Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 05:56 AM JST

PDB ID	:	7WTL
EMDB ID	:	EMD-32790
Title	:	Cryo-EM structure of a yeast pre-40S ribosomal subunit - State Dis-D
Authors	:	Cheng, J.; La Venuta, G.; Lau, B.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on	:	2022-02-05
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

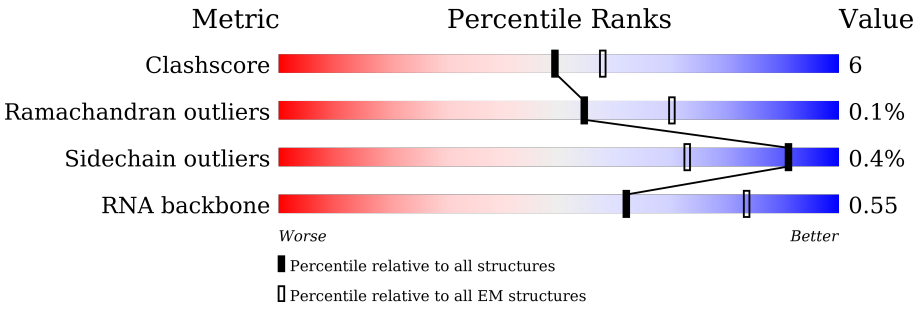
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	C2	1800	34% 23% 39%
2	SB	255	69% 15% 15%
3	SE	261	79% 21%
4	SG	236	74% 18% 8%
5	SH	190	78% 18%
6	SI	200	74% 20% 6%
7	SJ	197	72% 22% 6%

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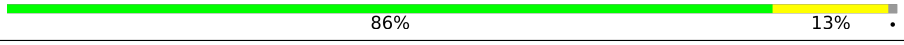
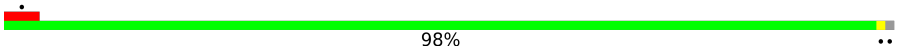
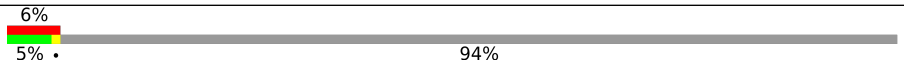
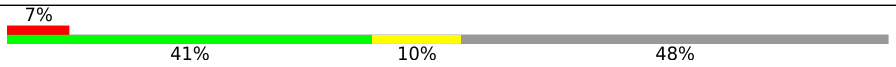
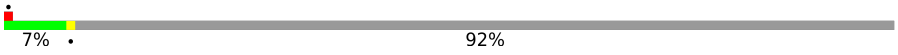
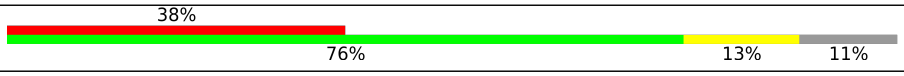
Mol	Chain	Length	Quality of chain
8	SL	156	
9	SN	151	
10	SO	137	
11	SW	130	
12	SX	145	
13	SY	135	
14	Sb	82	
15	CA	274	
16	CK	593	
17	CL	1183	
18	UC	610	
19	JL	318	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 49811 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C2	1102	23488	10508	4168	7710	1102	0	0

- Molecule 2 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	216	1722	1091	312	315	4	0	0

- Molecule 3 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SE	260	2068	1316	389	360	3	0	0

- Molecule 4 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SG	218	1755	1102	337	313	3	0	0

- Molecule 5 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	SH	185	1486	954	266	266	0	0

- Molecule 6 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SI	188	1489	925	298	264	2	0	0

- Molecule 7 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 8 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SL	146	Total	C	N	O	S	0	0
			1168	747	221	197	3		

- Molecule 9 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 10 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SO	128	Total	C	N	O	S	0	0
			949	582	188	176	3		

- Molecule 11 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 12 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SX	121	Total	C	N	O	S	0	0
			962	613	188	159	2		

- Molecule 13 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	SY	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 14 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Sb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 15 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CA	181	Total	C	N	O	S	0	0
			1436	917	261	254	4		

- Molecule 16 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	CK	36	Total	C	N	O	0	0
			299	188	52	59		

- Molecule 17 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CL	610	Total	C	N	O	S	0	0
			4910	3157	864	865	24		

- Molecule 18 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	UC	47	Total	C	N	O	0	0
			393	243	86	64		

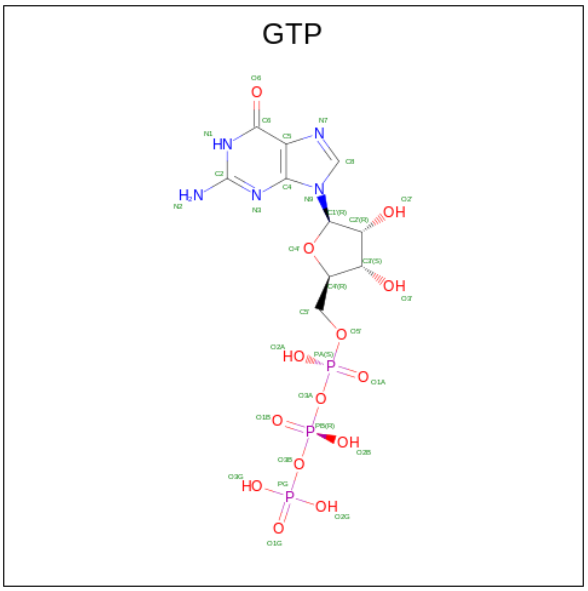
- Molecule 19 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	JL	283	Total	C	N	O	S	0	0
			2262	1439	401	408	14		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	Sb	1	Total	Zn	0
			1	1	

- Molecule 21 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
21	CL	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

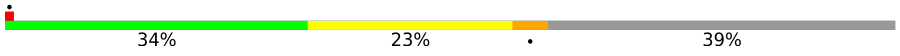
Mol	Chain	Residues	Atoms		AltConf
22	CL	1	Total	Mg	0
			1	1	

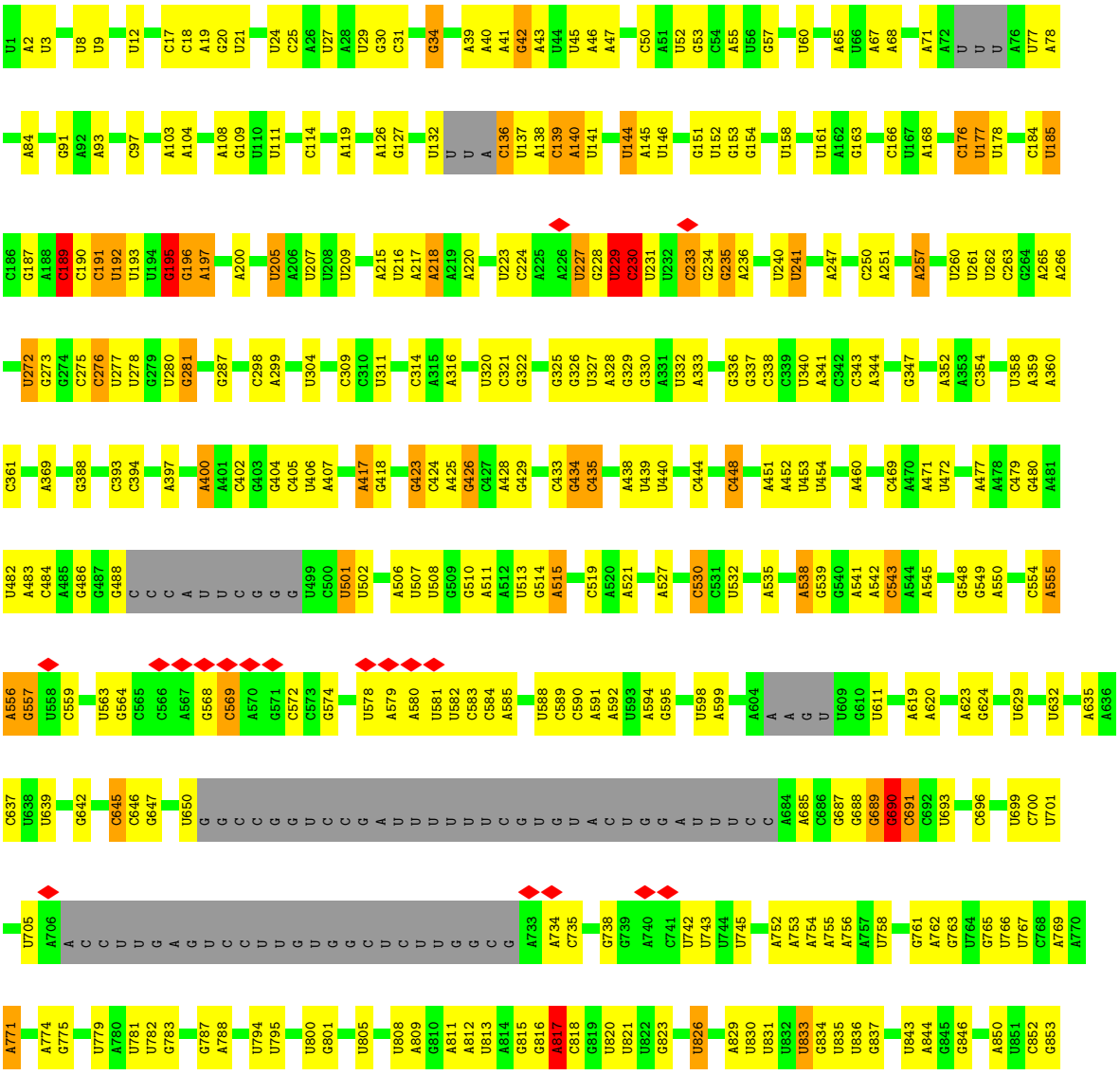
3 Residue-property plots (i)

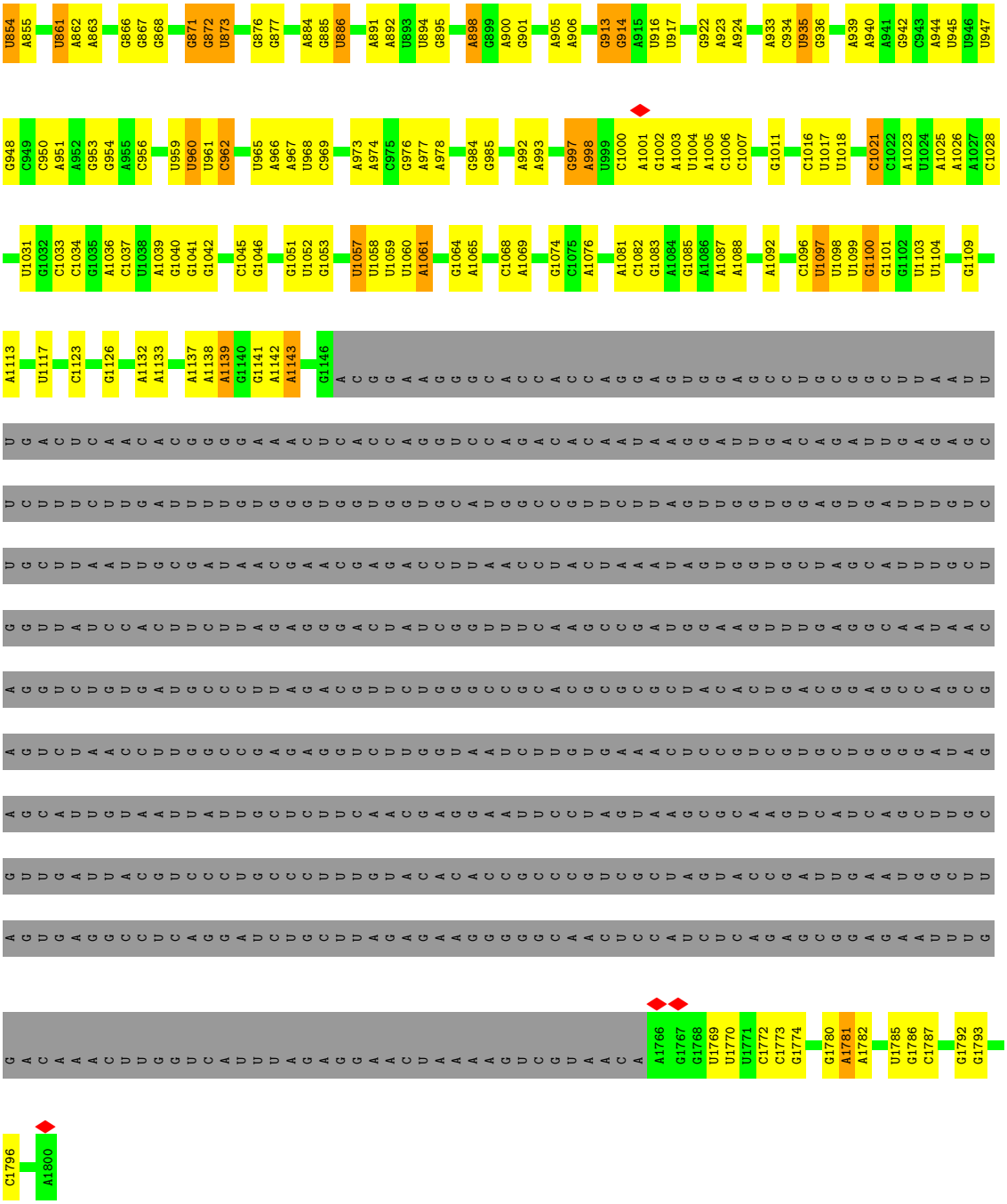
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 18S rRNA

Chain C2:

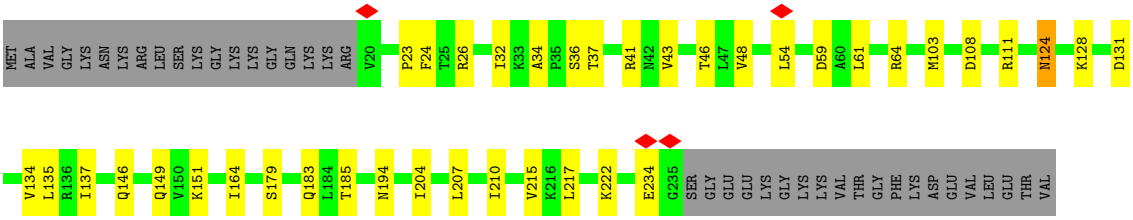






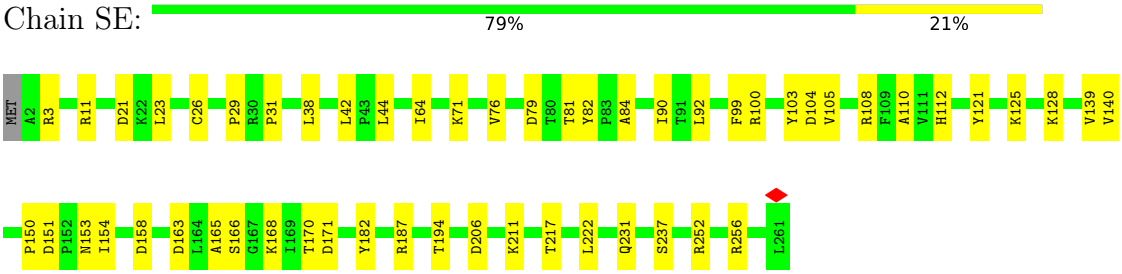
• Molecule 2: 40S ribosomal protein S1-A

Chain SB:



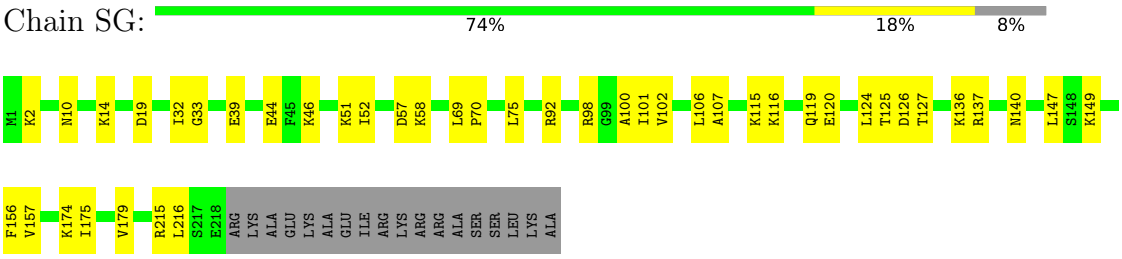
• Molecule 3: 40S ribosomal protein S4-A

Chain SE:



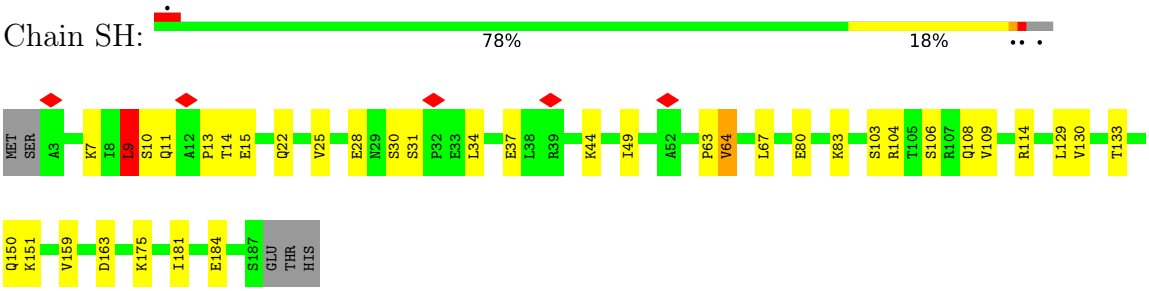
• Molecule 4: 40S ribosomal protein S6-A

