



Full wwPDB EM Validation Report ⓘ

Sep 15, 2026 – 02:23 pm BST

PDB ID : 5LL6 / pdb_00005ll6
EMDB ID : EMD-4071
Title : Structure of the 40S ABCE1 post-splitting complex in ribosome recycling and translation initiation
Authors : Heuer, A.; Gerovac, M.; Schmidt, C.; Trowitzsch, S.; Preis, A.; Koetter, P.; Berninghausen, O.; Becker, T.; Beckmann, R.; Tampe, R.
Deposited on : 2016-07-26
Resolution : 3.90 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:

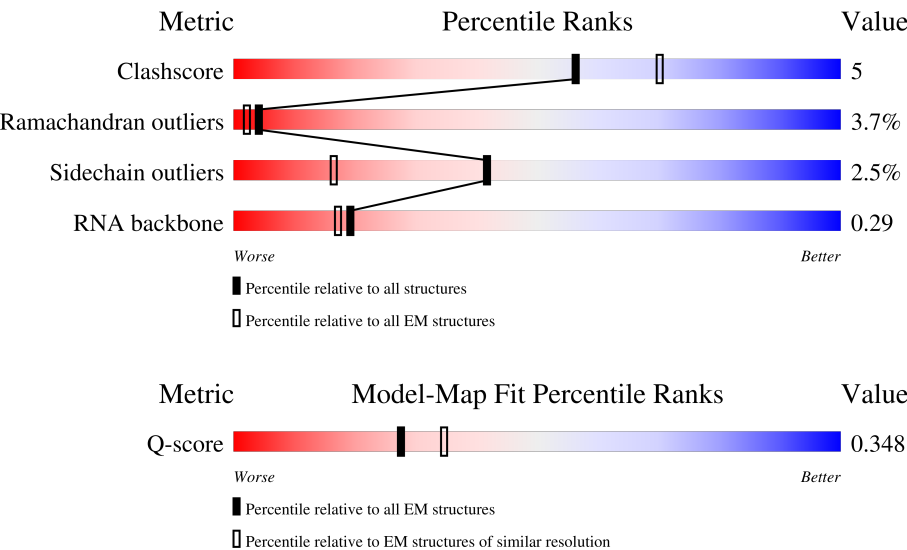
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	2	1798	5% 39% 29% 5% 26%
2	P	252	75% 6% 18%
3	Q	255	11% 73% 10% 16%

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Mol	Chain	Length	Quality of chain
4	R	254	
5	S	261	
6	T	236	
7	U	190	
8	V	200	
9	W	197	
10	X	156	
11	Y	151	
12	Z	137	
13	a	87	
14	b	130	
15	c	145	
16	d	135	
17	e	119	
18	f	82	
19	g	63	
20	h	608	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	SF4	h	701	-	-	X	-
21	SF4	h	702	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 55262 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1325	Total	C	N	O	P	0	0
			28237	12628	5001	9283	1325		

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	226	Total	C	N	O	S	0	0
			1717	1098	305	312	2		

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 6 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 7 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	U	184	Total	C	N	O		
			1481	951	265	265	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 9 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 10 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	155	Total	C	N	O	S		
			1213	774	230	206	3	0	0

- Molecule 11 is a protein called 40S ribosomal protein S13.

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

- Molecule 12 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	127	Total	C	N	O	S		
			891	545	182	163	1	0	0

- Molecule 13 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	87	Total	C	N	O	S		
			684	420	125	137	2	0	0

- Molecule 14 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 16 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	d	132	Total	C	N	O	S	0	0
			1060	669	206	185			

- Molecule 17 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 18 is a protein called 40S ribosomal protein S27-A.

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

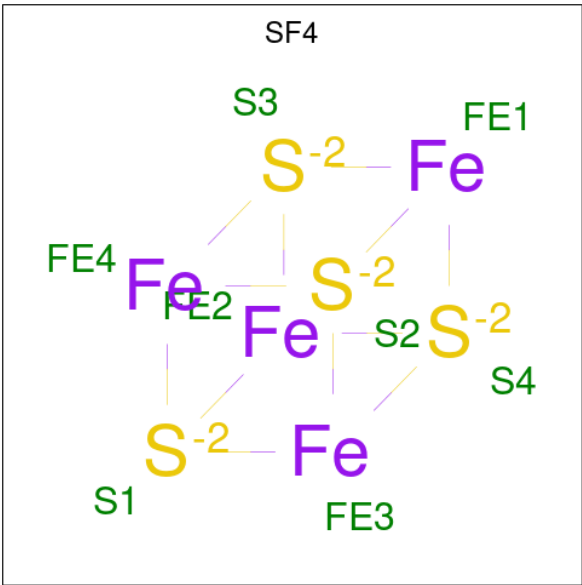
- Molecule 19 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	60	Total	C	N	O	S	0	0
			473	297	98	77	1		

- Molecule 20 is a protein called Translation initiation factor RLI1.

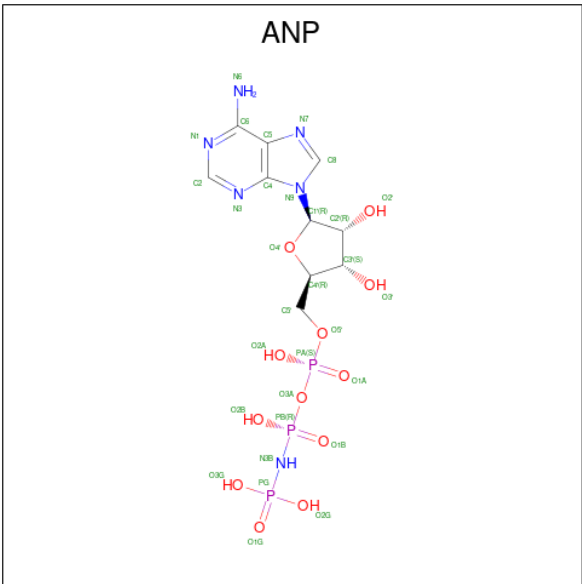
Mol	Chain	Residues	Atoms					AltConf	Trace
20	h	578	Total	C	N	O	S	0	0
			4578	2933	791	831	23		

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
21	h	1	Total	Fe	S	0
			8	4	4	
21	h	1	Total	Fe	S	0
			8	4	4	

- Molecule 22 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf
22	h	1	Total	C	N	O	P	0
			31	10	6	12	3	

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Mol	Chain	Residues	Atoms					AltConf
22	h	1	Total	C	N	O	P	0
			31	10	6	12	3	

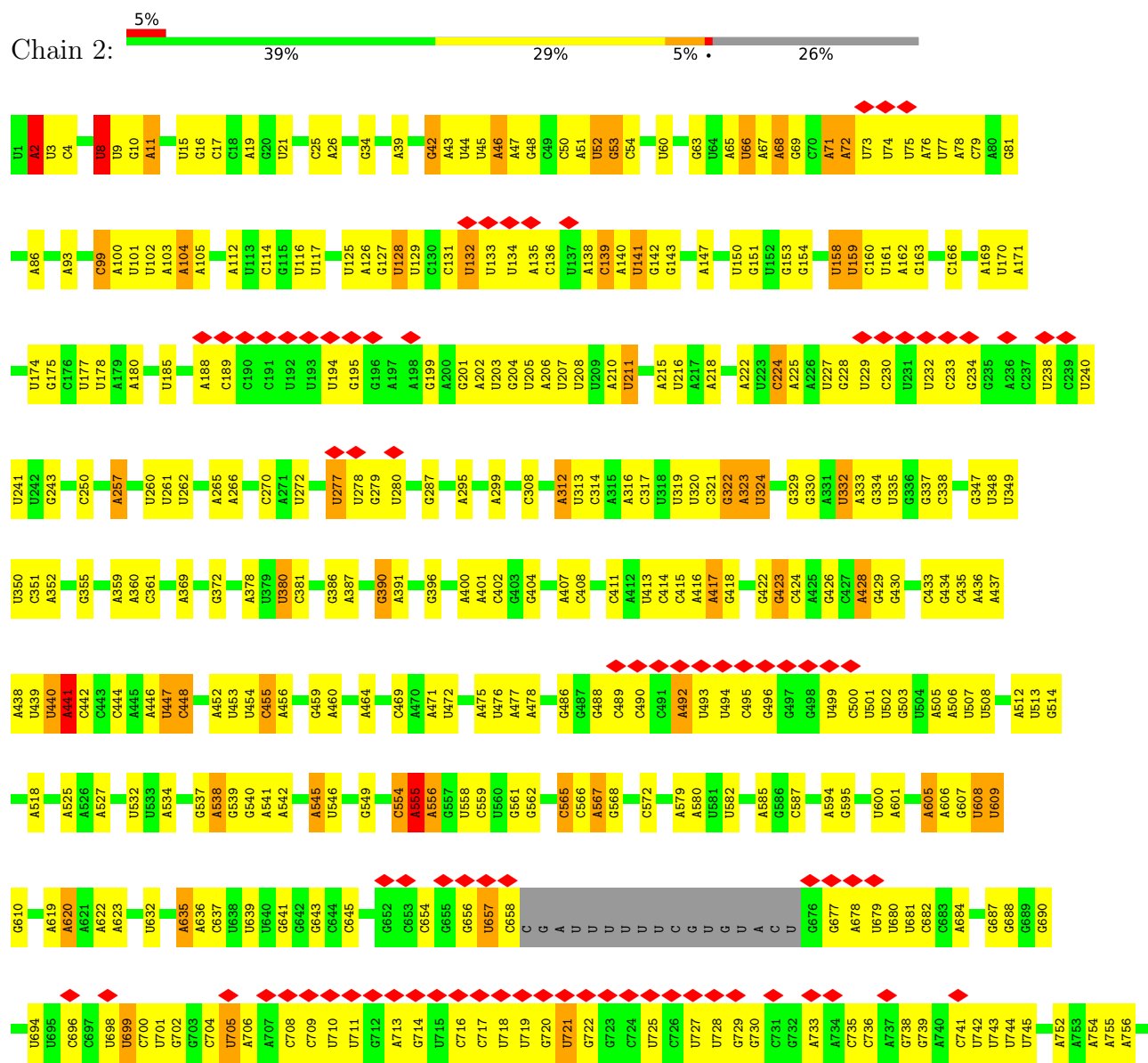
- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

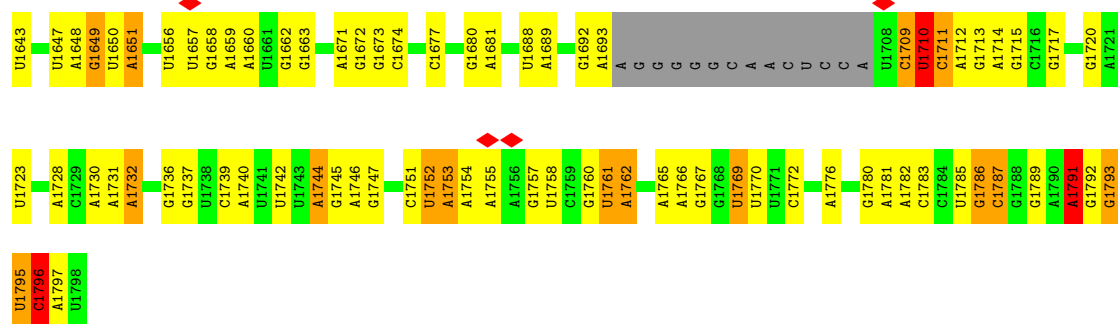
Mol	Chain	Residues	Atoms		AltConf
23	h	1	Total	Mg	0
			1	1	

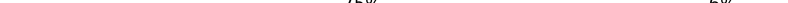
3 Residue-property plots

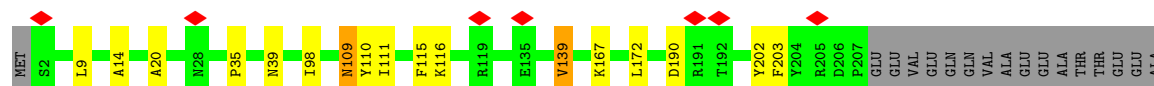
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

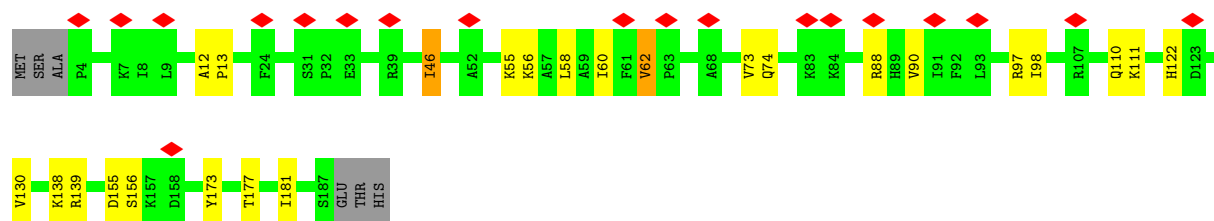
• Molecule 1: 18S ribosomal RNA



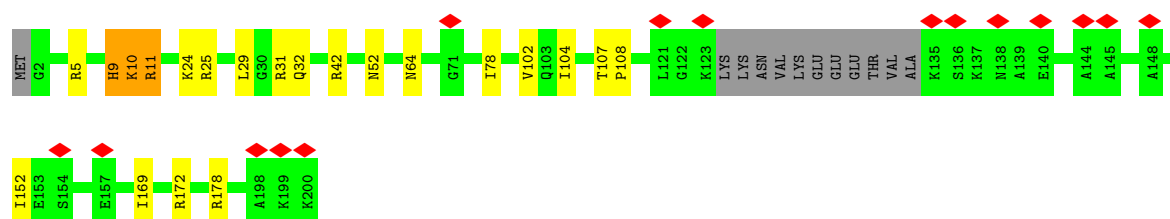
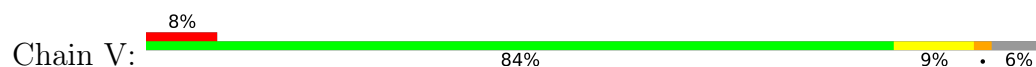


- Chain P:  75% 6% 18%

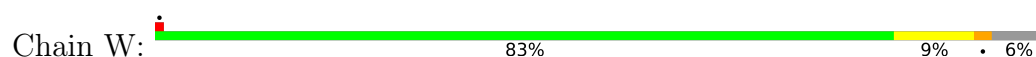




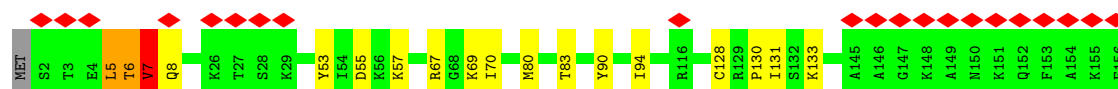
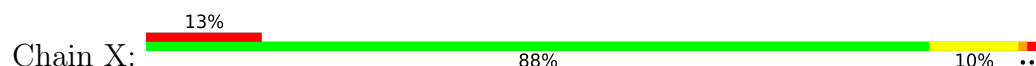
- Molecule 8: 40S ribosomal protein S8-A



- Molecule 9: 40S ribosomal protein S9-A



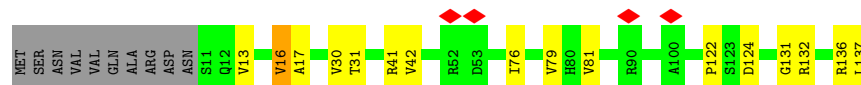
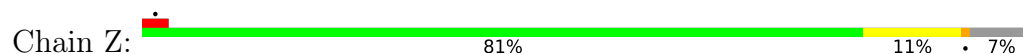
- Molecule 10: 40S ribosomal protein S11-A



- Molecule 11: 40S ribosomal protein S13

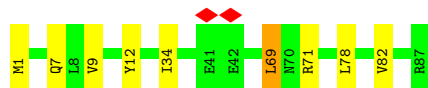


- Molecule 12: 40S ribosomal protein S14-A



- Molecule 13: 40S ribosomal protein S21-A

Chain a:  90% 9% .



- Molecule 14: 40S ribosomal protein S22-A

Chain b:  88% 10% ..



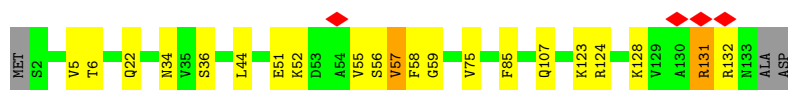
- Molecule 15: 40S ribosomal protein S23-A

Chain c:  83% 13% ..



