325:LEU:HD21	2.16	0.75
32:c:29:PRO:HG2	32:c:34:LEU:HD11	1.69	0.75
27:T:42:GLY:HA2	27:T:86:LEU:HD11	1.71	0.72
8:A:82:G:H1'	8:A:90:C:H2'	1.71	0.71
8:A:1530:G:H2'	8:A:1531:A:C8	2.27	0.70
17:J:48:ARG:HH12	21:N:101:TRP:HB3	1.57	0.70
30:a:568:U:H1'	30:a:2030:6MZ:H9C1	1.73	0.70
16:I:85:ARG:HA	16:I:88:MET:HE2	1.72	0.69
48:s:88:LYS:HB2	48:s:91:GLN:HG2	1.75	0.68
46:q:6:GLN:HG3	46:q:39:LEU:HD11	1.75	0.68
5:4:11:GLU:HA	5:4:25:ARG:HA	1.75	0.68
30:a:2305:U:H5''	35:f:131:GLY:HA3	1.76	0.67
18:K:87:LYS:HB2	18:K:113:VAL:HG23	1.76	0.67
8:A:538:G:P	19:L:112:GLN:HE22	2.18	0.67
29:W:309:PHE:HA	29:W:333:GLY:HA3	1.76	0.66
30:a:546:U:H3'	30:a:547:A:H8	1.60	0.66
8:A:420:U:C2'	8:A:421:U:H5''	2.26	0.66
17:J:65:TYR:OH	21:N:89:MET:HE2	1.96	0.66
60:W:703:FUA:H202	60:W:703:FUA:H5	1.77	0.66
14:G:75:VAL:HB	14:G:86:GLN:HB3	1.77	0.66
20:M:11:ASP:HA	20:M:45:ILE:HB	1.78	0.65
8:A:1013:G:H21	8:A:1015:G:H1'	1.62	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1166:G:H2'	8:A:1167:A:H2'	1.78	0.65
6:8:21:A:H61	6:8:46:G:H2'	1.60	0.65
11:D:124:MET:HE3	11:D:146:ARG:HG2	1.79	0.65
11:D:172:GLU:HG3	11:D:183:LYS:HD2	1.78	0.64
17:J:21:ALA:HB1	17:J:92:LEU:HD13	1.80	0.64
30:a:12:U:H2'	30:a:12:U:O2	1.97	0.64
20:M:33:ILE:HG23	20:M:59:GLU:HB2	1.81	0.63
8:A:1441:A:N3	44:o:114:LEU:HD11	2.13	0.63
44:o:33:VAL:HG22	44:o:38:LYS:HG3	1.81	0.63
17:J:63:ASP:OD1	21:N:98:LYS:NZ	2.32	0.62
19:L:55:VAL:HG21	19:L:80:ILE:HD11	1.79	0.62
29:W:106:LEU:HD21	29:W:116:THR:HG21	1.80	0.62
46:q:6:GLN:HG2	46:q:11:GLN:HG2	1.81	0.62
6:8:15:G:H3'	6:8:16:C:H5''	1.81	0.62
8:A:420:U:H2'	8:A:421:U:H5''	1.81	0.62
8:A:415:A:O2'	8:A:416:G:H5'	1.99	0.62
8:A:422:C:O4'	8:A:423:G:N2	2.33	0.62
29:W:355:LEU:HD13	29:W:369:VAL:HG23	1.82	0.62
8:A:416:G:O2'	8:A:417:C:H5'	2.00	0.62
9:B:117:LEU:HB3	9:B:141:LEU:HG	1.81	0.62
10:C:70:THR:HG21	10:C:76:VAL:HG21	1.80	0.62
32:c:271:ARG:O	32:c:272:SER:C	2.42	0.61
39:j:70:ARG:HD2	39:j:76:VAL:HG22	1.82	0.61
33:d:35:THR:HG22	33:d:73:VAL:HG21	1.83	0.61
8:A:413:G:H1'	8:A:428:G:H21	1.65	0.61
11:D:147:GLU:HA	11:D:150:LYS:HE2	1.83	0.60
8:A:77:A:H3'	8:A:78:A:H8	1.66	0.60
30:a:1079:C:H3'	30:a:1080:A:H8	1.64	0.60
8:A:1148:U:H2'	8:A:1149:C:O4'	2.01	0.60
8:A:538:G:OP2	19:L:112:GLN:NE2	2.34	0.60
49:t:14:LEU:HD11	49:t:71:ALA:HB2	1.82	0.60
8:A:769:G:H4'	8:A:1513:A:H4'	1.83	0.60
16:I:41:ARG:HD2	16:I:72:ILE:HD12	1.84	0.60
8:A:1328:C:H5''	20:M:28:THR:HG21	1.84	0.60
8:A:1287:A:H2'	8:A:1288:A:C8	2.37	0.59
29:W:492:VAL:HG21	29:W:591:GLU:HB2	1.83	0.59
12:E:90:THR:HG22	12:E:91:GLY:N	2.18	0.59
30:a:1434:A:H2'	30:a:1435:G:C8	2.37	0.59
19:L:110:ARG:HB3	19:L:119:VAL:HG21	1.84	0.59
24:Q:25:ILE:HB	24:Q:42:THR:HG23	1.85	0.59
35:f:43:ALA:HB2	35:f:50:LEU:HB2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1279:G:H4'	8:A:1281:C:H5	1.68	0.59
8:A:1129:C:H2'	8:A:1139:G:N7	2.18	0.59
8:A:1017:U:H2'	8:A:1018:G:H8	1.68	0.58
8:A:1356:G:H2'	8:A:1357:A:C8	2.38	0.58
29:W:523:GLU:HB2	29:W:563:LYS:HG2	1.84	0.58
8:A:269:C:H2'	8:A:270:A:C8	2.38	0.58
8:A:664:G:H22	8:A:741:G:H1	1.51	0.58
29:W:87:ASP:HB3	29:W:457:HIS:HB2	1.85	0.58
29:W:602:GLU:HB3	29:W:678:VAL:HG22	1.85	0.58
13:F:29:ILE:HG22	13:F:34:GLY:HA3	1.85	0.57
1:O:10:LYS:HG3	1:O:54:ILE:HA	1.87	0.57
12:E:38:VAL:HG11	12:E:114:VAL:HG22	1.86	0.57
5:4:24:ILE:HD12	35:f:102:ARG:HG2	1.86	0.57
8:A:1329:A:O2'	8:A:1330:U:H5'	2.04	0.57
20:M:84:GLY:HA2	20:M:92:ARG:HH22	1.68	0.57
8:A:1134:G:H2'	8:A:1135:U:H4'	1.85	0.57
14:G:107:ALA:HA	14:G:110:LYS:HE3	1.86	0.57
30:a:1028:A:N6	30:a:1125:G:H2'	2.20	0.57
8:A:1218:C:H2'	8:A:1219:A:C8	2.40	0.57
8:A:518:C:H2'	8:A:530:G:C8	2.40	0.57
8:A:415:A:H2'	8:A:416:G:O4'	2.04	0.56
8:A:993:G:H2'	8:A:993:G:N3	2.20	0.56
30:a:2327:A:H2'	30:a:2328:A:C8	2.41	0.56
8:A:216:U:H4'	8:A:464:U:H4'	1.86	0.56
8:A:415:A:H2'	8:A:416:G:C8	2.40	0.56
8:A:946:A:H2'	8:A:947:G:C8	2.40	0.56
19:L:50:ARG:HB3	19:L:66:TYR:HE1	1.70	0.56
35:f:61:SER:HB2	35:f:91:LEU:HD21	1.87	0.56
8:A:420:U:O2'	8:A:423:G:O6	2.23	0.56
34:e:21:ARG:HD3	34:e:106:LYS:HB3	1.88	0.56
8:A:454:G:H2'	8:A:455:G:H5''	1.88	0.56
17:J:48:ARG:HH12	21:N:101:TRP:CB	2.19	0.56
18:K:111:THR:HG23	28:U:3:VAL:HG22	1.87	0.56
30:a:2291:U:H2'	30:a:2292:U:C6	2.40	0.56
8:A:462:G:H2'	8:A:463:U:O5'	2.05	0.56
3:2:54:ASP:HB3	40:k:57:LEU:HD22	1.87	0.56
8:A:299:G:H2'	8:A:300:A:C8	2.41	0.56
8:A:425:G:H2'	8:A:426:U:C6	2.41	0.56
17:J:29:ALA:HA	17:J:83:THR:HG23	1.88	0.56
35:f:108:VAL:HG11	35:f:176:PRO:HG3	1.87	0.56
8:A:417:C:H2'	8:A:418:C:C6	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:498:ARG:O	29:W:504:GLY:HA2	2.05	0.56
30:a:2328:A:H2'	30:a:2329:U:C6	2.41	0.55
8:A:493:A:H2'	8:A:494:G:C8	2.41	0.55
8:A:1160:G:H4'	9:B:131:LYS:HE3	1.88	0.55
8:A:1043:G:H2'	8:A:1044:A:H8	1.70	0.55
30:a:851:C:H2'	30:a:852:U:C6	2.41	0.55
8:A:82:G:H1	8:A:89:U:H1'	1.72	0.55
8:A:216:U:H1'	8:A:466:A:N6	2.22	0.55
8:A:382:A:H2'	8:A:383:A:C8	2.42	0.55
30:a:2193:G:H2'	30:a:2194:U:C6	2.42	0.55
8:A:1017:U:H2'	8:A:1018:G:C8	2.42	0.54
8:A:1044:A:C6	8:A:1045:C:H1'	2.42	0.54
8:A:1131:G:H1	8:A:1143:G:H21	1.54	0.54
19:L:4:VAL:HG23	24:Q:34:TYR:HB3	1.89	0.54
30:a:547:A:H1'	30:a:548:G:C5	2.43	0.54
30:a:2314:A:H1'	35:f:155:THR:HG21	1.90	0.54
8:A:462:G:C2'	8:A:463:U:O5'	2.56	0.54
8:A:465:A:H2'	8:A:466:A:C8	2.42	0.54
8:A:1150:A:H4'	17:J:43:PRO:HG3	1.90	0.54
16:I:91:ASP:HB3	16:I:94:LEU:HG	1.88	0.54
30:a:910:A:H2'	30:a:911:A:C8	2.43	0.54
8:A:1060:U:H5''	10:C:3:GLN:HG2	1.90	0.54
60:W:703:FUA:H232	60:W:703:FUA:H121	1.90	0.54
8:A:1306:A:N6	8:A:1331:G:H1'	2.23	0.53
12:E:81:LEU:HB2	12:E:98:PRO:HG3	1.89	0.53
36:g:89:LEU:HD11	36:g:96:ALA:HB2	1.90	0.53
14:G:76:LYS:HG3	14:G:89:VAL:HG21	1.91	0.53
14:G:111:ARG:HD2	14:G:123:GLU:HB2	1.90	0.53
9:B:73:LYS:HG3	9:B:168:HIS:CD2	2.41	0.53
11:D:102:VAL:HG13	11:D:107:PHE:HB2	1.90	0.53
30:a:1131:G:O2'	30:a:2026:U:H5'	2.09	0.53
8:A:410:G:H2'	8:A:429:U:C4	2.43	0.53
30:a:927:A:H2'	30:a:928:A:C8	2.43	0.53
35:f:40:VAL:HG21	35:f:53:ALA:HB3	1.90	0.53
17:J:35:GLN:HG2	17:J:77:VAL:HB	1.91	0.53
8:A:1210:C:H4'	8:A:1214:C:C4	2.44	0.53
13:F:29:ILE:HD13	13:F:64:VAL:HG21	1.91	0.53
8:A:1001:C:H2'	8:A:1002:G:C8	2.44	0.53
36:g:94:TYR:HA	36:g:106:SER:O	2.09	0.53
8:A:8:A:C6	11:D:206:LYS:HA	2.44	0.53
8:A:711:G:O2'	8:A:712:A:H5'	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:624:THR:HG23	30:a:2473:U:H1'	1.91	0.53
36:g:18:LYS:HB3	36:g:25:THR:HG23	1.90	0.53
10:C:180:ALA:HA	10:C:206:GLU:HA	1.91	0.52
12:E:45:ARG:HG2	12:E:71:MET:HE2	1.91	0.52
8:A:594:U:H2'	8:A:595:A:O4'	2.10	0.52
30:a:1778:U:H2'	30:a:1784:A:N6	2.23	0.52
9:B:71:GLY:HA3	9:B:80:VAL:HG21	1.91	0.52
29:W:447:GLN:HE22	29:W:479:MET:H	1.57	0.52
30:a:479:A:N3	30:a:481:G:H5''	2.24	0.52
8:A:1277:C:H1'	8:A:1282:C:C2	2.44	0.52
29:W:616:MET:HE2	29:W:640:GLN:HG3	1.92	0.52
29:W:90:VAL:HG21	29:W:435:PRO:HD2	1.91	0.52
26:S:4:SER:HB2	26:S:7:LYS:HG3	1.92	0.52
30:a:644:A:H2'	30:a:645:C:O4'	2.09	0.52
8:A:666:G:H5'	8:A:726:C:H1'	1.91	0.52
8:A:991:U:H1'	8:A:993:G:H8	1.75	0.52
12:E:72:ILE:C	12:E:72:ILE:HD12	2.35	0.52
8:A:1297:G:O2'	14:G:114:LYS:NZ	2.37	0.51
9:B:97:LEU:HD11	9:B:147:SER:HB2	1.91	0.51
10:C:138:VAL:HA	10:C:149:ILE:HD13	1.91	0.51
29:W:228:LYS:HD2	29:W:235:ILE:HD13	1.91	0.51
30:a:811:U:H2'	40:k:21:ARG:HA	1.92	0.51
30:a:1102:C:H2'	30:a:1103:A:C8	2.45	0.51
36:g:164:TYR:HB2	36:g:167:GLU:HB3	1.93	0.51
8:A:414:A:C2	8:A:415:A:C8	2.99	0.51
8:A:469:C:H2'	8:A:470:C:O4'	2.09	0.51
12:E:56:VAL:N	12:E:57:PRO:HD2	2.25	0.51
20:M:40:ALA:HB3	20:M:43:VAL:HG23	1.92	0.51
8:A:1016:A:H1'	8:A:1017:U:C4'	2.30	0.51
11:D:9:LEU:HD13	11:D:32:CYS:HB3	1.90	0.51
30:a:2749:A:H3'	30:a:2750:A:H2'	1.93	0.51
8:A:467:U:O2'	8:A:468:A:OP1	2.26	0.51
30:a:1570:A:H2'	30:a:1571:A:C8	2.44	0.51
30:a:2273:A:H2'	30:a:2274:A:C8	2.45	0.51
8:A:413:G:H3'	8:A:414:A:H5'	1.93	0.51
8:A:1147:C:H2'	8:A:1148:U:C6	2.46	0.51
30:a:2615:U:C2	55:z:4:GLN:HA	2.46	0.51
41:l:66:ARG:NH1	41:l:104:GLU:OE2	2.44	0.51
8:A:1092:A:H2'	8:A:1093:A:C8	2.45	0.51
30:a:274:C:H2'	30:a:275:C:O4'	2.11	0.51
33:d:85:ALA:HB3	33:d:88:GLU:HG3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2014:A:H2'	30:a:2015:A:C8	2.46	0.51
30:a:2756:U:H1'	30:a:2757:A:H5''	1.92	0.51
8:A:422:C:O2	8:A:423:G:N2	2.43	0.51
8:A:713:G:H2'	8:A:714:G:C8	2.46	0.51
8:A:1015:G:H2'	8:A:1016:A:C4	2.45	0.51
8:A:1225:A:H2'	8:A:1226:C:C6	2.45	0.51
30:a:145:C:H2'	30:a:146:A:C8	2.46	0.51
30:a:1939:5MU:OP1	30:a:2604:PSU:O2'	2.29	0.51
34:e:87:ALA:O	34:e:88:ARG:NH2	2.42	0.51
14:G:88:PRO:HG2	14:G:149:LYS:HA	1.92	0.51
30:a:1105:U:H2'	30:a:1106:G:C8	2.46	0.51
37:h:8:LYS:HA	37:h:14:SER:HA	1.92	0.51
8:A:481:G:O2'	8:A:483:C:N4	2.42	0.50
8:A:1412:C:H2'	8:A:1413:A:C8	2.46	0.50
30:a:1287:A:H5'	42:m:103:ARG:HD2	1.92	0.50
30:a:2469:A:H4'	41:l:55:ARG:CD	2.41	0.50
8:A:160:A:H61	8:A:347:G:H1'	1.76	0.50
29:W:30:ILE:HG23	29:W:271:LEU:HD21	1.93	0.50
29:W:218:VAL:HG21	29:W:244:ILE:HG12	1.93	0.50
30:a:747:5MU:O2	30:a:2014:A:H1'	2.11	0.50
53:x:9:LYS:O	53:x:60:LYS:NZ	2.43	0.50
8:A:268:U:H2'	8:A:269:C:C6	2.47	0.50
8:A:376:G:H5''	23:P:5:ARG:HB2	1.94	0.50
8:A:1329:A:C2'	8:A:1330:U:H5'	2.40	0.50
8:A:1391:U:H2'	8:A:1392:G:C8	2.47	0.50
30:a:1105:U:H2'	30:a:1106:G:H8	1.75	0.50
35:f:135:GLN:HG2	35:f:141:ILE:HG21	1.92	0.50
20:M:33:ILE:HD13	20:M:60:VAL:HG22	1.93	0.50
29:W:309:PHE:CZ	29:W:335:MET:HE3	2.46	0.50
34:e:48:THR:HG23	34:e:88:ARG:NH1	2.27	0.50
40:k:79:LEU:HD11	40:k:112:LEU:HD12	1.92	0.50
6:8:21:A:H8	6:8:21:A:H5''	1.76	0.50
8:A:1237:C:H4'	8:A:1300:G:H22	1.75	0.50
15:H:11:LEU:HD22	15:H:75:ILE:HD11	1.92	0.50
32:c:232:HIS:HA	32:c:242:LYS:HD2	1.94	0.50
8:A:979:C:H1'	8:A:1317:C:H42	1.75	0.50
30:a:2377:A:H2'	30:a:2378:A:C8	2.46	0.50
8:A:1376:U:O4	14:G:10:ARG:NH1	2.45	0.50
30:a:534:U:O2'	45:p:49:ASP:OD2	2.26	0.50
48:s:25:GLU:HG3	48:s:26:LYS:HG3	1.93	0.50
8:A:328:C:H2'	8:A:328:C:O2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:590:U:H2'	8:A:591:U:C6	2.47	0.50
35:f:114:PHE:HZ	35:f:176:PRO:HB2	1.76	0.50
8:A:8:A:N6	11:D:202:GLU:O	2.44	0.49
8:A:475:C:H2'	8:A:476:U:C6	2.47	0.49
10:C:50:ALA:HB1	10:C:76:VAL:HG22	1.94	0.49
13:F:9:MET:HG3	13:F:85:ILE:HG13	1.94	0.49
30:a:1386:C:H2'	30:a:1387:A:C8	2.47	0.49
30:a:1607:C:H4'	30:a:1608:A:O5'	2.11	0.49
36:g:175:LYS:O	36:g:176:LYS:C	2.55	0.49
8:A:425:G:O2'	8:A:426:U:H5'	2.12	0.49
8:A:662:U:H2'	8:A:663:A:C8	2.48	0.49
8:A:1060:U:H4'	17:J:53:ILE:HG13	1.94	0.49
9:B:133:GLU:HA	9:B:136:MET:HE2	1.93	0.49
29:W:516:ASN:ND2	29:W:521:GLY:O	2.42	0.49
36:g:103:ILE:HD11	36:g:117:LEU:HD21	1.93	0.49
8:A:1187:G:H21	21:N:100:SER:HB3	1.78	0.49
14:G:107:ALA:O	14:G:111:ARG:HG3	2.12	0.49
30:a:476:G:H4'	30:a:502:A:N1	2.27	0.49
30:a:1932:A:H2'	30:a:1933:G:O4'	2.12	0.49
30:a:1506:U:H2'	30:a:1507:C:C6	2.46	0.49
30:a:1871:A:H2'	30:a:1872:A:C8	2.47	0.49
8:A:371:A:H2'	8:A:372:C:O4'	2.13	0.49
9:B:111:ILE:HD13	9:B:148:LEU:HB3	1.94	0.49
29:W:552:GLY:HA3	29:W:556:GLY:HA2	1.94	0.49
35:f:41:GLY:O	35:f:43:ALA:N	2.45	0.49
47:r:4:ILE:HD12	47:r:6:LYS:HE3	1.94	0.49
8:A:1300:G:HO2'	8:A:1301:U:P	2.36	0.49
32:c:107:PRO:HD2	32:c:110:LEU:HD22	1.94	0.49
5:4:27:THR:HG21	35:f:62:GLY:HA2	1.95	0.49
8:A:171:A:H2'	8:A:172:A:C8	2.47	0.49
29:W:592:ALA:O	29:W:596:CYS:N	2.45	0.49
41:l:50:ARG:HD3	41:l:65:ILE:HD11	1.95	0.49
8:A:436:C:H2'	8:A:437:U:C6	2.48	0.49
9:B:125:THR:HA	9:B:128:LYS:HD3	1.93	0.49
30:a:1528:A:H2'	30:a:1529:G:O4'	2.13	0.49
8:A:631:C:H3'	8:A:632:U:H5'	1.94	0.49
29:W:164:LEU:HG	29:W:178:LEU:HD11	1.95	0.49
60:W:703:FUA:H232	60:W:703:FUA:C12	2.42	0.49
8:A:420:U:O2'	8:A:421:U:H6	1.96	0.49
9:B:76:ALA:HB1	9:B:210:VAL:HG11	1.95	0.49
30:a:1434:A:H2'	30:a:1435:G:H8	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:51:G:H2'	31:b:52:A:C8	2.48	0.49
32:c:16:VAL:HG22	32:c:206:GLY:HA3	1.94	0.49
47:r:4:ILE:HG22	47:r:106:VAL:HG22	1.95	0.49
8:A:1323:G:H2'	8:A:1324:A:C8	2.48	0.48
8:A:1043:G:H2'	8:A:1044:A:C8	2.47	0.48
16:I:11:ARG:HB2	16:I:106:ARG:HE	1.78	0.48
30:a:191:A:H2'	30:a:192:C:C6	2.48	0.48
30:a:493:G:H2'	30:a:494:G:O4'	2.13	0.48
30:a:717:C:H3'	30:a:718:A:H8	1.78	0.48
34:e:41:GLN:HG2	34:e:43:THR:HG23	1.93	0.48
8:A:1005:A:H2'	8:A:1006:G:O4'	2.13	0.48
22:O:47:LYS:HA	22:O:53:ARG:HH22	1.78	0.48
29:W:619:ILE:HD11	29:W:662:THR:HG23	1.95	0.48
8:A:195:A:H2'	8:A:196:A:C8	2.48	0.48
21:N:10:GLU:HG3	21:N:63:ARG:HD2	1.96	0.48
30:a:1028:A:H2'	30:a:1029:A:C8	2.48	0.48
33:d:121:THR:HB	33:d:127:PHE:CD2	2.49	0.48
8:A:82:G:N3	8:A:82:G:H2'	2.29	0.48
8:A:211:G:C5	8:A:212:G:H1'	2.48	0.48
8:A:458:U:H2'	8:A:459:A:C8	2.49	0.48
30:a:2038:G:H2'	30:a:2039:U:O4'	2.14	0.48
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.95	0.48
8:A:475:C:O2'	8:A:476:U:H5'	2.14	0.48
32:c:135:ILE:O	32:c:167:ARG:NH1	2.47	0.48
6:8:18:G:H1	6:8:55:U:H6	1.62	0.48
8:A:1151:A:H5'	17:J:43:PRO:HA	1.95	0.48
30:a:1079:C:H3'	30:a:1080:A:C8	2.48	0.48
30:a:1171:G:N3	30:a:1171:G:H2'	2.28	0.48
30:a:2859:G:H2'	30:a:2860:A:C8	2.49	0.48
8:A:420:U:O2'	8:A:421:U:H5''	2.14	0.48
8:A:673:A:H2'	8:A:674:G:C8	2.48	0.48
8:A:1423:G:H5'	39:j:49:ARG:HH22	1.79	0.48
12:E:90:THR:HG22	12:E:91:GLY:H	1.78	0.48
23:P:12:LYS:HG2	23:P:13:LYS:HG2	1.96	0.48
30:a:90:U:H3'	30:a:91:A:H2'	1.96	0.48
1:0:13:SER:HB2	1:0:49:TYR:CZ	2.49	0.48
15:H:64:LYS:HE2	15:H:71:VAL:HG21	1.95	0.48
16:I:35:LEU:HD11	16:I:45:ARG:HA	1.96	0.48
30:a:2798:U:H6	30:a:2798:U:H5'	1.79	0.48
32:c:120:VAL:HG12	32:c:131:PRO:HG2	1.96	0.48
36:g:86:LYS:HG2	36:g:132:VAL:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:83:LEU:HD21	26:S:65:GLU:HB2	1.95	0.48
25:R:23:TYR:HA	25:R:29:LEU:HD11	1.96	0.48
34:e:21:ARG:HD3	34:e:106:LYS:CB	2.43	0.48
8:A:415:A:H2'	8:A:416:G:H8	1.77	0.47
8:A:1386:G:H2'	8:A:1387:G:C8	2.49	0.47
29:W:7:LEU:HD13	29:W:282:LEU:HD21	1.96	0.47
29:W:318:THR:HA	29:W:324:LYS:HA	1.95	0.47
30:a:308:G:H2'	30:a:309:A:C8	2.49	0.47
33:d:62:LYS:N	33:d:63:PRO:HD2	2.29	0.47
42:m:38:LEU:N	42:m:39:PRO:HD2	2.29	0.47
8:A:77:A:H3'	8:A:78:A:C8	2.47	0.47
8:A:958:A:N6	26:S:77:THR:O	2.47	0.47
8:A:1138:G:C8	8:A:1140:C:H1'	2.49	0.47
29:W:572:HIS:O	29:W:576:SER:N	2.47	0.47
32:c:5:LYS:HD2	32:c:17:VAL:HG22	1.95	0.47
8:A:1097:C:H2'	8:A:1098:C:C6	2.49	0.47
29:W:117:GLU:HA	29:W:155:LEU:HD21	1.97	0.47
29:W:151:LEU:HD23	29:W:155:LEU:HD12	1.95	0.47
29:W:166:ILE:HB	29:W:174:ALA:HB3	1.96	0.47
29:W:343:ASN:O	29:W:347:GLY:N	2.45	0.47
30:a:544:C:H3'	30:a:545:U:C6	2.49	0.47
30:a:1072:C:H2'	30:a:1093:G:O6	2.14	0.47
8:A:1016:A:H8	8:A:1017:U:H1'	1.78	0.47
9:B:185:ALA:HB3	9:B:196:VAL:HG11	1.95	0.47
43:n:83:LEU:HD11	43:n:114:GLY:HA3	1.95	0.47
3:2:62:LEU:HB3	3:2:65:ALA:HB3	1.95	0.47
8:A:1305:G:H1'	8:A:1332:A:N6	2.30	0.47
9:B:34:ALA:HB2	9:B:39:HIS:CD2	2.50	0.47
9:B:111:ILE:HD12	9:B:152:LYS:HA	1.96	0.47
23:P:19:VAL:HG21	23:P:52:LEU:HD21	1.95	0.47
30:a:161:A:H3'	30:a:162:U:H2'	1.96	0.47
30:a:588:U:H2'	30:a:589:U:C6	2.50	0.47
8:A:97:G:H2'	8:A:98:A:O4'	2.14	0.47
8:A:188:C:H2'	8:A:189:A:O4'	2.14	0.47
8:A:417:C:O2'	8:A:418:C:H5'	2.15	0.47
8:A:632:U:H3'	8:A:633:G:H5'	1.96	0.47
8:A:820:U:H4'	8:A:821:G:OP2	2.14	0.47
8:A:1051:C:H2'	8:A:1052:U:C6	2.50	0.47
8:A:1238:A:H2'	8:A:1239:A:H5''	1.97	0.47
8:A:1338:G:H2'	8:A:1339:A:C8	2.49	0.47
17:J:48:ARG:CG	17:J:66:GLU:HG3	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:34:LEU:HD13	20:M:41:GLU:HA	1.96	0.47
27:T:39:ILE:HA	27:T:86:LEU:HD22	1.97	0.47
29:W:181:MET:SD	29:W:211:ARG:HD2	2.55	0.47
29:W:533:VAL:HG13	29:W:581:PHE:HE1	1.79	0.47
30:a:351:C:H2'	30:a:352:A:C8	2.49	0.47
30:a:365:U:H2'	30:a:366:C:C6	2.50	0.47
30:a:2788:C:H2'	30:a:2789:C:C6	2.50	0.47
33:d:142:VAL:HB	33:d:143:PRO:HD2	1.97	0.47
34:e:12:LEU:HD11	34:e:194:LYS:HD3	1.96	0.47
8:A:81:A:H2	8:A:83:C:H1'	1.80	0.47
8:A:536:C:H2'	8:A:537:G:H8	1.79	0.47
8:A:1455:G:O2'	8:A:1456:A:H5'	2.15	0.47
11:D:139:PRO:HA	11:D:182:PHE:HD1	1.80	0.47
8:A:1251:A:HO2'	8:A:1369:C:HO2'	1.62	0.47
30:a:279:A:H2'	30:a:280:U:O4'	2.15	0.47
30:a:1728:C:H2'	30:a:1730:C:O2	2.15	0.47
30:a:2298:A:H2'	30:a:2299:U:O4'	2.15	0.47
46:q:5:PHE:HB3	46:q:59:ILE:HD12	1.97	0.47
8:A:235:C:H2'	8:A:236:A:C8	2.50	0.47
8:A:801:U:H2'	8:A:802:A:C8	2.51	0.47
30:a:547:A:H1'	30:a:548:G:C4	2.50	0.47
30:a:1081:U:H2'	30:a:1082:U:C6	2.50	0.47
31:b:36:C:N4	31:b:49:C:O2	2.45	0.47
43:n:39:VAL:HB	43:n:49:VAL:HG23	1.96	0.47
1:O:22:THR:HG21	30:a:2419:U:H4'	1.96	0.46
30:a:244:A:C2	30:a:255:A:C4	3.03	0.46
30:a:1094:U:H1'	30:a:1097:U:H5	1.80	0.46
30:a:2307:G:N1	35:f:39:GLY:O	2.47	0.46
8:A:208:U:H2'	8:A:209:U:H5''	1.98	0.46
17:J:6:ILE:HB	17:J:76:ILE:HB	1.97	0.46
30:a:1637:A:H5'	30:a:1760:C:O2'	2.15	0.46
30:a:2314:A:H5'	35:f:35:THR:HG21	1.96	0.46
35:f:138:PHE:CE2	35:f:152:LEU:HD21	2.51	0.46
16:I:21:ILE:HG12	16:I:63:LEU:HB3	1.97	0.46
40:k:91:ASP:H	40:k:94:THR:HG1	1.64	0.46
54:y:13:ALA:O	54:y:21:LYS:HE2	2.16	0.46
3:2:45:ARG:N	3:2:46:PRO:HD2	2.30	0.46
8:A:758:C:H4'	8:A:880:C:H4'	1.97	0.46
10:C:183:ASP:HB3	10:C:202:ILE:HB	1.97	0.46
30:a:1327:A:H2'	30:a:1328:A:O4'	2.16	0.46
30:a:1469:A:H2'	30:a:1470:A:C8	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2346:A:H3'	30:a:2347:C:H5''	1.96	0.46
12:E:77:ASN:O	12:E:80:THR:HG22	2.16	0.46
16:I:54:LEU:HD23	16:I:98:LEU:HD23	1.96	0.46
20:M:11:ASP:HB3	20:M:46:SER:HB3	1.96	0.46
29:W:228:LYS:HD3	29:W:233:GLU:HB2	1.98	0.46
29:W:290:HIS:ND1	29:W:298:GLU:OE1	2.47	0.46
29:W:552:GLY:HA3	29:W:556:GLY:CA	2.46	0.46
8:A:151:A:H2'	8:A:152:A:O4'	2.15	0.46
8:A:542:G:H5'	11:D:39:GLY:HA3	1.97	0.46
29:W:188:ASN:HD21	29:W:192:THR:HG23	1.81	0.46
30:a:1906:G:H2'	30:a:1907:G:H5''	1.97	0.46
30:a:2636:C:H2'	30:a:2637:U:C6	2.51	0.46
30:a:2750:A:H1'	30:a:2752:C:N4	2.31	0.46
31:b:49:C:H2'	31:b:50:A:C8	2.51	0.46
33:d:25:THR:HG21	33:d:193:VAL:HG22	1.97	0.46
8:A:1149:C:O2'	8:A:1150:A:H5'	2.15	0.46
8:A:1269:A:H1'	8:A:1326:U:H1'	1.98	0.46
14:G:53:ARG:HH22	14:G:121:ALA:C	2.24	0.46
15:H:108:LYS:HG2	15:H:121:LEU:CD1	2.46	0.46
17:J:77:VAL:HG12	17:J:78:GLU:HG2	1.97	0.46
24:Q:59:VAL:HB	24:Q:75:LEU:HD21	1.97	0.46
29:W:535:ARG:HA	29:W:538:ILE:HD12	1.97	0.46
30:a:634:C:H2'	30:a:635:C:C6	2.50	0.46
8:A:419:C:C2	8:A:425:G:N1	2.84	0.46
8:A:588:G:H2'	8:A:589:U:C6	2.51	0.46
12:E:81:LEU:HD11	12:E:96:MET:HB3	1.97	0.46
8:A:444:G:O2'	8:A:445:G:H5'	2.16	0.46
10:C:35:SER:OG	10:C:59:ARG:NH2	2.49	0.46
14:G:107:ALA:O	14:G:110:LYS:HG2	2.16	0.46
29:W:322:VAL:HG23	29:W:325:LEU:HD21	1.95	0.46
6:8:47:U:H4'	6:8:48:C:H5'	1.98	0.46
8:A:496:A:N3	8:A:496:A:H2'	2.30	0.46
8:A:751:U:H2'	8:A:752:G:O4'	2.16	0.46
12:E:76:LEU:HD21	12:E:120:VAL:HG22	1.98	0.46
14:G:2:PRO:HD2	14:G:5:ARG:HA	1.98	0.46
15:H:50:LYS:HG3	15:H:60:GLU:HB3	1.97	0.46
29:W:579:MET:SD	29:W:580:ALA:N	2.89	0.45
30:a:139:U:H5''	30:a:140:C:H5	1.80	0.45
30:a:729:G:C6	32:c:207:LYS:HB2	2.51	0.45
38:i:114:LEU:HG	38:i:118:MET:HE3	1.98	0.45
5:4:2:LYS:HB2	5:4:5:ILE:HG12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:169:C:H2'	8:A:170:U:C6	2.51	0.45
8:A:1170:A:H2'	8:A:1171:A:O4'	2.16	0.45
10:C:16:LYS:NZ	10:C:181:ASP:OD1	2.47	0.45
29:W:129:PRO:HG2	29:W:279:PRO:HG3	1.98	0.45
29:W:485:THR:HB	29:W:601:LEU:HD11	1.97	0.45
30:a:12:U:O2	30:a:12:U:C2'	2.63	0.45
8:A:31:G:O2'	8:A:48:C:N4	2.50	0.45
8:A:422:C:O4'	8:A:423:G:C2	2.70	0.45
8:A:1159:U:O2	8:A:1161:C:N4	2.49	0.45
8:A:17:U:H2'	8:A:18:C:C6	2.51	0.45
26:S:29:LYS:O	26:S:30:PRO:C	2.59	0.45
29:W:91:GLU:HG3	60:W:703:FUA:H212	1.98	0.45
30:a:609:A:H2'	30:a:610:C:O4'	2.16	0.45
44:o:29:LYS:HE3	44:o:40:LEU:HB3	1.99	0.45
8:A:634:C:H2'	8:A:635:A:H5''	1.99	0.45
8:A:868:C:H2'	8:A:869:G:O4'	2.16	0.45
8:A:1248:A:H2	8:A:1289:A:H62	1.65	0.45
29:W:456:LEU:HD21	60:W:703:FUA:H273	1.98	0.45
8:A:413:G:O5'	8:A:414:A:H5'	2.17	0.45
23:P:19:VAL:HG21	23:P:52:LEU:CD2	2.46	0.45
30:a:499:U:H5''	49:t:43:LYS:HE2	1.99	0.45
32:c:133:ARG:NH2	32:c:187:ASP:OD1	2.50	0.45
23:P:6:LEU:CD2	23:P:19:VAL:HG22	2.47	0.45
29:W:534:PRO:HB2	29:W:537:TYR:HD2	1.82	0.45
31:b:29:A:H2'	31:b:30:C:O4'	2.16	0.45
35:f:163:ASP:HB3	35:f:167:ARG:HH21	1.82	0.45
36:g:43:VAL:HA	36:g:51:THR:O	2.17	0.45
8:A:475:C:H2'	8:A:476:U:H6	1.80	0.45
8:A:945:G:H2'	8:A:945:G:N3	2.32	0.45
30:a:247:G:H4'	30:a:386:G:C5	2.52	0.45
35:f:38:MET:HG3	35:f:57:LEU:HD13	1.99	0.45
39:j:58:LEU:HD11	39:j:86:LEU:HD13	1.99	0.45
8:A:464:U:H3	8:A:467:U:P	2.40	0.45
8:A:932:C:H2'	8:A:933:G:C8	2.52	0.45
8:A:1237:C:H4'	8:A:1300:G:N2	2.32	0.45
8:A:1402:4OC:H6	8:A:1402:4OC:O5'	2.16	0.45
29:W:7:LEU:HB3	29:W:282:LEU:HG	1.99	0.45
29:W:160:ALA:HB3	29:W:253:PHE:HE1	1.82	0.45
30:a:354:A:H2'	30:a:355:U:C6	2.52	0.45
30:a:2547:A:H2'	30:a:2548:U:C6	2.52	0.45
8:A:131:A:H2'	8:A:132:C:C6	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:266:G:H3'	24:Q:69:LYS:HB2	1.98	0.45
8:A:1147:C:H1'	16:I:18:ARG:HH21	1.82	0.45
8:A:1160:G:H4'	9:B:131:LYS:CE	2.46	0.45
25:R:36:SER:HA	25:R:72:ASP:HB3	1.98	0.45
30:a:813:U:H2'	30:a:814:C:C6	2.52	0.45
35:f:41:GLY:C	35:f:43:ALA:N	2.76	0.45
51:v:38:VAL:HG12	51:v:59:LEU:HB2	1.98	0.45
8:A:859:G:H2'	8:A:860:A:C8	2.52	0.44
8:A:1010:U:H2'	8:A:1011:C:C6	2.52	0.44
8:A:1049:U:H4'	8:A:1050:G:H5''	1.99	0.44
9:B:162:PHE:CE1	9:B:217:VAL:HG11	2.53	0.44
14:G:129:GLU:HG3	14:G:131:LYS:HG3	1.99	0.44
30:a:1853:A:N1	30:a:2087:G:H1'	2.32	0.44
30:a:2794:C:H2'	30:a:2795:C:C6	2.52	0.44
36:g:64:GLN:O	36:g:67:THR:HG22	2.18	0.44
46:q:1:MET:HA	46:q:42:ALA:O	2.16	0.44
8:A:160:A:H2'	8:A:161:A:O4'	2.17	0.44
8:A:1367:C:H5''	16:I:116:VAL:HG13	1.99	0.44
29:W:579:MET:HA	29:W:582:LYS:HE2	2.00	0.44
32:c:31:ALA:HA	32:c:34:LEU:HD12	1.99	0.44
45:p:109:LEU:HD11	46:q:40:MET:HE1	1.98	0.44
8:A:51:A:N7	8:A:114:U:O2'	2.49	0.44
8:A:517:G:N2	8:A:531:U:H5'	2.31	0.44
8:A:675:A:O2'	18:K:116:ILE:O	2.34	0.44
8:A:1127:G:H5'	8:A:1280:A:O2'	2.16	0.44
8:A:1146:A:H2'	8:A:1146:A:N3	2.32	0.44
16:I:21:ILE:HD11	16:I:83:ILE:HG23	1.99	0.44
36:g:2:SER:O	36:g:6:LYS:HG2	2.17	0.44
36:g:24:ILE:HG21	36:g:72:LEU:HD21	1.99	0.44
8:A:205:A:H2'	8:A:205:A:N3	2.32	0.44
8:A:1236:A:H4'	8:A:1304:G:H4'	1.98	0.44
8:A:1372:U:H2'	8:A:1373:G:O4'	2.16	0.44
30:a:1727:C:H2'	30:a:1728:C:O4'	2.18	0.44
35:f:121:SER:HB2	35:f:128:TYR:CE1	2.53	0.44
8:A:499:A:H4'	8:A:500:G:OP1	2.18	0.44
35:f:43:ALA:HA	35:f:46:ASP:O	2.18	0.44
8:A:109:A:H2'	8:A:326:G:N2	2.32	0.44
8:A:1342:C:H2'	8:A:1343:G:C8	2.53	0.44
8:A:1397:C:H4'	8:A:1398:A:OP2	2.18	0.44
8:A:1428:A:H2'	8:A:1429:A:O4'	2.18	0.44
8:A:417:C:C4	8:A:418:C:C4	3.06	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1314:C:H2'	8:A:1315:U:C6	2.53	0.44
15:H:43:GLU:HG3	15:H:101:ILE:HD13	1.99	0.44
24:Q:27:ARG:HG3	24:Q:40:ARG:HB2	2.00	0.44
30:a:358:U:H2'	30:a:359:G:C8	2.53	0.44
30:a:1056:G:H4'	30:a:1086:A:C8	2.53	0.44
8:A:1307:U:H2'	8:A:1308:U:C6	2.53	0.44
26:S:50:ALA:HB1	26:S:57:HIS:HB3	2.00	0.44
30:a:2430:A:N3	30:a:2430:A:H2'	2.32	0.44
31:b:48:U:H2'	31:b:49:C:C6	2.52	0.44
8:A:429:U:H5'	11:D:9:LEU:HD12	1.99	0.44
8:A:1414:U:H2'	8:A:1415:G:H8	1.82	0.44
12:E:95:PHE:CZ	12:E:97:GLN:HB2	2.53	0.44
30:a:2646:C:H2'	30:a:2647:U:O4'	2.17	0.44
6:8:42:G:H2'	6:8:43:A:H5''	1.99	0.43
8:A:71:A:H61	8:A:99:C:H1'	1.82	0.43
8:A:82:G:N2	8:A:88:U:O2	2.50	0.43
8:A:860:A:H2'	8:A:861:G:O4'	2.17	0.43
8:A:801:U:H2'	8:A:802:A:H8	1.83	0.43
9:B:60:ILE:HD13	9:B:160:ALA:HB2	2.00	0.43
13:F:90:MET:HE1	25:R:61:ARG:HD3	2.00	0.43
14:G:26:PHE:CZ	14:G:120:LEU:HD11	2.52	0.43
29:W:484:GLU:HG3	29:W:557:TYR:HB2	2.00	0.43
30:a:494:G:H4'	47:r:6:LYS:HB2	2.00	0.43
30:a:2315:G:N3	35:f:125:ARG:NH2	2.66	0.43
30:a:2783:U:H2'	30:a:2784:U:C6	2.53	0.43
36:g:89:LEU:HD22	36:g:162:VAL:HG22	1.99	0.43
4:3:11:CYS:N	4:3:14:CYS:SG	2.91	0.43
16:I:6:TYR:CE2	16:I:90:TYR:HA	2.54	0.43
30:a:2556:C:H2'	30:a:2557:G:O4'	2.18	0.43
39:j:1:MET:HE3	39:j:32:TYR:CZ	2.53	0.43
8:A:677:U:H3	8:A:713:G:H22	1.66	0.43
8:A:744:C:H2'	8:A:745:G:C8	2.54	0.43
29:W:219:ALA:HB1	29:W:226:MET:HA	2.00	0.43
41:l:20:LEU:HD13	50:u:81:PRO:HG2	2.01	0.43
8:A:381:C:H2'	8:A:382:A:C8	2.53	0.43
8:A:486:U:H2'	8:A:487:A:H8	1.83	0.43
8:A:1031:C:H4'	8:A:1032:G:C4	2.53	0.43
10:C:70:THR:O	10:C:105:GLU:HA	2.19	0.43
30:a:1914:C:H2'	30:a:1915:3TD:O4'	2.18	0.43
7:9:18:G:H2'	7:9:19:G:C8	2.54	0.43
8:A:449:G:H2'	8:A:450:G:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:47:LEU:HB3	10:C:50:ALA:HB3	2.00	0.43
11:D:140:ASN:N	11:D:182:PHE:O	2.47	0.43
8:A:316:C:H2'	8:A:317:U:C6	2.54	0.43
8:A:974:A:P	21:N:69:ARG:HH22	2.41	0.43
13:F:18:VAL:HB	13:F:19:PRO:HD3	2.01	0.43
29:W:314:PHE:HA	29:W:401:MET:HE1	2.01	0.43
30:a:1585:C:H2'	30:a:1586:A:O4'	2.19	0.43
30:a:2376:A:H2'	30:a:2377:A:O4'	2.18	0.43
30:a:2684:U:H4'	39:j:76:VAL:CG2	2.48	0.43
30:a:2740:A:H2'	30:a:2741:A:C8	2.54	0.43
35:f:122:PHE:CE1	35:f:128:TYR:HB2	2.54	0.43
8:A:419:C:C2	8:A:425:G:C2	3.07	0.43
8:A:524:G:H2'	8:A:525:C:C6	2.54	0.43
17:J:92:LEU:HD12	17:J:98:VAL:HG22	2.01	0.43
30:a:279:A:N6	30:a:361:G:H1'	2.34	0.43
30:a:1182:G:H2'	30:a:1183:U:O4'	2.19	0.43
8:A:501:C:H2'	8:A:502:A:C8	2.54	0.43
8:A:937:A:H1'	8:A:1378:C:H42	1.84	0.43
8:A:1492:A:C2	30:a:1913:A:N3	2.86	0.43
8:A:1518:MA6:H103	8:A:1519:MA6:H102	2.01	0.43
17:J:7:ARG:N	17:J:101:SER:O	2.52	0.43
17:J:10:LEU:HD12	17:J:22:THR:HG22	2.01	0.43
19:L:114:ARG:HB3	19:L:119:VAL:HB	2.01	0.43
27:T:24:ARG:HH21	27:T:61:GLN:HE22	1.67	0.43
29:W:98:VAL:HG21	29:W:314:PHE:CG	2.54	0.43
30:a:340:A:H2'	30:a:341:C:O4'	2.18	0.43
30:a:639:U:H2'	30:a:640:C:C6	2.54	0.43
30:a:1064:C:H2'	30:a:1065:U:O4'	2.19	0.43
30:a:2243:U:H2'	30:a:2244:U:C6	2.54	0.43
48:s:22:THR:HA	48:s:25:GLU:HG2	2.01	0.43
8:A:190:A:H2'	8:A:191:G:O4'	2.19	0.43
8:A:1251:A:H2'	8:A:1252:A:C8	2.54	0.43
8:A:1486:G:H2'	8:A:1487:G:O4'	2.19	0.43
9:B:28:LYS:HB3	9:B:29:PRO:HD3	2.01	0.43
14:G:66:LEU:HD23	14:G:104:ILE:HD12	2.00	0.43
17:J:48:ARG:NH1	21:N:101:TRP:CD2	2.87	0.43
29:W:436:THR:HB	29:W:453:MET:HE3	2.00	0.43
19:L:86:ARG:HA	19:L:94:ARG:HA	2.00	0.42
30:a:1579:A:H2'	30:a:1580:A:C8	2.54	0.42
8:A:413:G:C3'	8:A:414:A:H5'	2.49	0.42
8:A:1147:C:H2'	8:A:1148:U:H6	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1376:U:H2'	8:A:1377:A:C8	2.53	0.42
20:M:86:TYR:O	20:M:90:ARG:HG2	2.19	0.42
29:W:98:VAL:HG11	29:W:314:PHE:HB3	1.99	0.42
30:a:94:A:H2'	30:a:95:A:C8	2.53	0.42
30:a:1225:G:OP1	46:q:73:LYS:NZ	2.49	0.42
30:a:2795:C:H2'	30:a:2796:U:C6	2.55	0.42
32:c:155:ALA:HB2	32:c:162:VAL:HG23	2.01	0.42
44:o:31:TRP:CE3	44:o:38:LYS:HG2	2.54	0.42
21:N:74:LEU:HD12	21:N:84:VAL:HG21	2.02	0.42
28:U:6:VAL:HG22	28:U:15:ALA:HB1	2.01	0.42
29:W:294:ASN:HB2	29:W:297:GLU:HB3	2.00	0.42
29:W:414:PRO:HD3	29:W:423:MET:HE2	2.01	0.42
30:a:74:A:H5''	30:a:74:A:N3	2.34	0.42
30:a:84:A:N3	30:a:85:G:H1'	2.34	0.42
30:a:280:U:H2'	30:a:281:C:C6	2.54	0.42
30:a:1412:U:H2'	30:a:1413:A:C8	2.54	0.42
39:j:102:PRO:HD2	44:o:68:GLU:HG3	2.01	0.42
8:A:635:A:H5''	8:A:635:A:H8	1.84	0.42
8:A:899:C:H2'	8:A:900:A:C8	2.54	0.42
10:C:68:ILE:HD13	10:C:101:ILE:HG23	2.01	0.42
13:F:18:VAL:HG21	13:F:58:HIS:CD2	2.54	0.42
15:H:29:SER:HB3	15:H:57:PRO:HB2	2.01	0.42
29:W:148:VAL:HA	29:W:151:LEU:HD12	2.00	0.42
30:a:454:A:H4'	30:a:455:C:OP2	2.20	0.42
30:a:861:A:H2'	30:a:862:G:O4'	2.19	0.42
30:a:1021:A:H3'	30:a:1021:A:N3	2.34	0.42
8:A:414:A:N3	8:A:414:A:H2'	2.35	0.42
8:A:416:G:O6	8:A:428:G:O6	2.36	0.42
8:A:530:G:N3	8:A:530:G:H3'	2.34	0.42
8:A:620:C:H2'	8:A:621:A:C8	2.55	0.42
17:J:76:ILE:HG21	17:J:87:LEU:HD11	2.00	0.42
30:a:244:A:H2'	30:a:245:G:O4'	2.19	0.42
30:a:593:U:H2'	30:a:594:U:C6	2.54	0.42
30:a:1198:U:H5'	45:p:9:ILE:HD11	2.02	0.42
37:h:31:VAL:N	37:h:32:PRO:HD2	2.35	0.42
42:m:55:ALA:HA	42:m:80:PHE:CE2	2.55	0.42
2:l:1:MET:H1	30:a:1619:G:H2'	1.83	0.42
2:l:29:GLN:NE2	30:a:210:C:OP1	2.51	0.42
6:8:32:C:O2	6:8:32:C:O4'	2.38	0.42
8:A:1134:G:C6	8:A:1135:U:H1'	2.54	0.42
20:M:83:LEU:HD21	26:S:65:GLU:CB	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:546:U:H3'	30:a:547:A:C8	2.48	0.42
50:u:21:ARG:HA	50:u:25:LYS:O	2.19	0.42
8:A:579:A:H2'	8:A:580:C:C6	2.54	0.42
8:A:1377:A:C5	14:G:7:ILE:HG21	2.54	0.42
13:F:51:ILE:HD11	25:R:66:SER:HB2	2.01	0.42
30:a:1088:A:H2'	30:a:1088:A:N3	2.35	0.42
30:a:2849:U:H4'	30:a:2868:A:C2	2.54	0.42
31:b:30:C:H1'	31:b:57:A:H61	1.84	0.42
8:A:413:G:H1'	8:A:428:G:N2	2.30	0.42
10:C:138:VAL:HG13	10:C:149:ILE:HG23	2.02	0.42
14:G:74:GLU:HG3	14:G:89:VAL:HG23	2.01	0.42
30:a:92:U:H2'	30:a:93:G:O4'	2.18	0.42
30:a:1721:G:N2	30:a:1738:G:O2'	2.53	0.42
30:a:1859:U:H2'	30:a:1860:G:C8	2.54	0.42
30:a:2591:C:H2'	30:a:2592:G:C8	2.54	0.42
35:f:36:LEU:HB2	35:f:57:LEU:HD11	2.02	0.42
6:8:55:U:O2	6:8:55:U:O4'	2.37	0.42
8:A:790:A:H2'	8:A:791:G:C8	2.55	0.42
16:I:118:LEU:HD22	16:I:124:ARG:HG2	2.01	0.42
30:a:2522:U:O2'	30:a:2647:U:OP1	2.37	0.42
35:f:58:ALA:HB2	35:f:65:PRO:HD3	2.02	0.42
6:8:19:G:N2	6:8:57:A:N3	2.68	0.42
6:8:38:A:H2'	6:8:39:C:O4'	2.20	0.42
8:A:49:U:O2	8:A:362:G:H1'	2.19	0.42
8:A:123:U:OP1	8:A:312:C:H5'	2.20	0.42
8:A:1259:C:H3'	8:A:1260:G:H5''	2.02	0.42
12:E:132:ASN:O	12:E:136:VAL:HG23	2.20	0.42
15:H:89:LYS:HA	15:H:92:LEU:HG	2.02	0.42
30:a:1869:G:H2'	30:a:1871:A:N7	2.35	0.42
35:f:44:ILE:HA	35:f:83:TYR:CE2	2.55	0.42
8:A:413:G:C1'	8:A:428:G:H21	2.32	0.41
8:A:1268:G:H2'	8:A:1269:A:C8	2.55	0.41
8:A:1277:C:H2'	8:A:1278:G:H5''	2.02	0.41
14:G:54:SER:HB3	14:G:56:LYS:HE2	2.01	0.41
18:K:35:THR:HG22	18:K:41:ALA:HA	2.02	0.41
19:L:30:LYS:HE2	19:L:59:ASN:HD22	1.85	0.41
29:W:335:MET:HE2	29:W:352:VAL:HG21	2.02	0.41
30:a:728:G:H4'	32:c:13:ARG:HD3	2.00	0.41
35:f:14:LYS:H	35:f:14:LYS:HD2	1.85	0.41
8:A:211:G:C4	8:A:212:G:H1'	2.56	0.41
8:A:1011:C:H2'	8:A:1012:A:C8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1295:U:H2'	8:A:1296:C:C6	2.55	0.41
22:O:43:PHE:HB3	22:O:53:ARG:HH21	1.85	0.41
22:O:88:ARG:NH1	30:a:716:A:OP1	2.53	0.41
29:W:280:SER:HB2	29:W:281:PRO:HD2	2.01	0.41
30:a:594:U:H2'	30:a:595:C:C6	2.55	0.41
30:a:2271:G:OP1	51:v:18:ALA:HB1	2.20	0.41
30:a:2680:U:H5'	33:d:194:PRO:HA	2.02	0.41
43:n:58:ILE:HG22	43:n:62:LEU:HD11	2.02	0.41
6:8:19:G:H4'	6:8:60:U:H3	1.84	0.41
8:A:736:C:H2'	8:A:737:C:C6	2.55	0.41
9:B:130:THR:O	9:B:132:LYS:N	2.50	0.41
17:J:65:TYR:OH	21:N:85:ARG:HG3	2.20	0.41
20:M:45:ILE:HD13	20:M:48:LEU:HD12	2.01	0.41
26:S:80:TYR:HE1	26:S:83:HIS:CE1	2.37	0.41
29:W:419:ASP:HB3	29:W:471:VAL:HG13	2.02	0.41
30:a:478:A:N1	30:a:500:G:H4'	2.34	0.41
31:b:104:A:H2'	31:b:105:G:O4'	2.20	0.41
32:c:76:ALA:HB2	32:c:96:TYR:CD2	2.55	0.41
6:8:18:G:N2	6:8:58:A:OP2	2.53	0.41
8:A:714:G:H2'	8:A:715:A:C8	2.54	0.41
8:A:1030:U:O2'	8:A:1031:C:OP2	2.37	0.41
13:F:7:VAL:HG22	13:F:61:LEU:HD13	2.02	0.41
29:W:19:ILE:HD12	29:W:19:ILE:H	1.85	0.41
30:a:2:G:H2'	30:a:3:U:C6	2.55	0.41
30:a:849:A:H2'	30:a:850:U:C6	2.56	0.41
35:f:40:VAL:CG2	35:f:53:ALA:HB3	2.51	0.41
8:A:22:G:O2'	8:A:913:A:N1	2.45	0.41
8:A:337:G:H2'	8:A:338:A:C8	2.55	0.41
8:A:595:A:H1'	8:A:596:A:N7	2.35	0.41
8:A:653:U:O2'	8:A:753:A:N6	2.53	0.41
8:A:1047:G:H21	8:A:1215:G:H5'	1.85	0.41
9:B:47:VAL:N	9:B:48:PRO:HD2	2.36	0.41
13:F:20:GLY:O	13:F:24:ARG:HG3	2.21	0.41
20:M:15:ALA:HB1	20:M:34:LEU:HD21	2.02	0.41
30:a:221:A:N1	30:a:265:A:O2'	2.48	0.41
30:a:1405:U:H2'	30:a:1406:U:C6	2.55	0.41
30:a:1682:G:H2'	30:a:1683:U:C6	2.55	0.41
30:a:1710:G:H4'	30:a:2858:C:O2	2.20	0.41
30:a:2286:G:N3	30:a:2286:G:H2'	2.35	0.41
30:a:2308:G:C2	35:f:77:PHE:CZ	3.08	0.41
30:a:2445:2MG:HM21	30:a:2449:H2U:O4	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2684:U:H4'	39:j:76:VAL:HG21	2.01	0.41
32:c:37:ASN:ND2	32:c:60:GLN:O	2.54	0.41
6:8:9:G:O2'	6:8:10:G:N7	2.50	0.41
8:A:87:C:H2'	8:A:88:U:O4'	2.21	0.41
8:A:701:U:H5''	8:A:703:G:O4'	2.20	0.41
8:A:1169:A:H2'	8:A:1170:A:O4'	2.20	0.41
8:A:1194:U:H2'	8:A:1195:C:C6	2.55	0.41
8:A:1250:A:H4'	8:A:1250:A:OP1	2.21	0.41
8:A:1273:C:H2'	8:A:1274:A:O4'	2.20	0.41
9:B:7:ARG:O	9:B:10:LEU:HG	2.21	0.41
11:D:61:VAL:HG21	11:D:200:ILE:HD11	2.03	0.41
29:W:572:HIS:O	29:W:573:ASP:C	2.63	0.41
30:a:357:C:H2'	30:a:358:U:C6	2.56	0.41
30:a:1790:C:H2'	30:a:1791:A:C5	2.56	0.41
30:a:2312:U:H5'	35:f:85:ILE:HG13	2.03	0.41
9:B:214:LEU:HA	9:B:217:VAL:HG22	2.02	0.41
15:H:39:VAL:O	15:H:42:GLU:HG2	2.21	0.41
29:W:354:ARG:HB3	29:W:378:VAL:HB	2.01	0.41
30:a:1090:A:C2	30:a:1102:C:H1'	2.55	0.41
39:j:114:LYS:HE3	39:j:118:LEU:HD11	2.03	0.41
17:J:6:ILE:HG12	17:J:102:LEU:HG	2.03	0.41
29:W:177:ASP:HB2	29:W:184:PHE:HE1	1.85	0.41
30:a:322:A:OP2	34:e:163:ASN:HB2	2.21	0.41
30:a:784:G:H5'	30:a:785:G:OP1	2.20	0.41
30:a:1061:U:H3'	30:a:1062:G:H5''	2.02	0.41
30:a:1361:G:H2'	30:a:1362:C:C6	2.56	0.41
30:a:1911:PSU:O2	30:a:1918:A:H2'	2.21	0.41
30:a:2461:A:H2'	30:a:2462:C:C6	2.56	0.41
8:A:408:A:H2'	8:A:409:U:O4'	2.21	0.41
8:A:1130:A:H2'	8:A:1131:G:C8	2.55	0.41
8:A:1305:G:H1'	8:A:1332:A:H61	1.86	0.41
9:B:6:MET:HG3	9:B:43:LEU:HB3	2.03	0.41
9:B:12:ALA:HB1	9:B:209:ALA:HA	2.02	0.41
9:B:23:TRP:CH2	9:B:25:PRO:HA	2.56	0.41
9:B:186:ILE:HG13	9:B:213:TYR:CD2	2.56	0.41
9:B:186:ILE:HG21	9:B:213:TYR:CE2	2.56	0.41
11:D:170:TRP:CD2	11:D:186:PRO:HB3	2.56	0.41
13:F:66:ALA:HB1	13:F:67:PRO:HD2	2.02	0.41
15:H:7:ILE:O	15:H:11:LEU:HG	2.20	0.41
17:J:64:GLN:NE2	21:N:101:TRP:CH2	2.89	0.41
25:R:32:TYR:HB3	25:R:55:LEU:HD21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:486:PHE:HB3	29:W:596:CYS:HB3	2.03	0.41
30:a:150:U:H2'	30:a:151:C:C6	2.55	0.41
30:a:614:A:H3'	30:a:615:U:C5'	2.50	0.41
30:a:871:U:H2'	30:a:872:U:C6	2.56	0.41
30:a:1102:C:H2'	30:a:1103:A:H8	1.86	0.41
30:a:1847:A:H1'	30:a:1848:A:N7	2.35	0.41
30:a:1927:A:H2'	30:a:1928:A:C8	2.56	0.41
30:a:2850:A:N7	30:a:2868:A:O2'	2.52	0.41
31:b:66:A:N6	31:b:107:G:H2'	2.35	0.41
45:p:41:LYS:HA	45:p:44:GLN:HE21	1.84	0.41
47:r:20:VAL:HG11	47:r:44:ALA:HA	2.01	0.41
8:A:600:A:H2'	8:A:601:G:C8	2.56	0.41
8:A:1444:U:H2'	8:A:1445:U:C6	2.55	0.41
30:a:645:C:H2'	30:a:647:G:C8	2.56	0.41
30:a:945:A:C4	30:a:2448:A:C2	3.09	0.41
30:a:1275:A:N1	30:a:1295:C:O2'	2.50	0.41
31:b:1:U:H2'	31:b:2:G:C8	2.55	0.41
35:f:42:GLU:HG3	35:f:49:LEU:HD13	2.02	0.41
8:A:381:C:H2'	8:A:382:A:O4'	2.21	0.40
8:A:455:G:H2'	8:A:456:A:C8	2.56	0.40
8:A:1162:C:H2'	8:A:1163:A:C8	2.55	0.40
10:C:50:ALA:HA	10:C:75:ILE:HD11	2.03	0.40
11:D:35:GLU:CD	11:D:35:GLU:H	2.29	0.40
11:D:173:VAL:HA	11:D:180:GLY:HA2	2.02	0.40
17:J:66:GLU:OE1	17:J:68:ARG:HG2	2.20	0.40
29:W:245:ARG:HD3	29:W:276:ASP:O	2.21	0.40
30:a:158:U:H2'	30:a:159:G:C8	2.56	0.40
30:a:1838:C:N4	30:a:1898:U:H2'	2.37	0.40
31:b:30:C:H2'	31:b:31:C:H5'	2.03	0.40
8:A:519:C:H2'	8:A:520:A:C8	2.56	0.40
8:A:1095:U:H2'	8:A:1096:C:C6	2.56	0.40
9:B:50:PHE:O	9:B:54:LEU:HG	2.21	0.40
17:J:48:ARG:HH12	21:N:101:TRP:CG	2.40	0.40
20:M:9:ILE:HD12	20:M:45:ILE:HD12	2.04	0.40
20:M:16:VAL:O	20:M:20:THR:HG23	2.21	0.40
29:W:247:ALA:HB1	29:W:253:PHE:HB3	2.01	0.40
29:W:314:PHE:CZ	29:W:327:PHE:HB3	2.55	0.40
30:a:833:A:H2'	30:a:834:G:C8	2.56	0.40
30:a:2358:A:H2'	30:a:2359:C:O4'	2.21	0.40
32:c:122:ALA:O	32:c:130:LEU:HD21	2.20	0.40
51:v:50:ASN:HB2	51:v:82:ILE:HB	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:27:ALA:O	3:2:28:ASN:HB2	2.22	0.40
8:A:640:A:H2'	8:A:641:U:O4'	2.21	0.40
8:A:1212:U:H5'	8:A:1213:A:C8	2.56	0.40
8:A:1504:G:H4'	8:A:1505:G:C4	2.55	0.40
9:B:31:ILE:HA	9:B:41:ILE:HA	2.02	0.40
9:B:41:ILE:HG21	9:B:201:PRO:HB2	2.03	0.40
16:I:88:MET:SD	16:I:95:ARG:HG3	2.61	0.40
30:a:101:A:N3	30:a:101:A:H2'	2.37	0.40
30:a:139:U:H3'	30:a:140:C:H6	1.86	0.40
30:a:288:U:H2'	30:a:289:G:O4'	2.20	0.40
30:a:1605:C:H2'	30:a:1606:C:O4'	2.21	0.40
30:a:2796:U:H3	30:a:2799:A:H61	1.69	0.40
43:n:43:ASN:OD1	43:n:44:GLY:N	2.54	0.40
52:w:32:ASN:OD1	52:w:34:HIS:NE2	2.54	0.40
8:A:1345:U:H5''	16:I:122:ARG:HH11	1.86	0.40
8:A:1401:G:H2'	8:A:1402:4OC:O4'	2.21	0.40
14:G:26:PHE:HZ	14:G:120:LEU:HD11	1.86	0.40
20:M:13:LYS:HD3	20:M:17:ILE:HG22	2.03	0.40
23:P:45:GLU:HG3	23:P:46:LYS:HG3	2.03	0.40
29:W:72:TRP:CD1	29:W:73:GLU:HG2	2.56	0.40
30:a:1180:U:H2'	30:a:1181:U:C6	2.56	0.40
30:a:1357:C:H2'	30:a:1358:G:O4'	2.21	0.40
30:a:1419:A:H5'	30:a:1579:A:H61	1.86	0.40
30:a:1680:U:H2'	30:a:1681:G:O4'	2.21	0.40
30:a:2305:U:H5''	35:f:131:GLY:CA	2.50	0.40
30:a:2308:G:C2	35:f:77:PHE:HZ	2.38	0.40
1:O:5:ILE:HD13	1:O:5:ILE:HA	1.96	0.40
8:A:451:A:H4'	8:A:452:A:O5'	2.21	0.40
14:G:113:ASP:HB2	14:G:119:ARG:CG	2.52	0.40
30:a:845:A:N3	30:a:845:A:H3'	2.37	0.40
30:a:1869:G:N2	30:a:1871:A:H3'	2.36	0.40
30:a:2552:OMU:HM23	30:a:2554:U:C6	2.57	0.40
31:b:37:C:H2'	31:b:38:C:O4'	2.22	0.40
33:d:48:ILE:HG21	33:d:90:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	48/55 (87%)	48 (100%)	0	0	100	100
2	1	43/46 (94%)	43 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	46/70 (66%)	45 (98%)	1 (2%)	0	100	100
9	B	220/241 (91%)	214 (97%)	5 (2%)	1 (0%)	24	23
10	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
11	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
12	E	152/167 (91%)	148 (97%)	4 (3%)	0	100	100
13	F	99/135 (73%)	95 (96%)	4 (4%)	0	100	100
14	G	148/179 (83%)	145 (98%)	3 (2%)	0	100	100
15	H	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	16	13
16	I	123/130 (95%)	118 (96%)	5 (4%)	0	100	100
17	J	92/103 (89%)	88 (96%)	3 (3%)	1 (1%)	11	7
18	K	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
19	L	118/124 (95%)	111 (94%)	7 (6%)	0	100	100
20	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
21	N	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	12	9
22	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
23	P	77/82 (94%)	74 (96%)	3 (4%)	0	100	100
24	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
25	R	62/75 (83%)	62 (100%)	0	0	100	100
26	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
27	T	84/87 (97%)	84 (100%)	0	0	100	100
28	U	53/71 (75%)	52 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	W	662/693 (96%)	647 (98%)	15 (2%)	0	100	100
32	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
33	d	204/209 (98%)	198 (97%)	6 (3%)	0	100	100
34	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
35	f	175/179 (98%)	170 (97%)	4 (2%)	1 (1%)	21	20
36	g	166/177 (94%)	164 (99%)	2 (1%)	0	100	100
37	h	39/149 (26%)	37 (95%)	2 (5%)	0	100	100
38	i	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
39	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
40	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	18	16
41	l	132/136 (97%)	129 (98%)	3 (2%)	0	100	100
42	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
43	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
44	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
45	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
46	q	101/103 (98%)	100 (99%)	0	1 (1%)	12	9
47	r	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
48	s	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
49	t	89/104 (86%)	88 (99%)	1 (1%)	0	100	100
50	u	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
51	v	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
52	w	75/78 (96%)	75 (100%)	0	0	100	100
53	x	58/63 (92%)	58 (100%)	0	0	100	100
54	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
55	z	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
All	All	6064/6606 (92%)	5915 (98%)	142 (2%)	7 (0%)	49	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	J	57	VAL
35	f	42	GLU
9	B	165	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	k	29	LYS
15	H	75	ILE
46	q	44	GLY
21	N	68	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	45 (98%)	1 (2%)	45	54
2	1	37/38 (97%)	37 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	44/62 (71%)	44 (100%)	0	100	100
9	B	184/199 (92%)	178 (97%)	6 (3%)	33	39
10	C	170/190 (90%)	168 (99%)	2 (1%)	63	72
11	D	172/173 (99%)	167 (97%)	5 (3%)	37	44
12	E	117/126 (93%)	116 (99%)	1 (1%)	70	78
13	F	88/116 (76%)	88 (100%)	0	100	100
14	G	124/147 (84%)	120 (97%)	4 (3%)	34	40
15	H	104/105 (99%)	103 (99%)	1 (1%)	68	76
16	I	103/107 (96%)	100 (97%)	3 (3%)	37	44
17	J	85/90 (94%)	84 (99%)	1 (1%)	63	72
18	K	89/98 (91%)	87 (98%)	2 (2%)	45	54
19	L	101/103 (98%)	98 (97%)	3 (3%)	36	43
20	M	93/96 (97%)	92 (99%)	1 (1%)	65	74
21	N	83/84 (99%)	83 (100%)	0	100	100
22	O	76/77 (99%)	76 (100%)	0	100	100
23	P	64/65 (98%)	64 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Q	73/78 (94%)	69 (94%)	4 (6%)	19	18
25	R	55/65 (85%)	55 (100%)	0	100	100
26	S	72/79 (91%)	72 (100%)	0	100	100
27	T	65/66 (98%)	64 (98%)	1 (2%)	57	66
28	U	48/61 (79%)	48 (100%)	0	100	100
29	W	556/579 (96%)	545 (98%)	11 (2%)	48	58
32	c	216/218 (99%)	215 (100%)	1 (0%)	81	86
33	d	162/163 (99%)	162 (100%)	0	100	100
34	e	165/165 (100%)	165 (100%)	0	100	100
35	f	148/150 (99%)	145 (98%)	3 (2%)	48	58
36	g	132/138 (96%)	128 (97%)	4 (3%)	36	43
37	h	32/114 (28%)	32 (100%)	0	100	100
38	i	115/116 (99%)	113 (98%)	2 (2%)	53	63
39	j	104/104 (100%)	104 (100%)	0	100	100
40	k	103/103 (100%)	102 (99%)	1 (1%)	68	76
41	l	107/107 (100%)	105 (98%)	2 (2%)	50	59
42	m	98/103 (95%)	98 (100%)	0	100	100
43	n	86/87 (99%)	83 (96%)	3 (4%)	32	37
44	o	99/100 (99%)	99 (100%)	0	100	100
45	p	89/90 (99%)	89 (100%)	0	100	100
46	q	84/84 (100%)	83 (99%)	1 (1%)	63	72
47	r	92/93 (99%)	92 (100%)	0	100	100
48	s	80/84 (95%)	80 (100%)	0	100	100
49	t	76/85 (89%)	76 (100%)	0	100	100
50	u	77/78 (99%)	77 (100%)	0	100	100
51	v	56/63 (89%)	56 (100%)	0	100	100
52	w	67/68 (98%)	67 (100%)	0	100	100
53	x	54/55 (98%)	54 (100%)	0	100	100
54	y	48/49 (98%)	48 (100%)	0	100	100
55	z	46/48 (96%)	46 (100%)	0	100	100
All	All	5070/5404 (94%)	5007 (99%)	63 (1%)	61	72

