



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:45 AM UTC

PDB ID : 6RBD / pdb_00006rbd
EMDB ID : EMD-4792
Title : State 1 of yeast Tsr1-TAP Rps20-Deltaloop pre-40S particles
Authors : Shayan, R.; Mitterer, V.; Ferreira-Cerca, S.; Murat, G.; Enne, T.; Rinaldi, D.; Weigl, S.; Omanic, H.; Gleizes, P.E.; Kressler, D.; Pertschy, B.; Plisson-Chastang, C.
Deposited on : 2019-04-10
Resolution : 3.47 Å(reported)
Based on initial models : 6EML, 6FAI, ?

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

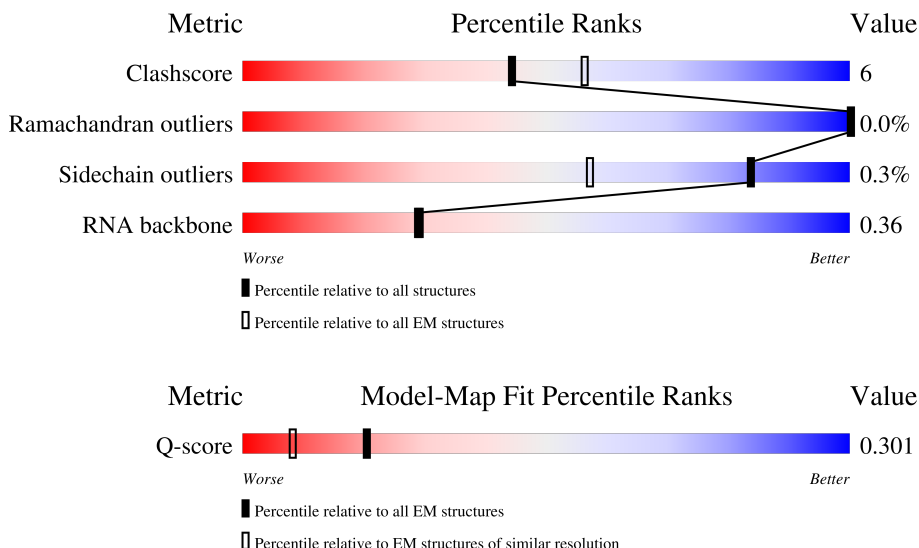
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.47 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	13733 (2.97 - 3.97)

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	b	82	
2	e	63	
3	2	1801	

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Mol	Chain	Length	Quality of chain
4	A	252	
5	B	255	
6	C	254	
7	E	261	
8	G	236	
9	H	190	
10	I	200	
11	J	197	
12	L	156	
13	N	151	
14	V	87	
15	W	130	
16	X	145	
17	Y	135	
18	c	67	
19	d	56	
20	h	274	
21	i	483	
22	k	788	
23	l	425	
24	y	318	
25	F	225	
26	M	143	
27	O	137	
28	P	142	

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Mol	Chain	Length	Quality of chain
29	Q	143	
30	R	136	
31	S	146	
32	T	144	
33	Z	108	
34	D	240	
35	U	121	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 81048 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 2 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	48	Total	C	N	O	S	0	0
			384	242	81	59	2		

- Molecule 3 is a RNA chain called 20S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	1777	Total	C	N	O	P	0	0
			37868	16929	6704	12458	1777		

- Molecule 4 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	206	Total	C	N	O	S	0	0
			1611	1036	285	288	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	PHE	ASP	conflict	UNP P32905

- Molecule 5 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 7 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	232	Total	C	N	O	S	0	0
			1873	1172	366	332	3		

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	H	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 12 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	140	Total	C	N	O	S	0	0
			1129	724	215	187	3		

- Molecule 13 is a protein called 40S ribosomal protein S13.

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

- Molecule 14 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 16 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 17 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 18 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	c	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 19 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	37	Total	C	N	O	S	0	0
			302	186	62	50	4		

- Molecule 20 is a protein called Pre-rRNA-processing protein PNO1.

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

- Molecule 21 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	139	Total	C	N	O	S	0	0
			1116	731	181	202	2		

- Molecule 22 is a protein called Ribosome biogenesis protein TSR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	k	605	Total	C	N	O	S	0	0
			4860	3112	849	885	14		

- Molecule 23 is a protein called Serine/threonine-protein kinase RIO2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	l	271	Total	C	N	O	S	0	0
			2199	1390	385	407	17		

- Molecule 24 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	154	Total	C	N	O	S	0	0
			1245	788	223	225	9		

- Molecule 25 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	125	Total	C	N	O	S	0	0
			941	591	166	182	2		

- Molecule 27 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	127	Total	C	N	O	S	0	0
			926	569	185	169	3		

- Molecule 28 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	P	114	Total	C	N	O	S	0	0
			902	574	166	155	7		

- Molecule 29 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Q	127	Total	C	N	O	S	0	0
			993	640	177	176			

- Molecule 30 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R	125	Total	C	N	O	S	0	0
			1000	625	188	185	2		

- Molecule 31 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S	104	Total	C	N	O	S	0	0
			840	528	154	156	2		

- Molecule 32 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	T	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 33 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	63	Total	C	N	O	S	0	0
			512	328	94	90			

- Molecule 34 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D	185	Total	C	N	O	S	0	0
			1442	911	266	259	6		

- Molecule 35 is a protein called 40S ribosomal protein S20.

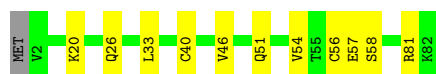
Mol	Chain	Residues	Atoms					AltConf	Trace
35	U	82	Total	C	N	O	S	0	0
			674	431	123	119	1		

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.

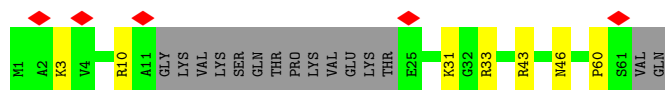
- Molecule 1: 40S ribosomal protein S27-A

Chain b: 



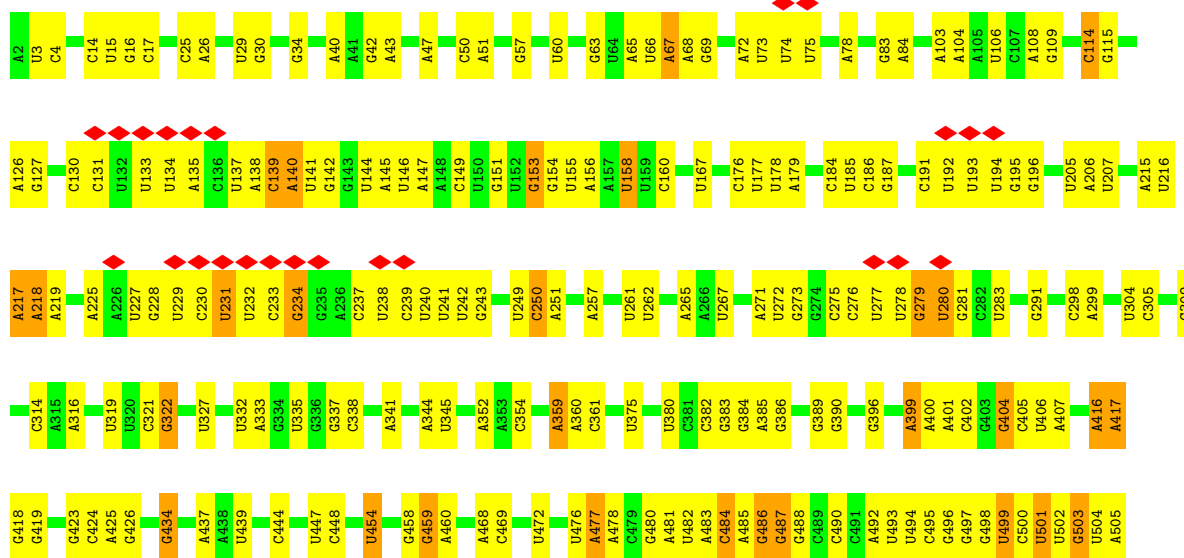
- Molecule 2: 40S ribosomal protein S30-A

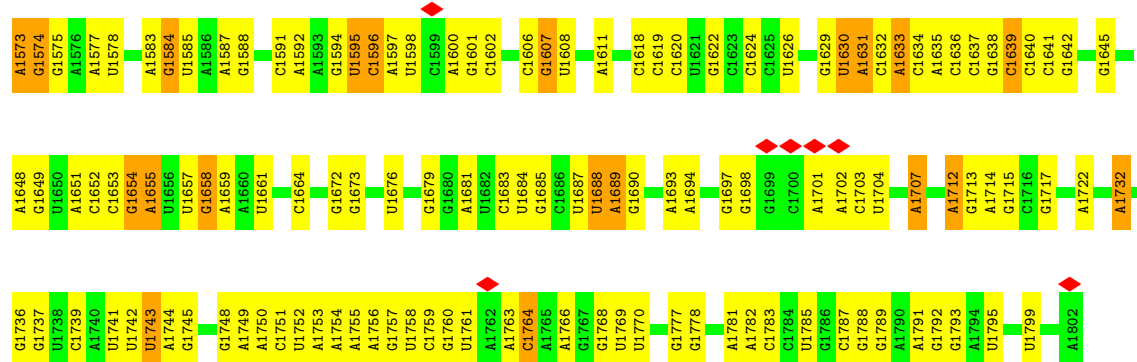
Chain e: 



- Molecule 3: 20S ribosomal RNA

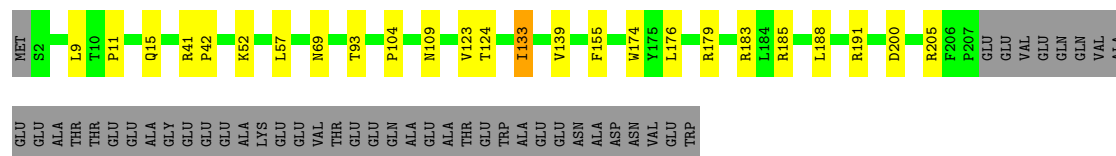
Chain 2: 





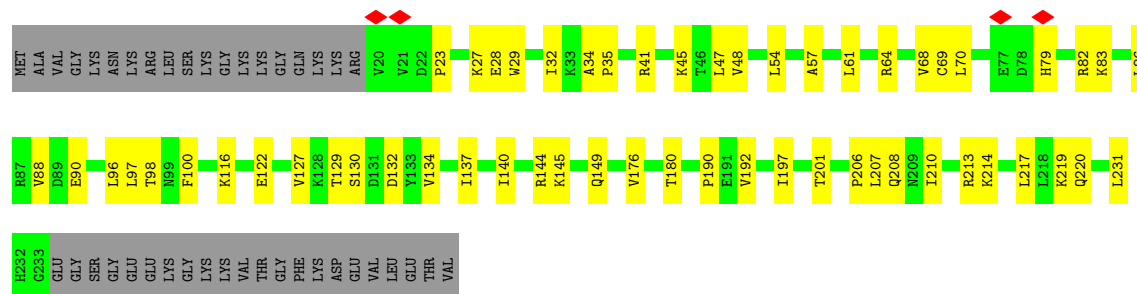
• Molecule 4: 40S ribosomal protein S0-A

Chain A: 72% 10% 18%



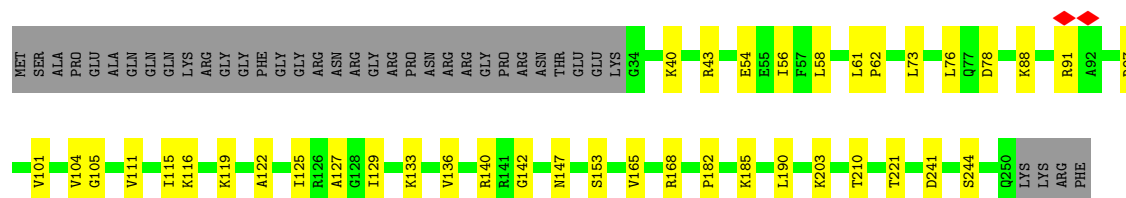
• Molecule 5: 40S ribosomal protein S1-A

Chain B: 62% 22% 16%



• Molecule 6: 40S ribosomal protein S2

Chain C: 70% 16% 15%



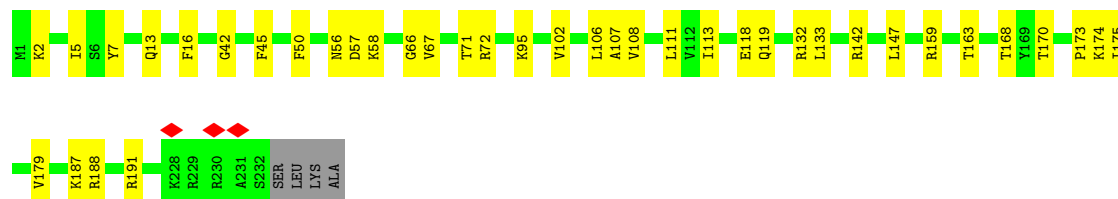
• Molecule 7: 40S ribosomal protein S4-A

Chain E: 87% 13%



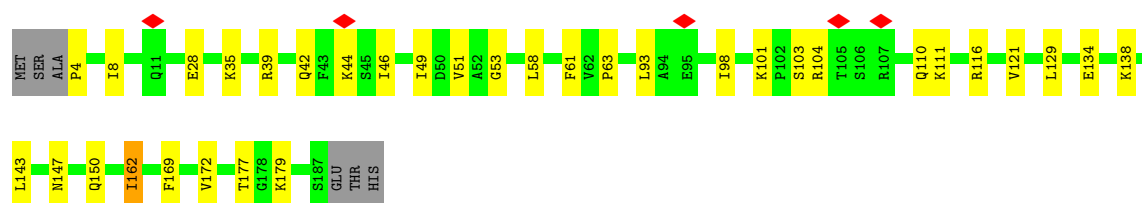
- Molecule 8: 40S ribosomal protein S6-A

Chain G: 82% 17% .