- Molecule 16: 40S ribosomal protein S24-A

Chain d:  82% 14% ..

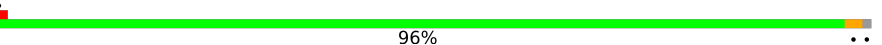


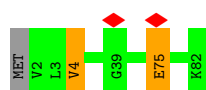
- Molecule 17: 40S ribosomal protein S26-A

Chain e:  69% 12% 18%

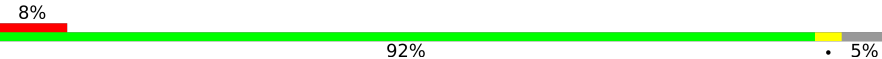


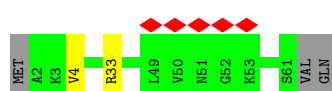
- Molecule 18: 40S ribosomal protein S27-A

Chain f:  96% ..

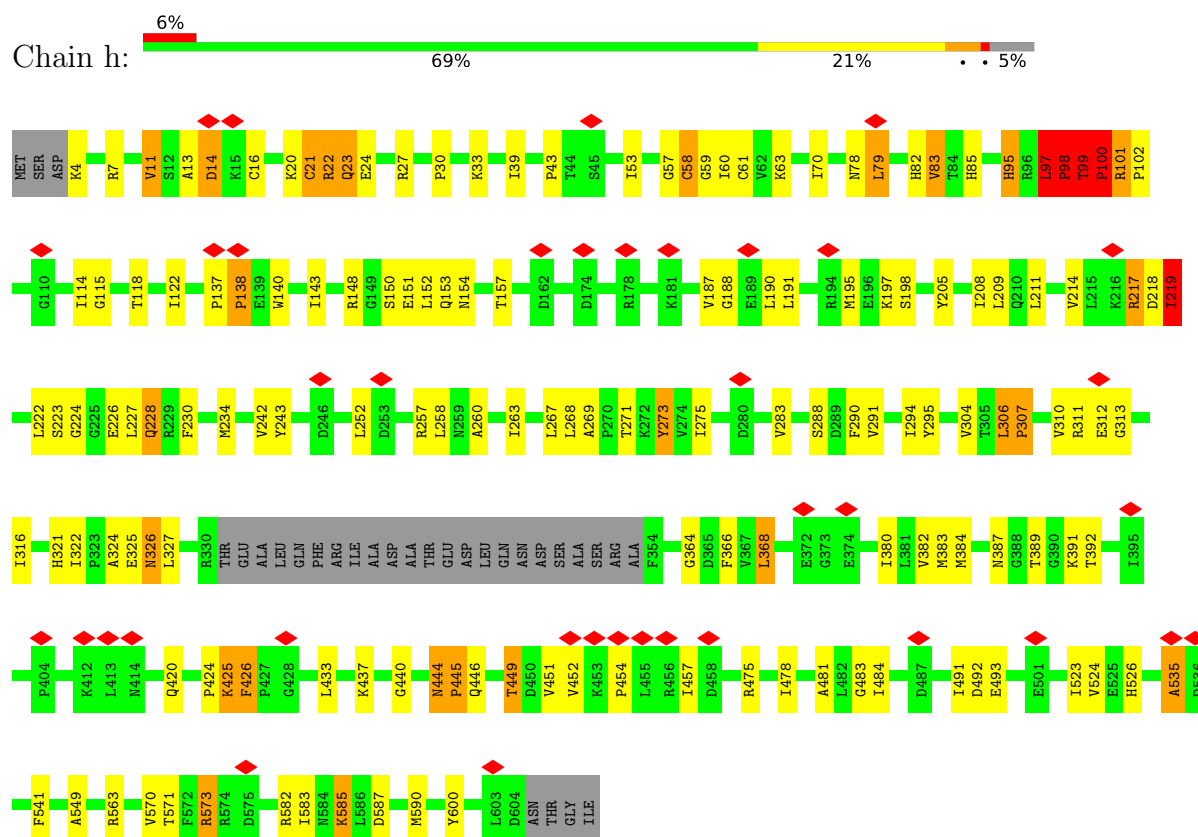


- Molecule 19: 40S ribosomal protein S30-A

Chain g:  8% 92% 5%



• Molecule 20: Translation initiation factor RLI1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.472	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.038	Depositor
Map size ($\text{\AA}$)	416.25598, 416.25598, 416.25598	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, SF4, MG

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	2	0.52	2/31584 (0.0%)	0.84	74/49203 (0.2%)
2	P	0.68	0/1617	0.88	0/2215
3	Q	0.63	0/1735	0.88	0/2335
4	R	0.69	0/1748	0.91	0/2371
5	S	0.66	0/2109	0.88	2/2839 (0.1%)
6	T	0.63	0/1823	0.85	0/2439
7	U	0.66	0/1506	0.90	2/2028 (0.1%)
8	V	0.62	0/1514	0.85	0/2021
9	W	0.66	0/1519	0.90	0/2035
10	X	0.68	0/1239	0.86	1/1673 (0.1%)
11	Y	0.65	0/1215	0.92	1/1638 (0.1%)
12	Z	0.66	0/901	0.95	0/1217
13	a	0.65	0/693	0.90	0/935
14	b	0.65	0/1038	0.93	1/1395 (0.1%)
15	c	0.70	0/1139	0.94	1/1518 (0.1%)
16	d	0.66	0/1074	0.83	0/1431
17	e	0.79	2/782 (0.3%)	0.92	1/1047 (0.1%)
18	f	0.60	0/620	0.79	0/838
19	g	0.65	0/481	0.90	0/640
20	h	1.58	7/4665 (0.2%)	1.30	31/6294 (0.5%)
All	All	0.71	11/59002 (0.0%)	0.90	114/86112 (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
1	2	0	2
7	U	0	2
20	h	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	h	14	ASP	CG-OD1	66.91	2.52	1.25
20	h	14	ASP	CG-OD2	60.63	2.40	1.25
1	2	1761	U	O3'-P	-35.78	1.07	1.61
1	2	1636	C	O3'-P	-24.42	1.24	1.61
20	h	101	ARG	CA-C	15.91	1.72	1.52
20	h	99	THR	N-CA	13.22	1.64	1.46
20	h	99	THR	C-O	-11.39	1.09	1.24
20	h	99	THR	CA-C	10.29	1.65	1.52
20	h	101	ARG	N-CA	9.60	1.59	1.46
17	e	95	ARG	CZ-NH1	8.42	1.44	1.32
17	e	95	ARG	CZ-NH2	5.66	1.40	1.33

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	h	14	ASP	CB-CG-OD2	-36.74	33.91	118.40
20	h	14	ASP	OD1-CG-OD2	-29.14	52.95	122.90
20	h	14	ASP	CB-CG-OD1	-28.97	51.77	118.40
1	2	1761	U	O3'-P-O5'	-15.27	81.10	104.00
20	h	99	THR	CA-C-O	-13.57	101.57	120.16
1	2	1636	C	O3'-P-O5'	-12.89	84.67	104.00
1	2	1761	U	P-O3'-C3'	-12.35	101.68	120.20
20	h	99	THR	O-C-N	-10.61	106.02	123.00
20	h	99	THR	N-CA-C	10.43	132.86	109.81
1	2	1023	A	C4'-C3'-O3'	10.37	124.96	109.40
1	2	1116	A	C1'-C2'-O2'	-9.94	93.48	108.40
20	h	99	THR	CA-C-N	9.60	138.97	121.70
20	h	99	THR	C-N-CA	9.60	138.97	121.70
1	2	42	G	C2'-C3'-O3'	9.54	123.81	109.50
20	h	11	VAL	N-CA-C	9.11	118.82	111.62
1	2	1636	C	OP1-P-O3'	8.92	134.75	108.00
1	2	99	C	C4'-C3'-O3'	8.52	122.19	109.40
1	2	1710	U	N1-C1'-C2'	-8.28	99.59	112.00
1	2	322	G	C2'-C3'-O3'	8.21	121.81	109.50
1	2	1028	C	C4'-C3'-O3'	8.12	121.58	109.40
1	2	811	A	C4'-C3'-O3'	8.09	121.53	109.40
1	2	132	U	C4'-C3'-O3'	8.06	121.48	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	721	U	C2'-C3'-O3'	7.95	121.43	109.50
1	2	52	U	C1'-C2'-O2'	-7.95	96.48	108.40
1	2	1081	A	C4'-C3'-O3'	7.90	121.25	109.40
1	2	53	G	C4'-C3'-O3'	7.81	124.72	113.00
1	2	1761	U	OP1-P-O3'	7.77	131.30	108.00
1	2	428	A	N9-C1'-C2'	-7.70	100.45	112.00
20	h	392	THR	N-CA-C	7.44	119.17	111.14
1	2	812	A	C4'-C3'-O3'	7.43	120.55	109.40
1	2	1054	U	C2'-C3'-O3'	7.40	124.80	113.70
1	2	1710	U	C4'-C3'-O3'	7.25	123.88	113.00
1	2	492	A	C4'-C3'-O3'	7.24	120.26	109.40
1	2	159	U	C4'-C3'-O3'	7.23	120.24	109.40
1	2	224	C	C4'-C3'-O3'	7.18	120.17	109.40
1	2	554	C	C4'-C3'-O3'	7.13	120.10	109.40
1	2	1114	G	C4'-C3'-O3'	7.09	120.04	109.40
1	2	52	U	C4'-C3'-O3'	7.05	123.58	113.00
1	2	1636	C	C2'-C3'-O3'	7.03	120.04	109.50
1	2	565	C	C4'-C3'-O3'	7.02	119.93	109.40
1	2	53	G	N9-C1'-C2'	-6.98	101.53	112.00
1	2	441	A	C4'-C3'-O3'	6.91	123.37	113.00
1	2	1765	A	C2'-C3'-O3'	-6.86	103.42	113.70
1	2	455	C	C4'-C3'-O3'	6.65	119.38	109.40
20	h	100	PRO	O-C-N	6.65	131.61	122.64
20	h	444	ASN	CA-C-N	6.56	128.04	119.84
20	h	444	ASN	C-N-CA	6.56	128.04	119.84
1	2	104	A	C3'-C2'-O2'	6.56	120.54	110.70
20	h	98	PRO	CA-C-N	6.51	137.69	121.80
20	h	98	PRO	C-N-CA	6.51	137.69	121.80
1	2	139	C	C2'-C3'-O3'	6.49	119.24	109.50
1	2	1003	A	C2'-C3'-O3'	6.48	119.22	109.50
1	2	139	C	C4'-C3'-O3'	6.47	119.10	109.40
20	h	101	ARG	CA-C-N	6.47	127.92	119.84
20	h	101	ARG	C-N-CA	6.47	127.92	119.84
1	2	46	A	C4'-C3'-O3'	6.47	119.10	109.40
1	2	441	A	N9-C1'-C2'	-6.37	102.45	112.00
1	2	417	A	C2'-C3'-O3'	-6.31	104.24	113.70
1	2	1114	G	C2'-C3'-O3'	6.30	118.95	109.50
1	2	1796	C	C4'-C3'-O3'	-6.30	103.55	113.00
1	2	46	A	C2'-C3'-O3'	6.26	118.89	109.50
1	2	158	U	C2'-C3'-O3'	6.20	122.99	113.70
20	h	100	PRO	CA-C-N	-6.16	106.77	121.80
20	h	100	PRO	C-N-CA	-6.16	106.77	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1791	A	C2'-C3'-O3'	-6.15	104.47	113.70
1	2	1026	A	C4'-C3'-O3'	-6.14	103.78	113.00
1	2	66	U	C4'-C3'-O3'	-6.13	103.81	113.00
1	2	555	A	C2'-C3'-O3'	6.05	122.78	113.70
1	2	2	A	C2'-C3'-O3'	6.01	118.52	109.50
20	h	217	ARG	N-CA-C	5.94	119.08	109.40
1	2	1099	U	C2'-C3'-O3'	-5.93	104.80	113.70
20	h	95	HIS	N-CA-C	5.90	120.53	112.68
1	2	128	U	C4'-C3'-O3'	5.89	118.24	109.40
1	2	53	G	C1'-C2'-O2'	-5.84	99.64	108.40
20	h	98	PRO	O-C-N	-5.81	114.80	122.64
20	h	219	ILE	CB-CA-C	-5.79	104.33	112.14
1	2	104	A	C2'-C3'-O3'	5.75	122.32	113.70
11	Y	83	GLU	N-CA-C	5.75	118.32	111.71
20	h	21	CYS	N-CA-C	5.70	119.96	112.89
1	2	1116	A	C4'-C3'-O3'	5.70	121.55	113.00
15	c	16	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	2	1710	U	C3'-C2'-O2'	5.64	119.16	110.70
1	2	1633	A	C2'-C3'-O3'	5.62	117.93	109.50
20	h	535	ALA	N-CA-C	5.58	117.75	110.43
1	2	699	U	C3'-C2'-O2'	5.58	119.06	110.70
1	2	605	A	C3'-C2'-O2'	5.55	119.02	110.70
1	2	277	U	C4'-C3'-O3'	5.54	121.31	113.00
1	2	1097	U	C3'-C2'-O2'	5.54	119.01	110.70
14	b	28	ARG	C-N-CD	-5.53	108.43	120.60
17	e	97	PRO	N-CA-C	5.53	117.44	110.70
7	U	56	LYS	N-CA-C	5.49	118.20	109.81
1	2	1113	A	C2'-C3'-O3'	5.48	117.71	109.50
10	X	90	TYR	N-CA-C	5.42	117.08	108.79
5	S	3	ARG	N-CA-C	5.40	119.16	112.24
7	U	97	ARG	N-CA-C	5.36	117.56	111.02
20	h	228	GLN	N-CA-C	-5.33	105.36	111.07
1	2	928	U	C2'-C3'-O3'	5.32	121.67	113.70
5	S	194	THR	N-CA-C	5.31	122.12	110.80
1	2	423	G	C4'-C3'-O3'	-5.26	105.11	113.00
20	h	137	PRO	CA-C-N	5.23	126.37	119.84
20	h	137	PRO	C-N-CA	5.23	126.37	119.84
20	h	97	LEU	N-CA-C	-5.18	101.56	109.64
1	2	705	U	C2'-C3'-O3'	-5.15	105.97	113.70
1	2	380	U	C4'-C3'-O3'	5.15	117.12	109.40
20	h	98	PRO	N-CA-C	5.13	123.03	112.47
1	2	428	A	C3'-C2'-O2'	5.12	118.38	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1769	U	C4'-C3'-O3'	5.11	117.07	109.40
1	2	312	A	C4'-C3'-O3'	-5.07	105.39	113.00
1	2	1108	G	C4'-C3'-O3'	-5.07	105.40	113.00
20	h	307	PRO	N-CA-C	5.06	119.15	111.11
1	2	452	A	C4'-C3'-O3'	-5.03	105.45	113.00
1	2	435	C	C4'-C3'-O3'	-5.02	105.47	113.00
1	2	103	A	C4'-C3'-O3'	-5.01	105.49	113.00
1	2	963	A	C4'-C3'-O3'	-5.00	105.49	113.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	1139	A	Sidechain
1	2	8	U	Sidechain
7	U	55	LYS	Peptide
7	U	88	ARG	Peptide
20	h	100	PRO	Mainchain
20	h	14	ASP	Sidechain
20	h	444	ASN	Peptide
20	h	98	PRO	Mainchain
20	h	99	THR	Mainchain

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	2	28237	0	14200	210	0
2	P	1577	0	1567	10	0
3	Q	1709	0	1784	10	0
4	R	1717	0	1809	17	0
5	S	2068	0	2154	21	0
6	T	1799	0	1878	11	0
7	U	1481	0	1572	11	0
8	V	1489	0	1525	18	0
9	W	1494	0	1573	9	0
10	X	1213	0	1257	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Y	1192	0	1255	10	0
12	Z	891	0	883	11	0
13	a	684	0	672	4	0
14	b	1021	0	1060	7	0
15	c	1121	0	1196	16	0
16	d	1060	0	1123	25	0
17	e	769	0	818	11	0
18	f	610	0	633	2	0
19	g	473	0	518	2	0
20	h	4578	0	4727	184	0
21	h	16	0	0	6	0
22	h	62	0	26	3	0
23	h	1	0	0	0	0
All	All	55262	0	42230	480	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 5.