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	5	ILE
9	B	23	TRP
9	B	133	GLU
9	B	143	LYS
9	B	163	VAL
9	B	192	ASP
9	B	196	VAL
10	C	58	GLU
10	C	70	THR
11	D	35	GLU
11	D	44	ARG
11	D	45	LYS
11	D	145	ILE
11	D	147	GLU
12	E	16	ILE
14	G	22	LEU
14	G	63	GLU
14	G	75	VAL
14	G	135	VAL
15	H	89	LYS
16	I	63	LEU
16	I	66	THR
16	I	72	ILE
17	J	63	ASP
18	K	37	ARG
18	K	86	VAL
19	L	52	VAL
19	L	112	GLN
19	L	120	LYS
20	M	93	ARG
24	Q	28	PHE
24	Q	42	THR
24	Q	52	GLU
24	Q	74	THR
27	T	49	LYS
29	W	90	VAL
29	W	260	THR
29	W	290	HIS
29	W	393	LYS
29	W	401	MET
29	W	447	GLN
29	W	448	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	W	472	GLU
29	W	492	VAL
29	W	609	ILE
29	W	619	ILE
32	c	37	ASN
35	f	40	VAL
35	f	144	ASP
35	f	150	ARG
36	g	25	THR
36	g	104	ASN
36	g	155	GLU
36	g	176	LYS
38	i	9	GLU
38	i	95	ARG
40	k	116	VAL
41	l	6	ARG
41	l	8	LYS
43	n	49	VAL
43	n	56	LYS
43	n	90	VAL
46	q	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	30	HIS
5	4	33	ASN
5	4	41	HIS
9	B	42	ASN
9	B	103	ASN
10	C	139	GLN
12	E	12	GLN
12	E	70	ASN
12	E	77	ASN
12	E	82	GLN
12	E	89	HIS
13	F	3	HIS
13	F	68	GLN
14	G	148	ASN
15	H	4	GLN
15	H	21	ASN
15	H	76	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	I	31	ASN
16	I	32	GLN
16	I	110	GLN
17	J	15	HIS
17	J	58	ASN
17	J	99	GLN
18	K	118	HIS
19	L	72	HIS
19	L	112	GLN
22	O	35	GLN
22	O	80	GLN
23	P	26	ASN
23	P	59	HIS
25	R	31	ASN
26	S	52	HIS
27	T	13	GLN
27	T	61	GLN
27	T	84	ASN
29	W	158	ASN
29	W	447	GLN
29	W	690	ASN
32	c	86	ASN
33	d	148	GLN
33	d	173	GLN
34	e	90	GLN
37	h	18	GLN
37	h	20	ASN
39	j	93	GLN
40	k	104	GLN
43	n	116	GLN
44	o	41	GLN
45	p	44	GLN
45	p	81	ASN
46	q	12	HIS
46	q	43	ASN
47	r	9	HIS
49	t	40	ASN
50	u	5	ASN
50	u	12	GLN
50	u	87	GLN
53	x	27	ASN
53	x	39	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	y	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	a	2778/2930 (94%)	309 (11%)	0
31	b	118/119 (99%)	7 (5%)	0
6	8	76/77 (98%)	15 (19%)	3 (3%)
7	9	4/24 (16%)	0	0
8	A	1524/1554 (98%)	240 (15%)	47 (3%)
All	All	4500/4704 (95%)	571 (12%)	50 (1%)