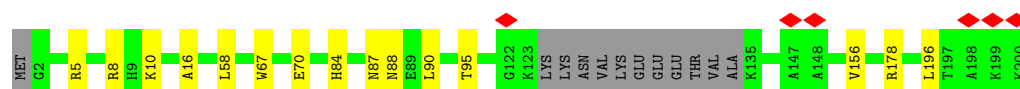
- Molecule 9: 40S ribosomal protein S7-A

Chain H: 79% 17% ..



- Molecule 10: 40S ribosomal protein S8-A

Chain I: 86% 8% 6%



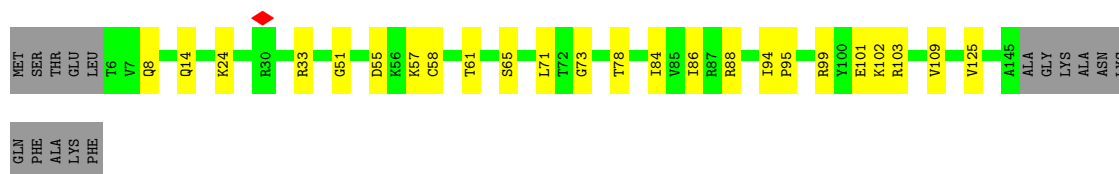
- Molecule 11: 40S ribosomal protein S9-A

Chain J: 77% 16% 6%

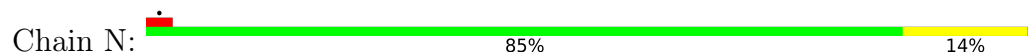


- Molecule 12: 40S ribosomal protein S11-A

Chain L: 74% 15% 10%



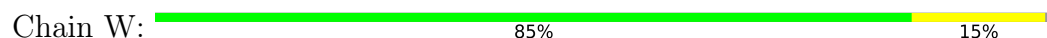
- Molecule 13: 40S ribosomal protein S13



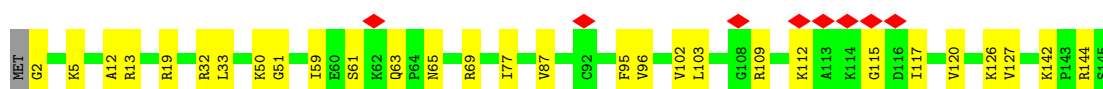
- Molecule 14: 40S ribosomal protein S21-A



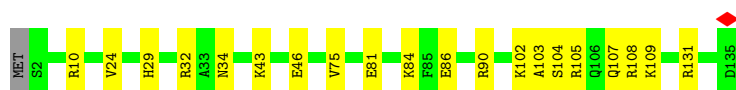
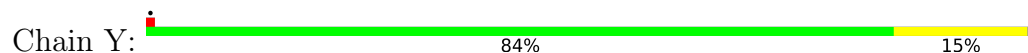
- Molecule 15: 40S ribosomal protein S22-A



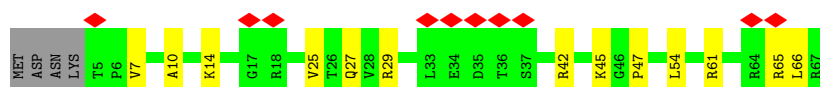
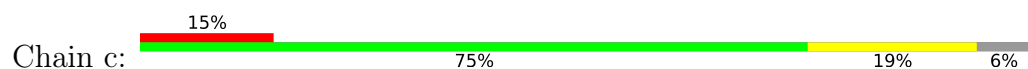
- Molecule 16: 40S ribosomal protein S23-A

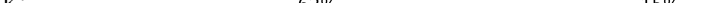


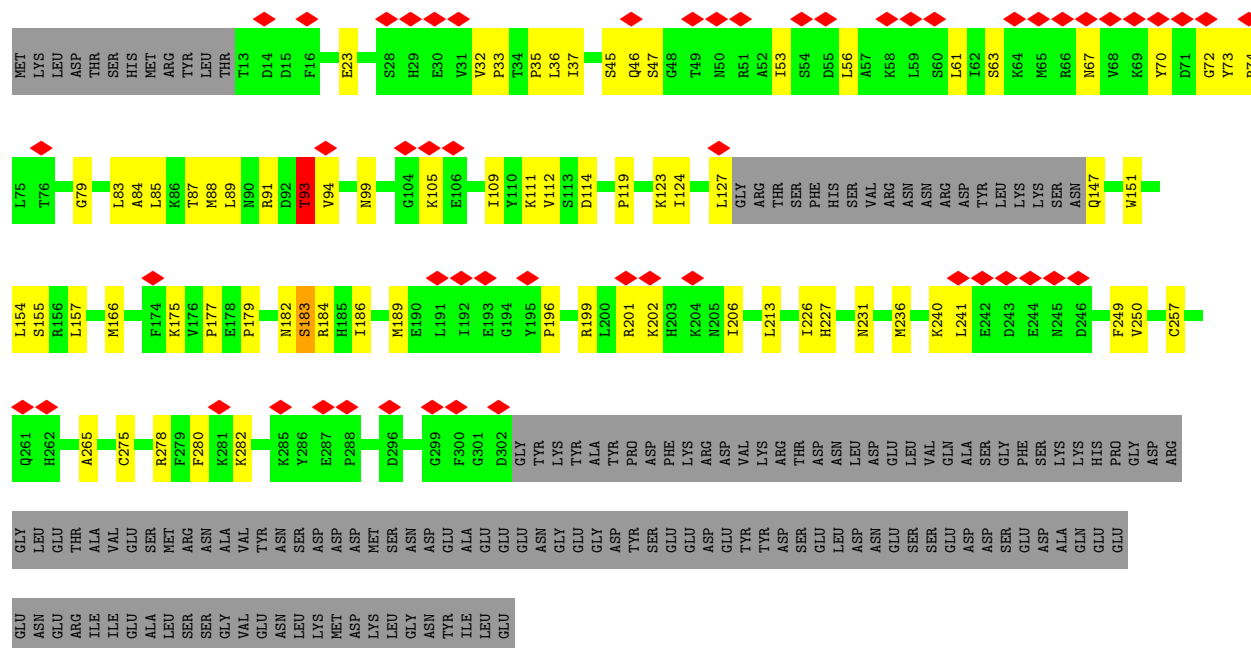
- Molecule 17: 40S ribosomal protein S24-A

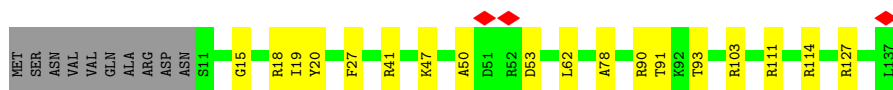


- Molecule 18: 40S ribosomal protein S28-A

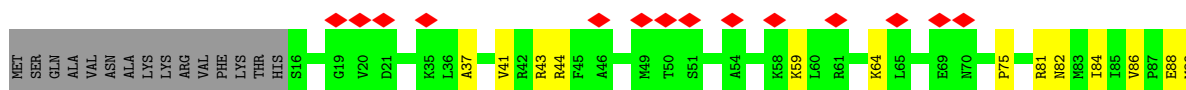


- Chain k: 





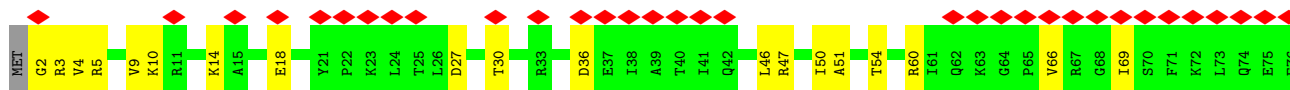
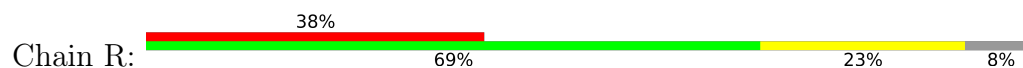
- Molecule 28: 40S ribosomal protein S15



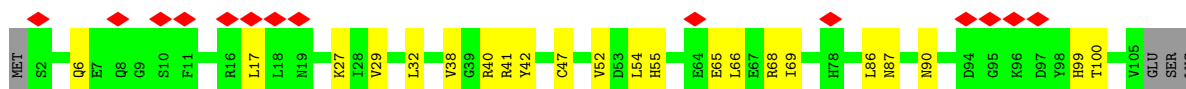
- Molecule 29: 40S ribosomal protein S16-A



- Molecule 30: 40S ribosomal protein S17-A



- Molecule 31: 40S ribosomal protein S18-A



- Molecule 32: 40S ribosomal protein S19-A

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54130	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.528	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	409.72803, 409.72803, 409.72803	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

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	b	0.26	0/620	0.51	0/838
2	e	0.30	0/390	0.58	0/517
3	2	0.29	0/42353	0.45	2/65990 (0.0%)
4	A	0.30	0/1653	0.61	2/2261 (0.1%)
5	B	0.29	0/1735	0.62	0/2335
6	C	0.30	0/1665	0.53	0/2263
7	E	0.35	0/2109	0.60	0/2839
8	G	0.29	0/1897	0.54	0/2532
9	H	0.24	0/1506	0.56	1/2028 (0.0%)
10	I	0.34	0/1514	0.57	0/2021
11	J	0.31	0/1519	0.61	0/2035
12	L	0.35	0/1155	0.56	0/1557
13	N	0.27	0/1215	0.56	0/1638
14	V	0.30	0/693	0.49	0/935
15	W	0.40	0/1038	0.68	0/1395
16	X	0.34	0/1139	0.64	0/1518
17	Y	0.32	0/1087	0.56	0/1449
18	c	0.19	0/499	0.55	0/670
19	d	0.20	0/305	0.53	0/401
20	h	0.24	0/1462	0.54	0/1969
21	i	0.23	0/1145	0.54	0/1556
22	k	0.22	0/4970	0.54	0/6718
23	l	0.24	0/2243	0.63	4/3014 (0.1%)
24	y	0.22	0/1265	0.63	0/1702
25	F	0.22	0/1629	0.55	0/2202
26	M	0.23	0/949	0.52	0/1284
27	O	0.23	0/937	0.54	0/1261
28	P	0.21	0/921	0.50	0/1237
29	Q	0.24	0/1011	0.57	0/1362
30	R	0.21	0/1010	0.54	0/1355
31	S	0.21	0/853	0.52	0/1154
32	T	0.23	0/1130	0.50	0/1517
33	Z	0.42	0/519	0.78	0/696
34	D	0.24	0/1459	0.57	0/1957

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	U	0.20	0/681	0.48	0/917
All	All	0.28	0/86276	0.51	9/125123 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
22	k	0	3
24	y	0	2
All	All	0	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	l	183	SER	CA-C-N	6.12	133.23	121.54
23	l	183	SER	C-N-CA	6.12	133.23	121.54
3	2	1343	U	P-O3'-C3'	5.46	128.38	120.20
3	2	1156	C	P-O3'-C3'	5.22	128.04	120.20
23	l	93	THR	CA-C-N	5.12	131.18	121.97
23	l	93	THR	C-N-CA	5.12	131.18	121.97
9	H	162	ILE	N-CA-C	-5.03	108.93	113.71
4	A	9	LEU	CA-C-N	5.02	135.51	120.69
4	A	9	LEU	C-N-CA	5.02	135.51	120.69