All (480) 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)
20:h:391:LYS:HG2	20:h:541:PHE:CE2	1.66	1.30
1:2:1636:C:C2'	1:2:1637:C:OP2	1.67	1.30
1:2:1636:C:O2'	1:2:1637:C:OP2	1.55	1.21
1:2:1636:C:N4	1:2:1638:G:N2	1.93	1.17
20:h:389:THR:OG1	20:h:541:PHE:HB3	1.44	1.15
20:h:424:PRO:HB2	20:h:426:PHE:CE2	1.81	1.14
20:h:325:GLU:OE1	20:h:327:LEU:HD22	1.46	1.13
1:2:1080:U:O4	1:2:1091:A:N1	1.81	1.12
20:h:426:PHE:HB3	20:h:433:LEU:HD21	1.25	1.12
1:2:1636:C:N4	1:2:1638:G:C2	2.18	1.11
1:2:1636:C:C4	1:2:1638:G:C2	2.37	1.11
1:2:8:U:H3	1:2:1139:A:N6	1.52	1.08
20:h:426:PHE:HB2	20:h:433:LEU:HD11	1.33	1.08
1:2:414:C:O2'	20:h:311:ARG:HD3	1.53	1.08
1:2:1038:U:N3	1:2:1092:A:N6	2.02	1.07
1:2:1145:U:O4	1:2:1633:A:N1	1.87	1.07
16:d:107:GLN:CD	20:h:271:THR:HG23	1.79	1.05
1:2:1636:C:C1'	1:2:1637:C:OP2	2.06	1.04
1:2:8:U:N3	1:2:1139:A:N6	2.06	1.02
16:d:107:GLN:NE2	20:h:271:THR:CG2	2.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:230:PHE:CZ	20:h:234:MET:CE	2.43	1.01
20:h:573:ARG:NH1	20:h:582:ARG:HD2	1.74	1.01
16:d:107:GLN:CD	20:h:271:THR:CG2	2.34	1.01
20:h:391:LYS:HG2	20:h:541:PHE:CD2	1.96	1.01
20:h:295:TYR:HB2	20:h:327:LEU:HG	1.42	0.98
1:2:1728:A:H1'	8:V:32:GLN:NE2	1.77	0.98
20:h:295:TYR:CG	20:h:327:LEU:HD21	1.98	0.98
1:2:1145:U:C4	1:2:1633:A:N1	2.30	0.98
20:h:426:PHE:CB	20:h:433:LEU:HD21	1.93	0.97
1:2:332:U:O2'	8:V:5:ARG:NH1	1.98	0.97
20:h:424:PRO:HB2	20:h:426:PHE:HE2	1.25	0.96
15:c:80:GLY:HA3	20:h:60:ILE:HD11	1.47	0.96
1:2:1038:U:O4	1:2:1092:A:N1	1.98	0.95
16:d:128:LYS:O	16:d:132:ARG:HG3	1.67	0.95
20:h:493:GLU:OE2	20:h:526:HIS:HD2	1.48	0.95
16:d:124:ARG:HE	16:d:128:LYS:HZ2	1.14	0.94
1:2:1057:U:O4	1:2:1062:A:N1	2.00	0.94
16:d:107:GLN:NE2	20:h:271:THR:HG23	1.80	0.94
1:2:1080:U:O4	1:2:1091:A:C2	2.21	0.94
20:h:295:TYR:CB	20:h:327:LEU:HG	1.97	0.93
20:h:573:ARG:HH11	20:h:582:ARG:HD2	1.24	0.93
20:h:230:PHE:CZ	20:h:234:MET:HE1	2.04	0.93
1:2:814:A:N1	1:2:857:U:O4	2.02	0.92
20:h:61:CYS:HG	21:h:701:SF4:FE3	0.74	0.92
20:h:325:GLU:OE1	20:h:327:LEU:CD2	2.18	0.91
20:h:295:TYR:HB2	20:h:327:LEU:CG	1.98	0.91
20:h:58:CYS:SG	21:h:701:SF4:FE4	1.65	0.87
20:h:493:GLU:OE2	20:h:526:HIS:CD2	2.27	0.87
20:h:21:CYS:HG	21:h:702:SF4:FE2	0.60	0.86
16:d:107:GLN:NE2	20:h:271:THR:HG22	1.91	0.86
1:2:414:C:O2'	20:h:311:ARG:CD	2.24	0.86
1:2:1636:C:H41	1:2:1638:G:N2	1.73	0.85
1:2:1636:C:C5	1:2:1638:G:N3	2.45	0.84
16:d:124:ARG:HE	16:d:128:LYS:NZ	1.74	0.84
20:h:21:CYS:SG	21:h:702:SF4:FE2	1.69	0.84
1:2:1636:C:H1'	1:2:1637:C:OP2	1.75	0.84
1:2:1080:U:C4	1:2:1091:A:N1	2.46	0.84
20:h:426:PHE:CB	20:h:433:LEU:HD11	2.07	0.84
1:2:1145:U:O4	1:2:1633:A:C6	2.31	0.83
20:h:391:LYS:CG	20:h:541:PHE:CD2	2.62	0.83
20:h:230:PHE:CZ	20:h:234:MET:HE2	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1730:A:OP1	8:V:24:LYS:NZ	2.12	0.82
1:2:1038:U:H3	1:2:1092:A:N6	1.76	0.81
1:2:1659:A:O3'	20:h:20:LYS:NZ	2.13	0.81
1:2:1745:G:H5''	20:h:27:ARG:HH11	1.46	0.81
20:h:573:ARG:NH1	20:h:582:ARG:CD	2.43	0.81
1:2:1135:U:O2'	1:2:1753:A:OP1	1.99	0.80
20:h:389:THR:HG1	20:h:541:PHE:HB3	1.47	0.80
1:2:433:C:O3'	20:h:63:LYS:NZ	2.15	0.79
1:2:1636:C:C4	1:2:1638:G:N3	2.50	0.79
20:h:295:TYR:HB2	20:h:327:LEU:CD1	2.13	0.78
16:d:107:GLN:CG	20:h:271:THR:HG23	2.12	0.78
22:h:705:ANP:H3'	22:h:705:ANP:O1A	1.84	0.78
15:c:80:GLY:CA	20:h:60:ILE:HD11	2.13	0.77
16:d:55:VAL:HG13	16:d:75:VAL:HG23	1.66	0.77
20:h:573:ARG:HH11	20:h:582:ARG:CD	1.98	0.77
1:2:1145:U:C4	1:2:1633:A:C2	2.74	0.76
20:h:58:CYS:SG	21:h:701:SF4:S2	2.84	0.75
1:2:391:A:O4'	1:2:1731:A:H5'	1.85	0.75
1:2:8:U:C4	1:2:1139:A:N6	2.54	0.74
1:2:1038:U:C4	1:2:1092:A:N1	2.54	0.74
1:2:391:A:O2'	1:2:1730:A:H4'	1.88	0.73
1:2:433:C:H5''	20:h:63:LYS:HZ1	1.55	0.72
1:2:433:C:H5''	20:h:63:LYS:NZ	2.04	0.72
20:h:424:PRO:CB	20:h:426:PHE:HE2	2.03	0.71
1:2:222:A:N6	1:2:833:U:C4	2.58	0.71
1:2:1145:U:O4	1:2:1633:A:C2	2.44	0.70
20:h:294:ILE:CG1	20:h:304:VAL:HG22	2.22	0.70
20:h:391:LYS:CG	20:h:541:PHE:CE2	2.61	0.70
1:2:1038:U:C2	1:2:1092:A:N6	2.60	0.69
1:2:1673:G:O3'	6:T:92:ARG:NH1	2.26	0.69
1:2:1728:A:H1'	8:V:32:GLN:HE22	1.55	0.68
1:2:222:A:C6	1:2:833:U:N3	2.60	0.68
2:P:139:VAL:HG23	4:R:62:PRO:CG	2.22	0.68
20:h:79:LEU:C	20:h:79:LEU:HD22	2.19	0.67
20:h:295:TYR:CD1	20:h:327:LEU:HD21	2.29	0.66
1:2:433:C:OP2	20:h:7:ARG:NH2	2.29	0.66
1:2:476:U:N3	1:2:545:A:C6	2.63	0.66
20:h:230:PHE:CE1	20:h:234:MET:HE1	2.30	0.66
16:d:128:LYS:O	16:d:132:ARG:CG	2.43	0.66
20:h:295:TYR:HB3	20:h:327:LEU:HG	1.78	0.66
9:W:123:HIS:CG	19:g:33:ARG:HH22	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:44:LEU:HD13	16:d:55:VAL:HG11	1.77	0.66
20:h:389:THR:O	20:h:541:PHE:CD1	2.49	0.65
20:h:426:PHE:CB	20:h:433:LEU:CD2	2.73	0.65
1:2:992:A:N6	1:2:1012:U:N3	2.45	0.65
20:h:79:LEU:HD13	20:h:79:LEU:O	1.97	0.65
20:h:391:LYS:HA	20:h:541:PHE:CZ	2.32	0.65
3:Q:201:THR:HG21	3:Q:207:LEU:HD22	1.79	0.65
15:c:57:LEU:HD22	19:g:4:VAL:HG13	1.78	0.64
1:2:414:C:H5'	20:h:312:GLU:HG3	1.79	0.64
20:h:295:TYR:HB2	20:h:327:LEU:HD11	1.79	0.64
20:h:426:PHE:CG	20:h:433:LEU:HD11	2.33	0.64
1:2:391:A:C4'	1:2:1731:A:H5'	2.28	0.64
20:h:493:GLU:CD	20:h:526:HIS:CD2	2.76	0.64
1:2:1680:G:C2	1:2:1720:G:C2	2.86	0.64
20:h:389:THR:O	20:h:541:PHE:HD1	1.81	0.64
1:2:414:C:H5'	20:h:312:GLU:CG	2.27	0.64
20:h:214:VAL:HG21	20:h:222:LEU:HD11	1.80	0.64
15:c:82:LYS:HE3	20:h:33:LYS:NZ	2.13	0.63
20:h:294:ILE:HG12	20:h:304:VAL:HG22	1.80	0.63
20:h:451:VAL:HG13	20:h:457:ILE:CG2	2.28	0.63
20:h:79:LEU:HD22	20:h:79:LEU:O	1.97	0.63
1:2:814:A:N6	1:2:857:U:N3	2.47	0.63
1:2:1760:G:HO2'	1:2:1781:A:H2	1.47	0.63
7:U:12:ALA:HB3	7:U:13:PRO:HD3	1.81	0.63
11:Y:22:ALA:HB1	11:Y:23:PRO:HA	1.81	0.63
20:h:493:GLU:CD	20:h:526:HIS:HD2	2.07	0.63
1:2:222:A:C5	1:2:833:U:C2	2.88	0.62
1:2:788:A:C6	5:S:19:LEU:HD13	2.34	0.62
16:d:124:ARG:O	16:d:128:LYS:HG2	2.00	0.62
1:2:407:A:O2'	1:2:1671:A:C2	2.52	0.62
2:P:139:VAL:HG23	4:R:62:PRO:HG3	1.81	0.62
1:2:407:A:O2'	1:2:1671:A:N3	2.31	0.62
1:2:1116:A:C4	1:2:1131:A:N6	2.55	0.62
1:2:1672:G:H2'	1:2:1673:G:C8	2.34	0.62
20:h:78:ASN:HD22	20:h:95:HIS:HE1	1.47	0.61
1:2:1038:U:N3	1:2:1092:A:C6	2.67	0.61
20:h:39:ILE:HD11	21:h:701:SF4:S4	2.40	0.61
7:U:46:ILE:HD13	7:U:60:ILE:HG12	1.83	0.61
16:d:107:GLN:HG2	20:h:271:THR:HG23	1.83	0.60
20:h:295:TYR:CB	20:h:327:LEU:CG	2.67	0.60
5:S:9:LEU:HD21	5:S:14:ALA:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:390:G:O2'	1:2:1731:A:H5''	2.00	0.60
1:2:324:U:OP2	10:X:133:LYS:NZ	2.23	0.60
4:R:228:ASN:HD22	13:a:1:MET:N	1.99	0.60
20:h:426:PHE:HB3	20:h:433:LEU:CD2	2.16	0.60
20:h:78:ASN:ND2	20:h:95:HIS:CE1	2.69	0.60
12:Z:16:VAL:HG23	12:Z:31:THR:HG23	1.84	0.59
20:h:426:PHE:CG	20:h:433:LEU:CD1	2.86	0.59
20:h:78:ASN:HD22	20:h:95:HIS:CE1	2.20	0.59
7:U:60:ILE:HG22	7:U:62:VAL:HG23	1.83	0.59
1:2:1080:U:O4	1:2:1091:A:C6	2.54	0.59
1:2:1139:A:H2'	1:2:1140:G:O4'	2.03	0.59
1:2:1650:U:H2'	1:2:1651:A:C8	2.38	0.59
20:h:426:PHE:HB2	20:h:433:LEU:CD1	2.20	0.58
1:2:609:U:O2'	15:c:19:ARG:NE	2.36	0.58
20:h:97:LEU:HD22	20:h:122:ILE:HG21	1.85	0.58
1:2:1785:U:OP1	12:Z:136:ARG:NH1	2.37	0.58
12:Z:131:GLY:O	17:e:22:ARG:NH2	2.38	0.57
1:2:896:U:O2'	12:Z:41:ARG:NH1	2.37	0.57
20:h:573:ARG:NH2	20:h:573:ARG:HB2	2.18	0.57
20:h:140:TRP:CE3	20:h:143:ILE:HD11	2.39	0.57
10:X:7:VAL:HG13	10:X:8:GLN:HE21	1.70	0.57
20:h:366:PHE:HB3	20:h:368:LEU:HD21	1.87	0.57
20:h:224:GLY:HA2	20:h:227:LEU:HB3	1.85	0.57
20:h:4:LYS:HA	20:h:79:LEU:HD12	1.87	0.57
20:h:99:THR:HG22	20:h:101:ARG:HG2	1.87	0.57
15:c:127:VAL:O	15:c:130:VAL:HG22	2.04	0.57
20:h:426:PHE:N	20:h:426:PHE:CD2	2.73	0.57
4:R:104:VAL:HG22	4:R:132:ALA:HB1	1.88	0.56
9:W:60:LEU:CD1	9:W:97:LEU:HD11	2.36	0.56
10:X:6:THR:O	10:X:7:VAL:HG12	2.05	0.56
15:c:76:LEU:O	20:h:60:ILE:HD12	2.04	0.56
1:2:861:U:OP1	11:Y:64:ARG:NH2	2.39	0.56
4:R:102:VAL:HG11	4:R:129:ILE:HG13	1.88	0.56
20:h:291:VAL:HG11	20:h:313:GLY:HA3	1.87	0.56
1:2:1795:U:O2	17:e:10:ARG:HD2	2.05	0.56
20:h:214:VAL:HG12	20:h:214:VAL:O	2.04	0.55
1:2:1789:G:OP2	12:Z:132:ARG:NH2	2.36	0.55
1:2:1674:C:P	6:T:92:ARG:HH12	2.29	0.55
1:2:814:A:N1	1:2:857:U:C4	2.72	0.55
1:2:1080:U:H3	1:2:1091:A:N6	2.05	0.55
1:2:1760:G:O2'	1:2:1781:A:C2	2.58	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:871:G:H2'	1:2:872:G:C8	2.42	0.55
1:2:1660:A:P	20:h:20:LYS:NZ	2.80	0.55
20:h:424:PRO:CB	20:h:426:PHE:CE2	2.73	0.55
1:2:1080:U:N3	1:2:1091:A:N6	2.55	0.54
1:2:933:A:OP2	17:e:37:LYS:NZ	2.36	0.54
5:S:9:LEU:HD23	5:S:28:ALA:HB3	1.89	0.54
1:2:609:U:O4	15:c:25:ALA:HB3	2.08	0.54
20:h:491:ILE:HG23	20:h:523:ILE:HA	1.90	0.54
1:2:1038:U:C4	1:2:1092:A:C6	2.96	0.54
1:2:1145:U:C5	1:2:1633:A:C2	2.95	0.54
20:h:230:PHE:CE1	20:h:234:MET:CE	2.89	0.54
1:2:207:U:H2'	1:2:208:U:C6	2.43	0.54
13:a:71:ARG:HE	18:f:4:VAL:HG11	1.73	0.54
20:h:295:TYR:CG	20:h:327:LEU:CD2	2.83	0.54
20:h:426:PHE:CB	20:h:433:LEU:CD1	2.84	0.53
3:Q:120:LEU:HD21	3:Q:122:GLU:HG3	1.91	0.53
8:V:102:VAL:HG21	8:V:169:ILE:HD11	1.90	0.53
20:h:294:ILE:HG13	20:h:304:VAL:HG22	1.89	0.53
20:h:306:LEU:HB3	20:h:307:PRO:HD2	1.89	0.53
1:2:1745:G:C5'	20:h:27:ARG:HH11	2.20	0.53
1:2:1116:A:H2'	1:2:1117:U:C6	2.43	0.53
20:h:205:TYR:HD1	20:h:263:ILE:HD11	1.73	0.53
1:2:1796:C:C5	17:e:93:LYS:HA	2.43	0.52
1:2:1116:A:H2'	1:2:1117:U:H6	1.74	0.52
20:h:268:LEU:HD12	20:h:269:ALA:HA	1.90	0.52
1:2:1057:U:C4	1:2:1062:A:N1	2.75	0.52
10:X:69:LYS:C	10:X:70:ILE:HD12	2.34	0.52
12:Z:17:ALA:HB3	12:Z:81:VAL:HA	1.91	0.52
16:d:44:LEU:CD1	16:d:55:VAL:HG11	2.39	0.52
1:2:21:U:N3	1:2:605:A:C2	2.77	0.52
3:Q:137:ILE:HG22	3:Q:215:VAL:HG23	1.91	0.52
20:h:368:LEU:HA	20:h:549:ALA:HB3	1.90	0.52
1:2:1710:U:H2'	1:2:1711:C:H4'	1.92	0.52
1:2:10:G:C6	1:2:1145:U:C4	2.98	0.52
12:Z:30:VAL:HG23	12:Z:79:VAL:HG21	1.91	0.51
20:h:58:CYS:SG	20:h:59:GLY:N	2.81	0.51
20:h:222:LEU:HD22	20:h:226:GLU:HB2	1.92	0.51
4:R:80:VAL:HG13	4:R:81:MET:N	2.25	0.51
20:h:382:VAL:HG21	20:h:535:ALA:CB	2.40	0.51
1:2:1709:C:O2'	1:2:1710:U:C5	2.60	0.51
1:2:1677:C:OP1	8:V:42:ARG:NH1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:54:TYR:HA	16:d:22:GLN:HE22	1.76	0.51
20:h:57:GLY:O	20:h:58:CYS:SG	2.69	0.51
1:2:21:U:O4	1:2:605:A:N1	2.44	0.51
1:2:804:A:N3	14:b:105:THR:HG22	2.26	0.51
20:h:83:VAL:HA	20:h:95:HIS:HD2	1.75	0.51
1:2:1793:G:O6	17:e:34:LYS:NZ	2.38	0.51
1:2:408:C:O2'	1:2:1732:A:O2'	2.24	0.51
1:2:1674:C:P	6:T:92:ARG:NH1	2.83	0.51
1:2:1787:C:OP2	12:Z:132:ARG:N	2.44	0.50
1:2:407:A:HO2'	1:2:1671:A:H2	1.54	0.50
1:2:967:A:OP2	11:Y:124:ARG:NH2	2.33	0.50
1:2:1294:G:H5'	2:P:109:ASN:HD22	1.77	0.50
1:2:1728:A:H1'	8:V:32:GLN:CD	2.36	0.50
1:2:112:A:O2'	10:X:67:ARG:NH1	2.44	0.50
1:2:413:U:O2'	20:h:312:GLU:OE2	2.29	0.50
4:R:169:LEU:HD23	4:R:198:THR:HG22	1.92	0.50
1:2:867:G:C5'	11:Y:4:MET:HE2	2.42	0.49
20:h:99:THR:CG2	20:h:100:PRO:HD2	2.42	0.49
1:2:414:C:O3'	20:h:311:ARG:HB3	2.11	0.49
1:2:433:C:C5'	20:h:63:LYS:HZ1	2.25	0.49
1:2:330:G:OP2	8:V:172:ARG:NH1	2.46	0.49
20:h:570:VAL:HB	20:h:583:ILE:HD11	1.94	0.49
1:2:1035:G:H4'	1:2:1035:G:OP1	2.10	0.49
2:P:98:ILE:HD11	2:P:116:LYS:CE	2.43	0.49
7:U:46:ILE:HD11	7:U:58:LEU:HB3	1.94	0.49
7:U:60:ILE:HG22	7:U:62:VAL:CG2	2.41	0.49