All (571) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	8	7	G
6	8	8	U
6	8	9	G
6	8	16	C
6	8	17(A)	U
6	8	19	G
6	8	20	U
6	8	21	A
6	8	22	G
6	8	43	A
6	8	46	G
6	8	47	U
6	8	55	U
6	8	58	A
6	8	76	A
8	A	3	A
8	A	4	U
8	A	5	U
8	A	6	G
8	A	7	A
8	A	8	A
8	A	9	G
8	A	32	A
8	A	39	G
8	A	47	C
8	A	48	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	A	49	U
8	A	50	A
8	A	51	A
8	A	66	A
8	A	72	A
8	A	76	G
8	A	77	A
8	A	78	A
8	A	80	A
8	A	81	A
8	A	82	G
8	A	83	C
8	A	84	U
8	A	85	U
8	A	86	G
8	A	87	C
8	A	90	C
8	A	94	G
8	A	95	C
8	A	96	U
8	A	97	G
8	A	120	A
8	A	122	G
8	A	130	A
8	A	131	A
8	A	137	U
8	A	143	A
8	A	144	G
8	A	159	G
8	A	163	C
8	A	164	G
8	A	170	U
8	A	182	A
8	A	196	A
8	A	197	A
8	A	207	C
8	A	208	U
8	A	209	U
8	A	210	C
8	A	226	G
8	A	240	G
8	A	245	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	A	247	G
8	A	250	A
8	A	251	G
8	A	253	A
8	A	266	G
8	A	267	C
8	A	289	G
8	A	305	G
8	A	306	A
8	A	321	A
8	A	328	C
8	A	329	A
8	A	330	C
8	A	332	G
8	A	352	C
8	A	354	G
8	A	367	U
8	A	372	C
8	A	398	U
8	A	406	G
8	A	411	A
8	A	412	A
8	A	413	G
8	A	414	A
8	A	421	U
8	A	422	C
8	A	429	U
8	A	455	G
8	A	457	G
8	A	458	U
8	A	463	U
8	A	467	U
8	A	468	A
8	A	482	A
8	A	484	G
8	A	486	U
8	A	495	A
8	A	499	A
8	A	500	G
8	A	511	C
8	A	518	C
8	A	524	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	A	527	G7M
8	A	530	G
8	A	532	A
8	A	547	A
8	A	559	A
8	A	562	U
8	A	572	A
8	A	573	A
8	A	576	C
8	A	589	U
8	A	595	A
8	A	596	A
8	A	607	A
8	A	615	G
8	A	619	U
8	A	635	A
8	A	642	A
8	A	650	G
8	A	665	A
8	A	687	A
8	A	695	A
8	A	702	A
8	A	703	G
8	A	721	G
8	A	723	U
8	A	724	G
8	A	755	G
8	A	777	A
8	A	793	U
8	A	794	A
8	A	815	A
8	A	817	C
8	A	829	G
8	A	849	G
8	A	874	G
8	A	884	U
8	A	885	G
8	A	890	G
8	A	902	G
8	A	914	A
8	A	926	G
8	A	927	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	A	934	C
8	A	935	A
8	A	942	G
8	A	958	A
8	A	960	U
8	A	965	U
8	A	969	A
8	A	975	A
8	A	976	G
8	A	977	A
8	A	989	U
8	A	991	U
8	A	992	U
8	A	993	G
8	A	994	A
8	A	1004	A
8	A	1013	G
8	A	1014	A
8	A	1015	G
8	A	1016	A
8	A	1017	U
8	A	1020	G
8	A	1021	A
8	A	1030	U
8	A	1031	C
8	A	1032	G
8	A	1056	U
8	A	1065	U
8	A	1085	U
8	A	1092	A
8	A	1094	G
8	A	1095	U
8	A	1101	A
8	A	1102	A
8	A	1104	G
8	A	1108	G
8	A	1109	C
8	A	1124	G
8	A	1125	U
8	A	1130	A
8	A	1135	U
8	A	1139	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	A	1141	C
8	A	1145	A
8	A	1146	A
8	A	1150	A
8	A	1152	A
8	A	1157	A
8	A	1158	C
8	A	1159	U
8	A	1160	G
8	A	1161	C
8	A	1183	U
8	A	1196	A
8	A	1197	A
8	A	1213	A
8	A	1226	C
8	A	1227	A
8	A	1238	A
8	A	1240	U
8	A	1250	A
8	A	1256	A
8	A	1257	A
8	A	1260	G
8	A	1268	G
8	A	1279	G
8	A	1280	A
8	A	1286	U
8	A	1287	A
8	A	1297	G
8	A	1298	U
8	A	1300	G
8	A	1305	G
8	A	1311	A
8	A	1312	G
8	A	1320	C
8	A	1331	G
8	A	1332	A
8	A	1336	C
8	A	1338	G
8	A	1346	A
8	A	1363	A
8	A	1364	U
8	A	1365	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	A	1379	G
8	A	1398	A
8	A	1419	G
8	A	1429	A
8	A	1441	A
8	A	1452	C
8	A	1453	G
8	A	1494	G
8	A	1497	G
8	A	1499	A
8	A	1503	A
8	A	1505	G
8	A	1506	U
8	A	1507	A
8	A	1517	G
8	A	1529	G
8	A	1530	G
8	A	1533	C
8	A	1534	A
30	a	10	A
30	a	12	U
30	a	15	G
30	a	34	U
30	a	71	A
30	a	74	A
30	a	75	G
30	a	101	A
30	a	118	A
30	a	119	A
30	a	120	U
30	a	131	A
30	a	139	U
30	a	142	A
30	a	162	U
30	a	181	A
30	a	196	A
30	a	199	A
30	a	200	U
30	a	215	G
30	a	216	A
30	a	221	A
30	a	222	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	248	G
30	a	272	A
30	a	278	A
30	a	279	A
30	a	281	C
30	a	285	G
30	a	289	G
30	a	310	A
30	a	311	A
30	a	330	A
30	a	345	A
30	a	346	A
30	a	354	A
30	a	361	G
30	a	362	A
30	a	386	G
30	a	411	G
30	a	448	U
30	a	451	U
30	a	481	G
30	a	491	G
30	a	503	A
30	a	504	A
30	a	505	A
30	a	509	C
30	a	531	C
30	a	532	A
30	a	533	G
30	a	544	C
30	a	545	U
30	a	547	A
30	a	548	G
30	a	549	G
30	a	555	G
30	a	556	A
30	a	563	A
30	a	573	U
30	a	574	A
30	a	575	A
30	a	586	A
30	a	603	A
30	a	615	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	627	A
30	a	637	A
30	a	645	C
30	a	647	G
30	a	653	U
30	a	654	A
30	a	655	A
30	a	686	U
30	a	716	A
30	a	717	C
30	a	730	A
30	a	747	5MU
30	a	764	A
30	a	765	C
30	a	775	G
30	a	776	G
30	a	782	A
30	a	784	G
30	a	785	G
30	a	792	A
30	a	805	G
30	a	812	C
30	a	827	U
30	a	828	U
30	a	845	A
30	a	846	U
30	a	858	G
30	a	869	G
30	a	910	A
30	a	914	G
30	a	915	C
30	a	931	U
30	a	934	U
30	a	946	C
30	a	961	C
30	a	974	G
30	a	983	A
30	a	984	A
30	a	985	C
30	a	996	A
30	a	1012	U
30	a	1013	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1022	G
30	a	1026	G
30	a	1033	U
30	a	1041	G
30	a	1047	G
30	a	1059	G
30	a	1060	U
30	a	1069	A
30	a	1070	A
30	a	1077	A
30	a	1080	A
30	a	1083	U
30	a	1087	G
30	a	1088	A
30	a	1097	U
30	a	1101	U
30	a	1112	G
30	a	1116	G
30	a	1128	G
30	a	1129	A
30	a	1130	U
30	a	1132	U
30	a	1133	A
30	a	1134	A
30	a	1135	C
30	a	1142	A
30	a	1144	A
30	a	1151	A
30	a	1169	A
30	a	1170	C
30	a	1179	G
30	a	1187	G
30	a	1188	U
30	a	1253	A
30	a	1256	G
30	a	1271	G
30	a	1272	A
30	a	1300	G
30	a	1301	A
30	a	1321	A
30	a	1352	U
30	a	1365	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1378	A
30	a	1379	U
30	a	1383	A
30	a	1386	C
30	a	1409	U
30	a	1416	G
30	a	1419	A
30	a	1428	C
30	a	1451	C
30	a	1452	G
30	a	1453	A
30	a	1455	G
30	a	1458	U
30	a	1459	G
30	a	1460	U
30	a	1482	G
30	a	1490	A
30	a	1493	C
30	a	1508	A
30	a	1509	A
30	a	1510	G
30	a	1515	A
30	a	1534	U
30	a	1535	A
30	a	1536	C
30	a	1537	G
30	a	1538	G
30	a	1569	A
30	a	1578	U
30	a	1585	C
30	a	1608	A
30	a	1609	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1674	G
30	a	1698	A
30	a	1715	G
30	a	1729	U
30	a	1730	C
30	a	1734	G
30	a	1737	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1738	G
30	a	1744	A
30	a	1764	C
30	a	1773	A
30	a	1782	U
30	a	1800	C
30	a	1801	A
30	a	1808	A
30	a	1816	C
30	a	1829	A
30	a	1847	A
30	a	1848	A
30	a	1858	A
30	a	1870	C
30	a	1871	A
30	a	1872	A
30	a	1906	G
30	a	1907	G
30	a	1913	A
30	a	1914	C
30	a	1929	G
30	a	1930	G
30	a	1931	U
30	a	1937	A
30	a	1955	U
30	a	1967	C
30	a	1970	A
30	a	1971	U
30	a	1972	G
30	a	1991	U
30	a	1993	U
30	a	2020	A
30	a	2023	C
30	a	2031	A
30	a	2033	A
30	a	2043	C
30	a	2055	C
30	a	2056	G
30	a	2060	A
30	a	2061	G
30	a	2062	A
30	a	2069	G7M