Chain SG:



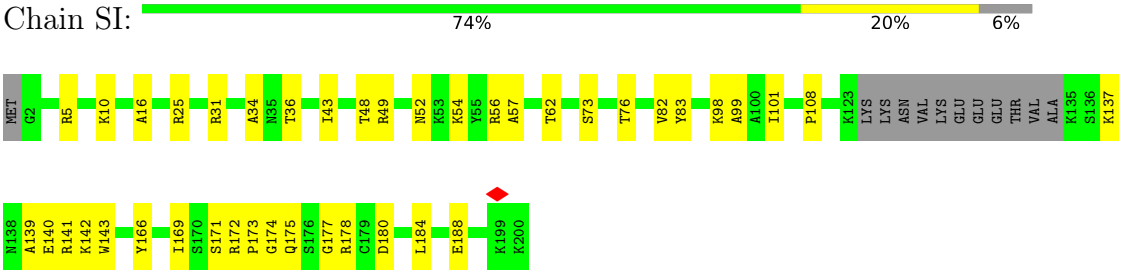
• Molecule 5: 40S ribosomal protein S7-A

Chain SH:



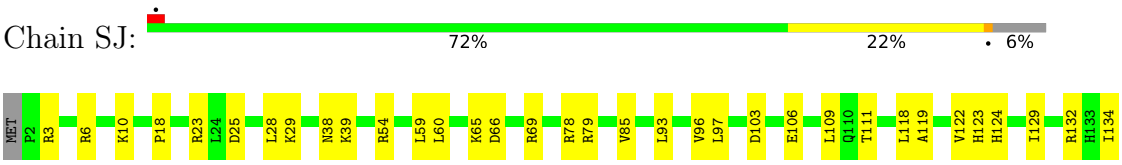
• Molecule 6: 40S ribosomal protein S8-A

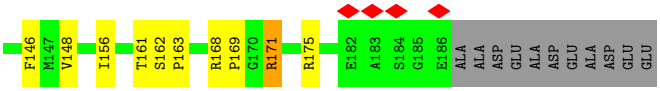
Chain SI:



• Molecule 7: 40S ribosomal protein S9-A

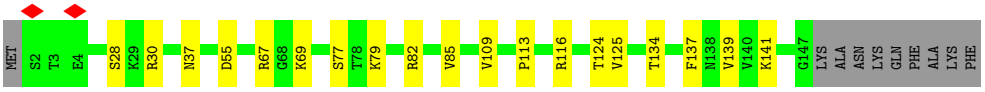
Chain SJ:





• Molecule 8: 40S ribosomal protein S11-A

Chain SL:

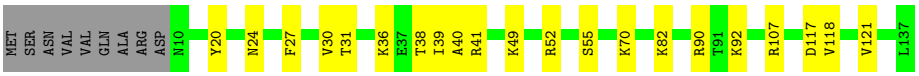


• Molecule 9: 40S ribosomal protein S13

Chain SN:

• Molecule 10: 40S ribosomal protein S14-A

Chain SO:

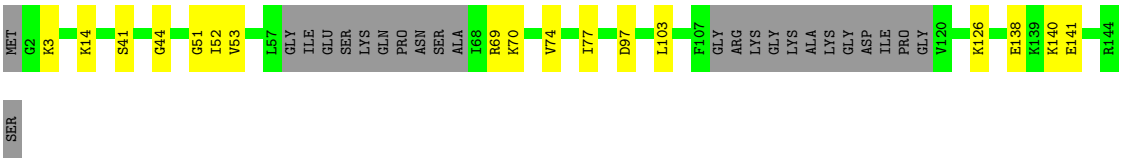


• Molecule 11: 40S ribosomal protein S22-A

Chain SW:

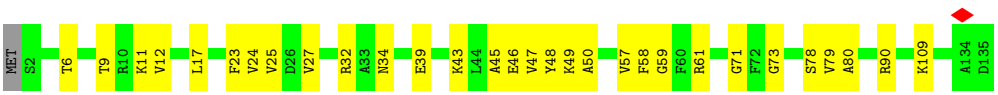
• Molecule 12: 40S ribosomal protein S23-A

Chain SX:



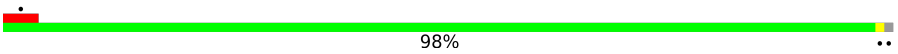
• Molecule 13: 40S ribosomal protein S24-A

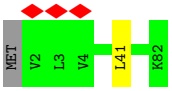
Chain SY:



• Molecule 14: 40S ribosomal protein S27-A

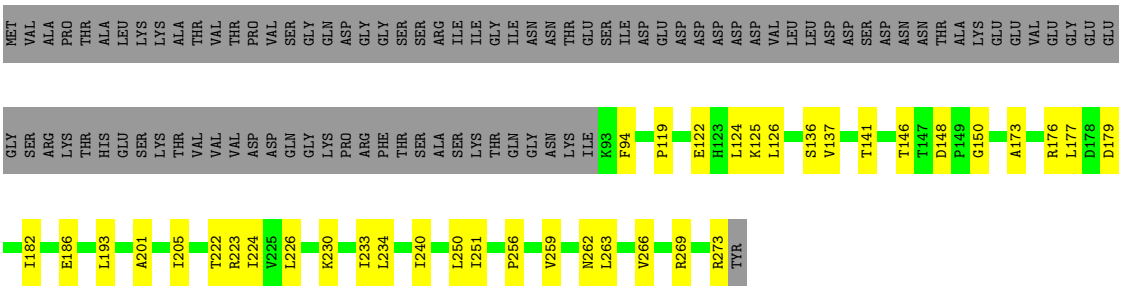
Chain Sb:





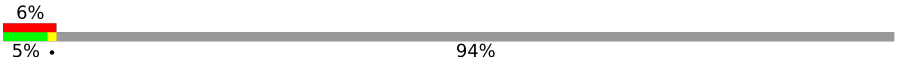
• Molecule 15: Pre-rRNA-processing protein PNO1

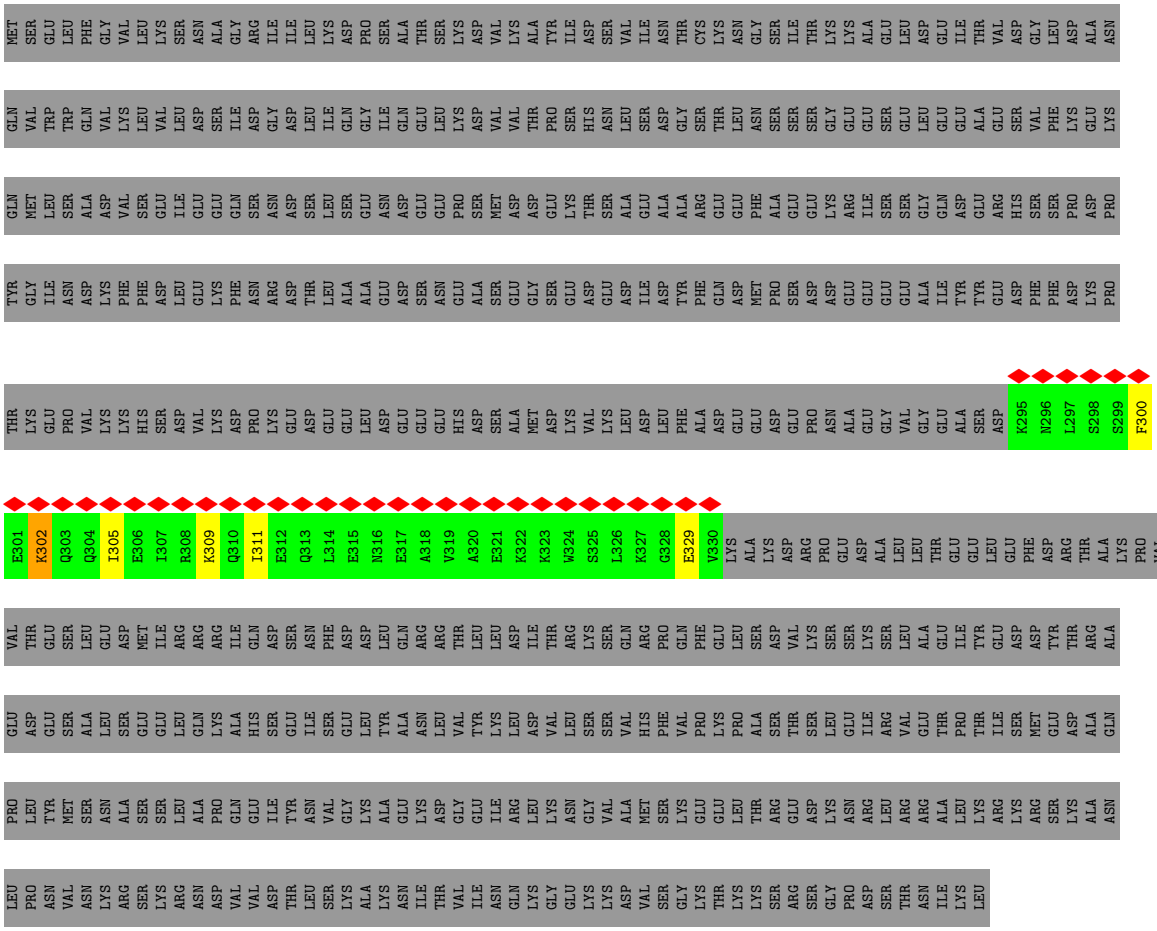
Chain CA:



• Molecule 16: U3 small nucleolar RNA-associated protein MPP10

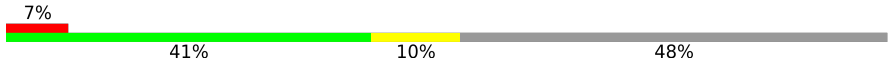
Chain CK:

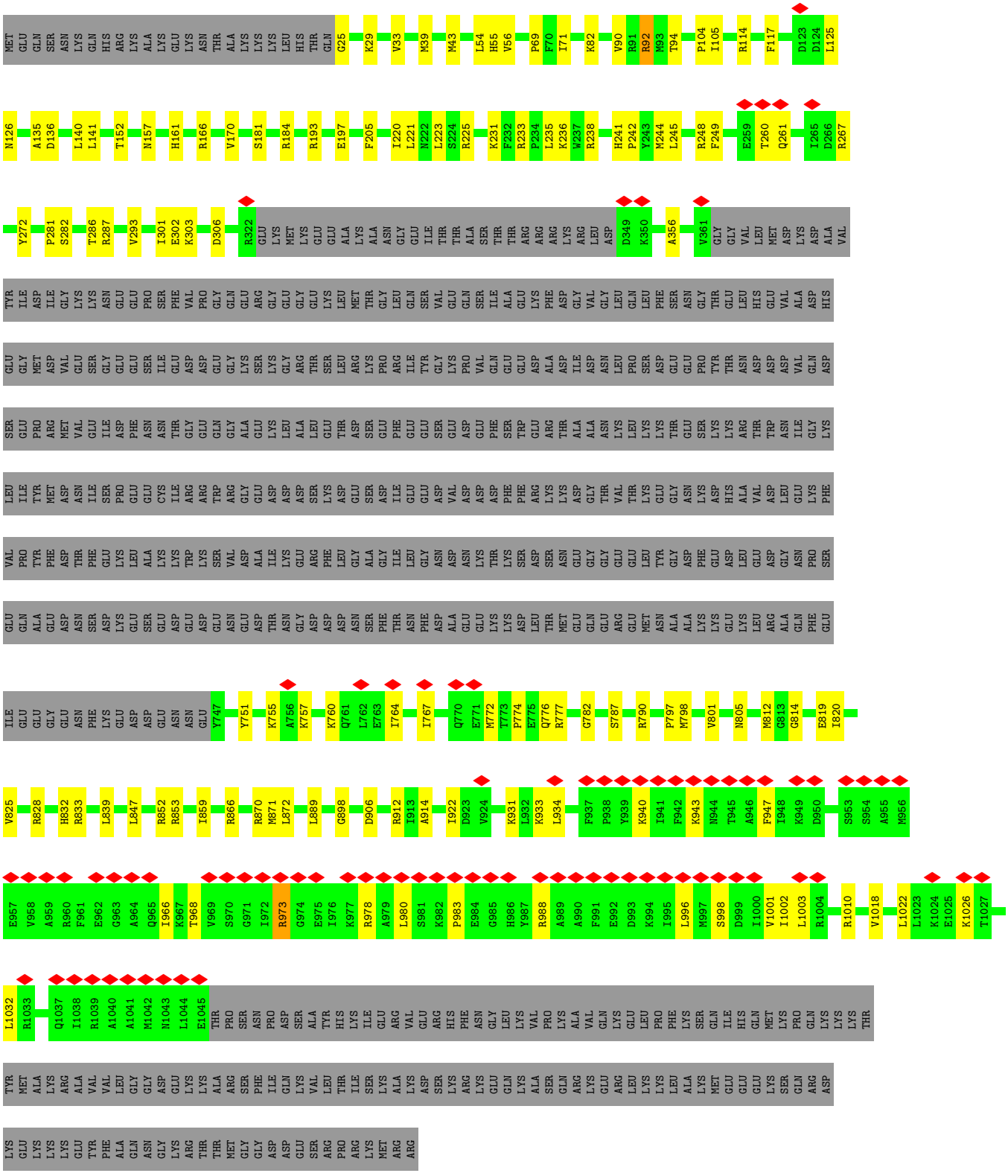




• Molecule 17: Ribosome biogenesis protein BMS1

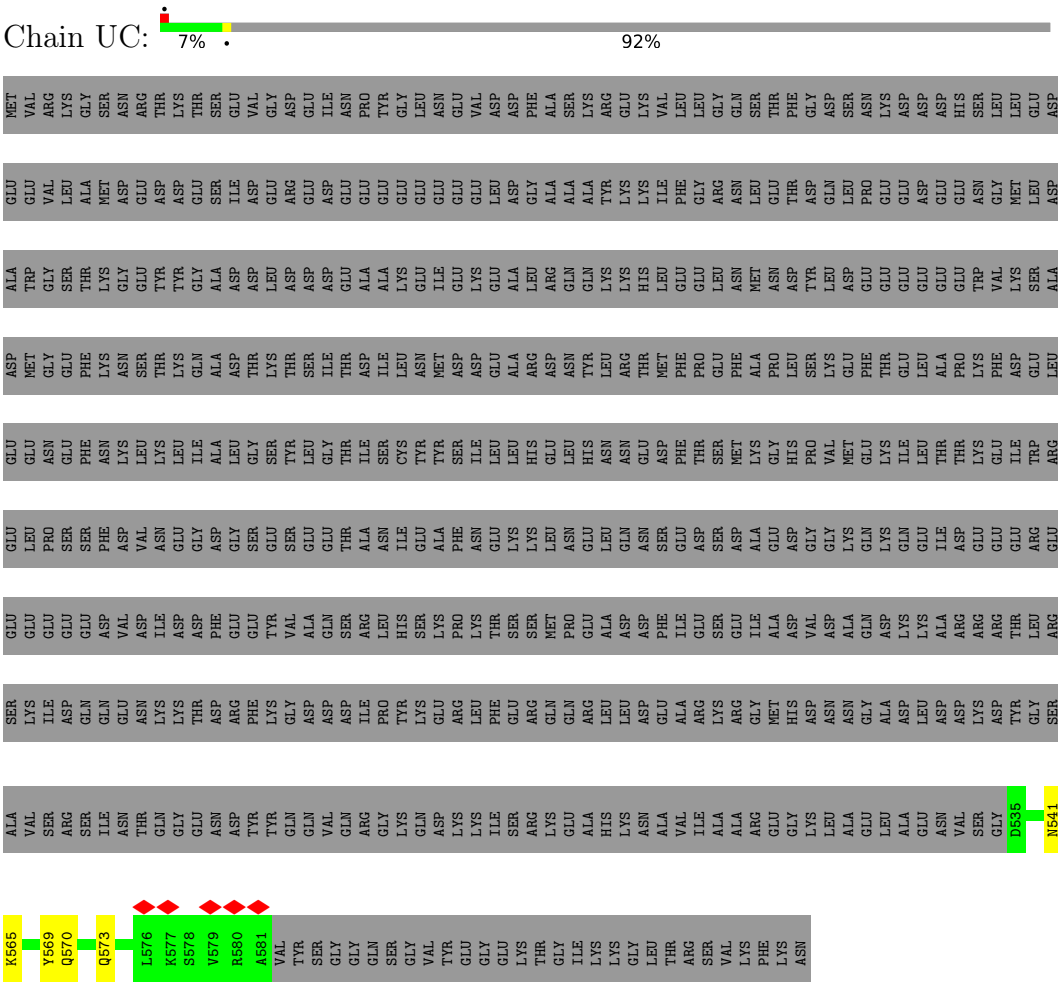
Chain CL:





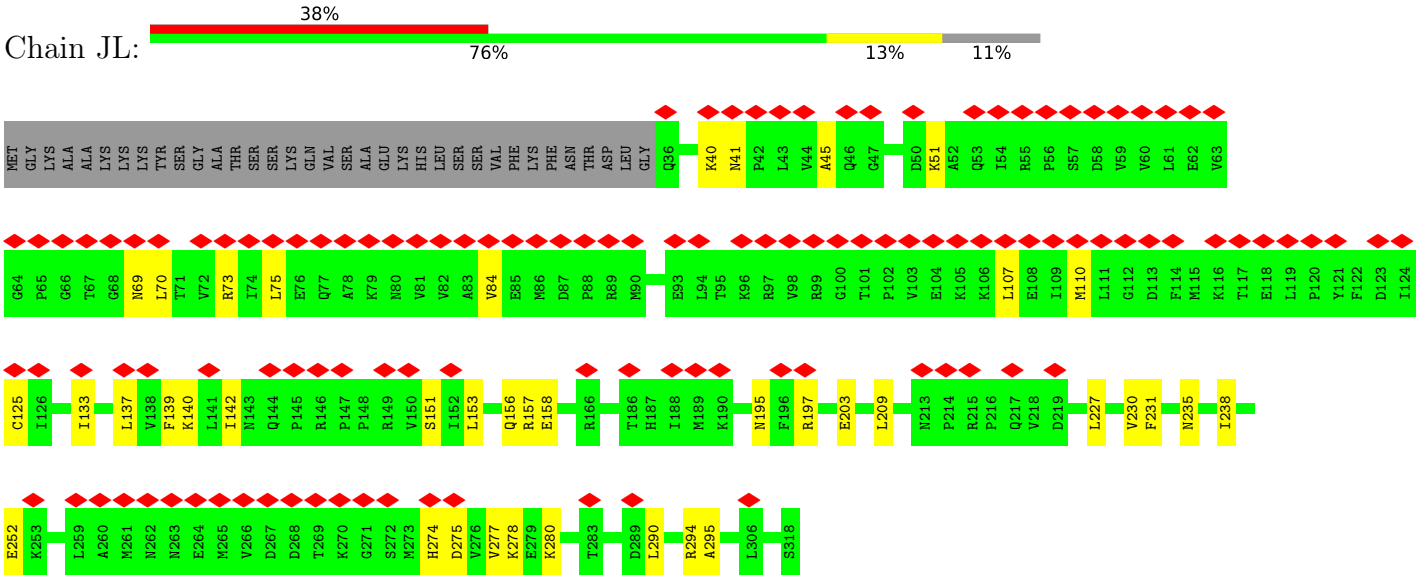
• Molecule 18: Something about silencing protein 10

Chain UC:



• Molecule 19: Dimethyladenosine transferase

Chain JL:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.397	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	376.92, 376.92, 376.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GTP

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	C2	0.30	0/26274	0.97	66/40922 (0.2%)
2	SB	0.27	0/1748	0.60	1/2352 (0.0%)
3	SE	0.28	0/2109	0.63	0/2839
4	SG	0.26	0/1779	0.61	1/2379 (0.0%)
5	SH	0.27	0/1511	0.68	1/2036 (0.0%)
6	SI	0.30	0/1514	0.66	0/2021
7	SJ	0.27	0/1519	0.62	1/2035 (0.0%)
8	SL	0.30	0/1194	0.59	0/1610
9	SN	0.29	0/1215	0.59	0/1638
10	SO	0.28	0/960	0.69	1/1290 (0.1%)
11	SW	0.28	0/1038	0.60	0/1395
12	SX	0.26	0/976	0.56	0/1299
13	SY	0.29	0/1087	0.69	1/1449 (0.1%)
14	Sb	0.28	0/620	0.71	1/838 (0.1%)
15	CA	0.27	0/1462	0.62	1/1969 (0.1%)
16	CK	0.24	0/301	0.48	0/399
17	CL	0.27	0/5026	0.59	0/6791
18	UC	0.27	0/395	0.59	0/517
19	JL	0.26	0/2305	0.56	0/3116
All	All	0.29	0/53033	0.82	74/76895 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	SH	0	2
13	SY	0	1
All	All	0	3

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C2	190	C	N3-C2-O2	-12.07	113.45	121.90
1	C2	645	C	N3-C2-O2	-11.45	113.89	121.90
1	C2	646	C	N3-C2-O2	-9.62	115.17	121.90
1	C2	190	C	N1-C2-O2	9.09	124.35	118.90
4	SG	69	LEU	CA-CB-CG	8.76	135.44	115.30
1	C2	956	C	N3-C2-O2	-8.60	115.88	121.90
1	C2	645	C	N1-C2-O2	8.32	123.89	118.90
1	C2	646	C	C6-N1-C2	-7.96	117.11	120.30
1	C2	479	C	N3-C2-O2	-7.72	116.50	121.90
10	SO	117	ASP	CB-CG-OD1	7.51	125.06	118.30
1	C2	767	U	N3-C2-O2	-7.46	116.97	122.20
1	C2	767	U	N1-C2-O2	7.28	127.90	122.80
1	C2	956	C	N1-C2-O2	7.14	123.18	118.90
15	CA	179	ASP	CB-CG-OD1	7.04	124.64	118.30
1	C2	965	U	C2-N1-C1'	7.04	126.15	117.70
1	C2	861	U	C2-N1-C1'	6.96	126.05	117.70
1	C2	189	C	N1-C2-O2	6.96	123.07	118.90
1	C2	767	U	C2-N1-C1'	6.92	126.01	117.70
1	C2	934	C	C2-N1-C1'	6.75	126.22	118.80
1	C2	795	U	N3-C2-O2	-6.66	117.54	122.20
1	C2	795	U	C2-N1-C1'	6.60	125.62	117.70
1	C2	224	C	N3-C2-O2	-6.51	117.34	121.90
1	C2	795	U	N1-C2-O2	6.50	127.35	122.80
1	C2	42	G	P-O3'-C3'	6.50	127.50	119.70
1	C2	645	C	C6-N1-C2	-6.48	117.71	120.30
1	C2	569	C	N1-C2-O2	6.44	122.76	118.90
14	Sb	41	LEU	CA-CB-CG	6.43	130.09	115.30
1	C2	1021	C	C2-N1-C1'	6.31	125.74	118.80
1	C2	272	U	P-O3'-C3'	6.27	127.23	119.70
1	C2	184	C	N1-C2-O2	6.21	122.63	118.90
1	C2	479	C	N1-C2-O2	6.19	122.61	118.90
1	C2	195	G	N1-C2-N2	-6.15	110.67	116.20
1	C2	1016	C	N3-C2-O2	-6.13	117.61	121.90
1	C2	934	C	N1-C2-O2	6.07	122.54	118.90
1	C2	1021	C	C6-N1-C2	-6.03	117.89	120.30
1	C2	276	C	N3-C2-O2	-5.96	117.73	121.90
1	C2	195	G	N3-C2-N2	5.94	124.06	119.90
1	C2	691	C	C2-N1-C1'	5.93	125.33	118.80
1	C2	191	C	O4'-C1'-N1	5.92	112.94	108.20
5	SH	9	LEU	CA-CB-CG	5.90	128.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C2	144	U	C2-N1-C1'	5.72	124.56	117.70
2	SB	54	LEU	CA-CB-CG	5.67	128.34	115.30
1	C2	184	C	N3-C2-O2	-5.66	117.94	121.90
1	C2	689	G	N1-C6-O6	-5.64	116.51	119.90
7	SJ	118	LEU	CA-CB-CG	5.64	128.27	115.30
1	C2	758	U	N1-C2-O2	5.64	126.75	122.80
1	C2	190	C	C6-N1-C2	-5.56	118.08	120.30
1	C2	690	G	C8-N9-C4	-5.54	104.18	106.40
1	C2	229	U	C2-N1-C1'	5.48	124.27	117.70
1	C2	1097	U	P-O3'-C3'	5.37	126.14	119.70
1	C2	689	G	N1-C2-N2	-5.37	111.37	116.20
1	C2	136	C	P-O3'-C3'	5.33	126.10	119.70
1	C2	962	C	N3-C2-O2	-5.33	118.17	121.90
1	C2	417	A	P-O3'-C3'	5.32	126.08	119.70
1	C2	646	C	N1-C2-O2	5.29	122.07	118.90
1	C2	184	C	C2-N1-C1'	5.28	124.61	118.80
1	C2	935	U	N1-C2-O2	5.28	126.49	122.80
1	C2	758	U	N3-C2-O2	-5.24	118.53	122.20
1	C2	965	U	N1-C2-O2	5.24	126.47	122.80
1	C2	205	U	N3-C2-O2	-5.23	118.54	122.20
1	C2	817	A	P-O3'-C3'	5.23	125.98	119.70
1	C2	275	C	N1-C2-O2	5.15	121.99	118.90
13	SY	49	LYS	CA-CB-CG	5.11	124.65	113.40
1	C2	50	C	N3-C2-O2	-5.11	118.33	121.90
1	C2	189	C	N3-C2-O2	-5.11	118.32	121.90
1	C2	871	G	N3-C4-N9	5.11	129.06	126.00
1	C2	1781	A	P-O3'-C3'	5.10	125.83	119.70
1	C2	230	C	N1-C2-O2	5.09	121.95	118.90
1	C2	139	C	P-O3'-C3'	5.09	125.80	119.70
1	C2	530	C	N1-C2-O2	5.08	121.95	118.90
1	C2	281	G	N1-C2-N2	-5.07	111.63	116.20
1	C2	872	G	C5-C6-O6	5.05	131.63	128.60
1	C2	185	U	C2-N1-C1'	5.04	123.75	117.70
1	C2	260	U	C2-N1-C1'	5.03	123.74	117.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	SH	64	VAL	Peptide
5	SH	9	LEU	Peptide
13	SY	48	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C2	23488	0	11812	224	0
2	SB	1722	0	1793	24	0
3	SE	2068	0	2154	34	0
4	SG	1755	0	1846	29	0
5	SH	1486	0	1576	21	0
6	SI	1489	0	1525	33	0
7	SJ	1494	0	1573	30	0
8	SL	1168	0	1233	12	0
9	SN	1192	0	1255	14	0
10	SO	949	0	985	18	0
11	SW	1021	0	1060	15	0
12	SX	962	0	1029	17	0
13	SY	1073	0	1132	18	0
14	Sb	610	0	633	0	0
15	CA	1436	0	1515	25	0
16	CK	299	0	307	4	0
17	CL	4910	0	5018	83	0
18	UC	393	0	444	5	0
19	JL	2262	0	2330	23	0
20	Sb	1	0	0	0	0
21	CL	32	0	12	0	0
22	CL	1	0	0	0	0
All	All	49811	0	39232	530	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 6.