11:Y:66:ILE:HG23	11:Y:67:THR:HG23	1.94	0.49
20:h:424:PRO:HB2	20:h:426:PHE:CZ	2.43	0.49
1:2:257:A:O2'	8:V:64:ASN:OD1	2.31	0.49
1:2:1636:C:C5	1:2:1638:G:C4	3.00	0.49
1:2:1728:A:C1'	8:V:32:GLN:HE22	2.24	0.49
1:2:608:U:O2	1:2:608:U:O4'	2.29	0.49
20:h:223:SER:N	22:h:705:ANP:O2'	2.46	0.49
1:2:1641:C:H1'	1:2:1762:A:C2	2.47	0.49
20:h:187:VAL:HG23	20:h:214:VAL:O	2.13	0.49
8:V:78:ILE:HA	8:V:104:ILE:HG22	1.94	0.48
2:P:98:ILE:HD11	2:P:116:LYS:HE3	1.94	0.48
20:h:573:ARG:HB2	20:h:573:ARG:HH21	1.78	0.48
1:2:1038:U:C4	1:2:1092:A:N6	2.76	0.48
1:2:323:A:OP2	8:V:10:LYS:NZ	2.40	0.48
20:h:383:MET:HB3	20:h:391:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:55:VAL:HG13	16:d:75:VAL:CG2	2.40	0.48
20:h:295:TYR:CB	20:h:327:LEU:CD2	2.90	0.48
1:2:567:A:OP1	15:c:70:LYS:NZ	2.47	0.48
1:2:1786:G:OP2	12:Z:136:ARG:NH2	2.47	0.48
11:Y:21:ASN:O	11:Y:22:ALA:HB3	2.14	0.48
20:h:227:LEU:O	20:h:227:LEU:HD12	2.14	0.48
20:h:273:TYR:N	20:h:273:TYR:CD2	2.82	0.48
1:2:68:A:OP1	6:T:160:ARG:NH2	2.40	0.48
1:2:154:G:OP1	6:T:2:LYS:NZ	2.41	0.48
1:2:386:G:OP2	8:V:25:ARG:NH2	2.47	0.48
1:2:1080:U:C4	1:2:1091:A:C6	3.02	0.48
3:Q:139:ALA:HB2	3:Q:212:VAL:HG12	1.94	0.48
20:h:316:ILE:HD13	20:h:322:ILE:HG21	1.95	0.48
1:2:222:A:C6	1:2:833:U:C2	3.02	0.47
1:2:1636:C:C6	1:2:1638:G:H1'	2.49	0.47
1:2:1641:C:C2	1:2:1762:A:C6	3.01	0.47
1:2:1745:G:H5''	20:h:27:ARG:NH1	2.23	0.47
20:h:214:VAL:HG11	20:h:222:LEU:HD11	1.96	0.47
1:2:207:U:O2'	8:V:178:ARG:NH2	2.48	0.47
5:S:28:ALA:HB1	5:S:29:PRO:HD2	1.96	0.47
20:h:57:GLY:O	20:h:59:GLY:N	2.47	0.47
1:2:391:A:HO2'	1:2:1730:A:H4'	1.78	0.47
1:2:429:G:H2'	1:2:430:G:H8	1.80	0.47
1:2:1744:A:H2	20:h:22:ARG:NH1	2.12	0.47
2:P:9:LEU:HD21	2:P:14:ALA:HB2	1.97	0.47
15:c:82:LYS:HE3	20:h:33:LYS:HZ3	1.78	0.47
20:h:154:ASN:O	20:h:157:THR:HG22	2.15	0.47
1:2:222:A:C6	1:2:833:U:C4	3.03	0.47
1:2:414:C:H5'	20:h:312:GLU:HG2	1.95	0.47
15:c:82:LYS:HE3	20:h:33:LYS:HZ1	1.79	0.47
16:d:55:VAL:HG12	16:d:56:SER:O	2.15	0.47
20:h:99:THR:CG2	20:h:101:ARG:HG2	2.45	0.47
4:R:139:ILE:HD12	4:R:191:ALA:HB1	1.97	0.47
13:a:71:ARG:NE	18:f:4:VAL:HG11	2.29	0.47
15:c:57:LEU:HD11	15:c:73:ARG:HG2	1.97	0.47
20:h:99:THR:HG23	20:h:100:PRO:HD2	1.97	0.46
1:2:391:A:O4'	1:2:1731:A:C5'	2.61	0.46
1:2:1681:A:H8	6:T:66:GLY:HA3	1.79	0.46
1:2:150:U:P	16:d:123:LYS:HE3	2.54	0.46
1:2:323:A:OP1	8:V:11:ARG:HB2	2.15	0.46
2:P:139:VAL:HG23	4:R:62:PRO:HG2	1.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:110:ASP:O	11:Y:114:ARG:HG2	2.16	0.46
14:b:11:LEU:HD21	14:b:37:PHE:CZ	2.51	0.46
1:2:1794:A:O2'	17:e:79:ILE:HD13	2.15	0.46
9:W:109:LEU:HD23	9:W:129:ILE:HD13	1.98	0.46
17:e:74:CYS:SG	17:e:77:CYS:SG	3.14	0.46
20:h:230:PHE:HZ	20:h:234:MET:HE1	1.73	0.46
20:h:115:GLY:C	22:h:703:ANP:O1A	2.59	0.46
20:h:585:LYS:HE2	20:h:585:LYS:HB2	1.58	0.46
1:2:1146:G:C2	1:2:1633:A:C2	3.04	0.46
1:2:1791:A:H5''	17:e:8:ASN:HB3	1.97	0.46
20:h:475:ARG:HA	20:h:478:ILE:HD12	1.98	0.46
20:h:384:MET:O	20:h:391:LYS:HD3	2.15	0.46
4:R:183:ALA:HB1	4:R:211:LEU:HD21	1.99	0.45
20:h:451:VAL:HG13	20:h:457:ILE:HG21	1.98	0.45
1:2:2:A:H3'	4:R:179:VAL:HG11	1.98	0.45
1:2:414:C:O3'	20:h:311:ARG:HD3	2.15	0.45
4:R:102:VAL:HG11	4:R:129:ILE:CG1	2.46	0.45
6:T:32:ILE:HD11	6:T:63:MET:HE3	1.98	0.45
1:2:15:U:O2'	1:2:620:A:N6	2.49	0.45
1:2:222:A:N6	1:2:833:U:C5	2.84	0.45
7:U:122:HIS:NE2	7:U:177:THR:HG22	2.32	0.45
20:h:151:GLU:C	20:h:151:GLU:CD	2.84	0.45
2:P:139:VAL:HG22	2:P:139:VAL:O	2.15	0.45
5:S:14:ALA:HB1	5:S:15:PRO:HD2	1.98	0.45
1:2:1087:A:H2'	1:2:1088:A:C8	2.51	0.45
4:R:80:VAL:HG22	4:R:81:MET:H	1.81	0.45
5:S:47:PHE:CE2	5:S:52:LEU:HD11	2.52	0.45
1:2:1722:A:H2'	1:2:1723:U:O4'	2.16	0.45
5:S:147:ILE:HG21	5:S:169:ILE:HG13	1.97	0.45
1:2:16:G:H2'	1:2:17:C:C6	2.51	0.45
1:2:150:U:OP2	16:d:123:LYS:HE3	2.16	0.45
1:2:1796:C:N4	17:e:93:LYS:HG2	2.31	0.45
20:h:295:TYR:CB	20:h:327:LEU:HD21	2.45	0.45
10:X:7:VAL:HG13	10:X:8:GLN:NE2	2.32	0.45
10:X:94:ILE:N	10:X:94:ILE:HD12	2.32	0.45
20:h:57:GLY:C	20:h:58:CYS:SG	3.00	0.45
1:2:865:A:OP1	14:b:28:ARG:NH2	2.50	0.45
1:2:952:A:H5'	11:Y:98:VAL:HG22	1.98	0.45
5:S:59:ARG:NH1	16:d:85:PHE:O	2.48	0.45
8:V:9:HIS:O	8:V:10:LYS:HB2	2.17	0.45
1:2:499:U:O2	1:2:499:U:O4'	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:160:VAL:HG13	5:S:169:ILE:HG23	1.99	0.44
7:U:58:LEU:HD12	7:U:90:VAL:HG13	1.99	0.44
1:2:53:G:H5'	20:h:290:PHE:HZ	1.83	0.44
1:2:1301:U:H2'	1:2:1302:U:O4'	2.17	0.44
7:U:138:LYS:HB2	14:b:54:ASP:HB3	1.98	0.44
20:h:214:VAL:CG2	20:h:222:LEU:HD21	2.48	0.44
1:2:1660:A:OP1	20:h:20:LYS:CE	2.65	0.44
5:S:141:THR:HG21	5:S:162:ILE:HD11	1.98	0.44
10:X:80:MET:HB2	10:X:83:THR:HG23	1.99	0.44
1:2:141:U:O2'	1:2:266:A:N3	2.50	0.44
10:X:57:LYS:HG2	10:X:131:ILE:HD11	1.98	0.44
15:c:43:PHE:CE1	15:c:49:ALA:HB3	2.52	0.44
20:h:389:THR:CB	20:h:541:PHE:HB3	2.42	0.44
1:2:472:U:O2'	1:2:769:A:N3	2.47	0.44
1:2:512:A:H2'	1:2:513:U:O4'	2.17	0.44
1:2:1636:C:C4	1:2:1638:G:C4	3.05	0.44
3:Q:47:LEU:CD1	12:Z:76:ILE:HD11	2.48	0.44
17:e:74:CYS:HG	17:e:77:CYS:HG	1.65	0.44
20:h:426:PHE:CD1	20:h:433:LEU:HD22	2.51	0.44
20:h:585:LYS:O	20:h:587:ASP:N	2.50	0.44
15:c:52:ILE:HD13	20:h:30:PRO:HG3	2.00	0.44
20:h:387:ASN:N	20:h:387:ASN:OD1	2.51	0.44
1:2:632:U:H4'	15:c:11:SER:HB3	1.99	0.44
1:2:868:G:N2	11:Y:48:SER:OG	2.50	0.44
1:2:980:G:H4'	1:2:1776:A:H4'	1.98	0.44
1:2:635:A:H2'	1:2:636:A:O4'	2.18	0.44
1:2:1038:U:O4	1:2:1092:A:C2	2.69	0.44
1:2:79:C:H5'	6:T:172:ALA:HB3	2.00	0.43
5:S:181:VAL:HA	5:S:227:VAL:HA	2.00	0.43
20:h:316:ILE:HD13	20:h:322:ILE:CG2	2.48	0.43
1:2:8:U:O4	1:2:15:U:O4	2.36	0.43
1:2:555:A:C2	1:2:556:A:C6	3.07	0.43
1:2:1142:A:OP1	17:e:2:PRO:N	2.51	0.43
1:2:1635:A:H4'	1:2:1638:G:O2'	2.19	0.43
20:h:214:VAL:HG21	20:h:222:LEU:HD21	2.01	0.43
1:2:93:A:O4'	5:S:3:ARG:NH1	2.51	0.43
6:T:113:ILE:HG22	6:T:114:VAL:N	2.34	0.43
20:h:585:LYS:O	20:h:585:LYS:HD3	2.19	0.43
4:R:158:THR:HG21	4:R:221:THR:HG22	2.00	0.43
5:S:14:ALA:HB1	5:S:18:TRP:CZ3	2.54	0.43
7:U:139:ARG:HB3	14:b:51:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:275:ILE:O	20:h:275:ILE:HG23	2.19	0.43
1:2:71:A:H2'	1:2:72:A:O4'	2.19	0.43
1:2:162:A:H62	16:d:124:ARG:NH2	2.17	0.43
8:V:107:THR:N	8:V:108:PRO:CD	2.82	0.43
9:W:104:PHE:O	9:W:147:MET:HE1	2.19	0.43
20:h:11:VAL:HA	20:h:70:ILE:HG22	2.01	0.43
20:h:102:PRO:HB3	20:h:273:TYR:CD1	2.53	0.43
1:2:1146:G:N3	1:2:1633:A:C2	2.87	0.42
1:2:150:U:OP1	16:d:123:LYS:NZ	2.47	0.42
1:2:1744:A:C2	20:h:22:ARG:NH1	2.87	0.42
5:S:65:LEU:HD23	5:S:70:VAL:CG1	2.49	0.42
20:h:243:TYR:CD1	20:h:267:LEU:HD23	2.53	0.42
1:2:886:U:O2'	12:Z:122:PRO:HA	2.19	0.42
7:U:173:TYR:CE2	7:U:181:ILE:HD11	2.54	0.42
9:W:136:VAL:HG23	9:W:141:VAL:HG21	2.00	0.42
20:h:4:LYS:N	20:h:79:LEU:HG	2.33	0.42
1:2:53:G:H2'	1:2:54:C:C6	2.54	0.42
20:h:291:VAL:CG1	20:h:313:GLY:HA3	2.49	0.42
1:2:210:A:H2'	1:2:211:U:O4'	2.19	0.42
1:2:1648:A:H2'	1:2:1649:G:O4'	2.19	0.42
3:Q:135:LEU:HD13	3:Q:137:ILE:HG23	2.00	0.42
5:S:181:VAL:HG22	5:S:227:VAL:HG12	2.01	0.42
20:h:217:ARG:NH1	20:h:366:PHE:CE2	2.88	0.42
20:h:257:ARG:HG2	20:h:283:VAL:HG11	2.01	0.42
1:2:441:A:H2'	1:2:442:C:C6	2.55	0.42
1:2:600:U:N3	1:2:601:A:N7	2.68	0.42
1:2:992:A:N3	1:2:992:A:O4'	2.53	0.42
20:h:258:LEU:HD23	20:h:283:VAL:HG13	2.01	0.42
20:h:571:THR:HG22	20:h:600:TYR:CD1	2.55	0.42
1:2:637:C:OP1	14:b:32:LYS:N	2.53	0.42
1:2:992:A:C6	1:2:1012:U:N3	2.88	0.42
5:S:100:ARG:HB2	5:S:114:ILE:HD13	2.02	0.42
1:2:414:C:C2'	20:h:311:ARG:HD3	2.43	0.42
1:2:433:C:C3'	20:h:63:LYS:HZ1	2.33	0.42
6:T:55:GLY:HA3	6:T:63:MET:HE2	2.02	0.42
1:2:657:U:C4	1:2:677:G:C2	3.08	0.41
20:h:321:HIS:CB	20:h:326:ASN:HD22	2.33	0.41
20:h:445:PRO:CB	20:h:449:THR:HG23	2.49	0.41
11:Y:4:MET:HE3	11:Y:121:ARG:CG	2.50	0.41
20:h:260:ALA:O	20:h:263:ILE:HG22	2.21	0.41
1:2:1038:U:O3'	14:b:20:THR:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:248:ILE:HD12	9:W:71:PHE:CG	2.56	0.41
8:V:29:LEU:HD21	8:V:31:ARG:HG3	2.01	0.41
20:h:85:HIS:CE1	20:h:118:THR:HG21	2.54	0.41
1:2:1751:C:H2'	1:2:1752:U:O4'	2.21	0.41
20:h:4:LYS:HA	20:h:79:LEU:CD1	2.49	0.41
9:W:122:VAL:HG23	9:W:123:HIS:HD2	1.86	0.41
20:h:368:LEU:N	20:h:368:LEU:HD23	2.36	0.41
1:2:924:A:H2'	1:2:925:G:C8	2.56	0.41
1:2:962:C:N4	1:2:963:A:C2	2.88	0.41
1:2:1641:C:C2	1:2:1762:A:N6	2.88	0.41
3:Q:120:LEU:HD23	3:Q:120:LEU:C	2.46	0.41
3:Q:129:THR:HG21	3:Q:133:TYR:HB2	2.02	0.41
4:R:116:LYS:HG2	4:R:127:ALA:HB3	2.02	0.41
5:S:136:VAL:HG13	5:S:149:TYR:CE1	2.55	0.41
20:h:13:ALA:HB3	20:h:16:CYS:HB2	2.03	0.41
20:h:190:LEU:HD12	20:h:191:LEU:N	2.36	0.41
20:h:424:PRO:O	20:h:425:LYS:HG2	2.20	0.41
1:2:447:U:H2'	1:2:448:C:O4'	2.21	0.41
1:2:538:A:OP2	9:W:175:ARG:NH1	2.54	0.41
1:2:1739:C:H2'	1:2:1740:A:O4'	2.21	0.41
2:P:115:PHE:CZ	4:R:39:THR:HG22	2.56	0.41
20:h:148:ARG:C	20:h:150:SER:N	2.78	0.41
1:2:428:A:H2	1:2:440:U:O2	2.04	0.41
1:2:992:A:N6	1:2:1012:U:C4	2.89	0.41
2:P:20:ALA:HB2	2:P:172:LEU:HD13	2.03	0.41
3:Q:214:LYS:O	3:Q:215:VAL:C	2.63	0.41
4:R:148:LEU:HD11	9:W:94:ASP:CB	2.50	0.41
5:S:68:ARG:O	5:S:70:VAL:N	2.54	0.41
20:h:219:ILE:H	20:h:219:ILE:HG13	1.60	0.41
20:h:288:SER:O	20:h:310:VAL:HG21	2.21	0.41
20:h:492:ASP:HA	20:h:524:VAL:HB	2.03	0.41
1:2:153:G:OP2	16:d:131:ARG:CD	2.68	0.41
13:a:34:ILE:HG13	13:a:69:LEU:HD11	2.03	0.41
20:h:208:ILE:CG2	20:h:263:ILE:HD13	2.51	0.41
1:2:10:G:C6	1:2:11:A:C5	3.09	0.40
1:2:811:A:N7	7:U:111:LYS:CB	2.84	0.40
20:h:23:GLN:HE22	20:h:43:PRO:HG3	1.86	0.40
1:2:391:A:H4'	1:2:1730:A:O3'	2.21	0.40
1:2:1081:A:C2	1:2:1091:A:C6	3.09	0.40
3:Q:171:ILE:HD13	3:Q:197:ILE:HD13	2.01	0.40
15:c:124:VAL:HG12	15:c:125:VAL:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:228:GLN:HG2	20:h:252:LEU:HD11	2.03	0.40
20:h:437:LYS:NZ	20:h:484:ILE:HG23	2.37	0.40
1:2:150:U:P	16:d:123:LYS:CE	3.10	0.40
1:2:162:A:H2'	1:2:163:G:O4'	2.22	0.40
1:2:208:U:N3	1:2:257:A:C2	2.89	0.40
1:2:1636:C:C6	1:2:1638:G:C4	3.10	0.40
1:2:151:G:N3	6:T:13:GLN:NE2	2.57	0.40
1:2:447:U:O2'	5:S:27:TYR:O	2.39	0.40
1:2:1745:G:C5'	20:h:27:ARG:NH1	2.82	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	
2	P	204/252 (81%)	175 (86%)	19 (9%)	10 (5%)	1	18
3	Q	212/255 (83%)	163 (77%)	35 (16%)	14 (7%)	1	14
4	R	224/254 (88%)	192 (86%)	21 (9%)	11 (5%)	1	18
5	S	258/261 (99%)	226 (88%)	22 (8%)	10 (4%)	2	21
6	T	224/236 (95%)	207 (92%)	13 (6%)	4 (2%)	6	34
7	U	182/190 (96%)	161 (88%)	15 (8%)	6 (3%)	3	24
8	V	184/200 (92%)	158 (86%)	21 (11%)	5 (3%)	4	28
9	W	183/197 (93%)	162 (88%)	14 (8%)	7 (4%)	2	21
10	X	153/156 (98%)	133 (87%)	14 (9%)	6 (4%)	2	21
11	Y	148/151 (98%)	134 (90%)	13 (9%)	1 (1%)	18	53
12	Z	125/137 (91%)	105 (84%)	18 (14%)	2 (2%)	7	36
13	a	85/87 (98%)	73 (86%)	8 (9%)	4 (5%)	2	19
14	b	127/130 (98%)	115 (91%)	8 (6%)	4 (3%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	c	142/145 (98%)	116 (82%)	20 (14%)	6 (4%)	2	20
16	d	130/135 (96%)	112 (86%)	10 (8%)	8 (6%)	1	15
17	e	95/119 (80%)	78 (82%)	13 (14%)	4 (4%)	2	20
18	f	79/82 (96%)	70 (89%)	7 (9%)	2 (2%)	4	29
19	g	58/63 (92%)	51 (88%)	7 (12%)	0	100	100
20	h	574/608 (94%)	472 (82%)	82 (14%)	20 (4%)	3	23
All	All	3387/3658 (93%)	2903 (86%)	360 (11%)	124 (4%)	4	22