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2093	G
30	a	2096	C
30	a	2193	G
30	a	2198	A
30	a	2204	G
30	a	2211	A
30	a	2225	A
30	a	2238	G
30	a	2268	A
30	a	2273	A
30	a	2278	A
30	a	2283	C
30	a	2287	A
30	a	2305	U
30	a	2308	G
30	a	2311	A
30	a	2312	U
30	a	2322	A
30	a	2325	G
30	a	2333	A
30	a	2335	A
30	a	2347	C
30	a	2350	C
30	a	2366	A
30	a	2383	G
30	a	2385	C
30	a	2402	U
30	a	2406	A
30	a	2425	A
30	a	2429	G
30	a	2430	A
30	a	2431	U
30	a	2435	A
30	a	2441	U
30	a	2448	A
30	a	2459	A
30	a	2468	A
30	a	2469	A
30	a	2476	A
30	a	2478	A
30	a	2491	U
30	a	2502	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2505	G
30	a	2518	A
30	a	2529	G
30	a	2530	A
30	a	2547	A
30	a	2566	A
30	a	2567	G
30	a	2573	C
30	a	2602	A
30	a	2609	U
30	a	2613	U
30	a	2629	U
30	a	2661	G
30	a	2663	G
30	a	2689	U
30	a	2690	U
30	a	2714	G
30	a	2716	C
30	a	2726	A
30	a	2744	G
30	a	2748	A
30	a	2750	A
30	a	2757	A
30	a	2765	A
30	a	2778	A
30	a	2798	U
30	a	2799	A
30	a	2803	G
30	a	2809	A
30	a	2818	U
30	a	2820	A
30	a	2821	A
30	a	2883	A
30	a	2884	U
31	b	35	C
31	b	36	C
31	b	37	C
31	b	44	G
31	b	45	A
31	b	89	U
31	b	109	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	8	7	G
6	8	17(A)	U
6	8	20	U
8	A	7	A
8	A	30	U
8	A	84	U
8	A	86	G
8	A	182	A
8	A	199	A
8	A	305	G
8	A	329	A
8	A	345	C
8	A	411	A
8	A	428	G
8	A	434	U
8	A	446	G
8	A	499	A
8	A	575	G
8	A	595	A
8	A	702	A
8	A	776	G
8	A	827	U
8	A	884	U
8	A	958	A
8	A	974	A
8	A	991	U
8	A	993	G
8	A	1013	G
8	A	1031	C
8	A	1092	A
8	A	1101	A
8	A	1108	G
8	A	1124	G
8	A	1129	C
8	A	1145	A
8	A	1157	A
8	A	1159	U
8	A	1160	G
8	A	1187	G
8	A	1256	A
8	A	1297	G
8	A	1320	C
8	A	1331	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	A	1364	U
8	A	1380	U
8	A	1397	C
8	A	1447	A
8	A	1452	C
8	A	1459	G
8	A	1505	G