All (530) 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)
1:C2:895:G:H1	1:C2:917:U:H3	1.03	0.97
1:C2:486:G:H1	1:C2:501:U:H3	1.00	0.93
1:C2:451:A:C6	1:C2:453:U:O2	2.22	0.92
19:JL:275:ASP:O	19:JL:278:LYS:HB3	1.77	0.85
1:C2:826:U:H3	1:C2:846:G:H1	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:868:G:H1	1:C2:960:U:H3	1.30	0.79
6:SI:62:THR:HA	6:SI:76:THR:O	1.86	0.74
2:SB:149:GLN:HE21	2:SB:151:LYS:HB3	1.55	0.72
1:C2:873:U:O4	1:C2:954:G:O6	2.10	0.70
1:C2:229:U:O4	1:C2:235:G:O6	2.11	0.68
15:CA:205:ILE:HD13	15:CA:250:LEU:HD22	1.75	0.68
6:SI:172:ARG:HE	6:SI:175:GLN:HG3	1.57	0.68
15:CA:94:PHE:HA	15:CA:141:THR:O	1.94	0.68
16:CK:300:PHE:HB2	17:CL:797:PRO:HB3	1.75	0.67
1:C2:1004:U:H3	15:CA:269:ARG:HH22	1.43	0.67
1:C2:532:U:OP1	7:SJ:132:ARG:NH2	2.28	0.66
1:C2:1034:C:HO2'	11:SW:2:THR:N	1.94	0.66
17:CL:996:LEU:HD23	17:CL:998:SER:H	1.61	0.66
1:C2:358:U:H4'	17:CL:33:VAL:HG12	1.79	0.65
1:C2:584:C:OP1	12:SX:70:LYS:NZ	2.27	0.65
5:SH:151:LYS:HE3	5:SH:184:GLU:HG3	1.77	0.65
17:CL:170:VAL:HG12	17:CL:205:PHE:HB2	1.79	0.65
5:SH:150:GLN:HB3	5:SH:181:ILE:HG22	1.78	0.64
6:SI:99:ALA:N	6:SI:169:ILE:O	2.30	0.64
15:CA:119:PRO:HA	15:CA:122:GLU:HG2	1.80	0.64
4:SG:157:VAL:HG21	4:SG:175:ILE:HD11	1.80	0.63
17:CL:825:VAL:HG12	17:CL:922:ILE:HG22	1.79	0.63
1:C2:564:G:H1	1:C2:578:U:H3	1.36	0.63
1:C2:894:U:O2	10:SO:36:LYS:NZ	2.31	0.63
6:SI:184:LEU:HD22	6:SI:188:GLU:HB3	1.81	0.63
1:C2:451:A:C5	1:C2:453:U:O2	2.53	0.62
7:SJ:122:VAL:HG23	7:SJ:123:HIS:HD2	1.63	0.62
1:C2:228:G:N1	1:C2:236:A:N6	2.47	0.62
1:C2:752:A:OP1	3:SE:187:ARG:NH1	2.32	0.62
7:SJ:109:LEU:HB2	7:SJ:146:PHE:HB3	1.82	0.62
10:SO:107:ARG:NH2	15:CA:148:ASP:OD1	2.32	0.62
1:C2:218:A:H61	1:C2:844:A:H1'	1.65	0.62
11:SW:15:ASN:ND2	11:SW:72:CYS:SG	2.72	0.62
5:SH:44:LYS:HG3	5:SH:63:PRO:HG3	1.81	0.62
17:CL:282:SER:HA	17:CL:301:ILE:HD11	1.82	0.62
1:C2:993:A:H62	1:C2:1011:G:H21	1.46	0.62
1:C2:231:U:C2	1:C2:234:G:O6	2.53	0.61
17:CL:242:PRO:HG2	17:CL:814:GLY:HA3	1.82	0.61
19:JL:45:ALA:HB1	19:JL:73:ARG:HH22	1.65	0.61
1:C2:900:A:H3'	1:C2:901:G:H21	1.65	0.61
19:JL:238:ILE:HD12	19:JL:290:LEU:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:1101:G:HO2'	11:SW:4:SER:HG	1.48	0.61
1:C2:647:G:H21	1:C2:687:G:H1	1.48	0.61
6:SI:139:ALA:HA	6:SI:142:LYS:HE3	1.82	0.60
5:SH:103:SER:HG	5:SH:106:SER:HG	1.47	0.60
1:C2:189:C:N4	1:C2:197:A:N6	2.49	0.60
17:CL:302:GLU:OE2	17:CL:790:ARG:NH1	2.31	0.60
1:C2:689:G:H2'	1:C2:690:G:C8	2.37	0.60
11:SW:48:GLY:HA3	11:SW:64:GLN:O	2.01	0.60
1:C2:388:G:N7	1:C2:423:G:C2	2.71	0.59
1:C2:1081:A:O2'	1:C2:1083:G:N7	2.34	0.59
1:C2:530:C:O2	13:SY:61:ARG:NH1	2.35	0.59
13:SY:59:GLY:O	13:SY:71:GLY:HA3	2.02	0.59
12:SX:103:LEU:HB3	12:SX:126:LYS:HB2	1.85	0.59
1:C2:535:A:OP1	7:SJ:168:ARG:NH2	2.36	0.59
1:C2:393:C:O2'	4:SG:92:ARG:NH2	2.36	0.58
1:C2:1117:U:HO2'	17:CL:25:GLY:N	2.00	0.58
8:SL:124:THR:HB	8:SL:141:LYS:HB3	1.85	0.58
9:SN:35:GLU:HA	9:SN:38:VAL:HG22	1.86	0.58
17:CL:166:ARG:NH1	17:CL:231:LYS:O	2.36	0.58
2:SB:23:PRO:HB3	2:SB:26:ARG:HH21	1.68	0.58
1:C2:1123:C:O2	19:JL:294:ARG:NH2	2.37	0.57
1:C2:207:U:O2	6:SI:178:ARG:NH2	2.38	0.57
1:C2:480:G:H1	1:C2:508:U:H3	1.53	0.57
1:C2:1132:A:H2'	1:C2:1133:A:H8	1.68	0.57
1:C2:1064:G:O2'	2:SB:204:ILE:O	2.23	0.57
17:CL:235:LEU:HB2	17:CL:238:ARG:HD2	1.85	0.57
17:CL:940:LYS:HB3	17:CL:947:PHE:HB2	1.86	0.57
3:SE:11:ARG:NH1	3:SE:21:ASP:O	2.35	0.57
11:SW:90:THR:HG23	11:SW:94:LEU:HD12	1.86	0.57
12:SX:138:GLU:HB3	17:CL:833:ARG:HD2	1.86	0.57
1:C2:231:U:O2	1:C2:234:G:O6	2.22	0.57
1:C2:689:G:H2'	1:C2:690:G:H8	1.69	0.57
1:C2:862:A:H3'	9:SN:16:ILE:HD13	1.87	0.57
4:SG:10:ASN:ND2	4:SG:127:THR:O	2.37	0.57
10:SO:107:ARG:HH21	15:CA:150:GLY:H	1.51	0.57
1:C2:241:U:H5'	4:SG:216:LEU:HD21	1.85	0.57
15:CA:269:ARG:HB3	15:CA:273:ARG:HH21	1.69	0.57
6:SI:137:LYS:HE2	6:SI:141:ARG:NH1	2.20	0.56
12:SX:138:GLU:O	17:CL:833:ARG:NH1	2.38	0.56
1:C2:187:G:OP2	6:SI:142:LYS:NZ	2.37	0.56
1:C2:347:G:OP2	8:SL:79:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SL:77:SER:HB3	8:SL:85:VAL:HB	1.87	0.56
19:JL:235:ASN:O	19:JL:294:ARG:NH1	2.36	0.56
3:SE:153:ASN:OD1	4:SG:215:ARG:NH1	2.39	0.56
19:JL:70:LEU:HA	19:JL:73:ARG:HH21	1.71	0.56
1:C2:564:G:N2	1:C2:578:U:O2	2.39	0.56
1:C2:629:U:OP1	9:SN:127:ARG:NH2	2.38	0.56
3:SE:151:ASP:HB3	3:SE:154:ILE:HG13	1.87	0.56
4:SG:14:LYS:HB2	4:SG:124:LEU:HD12	1.88	0.56
4:SG:33:GLY:HA2	4:SG:51:LYS:HE2	1.88	0.56
17:CL:71:ILE:HG23	17:CL:136:ASP:H	1.69	0.56
1:C2:816:G:H2'	1:C2:817:A:H8	1.72	0.56
3:SE:90:ILE:HG23	3:SE:99:PHE:HB2	1.86	0.56
6:SI:137:LYS:HG3	6:SI:141:ARG:HH12	1.71	0.56
7:SJ:18:PRO:O	7:SJ:23:ARG:NH2	2.39	0.55
8:SL:109:VAL:HG12	8:SL:137:PHE:HB2	1.88	0.55
10:SO:30:VAL:HG13	10:SO:39:ILE:HB	1.88	0.55
1:C2:967:A:OP2	9:SN:124:ARG:NH2	2.39	0.55
1:C2:976:G:H1	1:C2:1023:A:HO2'	1.48	0.55
19:JL:84:VAL:HG22	19:JL:110:MET:HB2	1.87	0.55
1:C2:228:G:H1	1:C2:236:A:N6	2.04	0.55
1:C2:434:G:H1'	17:CL:233:ARG:HG3	1.89	0.55
1:C2:1065:A:N3	2:SB:146:GLN:NE2	2.51	0.55
1:C2:1785:U:H2'	1:C2:1786:G:H8	1.71	0.55
1:C2:168:A:OP1	4:SG:140:ASN:ND2	2.39	0.55
1:C2:557:G:C2	1:C2:588:U:O2	2.59	0.55
19:JL:227:LEU:O	19:JL:231:PHE:HB2	2.05	0.55
3:SE:104:ASP:OD1	3:SE:105:VAL:N	2.40	0.55
12:SX:52:ILE:HG12	17:CL:56:VAL:HG22	1.89	0.55
1:C2:235:G:H2'	1:C2:236:A:C8	2.41	0.55
1:C2:950:C:O2'	9:SN:104:ARG:NH2	2.39	0.55
3:SE:121:TYR:HA	3:SE:163:ASP:HA	1.88	0.55
10:SO:20:TYR:HB3	10:SO:27:PHE:HB2	1.89	0.55
17:CL:934:LEU:O	17:CL:1002:ILE:HA	2.07	0.55
2:SB:46:THR:OG1	2:SB:64:ARG:NH1	2.40	0.55
1:C2:843:U:H2'	1:C2:844:A:H8	1.72	0.54
2:SB:34:ALA:HB3	2:SB:41:ARG:HA	1.89	0.54
1:C2:78:A:H2	4:SG:174:LYS:HG3	1.72	0.54
1:C2:231:U:O2	1:C2:234:G:C6	2.60	0.54
1:C2:961:U:H5"	9:SN:71:ILE:HD13	1.90	0.54
13:SY:9:THR:HG22	13:SY:25:VAL:HG12	1.88	0.54
19:JL:125:CYS:O	19:JL:151:SER:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:8:U:O2'	1:C2:1139:A:N7	2.39	0.53
5:SH:80:GLU:HG2	5:SH:83:LYS:HE3	1.91	0.53
7:SJ:161:THR:HG22	7:SJ:162:SER:H	1.72	0.53
1:C2:836:U:H2'	1:C2:837:G:H8	1.73	0.53
17:CL:244:MET:HB3	17:CL:812:MET:HB3	1.90	0.53
3:SE:170:THR:HG22	3:SE:171:ASP:H	1.73	0.53
17:CL:980:LEU:HB3	17:CL:983:PRO:HD2	1.89	0.53
19:JL:69:ASN:O	19:JL:73:ARG:NH2	2.39	0.53
1:C2:572:C:OP1	17:CL:973:ARG:NH1	2.41	0.53
1:C2:861:U:O2'	11:SW:56:HIS:O	2.26	0.53
4:SG:32:ILE:HA	4:SG:52:ILE:HG23	1.90	0.53
1:C2:905:A:OP2	10:SO:52:ARG:NH1	2.42	0.53
3:SE:100:ARG:NH2	3:SE:121:TYR:O	2.40	0.53
4:SG:147:LEU:HD21	4:SG:156:PHE:HD2	1.72	0.53
1:C2:227:U:O2	1:C2:834:G:O6	2.26	0.53
1:C2:953:G:H2'	1:C2:954:G:C8	2.44	0.53
1:C2:1099:U:OP1	11:SW:71:LYS:NZ	2.39	0.53
10:SO:82:LYS:HD3	10:SO:118:VAL:HG21	1.90	0.53
19:JL:157:ARG:NH1	19:JL:203:GLU:OE1	2.42	0.53
1:C2:325:G:OP1	8:SL:134:THR:OG1	2.27	0.52
3:SE:103:TYR:O	3:SE:182:TYR:OH	2.27	0.52
17:CL:125:LEU:HD22	17:CL:912:ARG:HE	1.74	0.52
1:C2:91:G:OP1	1:C2:397:A:N6	2.43	0.52
3:SE:104:ASP:HB2	3:SE:110:ALA:HB2	1.91	0.52
3:SE:112:HIS:NE2	3:SE:237:SER:O	2.41	0.52
1:C2:8:U:H4'	1:C2:1138:A:H5'	1.91	0.52
1:C2:257:A:H1'	6:SI:73:SER:HB2	1.91	0.52
19:JL:156:GLN:NE2	19:JL:158:GLU:OE1	2.39	0.52
1:C2:152:U:O2	1:C2:163:G:N2	2.43	0.52
9:SN:54:LEU:HG	9:SN:60:VAL:HB	1.91	0.52
15:CA:222:THR:O	15:CA:223:ARG:NH1	2.39	0.52
17:CL:267:ARG:NH1	17:CL:798:MET:SD	2.82	0.52
2:SB:108:ASP:HA	2:SB:111:ARG:HD2	1.91	0.52
5:SH:34:LEU:HA	5:SH:37:GLU:HG3	1.91	0.52
5:SH:108:GLN:NE2	5:SH:109:VAL:O	2.43	0.52
7:SJ:163:PRO:HB3	7:SJ:169:PRO:HA	1.92	0.52
4:SG:58:LYS:HA	4:SG:107:ALA:HB2	1.90	0.52
7:SJ:93:LEU:HA	7:SJ:96:VAL:HG12	1.92	0.52
12:SX:69:ARG:HH21	17:CL:866:ARG:HH21	1.58	0.52
11:SW:100:GLY:HA2	11:SW:130:TYR:HB3	1.92	0.51
1:C2:406:U:H2'	1:C2:407:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SH:9:LEU:HG	5:SH:10:SER:H	1.75	0.51
7:SJ:38:ASN:HA	18:UC:565:LYS:HE3	1.92	0.51
1:C2:451:A:C5	1:C2:453:U:C2	2.99	0.51
1:C2:434:G:N7	17:CL:755:LYS:NZ	2.59	0.51
1:C2:761:G:OP1	7:SJ:54:ARG:NH2	2.43	0.51
4:SG:70:PRO:HB3	4:SG:101:ILE:HB	1.92	0.51
11:SW:15:ASN:ND2	11:SW:72:CYS:O	2.42	0.51
15:CA:173:ALA:HA	15:CA:176:ARG:HG2	1.92	0.51
16:CK:311:ILE:HG23	17:CL:1032:LEU:HD23	1.91	0.51
17:CL:71:ILE:HD12	17:CL:245:LEU:HD22	1.92	0.51
1:C2:1100:G:OP1	12:SX:3:LYS:NZ	2.43	0.51
15:CA:176:ARG:HG3	15:CA:177:LEU:HG	1.93	0.51
1:C2:154:G:OP1	4:SG:2:LYS:NZ	2.39	0.50
1:C2:340:U:H2'	1:C2:341:A:C8	2.46	0.50
1:C2:564:G:O6	1:C2:578:U:O4	2.29	0.50
3:SE:31:PRO:HA	3:SE:81:THR:HB	1.91	0.50
8:SL:125:VAL:HG12	8:SL:139:VAL:HA	1.93	0.50
17:CL:281:PRO:HG2	17:CL:286:THR:HG21	1.93	0.50
19:JL:230:VAL:HG22	19:JL:295:ALA:HB2	1.94	0.50
17:CL:287:ARG:HD3	17:CL:820:ILE:HG12	1.93	0.50
1:C2:31:C:OP1	12:SX:140:LYS:NZ	2.37	0.50
2:SB:108:ASP:OD1	2:SB:108:ASP:N	2.45	0.50
2:SB:194:ASN:HD22	2:SB:210:ILE:HG22	1.76	0.50
11:SW:81:VAL:O	11:SW:122:SER:OG	2.30	0.50
15:CA:224:ILE:HG12	15:CA:233:ILE:HG12	1.93	0.50
17:CL:241:HIS:NE2	17:CL:819:GLU:OE2	2.44	0.50
17:CL:281:PRO:HA	17:CL:782:GLY:HA3	1.94	0.50
1:C2:406:U:H2'	1:C2:407:A:H8	1.77	0.50
1:C2:688:G:H2'	1:C2:689:G:C8	2.47	0.50
1:C2:228:G:C6	1:C2:236:A:N6	2.79	0.50
1:C2:762:A:OP1	7:SJ:79:ARG:NH1	2.43	0.50
6:SI:99:ALA:CA	6:SI:169:ILE:O	2.60	0.50
17:CL:140:LEU:HD11	17:CL:152:THR:HG23	1.94	0.50
17:CL:193:ARG:NH1	17:CL:197:GLU:OE2	2.40	0.50
12:SX:97:ASP:OD1	17:CL:828:ARG:NH2	2.44	0.50
17:CL:181:SER:HA	17:CL:184:ARG:HH21	1.77	0.50
1:C2:144:U:H5	4:SG:137:ARG:HH22	1.60	0.49
1:C2:329:G:H2'	1:C2:330:G:H8	1.77	0.49
3:SE:165:ALA:HB3	3:SE:168:LYS:HZ1	1.77	0.49
4:SG:44:GLU:O	4:SG:119:GLN:NE2	2.45	0.49
6:SI:34:ALA:HB2	6:SI:56:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SO:31:THR:HG22	10:SO:38:THR:HA	1.94	0.49
1:C2:1005:A:OP2	15:CA:262:ASN:ND2	2.44	0.49
6:SI:99:ALA:HA	6:SI:169:ILE:O	2.12	0.49
19:JL:41:ASN:ND2	19:JL:195:ASN:OD1	2.44	0.49
1:C2:763:G:OP1	7:SJ:78:ARG:NH2	2.45	0.49
6:SI:36:THR:HG21	6:SI:173:PRO:HB2	1.93	0.49
7:SJ:148:VAL:HG11	7:SJ:156:ILE:HD11	1.93	0.49
17:CL:141:LEU:HA	17:CL:170:VAL:O	2.13	0.49
1:C2:877:G:H22	1:C2:951:A:H2	1.60	0.49
7:SJ:129:ILE:HG12	7:SJ:134:ILE:HG13	1.95	0.49
11:SW:31:SER:HB2	11:SW:34:ILE:HG13	1.95	0.49
1:C2:354:C:H5"	6:SI:16:ALA:HB2	1.94	0.49
1:C2:1041:G:H2'	1:C2:1042:G:C8	2.47	0.49
17:CL:859:ILE:HD11	17:CL:871:MET:HG2	1.95	0.49
1:C2:29:U:H2'	1:C2:30:G:H8	1.78	0.49
1:C2:230:C:N4	1:C2:233:C:N3	2.61	0.49
1:C2:985:G:N1	1:C2:1017:U:C2	2.81	0.49
3:SE:42:LEU:N	3:SE:84:ALA:O	2.42	0.49
16:CK:302:LYS:HA	16:CK:305:ILE:HG22	1.93	0.49
1:C2:502:U:O3'	18:UC:570:GLN:NE2	2.46	0.48
6:SI:56:ARG:NH1	6:SI:174:GLY:O	2.46	0.48
1:C2:836:U:H2'	1:C2:837:G:C8	2.48	0.48
3:SE:92:LEU:HD12	13:SY:17:LEU:HD11	1.95	0.48
3:SE:194:THR:OG1	3:SE:231:GLN:OE1	2.28	0.48
1:C2:93:A:H1'	3:SE:3:ARG:HG2	1.95	0.48
3:SE:64:ILE:HG23	13:SY:17:LEU:HD12	1.95	0.48
6:SI:57:ALA:HB2	6:SI:177:GLY:HA2	1.93	0.48
6:SI:76:THR:HG22	6:SI:108:PRO:HG2	1.94	0.48
12:SX:41:SER:OG	12:SX:44:GLY:O	2.31	0.48
1:C2:808:U:H2'	1:C2:809:A:C8	2.48	0.48
1:C2:854:U:O4	1:C2:855:A:N6	2.45	0.48
1:C2:1796:C:H42	15:CA:226:LEU:HB2	1.79	0.48
1:C2:191:C:O2'	1:C2:192:U:O4'	2.30	0.48
3:SE:79:ASP:HB3	3:SE:82:TYR:HB2	1.95	0.48
4:SG:57:ASP:HA	4:SG:106:LEU:HA	1.96	0.48
1:C2:771:A:O2'	7:SJ:6:ARG:NH2	2.38	0.48
1:C2:978:A:O2'	1:C2:1787:C:O2	2.26	0.48
1:C2:800:U:H2'	1:C2:801:G:H8	1.79	0.48
3:SE:23:LEU:HD21	7:SJ:6:ARG:HD2	1.94	0.48
1:C2:953:G:H2'	1:C2:954:G:H8	1.77	0.48
15:CA:186:GLU:HG2	15:CA:230:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:JL:153:LEU:HD12	19:JL:209:LEU:HD23	1.95	0.48
19:JL:139:PHE:HA	19:JL:142:ILE:HD12	1.95	0.48
1:C2:52:U:H2'	1:C2:53:G:H8	1.79	0.47
7:SJ:119:ALA:O	7:SJ:124:HIS:ND1	2.42	0.47
15:CA:125:LYS:HD2	15:CA:146:THR:HG23	1.95	0.47
17:CL:82:LYS:HB3	17:CL:141:LEU:HD21	1.95	0.47
1:C2:336:G:O6	6:SI:5:ARG:NH1	2.38	0.47
1:C2:564:G:N1	1:C2:578:U:N3	2.46	0.47
5:SH:11:GLN:HG3	5:SH:13:PRO:HD2	1.95	0.47
7:SJ:106:GLU:O	7:SJ:111:THR:OG1	2.31	0.47
1:C2:18:C:H2'	1:C2:19:A:H8	1.79	0.47
1:C2:1141:G:H2'	1:C2:1142:A:H8	1.79	0.47
5:SH:129:LEU:HD23	5:SH:130:VAL:HG13	1.95	0.47
17:CL:135:ALA:O	17:CL:238:ARG:NH2	2.46	0.47
2:SB:59:ASP:OD2	2:SB:59:ASP:N	2.44	0.47
17:CL:805:ASN:OD1	17:CL:1026:LYS:NZ	2.37	0.47
1:C2:482:U:H2'	1:C2:483:A:C8	2.50	0.47
1:C2:977:A:H61	1:C2:1774:G:H1'	1.79	0.47
6:SI:83:TYR:HB3	6:SI:101:ILE:HB	1.96	0.47
17:CL:39:MET:O	17:CL:43:MET:HB3	2.15	0.47
6:SI:140:GLU:HA	6:SI:143:TRP:HB2	1.97	0.47
2:SB:37:THR:HG21	2:SB:185:THR:HG23	1.97	0.47
2:SB:124:ASN:HA	2:SB:137:ILE:O	2.14	0.47
4:SG:115:LYS:NZ	4:SG:116:LYS:O	2.47	0.47
12:SX:141:GLU:OE2	17:CL:161:HIS:NE2	2.43	0.47
1:C2:55:A:H5'	13:SY:109:LYS:HE2	1.97	0.47
17:CL:293:VAL:HG13	17:CL:1022:LEU:HD21	1.97	0.47
17:CL:889:LEU:HD22	17:CL:922:ILE:HB	1.97	0.47
1:C2:435:C:H2'	17:CL:55:HIS:HE1	1.80	0.46
1:C2:632:U:O2'	1:C2:1103:U:OP1	2.30	0.46
13:SY:59:GLY:O	13:SY:71:GLY:CA	2.62	0.46
15:CA:256:PRO:HA	15:CA:259:VAL:HG22	1.97	0.46
18:UC:570:GLN:HG3	18:UC:573:GLN:HE21	1.79	0.46
1:C2:65:A:OP1	4:SG:136:LYS:NZ	2.39	0.46
3:SE:139:VAL:HG13	3:SE:150:PRO:HG3	1.97	0.46
8:SL:82:ARG:HE	8:SL:113:PRO:HG3	1.79	0.46