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	k	118	VAL	Peptide
22	k	710	PHE	Peptide
22	k	711	HIS	Peptide
24	y	270	LYS	Peptide
24	y	275	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	610	0	633	7	0
2	e	384	0	423	8	0
3	2	37868	0	19053	364	0
4	A	1611	0	1616	19	0
5	B	1709	0	1784	32	0
6	C	1635	0	1723	28	0
7	E	2068	0	2154	21	0
8	G	1873	0	1980	26	0
9	H	1481	0	1572	23	0
10	I	1489	0	1525	13	0
11	J	1494	0	1573	24	0
12	L	1129	0	1196	16	0
13	N	1192	0	1255	16	0
14	V	684	0	672	7	0
15	W	1021	0	1060	15	0
16	X	1121	0	1196	23	0
17	Y	1073	0	1132	12	0
18	c	497	0	535	8	0
19	d	302	0	300	8	0
20	h	1436	0	1515	32	0
21	i	1116	0	1134	13	0
22	k	4860	0	4795	66	0
23	l	2199	0	2182	42	0
24	y	1245	0	1284	17	0
25	F	1609	0	1675	34	0
26	M	941	0	982	27	0
27	O	926	0	950	15	0
28	P	902	0	933	17	0
29	Q	993	0	1051	24	0
30	R	1000	0	1063	21	0
31	S	840	0	849	14	0
32	T	1112	0	1124	21	0
33	Z	512	0	551	10	0
34	D	1442	0	1495	19	0
35	U	674	0	740	10	0
All	All	81048	0	63705	886	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 (886) 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)
3:2:1658:G:H1	3:2:1743:U:H3	1.03	0.96
3:2:1213:G:H1	3:2:1450:U:H3	0.97	0.96
3:2:1158:C:N4	3:2:1163:A:H61	1.62	0.95
3:2:1158:C:H42	3:2:1163:A:N6	1.64	0.95
3:2:1167:G:H1	3:2:1578:U:H3	1.10	0.95
3:2:1158:C:H42	3:2:1163:A:H61	0.93	0.92
3:2:1499:G:H1	3:2:1508:U:H3	0.99	0.92
3:2:1335:U:H3	3:2:1416:G:H1	1.11	0.91
3:2:1541:G:H21	3:2:1570:A:H62	1.19	0.89
3:2:699:U:H3	3:2:739:G:H1	1.26	0.84
28:P:75:PRO:HA	28:P:93:VAL:O	1.78	0.83
3:2:766:U:H3	3:2:770:A:H62	1.26	0.81
23:l:67:ASN:O	23:l:70:TYR:HB3	1.83	0.78
5:B:28:GLU:HB3	5:B:48:VAL:O	1.85	0.77
3:2:1356:U:H3	3:2:1367:G:H1	1.32	0.77
20:h:94:PHE:HA	20:h:141:THR:O	1.85	0.77
3:2:976:G:H1	3:2:1023:A:HO2'	1.31	0.76
3:2:1278:G:H22	3:2:1430:U:H3	1.31	0.76
15:W:24:GLN:HA	15:W:63:VAL:O	1.86	0.75
3:2:1174:C:H42	3:2:1465:C:H42	1.33	0.74
3:2:1295:G:H1	3:2:1302:U:H3	1.34	0.73
3:2:1588:G:H1	3:2:1608:U:H3	1.36	0.73
3:2:1688:U:H3	3:2:1713:G:H1	1.35	0.73
17:Y:102:LYS:HB3	17:Y:108:ARG:HH22	1.53	0.71
3:2:488:G:H1	3:2:499:U:H3	1.38	0.70
3:2:1034:C:HO2'	15:W:2:THR:N	1.88	0.70
3:2:1276:U:H3	3:2:1433:G:H1	1.39	0.70
3:2:1541:G:N2	3:2:1570:A:H62	1.90	0.70
23:l:99:ASN:HB3	23:l:111:LYS:HB3	1.73	0.69
20:h:182:ILE:HA	20:h:233:ILE:O	1.93	0.69
3:2:151:G:N3	8:G:13:GLN:NE2	2.40	0.69
3:2:1175:U:H3	3:2:1464:G:H1	1.40	0.69
3:2:650:U:H3	3:2:684:A:H61	1.41	0.68
1:b:26:GLN:HE22	13:N:16:ILE:H	1.39	0.68
3:2:1584:G:N7	29:Q:122:ARG:NH1	2.42	0.68
3:2:984:G:H1	3:2:1017:U:H3	1.42	0.67
3:2:568:G:H5''	3:2:576:G:H1	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1482:C:OP2	3:2:1521:G:N2	2.29	0.66
15:W:3:ARG:HH22	15:W:28:ARG:HH21	1.42	0.66
23:l:109:ILE:HG12	23:l:123:LYS:HG2	1.77	0.65
24:y:271:GLY:HA3	24:y:278:LYS:H	1.62	0.65
25:F:54:LYS:HB2	25:F:138:THR:HG21	1.78	0.65
3:2:1170:G:H1	3:2:1469:A:H61	1.43	0.65
23:l:236:MET:HB3	23:l:250:VAL:HB	1.77	0.65
3:2:715:U:H3	3:2:723:G:H1	1.42	0.65
8:G:57:ASP:HA	8:G:106:LEU:HA	1.78	0.65
9:H:51:VAL:HG23	9:H:53:GLY:H	1.62	0.64
23:l:33:PRO:HA	23:l:72:GLY:HA2	1.80	0.64
3:2:1335:U:O2	3:2:1416:G:N2	2.27	0.64
3:2:1488:G:H3'	3:2:1515:A:H61	1.63	0.64
3:2:153:G:H21	8:G:56:ASN:HD21	1.45	0.64
3:2:1349:G:H21	3:2:1379:C:H42	1.45	0.64
22:k:647:HIS:HD2	22:k:650:THR:H	1.46	0.63
7:E:79:ASP:HB3	7:E:82:TYR:HB2	1.79	0.63
3:2:1286:U:O2	3:2:1422:A:N7	2.30	0.63
13:N:54:LEU:HB3	13:N:60:VAL:HB	1.80	0.63
3:2:1548:G:H4'	31:S:90:ASN:HB2	1.81	0.63
18:c:45:LYS:HB3	25:F:162:VAL:HG12	1.78	0.63
3:2:639:U:H5'	9:H:101:LYS:HD2	1.79	0.63
5:B:70:LEU:HD22	5:B:82:ARG:HD2	1.78	0.63
3:2:1167:G:N2	3:2:1578:U:O2	2.30	0.63
3:2:1358:G:H5'	32:T:126:GLU:HB2	1.79	0.62
3:2:1689:A:H61	3:2:1712:A:H62	1.47	0.62
24:y:154:MET:HB3	24:y:206:VAL:HG22	1.81	0.62
5:B:69:CYS:SG	27:O:114:ARG:NH1	2.73	0.62
8:G:118:GLU:HG3	8:G:119:GLN:HG2	1.79	0.62
3:2:748:U:H3	3:2:801:G:H1	1.47	0.62
25:F:139:ASN:ND2	25:F:202:ALA:O	2.31	0.62
3:2:1681:A:H1'	8:G:66:GLY:HA2	1.81	0.62
11:J:17:ARG:O	11:J:23:ARG:NH2	2.32	0.62
22:k:617:GLN:O	22:k:667:ALA:HA	2.00	0.62
4:A:41:ARG:NH1	30:R:103:ASP:OD2	2.30	0.62
3:2:65:A:H2	3:2:84:A:H62	1.48	0.62
20:h:95:GLU:O	20:h:140:ARG:HA	1.99	0.61
22:k:86:ILE:HG13	22:k:157:PHE:HB2	1.83	0.61
16:X:61:SER:HB3	16:X:69:ARG:HD2	1.81	0.61
34:D:105:MET:HE3	34:D:136:VAL:HG11	1.82	0.61
3:2:1584:G:N1	3:2:1611:A:OP2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1501:C:OP2	32:T:102:ARG:NH1	2.34	0.61
12:L:101:GLU:OE2	12:L:103:ARG:NH2	2.33	0.61
22:k:525:TRP:O	22:k:530:ARG:NH2	2.34	0.61
3:2:1345:A:O2'	3:2:1348:A:N6	2.34	0.60
21:i:307:VAL:HG12	21:i:341:VAL:HG11	1.82	0.60
22:k:703:LEU:O	22:k:770:ALA:HA	2.01	0.60
26:M:63:VAL:HG12	26:M:65:SER:H	1.65	0.60
21:i:256:PRO:HB2	21:i:302:HIS:HB2	1.82	0.60
17:Y:86:GLU:OE1	17:Y:90:ARG:NH1	2.33	0.60
25:F:128:ASN:ND2	25:F:131:GLN:OE1	2.34	0.60
3:2:1535:U:O2'	3:2:1536:G:N3	2.34	0.60
3:2:777:C:H3'	3:2:778:G:H21	1.67	0.60
7:E:87:MET:HE2	7:E:123:LEU:HB2	1.84	0.60
12:L:8:GLN:HE22	12:L:14:GLN:H	1.50	0.60
20:h:205:ILE:HA	20:h:250:LEU:HD13	1.84	0.60
20:h:101:VAL:HB	20:h:135:LYS:HB3	1.83	0.59
3:2:1213:G:N2	3:2:1450:U:O2	2.31	0.59
4:A:11:PRO:HG3	30:R:115:LEU:HD11	1.83	0.59
3:2:1310:U:O2'	3:2:1401:A:N1	2.34	0.59
3:2:1541:G:H21	3:2:1570:A:N6	1.97	0.59
3:2:231:U:H3	3:2:234:G:H22	1.50	0.59
3:2:1267:G:H1	3:2:1442:U:HO2'	1.49	0.59
29:Q:44:LEU:HB3	29:Q:78:VAL:HG11	1.84	0.59
33:Z:54:VAL:HG13	33:Z:60:VAL:HG11	1.85	0.59
20:h:178:ASP:O	27:O:103:ARG:NH1	2.36	0.59
3:2:859:A:N1	13:N:76:LYS:NZ	2.50	0.59
3:2:1241:G:H5''	28:P:59:LYS:HZ1	1.66	0.59
16:X:96:VAL:HG22	16:X:127:VAL:HG11	1.84	0.59
11:J:169:PRO:O	11:J:174:ARG:NH1	2.35	0.59
3:2:486:G:H1	3:2:501:U:H3	1.50	0.59
3:2:763:G:OP1	11:J:78:ARG:NH1	2.35	0.59
11:J:109:LEU:HB2	11:J:146:PHE:HB3	1.84	0.59
25:F:92:ARG:NH2	25:F:169:ASN:OD1	2.32	0.59
6:C:54:GLU:O	6:C:58:LEU:HB2	2.03	0.59
16:X:95:PHE:O	16:X:142:LYS:NZ	2.35	0.59
30:R:88:VAL:O	30:R:95:ARG:NH2	2.36	0.59
32:T:86:ARG:HB2	32:T:89:ARG:HB2	1.85	0.59
22:k:513:GLN:HB3	22:k:516:GLU:HG3	1.84	0.58
3:2:953:G:H2'	3:2:954:G:H8	1.68	0.58
20:h:227:ALA:HB3	20:h:230:LYS:HB2	1.83	0.58
5:B:79:HIS:HD2	20:h:98:LYS:HE2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:122:GLU:HG2	5:B:140:ILE:HG22	1.85	0.58
3:2:1294:G:H3'	3:2:1295:G:H8	1.68	0.58
8:G:2:LYS:HB3	8:G:108:VAL:HG22	1.86	0.58
18:c:25:VAL:HG21	18:c:66:LEU:HD22	1.86	0.58
3:2:1356:U:O2	3:2:1367:G:N2	2.34	0.58
5:B:34:ALA:HB3	5:B:41:ARG:HA	1.86	0.58
3:2:1099:U:O4	6:C:168:ARG:NH1	2.36	0.58
3:2:1552:U:OP2	28:P:43:ARG:NH2	2.36	0.58
15:W:23:ARG:NH1	15:W:66:ASN:O	2.37	0.58
23:l:196:PRO:HD2	23:l:199:ARG:HH21	1.69	0.58
24:y:151:SER:O	24:y:208:ARG:HA	2.03	0.58
3:2:925:G:H2'	3:2:926:A:H8	1.69	0.58
9:H:143:LEU:HD12	9:H:147:ASN:HB2	1.85	0.58
19:d:20:GLN:HG3	19:d:27:HIS:HE1	1.68	0.58
9:H:46:ILE:HD11	9:H:58:LEU:HB3	1.86	0.57
3:2:327:U:OP2	12:L:57:LYS:NZ	2.34	0.57
3:2:1294:G:O2'	4:A:109:ASN:ND2	2.37	0.57
5:B:29:TRP:HE1	5:B:45:LYS:HD2	1.68	0.57
22:k:227:TYR:HB3	22:k:234:ASP:HB3	1.85	0.57
29:Q:25:GLY:HA3	29:Q:64:ASP:HB2	1.86	0.57
3:2:1377:U:O2	3:2:1379:C:N4	2.37	0.57
4:A:52:LYS:NZ	14:V:81:ASN:O	2.37	0.57
5:B:90:GLU:HB2	5:B:97:LEU:HB3	1.87	0.57
26:M:131:ASP:O	26:M:134:SER:HB2	2.05	0.57
3:2:1502:G:N7	32:T:102:ARG:NH2	2.53	0.57
9:H:162:ILE:HG23	9:H:169:PHE:HE2	1.68	0.57
16:X:102:VAL:HG22	16:X:127:VAL:HG12	1.86	0.57
26:M:42:ALA:HB3	26:M:122:VAL:HB	1.86	0.57
34:D:59:LEU:O	34:D:64:ARG:N	2.37	0.57
3:2:629:U:OP2	3:2:969:C:N4	2.35	0.57
3:2:918:U:O2'	27:O:18:ARG:NH1	2.38	0.57
3:2:1103:U:O4	16:X:2:GLY:N	2.38	0.57
16:X:63:GLN:HB2	16:X:115:GLY:HA3	1.86	0.57
27:O:20:TYR:HB3	27:O:27:PHE:HB2	1.86	0.57
3:2:594:A:OP2	11:J:37:LYS:NZ	2.37	0.57
3:2:861:U:O2'	15:W:56:HIS:O	2.23	0.57
3:2:967:A:OP2	13:N:124:ARG:NH2	2.33	0.57
3:2:1781:A:OP2	24:y:156:GLN:NE2	2.38	0.57
6:C:73:LEU:HB3	6:C:76:LEU:HB2	1.87	0.57
26:M:62:LEU:HD11	26:M:88:LEU:HD13	1.87	0.57
3:2:1415:U:OP1	30:R:3:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1498:G:H5''	32:T:72:GLY:HA3	1.87	0.56
29:Q:94:GLN:HB2	29:Q:102:LYS:HG3	1.87	0.56
3:2:153:G:OP2	17:Y:131:ARG:NH1	2.32	0.56
3:2:950:C:O2'	13:N:104:ARG:NH1	2.36	0.56
10:I:87:ASN:HB3	10:I:90:LEU:HD23	1.86	0.56
3:2:1658:G:N2	3:2:1743:U:O2	2.31	0.56
16:X:144:ARG:NH2	22:k:687:THR:OG1	2.38	0.56
23:l:179:PRO:HA	23:l:189:MET:HG2	1.87	0.56
30:R:5:ARG:O	30:R:10:LYS:NZ	2.38	0.56
3:2:1005:A:H2'	3:2:1006:C:H4'	1.87	0.56
6:C:165:VAL:HG11	6:C:210:THR:HA	1.88	0.56
22:k:90:PRO:HD2	22:k:142:MET:HE3	1.87	0.56
3:2:538:A:OP1	11:J:175:ARG:NH1	2.37	0.56
3:2:139:C:O2'	8:G:187:LYS:NZ	2.38	0.56
3:2:1272:U:H3	3:2:1438:G:H1	1.54	0.56
22:k:613:PRO:HG3	22:k:626:GLN:HE21	1.71	0.56
25:F:82:PHE:O	25:F:86:GLN:NE2	2.39	0.56
32:T:16:ASN:OD1	32:T:56:LYS:NZ	2.37	0.56
3:2:609:U:O2	16:X:19:ARG:NH2	2.38	0.56
3:2:1573:A:OP1	3:2:1574:G:N2	2.39	0.56
6:C:111:VAL:O	6:C:136:VAL:HA	2.06	0.56
30:R:14:LYS:NZ	30:R:18:GLU:OE2	2.37	0.56
4:A:155:PHE:HA	14:V:60:ARG:HG2	1.88	0.55
20:h:127:GLN:HB3	20:h:140:ARG:O	2.05	0.55
20:h:131:ASN:ND2	20:h:138:GLU:OE2	2.39	0.55
28:P:37:ALA:HB1	28:P:41:VAL:HB	1.88	0.55
3:2:322:G:O2'	10:I:10:LYS:NZ	2.40	0.55
20:h:93:LYS:HB2	20:h:143:PRO:HG3	1.86	0.55
20:h:222:THR:HG22	20:h:235:GLY:HA3	1.89	0.55
3:2:900:A:H3'	3:2:901:G:H21	1.71	0.55
11:J:107:ARG:NH1	11:J:153:GLU:OE2	2.39	0.55
3:2:810:G:H2'	9:H:111:LYS:HB2	1.88	0.55
3:2:687:G:OP1	15:W:118:ARG:NH1	2.38	0.55
22:k:149:LEU:HD23	22:k:180:LEU:HD23	1.89	0.55
3:2:1273:G:O6	3:2:1437:U:O4	2.25	0.55
3:2:707:A:H61	3:2:731:C:H42	1.53	0.55
29:Q:8:GLN:HG2	29:Q:21:HIS:HD2	1.70	0.55
3:2:779:U:OP2	3:2:780:A:N6	2.39	0.55
17:Y:29:HIS:HB2	17:Y:32:ARG:HB2	1.89	0.55
29:Q:13:LYS:O	29:Q:16:ALA:HB3	2.07	0.55
3:2:704:C:H42	3:2:734:A:H61	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:706:A:H2	3:2:732:G:H1	1.52	0.55
3:2:1788:G:OP1	27:O:127:ARG:NH2	2.39	0.55
22:k:749:LEU:H	22:k:755:PHE:HA	1.71	0.55
34:D:28:GLU:O	34:D:65:ARG:NH2	2.40	0.55
3:2:17:C:O2'	3:2:1137:A:N1	2.36	0.54
28:P:98:ASN:HB2	28:P:122:THR:HA	1.89	0.54
5:B:144:ARG:HE	5:B:206:PRO:HB2	1.72	0.54
3:2:454:U:H5'	7:E:66:MET:HE3	1.89	0.54
3:2:1414:U:OP1	30:R:2:GLY:N	2.40	0.54
7:E:37:LYS:HB2	7:E:40:GLU:HG2	1.88	0.54
3:2:511:A:OP2	11:J:176:ASN:ND2	2.40	0.54
3:2:1290:U:OP1	6:C:91:ARG:NH1	2.39	0.54
20:h:98:LYS:HG2	20:h:138:GLU:HG2	1.89	0.54
3:2:16:G:O6	6:C:203:LYS:NZ	2.40	0.54
3:2:916:U:O2	27:O:41:ARG:NH2	2.36	0.54
9:H:134:GLU:OE1	13:N:21:ASN:ND2	2.39	0.54
15:W:25:VAL:HG22	15:W:63:VAL:HB	1.90	0.54
3:2:40:A:OP1	11:J:3:ARG:NH1	2.41	0.54
3:2:1211:A:H1'	28:P:100:LYS:HA	1.89	0.54
3:2:1382:A:O2'	35:U:89:ARG:NH2	2.41	0.54
29:Q:29:ILE:HG12	29:Q:65:ILE:HD12	1.89	0.54
3:2:1243:G:N2	3:2:1451:C:O2	2.40	0.54
3:2:1295:G:O6	3:2:1302:U:O4	2.25	0.54
3:2:1300:A:H5''	6:C:88:LYS:HE3	1.90	0.54
3:2:1556:A:OP1	28:P:115:TYR:OH	2.25	0.54
3:2:78:A:H1'	8:G:175:ILE:HG12	1.90	0.54
3:2:1587:A:O2'	25:F:104:ASN:ND2	2.41	0.54
12:L:33:ARG:NH2	12:L:51:GLY:O	2.40	0.54
20:h:184:THR:HA	20:h:231:ILE:O	2.07	0.54
23:l:85:LEU:O	23:l:89:LEU:N	2.40	0.54
3:2:153:G:H2'	3:2:154:G:H8	1.72	0.54
3:2:177:U:O2	8:G:191:ARG:NH1	2.41	0.54
3:2:1577:A:O3'	23:l:105:LYS:NZ	2.41	0.54
5:B:129:THR:O	5:B:132:ASP:N	2.40	0.54
7:E:11:ARG:NH1	7:E:27:TYR:O	2.41	0.54
20:h:95:GLU:OE1	27:O:111:ARG:NH1	2.40	0.54
3:2:1521:G:O2'	3:2:1523:G:OP2	2.26	0.54
5:B:217:LEU:HD13	5:B:220:GLN:HE21	1.73	0.54
11:J:83:VAL:HA	11:J:149:ARG:HA	1.90	0.54
22:k:103:LYS:NZ	22:k:193:SER:O	2.41	0.54
23:l:88:MET:HB3	23:l:93:THR:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1177:C:H5''	3:2:1189:A:H61	1.73	0.53
26:M:91:VAL:HG21	26:M:97:LEU:HD13	1.89	0.53
26:M:99:GLU:HA	26:M:105:LYS:H	1.73	0.53
2:e:33:ARG:HB3	11:J:37:LYS:HB3	1.90	0.53
34:D:45:LYS:NZ	34:D:82:GLY:O	2.41	0.53
3:2:458:G:OP1	17:Y:109:LYS:NZ	2.41	0.53
5:B:32:ILE:HA	5:B:96:LEU:HB2	1.89	0.53
22:k:169:ASP:HB3	22:k:173:GLY:H	1.73	0.53
3:2:1243:G:H21	3:2:1451:C:H1'	1.73	0.53
3:2:1575:G:O2'	23:l:231:ASN:ND2	2.41	0.53
31:S:47:CYS:HB3	31:S:52:VAL:HB	1.89	0.53
3:2:1035:G:OP2	13:N:9:LYS:NZ	2.41	0.53
3:2:1183:A:N6	28:P:122:THR:O	2.42	0.53
4:A:176:LEU:HD23	4:A:179:ARG:HD3	1.89	0.53
9:H:44:LYS:HG3	9:H:63:PRO:HD3	1.90	0.53
25:F:208:SER:O	25:F:212:LYS:NZ	2.40	0.53
31:S:86:LEU:HD22	31:S:99:HIS:HB2	1.90	0.53
5:B:145:LYS:HB2	5:B:149:GLN:HG3	1.89	0.53
3:2:1499:G:OP1	32:T:122:ARG:NH1	2.42	0.53
5:B:213:ARG:HG2	5:B:214:LYS:HG3	1.90	0.53
26:M:106:ILE:HD12	26:M:113:ARG:HD2	1.90	0.53
21:i:283:LEU:O	21:i:287:PHE:HB2	2.08	0.53
29:Q:50:GLU:OE1	29:Q:82:ARG:NH2	2.41	0.53
22:k:537:THR:HG23	22:k:540:ARG:HH21	1.74	0.53
12:L:99:ARG:HG3	16:X:12:ALA:HB2	1.89	0.53
23:l:177:PRO:HD3	23:l:250:VAL:HG13	1.91	0.53
31:S:6:GLN:HB3	33:Z:43:ASP:HB2	1.90	0.53
34:D:55:THR:HG21	34:D:90:ARG:HA	1.90	0.53
4:A:42:PRO:HB2	30:R:126:ALA:H	1.74	0.52
4:A:93:THR:O	4:A:185:ARG:NH1	2.40	0.52
14:V:17:CYS:SG	14:V:18:SER:N	2.82	0.52
11:J:62:ARG:O	11:J:69:ARG:NH1	2.42	0.52
3:2:354:C:H5''	10:I:16:ALA:HB2	1.90	0.52
3:2:389:G:N2	3:2:1732:A:OP1	2.36	0.52
3:2:1310:U:H4'	3:2:1400:A:H61	1.73	0.52
11:J:110:GLN:HE22	11:J:126:ARG:HB2	1.74	0.52
14:V:8:LEU:HD23	14:V:10:GLU:H	1.73	0.52
16:X:144:ARG:HD3	22:k:666:PRO:HB3	1.89	0.52
26:M:63:VAL:HG21	26:M:94:ALA:HA	1.91	0.52
3:2:1537:C:O2'	3:2:1540:G:O6	2.22	0.52
22:k:671:LYS:HB2	22:k:683:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Q:13:LYS:O	29:Q:76:SER:OG	2.27	0.52
34:D:104:SER:OG	34:D:108:LYS:NZ	2.43	0.52
3:2:298:C:H5'	7:E:38:LEU:HB2	1.91	0.52
3:2:434:G:OP1	22:k:65:ARG:NH1	2.41	0.52
3:2:1280:C:O2'	19:d:41:GLN:O	2.26	0.52
9:H:177:THR:HG23	9:H:179:LYS:H	1.75	0.52
23:l:182:ASN:O	23:l:184:ARG:N	2.43	0.52
29:Q:16:ALA:HB2	29:Q:72:GLY:HA3	1.91	0.52
8:G:50:PHE:HB3	8:G:111:LEU:HD22	1.91	0.52
16:X:109:ARG:HH22	16:X:117:ILE:HD12	1.74	0.52
10:I:84:HIS:HD2	10:I:87:ASN:H	1.56	0.52
29:Q:39:VAL:HG12	29:Q:41:PRO:HD2	1.91	0.52
3:2:871:G:H2'	3:2:872:G:C8	2.45	0.52
3:2:1267:G:N1	3:2:1442:U:O2'	2.37	0.52
27:O:47:LYS:HE2	27:O:62:LEU:HB3	1.92	0.52
1:b:56:CYS:SG	1:b:57:GLU:N	2.83	0.51
3:2:273:G:H1	3:2:283:U:H3	1.56	0.51
3:2:359:A:OP2	22:k:51:LYS:NZ	2.44	0.51
22:k:339:SER:O	22:k:343:ARG:NH2	2.38	0.51
17:Y:103:ALA:O	17:Y:108:ARG:NH2	2.43	0.51
18:c:14:LYS:HB2	18:c:29:ARG:HB2	1.93	0.51
3:2:1387:G:H2'	3:2:1388:A:H2'	1.91	0.51
22:k:73:ARG:NH2	22:k:244:GLN:O	2.44	0.51
23:l:88:MET:HE1	23:l:91:ARG:HD2	1.91	0.51
24:y:157:ARG:HE	24:y:203:GLU:HB2	1.74	0.51
3:2:1367:G:H2'	3:2:1368:G:H8	1.75	0.51
3:2:1561:U:H2'	3:2:1562:G:H8	1.75	0.51
22:k:642:TYR:HA	22:k:697:LEU:HD23	1.92	0.51
29:Q:37:THR:O	29:Q:45:ARG:NH1	2.43	0.51
6:C:40:LYS:HA	6:C:43:ARG:HG2	1.93	0.51
26:M:52:LEU:HD21	26:M:60:VAL:HG21	1.92	0.51
26:M:73:LYS:HA	26:M:76:GLU:HG2	1.93	0.51
7:E:212:ASP:OD1	7:E:216:ASN:N	2.44	0.51
19:d:26:SER:OG	19:d:39:CYS:SG	2.67	0.51
31:S:17:LEU:HD22	31:S:66:LEU:HD22	1.92	0.51
6:C:56:ILE:HG23	6:C:61:LEU:HB2	1.93	0.51
6:C:116:LYS:HG2	6:C:127:ALA:HB3	1.93	0.51
19:d:44:ARG:NH1	35:U:82:TYR:OH	2.44	0.51
23:l:33:PRO:HB2	23:l:35:PRO:HD2	1.93	0.51
3:2:205:U:H2'	3:2:206:A:H8	1.76	0.51
3:2:773:C:O2'	3:2:787:G:N2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:873:U:O2'	3:2:1047:G:OP1	2.29	0.51
22:k:124:PHE:O	22:k:136:LYS:HA	2.11	0.51
26:M:42:ALA:HB2	26:M:124:LYS:HE3	1.93	0.51
1:b:33:LEU:HD23	1:b:81:ARG:HA	1.92	0.51
3:2:126:A:H62	3:2:291:G:H21	1.59	0.51
3:2:1688:U:O2	3:2:1713:G:N2	2.36	0.51
23:l:37:ILE:HD12	23:l:73:TYR:HD2	1.76	0.51
24:y:276:VAL:HA	24:y:280:LYS:HB3	1.93	0.51
3:2:1213:G:O6	3:2:1450:U:O4	2.28	0.50
30:R:18:GLU:HG2	30:R:69:ILE:H	1.76	0.50
3:2:570:A:OP2	16:X:65:ASN:ND2	2.44	0.50
3:2:992:A:O2'	3:2:1785:U:O2	2.29	0.50
23:l:226:ILE:HD12	23:l:265:ALA:HB1	1.93	0.50
35:U:35:GLU:OE2	35:U:89:ARG:NH2	2.44	0.50
3:2:811:A:N6	9:H:111:LYS:O	2.42	0.50
23:l:201:ARG:HD3	23:l:202:LYS:HG2	1.93	0.50
29:Q:31:VAL:HA	29:Q:67:VAL:HB	1.93	0.50
5:B:190:PRO:HG2	5:B:192:VAL:HG23	1.93	0.50
18:c:42:ARG:NH1	18:c:61:ARG:O	2.44	0.50
3:2:656:G:O2'	3:2:657:U:O4'	2.30	0.50
3:2:1594:G:OP2	3:2:1596:C:N4	2.41	0.50
12:L:71:LEU:HD22	12:L:88:ARG:HH12	1.76	0.50
20:h:127:GLN:OE1	20:h:142:ASN:ND2	2.37	0.50
3:2:1600:A:OP1	32:T:86:ARG:NH1	2.44	0.50
11:J:107:ARG:NH2	11:J:148:VAL:O	2.41	0.50
16:X:32:ARG:HD3	16:X:33:LEU:HG	1.93	0.50
20:h:213:LYS:O	20:h:216:ILE:HB	2.12	0.50
3:2:1197:C:OP1	3:2:1602:C:O2'	2.28	0.50
1:b:40:CYS:SG	1:b:58:SER:OG	2.69	0.50
3:2:1081:A:O2'	3:2:1083:G:N7	2.40	0.50
3:2:1328:G:H3'	3:2:1329:A:H8	1.76	0.50
18:c:10:ALA:HB3	18:c:54:LEU:HB2	1.93	0.50
23:l:23:GLU:HB2	23:l:83:LEU:HD13	1.93	0.50
26:M:62:LEU:HB2	26:M:90:LYS:HD3	1.94	0.50
3:2:1082:C:O2'	3:2:1083:G:O4'	2.30	0.49
5:B:35:PRO:HB3	5:B:231:LEU:HG	1.94	0.49
29:Q:83:GLN:HE22	29:Q:119:ALA:HA	1.76	0.49
6:C:97:ARG:HG2	6:C:119:LYS:HA	1.93	0.49
3:2:566:C:H4'	3:2:567:A:C8	2.47	0.49
3:2:1345:A:N6	3:2:1377:U:O2'	2.46	0.49
9:H:8:ILE:HA	9:H:42:GLN:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:49:ILE:HD11	9:H:172:VAL:HG22	1.94	0.49
16:X:51:GLY:HA2	16:X:77:ILE:HG13	1.94	0.49
22:k:616:VAL:O	22:k:622:ARG:HA	2.13	0.49
26:M:103:LEU:HD12	26:M:118:ALA:HB2	1.95	0.49
3:2:1160:A:O2'	3:2:1620:C:N3	2.44	0.49
3:2:1313:A:H61	30:R:4:VAL:HG11	1.76	0.49
3:2:1471:A:OP1	25:F:185:ARG:NH2	2.44	0.49
14:V:38:LYS:HD2	14:V:49:GLU:HB3	1.94	0.49
22:k:89:VAL:HG22	22:k:140:PRO:HG2	1.94	0.49
24:y:149:ARG:HD3	24:y:150:VAL:HG13	1.94	0.49
3:2:539:G:N2	3:2:539:G:OP2	2.46	0.49
6:C:78:ASP:HA	6:C:104:VAL:HA	1.94	0.49
28:P:41:VAL:HG13	28:P:84:ILE:HG13	1.93	0.49
34:D:105:MET:HE1	34:D:119:ALA:HA	1.95	0.49
3:2:106:U:OP1	10:I:8:ARG:NH2	2.44	0.49
3:2:856:A:H2'	9:H:116:ARG:HH21	1.78	0.49
24:y:151:SER:HB2	24:y:209:LEU:HB2	1.93	0.49
32:T:84:LYS:O	32:T:91:TYR:HA	2.13	0.49
3:2:775:G:O6	3:2:785:U:O2	2.31	0.49
12:L:102:LYS:O	16:X:13:ARG:NH2	2.39	0.49
23:l:84:ALA:O	23:l:88:MET:N	2.45	0.49
2:e:60:PRO:HD2	3:2:559:C:H4'	1.93	0.49
3:2:1151:A:OP2	3:2:1629:G:N2	2.46	0.49
6:C:142:GLY:N	6:C:153:SER:O	2.46	0.49
7:E:46:VAL:HG13	7:E:50:ASN:HD22	1.77	0.49
20:h:116:ILE:HG23	20:h:158:PHE:HE2	1.78	0.49
1:b:51:GLN:NE2	3:2:958:U:O2	2.44	0.49
2:e:10:ARG:NE	3:2:516:G:O3'	2.41	0.49
4:A:139:VAL:HA	6:C:62:PRO:HG3	1.94	0.49
2:e:3:LYS:NZ	22:k:214:SER:OG	2.40	0.49
21:i:315:SER:OG	21:i:351:HIS:NE2	2.45	0.49
25:F:192:GLU:OE1	33:Z:63:SER:OG	2.30	0.49
32:T:70:GLN:HG3	32:T:121:GLY:HA3	1.94	0.49
3:2:3:U:O2'	11:J:17:ARG:NH2	2.45	0.48
3:2:1679:G:H21	3:2:1722:A:H62	1.60	0.48
3:2:1697:G:H1	3:2:1704:U:H3	1.59	0.48
20:h:153:GLN:HG2	27:O:103:ARG:HA	1.94	0.48
28:P:81:ARG:HH12	28:P:120:SER:HB3	1.77	0.48
3:2:1473:U:O2'	25:F:103:ASN:OD1	2.26	0.48
7:E:230:GLU:HB2	7:E:233:LYS:HB2	1.93	0.48
9:H:143:LEU:O	15:W:42:GLN:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:183:GLU:HG2	20:h:240:ILE:HD12	1.94	0.48
3:2:936:G:OP1	3:2:1074:G:N2	2.38	0.48
8:G:7:TYR:HB2	8:G:113:ILE:HD12	1.96	0.48
22:k:596:PHE:HB2	22:k:654:ALA:HB3	1.94	0.48
26:M:132:GLU:O	26:M:135:MET:HB3	2.13	0.48
31:S:29:VAL:HG23	31:S:54:LEU:HD22	1.95	0.48
3:2:566:C:OP1	22:k:633:SER:OG	2.32	0.48
8:G:58:LYS:HA	8:G:107:ALA:HB2	1.94	0.48
22:k:573:ASP:HB3	22:k:576:GLN:HB3	1.95	0.48
22:k:699:LYS:O	22:k:774:TYR:HA	2.13	0.48
31:S:41:ARG:NH2	32:T:36:ILE:O	2.46	0.48
32:T:40:SER:OG	32:T:43:ASN:ND2	2.46	0.48
3:2:375:U:H5''	16:X:32:ARG:HH22	1.77	0.48
3:2:1676:U:H5''	10:I:58:LEU:HD11	1.96	0.48
5:B:144:ARG:HB3	5:B:208:GLN:HB3	1.94	0.48
3:2:953:G:H2'	3:2:954:G:C8	2.46	0.48
29:Q:20:ALA:HA	29:Q:66:ARG:O	2.14	0.48
31:S:38:VAL:HG13	31:S:42:TYR:HD2	1.79	0.48
4:A:200:ASP:HB3	30:R:86:PRO:HD2	1.96	0.48
34:D:63:GLY:O	34:D:67:ASN:ND2	2.46	0.48
26:M:60:VAL:HG22	26:M:122:VAL:HG22	1.95	0.48
31:S:41:ARG:HH12	32:T:38:LYS:HB3	1.78	0.48
3:2:114:C:HO2'	12:L:65:SER:HG	1.62	0.48
3:2:1403:C:OP1	30:R:3:ARG:N	2.47	0.48
4:A:124:THR:HG22	4:A:174:TRP:HE1	1.79	0.48
32:T:77:ASN:HB3	32:T:95:ASP:HB3	1.95	0.48
3:2:283:U:H5''	8:G:188:ARG:HD3	1.96	0.47
3:2:1397:U:O2'	3:2:1400:A:N6	2.47	0.47
3:2:1672:G:H2'	3:2:1673:G:C8	2.48	0.47
31:S:32:LEU:HD11	31:S:69:ILE:HD13	1.96	0.47
32:T:49:ASP:O	32:T:53:TRP:N	2.47	0.47
1:b:20:LYS:NZ	13:N:13:SER:O	2.38	0.47
9:H:138:LYS:HD2	9:H:150:GLN:HE21	1.79	0.47
21:i:288:ARG:O	21:i:292:GLU:HB3	2.14	0.47
23:l:33:PRO:HD2	23:l:36:LEU:HD12	1.96	0.47
31:S:40:ARG:NH1	32:T:44:GLU:OE2	2.46	0.47
3:2:29:U:H2'	3:2:30:G:H8	1.78	0.47
3:2:250:C:H2'	3:2:251:A:H8	1.80	0.47
3:2:917:U:H1'	27:O:41:ARG:HH21	1.79	0.47
3:2:1170:G:H1	3:2:1469:A:N6	2.10	0.47
3:2:1287:A:H4'	3:2:1328:G:H21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1654:G:H4'	3:2:1655:A:H5'	1.96	0.47
6:C:78:ASP:HB3	6:C:104:VAL:HG12	1.95	0.47
21:i:283:LEU:HD21	21:i:307:VAL:HG22	1.95	0.47
3:2:577:G:N7	23:l:47:SER:HB3	2.30	0.47
3:2:751:G:H2'	3:2:752:A:C8	2.50	0.47