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$
30	6MZ	a	2030	30	22,25,26	0.30	0	30,36,39	0.59	0
30	5MU	a	1939	30,57	19,22,23	0.30	0	28,32,35	0.37	0
30	PSU	a	2457	30	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
30	3TD	a	1915	30	18,22,23	0.98	1 (5%)	22,32,35	0.62	0
8	5MC	A	1407	8	18,22,23	0.32	0	26,32,35	0.54	0
30	PSU	a	1911	30	18,21,22	0.92	1 (5%)	22,30,33	0.66	0
30	PSU	a	2605	30	18,21,22	0.90	1 (5%)	22,30,33	0.75	0
8	PSU	A	516	8	18,21,22	0.91	1 (5%)	22,30,33	0.59	0
41	4D4	l	81	41	9,11,12	0.55	0	8,13,15	0.70	0
30	PSU	a	2580	30,57	18,21,22	0.90	1 (5%)	22,30,33	0.85	1 (4%)
30	2MA	a	2503	30,58,57	22,25,26	0.91	1 (4%)	33,37,40	1.07	4 (12%)
30	5MU	a	747	30	19,22,23	0.26	0	28,32,35	0.42	0
8	MA6	A	1519	8	23,26,27	0.25	0	34,38,41	0.72	1 (2%)
8	4OC	A	1402	8	20,23,24	0.39	0	26,32,35	0.42	0
30	1MG	a	745	30	22,26,27	0.52	0	33,39,42	0.46	0
8	G7M	A	527	8	23,26,27	0.71	1 (4%)	35,39,42	0.55	0
30	PSU	a	1917	30	18,21,22	0.89	1 (5%)	22,30,33	0.52	0
8	MA6	A	1518	8	23,26,27	0.26	0	34,38,41	0.65	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	MEQ	d	150	33	8,9,10	0.43	0	5,10,12	0.54	0
18	IAS	K	119	18	6,7,8	0.91	0	6,8,10	0.99	0
30	6MZ	a	1618	30	22,25,26	0.39	0	30,36,39	0.57	0
8	5MC	A	967	8	18,22,23	0.33	0	26,32,35	0.49	0
30	H2U	a	2449	30	18,21,22	0.60	0	21,30,33	0.88	2 (9%)
30	PSU	a	746	30,58	18,21,22	0.95	1 (5%)	22,30,33	0.60	0
30	5MC	a	1962	30	18,22,23	0.34	0	26,32,35	0.50	0
30	OMG	a	2251	30,57	23,26,27	0.32	0	33,38,41	0.39	0
30	PSU	a	2504	30,57	18,21,22	0.85	1 (5%)	22,30,33	0.76	0
30	PSU	a	955	30	18,21,22	0.88	1 (5%)	22,30,33	0.65	0
30	2MG	a	1835	30	23,26,27	0.39	0	32,38,41	0.36	0
30	G7M	a	2069	30	23,26,27	0.69	1 (4%)	35,39,42	0.64	0
30	2MG	a	2445	30	23,26,27	0.39	0	32,38,41	0.42	0
19	D2T	L	89	19	7,9,10	0.94	0	6,11,13	1.85	4 (66%)
41	MS6	l	82	41	5,7,8	0.22	0	2,7,9	0.01	0
8	2MG	A	966	8	23,26,27	0.41	0	32,38,41	0.35	0
30	OMU	a	2552	30	19,22,23	0.21	0	26,31,34	0.40	0
8	UR3	A	1498	8	19,22,23	0.28	0	26,32,35	0.64	0
8	2MG	A	1516	8	23,26,27	0.39	0	32,38,41	0.49	0
30	OMC	a	2498	30,58	19,22,23	0.28	0	26,31,34	0.53	0
8	2MG	A	1207	8	23,26,27	0.40	0	32,38,41	0.38	0
30	PSU	a	2604	30	18,21,22	0.91	1 (5%)	22,30,33	0.75	1 (4%)