9:SN:87:ASP:OD1	9:SN:87:ASP:N	2.47	0.46
1:C2:1104:U:OP1	12:SX:14:LYS:NZ	2.42	0.46
7:SJ:59:LEU:HD22	7:SJ:69:ARG:HA	1.97	0.46
9:SN:138:ASN:OD1	9:SN:139:TRP:N	2.39	0.46
1:C2:343:C:H2'	1:C2:344:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:985:G:N1	1:C2:1017:U:N3	2.64	0.46
2:SB:135:LEU:HD23	2:SB:217:LEU:HA	1.96	0.46
1:C2:65:A:H2	1:C2:84:A:H62	1.62	0.46
1:C2:429:G:O2'	17:CL:225:ARG:NH2	2.48	0.46
1:C2:961:U:H2'	1:C2:962:C:C6	2.51	0.46
17:CL:157:ASN:O	17:CL:161:HIS:ND1	2.48	0.46
18:UC:541:ASN:HB3	18:UC:544:ILE:HG12	1.96	0.46
7:SJ:65:LYS:HA	7:SJ:65:LYS:HD3	1.74	0.46
1:C2:311:U:H4'	17:CL:29:LYS:HB3	1.98	0.46
1:C2:538:A:H5'	1:C2:543:C:H41	1.81	0.46
1:C2:947:U:H2'	1:C2:948:G:H8	1.80	0.46
17:CL:260:THR:OG1	17:CL:261:GLN:OE1	2.25	0.46
4:SG:32:ILE:HG12	4:SG:100:ALA:HB1	1.97	0.46
17:CL:126:ASN:OD1	17:CL:853:ARG:NH1	2.49	0.46
1:C2:984:G:C6	1:C2:1018:U:N3	2.84	0.46
13:SY:43:LYS:HA	13:SY:46:GLU:HG3	1.97	0.46
19:JL:133:ILE:HB	19:JL:137:LEU:HD23	1.97	0.46
1:C2:805:U:O4	5:SH:104:ARG:NH2	2.49	0.45
10:SO:40:ALA:HB2	10:SO:70:LYS:HG2	1.97	0.45
16:CK:329:GLU:HA	17:CL:933:LYS:HG3	1.98	0.45
17:CL:104:PRO:HA	17:CL:117:PHE:O	2.15	0.45
17:CL:757:LYS:HA	17:CL:760:LYS:HG2	1.98	0.45
1:C2:619:A:HO2'	1:C2:1141:G:HO2'	1.64	0.45
1:C2:936:G:OP1	1:C2:1074:G:N2	2.40	0.45
10:SO:52:ARG:HA	10:SO:52:ARG:HD3	1.80	0.45
17:CL:220:ILE:HD13	17:CL:223:LEU:HD12	1.99	0.45
2:SB:24:PHE:HE2	10:SO:70:LYS:HE3	1.82	0.45
11:SW:72:CYS:HB3	11:SW:129:VAL:HG23	1.98	0.45
3:SE:44:LEU:HG	3:SE:82:TYR:HB3	1.98	0.45
2:SB:64:ARG:HG2	10:SO:36:LYS:HG3	1.99	0.45
6:SI:82:VAL:HG21	6:SI:166:TYR:HE1	1.81	0.45
17:CL:90:VAL:O	17:CL:94:THR:OG1	2.27	0.45
17:CL:249:PHE:HZ	17:CL:801:VAL:HG22	1.80	0.45
19:JL:75:LEU:HD11	19:JL:107:LEU:HB2	1.98	0.45
1:C2:304:U:O2	8:SL:69:LYS:NZ	2.35	0.45
1:C2:800:U:H2'	1:C2:801:G:C8	2.52	0.45
1:C2:29:U:H2'	1:C2:30:G:C8	2.52	0.45
1:C2:325:G:H2'	1:C2:326:G:H8	1.80	0.45
1:C2:329:G:H5"	6:SI:98:LYS:HB3	1.99	0.45
5:SH:22:GLN:HA	5:SH:25:VAL:HG22	1.99	0.45
10:SO:24:ASN:HA	10:SO:55:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:CL:774:PRO:HA	17:CL:777:ARG:HD3	1.97	0.45
1:C2:997:G:H2'	1:C2:998:A:C8	2.52	0.45
6:SI:137:LYS:HE2	6:SI:141:ARG:HH12	1.80	0.45
12:SX:77:ILE:HB	17:CL:54:LEU:HD23	1.97	0.45
15:CA:193:LEU:HD22	15:CA:201:ALA:HB2	1.98	0.45
15:CA:263:LEU:HA	15:CA:266:VAL:HG12	1.99	0.45
1:C2:235:G:H2'	1:C2:236:A:H8	1.82	0.45
1:C2:939:A:H2'	1:C2:940:A:C8	2.52	0.45
1:C2:1087:A:H2'	1:C2:1088:A:C8	2.52	0.45
17:CL:69:PRO:HD3	17:CL:114:ARG:HH21	1.82	0.45
1:C2:923:A:H2'	1:C2:924:A:C8	2.52	0.45
6:SI:49:ARG:O	6:SI:52:ASN:ND2	2.50	0.45
17:CL:92:ARG:HH21	17:CL:221:LEU:HD13	1.81	0.45
1:C2:1057:U:C4	1:C2:1061:A:N1	2.85	0.44
9:SN:46:THR:HG22	9:SN:49:GLN:HE22	1.82	0.44
1:C2:973:A:H2'	1:C2:974:A:H8	1.82	0.44
9:SN:91:LEU:HB3	9:SN:122:ILE:HG12	1.98	0.44
12:SX:53:VAL:HA	12:SX:74:VAL:HG22	2.00	0.44
9:SN:55:ARG:NH1	9:SN:56:ASP:OD1	2.51	0.44
19:JL:137:LEU:HA	19:JL:140:LYS:HB2	2.00	0.44
1:C2:332:U:OP1	6:SI:31:ARG:NH1	2.42	0.44
1:C2:189:C:N3	1:C2:197:A:C6	2.85	0.44
1:C2:513:U:H2'	1:C2:514:G:C8	2.52	0.44
2:SB:36:SER:OG	2:SB:234:GLU:OE1	2.36	0.44
3:SE:125:LYS:HA	3:SE:158:ASP:O	2.18	0.44
9:SN:136:PRO:HG2	9:SN:139:TRP:HD1	1.82	0.44
15:CA:182:ILE:HG13	15:CA:234:LEU:HD13	1.99	0.44
1:C2:250:C:H2'	1:C2:251:A:H8	1.82	0.44
1:C2:329:G:H2'	1:C2:330:G:C8	2.53	0.44
1:C2:637:C:O2	5:SH:114:ARG:NH2	2.40	0.44
7:SJ:85:VAL:HG13	7:SJ:103:ASP:HB3	1.99	0.44
7:SJ:171:ARG:HH21	7:SJ:175:ARG:HH22	1.65	0.44
1:C2:922:G:H2'	1:C2:923:A:C8	2.53	0.44
17:CL:966:ILE:HG22	17:CL:1003:LEU:HB2	1.99	0.44
4:SG:126:ASP:OD1	4:SG:126:ASP:N	2.50	0.44
5:SH:30:SER:N	5:SH:31:SER:HA	2.33	0.44
12:SX:141:GLU:OE1	17:CL:832:HIS:NE2	2.51	0.44
1:C2:17:C:H2'	1:C2:18:C:H6	1.82	0.44
1:C2:108:A:H2'	1:C2:109:G:C8	2.53	0.44
1:C2:332:U:P	6:SI:56:ARG:HH22	2.41	0.44
1:C2:1068:C:H2'	1:C2:1069:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SG:120:GLU:OE2	4:SG:125:THR:OG1	2.34	0.44
5:SH:13:PRO:HA	5:SH:14:THR:HA	1.74	0.44
13:SY:6:THR:O	13:SY:27:VAL:HA	2.17	0.44
17:CL:839:LEU:HD21	17:CL:914:ALA:HB1	1.99	0.43
1:C2:176:C:O2'	1:C2:177:U:O4'	2.31	0.43
1:C2:230:C:H2'	1:C2:231:U:H6	1.83	0.43
1:C2:405:C:O2'	4:SG:92:ARG:O	2.32	0.43
13:SY:58:PHE:HB3	13:SY:90:ARG:HD3	2.00	0.43
17:CL:236:LYS:HE3	17:CL:236:LYS:HB3	1.88	0.43
1:C2:138:A:H62	1:C2:266:A:H61	1.66	0.43
1:C2:1085:G:N2	1:C2:1088:A:OP2	2.37	0.43
3:SE:26:CYS:HB3	7:SJ:3:ARG:HG3	1.99	0.43
5:SH:64:VAL:HG23	5:SH:67:LEU:HD23	2.00	0.43
8:SL:28:SER:O	8:SL:30:ARG:NH2	2.45	0.43
15:CA:124:LEU:HG	15:CA:126:LEU:HD23	2.00	0.43
15:CA:205:ILE:HD11	15:CA:251:ILE:HG13	2.00	0.43
1:C2:557:G:N1	1:C2:588:U:C2	2.87	0.43
1:C2:866:G:H2'	1:C2:867:G:C8	2.53	0.43
1:C2:913:G:OP1	1:C2:913:G:N2	2.50	0.43
1:C2:984:G:N1	1:C2:1018:U:C2	2.86	0.43
1:C2:20:G:H2'	1:C2:21:U:C6	2.54	0.43
1:C2:590:C:H2'	1:C2:591:A:H8	1.83	0.43
2:SB:124:ASN:HD22	2:SB:124:ASN:C	2.19	0.43
2:SB:164:ILE:HD13	2:SB:207:LEU:HD21	2.00	0.43
4:SG:149:LYS:HB3	4:SG:149:LYS:HE3	1.89	0.43
17:CL:978:ARG:HB2	17:CL:988:ARG:HH11	1.84	0.43
19:JL:51:LYS:HA	19:JL:51:LYS:HD2	1.80	0.43
1:C2:1773:C:H2'	1:C2:1774:G:C8	2.54	0.43
2:SB:48:VAL:HG21	2:SB:61:LEU:HD11	2.01	0.43
7:SJ:29:LYS:HD2	18:UC:569:TYR:HE1	1.83	0.43
17:CL:303:LYS:HG3	17:CL:787:SER:HB3	2.01	0.43
17:CL:870:ARG:HH22	17:CL:931:LYS:H	1.64	0.43
1:C2:871:G:H2'	1:C2:872:G:C8	2.54	0.43
7:SJ:97:LEU:HD23	7:SJ:97:LEU:HA	1.90	0.43
13:SY:12:VAL:HG22	13:SY:23:PHE:HB3	2.01	0.43
13:SY:57:VAL:HG12	13:SY:73:GLY:HA3	1.99	0.43
1:C2:52:U:H2'	1:C2:53:G:C8	2.54	0.43
1:C2:555:A:H2'	1:C2:556:A:C8	2.54	0.43
1:C2:884:A:H2'	1:C2:885:G:C8	2.53	0.43
1:C2:906:A:OP2	10:SO:52:ARG:NE	2.42	0.43
1:C2:298:C:H5"	3:SE:38:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:1037:C:O2	11:SW:16:ASN:ND2	2.52	0.43
13:SY:78:SER:O	13:SY:80:ALA:N	2.51	0.43
2:SB:128:LYS:HB2	2:SB:134:VAL:HG22	2.01	0.42
4:SG:75:LEU:HD23	4:SG:75:LEU:HA	1.92	0.42
17:CL:772:MET:SD	17:CL:776:GLN:HB3	2.59	0.42
17:CL:906:ASP:OD1	17:CL:906:ASP:N	2.46	0.42
1:C2:563:U:H2'	1:C2:564:G:H8	1.84	0.42
1:C2:592:A:OP1	7:SJ:39:LYS:NZ	2.42	0.42
1:C2:891:A:H2'	1:C2:892:A:H8	1.84	0.42
4:SG:52:ILE:HD11	4:SG:102:VAL:HG21	2.02	0.42
17:CL:306:ASP:N	17:CL:306:ASP:OD1	2.50	0.42
17:CL:819:GLU:O	17:CL:852:ARG:NH2	2.51	0.42
1:C2:813:U:O2'	1:C2:815:G:OP1	2.36	0.42
1:C2:985:G:C2	1:C2:1017:U:C2	3.07	0.42
8:SL:116:ARG:HA	8:SL:116:ARG:NH1	2.34	0.42
15:CA:250:LEU:HD12	15:CA:259:VAL:HG21	2.00	0.42
17:CL:933:LYS:HA	17:CL:1003:LEU:O	2.19	0.42
19:JL:252:GLU:HB2	19:JL:274:HIS:HB3	2.01	0.42
1:C2:209:U:H5'	6:SI:171:SER:HB2	2.01	0.42
1:C2:428:A:N3	1:C2:440:U:O2'	2.45	0.42
1:C2:898:A:H62	1:C2:914:G:N2	2.16	0.42
1:C2:1132:A:H2'	1:C2:1133:A:C8	2.52	0.42
4:SG:19:ASP:OD1	4:SG:19:ASP:N	2.52	0.42
17:CL:847:LEU:HA	17:CL:898:GLY:HA2	2.02	0.42
1:C2:41:A:H2'	1:C2:438:A:H62	1.84	0.42
1:C2:388:G:OP2	1:C2:423:G:O2'	2.37	0.42
1:C2:642:G:N1	1:C2:693:U:C2	2.88	0.42
1:C2:916:U:H3	10:SO:41:ARG:HH12	1.67	0.42
1:C2:922:G:H2'	1:C2:923:A:H8	1.85	0.42
1:C2:968:U:OP1	1:C2:1033:C:O2'	2.37	0.42
1:C2:993:A:H62	1:C2:1011:G:N2	2.14	0.42
5:SH:25:VAL:HA	5:SH:28:GLU:HB2	2.02	0.42
10:SO:49:LYS:HE3	10:SO:49:LYS:HB3	1.83	0.42
1:C2:393:C:H2'	1:C2:394:C:C6	2.54	0.42
1:C2:950:C:H2'	1:C2:951:A:C8	2.55	0.42
1:C2:1142:A:C6	1:C2:1143:A:N6	2.88	0.42
6:SI:43:ILE:HG12	6:SI:57:ALA:HA	2.01	0.42
11:SW:24:GLN:HE21	11:SW:64:GLN:HG3	1.83	0.42
1:C2:549:G:H2'	1:C2:550:A:C8	2.54	0.42
4:SG:39:GLU:HA	4:SG:46:LYS:HZ1	1.85	0.42
1:C2:97:C:H1'	1:C2:426:G:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:195:G:H2'	1:C2:196:G:C8	2.55	0.42
1:C2:247:A:O2'	8:SL:37:ASN:O	2.33	0.42
1:C2:327:U:H2'	1:C2:328:A:C8	2.55	0.42
1:C2:886:U:O2'	10:SO:121:VAL:O	2.28	0.42
2:SB:131:ASP:OD1	2:SB:131:ASP:N	2.44	0.42
3:SE:211:LYS:HB2	3:SE:217:THR:HG22	2.01	0.42
13:SY:39:GLU:HG2	13:SY:43:LYS:HE2	2.02	0.42
13:SY:43:LYS:O	13:SY:47:VAL:HG23	2.20	0.42
17:CL:1010:ARG:HD2	17:CL:1010:ARG:HA	1.84	0.42
1:C2:833:U:H5'	1:C2:834:G:H5"	2.02	0.42
17:CL:105:ILE:HG13	17:CL:356:ALA:HB2	2.02	0.42
17:CL:248:ARG:HG2	17:CL:272:TYR:HB2	2.02	0.42
17:CL:820:ILE:HD12	17:CL:820:ILE:HA	1.87	0.42
1:C2:151:G:H22	1:C2:163:G:H1	1.68	0.41
1:C2:642:G:C2	1:C2:693:U:O2	2.72	0.41
1:C2:1045:C:H2'	1:C2:1046:G:H8	1.85	0.41
3:SE:206:ASP:HB2	3:SE:222:LEU:HD22	2.01	0.41
6:SI:171:SER:HB3	6:SI:180:ASP:H	1.84	0.41
15:CA:233:ILE:HG22	15:CA:240:ILE:HG22	2.01	0.41
19:JL:40:LYS:HD3	19:JL:197:ARG:HB2	2.02	0.41
1:C2:340:U:H2'	1:C2:341:A:H8	1.85	0.41
8:SL:55:ASP:OD1	8:SL:82:ARG:HD3	2.19	0.41
11:SW:48:GLY:CA	11:SW:64:GLN:O	2.68	0.41
17:CL:968:THR:HG22	17:CL:1001:VAL:HG12	2.02	0.41
1:C2:873:U:H3	1:C2:954:G:H1	1.68	0.41
5:SH:163:ASP:N	5:SH:163:ASP:OD1	2.52	0.41
1:C2:119:A:H1'	1:C2:397:A:C5	2.55	0.41
5:SH:133:THR:HG21	5:SH:159:VAL:HA	2.01	0.41
1:C2:140:A:H1'	4:SG:179:VAL:HG11	2.03	0.41
1:C2:556:A:HO2'	1:C2:589:C:HO2'	1.66	0.41
2:SB:103:MET:HB3	2:SB:215:VAL:HG22	2.03	0.41
1:C2:862:A:OP2	9:SN:64:ARG:NH1	2.53	0.41
1:C2:1773:C:H2'	1:C2:1774:G:H8	1.85	0.41
3:SE:252:ARG:O	3:SE:256:ARG:HG3	2.20	0.41
13:SY:45:ALA:HA	13:SY:50:ALA:HB3	2.02	0.41
5:SH:14:THR:OG1	5:SH:15:GLU:N	2.52	0.41
1:C2:400:A:H5"	6:SI:25:ARG:HA	2.03	0.41
1:C2:34:G:O2'	1:C2:515:A:O2'	2.36	0.41
1:C2:97:C:O2	1:C2:425:A:O2'	2.34	0.41
1:C2:205:U:O2	1:C2:263:C:N3	2.53	0.41
1:C2:482:U:H2'	1:C2:483:A:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:486:G:N2	1:C2:501:U:O2	2.37	0.41
1:C2:598:U:H2'	1:C2:599:A:C8	2.56	0.41
1:C2:976:G:N1	1:C2:1023:A:O2'	2.37	0.41
15:CA:201:ALA:O	15:CA:205:ILE:HG12	2.21	0.41
19:JL:277:VAL:O	19:JL:280:LYS:HB3	2.21	0.41
1:C2:448:C:H5'	3:SE:29:PRO:HA	2.03	0.41
1:C2:471:A:H5"	7:SJ:10:LYS:HG2	2.03	0.41
6:SI:48:THR:HG21	6:SI:54:LYS:HD2	2.03	0.41
7:SJ:66:ASP:HB3	7:SJ:69:ARG:HB3	2.02	0.41
17:CL:140:LEU:HD21	17:CL:152:THR:HG23	2.03	0.41
17:CL:853:ARG:NH1	17:CL:1018:VAL:HG21	2.36	0.41
1:C2:472:U:O2'	1:C2:769:A:N3	2.50	0.40
1:C2:1057:U:N3	1:C2:1061:A:C6	2.89	0.40
3:SE:128:LYS:HG2	3:SE:140:VAL:HG12	2.03	0.40
7:SJ:60:LEU:HD23	7:SJ:60:LEU:HA	1.84	0.40
12:SX:51:GLY:HA2	12:SX:77:ILE:HG13	2.02	0.40
13:SY:11:LYS:HB2	13:SY:24:VAL:HG12	2.03	0.40
15:CA:136:SER:OG	15:CA:137:VAL:N	2.55	0.40
1:C2:788:A:OP2	3:SE:108:ARG:NH2	2.40	0.40
2:SB:179:SER:HB2	2:SB:183:GLN:HE21	1.86	0.40
3:SE:71:LYS:HG2	3:SE:76:VAL:HG22	2.02	0.40
17:CL:764:ILE:HA	17:CL:767:ILE:HG22	2.04	0.40
1:C2:521:A:N3	13:SY:34:ASN:ND2	2.69	0.40
5:SH:49:ILE:HD12	5:SH:175:LYS:HG2	2.03	0.40
6:SI:10:LYS:HB3	6:SI:10:LYS:HE3	1.85	0.40
7:SJ:25:ASP:HA	7:SJ:28:LEU:HB3	2.03	0.40
1:C2:947:U:H2'	1:C2:948:G:C8	2.56	0.40
1:C2:1036:A:H2'	1:C2:1037:C:C6	2.57	0.40
2:SB:32:ILE:HG13	2:SB:43:VAL:HB	2.04	0.40
3:SE:166:SER:OG	3:SE:168:LYS:NZ	2.48	0.40
10:SO:92:LYS:HD3	10:SO:121:VAL:HA	2.04	0.40
12:SX:77:ILE:HG22	17:CL:751:TYR:HB2	2.03	0.40
17:CL:872:LEU:HD23	17:CL:872:LEU:HA	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SB	214/255 (84%)	199 (93%)	15 (7%)	0	100	100
3	SE	258/261 (99%)	239 (93%)	19 (7%)	0	100	100
4	SG	216/236 (92%)	204 (94%)	12 (6%)	0	100	100
5	SH	183/190 (96%)	163 (89%)	20 (11%)	0	100	100
6	SI	184/200 (92%)	179 (97%)	5 (3%)	0	100	100
7	SJ	183/197 (93%)	167 (91%)	16 (9%)	0	100	100
8	SL	144/156 (92%)	130 (90%)	14 (10%)	0	100	100
9	SN	148/151 (98%)	138 (93%)	10 (7%)	0	100	100
10	SO	126/137 (92%)	112 (89%)	14 (11%)	0	100	100
11	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
12	SX	115/145 (79%)	108 (94%)	7 (6%)	0	100	100
13	SY	132/135 (98%)	118 (89%)	12 (9%)	2 (2%)	10	38
14	Sb	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
15	CA	179/274 (65%)	174 (97%)	5 (3%)	0	100	100
16	CK	34/593 (6%)	33 (97%)	1 (3%)	0	100	100
17	CL	604/1183 (51%)	581 (96%)	23 (4%)	0	100	100
18	UC	45/610 (7%)	43 (96%)	2 (4%)	0	100	100
19	JL	281/318 (88%)	271 (96%)	10 (4%)	0	100	100
All	All	3252/5253 (62%)	3048 (94%)	202 (6%)	2 (0%)	54	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	SY	32	ARG
13	SY	79	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	SB	192/224 (86%)	190 (99%)	2 (1%)	76 86
3	SE	221/222 (100%)	221 (100%)	0	100 100
4	SG	187/201 (93%)	186 (100%)	1 (0%)	88 93
5	SH	165/170 (97%)	164 (99%)	1 (1%)	86 91
6	SI	150/161 (93%)	150 (100%)	0	100 100
7	SJ	158/166 (95%)	157 (99%)	1 (1%)	86 91
8	SL	129/137 (94%)	128 (99%)	1 (1%)	81 89
9	SN	127/128 (99%)	127 (100%)	0	100 100
10	SO	97/105 (92%)	96 (99%)	1 (1%)	76 86
11	SW	110/111 (99%)	110 (100%)	0	100 100
12	SX	103/120 (86%)	103 (100%)	0	100 100
13	SY	112/113 (99%)	112 (100%)	0	100 100
14	Sb	70/71 (99%)	70 (100%)	0	100 100
15	CA	158/238 (66%)	158 (100%)	0	100 100
16	CK	33/535 (6%)	31 (94%)	2 (6%)	18 48
17	CL	534/1039 (51%)	531 (99%)	3 (1%)	86 91
18	UC	42/538 (8%)	42 (100%)	0	100 100
19	JL	255/283 (90%)	255 (100%)	0	100 100
All	All	2843/4562 (62%)	2831 (100%)	12 (0%)	91 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	124	ASN
2	SB	222	LYS
4	SG	98	ARG
5	SH	7	LYS
7	SJ	171	ARG
8	SL	67	ARG