3:2:1572:G:H3'	23:l:282:LYS:HD2	1.96	0.47
3:2:1611:A:O2'	25:F:95:ASN:O	2.31	0.47
17:Y:81:GLU:HA	17:Y:84:LYS:HG2	1.96	0.47
22:k:246:LEU:HD12	22:k:247:PRO:HD2	1.95	0.47
33:Z:60:VAL:HG23	33:Z:101:TYR:HB2	1.96	0.47
3:2:868:G:H1	3:2:960:U:H3	1.62	0.47
5:B:88:VAL:HG22	5:B:98:THR:HG23	1.95	0.47
7:E:87:MET:HE1	7:E:236:ILE:HD13	1.96	0.47
22:k:275:ASP:OD1	22:k:304:ASN:ND2	2.44	0.47
3:2:167:U:H1'	8:G:133:LEU:HD23	1.97	0.47
3:2:1484:G:N3	3:2:1606:C:O2'	2.41	0.47
4:A:183:ARG:NH2	4:A:191:ARG:O	2.47	0.47
20:h:181:TYR:O	20:h:234:LEU:HA	2.15	0.47
22:k:128:ILE:HD13	22:k:135:LEU:HD13	1.97	0.47
22:k:257:GLY:HA2	22:k:284:GLY:HA3	1.95	0.47
26:M:42:ALA:HB1	26:M:47:GLU:HG2	1.96	0.47
29:Q:44:LEU:O	29:Q:47:LYS:HB2	2.14	0.47
34:D:52:ALA:HB3	34:D:55:THR:HG22	1.97	0.47
3:2:829:A:H4'	3:2:830:U:H5'	1.97	0.47
3:2:1532:U:OP2	33:Z:77:ARG:NH1	2.37	0.47
17:Y:104:SER:HB2	17:Y:107:GLN:HG2	1.96	0.47
21:i:311:LEU:HA	21:i:317:PHE:HB2	1.97	0.47
22:k:639:VAL:HG22	22:k:696:ILE:HD11	1.96	0.47
34:D:164:VAL:HG13	34:D:168:ILE:HD11	1.96	0.47
3:2:114:C:O2'	12:L:65:SER:OG	2.32	0.47
3:2:434:G:N2	3:2:437:A:OP2	2.38	0.47
3:2:790:U:H2'	3:2:791:A:H8	1.79	0.47
3:2:1472:C:H4'	3:2:1473:U:H5'	1.96	0.47
5:B:127:VAL:HG21	5:B:137:ILE:HD12	1.95	0.47
23:l:154:LEU:HD23	23:l:157:LEU:HD12	1.97	0.47
29:Q:21:HIS:HB2	29:Q:66:ARG:HB2	1.96	0.47
2:e:31:LYS:HB2	3:2:476:U:H2'	1.96	0.47
3:2:766:U:O4	3:2:770:A:N7	2.48	0.47
7:E:87:MET:HE1	7:E:236:ILE:HG21	1.97	0.47
33:Z:82:HIS:NE2	33:Z:86:GLU:OE2	2.48	0.47
22:k:705:GLY:HA3	22:k:720:MET:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:57:TYR:OH	33:Z:68:ARG:NH1	2.48	0.46
2:e:46:ASN:OD1	3:2:502:U:O2'	2.34	0.46
3:2:513:U:H2'	3:2:514:G:C8	2.50	0.46
3:2:925:G:H2'	3:2:926:A:C8	2.50	0.46
24:y:177:ALA:HA	24:y:300:GLN:HE21	1.80	0.46
31:S:27:LYS:NZ	31:S:55:HIS:O	2.40	0.46
22:k:78:GLY:HA3	22:k:133:SER:HA	1.97	0.46
22:k:297:ASP:OD1	22:k:622:ARG:NH2	2.48	0.46
24:y:179:VAL:O	24:y:183:ALA:N	2.45	0.46
26:M:87:PRO:HG3	26:M:137:MET:HG3	1.97	0.46
3:2:1480:G:OP1	32:T:60:SER:OG	2.27	0.46
22:k:302:GLN:HG3	22:k:562:ARG:HD2	1.97	0.46
24:y:233:ARG:HB3	24:y:236:ARG:HB3	1.96	0.46
3:2:67:A:N6	3:2:83:G:O2'	2.47	0.46
3:2:803:A:C5	9:H:104:ARG:HG3	2.50	0.46
25:F:37:GLN:HB2	29:Q:53:LEU:HD13	1.97	0.46
3:2:140:A:H1'	8:G:179:VAL:HG21	1.98	0.46
3:2:1511:U:H2'	3:2:1512:G:H8	1.80	0.46
4:A:15:GLN:HG3	30:R:117:LEU:HD22	1.97	0.46
5:B:197:ILE:O	5:B:201:THR:CB	2.64	0.46
22:k:103:LYS:HB3	22:k:229:LEU:HB3	1.96	0.46
22:k:502:ARG:NH1	22:k:516:GLU:OE2	2.48	0.46
3:2:146:U:H2'	3:2:147:A:H8	1.81	0.46
3:2:568:G:N2	3:2:582:U:O2'	2.48	0.46
3:2:1149:G:O2'	3:2:1150:G:N2	2.49	0.46
11:J:81:VAL:HG21	11:J:91:LYS:HE2	1.96	0.46
22:k:668:ILE:HA	22:k:685:HIS:HA	1.96	0.46
27:O:15:GLY:N	27:O:78:ALA:O	2.48	0.46
35:U:58:LEU:HB2	35:U:88:LYS:HB2	1.98	0.46
3:2:585:A:H2'	3:2:586:G:H8	1.80	0.46
3:2:612:U:OP2	16:X:5:LYS:NZ	2.46	0.46
3:2:1294:G:H3'	3:2:1295:G:C8	2.50	0.46
22:k:565:LYS:HD2	22:k:568:LEU:HD12	1.97	0.46
3:2:1087:A:H2'	3:2:1088:A:C8	2.51	0.46
3:2:1309:C:H1'	3:2:1398:U:H3	1.81	0.46
8:G:102:VAL:HG13	8:G:106:LEU:HD12	1.97	0.46
21:i:288:ARG:O	21:i:292:GLU:CB	2.64	0.46
22:k:609:PRO:HA	22:k:645:PHE:HA	1.97	0.46
3:2:837:G:H2'	3:2:838:G:H8	1.80	0.45
3:2:1469:A:H4'	3:2:1541:G:H4'	1.98	0.45
19:d:52:PHE:HB3	35:U:82:TYR:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:k:670:PHE:HB3	22:k:682:LEU:HD23	1.98	0.45
26:M:33:ARG:HB2	26:M:100:TRP:HE3	1.80	0.45
3:2:67:A:O2'	3:2:69:G:OP1	2.33	0.45
3:2:1377:U:H1'	3:2:1379:C:H41	1.81	0.45
3:2:1684:U:H2'	3:2:1685:G:H8	1.80	0.45
20:h:236:GLY:HA3	20:h:239:HIS:HD2	1.81	0.45
22:k:83:ALA:HB3	22:k:283:ARG:HD2	1.97	0.45
23:l:166:MET:HE3	23:l:189:MET:HE1	1.99	0.45
25:F:51:VAL:HG13	25:F:134:VAL:HG21	1.98	0.45
34:D:137:VAL:HB	34:D:185:LYS:HB2	1.98	0.45
27:O:50:ALA:HB3	27:O:53:ASP:HB2	1.97	0.45
2:e:43:ARG:HH22	3:2:591:A:P	2.39	0.45
3:2:649:U:O2'	3:2:650:U:O5'	2.34	0.45
3:2:1639:C:O2	3:2:1764:C:N4	2.45	0.45
27:O:19:ILE:HA	27:O:27:PHE:O	2.17	0.45
3:2:1042:G:H2'	3:2:1043:A:H8	1.82	0.45
3:2:1645:G:H22	3:2:1756:A:H2	1.65	0.45
3:2:1788:G:H2'	3:2:1789:G:H8	1.82	0.45
17:Y:43:LYS:HA	17:Y:46:GLU:HG2	1.97	0.45
22:k:265:ASP:N	22:k:265:ASP:OD1	2.49	0.45
23:l:61:LEU:HB3	23:l:79:GLY:HA3	1.98	0.45
5:B:64:ARG:HB2	5:B:88:VAL:HB	1.97	0.45
7:E:48:LEU:HD12	7:E:61:VAL:HG13	1.99	0.45
21:i:279:ILE:HG23	21:i:283:LEU:HD22	1.99	0.45
22:k:189:ILE:HD13	22:k:238:VAL:HG13	1.99	0.45
23:l:275:CYS:HA	23:l:278:ARG:HG2	1.97	0.45
3:2:1147:A:N1	3:2:1633:A:N6	2.64	0.45
3:2:1584:G:N2	3:2:1585:U:O4	2.36	0.45
18:c:27:GLN:HE22	18:c:65:ARG:HD2	1.80	0.45
22:k:667:ALA:O	22:k:686:GLY:N	2.47	0.45
24:y:139:PHE:HA	24:y:142:ILE:HD12	1.99	0.45
30:R:101:ASN:OD1	30:R:120:SER:OG	2.33	0.45
3:2:1357:A:H2'	3:2:1358:G:C8	2.52	0.45
3:2:1591:C:H2'	3:2:1592:A:H8	1.81	0.45
10:I:90:LEU:HD13	10:I:95:THR:HB	1.99	0.45
22:k:278:ILE:O	22:k:558:ARG:HA	2.16	0.45
22:k:306:ILE:HB	22:k:337:PHE:HB2	1.98	0.45
11:J:53:ARG:HH11	11:J:57:ARG:HH21	1.64	0.45
21:i:315:SER:HG	21:i:351:HIS:CD2	2.35	0.45
22:k:265:ASP:O	22:k:277:VAL:N	2.36	0.45
3:2:878:G:H2'	3:2:879:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1374:C:H2'	3:2:1375:A:C8	2.52	0.45
3:2:1591:C:H2'	3:2:1592:A:C8	2.52	0.45
3:2:1658:G:O6	3:2:1743:U:O4	2.35	0.45
13:N:99:ARG:NH2	13:N:119:GLU:OE2	2.50	0.45
21:i:304:TYR:CZ	21:i:308:LYS:HD2	2.52	0.45
23:l:94:VAL:HA	23:l:114:ASP:HA	1.98	0.45
26:M:28:LEU:HD13	26:M:136:ILE:HG21	1.99	0.45
26:M:98:GLY:O	26:M:103:LEU:N	2.49	0.45
3:2:477:A:H2'	3:2:478:A:H8	1.82	0.44
3:2:484:C:H2'	3:2:485:A:H8	1.81	0.44
3:2:546:U:H2'	3:2:547:U:C6	2.53	0.44
3:2:1152:A:H2'	3:2:1153:G:H8	1.82	0.44
3:2:1354:G:O6	3:2:1369:U:O2	2.35	0.44
22:k:540:ARG:NH1	22:k:544:GLU:OE2	2.50	0.44
3:2:14:C:H2'	3:2:15:U:C6	2.52	0.44
3:2:632:U:O2'	3:2:1103:U:OP1	2.31	0.44
3:2:890:C:H2'	3:2:891:A:H8	1.82	0.44
3:2:1409:G:N1	3:2:1412:G:OP2	2.48	0.44
12:L:78:THR:HG23	12:L:84:ILE:HG22	1.99	0.44
33:Z:48:ASP:O	33:Z:52:LYS:HE2	2.17	0.44
3:2:207:U:O2	10:I:178:ARG:NH1	2.48	0.44
3:2:647:G:H22	3:2:687:G:H1	1.65	0.44
3:2:1155:G:H2'	3:2:1156:C:C6	2.53	0.44
21:i:308:LYS:HA	21:i:341:VAL:HG13	1.99	0.44
23:l:202:LYS:HD2	23:l:206:ILE:HD11	2.00	0.44
34:D:172:THR:O	34:D:173:ARG:NH1	2.41	0.44
2:e:46:ASN:HD21	3:2:503:G:H5'	1.81	0.44
3:2:459:G:OP2	17:Y:105:ARG:NH2	2.48	0.44
12:L:55:ASP:HB3	12:L:58:CYS:HB2	1.98	0.44
3:2:279:G:H8	3:2:280:U:H4'	1.83	0.44
3:2:804:A:N3	15:W:105:THR:HG22	2.33	0.44
16:X:112:LYS:H	16:X:117:ILE:HG13	1.83	0.44
20:h:193:LEU:HD22	20:h:197:HIS:HB3	1.99	0.44
21:i:260:TYR:CZ	21:i:264:LYS:HD2	2.52	0.44
23:l:213:LEU:HD12	23:l:280:PHE:HZ	1.82	0.44
35:U:42:VAL:O	35:U:52:LYS:NZ	2.50	0.44
3:2:78:A:H2	8:G:174:LYS:HG3	1.81	0.44
3:2:108:A:H2'	3:2:109:G:C8	2.53	0.44
3:2:1427:A:H5'	3:2:1428:G:C8	2.53	0.44
3:2:1474:G:H2'	3:2:1475:A:C8	2.52	0.44
6:C:241:ASP:HA	6:C:244:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:98:ILE:HG22	9:H:121:VAL:HG21	2.00	0.44
16:X:69:ARG:HH22	16:X:120:VAL:HG22	1.82	0.44
20:h:184:THR:HB	27:O:93:THR:HG21	1.99	0.44
25:F:192:GLU:OE2	33:Z:61:SER:OG	2.29	0.44
30:R:27:ASP:HB3	30:R:30:THR:HG22	1.99	0.44
3:2:1151:A:OP2	20:h:264:ARG:NH2	2.46	0.44
3:2:1482:C:O2'	29:Q:72:GLY:O	2.36	0.44
3:2:982:U:H2'	3:2:983:A:C8	2.53	0.44
3:2:1279:C:N4	3:2:1428:G:O6	2.51	0.44
3:2:1432:U:H5'	3:2:1433:G:H5'	1.99	0.44
3:2:1461:C:H2'	3:2:1462:G:H8	1.83	0.44
8:G:163:THR:HG22	8:G:168:THR:HG23	1.99	0.44
19:d:39:CYS:O	19:d:43:PHE:N	2.41	0.44
22:k:192:ILE:HG13	22:k:226:VAL:HG12	1.99	0.44
32:T:22:LEU:HD13	32:T:28:LEU:HD11	1.99	0.44
3:2:149:C:O2'	8:G:132:ARG:NH1	2.48	0.44
9:H:4:PRO:HB2	9:H:39:ARG:HH12	1.82	0.44
13:N:103:GLU:OE1	13:N:106:ARG:NH1	2.39	0.44
23:l:240:LYS:HG3	23:l:241:LEU:HG	2.00	0.44
25:F:34:GLN:O	25:F:38:THR:CB	2.66	0.44
28:P:44:ARG:NH1	28:P:82:ASN:O	2.42	0.44
31:S:87:ASN:HD22	31:S:100:THR:N	2.16	0.44
3:2:688:G:H2'	3:2:689:G:H8	1.83	0.43
7:E:103:TYR:O	7:E:182:TYR:OH	2.35	0.43
11:J:53:ARG:NH2	11:J:97:LEU:O	2.51	0.43
22:k:510:CYS:O	22:k:637:ASN:ND2	2.39	0.43
25:F:42:LEU:HD12	25:F:48:PHE:H	1.83	0.43
25:F:133:VAL:HG22	25:F:198:LEU:HD13	2.00	0.43
3:2:540:G:O2'	3:2:543:C:OP2	2.34	0.43
3:2:1321:A:C6	4:A:104:PRO:HB2	2.53	0.43
3:2:1483:A:N3	3:2:1607:G:O2'	2.42	0.43
3:2:1630:U:H2'	3:2:1631:A:H4'	2.00	0.43
3:2:1630:U:O2'	3:2:1632:C:OP1	2.31	0.43
24:y:227:LEU:HA	24:y:230:VAL:HG22	2.00	0.43
25:F:110:ALA:HA	25:F:113:ILE:HD12	2.00	0.43
34:D:53:THR:HA	34:D:93:ASP:HB2	1.99	0.43
34:D:99:VAL:HG13	34:D:173:ARG:HH21	1.82	0.43
22:k:103:LYS:NZ	22:k:230:GLU:OE2	2.44	0.43
22:k:292:LEU:HB2	22:k:584:LEU:HB2	2.00	0.43
29:Q:13:LYS:HG2	29:Q:79:TYR:HB2	2.00	0.43
34:D:163:PRO:HA	34:D:166:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1387:G:O2'	3:2:1411:A:N1	2.48	0.43
4:A:69:ASN:ND2	6:C:244:SER:OG	2.51	0.43
3:2:1535:U:H5''	25:F:187:ILE:HD11	1.99	0.43
4:A:205:ARG:NH2	30:R:84:TYR:O	2.51	0.43
23:l:63:SER:HB2	23:l:74:ARG:HB3	2.01	0.43
24:y:176:SER:HA	24:y:179:VAL:HG12	2.01	0.43
33:Z:80:LEU:HD13	33:Z:101:TYR:HE2	1.83	0.43
3:2:1777:G:H2'	3:2:1778:G:C8	2.54	0.43
10:I:67:TRP:HH2	10:I:156:VAL:HG11	1.83	0.43
13:N:135:LEU:HD12	13:N:136:PRO:HD2	2.00	0.43
25:F:80:LYS:HE2	25:F:83:ARG:HB2	2.00	0.43
26:M:41:LEU:HB2	26:M:43:ARG:HH11	1.82	0.43
3:2:728:U:H2'	3:2:729:G:H8	1.83	0.43
3:2:1082:C:N4	3:2:1091:A:H62	2.16	0.43
3:2:1595:U:O3'	19:d:32:ARG:NH2	2.44	0.43
11:J:83:VAL:HG12	11:J:149:ARG:HG2	2.01	0.43
23:l:45:SER:OG	23:l:46:GLN:N	2.51	0.43
23:l:127:LEU:HD13	23:l:155:SER:HA	2.00	0.43
28:P:90:ILE:HD11	28:P:112:LEU:HD11	2.00	0.43
3:2:385:A:H2'	3:2:386:G:C8	2.54	0.43
3:2:1041:G:H2'	3:2:1042:G:C8	2.53	0.43
6:C:182:PRO:HA	6:C:185:LYS:HB3	2.00	0.43
7:E:160:VAL:HG13	7:E:169:ILE:HG23	2.01	0.43
11:J:89:ASP:OD1	11:J:89:ASP:N	2.51	0.43
20:h:233:ILE:HG22	20:h:240:ILE:HG22	2.01	0.43
26:M:25:GLU:HG2	26:M:91:VAL:HA	2.01	0.43
28:P:94:VAL:O	28:P:104:GLN:HA	2.19	0.43
3:2:521:A:N3	17:Y:34:ASN:ND2	2.62	0.43
13:N:87:ASP:N	13:N:87:ASP:OD1	2.49	0.43
15:W:25:VAL:O	15:W:62:VAL:HA	2.19	0.43
28:P:64:LYS:NZ	28:P:88:GLU:O	2.52	0.43
3:2:1211:A:N3	28:P:97:TYR:OH	2.41	0.43
3:2:1511:U:H2'	3:2:1512:G:C8	2.52	0.43
5:B:129:THR:HG22	5:B:176:VAL:HG22	2.00	0.43
12:L:33:ARG:HH11	12:L:61:THR:HG21	1.84	0.43
23:l:147:GLN:HG2	23:l:151:TRP:CD1	2.53	0.43
24:y:136:PRO:HA	24:y:139:PHE:HB3	2.00	0.43
25:F:34:GLN:O	25:F:38:THR:HB	2.19	0.43
30:R:51:ALA:O	30:R:54:THR:OG1	2.31	0.43
34:D:29:LEU:HD21	34:D:69:LEU:HD11	2.01	0.43
3:2:1199:G:N2	3:2:1594:G:O2'	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1500:C:OP1	32:T:122:ARG:NH2	2.51	0.42
8:G:71:THR:HG22	8:G:72:ARG:H	1.84	0.42
11:J:105:LEU:HD12	11:J:108:ARG:HD2	2.01	0.42
23:l:53:ILE:HA	23:l:56:LEU:HD12	2.01	0.42
3:2:966:A:H5''	13:N:4:MET:HE1	2.00	0.42
3:2:1217:A:H3'	3:2:1218:G:H3'	2.01	0.42
3:2:1365:C:OP1	29:Q:66:ARG:NH2	2.52	0.42
5:B:27:LYS:HB3	5:B:47:LEU:HD11	2.00	0.42
13:N:66:ILE:HG23	13:N:67:THR:HG23	2.00	0.42
3:2:959:U:H6	13:N:61:THR:HB	1.85	0.42
3:2:1114:G:O2'	3:2:1130:G:O6	2.29	0.42
9:H:28:GLU:HB3	9:H:35:LYS:HG3	2.02	0.42
17:Y:10:ARG:HB2	17:Y:24:VAL:HB	2.01	0.42
23:l:83:LEU:O	23:l:87:THR:N	2.40	0.42
3:2:1145:U:H5''	3:2:1146:G:H21	1.84	0.42
3:2:1305:U:H5	6:C:91:ARG:HH22	1.67	0.42
3:2:1787:C:H2'	3:2:1788:G:C8	2.54	0.42
6:C:101:VAL:HG22	6:C:115:ILE:HG12	2.01	0.42
8:G:42:GLY:HA3	8:G:45:PHE:HD2	1.84	0.42
11:J:120:LYS:H	11:J:124:HIS:HD2	1.66	0.42
34:D:132:LYS:HB3	34:D:189:MET:HG3	2.01	0.42
3:2:126:A:H62	3:2:291:G:N2	2.17	0.42
3:2:1474:G:H2'	3:2:1475:A:H8	1.84	0.42
6:C:88:LYS:HE2	6:C:97:ARG:HD2	2.02	0.42
7:E:101:LEU:HD23	7:E:101:LEU:HA	1.88	0.42
25:F:166:ARG:HA	25:F:169:ASN:HD22	1.85	0.42
3:2:375:U:O3'	16:X:32:ARG:NH2	2.52	0.42
3:2:699:U:O2	3:2:739:G:N2	2.43	0.42
3:2:811:A:O2'	3:2:858:G:N2	2.49	0.42
5:B:86:LEU:HD13	5:B:100:PHE:HA	2.00	0.42
7:E:21:ASP:N	7:E:21:ASP:OD1	2.52	0.42
22:k:304:ASN:HB2	22:k:562:ARG:HG3	2.01	0.42
23:l:175:LYS:HD3	23:l:249:PHE:H	1.85	0.42
30:R:60:ARG:HH12	30:R:66:VAL:HG11	1.84	0.42
3:2:472:U:O2'	3:2:769:A:N3	2.44	0.42
3:2:762:A:OP1	11:J:79:ARG:NH2	2.51	0.42
3:2:906:A:H2'	3:2:907:A:C8	2.54	0.42
3:2:1367:G:H2'	3:2:1368:G:C8	2.55	0.42
3:2:1533:C:H4'	3:2:1539:G:N1	2.35	0.42
20:h:171:SER:HA	20:h:174:LEU:HD12	2.00	0.42
34:D:53:THR:OG1	34:D:54:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:158:U:O2'	3:2:160:C:OP2	2.27	0.42
3:2:160:C:O3'	8:G:95:LYS:NZ	2.52	0.42
3:2:1295:G:N1	3:2:1302:U:N3	2.50	0.42
3:2:1502:G:N2	3:2:1504:G:H3'	2.34	0.42
5:B:130:SER:HB2	5:B:180:THR:HG22	2.02	0.42
6:C:147:ASN:ND2	14:V:2:GLU:O	2.44	0.42
8:G:142:ARG:HA	8:G:147:LEU:HD12	2.02	0.42
20:h:237:PHE:HA	20:h:240:ILE:HG12	2.01	0.42
1:b:46:VAL:HG22	1:b:54:VAL:HG11	2.00	0.42
3:2:817:A:O4'	9:H:110:GLN:NE2	2.53	0.42
3:2:922:G:H2'	3:2:923:A:H8	1.84	0.42
3:2:1661:U:H1'	22:k:60:GLN:HE21	1.84	0.42
25:F:66:GLN:HA	25:F:67:PRO:HD3	1.88	0.42
28:P:95:GLY:HA2	28:P:103:ASN:O	2.20	0.42
3:2:745:U:H2'	3:2:746:A:H8	1.85	0.42
3:2:1242:A:H2	3:2:1452:U:H1'	1.84	0.42
3:2:1321:A:C5	4:A:104:PRO:HB2	2.55	0.42
3:2:1654:G:H4'	3:2:1655:A:H8	1.85	0.42
5:B:61:LEU:HD22	5:B:96:LEU:HD13	2.02	0.42
7:E:182:TYR:HB2	7:E:228:ILE:HD11	2.01	0.42
8:G:5:ILE:HD12	8:G:16:PHE:HD2	1.84	0.42
20:h:174:LEU:HD11	20:h:234:LEU:HD11	2.01	0.42
23:l:112:VAL:O	23:l:119:PRO:HA	2.19	0.42
3:2:1206:U:H3'	3:2:1207:C:H5''	2.00	0.41
3:2:1349:G:N2	3:2:1379:C:H42	2.14	0.41
3:2:1561:U:H2'	3:2:1562:G:C8	2.54	0.41
4:A:123:VAL:HG11	4:A:133:ILE:HD11	2.02	0.41
4:A:183:ARG:HA	4:A:188:LEU:HB2	2.01	0.41
5:B:134:VAL:HB	5:B:219:LYS:HB2	2.00	0.41
7:E:195:ILE:HG22	7:E:210:ILE:HG12	2.01	0.41
10:I:196:LEU:HD23	10:I:196:LEU:HA	1.90	0.41
16:X:59:ILE:HB	16:X:69:ARG:HB2	2.02	0.41
16:X:103:LEU:HB3	16:X:126:LYS:HB2	2.01	0.41
25:F:103:ASN:HA	25:F:106:LYS:HD2	2.02	0.41
26:M:72:ILE:HA	26:M:75:VAL:HB	2.02	0.41
30:R:9:VAL:HG13	30:R:50:ILE:HA	2.01	0.41
3:2:1273:G:H1	3:2:1437:U:H3	1.62	0.41
3:2:1289:U:H2'	3:2:1290:U:C6	2.54	0.41
10:I:87:ASN:HD22	10:I:88:ASN:H	1.66	0.41
22:k:152:ALA:HB3	22:k:180:LEU:HD22	2.02	0.41
3:2:384:G:H2'	3:2:385:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:717:C:H42	3:2:720:G:N2	2.18	0.41
3:2:843:U:O4	3:2:844:A:N6	2.53	0.41
6:C:140:ARG:HB3	6:C:221:THR:HG22	2.02	0.41
22:k:657:ILE:HG13	22:k:779:PRO:HB2	2.01	0.41
25:F:46:TRP:HE1	25:F:129:PRO:HG2	1.85	0.41
28:P:86:VAL:HG12	28:P:89:MET:HE3	2.01	0.41
29:Q:44:LEU:HD11	29:Q:75:VAL:HG22	2.01	0.41
3:2:484:C:H2'	3:2:485:A:C8	2.55	0.41
6:C:140:ARG:HH21	14:V:1:MET:HB2	1.85	0.41
10:I:70:GLU:OE2	12:L:24:LYS:NZ	2.53	0.41
18:c:47:PRO:HG2	25:F:165:LEU:HD23	2.03	0.41
25:F:43:PHE:HB3	25:F:46:TRP:HE3	1.84	0.41
32:T:77:ASN:OD1	32:T:101:ASN:ND2	2.53	0.41
22:k:718:ARG:HG2	22:k:719:TYR:CD2	2.56	0.41
26:M:72:ILE:O	26:M:76:GLU:N	2.40	0.41
26:M:99:GLU:HG3	26:M:105:LYS:HB2	2.02	0.41
35:U:60:THR:HA	35:U:86:ILE:O	2.20	0.41
3:2:939:A:H2'	3:2:940:A:C8	2.55	0.41
3:2:1145:U:H3'	3:2:1146:G:H21	1.86	0.41
6:C:122:ALA:HA	6:C:125:ILE:HD12	2.02	0.41
7:E:82:TYR:HA	7:E:83:PRO:HD3	1.86	0.41
9:H:61:PHE:HA	9:H:93:LEU:O	2.21	0.41
20:h:220:THR:HG21	20:h:243:ALA:HB2	2.02	0.41
26:M:106:ILE:HB	26:M:113:ARG:HB3	2.02	0.41
30:R:100:LEU:HB2	30:R:119:LEU:HD23	2.01	0.41
3:2:706:A:N1	3:2:732:G:O6	2.53	0.41
3:2:823:G:O6	3:2:850:A:N6	2.54	0.41
15:W:103:ILE:HD11	15:W:126:LEU:HB2	2.02	0.41
18:c:7:VAL:HG22	25:F:143:ARG:HH12	1.85	0.41
22:k:513:GLN:HG3	22:k:515:ASP:H	1.86	0.41
25:F:88:PRO:O	25:F:92:ARG:N	2.42	0.41
27:O:90:ARG:HG2	27:O:91:THR:H	1.85	0.41
3:2:577:G:O2'	3:2:579:A:OP1	2.37	0.41
3:2:890:C:H2'	3:2:891:A:C8	2.56	0.41
3:2:1167:G:O6	3:2:1578:U:O4	2.39	0.41
3:2:1280:C:N4	3:2:1428:G:H22	2.18	0.41
3:2:1339:C:H2'	3:2:1341:A:H62	1.86	0.41
3:2:1694:A:H61	3:2:1707:A:H62	1.69	0.41
7:E:185:GLY:H	7:E:224:ASN:HB3	1.85	0.41
22:k:124:PHE:HB2	22:k:137:ILE:HB	2.03	0.41
31:S:65:GLU:OE2	31:S:68:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:D:13:ALA:H	34:D:41:VAL:HG21	1.85	0.41
3:2:217:A:H3'	3:2:218:A:H5''	2.03	0.41
3:2:396:G:N1	3:2:399:A:OP2	2.50	0.41
3:2:406:U:H2'	3:2:407:A:C8	2.56	0.41
3:2:836:U:H2'	3:2:837:G:C8	2.55	0.41
3:2:878:G:H2'	3:2:879:G:C8	2.56	0.41
3:2:1057:U:O2'	3:2:1059:U:OP2	2.33	0.41
3:2:1345:A:H1'	35:U:56:VAL:HG13	2.03	0.41
3:2:1381:U:H4'	35:U:59:PRO:HG3	2.03	0.41
5:B:23:PRO:HB2	5:B:27:LYS:HE3	2.03	0.41
5:B:54:LEU:HA	5:B:57:ALA:HB3	2.03	0.41
5:B:68:VAL:O	5:B:83:LYS:HA	2.21	0.41
5:B:207:LEU:HB2	5:B:210:ILE:HD11	2.03	0.41
8:G:159:ARG:HH21	8:G:170:THR:HG23	1.86	0.41
11:J:87:SER:OG	11:J:89:ASP:OD1	2.29	0.41
12:L:73:GLY:HA3	12:L:86:ILE:HD12	2.02	0.41
13:N:20:ARG:HE	15:W:56:HIS:CG	2.39	0.41
15:W:105:THR:HG23	15:W:110:ILE:HG12	2.02	0.41
23:I:227:HIS:CD2	23:I:257:CYS:HB3	2.56	0.41
26:M:29:LYS:HB3	26:M:100:TRP:CG	2.55	0.41
30:R:36:ASP:OD1	30:R:47:ARG:NE	2.53	0.41
3:2:29:U:H2'	3:2:30:G:C8	2.55	0.41
3:2:332:U:O2'	10:I:5:ARG:NH2	2.54	0.41
3:2:416:A:H3'	3:2:417:A:H8	1.86	0.41
3:2:829:A:N1	3:2:842:C:N4	2.69	0.41
3:2:1122:G:N2	3:2:1125:A:OP2	2.47	0.41
3:2:1321:A:H1'	3:2:1322:A:C8	2.56	0.41
3:2:1443:U:H4'	3:2:1445:G:C4	2.56	0.41
9:H:103:SER:OG	9:H:104:ARG:N	2.52	0.41
9:H:129:LEU:HD21	9:H:172:VAL:HG11	2.03	0.41
12:L:109:VAL:HG21	12:L:125:VAL:HG11	2.03	0.41
22:k:50:SER:HB2	22:k:53:GLN:HG3	2.03	0.41
3:2:1469:A:O2'	3:2:1540:G:N2	2.51	0.40
3:2:1504:G:N3	3:2:1563:C:O2'	2.53	0.40
3:2:1777:G:OP1	24:y:235:ASN:ND2	2.42	0.40
15:W:52:TYR:CE1	15:W:59:GLY:HA3	2.56	0.40
16:X:50:LYS:HA	16:X:102:VAL:O	2.21	0.40
25:F:117:THR:HG23	25:F:195:ALA:HB2	2.03	0.40
3:2:78:A:O2'	8:G:173:PRO:O	2.28	0.40
3:2:404:G:H2'	3:2:405:C:H6	1.86	0.40
3:2:1101:G:H5''	15:W:76:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:105:GLY:HA3	6:C:190:LEU:HB3	2.03	0.40
6:C:129:ILE:O	6:C:133:LYS:HG2	2.22	0.40
19:d:21:CYS:HB2	19:d:30:LEU:HD21	2.03	0.40
20:h:224:ILE:HA	20:h:232:HIS:O	2.21	0.40
24:y:278:LYS:NZ	24:y:279:GLU:OE2	2.34	0.40
25:F:97:LEU:O	25:F:180:ARG:NH2	2.52	0.40
3:2:382:C:H2'	3:2:383:G:C8	2.57	0.40
3:2:406:U:H2'	3:2:407:A:H8	1.87	0.40
3:2:487:G:H2'	3:2:488:G:C8	2.56	0.40
3:2:931:C:H5''	5:B:116:LYS:HA	2.02	0.40
3:2:1054:U:H2'	3:2:1055:U:C6	2.57	0.40
3:2:1106:U:H2'	3:2:1107:G:H8	1.86	0.40
3:2:1382:A:H1'	35:U:57:ARG:HD3	2.04	0.40
23:l:32:VAL:O	23:l:73:TYR:N	2.50	0.40
25:F:61:TYR:HE2	25:F:164:PRO:HG2	1.87	0.40
3:2:555:A:N3	3:2:590:C:O2'	2.53	0.40
3:2:585:A:H2'	3:2:586:G:C8	2.55	0.40
3:2:1171:A:H2'	3:2:1172:G:C8	2.56	0.40
3:2:1520:U:OP2	32:T:75:LYS:NZ	2.39	0.40
7:E:31:PRO:HA	7:E:81:THR:HB	2.03	0.40
12:L:94:ILE:HA	12:L:95:PRO:HD3	1.86	0.40
25:F:100:ASN:HB3	25:F:103:ASN:HD22	1.85	0.40
3:2:590:C:H2'	3:2:591:A:C8	2.56	0.40
3:2:1394:G:H2'	3:2:1395:G:H8	1.86	0.40
20:h:266:VAL:HA	20:h:269:ARG:HG2	2.02	0.40
22:k:82:ALA:HB3	22:k:134:ASN:HB2	2.04	0.40
23:l:124:ILE:HA	23:l:186:ILE:HG12	2.03	0.40
29:Q:13:LYS:NZ	29:Q:120:ASP:OD2	2.54	0.40
29:Q:54:LEU:HD23	29:Q:109:PHE:HD1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
2	e	44/63 (70%)	40 (91%)	4 (9%)	0	100	100
4	A	204/252 (81%)	189 (93%)	15 (7%)	0	100	100
5	B	212/255 (83%)	197 (93%)	15 (7%)	0	100	100
6	C	215/254 (85%)	208 (97%)	7 (3%)	0	100	100
7	E	258/261 (99%)	249 (96%)	9 (4%)	0	100	100
8	G	230/236 (98%)	224 (97%)	6 (3%)	0	100	100
9	H	182/190 (96%)	168 (92%)	14 (8%)	0	100	100
10	I	184/200 (92%)	175 (95%)	9 (5%)	0	100	100
11	J	183/197 (93%)	172 (94%)	11 (6%)	0	100	100
12	L	138/156 (88%)	136 (99%)	2 (1%)	0	100	100
13	N	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
14	V	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
15	W	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
16	X	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
17	Y	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
18	c	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
19	d	33/56 (59%)	29 (88%)	4 (12%)	0	100	100
20	h	179/274 (65%)	174 (97%)	5 (3%)	0	100	100
21	i	137/483 (28%)	133 (97%)	4 (3%)	0	100	100
22	k	597/788 (76%)	562 (94%)	34 (6%)	1 (0%)	43	74
23	l	267/425 (63%)	233 (87%)	33 (12%)	1 (0%)	30	62
24	y	150/318 (47%)	128 (85%)	22 (15%)	0	100	100
25	F	204/225 (91%)	195 (96%)	9 (4%)	0	100	100
26	M	123/143 (86%)	117 (95%)	6 (5%)	0	100	100
27	O	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
28	P	112/142 (79%)	108 (96%)	4 (4%)	0	100	100
29	Q	125/143 (87%)	120 (96%)	5 (4%)	0	100	100
30	R	123/136 (90%)	120 (98%)	3 (2%)	0	100	100
31	S	102/146 (70%)	92 (90%)	10 (10%)	0	100	100
32	T	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
33	Z	61/108 (56%)	60 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	D	179/240 (75%)	173 (97%)	6 (3%)	0	100	100
35	U	78/121 (64%)	76 (97%)	2 (3%)	0	100	100
All	All	5360/6890 (78%)	5072 (95%)	286 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	l	183	SER
22	k	483	PRO