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
30	6MZ	a	2030	30	-	2/9/27/28	0/3/3/3
30	5MU	a	1939	30,57	-	0/7/25/26	0/2/2/2
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
30	3TD	a	1915	30	-	0/7/25/26	0/2/2/2
8	5MC	A	1407	8	-	0/7/25/26	0/2/2/2
30	PSU	a	1911	30	-	2/7/25/26	0/2/2/2
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
8	PSU	A	516	8	-	0/7/25/26	0/2/2/2
41	4D4	l	81	41	-	1/11/12/14	-
30	PSU	a	2580	30,57	-	0/7/25/26	0/2/2/2
30	2MA	a	2503	30,58,57	-	1/7/25/26	0/3/3/3
30	5MU	a	747	30	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MA6	A	1519	8	-	0/11/29/30	0/3/3/3
8	4OC	A	1402	8	-	0/9/29/30	0/2/2/2
30	1MG	a	745	30	-	0/7/25/26	0/3/3/3
8	G7M	A	527	8	-	2/7/25/26	0/3/3/3
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
8	MA6	A	1518	8	-	0/11/29/30	0/3/3/3
33	MEQ	d	150	33	-	2/8/9/11	-
18	IAS	K	119	18	-	2/7/7/8	-
30	6MZ	a	1618	30	-	0/9/27/28	0/3/3/3
8	5MC	A	967	8	-	0/7/25/26	0/2/2/2
30	H2U	a	2449	30	-	0/7/38/39	0/2/2/2
30	PSU	a	746	30,58	-	2/7/25/26	0/2/2/2
30	5MC	a	1962	30	-	2/7/25/26	0/2/2/2
30	OMG	a	2251	30,57	-	1/9/27/28	0/3/3/3
30	PSU	a	2504	30,57	-	2/7/25/26	0/2/2/2
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
30	2MG	a	1835	30	-	0/9/27/28	0/3/3/3
30	G7M	a	2069	30	-	2/7/25/26	0/3/3/3
30	2MG	a	2445	30	-	1/9/27/28	0/3/3/3
19	D2T	L	89	19	-	4/7/12/14	-
41	MS6	l	82	41	-	1/4/6/8	-
8	2MG	A	966	8	-	2/9/27/28	0/3/3/3
30	OMU	a	2552	30	-	0/9/27/28	0/2/2/2
8	UR3	A	1498	8	-	0/7/25/26	0/2/2/2
8	2MG	A	1516	8	-	0/9/27/28	0/3/3/3
30	OMC	a	2498	30,58	-	0/9/27/28	0/2/2/2
8	2MG	A	1207	8	-	0/9/27/28	0/3/3/3
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	746	PSU	C6-C5	3.77	1.39	1.35
30	a	1915	3TD	C6-C5	3.71	1.39	1.35
30	a	1911	PSU	C6-C5	3.65	1.39	1.35
8	A	516	PSU	C6-C5	3.58	1.39	1.35
30	a	2580	PSU	C6-C5	3.58	1.39	1.35
30	a	2604	PSU	C6-C5	3.53	1.39	1.35
30	a	1917	PSU	C6-C5	3.52	1.39	1.35
30	a	2605	PSU	C6-C5	3.49	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2457	PSU	C6-C5	3.47	1.39	1.35
30	a	955	PSU	C6-C5	3.41	1.39	1.35
30	a	2504	PSU	C6-C5	3.36	1.39	1.35
8	A	527	G7M	C8-N7	2.53	1.37	1.33
30	a	2069	G7M	C8-N7	2.43	1.37	1.33
30	a	2503	2MA	C6-N6	-2.35	1.28	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2503	2MA	C5-C4-N3	-2.99	123.83	127.19
8	A	1518	MA6	C2-N1-C6	2.92	118.65	111.75
8	A	1519	MA6	C2-N1-C6	2.91	118.64	111.75
30	a	2580	PSU	C3'-C2'-C1'	2.75	104.84	101.64
19	L	89	D2T	OD1-CG-CB	-2.58	117.03	122.44
30	a	2503	2MA	CM2-C2-N1	2.37	120.85	117.15
30	a	2449	H2U	O2-C2-N1	-2.36	120.15	123.11
30	a	2449	H2U	N3-C2-N1	2.28	119.06	116.65
30	a	2503	2MA	C2-N1-C6	2.27	121.62	118.08
19	L	89	D2T	CB-CA-N	2.24	113.87	109.10
30	a	2503	2MA	N3-C2-N1	-2.21	121.65	125.72
19	L	89	D2T	OD2-CG-CB	2.07	117.62	113.15
19	L	89	D2T	O-C-CA	-2.03	119.46	124.78
30	a	2604	PSU	C2'-C3'-C4'	-2.01	98.74	102.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	L	89	D2T	CA-CB-CG-OD1
19	L	89	D2T	CA-CB-CG-OD2
30	a	746	PSU	C2'-C1'-C5-C4
30	a	1911	PSU	O4'-C1'-C5-C4
30	a	1911	PSU	O4'-C1'-C5-C6
30	a	2030	6MZ	O4'-C4'-C5'-O5'
30	a	2251	OMG	C1'-C2'-O2'-CM2
8	A	527	G7M	O4'-C4'-C5'-O5'
8	A	527	G7M	C3'-C4'-C5'-O5'
33	d	150	MEQ	OE1-CD-CG-CB
30	a	2030	6MZ	C3'-C4'-C5'-O5'
33	d	150	MEQ	NE2-CD-CG-CB
19	L	89	D2T	CG-CB-SB-CB1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	2445	2MG	C3'-C4'-C5'-O5'
30	a	2504	PSU	O4'-C4'-C5'-O5'
8	A	966	2MG	O4'-C4'-C5'-O5'
41	l	82	MS6	CB-CG-SD-CE
18	K	119	IAS	CA-CB-CG-OD1
18	K	119	IAS	O-C-CA-N
30	a	2069	G7M	C4'-C5'-O5'-P
30	a	1962	5MC	C2'-C1'-N1-C6
8	A	966	2MG	C3'-C4'-C5'-O5'
19	L	89	D2T	SB-CB-CG-OD2
30	a	1962	5MC	O4'-C1'-N1-C6
30	a	747	5MU	C3'-C4'-C5'-O5'
30	a	746	PSU	O4'-C1'-C5-C6
30	a	2504	PSU	C3'-C4'-C5'-O5'
30	a	2069	G7M	O4'-C4'-C5'-O5'
30	a	2503	2MA	O4'-C4'-C5'-O5'
41	l	81	4D4	O-C-CA-CB

There are no ring outliers.

12 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	a	2030	6MZ	1	0
30	a	1939	5MU	1	0
30	a	1915	3TD	1	0
30	a	1911	PSU	1	0
30	a	747	5MU	1	0
8	A	1519	MA6	1	0
8	A	1402	4OC	2	0
8	A	1518	MA6	1	0
30	a	2449	H2U	1	0
30	a	2445	2MG	1	0
30	a	2552	OMU	1	0
30	a	2604	PSU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 369 ligands modelled in this entry, 367 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	GDP	W	701	58	28,30,30	0.46	0	44,47,47	0.41	0
60	FUA	W	703	-	39,40,40	1.48	2 (5%)	49,64,64	0.91	2 (4%)

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
59	GDP	W	701	58	-	1/16/32/32	0/3/3/3
60	FUA	W	703	-	-	7/15/92/92	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	W	703	FUA	C29-C22	-8.49	1.35	1.47
60	W	703	FUA	O5-C29	-2.32	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	W	703	FUA	C14-C8-C9	-2.20	105.10	109.40
60	W	703	FUA	C16-O2-C31	2.16	120.34	117.06

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	W	703	FUA	C13-C17-C22-C29
60	W	703	FUA	C32-C31-O2-C16

Continued on next page...

Continued from previous page...

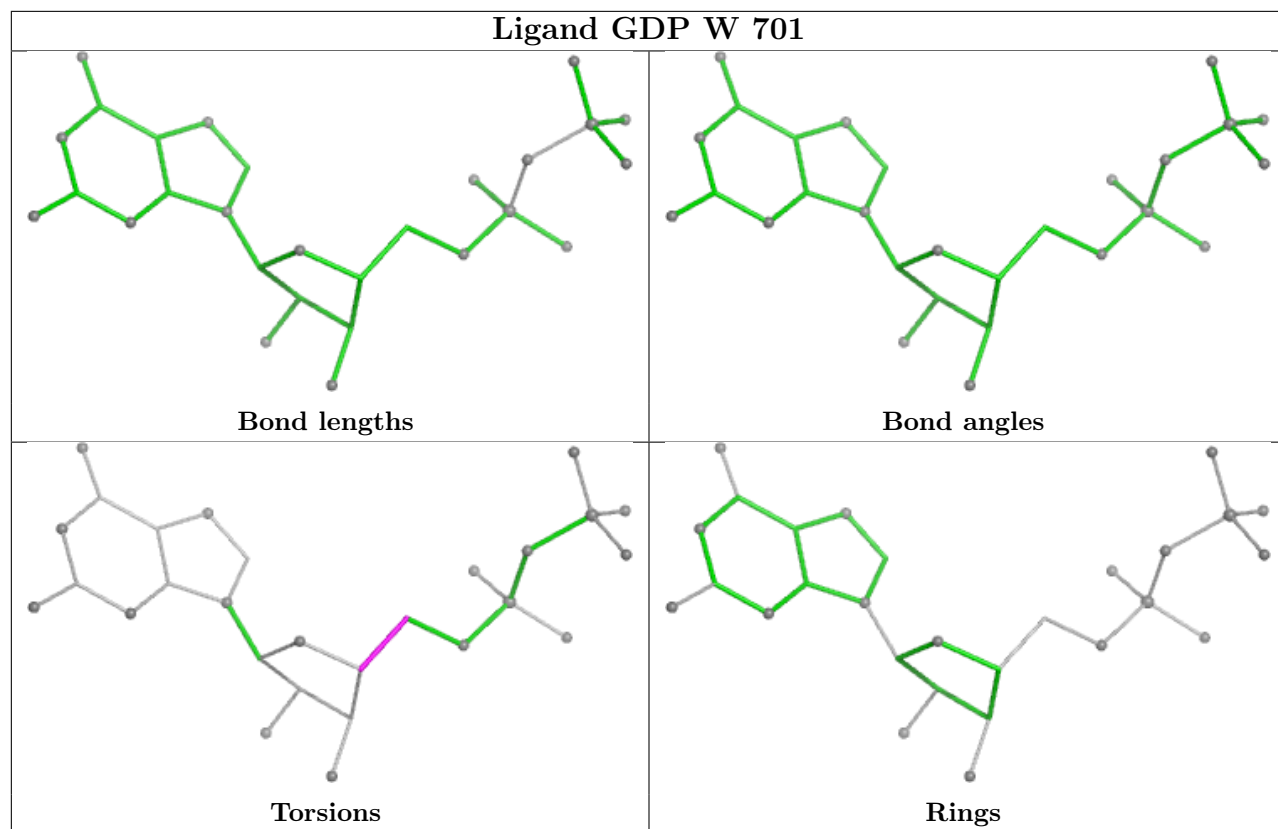
Mol	Chain	Res	Type	Atoms
60	W	703	FUA	O3-C31-O2-C16
60	W	703	FUA	C29-C22-C23-C24
60	W	703	FUA	C17-C22-C29-O4
60	W	703	FUA	C17-C22-C29-O5
59	W	701	GDP	O4'-C4'-C5'-O5'
60	W	703	FUA	C17-C16-O2-C31

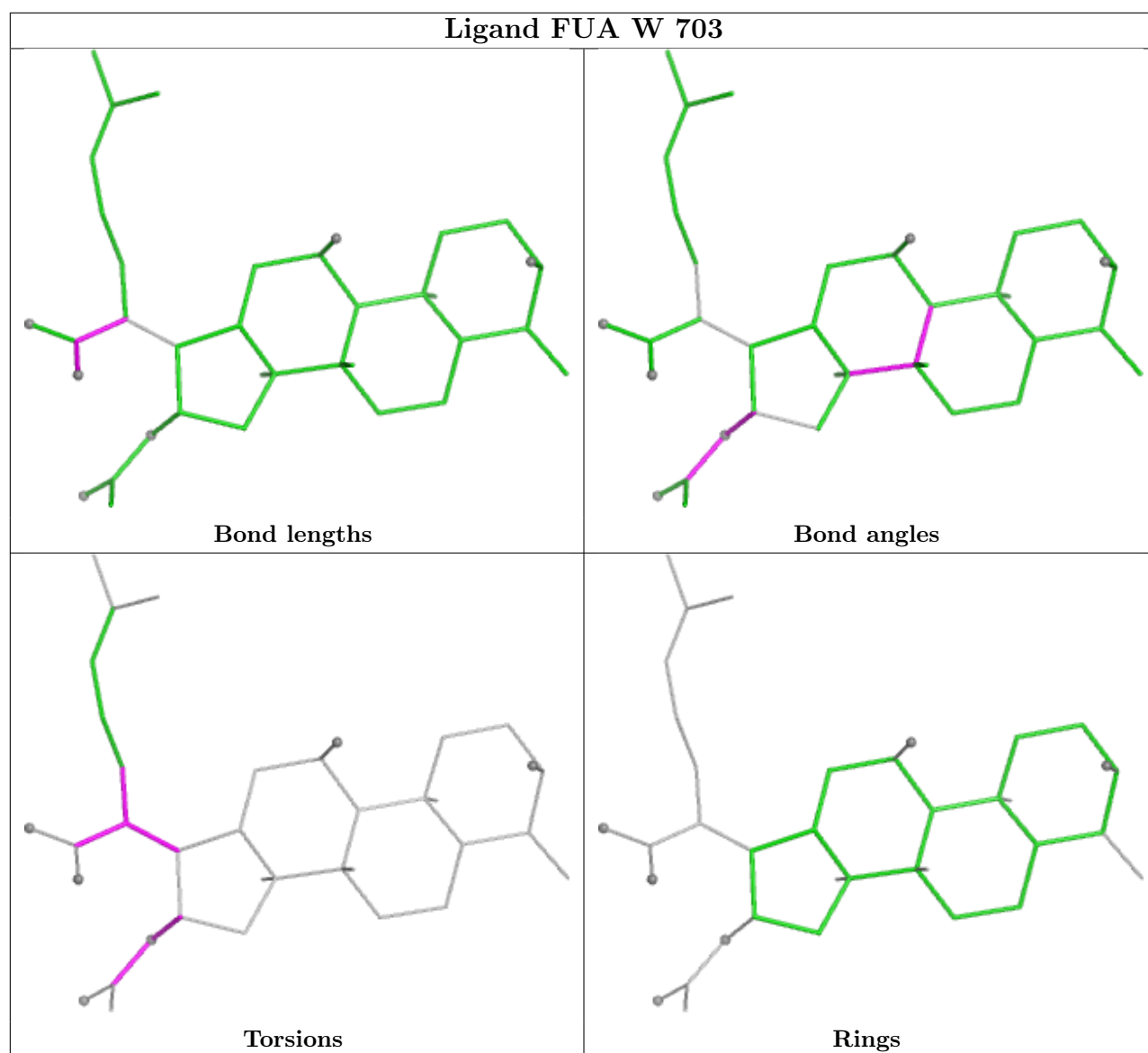
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	W	703	FUA	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

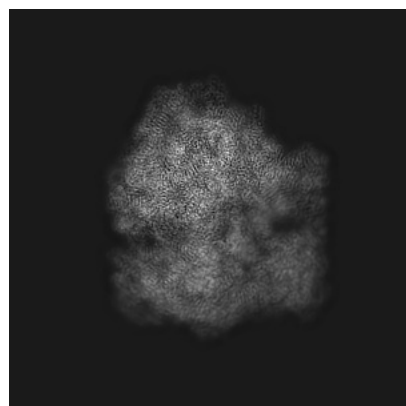
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51350. These allow visual inspection of the internal detail of the map and identification of artifacts.

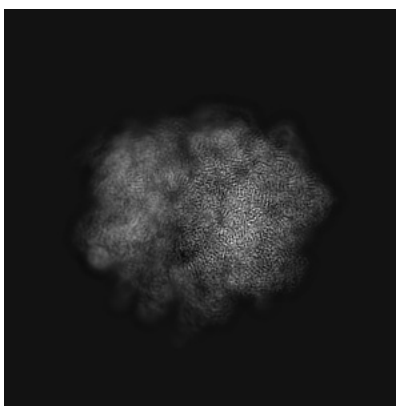
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

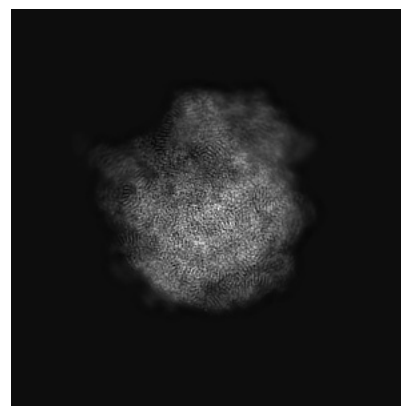
6.1.1 Primary map



X

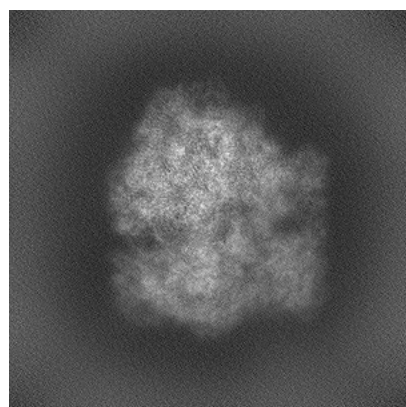


Y

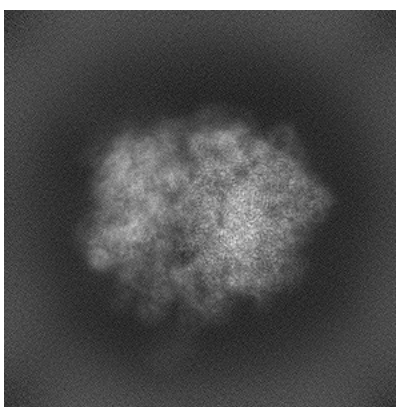


Z

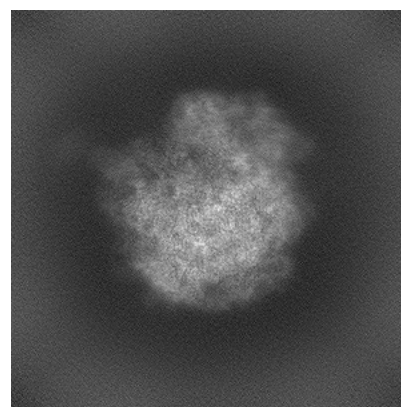
6.1.2 Raw map



X



Y

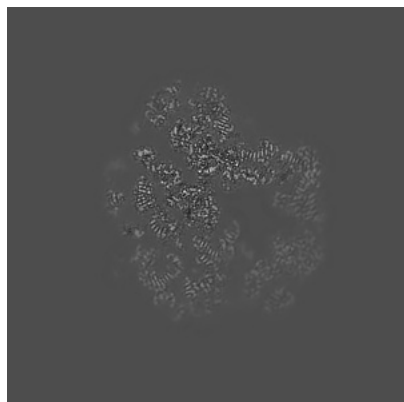


Z

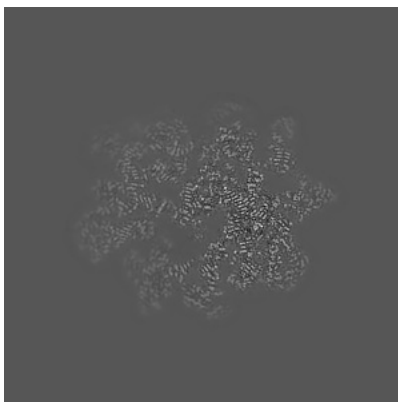
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