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Mol	Chain	Res	Type
10	SO	90	ARG
16	CK	302	LYS
16	CK	309	LYS
17	CL	92	ARG
17	CL	943	LYS
17	CL	973	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	149	GLN
2	SB	183	GLN
2	SB	194	ASN
7	SJ	123	HIS
11	SW	24	GLN
18	UC	573	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C2	1095/1800 (60%)	250 (22%)	12 (1%)

All (250) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C2	2	A
1	C2	3	U
1	C2	9	U
1	C2	12	U
1	C2	24	U
1	C2	25	C
1	C2	27	U
1	C2	34	G
1	C2	39	A
1	C2	40	A
1	C2	42	G
1	C2	43	A
1	C2	45	U
1	C2	46	A
1	C2	47	A

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Mol	Chain	Res	Type
1	C2	57	G
1	C2	60	U
1	C2	67	A
1	C2	68	A
1	C2	71	A
1	C2	77	U
1	C2	103	A
1	C2	104	A
1	C2	111	U
1	C2	114	C
1	C2	126	A
1	C2	127	G
1	C2	132	U
1	C2	137	U
1	C2	140	A
1	C2	141	U
1	C2	145	A
1	C2	146	U
1	C2	153	G
1	C2	158	U
1	C2	161	U
1	C2	166	C
1	C2	176	C
1	C2	177	U
1	C2	178	U
1	C2	185	U
1	C2	189	C
1	C2	192	U
1	C2	193	U
1	C2	195	G
1	C2	196	G
1	C2	197	A
1	C2	200	A
1	C2	215	A
1	C2	216	U
1	C2	217	A
1	C2	218	A
1	C2	220	A
1	C2	223	U
1	C2	227	U
1	C2	229	U
1	C2	230	C

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Mol	Chain	Res	Type
1	C2	233	C
1	C2	235	G
1	C2	240	U
1	C2	241	U
1	C2	257	A
1	C2	261	U
1	C2	262	U
1	C2	265	A
1	C2	273	G
1	C2	276	C
1	C2	277	U
1	C2	278	U
1	C2	280	U
1	C2	281	G
1	C2	287	G
1	C2	299	A
1	C2	309	C
1	C2	314	C
1	C2	316	A
1	C2	320	U
1	C2	321	C
1	C2	322	G
1	C2	333	A
1	C2	337	G
1	C2	338	C
1	C2	352	A
1	C2	359	A
1	C2	360	A
1	C2	361	C
1	C2	369	A
1	C2	400	A
1	C2	402	C
1	C2	404	G
1	C2	417	A
1	C2	418	G
1	C2	423	G
1	C2	424	C
1	C2	426	G
1	C2	433	C
1	C2	434	G
1	C2	435	C
1	C2	439	U

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Mol	Chain	Res	Type
1	C2	444	C
1	C2	448	C
1	C2	452	A
1	C2	454	U
1	C2	460	A
1	C2	469	C
1	C2	477	A
1	C2	484	C
1	C2	488	G
1	C2	501	U
1	C2	506	A
1	C2	507	U
1	C2	510	G
1	C2	511	A
1	C2	515	A
1	C2	519	C
1	C2	527	A
1	C2	538	A
1	C2	539	G
1	C2	541	A
1	C2	542	A
1	C2	543	C
1	C2	545	A
1	C2	548	G
1	C2	554	C
1	C2	556	A
1	C2	557	G
1	C2	559	C
1	C2	568	G
1	C2	569	C
1	C2	574	G
1	C2	579	A
1	C2	580	A
1	C2	581	U
1	C2	582	U
1	C2	583	C
1	C2	585	A
1	C2	594	A
1	C2	595	G
1	C2	611	U
1	C2	620	A
1	C2	623	A

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Mol	Chain	Res	Type
1	C2	624	G
1	C2	635	A
1	C2	639	U
1	C2	645	C
1	C2	650	U
1	C2	685	A
1	C2	690	G
1	C2	691	C
1	C2	696	C
1	C2	699	U
1	C2	700	C
1	C2	701	U
1	C2	705	U
1	C2	734	A
1	C2	735	C
1	C2	738	G
1	C2	742	U
1	C2	743	U
1	C2	745	U
1	C2	753	A
1	C2	754	A
1	C2	755	A
1	C2	756	A
1	C2	765	G
1	C2	766	U
1	C2	771	A
1	C2	774	A
1	C2	775	G
1	C2	779	U
1	C2	781	U
1	C2	782	U
1	C2	783	G
1	C2	787	G
1	C2	794	U
1	C2	811	A
1	C2	812	A
1	C2	818	C
1	C2	820	U
1	C2	821	U
1	C2	823	G
1	C2	826	U
1	C2	829	A

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Mol	Chain	Res	Type
1	C2	830	U
1	C2	831	U
1	C2	833	U
1	C2	835	U
1	C2	850	A
1	C2	852	C
1	C2	853	G
1	C2	854	U
1	C2	863	A
1	C2	873	U
1	C2	876	G
1	C2	886	U
1	C2	898	A
1	C2	913	G
1	C2	914	G
1	C2	933	A
1	C2	935	U
1	C2	942	G
1	C2	944	A
1	C2	945	U
1	C2	959	U
1	C2	960	U
1	C2	966	A
1	C2	969	C
1	C2	992	A
1	C2	998	A
1	C2	1000	C
1	C2	1001	A
1	C2	1002	G
1	C2	1003	A
1	C2	1006	C
1	C2	1007	C
1	C2	1021	C
1	C2	1025	A
1	C2	1026	A
1	C2	1028	C
1	C2	1031	U
1	C2	1039	A
1	C2	1040	G
1	C2	1052	U
1	C2	1053	G
1	C2	1057	U

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Mol	Chain	Res	Type
1	C2	1058	U
1	C2	1059	U
1	C2	1060	U
1	C2	1061	A
1	C2	1076	A
1	C2	1082	C
1	C2	1092	A
1	C2	1096	C
1	C2	1097	U
1	C2	1098	U
1	C2	1100	G
1	C2	1109	G
1	C2	1113	A
1	C2	1126	G
1	C2	1137	A
1	C2	1139	A
1	C2	1143	A
1	C2	1769	U
1	C2	1770	U
1	C2	1772	C
1	C2	1780	G
1	C2	1781	A
1	C2	1782	A
1	C2	1792	G
1	C2	1793	G

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C2	42	G
1	C2	136	C
1	C2	139	C
1	C2	261	U
1	C2	272	U
1	C2	417	A
1	C2	555	A
1	C2	817	A
1	C2	997	G
1	C2	1051	G
1	C2	1097	U
1	C2	1781	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	GTP	CL	2001	22	26,34,34	1.12	2 (7%)	32,54,54	1.52	7 (21%)

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
21	GTP	CL	2001	22	-	7/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	CL	2001	GTP	C5-C6	-3.99	1.39	1.47
21	CL	2001	GTP	C2-N3	2.21	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	CL	2001	GTP	PB-O3B-PG	-3.66	120.26	132.83
21	CL	2001	GTP	C5-C6-N1	3.22	119.63	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	CL	2001	GTP	C8-N7-C5	3.02	108.74	102.99
21	CL	2001	GTP	C3'-C2'-C1'	2.89	105.33	100.98
21	CL	2001	GTP	C2-N1-C6	-2.81	119.92	125.10
21	CL	2001	GTP	O6-C6-C5	-2.16	120.16	124.37
21	CL	2001	GTP	PA-O3A-PB	-2.01	125.93	132.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