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	
1	b	70/71 (99%)	70 (100%)	0	100	100
2	e	40/54 (74%)	40 (100%)	0	100	100
4	A	171/210 (81%)	169 (99%)	2 (1%)	63	73
5	B	191/224 (85%)	191 (100%)	0	100	100
6	C	176/205 (86%)	176 (100%)	0	100	100
7	E	221/222 (100%)	221 (100%)	0	100	100
8	G	198/201 (98%)	197 (100%)	1 (0%)	81	80
9	H	165/170 (97%)	165 (100%)	0	100	100
10	I	150/161 (93%)	150 (100%)	0	100	100
11	J	158/166 (95%)	156 (99%)	2 (1%)	61	72
12	L	125/137 (91%)	125 (100%)	0	100	100
13	N	127/128 (99%)	127 (100%)	0	100	100
14	V	74/74 (100%)	74 (100%)	0	100	100
15	W	110/111 (99%)	110 (100%)	0	100	100
16	X	119/120 (99%)	118 (99%)	1 (1%)	73	76
17	Y	112/113 (99%)	111 (99%)	1 (1%)	70	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	c	56/60 (93%)	56 (100%)	0	100	100
19	d	33/49 (67%)	32 (97%)	1 (3%)	36	60
20	h	158/238 (66%)	158 (100%)	0	100	100
21	i	125/424 (30%)	125 (100%)	0	100	100
22	k	523/703 (74%)	523 (100%)	0	100	100
23	l	246/384 (64%)	245 (100%)	1 (0%)	84	81
24	y	141/283 (50%)	141 (100%)	0	100	100
25	F	173/191 (91%)	172 (99%)	1 (1%)	78	79
26	M	101/119 (85%)	100 (99%)	1 (1%)	68	75
27	O	91/105 (87%)	91 (100%)	0	100	100
28	P	95/118 (80%)	95 (100%)	0	100	100
29	Q	107/119 (90%)	107 (100%)	0	100	100
30	R	113/124 (91%)	112 (99%)	1 (1%)	70	75
31	S	93/129 (72%)	93 (100%)	0	100	100
32	T	115/116 (99%)	115 (100%)	0	100	100
33	Z	56/89 (63%)	55 (98%)	1 (2%)	51	69
34	D	149/195 (76%)	149 (100%)	0	100	100
35	U	79/114 (69%)	79 (100%)	0	100	100
All	All	4661/5927 (79%)	4648 (100%)	13 (0%)	84	83