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	111	ILE
3	Q	215	VAL
3	Q	216	LYS
7	U	110	GLN
9	W	98	ALA
9	W	134	ILE
10	X	6	THR
12	Z	42	VAL
13	a	7	GLN
14	b	78	ARG
14	b	83	ILE
16	d	57	VAL
17	e	84	VAL
18	f	75	GLU
20	h	58	CYS
20	h	98	PRO
20	h	99	THR
20	h	100	PRO
20	h	138	PRO
20	h	197	LYS
20	h	324	ALA
20	h	326	ASN
20	h	445	PRO
20	h	446	GLN
2	P	109	ASN
2	P	203	PHE
3	Q	62	LYS
4	R	77	GLN
4	R	145	GLY

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Mol	Chain	Res	Type
5	S	69	HIS
5	S	76	VAL
5	S	195	ILE
5	S	227	VAL
7	U	156	SER
8	V	152	ILE
10	X	7	VAL
13	a	82	VAL
14	b	57	ARG
15	c	52	ILE
15	c	53	VAL
20	h	23	GLN
20	h	83	VAL
20	h	188	GLY
20	h	452	VAL
20	h	481	ALA
2	P	39	ASN
2	P	110	TYR
3	Q	94	LYS
3	Q	147	ALA
3	Q	217	LEU
4	R	79	GLU
4	R	81	MET
4	R	252	LYS
5	S	185	GLY
5	S	201	HIS
5	S	257	ALA
6	T	69	LEU
7	U	155	ASP
8	V	9	HIS
8	V	10	LYS
8	V	11	ARG
9	W	120	LYS
10	X	5	LEU
10	X	55	ASP
13	a	12	TYR
16	d	6	THR
16	d	52	LYS
16	d	58	PHE
17	e	63	ALA
18	f	4	VAL
20	h	82	HIS

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Mol	Chain	Res	Type
20	h	440	GLY
2	P	35	PRO
2	P	139	VAL
2	P	167	LYS
2	P	190	ASP
3	Q	39	GLU
3	Q	176	VAL
3	Q	209	ASN
3	Q	218	LEU
4	R	150	GLN
7	U	74	GLN
9	W	99	LEU
9	W	118	LEU
9	W	146	PHE
10	X	53	TYR
15	c	25	ALA
15	c	99	ASN
15	c	115	GLY
17	e	8	ASN
20	h	483	GLY
2	P	202	TYR
4	R	80	VAL
4	R	235	LEU
6	T	20	ASP
8	V	52	ASN
11	Y	144	ALA
12	Z	124	ASP
15	c	131	SER
16	d	36	SER
16	d	51	GLU
3	Q	53	GLY
4	R	231	ALA
5	S	164	LEU
5	S	245	LYS
6	T	132	ARG
7	U	73	VAL
7	U	98	ILE
9	W	169	PRO
14	b	30	SER
16	d	59	GLY
20	h	364	GLY
20	h	454	PRO

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Mol	Chain	Res	Type
3	Q	210	ILE
16	d	5	VAL
4	R	109	GLY
13	a	9	VAL
4	R	93	GLY
6	T	112	VAL
10	X	130	PRO
17	e	59	TYR
3	Q	43	VAL
3	Q	204	ILE
5	S	228	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	164/210 (78%)	164 (100%)	0	100	100
3	Q	191/224 (85%)	186 (97%)	5 (3%)	40	60
4	R	185/205 (90%)	182 (98%)	3 (2%)	55	69
5	S	221/222 (100%)	219 (99%)	2 (1%)	70	75
6	T	188/201 (94%)	185 (98%)	3 (2%)	55	69
7	U	165/170 (97%)	162 (98%)	3 (2%)	51	67
8	V	150/161 (93%)	150 (100%)	0	100	100
9	W	158/166 (95%)	153 (97%)	5 (3%)	34	56
10	X	129/137 (94%)	126 (98%)	3 (2%)	44	63
11	Y	127/128 (99%)	126 (99%)	1 (1%)	73	77
12	Z	81/105 (77%)	78 (96%)	3 (4%)	30	53
13	a	74/74 (100%)	72 (97%)	2 (3%)	39	60
14	b	110/111 (99%)	106 (96%)	4 (4%)	31	54
15	c	119/120 (99%)	113 (95%)	6 (5%)	22	47
16	d	111/113 (98%)	108 (97%)	3 (3%)	39	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	e	83/101 (82%)	83 (100%)	0	100	100
18	f	70/71 (99%)	69 (99%)	1 (1%)	59	71
19	g	50/54 (93%)	50 (100%)	0	100	100
20	h	513/537 (96%)	484 (94%)	29 (6%)	18	44
All	All	2889/3110 (93%)	2816 (98%)	73 (2%)	42	62

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	137	ILE
3	Q	149	GLN
3	Q	176	VAL
3	Q	215	VAL
3	Q	218	LEU
4	R	53	ILE
4	R	91	ARG
4	R	139	ILE
5	S	189	LEU
5	S	228	ILE
6	T	24	ILE
6	T	78	THR
6	T	112	VAL
7	U	46	ILE
7	U	62	VAL
7	U	130	VAL
9	W	33	GLU
9	W	99	LEU
9	W	118	LEU
9	W	120	LYS
9	W	134	ILE
10	X	5	LEU
10	X	7	VAL
10	X	128	CYS
11	Y	71	ILE
12	Z	13	VAL
12	Z	16	VAL
12	Z	137	LEU
13	a	69	LEU
13	a	78	LEU
14	b	82	LYS
14	b	83	ILE

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Mol	Chain	Res	Type
14	b	93	LEU
14	b	103	ILE
15	c	9	LEU
15	c	19	ARG
15	c	26	GLU
15	c	53	VAL
15	c	100	ASP
15	c	124	VAL
16	d	34	ASN
16	d	57	VAL
16	d	131	ARG
18	f	75	GLU
20	h	22	ARG
20	h	24	GLU
20	h	53	ILE
20	h	79	LEU
20	h	97	LEU
20	h	99	THR
20	h	114	ILE
20	h	138	PRO
20	h	152	LEU
20	h	153	GLN
20	h	195	MET
20	h	198	SER
20	h	209	LEU
20	h	211	LEU
20	h	218	ASP
20	h	219	ILE
20	h	242	VAL
20	h	273	TYR
20	h	306	LEU
20	h	368	LEU
20	h	380	ILE
20	h	420	GLN
20	h	425	LYS
20	h	426	PHE
20	h	449	THR
20	h	563	ARG
20	h	573	ARG
20	h	585	LYS
20	h	590	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52)

such sidechains are listed below:

Mol	Chain	Res	Type
2	P	28	ASN
2	P	69	ASN
2	P	131	GLN
3	Q	146	GLN
3	Q	211	HIS
4	R	87	GLN
4	R	89	GLN
4	R	228	ASN
4	R	233	GLN
5	S	197	HIS
6	T	34	GLN
6	T	119	GLN
6	T	190	GLN
7	U	74	GLN
7	U	108	GLN
8	V	20	GLN
8	V	32	GLN
9	W	139	GLN
9	W	176	ASN
10	X	8	GLN
10	X	127	GLN
11	Y	5	HIS
11	Y	58	HIS
11	Y	105	ASN
11	Y	138	ASN
13	a	3	ASN
13	a	29	HIS
13	a	33	GLN
13	a	35	ASN
14	b	15	ASN
14	b	64	GLN
14	b	113	HIS
15	c	18	HIS
15	c	99	ASN
16	d	22	GLN
16	d	107	GLN
16	d	133	ASN
17	e	11	ASN
17	e	43	ASN
18	f	9	HIS
20	h	78	ASN
20	h	95	HIS

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Mol	Chain	Res	Type
20	h	185	GLN
20	h	210	GLN
20	h	326	ASN
20	h	363	GLN
20	h	420	GLN
20	h	432	GLN
20	h	446	GLN
20	h	463	GLN
20	h	526	HIS
20	h	562	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1319/1798 (73%)	503 (38%)	65 (4%)