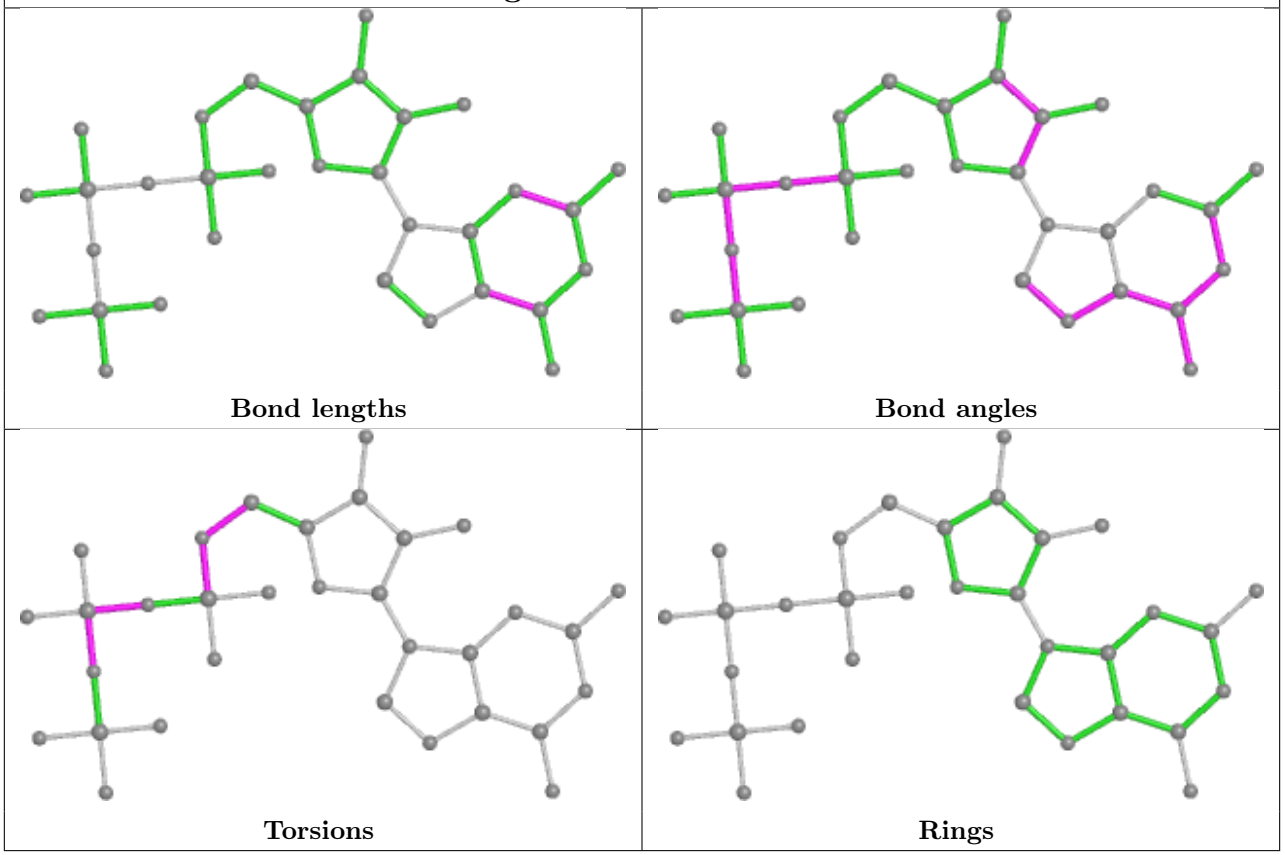
Mol	Chain	Res	Type	Atoms
21	CL	2001	GTP	C5'-O5'-PA-O3A
21	CL	2001	GTP	C5'-O5'-PA-O1A
21	CL	2001	GTP	C4'-C5'-O5'-PA
21	CL	2001	GTP	PG-O3B-PB-O1B
21	CL	2001	GTP	PG-O3B-PB-O2B
21	CL	2001	GTP	PA-O3A-PB-O2B
21	CL	2001	GTP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand GTP CL 2001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

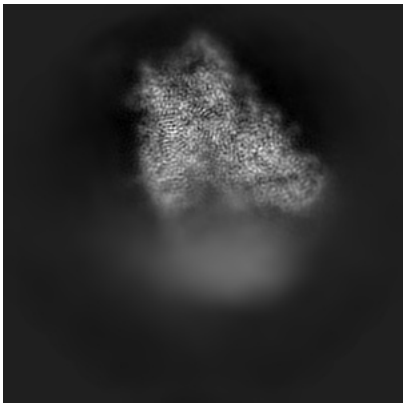
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32790. These allow visual inspection of the internal detail of the map and identification of artifacts.

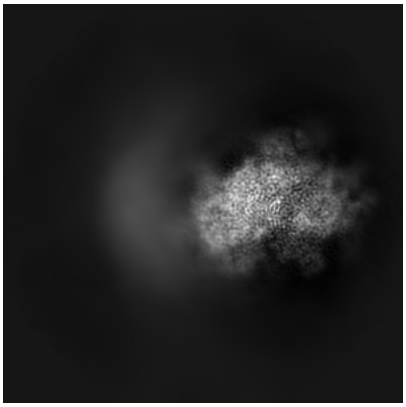
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

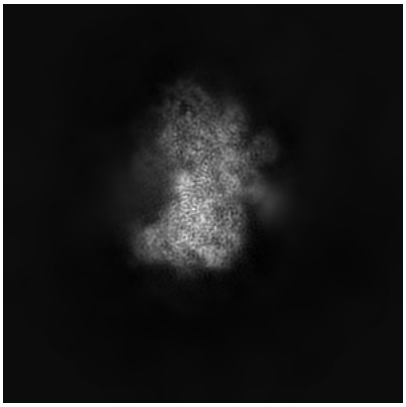
6.1.1 Primary map



X



Y

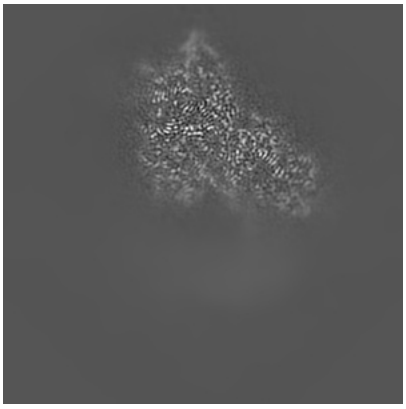


Z

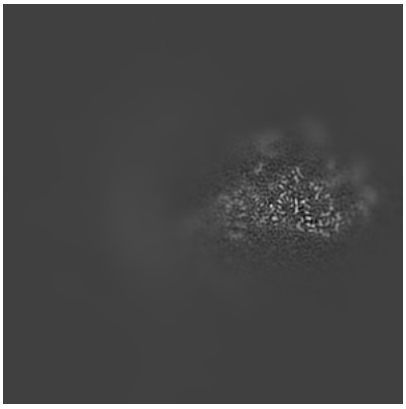
The images above show the map projected in three orthogonal directions.

6.2 Central slices

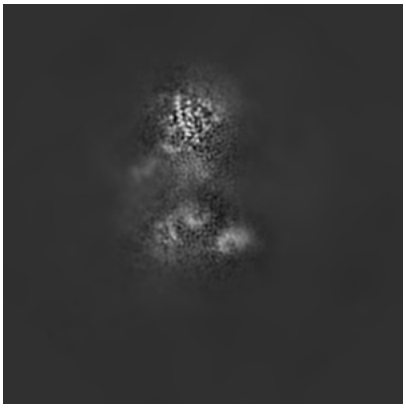
6.2.1 Primary map



X Index: 180



Y Index: 180

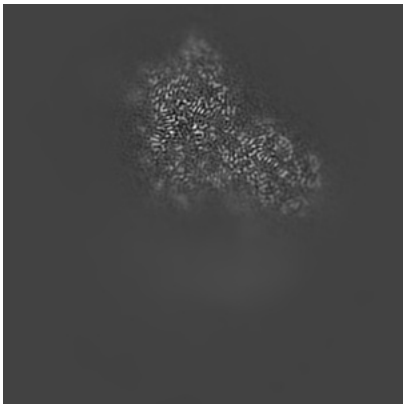


Z Index: 180

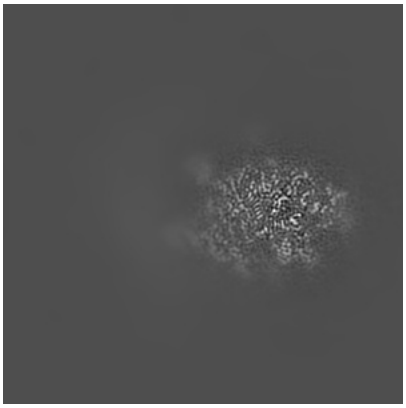
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

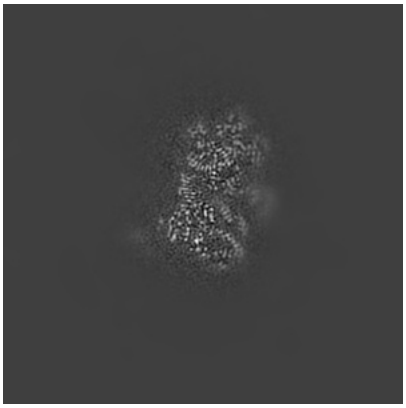
6.3.1 Primary map



X Index: 176



Y Index: 155

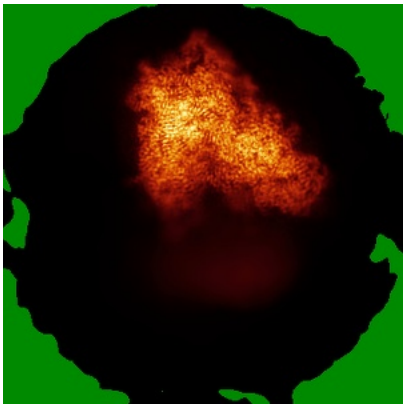


Z Index: 240

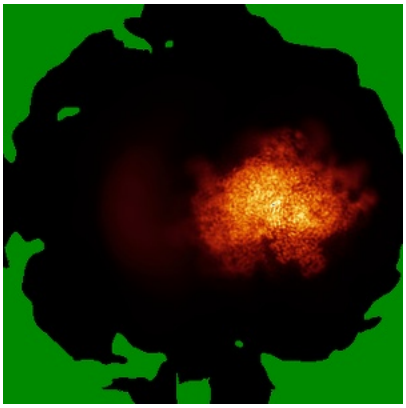
The images above show the largest variance slices of the map in three orthogonal directions.

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

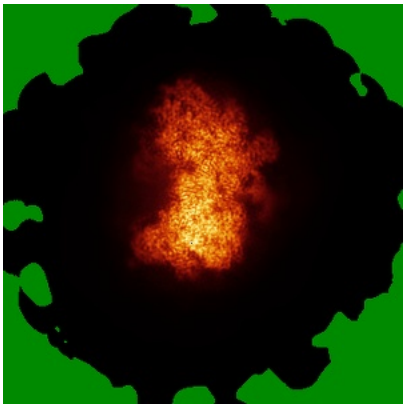
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

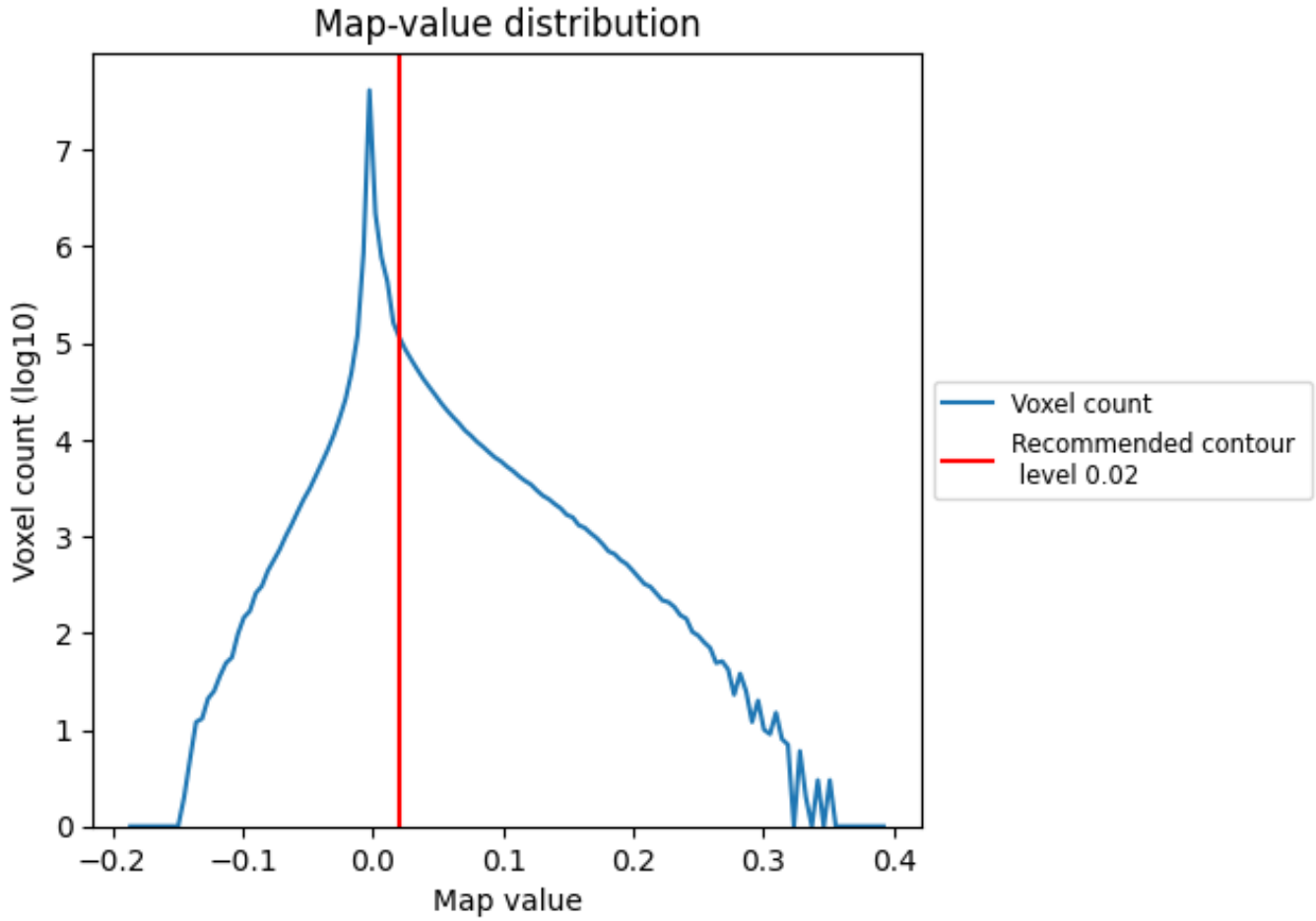
6.6 Mask visualisation (i)

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

7 Map analysis

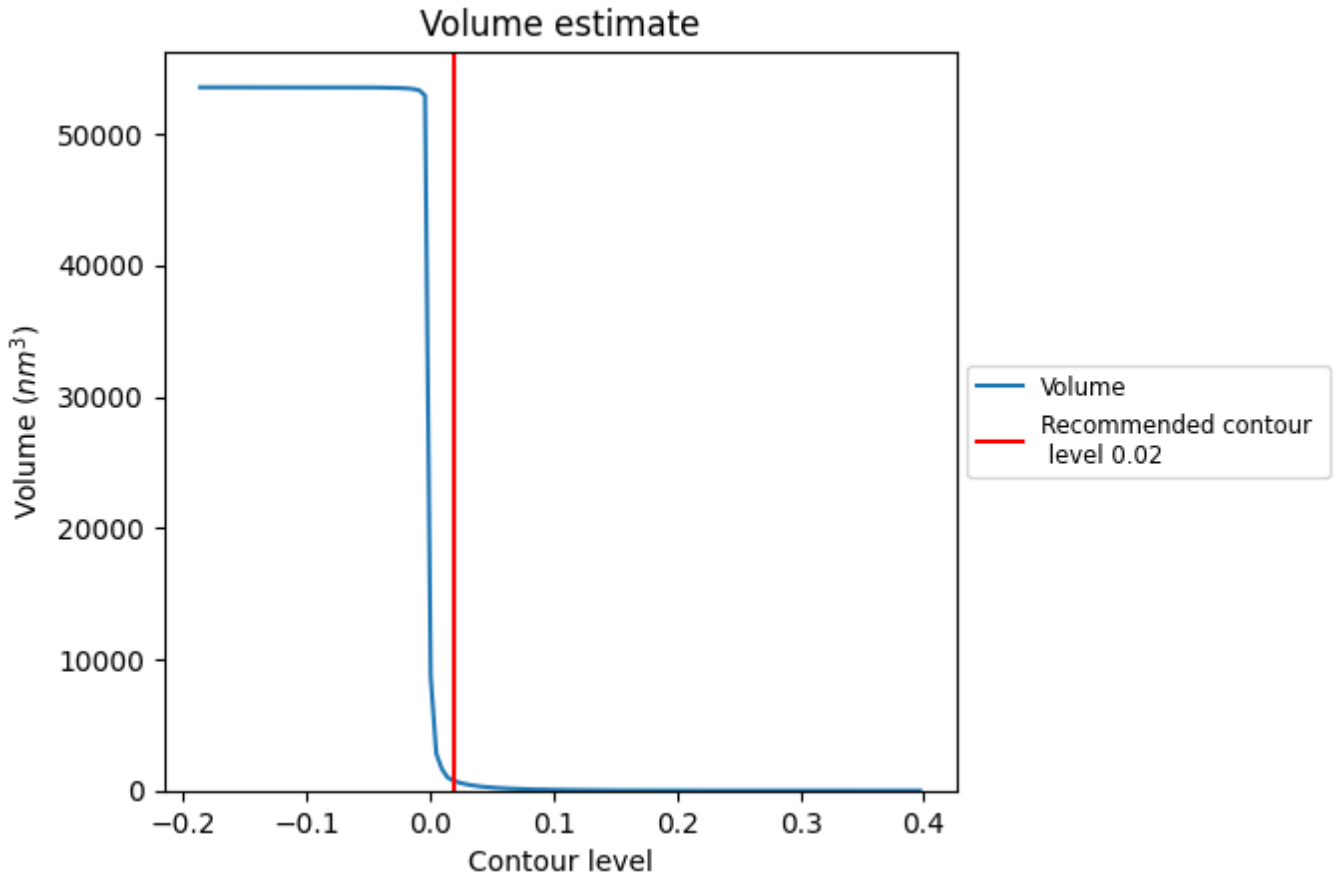
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