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	57	LEU
4	A	133	ILE
8	G	67	VAL
11	J	109	LEU
11	J	143	ILE
16	X	87	VAL
17	Y	75	VAL
19	d	28	THR
23	l	93	THR
25	F	43	PHE
26	M	115	VAL
30	R	46	LEU
33	Z	50	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	9	HIS
1	b	26	GLN
2	e	46	ASN
4	A	46	HIS
4	A	69	ASN
4	A	109	ASN
5	B	79	HIS
5	B	146	GLN
5	B	208	GLN
5	B	220	GLN
6	C	82	ASN
6	C	87	GLN
6	C	108	ASN
6	C	110	HIS
7	E	50	ASN
7	E	98	ASN
7	E	112	HIS
8	G	34	GLN
8	G	189	HIS
8	G	190	GLN
8	G	201	GLN
9	H	42	GLN
9	H	150	GLN
10	I	32	GLN
10	I	84	HIS
10	I	87	ASN
10	I	94	ASN
10	I	138	ASN
11	J	139	GLN
12	L	8	GLN
12	L	92	HIS
13	N	36	GLN
15	W	42	GLN
15	W	44	HIS
15	W	80	ASN
16	X	22	ASN
16	X	99	ASN
18	c	27	GLN
18	c	43	ASN
19	d	27	HIS
20	h	104	HIS