All (503) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	8	U
1	2	9	U
1	2	11	A
1	2	19	A
1	2	25	C
1	2	26	A
1	2	34	G
1	2	39	A
1	2	42	G
1	2	43	A
1	2	44	U
1	2	45	U
1	2	46	A
1	2	47	A
1	2	48	G
1	2	50	C
1	2	51	A
1	2	52	U
1	2	60	U

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Mol	Chain	Res	Type
1	2	63	G
1	2	65	A
1	2	66	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	71	A
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	77	U
1	2	78	A
1	2	81	G
1	2	86	A
1	2	99	C
1	2	100	A
1	2	101	U
1	2	102	U
1	2	104	A
1	2	105	A
1	2	114	C
1	2	116	U
1	2	117	U
1	2	125	U
1	2	126	A
1	2	127	G
1	2	128	U
1	2	129	U
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	138	A
1	2	139	C
1	2	140	A
1	2	141	U
1	2	142	G
1	2	143	G

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Mol	Chain	Res	Type
1	2	147	A
1	2	159	U
1	2	160	C
1	2	161	U
1	2	166	C
1	2	170	U
1	2	171	A
1	2	174	U
1	2	175	G
1	2	177	U
1	2	178	U
1	2	180	A
1	2	185	U
1	2	188	A
1	2	189	C
1	2	194	U
1	2	195	G
1	2	199	G
1	2	201	G
1	2	202	A
1	2	203	U
1	2	204	G
1	2	205	U
1	2	206	A
1	2	211	U
1	2	215	A
1	2	216	U
1	2	218	A
1	2	225	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	230	C
1	2	232	U
1	2	233	C
1	2	234	G
1	2	238	U
1	2	240	U
1	2	241	U
1	2	243	G
1	2	250	C
1	2	257	A

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Mol	Chain	Res	Type
1	2	260	U
1	2	261	U
1	2	262	U
1	2	270	C
1	2	272	U
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	287	G
1	2	295	A
1	2	299	A
1	2	308	C
1	2	312	A
1	2	313	U
1	2	314	C
1	2	316	A
1	2	317	C
1	2	319	U
1	2	320	U
1	2	321	C
1	2	322	G
1	2	323	A
1	2	324	U
1	2	329	G
1	2	332	U
1	2	333	A
1	2	334	G
1	2	335	U
1	2	337	G
1	2	338	C
1	2	347	G
1	2	348	U
1	2	349	U
1	2	350	U
1	2	351	C
1	2	352	A
1	2	355	G
1	2	359	A
1	2	360	A
1	2	361	C
1	2	369	A

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Mol	Chain	Res	Type
1	2	372	G
1	2	378	A
1	2	381	C
1	2	387	A
1	2	390	G
1	2	396	G
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	411	C
1	2	415	C
1	2	416	A
1	2	417	A
1	2	418	G
1	2	422	G
1	2	423	G
1	2	424	C
1	2	426	G
1	2	434	G
1	2	436	A
1	2	437	A
1	2	439	U
1	2	440	U
1	2	441	A
1	2	444	C
1	2	446	A
1	2	447	U
1	2	448	C
1	2	453	U
1	2	454	U
1	2	455	C
1	2	456	A
1	2	459	G
1	2	460	A
1	2	464	A
1	2	469	C
1	2	471	A
1	2	475	A
1	2	477	A
1	2	478	A
1	2	486	G

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Mol	Chain	Res	Type
1	2	488	G
1	2	489	C
1	2	490	C
1	2	492	A
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	500	C
1	2	501	U
1	2	502	U
1	2	503	G
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	514	G
1	2	518	A
1	2	525	A
1	2	527	A
1	2	532	U
1	2	534	A
1	2	537	G
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	545	A
1	2	546	U
1	2	549	G
1	2	554	C
1	2	555	A
1	2	556	A
1	2	558	U
1	2	559	C
1	2	561	G
1	2	562	G
1	2	565	C
1	2	566	C
1	2	567	A
1	2	568	G

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Mol	Chain	Res	Type
1	2	572	C
1	2	579	A
1	2	580	A
1	2	582	U
1	2	585	A
1	2	587	C
1	2	594	A
1	2	595	G
1	2	606	A
1	2	607	G
1	2	608	U
1	2	610	G
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	635	A
1	2	639	U
1	2	641	G
1	2	643	G
1	2	645	C
1	2	654	C
1	2	656	G
1	2	657	U
1	2	658	C
1	2	678	A
1	2	679	U
1	2	680	U
1	2	681	U
1	2	682	C
1	2	684	A
1	2	687	G
1	2	688	G
1	2	690	G
1	2	694	U
1	2	696	C
1	2	698	U
1	2	700	C
1	2	701	U
1	2	702	G
1	2	704	C
1	2	705	U

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Mol	Chain	Res	Type
1	2	706	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	711	U
1	2	713	A
1	2	714	G
1	2	716	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	729	G
1	2	730	G
1	2	733	A
1	2	735	C
1	2	736	C
1	2	738	G
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	744	U
1	2	745	U
1	2	752	A
1	2	754	A
1	2	755	A
1	2	756	A
1	2	763	G
1	2	766	U
1	2	767	U
1	2	771	A
1	2	774	A
1	2	775	G
1	2	776	G
1	2	778	G
1	2	780	A

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Mol	Chain	Res	Type
1	2	781	U
1	2	782	U
1	2	783	G
1	2	788	A
1	2	795	U
1	2	798	C
1	2	803	A
1	2	805	U
1	2	806	A
1	2	809	A
1	2	811	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	816	G
1	2	817	A
1	2	818	C
1	2	819	G
1	2	821	U
1	2	823	G
1	2	826	U
1	2	827	C
1	2	828	U
1	2	830	U
1	2	833	U
1	2	835	U
1	2	836	U
1	2	838	G
1	2	839	U
1	2	844	A
1	2	845	G
1	2	846	G
1	2	854	U
1	2	857	U
1	2	863	A
1	2	864	U
1	2	865	A
1	2	877	G
1	2	891	A
1	2	895	G
1	2	901	G

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Mol	Chain	Res	Type
1	2	903	U
1	2	904	G
1	2	906	A
1	2	911	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	917	U
1	2	922	G
1	2	929	A
1	2	931	C
1	2	932	U
1	2	933	A
1	2	934	C
1	2	935	U
1	2	940	A
1	2	942	G
1	2	951	A
1	2	959	U
1	2	960	U
1	2	965	U
1	2	966	A
1	2	970	A
1	2	987	G
1	2	988	A
1	2	998	A
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1006	C
1	2	1007	C
1	2	1013	A
1	2	1014	G
1	2	1023	A
1	2	1024	U
1	2	1025	A
1	2	1026	A
1	2	1027	A
1	2	1028	C
1	2	1029	U
1	2	1030	A
1	2	1032	G

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Mol	Chain	Res	Type
1	2	1035	G
1	2	1039	A
1	2	1051	G
1	2	1052	U
1	2	1053	G
1	2	1055	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1062	A
1	2	1064	G
1	2	1072	C
1	2	1074	G
1	2	1076	A
1	2	1082	C
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1098	U
1	2	1099	U
1	2	1100	G
1	2	1108	G
1	2	1113	A
1	2	1114	G
1	2	1115	U
1	2	1116	A
1	2	1119	G
1	2	1124	A
1	2	1138	A
1	2	1150	G
1	2	1152	A
1	2	1291	G
1	2	1299	G
1	2	1301	U
1	2	1305	U
1	2	1306	C
1	2	1307	U
1	2	1321	A
1	2	1322	A
1	2	1324	G
1	2	1628	U
1	2	1631	A

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Mol	Chain	Res	Type
1	2	1632	C
1	2	1634	C
1	2	1636	C
1	2	1637	C
1	2	1639	C
1	2	1640	C
1	2	1642	G
1	2	1643	U
1	2	1647	U
1	2	1649	G
1	2	1651	A
1	2	1656	U
1	2	1657	U
1	2	1658	G
1	2	1662	G
1	2	1663	G
1	2	1688	U
1	2	1689	A
1	2	1692	G
1	2	1693	A
1	2	1709	C
1	2	1710	U
1	2	1711	C
1	2	1712	A
1	2	1713	G
1	2	1714	A
1	2	1715	G
1	2	1717	G
1	2	1722	A
1	2	1732	A
1	2	1736	G
1	2	1737	G
1	2	1742	U
1	2	1744	A
1	2	1746	A
1	2	1747	G
1	2	1752	U
1	2	1753	A
1	2	1754	A
1	2	1755	A
1	2	1757	G
1	2	1758	U

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Mol	Chain	Res	Type
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1767	G
1	2	1769	U
1	2	1770	U
1	2	1772	C
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1786	G
1	2	1787	C
1	2	1791	A
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
1	2	1797	A

All (65) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	42	G
1	2	46	A
1	2	47	A
1	2	51	A
1	2	68	A
1	2	99	C
1	2	104	A
1	2	126	A
1	2	128	U
1	2	132	U
1	2	139	C
1	2	158	U
1	2	159	U
1	2	169	A
1	2	170	U
1	2	224	C
1	2	232	U

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Mol	Chain	Res	Type
1	2	265	A
1	2	277	U
1	2	312	A
1	2	313	U
1	2	322	G
1	2	380	U
1	2	400	A
1	2	401	A
1	2	438	A
1	2	439	U
1	2	440	U
1	2	455	C
1	2	492	A
1	2	541	A
1	2	554	C
1	2	555	A
1	2	565	C
1	2	606	A
1	2	609	U
1	2	622	A
1	2	699	U
1	2	705	U
1	2	721	U
1	2	754	A
1	2	755	A
1	2	804	A
1	2	811	A
1	2	812	A
1	2	814	A
1	2	928	U
1	2	959	U
1	2	997	G
1	2	1003	A
1	2	1023	A
1	2	1028	C
1	2	1054	U
1	2	1058	U
1	2	1081	A
1	2	1097	U
1	2	1113	A
1	2	1114	G
1	2	1633	A

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Mol	Chain	Res	Type
1	2	1636	C
1	2	1766	A
1	2	1769	U
1	2	1793	G

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	SF4	h	701	20	0,12,12	-	-	-		
21	SF4	h	702	20	0,12,12	-	-	-		
22	ANP	h	703	23	32,33,33	1.66	8 (25%)	44,52,52	2.47	14 (31%)
22	ANP	h	705	-	32,33,33	2.02	11 (34%)	44,52,52	2.49	16 (36%)

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	SF4	h	701	20	-	-	0/6/5/5
21	SF4	h	702	20	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	ANP	h	705	-	-	5/18/38/38	0/3/3/3
22	ANP	h	703	23	-	5/18/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	h	705	ANP	C5-C4	4.59	1.47	1.39
22	h	703	ANP	C5-C4	4.48	1.47	1.39
22	h	705	ANP	PG-N3B	4.44	1.75	1.63
22	h	705	ANP	PB-N3B	3.98	1.73	1.63
22	h	703	ANP	C5-C6	3.46	1.50	1.41
22	h	705	ANP	PB-O3A	3.18	1.63	1.59
22	h	705	ANP	PB-O1B	3.18	1.51	1.46
22	h	705	ANP	C5-C6	2.93	1.49	1.41
22	h	703	ANP	PG-O1G	2.71	1.50	1.46
22	h	703	ANP	PB-O1B	2.69	1.50	1.46
22	h	705	ANP	PG-O1G	2.67	1.50	1.46
22	h	703	ANP	PB-O3A	2.52	1.62	1.59
22	h	705	ANP	C5-N7	-2.47	1.34	1.39
22	h	705	ANP	PB-O2B	-2.42	1.50	1.56
22	h	703	ANP	PG-O2G	-2.19	1.50	1.56
22	h	703	ANP	C8-N7	2.12	1.35	1.31
22	h	703	ANP	C5-N7	-2.09	1.35	1.39
22	h	705	ANP	PG-O3G	-2.08	1.51	1.56
22	h	705	ANP	C8-N7	2.01	1.35	1.31

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	h	705	ANP	C5-C4-N3	-7.17	117.40	126.75
22	h	703	ANP	C5-C4-N3	-7.10	117.49	126.75
22	h	703	ANP	O1G-PG-N3B	-6.89	101.62	111.77
22	h	703	ANP	N3-C4-N9	5.47	136.10	127.08
22	h	705	ANP	O1G-PG-N3B	-5.43	103.77	111.77
22	h	705	ANP	N3-C4-N9	5.35	135.90	127.08
22	h	703	ANP	C2-N3-C4	4.73	122.92	111.75
22	h	705	ANP	C2-N3-C4	4.48	122.33	111.75
22	h	703	ANP	O2B-PB-O1B	4.44	119.23	109.92
22	h	705	ANP	O2B-PB-O1B	4.35	119.04	109.92
22	h	705	ANP	C4-C5-N7	-4.15	105.56	110.62
22	h	703	ANP	N3-C2-N1	-3.86	122.56	128.60
22	h	705	ANP	C5-N7-C8	3.71	108.79	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	h	703	ANP	C4-C5-N7	-3.57	106.27	110.62
22	h	705	ANP	N3-C2-N1	-3.54	123.07	128.60
22	h	703	ANP	O1B-PB-N3B	-3.32	106.88	111.77
22	h	705	ANP	O1B-PB-N3B	-3.15	107.13	111.77
22	h	703	ANP	C5-N7-C8	2.99	107.76	103.51
22	h	705	ANP	PB-O3A-PA	-2.84	122.63	132.62
22	h	703	ANP	O2G-PG-O3G	2.74	114.94	107.64
22	h	703	ANP	C3'-C2'-C1'	2.63	106.42	101.43
22	h	705	ANP	C4-N9-C8	2.56	108.50	105.73
22	h	705	ANP	N9-C8-N7	-2.54	110.44	113.91
22	h	703	ANP	C4-N9-C8	2.54	108.48	105.73
22	h	705	ANP	C6-C5-N7	2.50	136.68	132.02
22	h	703	ANP	C6-C5-N7	2.43	136.55	132.02
22	h	705	ANP	C2'-C3'-C4'	2.34	107.19	102.64
22	h	705	ANP	O2G-PG-O3G	2.27	113.68	107.64
22	h	705	ANP	O4'-C1'-N9	2.14	112.27	108.06
22	h	703	ANP	N9-C8-N7	-2.07	111.08	113.91

There are no chirality outliers.