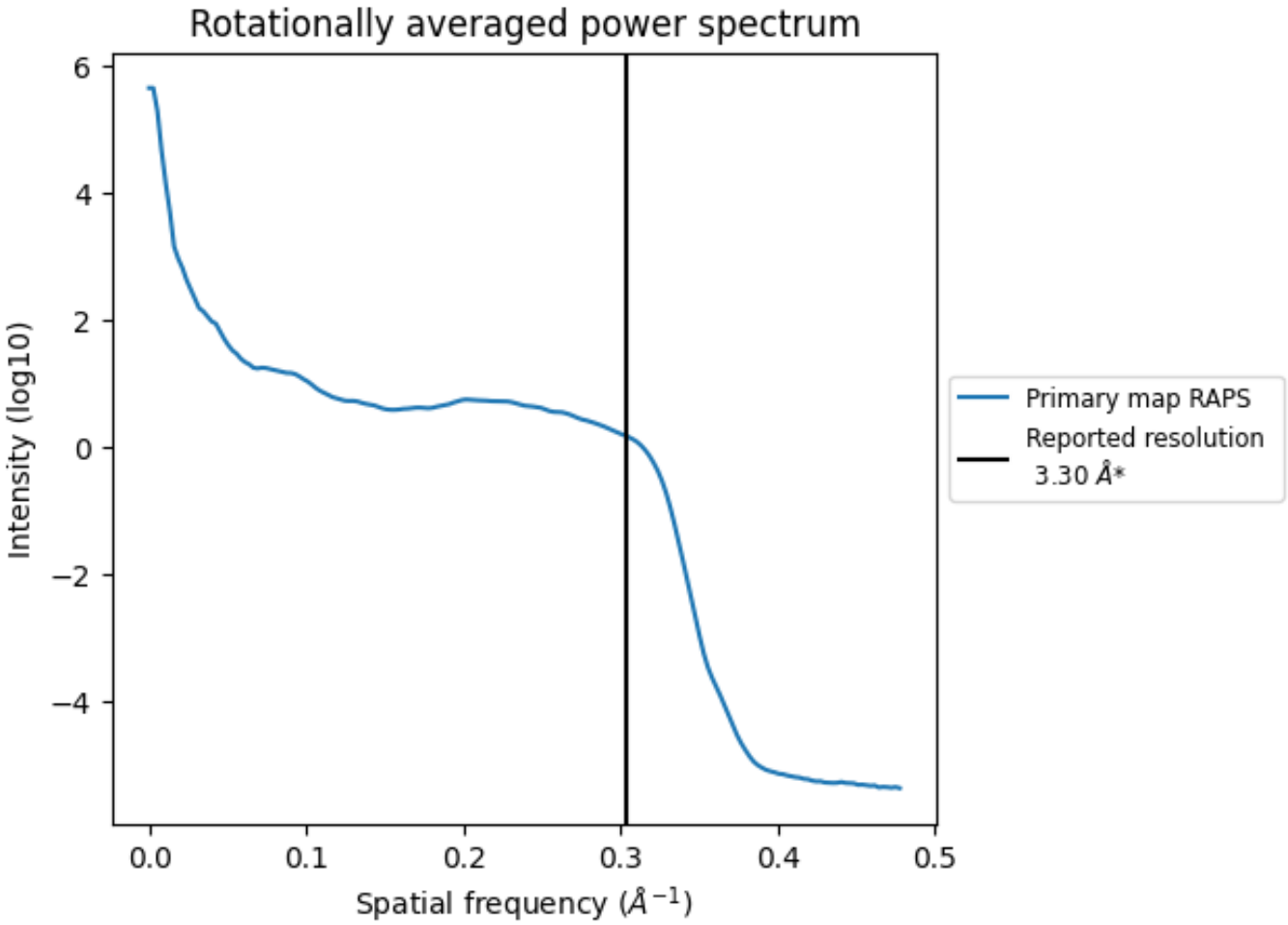
7.2 Volume estimate



The volume at the recommended contour level is 720 nm^3; this corresponds to an approximate mass of 650 kDa.

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

7.3 Rotationally averaged power spectrum (i)

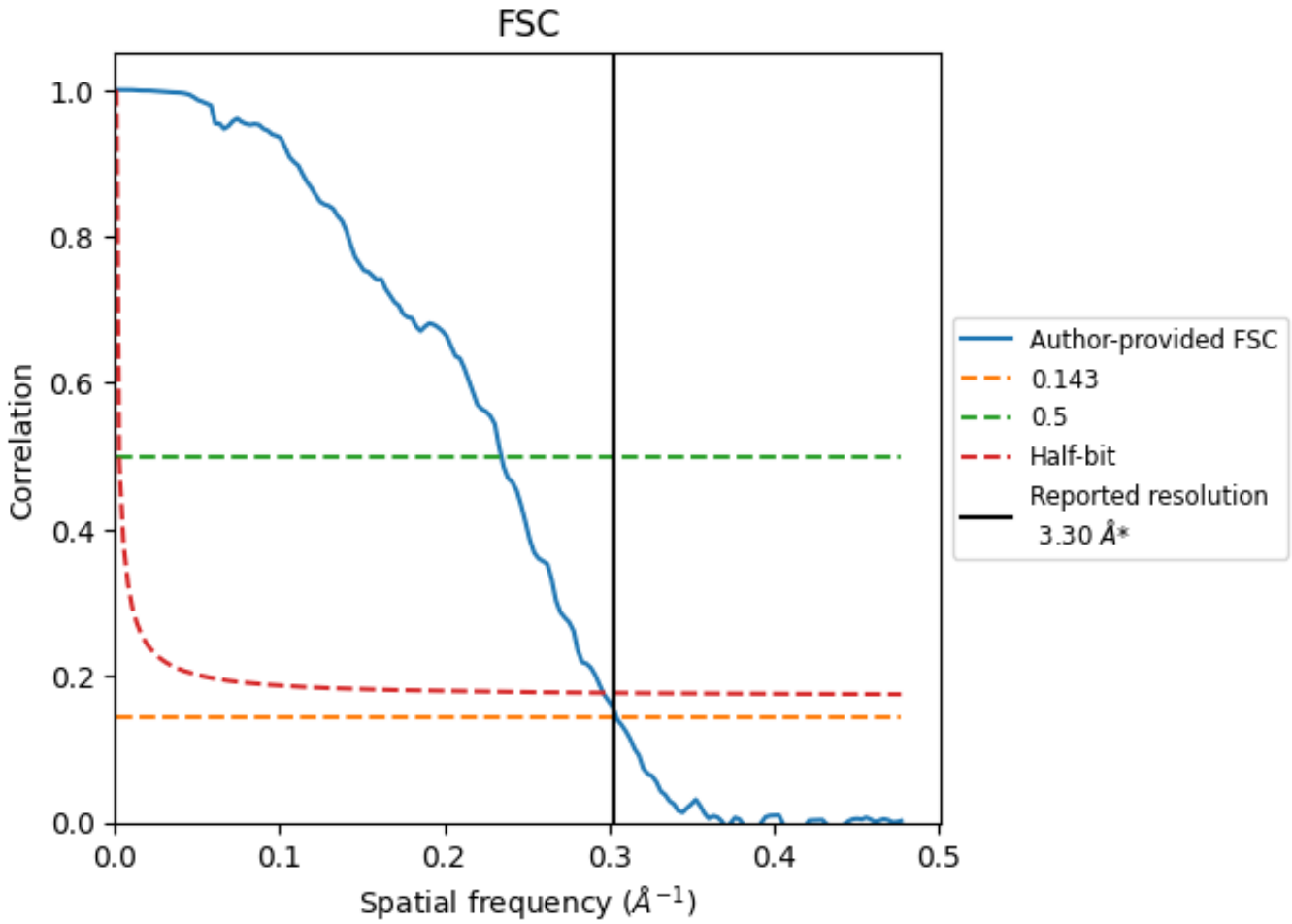


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

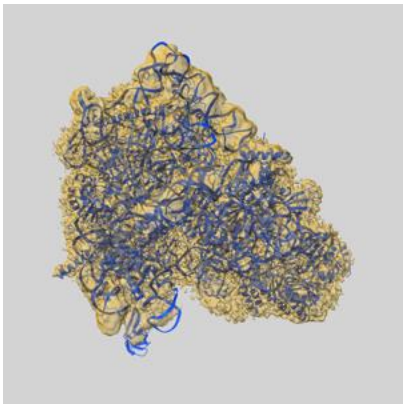
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	4.26	3.37
Unmasked-calculated*	-	-	-

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

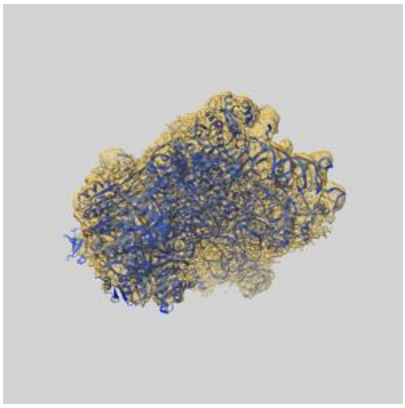
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32790 and PDB model 7WTL. Per-residue inclusion information can be found in section 3 on page 8.

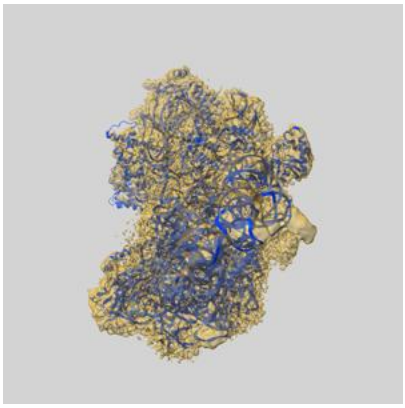
9.1 Map-model overlay



X



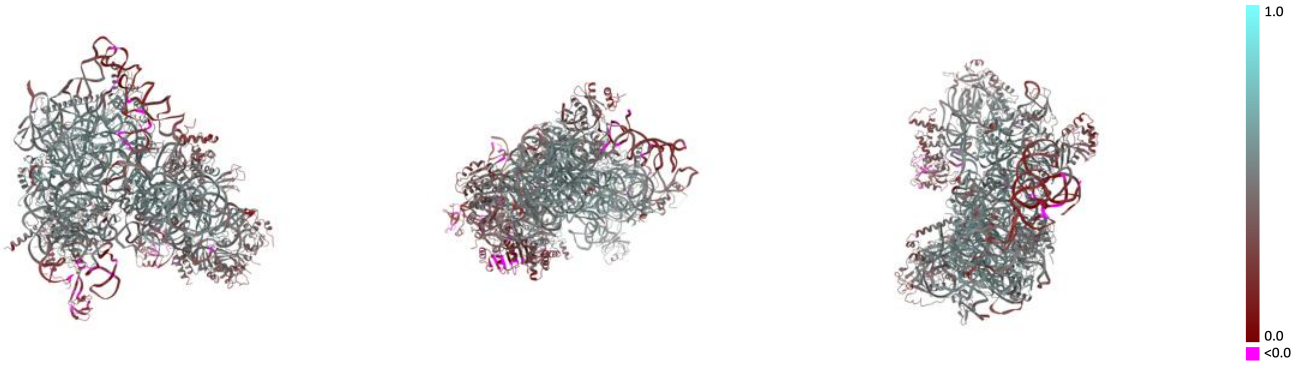
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

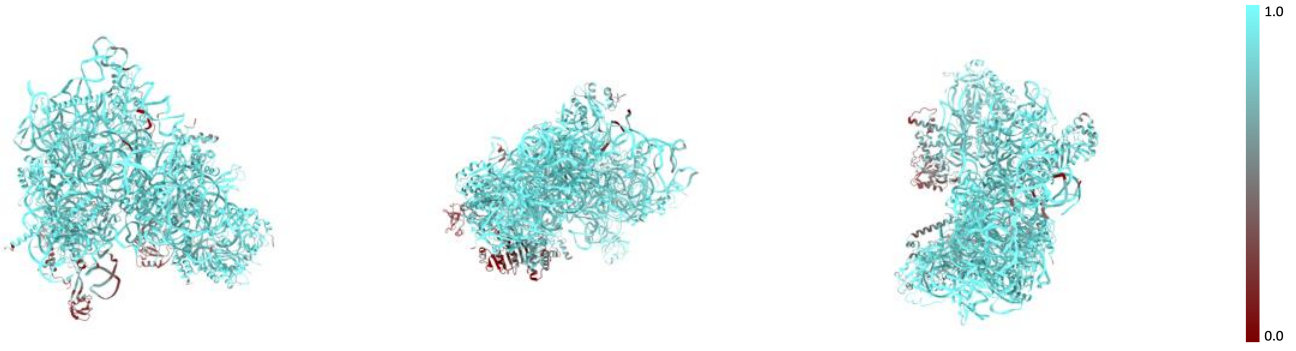
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

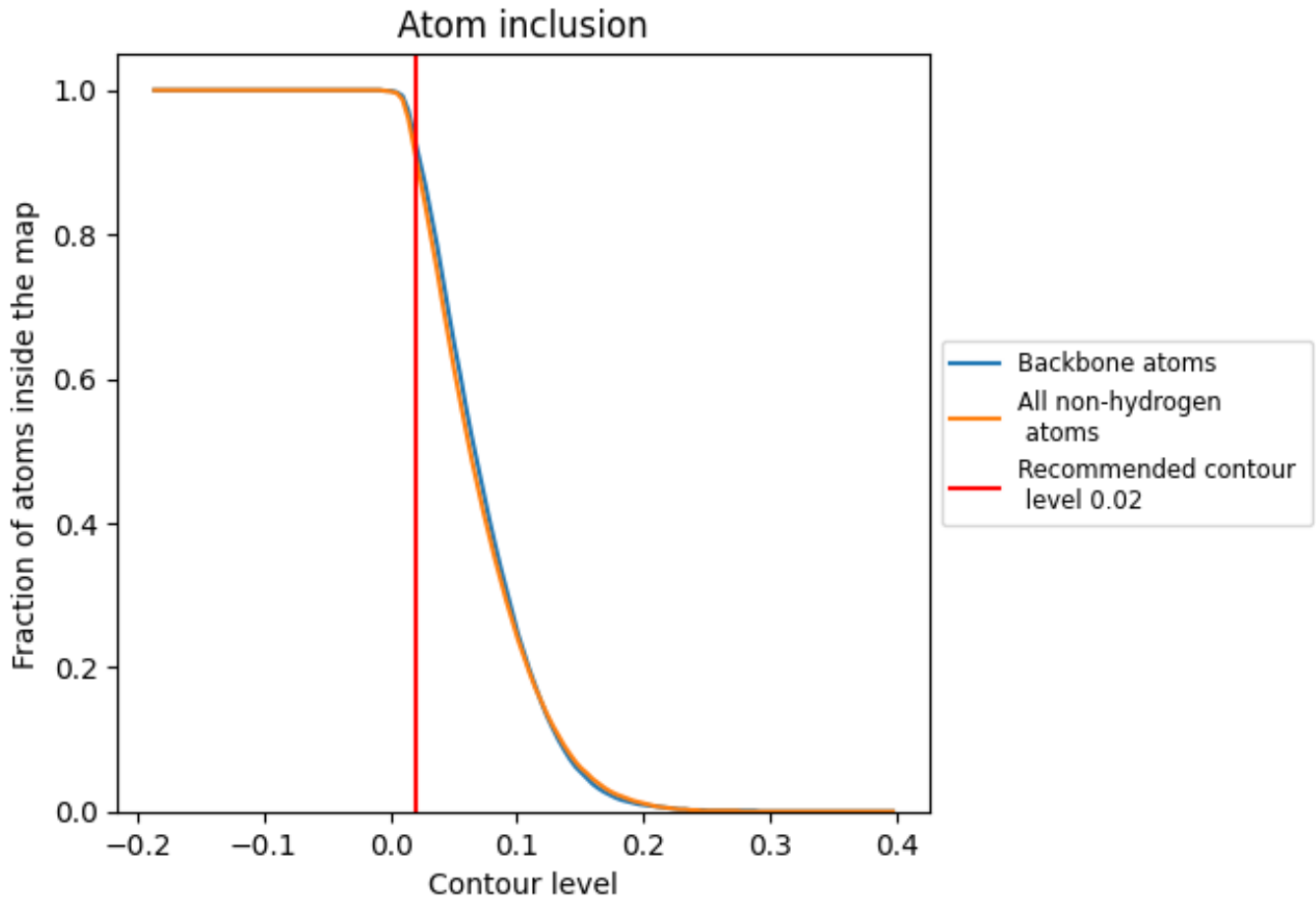
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 91% 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	0.9090	0.4440
C2	0.9580	0.4600
CA	0.9400	0.4090
CK	0.0640	0.1220
CL	0.7790	0.3680
JL	0.4610	0.2130
SB	0.9330	0.4380
SE	0.9720	0.5480
SG	0.9570	0.4630
SH	0.8720	0.3710
SI	0.9610	0.5060
SJ	0.9550	0.4850
SL	0.9600	0.5300
SN	0.9700	0.4910
SO	0.9610	0.4450
SW	0.9790	0.5420
SX	0.9590	0.4890
SY	0.9710	0.5170
Sb	0.9200	0.4530
UC	0.8500	0.4050