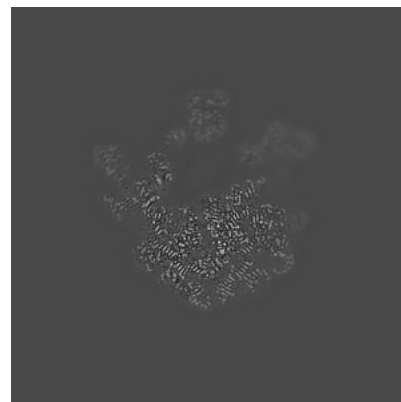
6.2.1 Primary map



X Index: 300

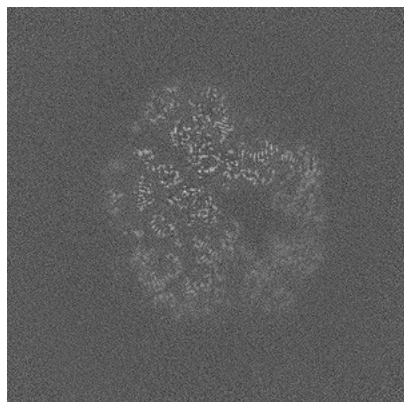


Y Index: 300

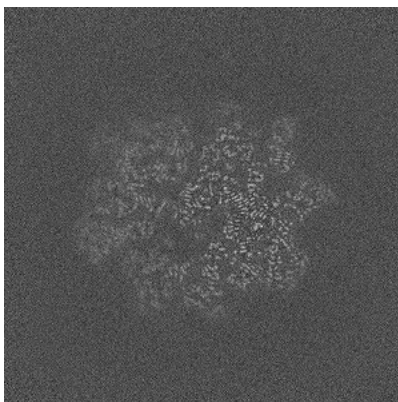


Z Index: 300

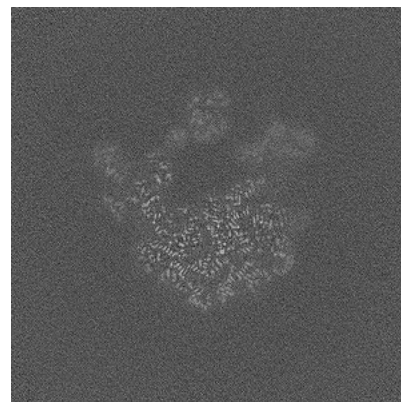
6.2.2 Raw map



X Index: 300



Y Index: 300

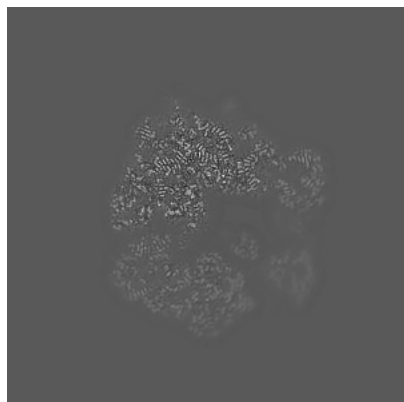


Z Index: 300

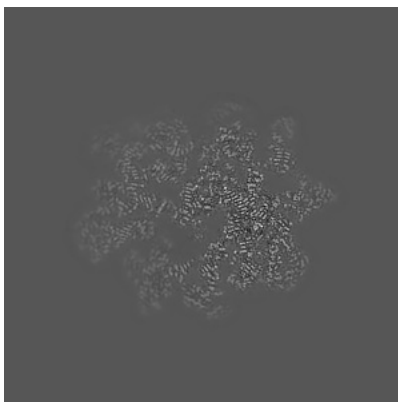
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

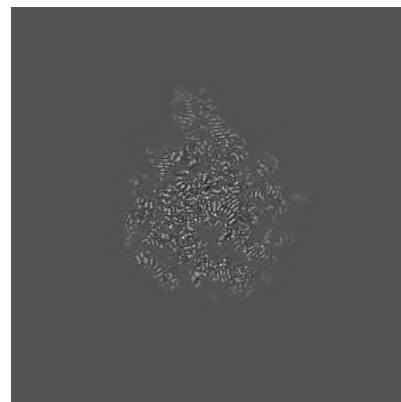
6.3.1 Primary map



X Index: 268

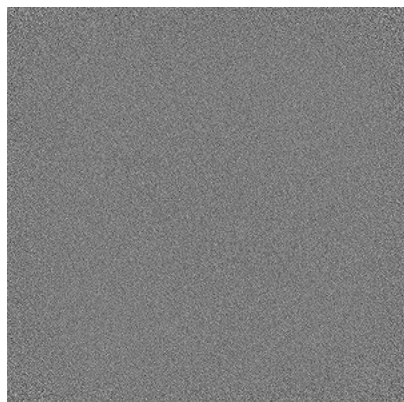


Y Index: 300

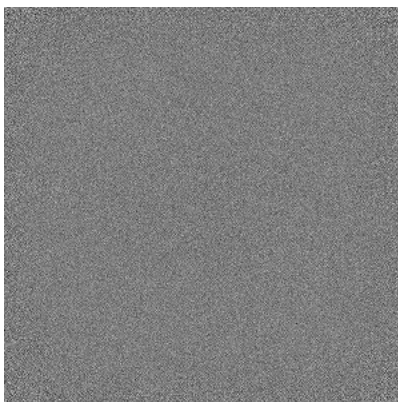


Z Index: 372

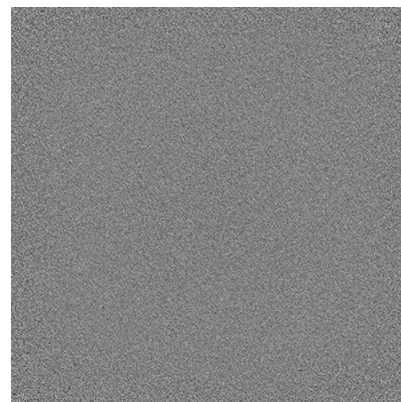
6.3.2 Raw map



X Index: 0



Y Index: 0

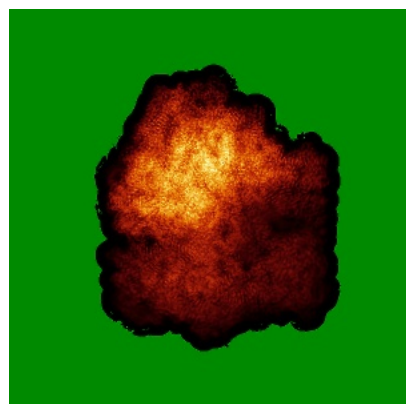


Z Index: 0

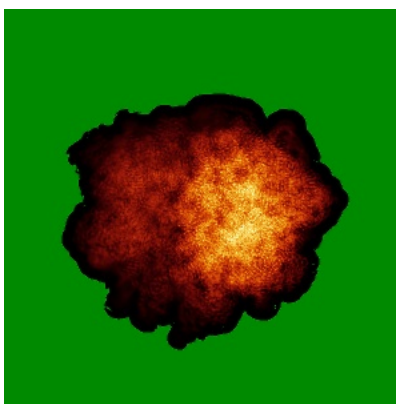
The images above show the largest variance slices of the map in three orthogonal directions.

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

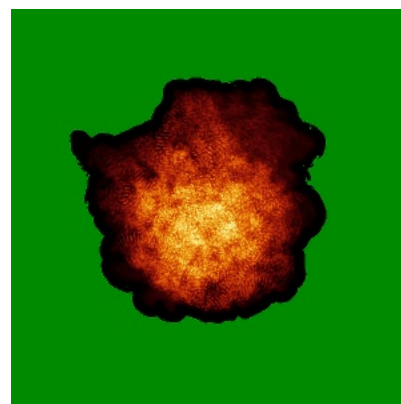
6.4.1 Primary map



X

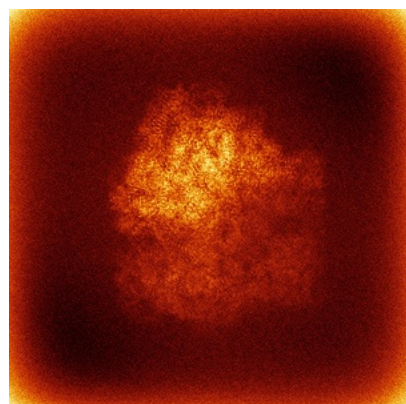


Y

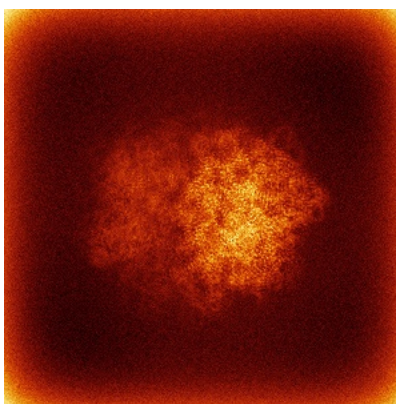


Z

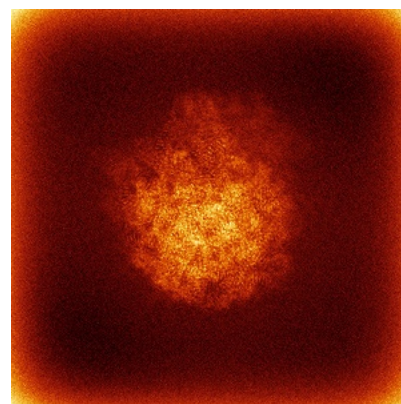
6.4.2 Raw map



X



Y



Z

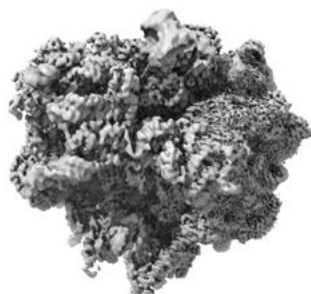
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

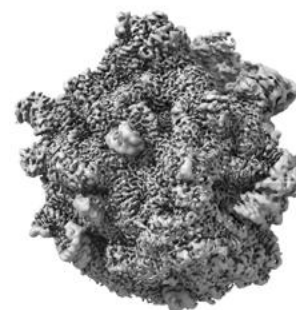
6.5.1 Primary map



X



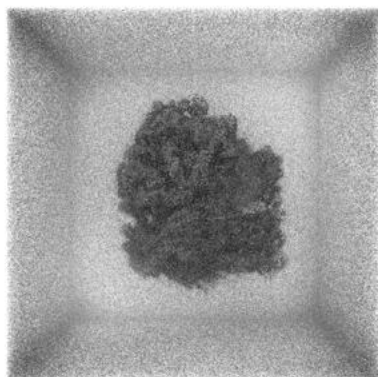
Y



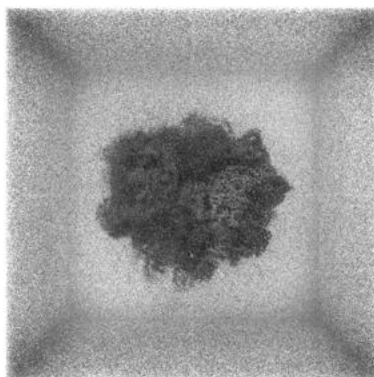
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

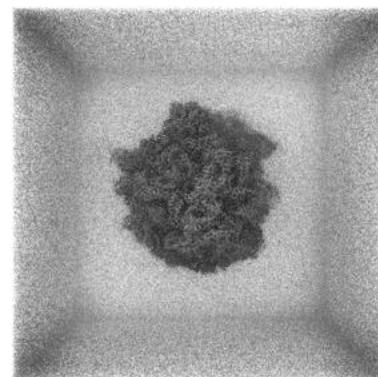
6.5.2 Raw map



X



Y



Z

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

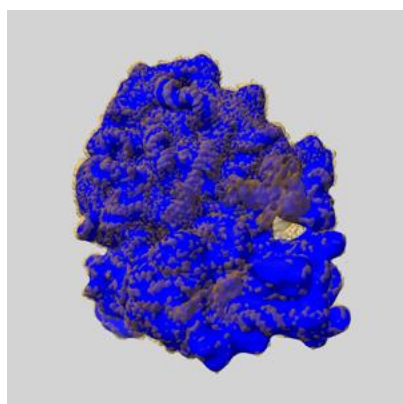
6.6 Mask visualisation [i](#)

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

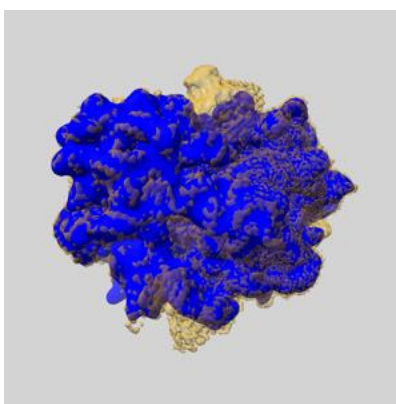
A mask typically either:

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

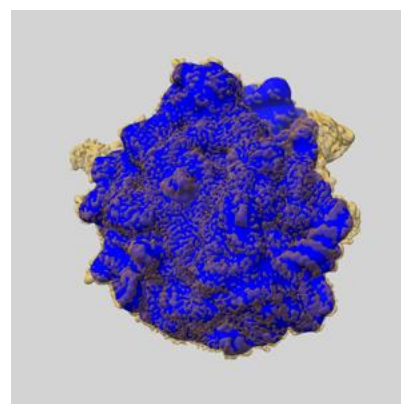
6.6.1 emd_51350_msk_1.map [i](#)



X



Y

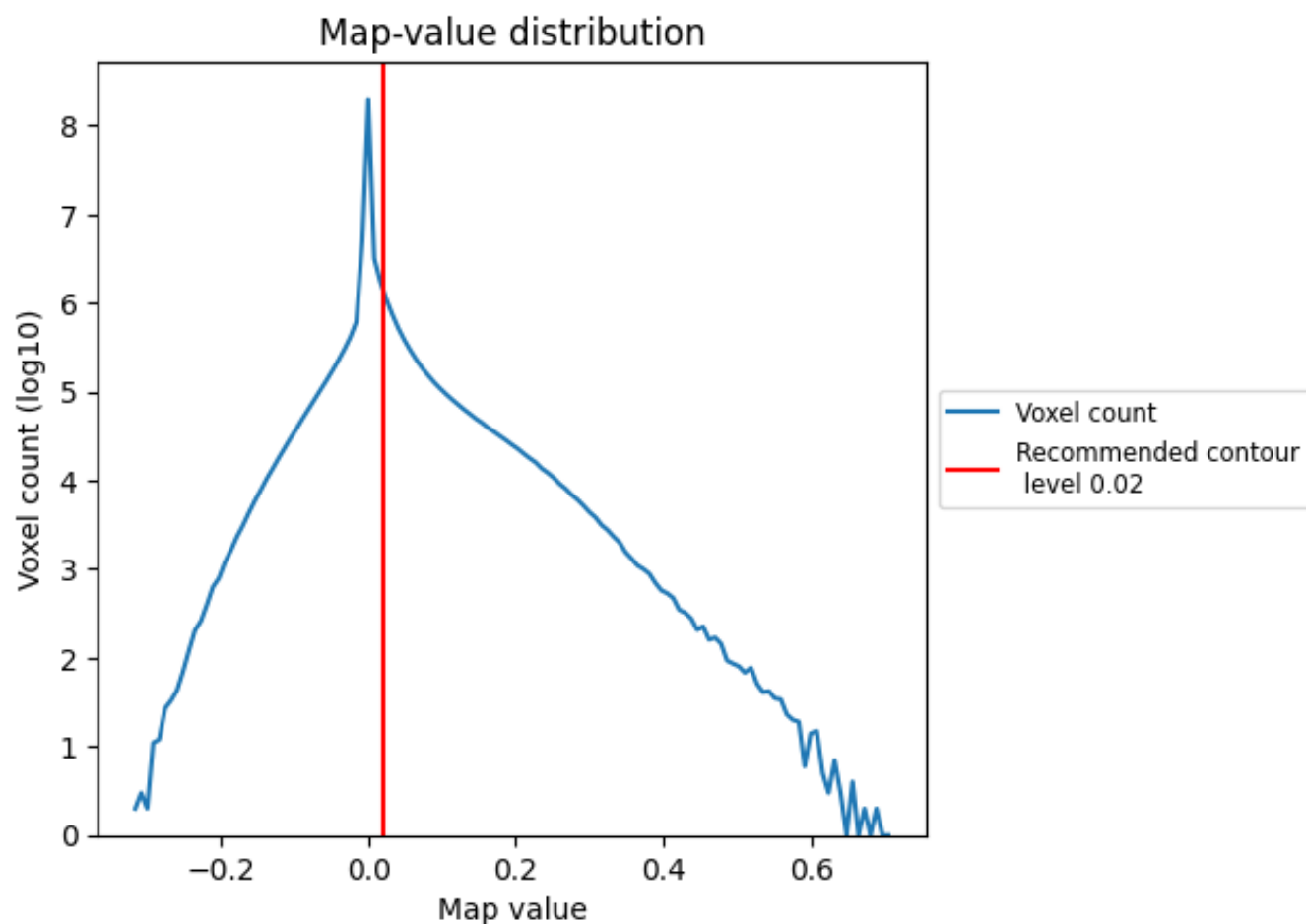


Z

7 Map analysis [i](#)

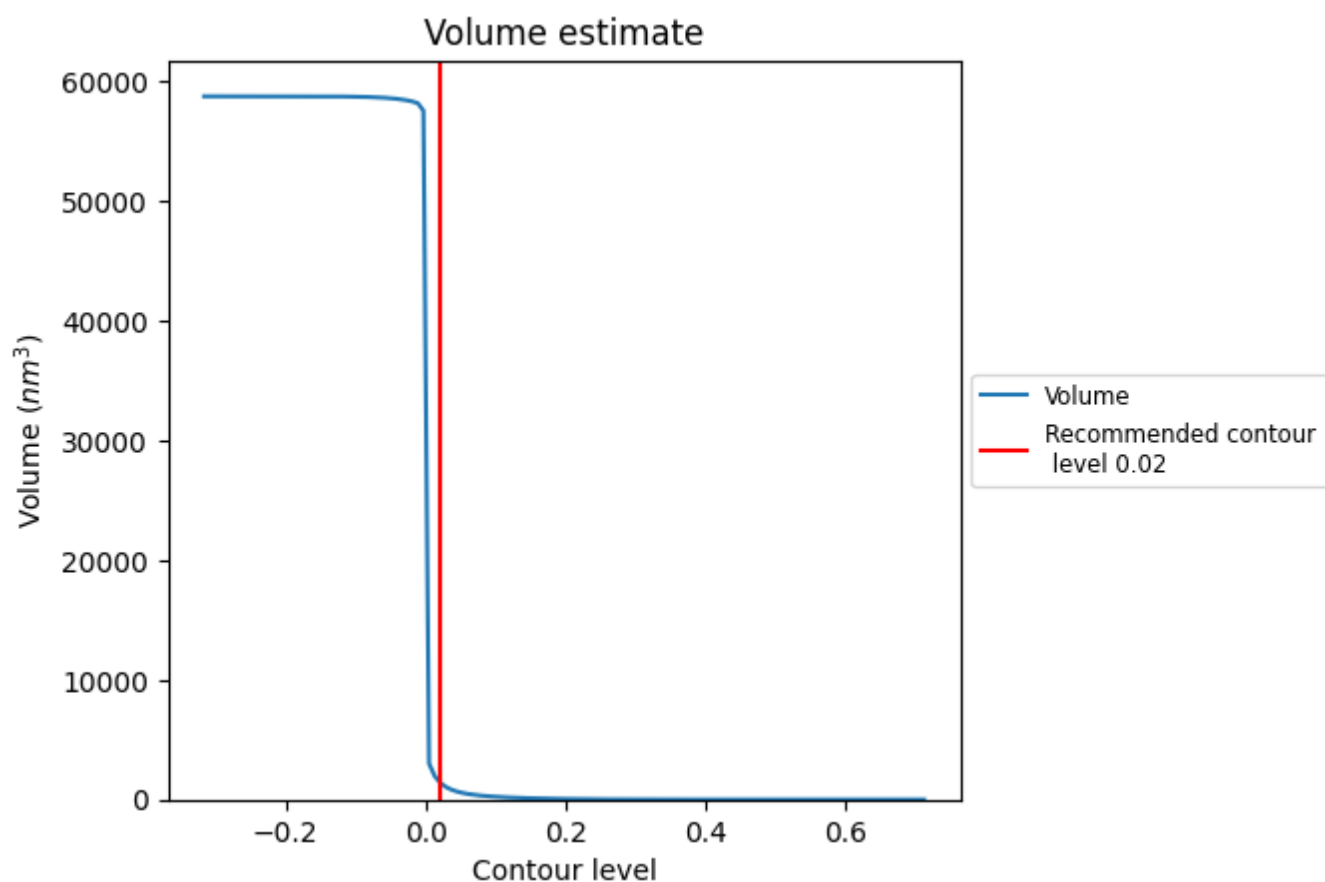
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