All (10) torsion outliers are listed below:

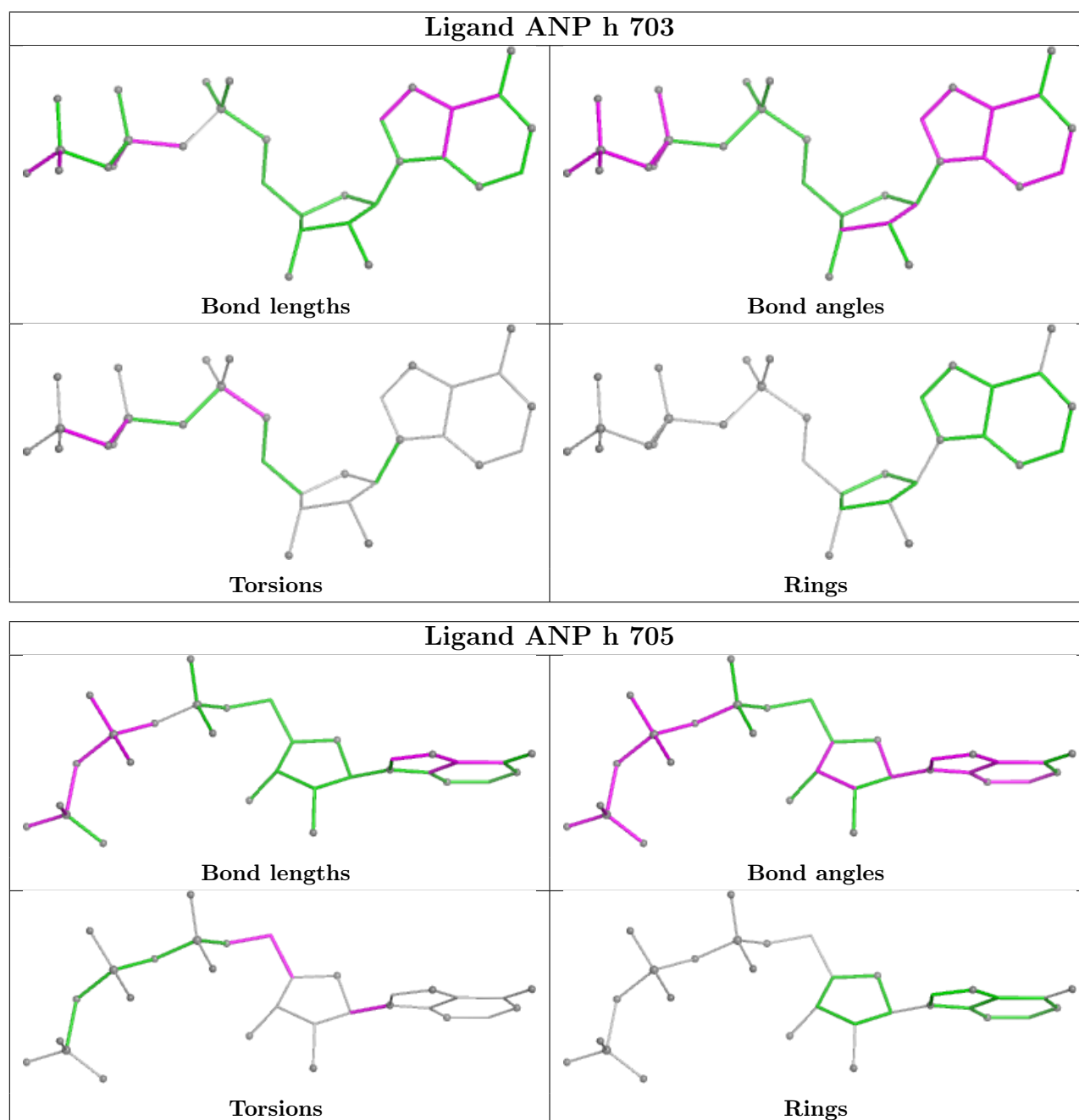
Mol	Chain	Res	Type	Atoms
22	h	703	ANP	PB-N3B-PG-O1G
22	h	703	ANP	PG-N3B-PB-O1B
22	h	703	ANP	C5'-O5'-PA-O1A
22	h	703	ANP	C5'-O5'-PA-O3A
22	h	705	ANP	C2'-C1'-N9-C8
22	h	705	ANP	C4'-C5'-O5'-PA
22	h	705	ANP	O4'-C1'-N9-C8
22	h	703	ANP	C5'-O5'-PA-O2A
22	h	705	ANP	O4'-C4'-C5'-O5'
22	h	705	ANP	C2'-C1'-N9-C4

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	h	701	SF4	4	0
21	h	702	SF4	2	0
22	h	703	ANP	1	0
22	h	705	ANP	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1636:C	O3'	1637:C	P	1.24
1	2	1761:U	O3'	1762:A	P	1.07

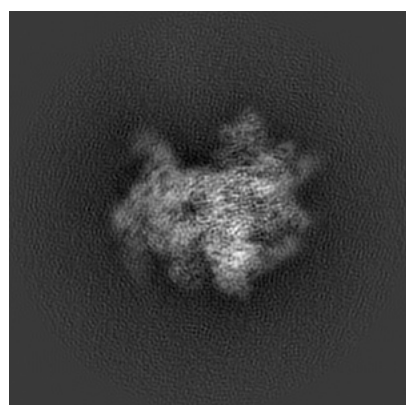
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4071. These allow visual inspection of the internal detail of the map and identification of artifacts.

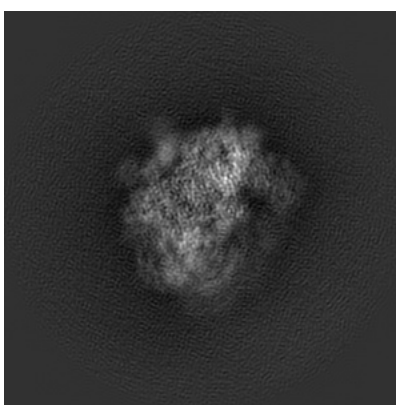
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

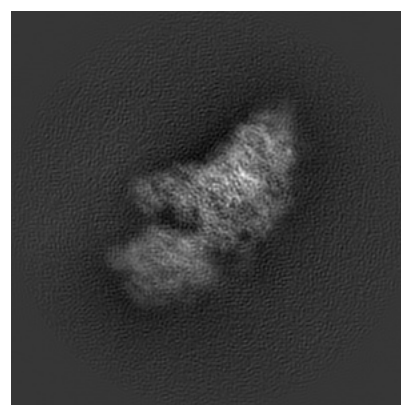
6.1.1 Primary map



X



Y

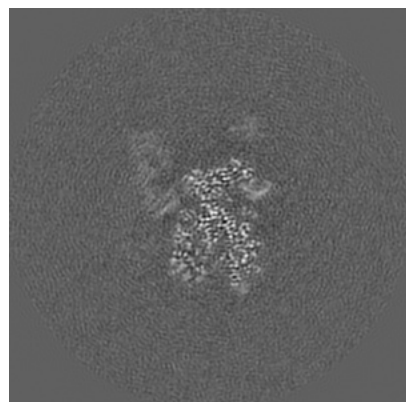


Z

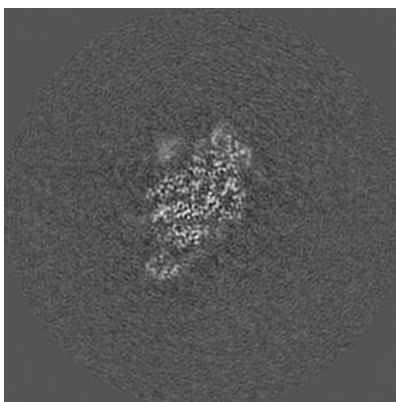
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

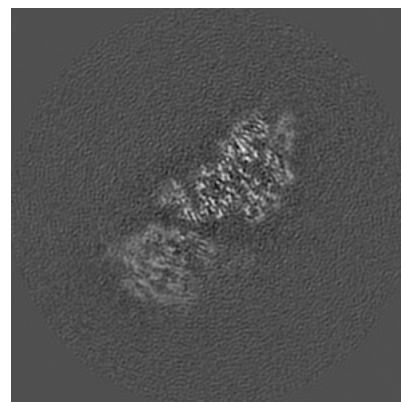
6.2.1 Primary map



X Index: 192



Y Index: 192

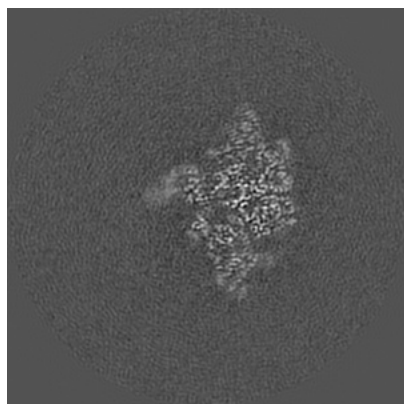


Z Index: 192

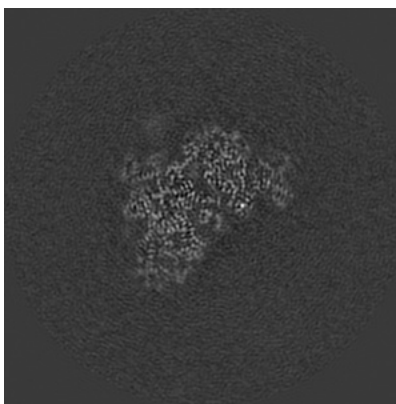
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

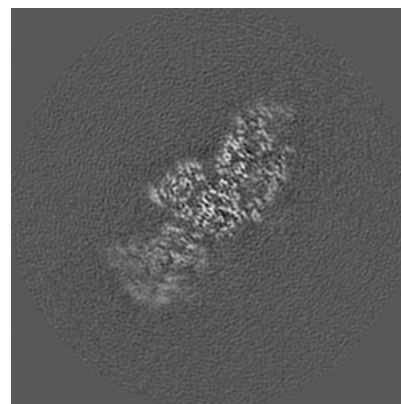
6.3.1 Primary map



X Index: 223



Y Index: 216

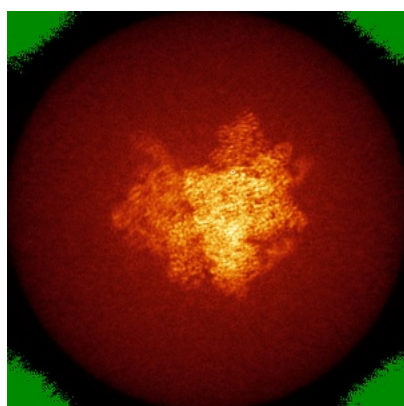


Z Index: 181

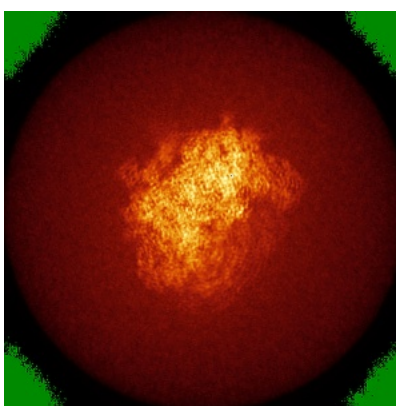
The images above show the largest variance slices of the map in three orthogonal directions.

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

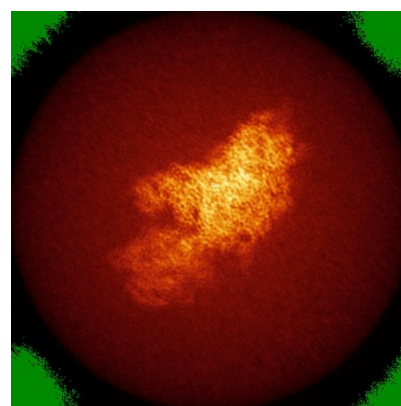
6.4.1 Primary map



X



Y

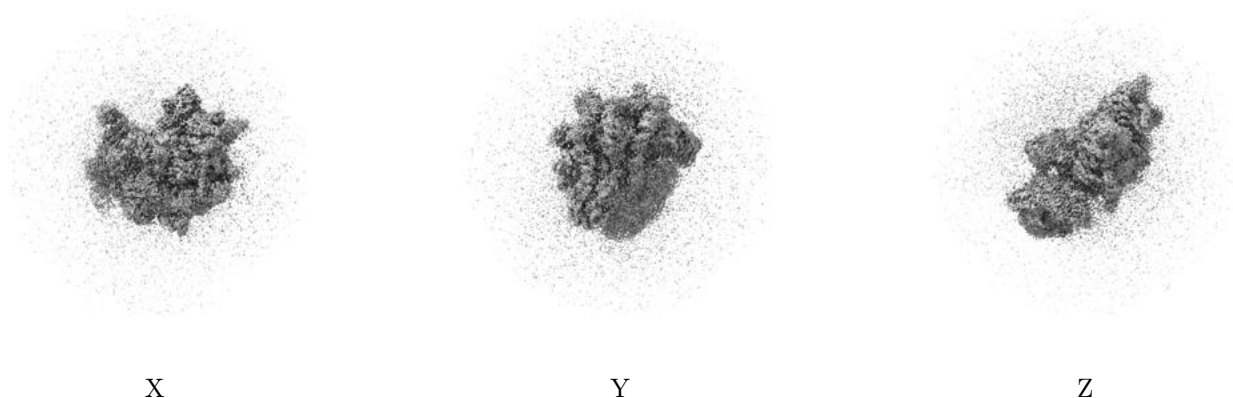


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

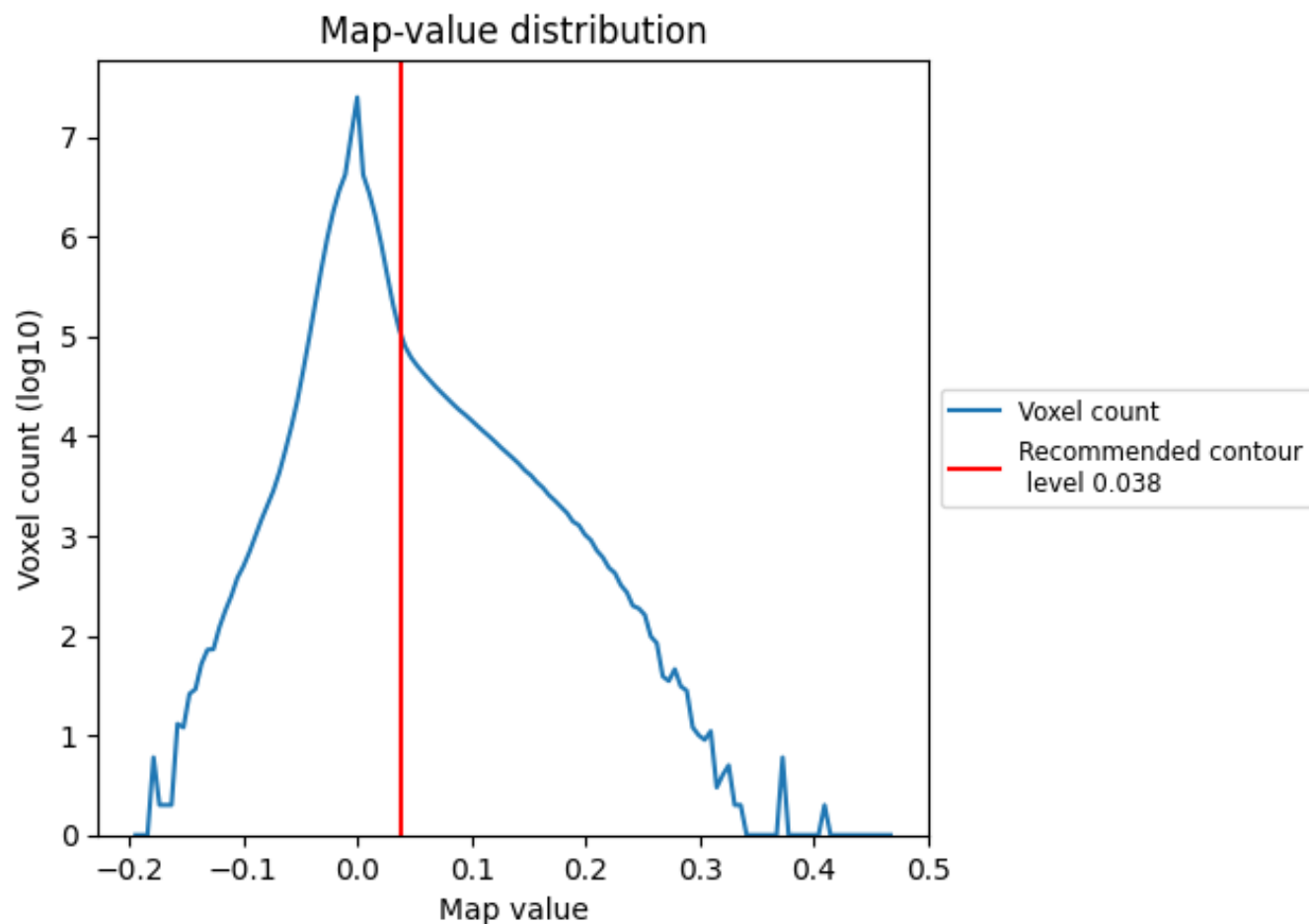
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