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Mol	Chain	Res	Type
20	h	239	HIS
21	i	297	HIS
22	k	60	GLN
22	k	147	ASN
22	k	218	HIS
22	k	228	ASN
22	k	251	ASN
22	k	288	ASN
22	k	547	ASN
22	k	576	GLN
22	k	591	ASN
22	k	626	GLN
22	k	647	HIS
22	k	706	HIS
23	l	29	HIS
23	l	46	GLN
23	l	90	ASN
23	l	153	HIS
23	l	203	HIS
23	l	227	HIS
23	l	262	HIS
24	y	213	ASN
24	y	300	GLN
25	F	34	GLN
25	F	72	HIS
25	F	103	ASN
25	F	104	ASN
25	F	116	HIS
25	F	139	ASN
25	F	170	GLN
26	M	96	GLN
29	Q	83	GLN
29	Q	103	ASN
30	R	123	ASN
31	S	55	HIS
31	S	87	ASN
32	T	43	ASN
32	T	64	HIS
32	T	101	ASN
34	D	111	ASN
34	D	159	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	1774/1801 (98%)	619 (34%)	17 (0%)

All (619) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	4	C
3	2	25	C
3	2	26	A
3	2	34	G
3	2	42	G
3	2	43	A
3	2	47	A
3	2	50	C
3	2	51	A
3	2	57	G
3	2	60	U
3	2	63	G
3	2	66	U
3	2	67	A
3	2	68	A
3	2	72	A
3	2	73	U
3	2	74	U
3	2	75	U
3	2	103	A
3	2	104	A
3	2	114	C
3	2	115	G
3	2	127	G
3	2	130	C
3	2	131	C
3	2	133	U
3	2	134	U
3	2	135	A
3	2	137	U
3	2	138	A
3	2	139	C
3	2	140	A
3	2	141	U
3	2	142	G
3	2	144	U