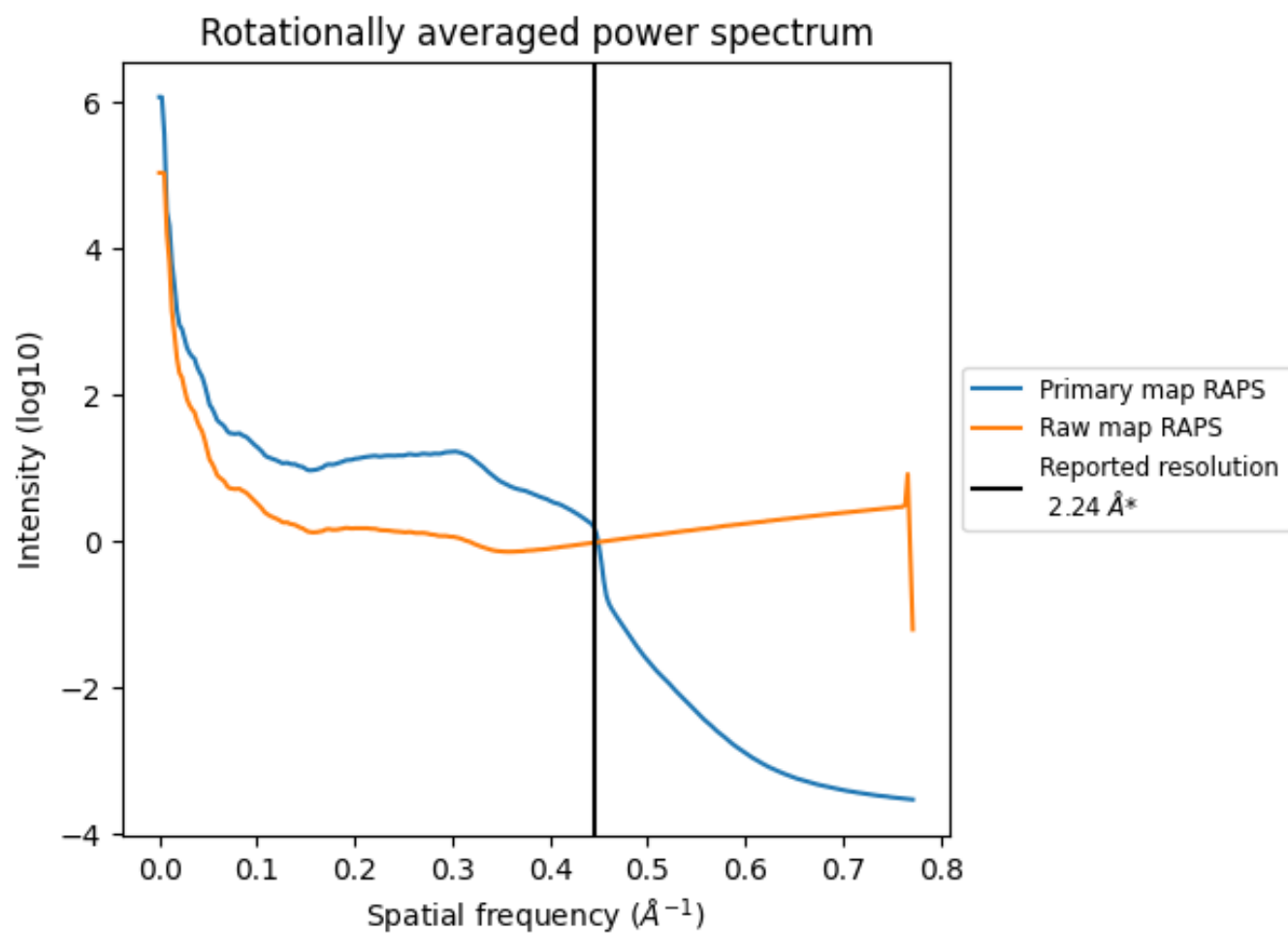
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1500 nm³; this corresponds to an approximate mass of 1355 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

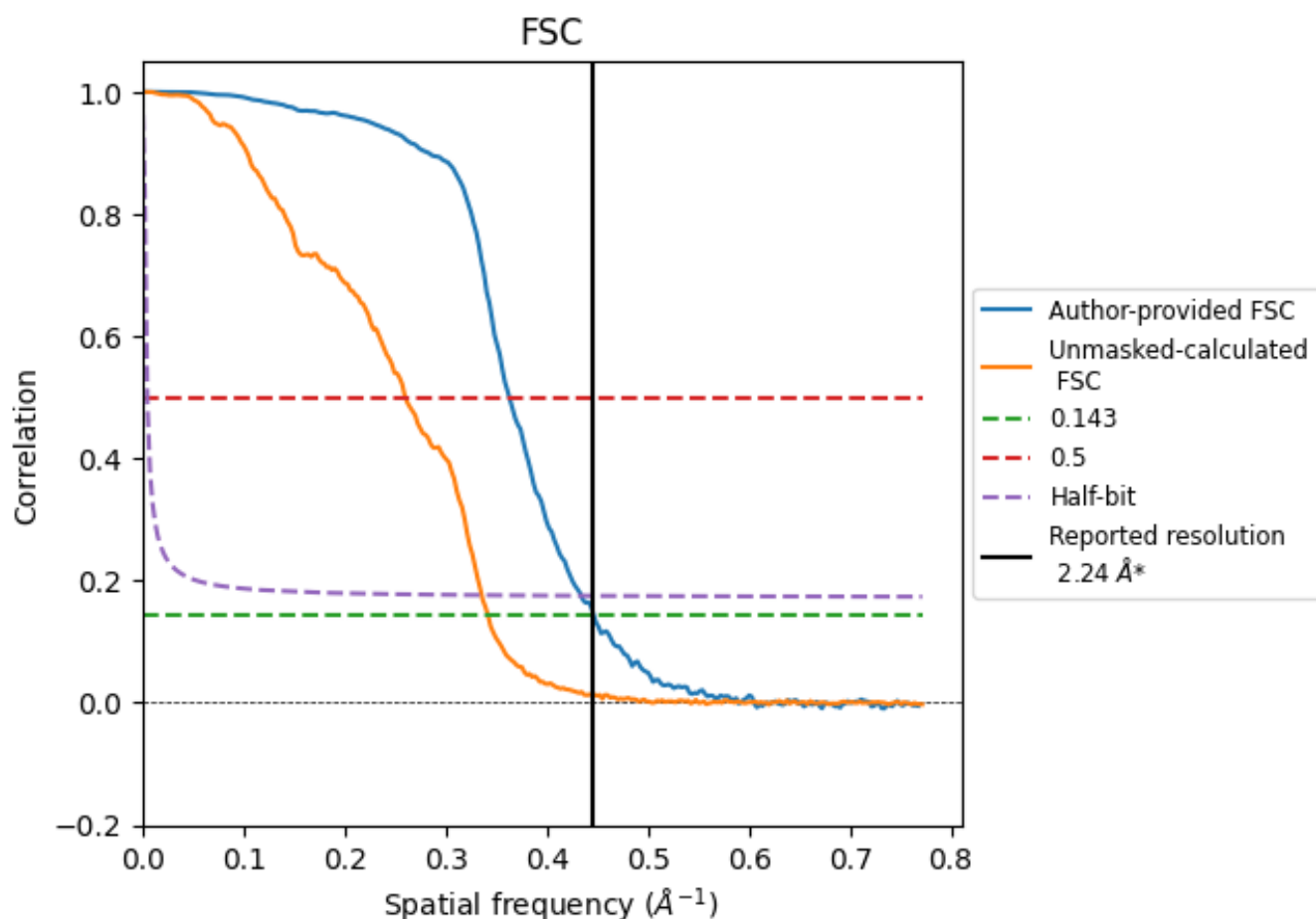


*Reported resolution corresponds to spatial frequency of 0.446 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.446 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

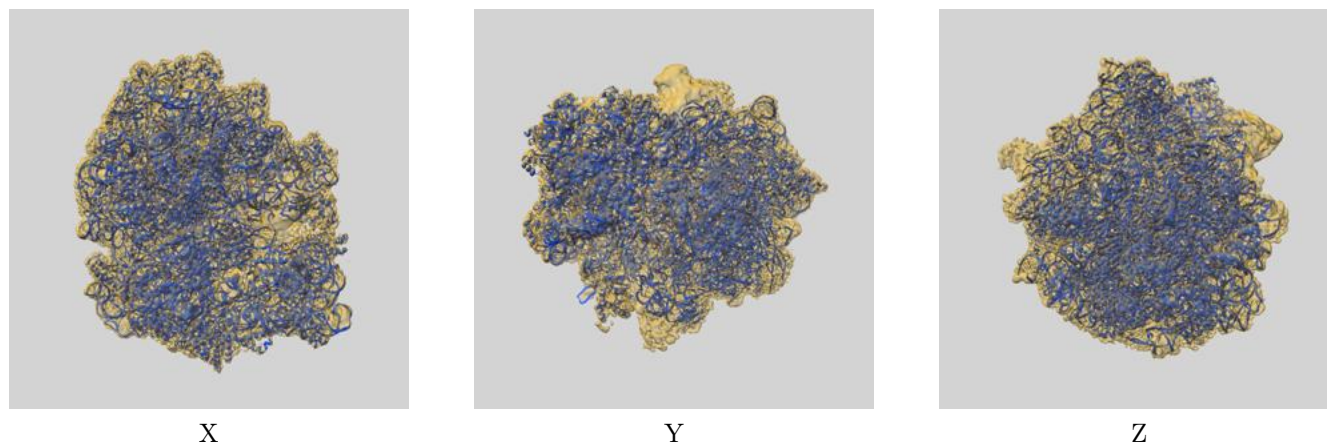
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.24	2.75	2.30
Unmasked-calculated*	2.92	3.84	2.98

*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 2.92 differs from the reported value 2.24 by more than 10 %

9 Map-model fit [i](#)

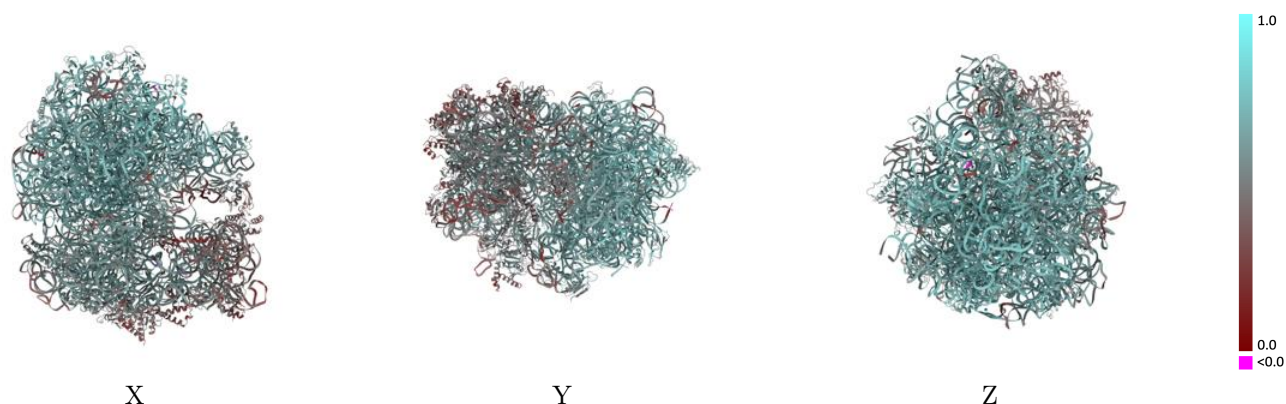
This section contains information regarding the fit between EMDB map EMD-51350 and PDB model 9GHA. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



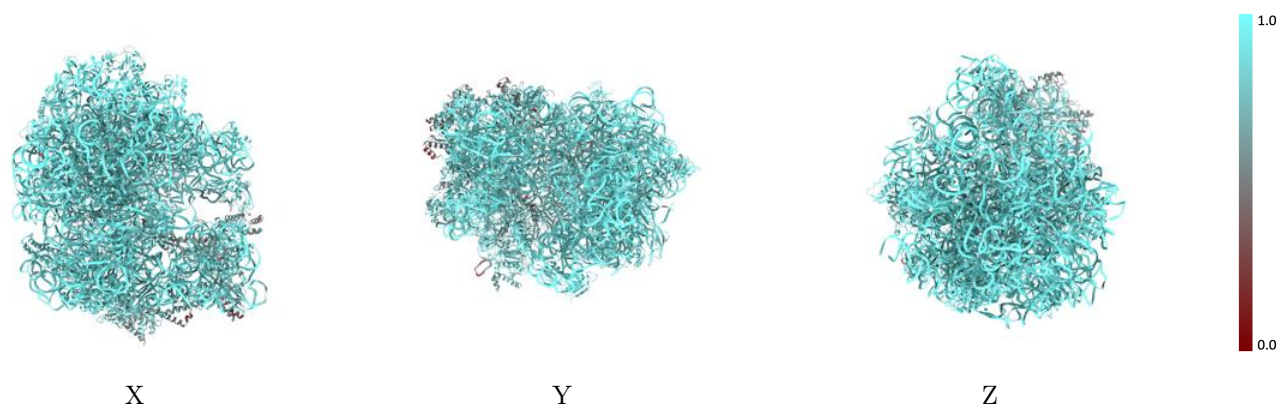
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



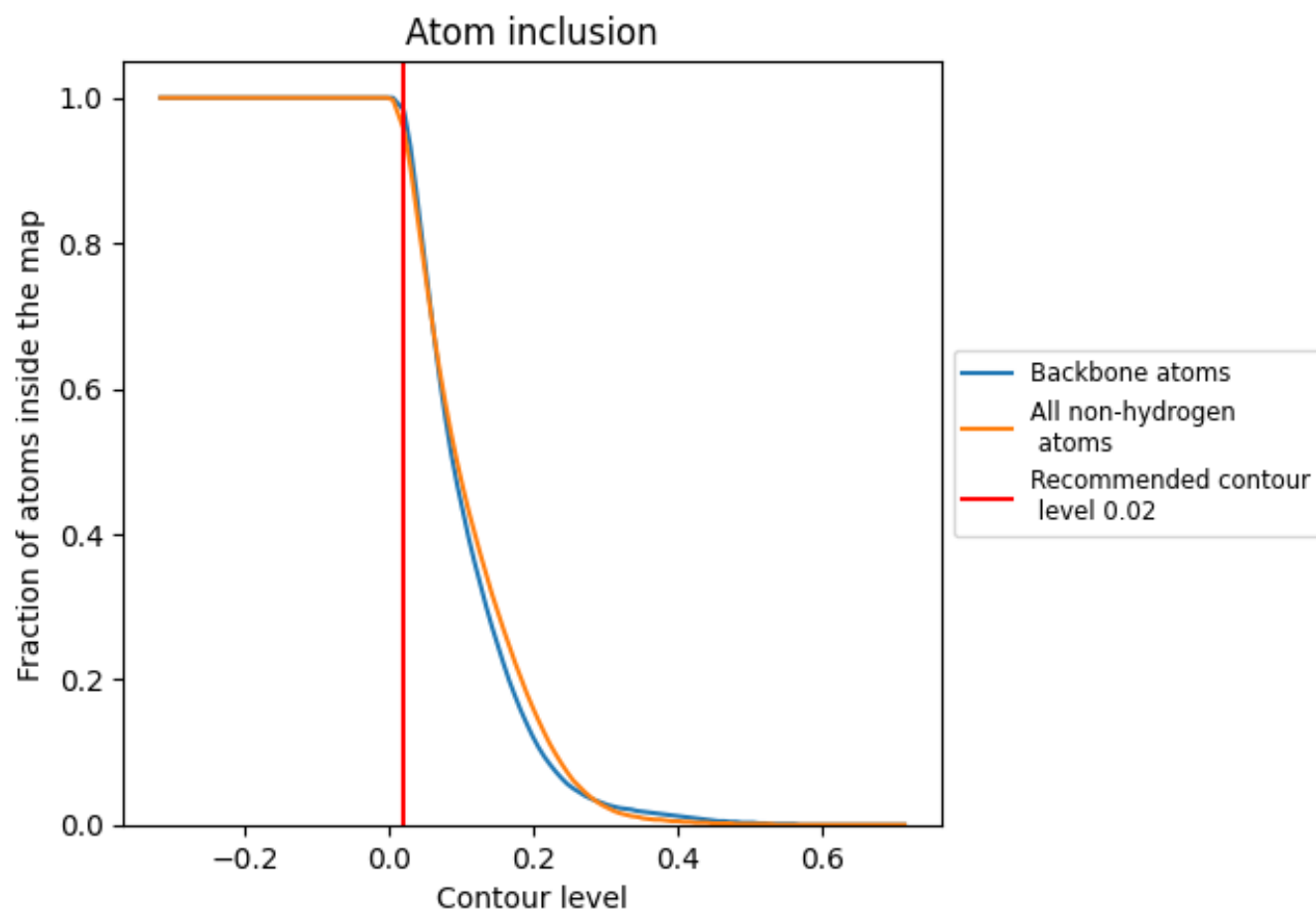
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.6150
0	 0.9460	 0.6380
1	 0.9970	 0.7540
2	 0.9940	 0.7340
3	 0.9930	 0.6730
4	 0.7980	 0.3930
8	 0.9290	 0.4840
9	 0.8730	 0.5040
A	 0.9740	 0.5540
B	 0.6740	 0.3880
C	 0.8280	 0.4780
D	 0.8720	 0.4780
E	 0.9200	 0.5390
F	 0.8780	 0.4970
G	 0.6590	 0.3370
H	 0.9170	 0.5450
I	 0.8110	 0.4350
J	 0.7150	 0.4190
K	 0.9040	 0.5440
L	 0.9340	 0.5650
M	 0.7040	 0.4140
N	 0.8820	 0.4880
O	 0.9250	 0.5580
P	 0.9490	 0.5510
Q	 0.9330	 0.5690
R	 0.9180	 0.5330
S	 0.8220	 0.4580
T	 0.9360	 0.5530
U	 0.8500	 0.5020
W	 0.8390	 0.4790
a	 0.9930	 0.6860
b	 0.9950	 0.6280
c	 0.9890	 0.7120
d	 0.9730	 0.7060
e	 0.9590	 0.6740



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.8550	 0.4730
g	 0.9410	 0.5910
h	 0.9430	 0.5840
i	 0.9790	 0.7090
j	 0.9780	 0.6920
k	 0.9800	 0.7030
l	 0.9760	 0.6830
m	 0.9970	 0.7360
n	 0.9570	 0.6110
o	 0.9550	 0.6700
p	 0.9920	 0.7360
q	 0.9510	 0.6680
r	 0.9810	 0.7100
s	 0.9520	 0.6460
t	 0.9660	 0.6480
u	 0.9340	 0.6210
v	 0.9730	 0.6990
w	 0.9770	 0.6920
x	 0.9400	 0.6260
y	 0.9660	 0.6950
z	 0.9830	 0.7150