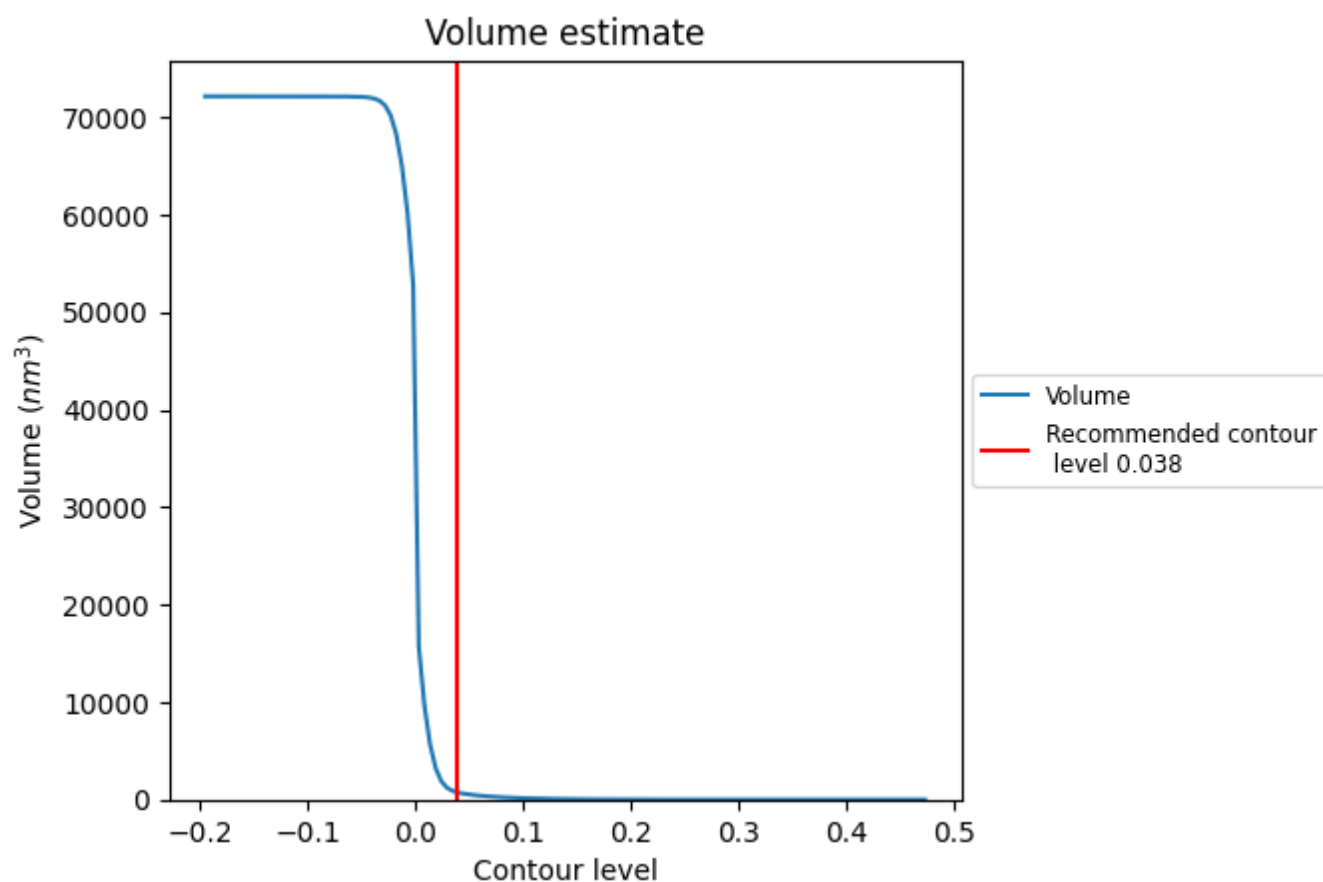
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

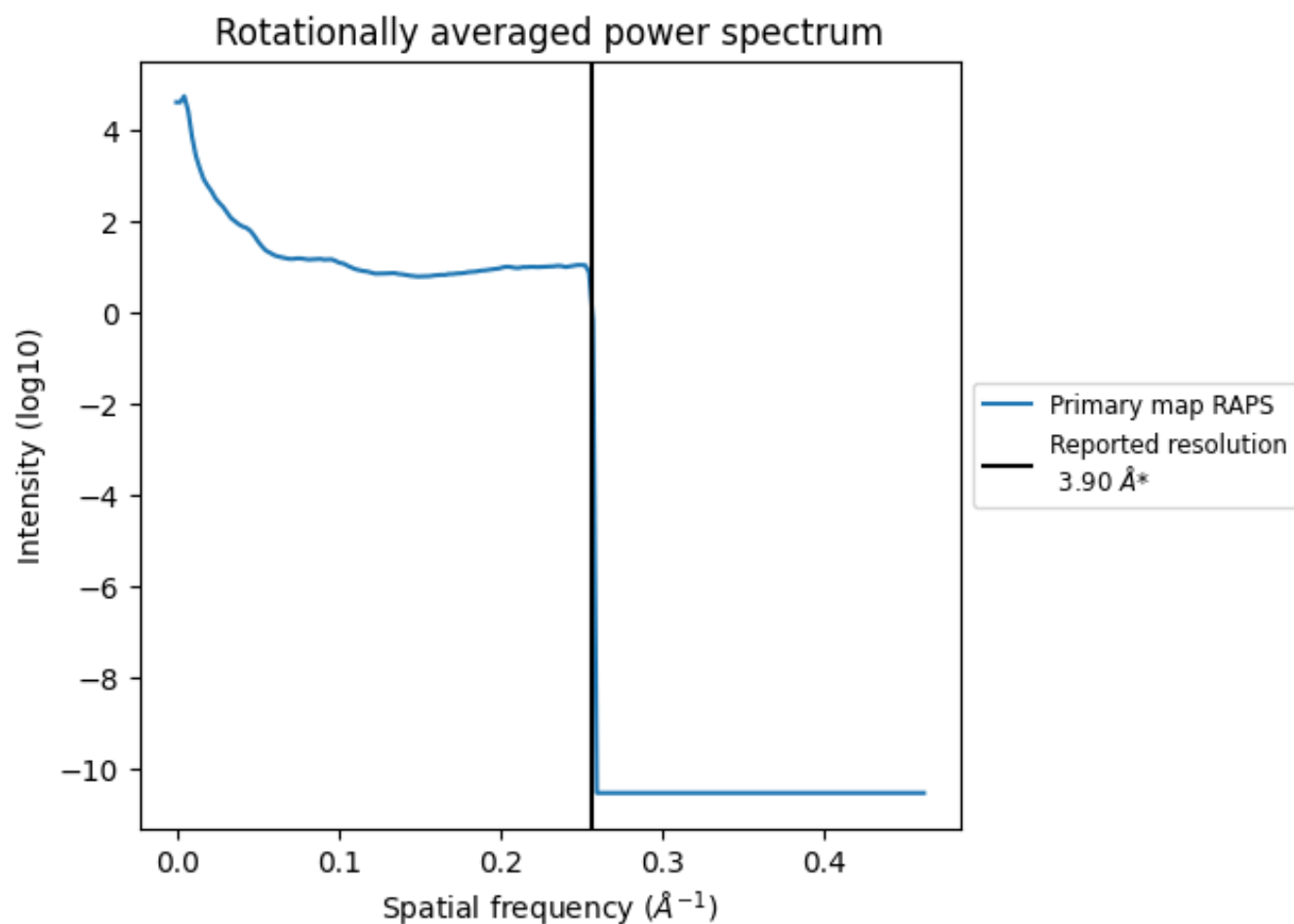
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 774 nm^3 ; this corresponds to an approximate mass of 699 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 0.256 Å⁻¹

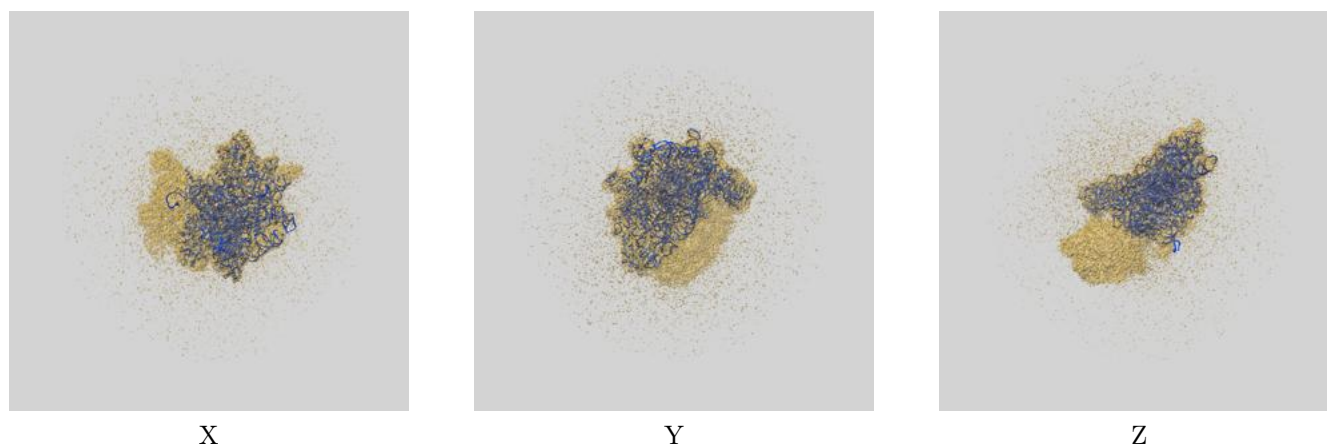
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

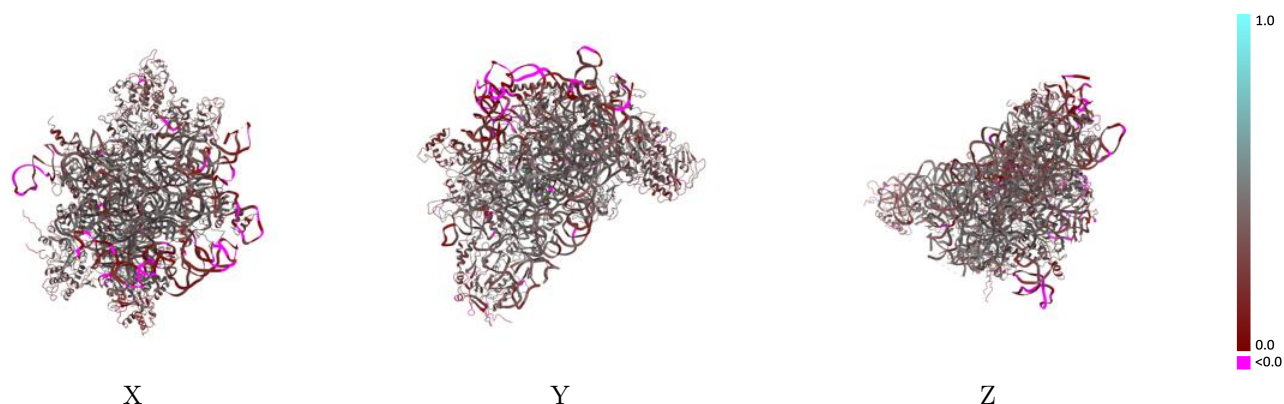
This section contains information regarding the fit between EMDB map EMD-4071 and PDB model 5LL6. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



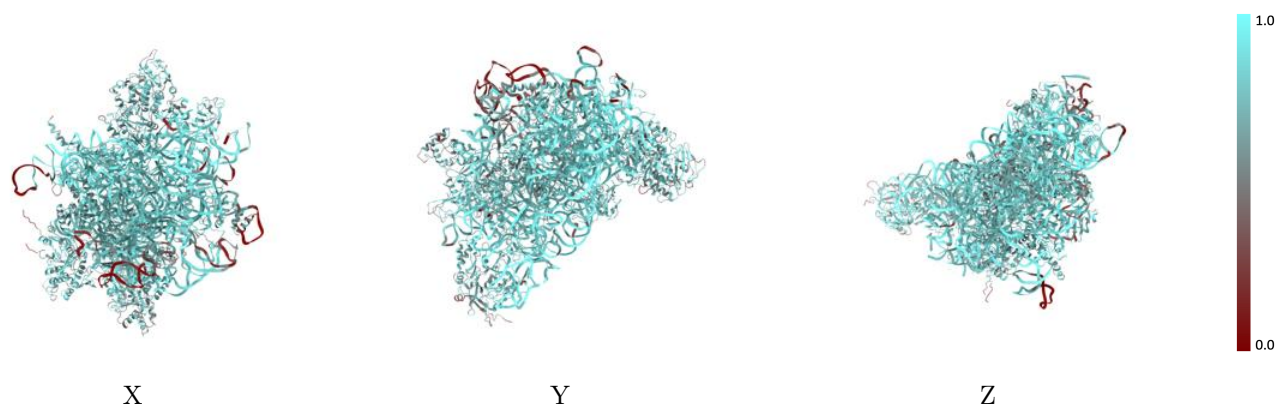
The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



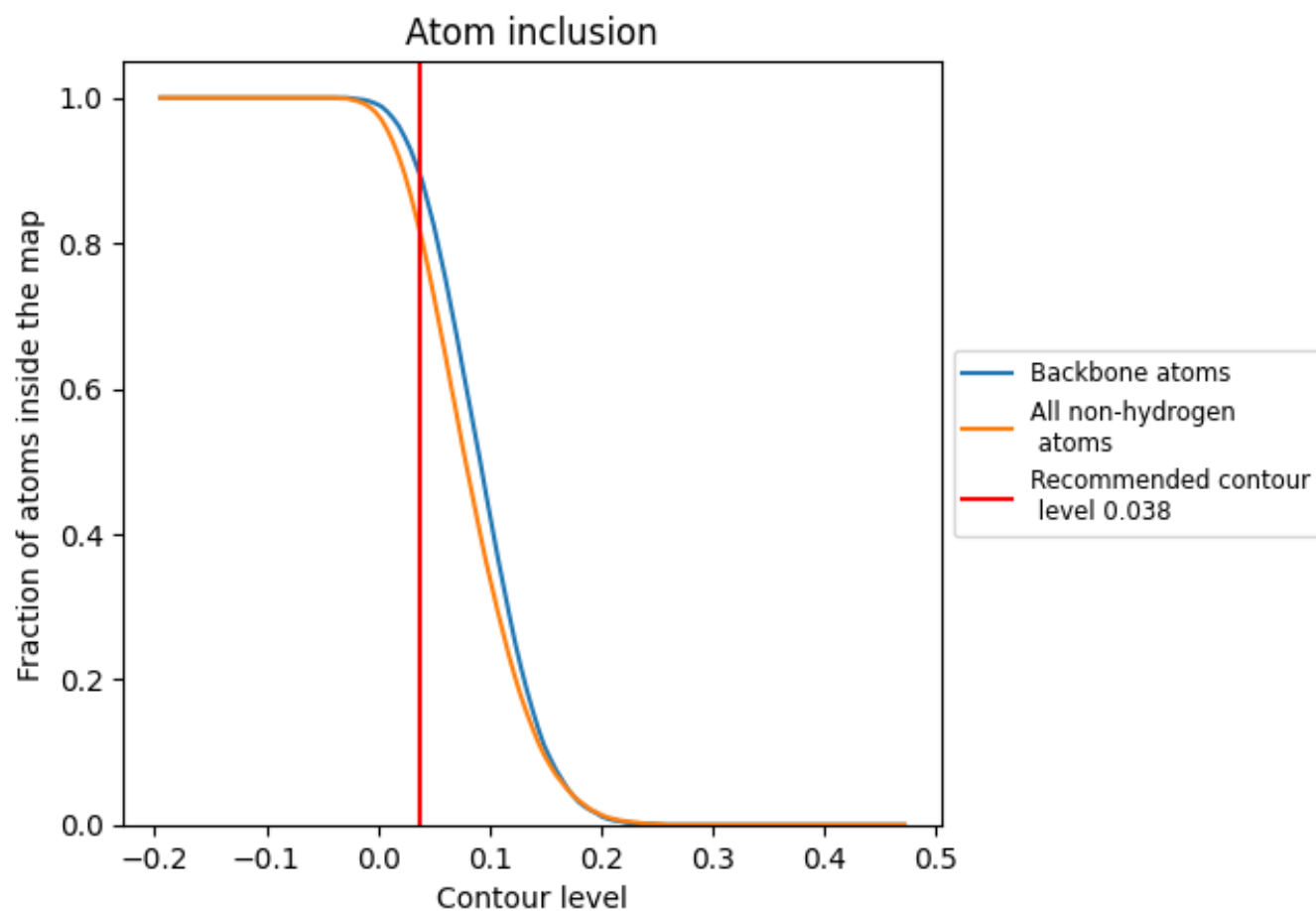
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.038).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8150	 0.3480
2	 0.8580	 0.3360
P	 0.7900	 0.3560
Q	 0.6750	 0.2900
R	 0.7490	 0.3770
S	 0.8140	 0.3970
T	 0.8060	 0.3540
U	 0.6700	 0.2800
V	 0.7940	 0.3660
W	 0.8080	 0.3860
X	 0.7650	 0.3960
Y	 0.8250	 0.3680
Z	 0.7750	 0.3470
a	 0.7970	 0.3800
b	 0.8320	 0.4310
c	 0.7820	 0.4090
d	 0.8020	 0.3700
e	 0.7820	 0.3880
f	 0.7700	 0.3740
g	 0.7570	 0.3570
h	 0.7400	 0.3380