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Mol	Chain	Res	Type
3	2	145	A
3	2	153	G
3	2	155	U
3	2	156	A
3	2	158	U
3	2	176	C
3	2	178	U
3	2	179	A
3	2	184	C
3	2	185	U
3	2	186	C
3	2	187	G
3	2	191	C
3	2	192	U
3	2	193	U
3	2	194	U
3	2	195	G
3	2	196	G
3	2	215	A
3	2	217	A
3	2	218	A
3	2	219	A
3	2	225	A
3	2	227	U
3	2	228	G
3	2	229	U
3	2	230	C
3	2	231	U
3	2	232	U
3	2	233	C
3	2	234	G
3	2	237	C
3	2	238	U
3	2	239	C
3	2	240	U
3	2	241	U
3	2	242	U
3	2	243	G
3	2	249	U
3	2	250	C
3	2	257	A
3	2	261	U

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Mol	Chain	Res	Type
3	2	262	U
3	2	265	A
3	2	267	U
3	2	271	A
3	2	272	U
3	2	275	C
3	2	276	C
3	2	277	U
3	2	278	U
3	2	279	G
3	2	280	U
3	2	281	G
3	2	299	A
3	2	304	U
3	2	305	C
3	2	309	C
3	2	314	C
3	2	316	A
3	2	319	U
3	2	321	C
3	2	322	G
3	2	333	A
3	2	335	U
3	2	337	G
3	2	338	C
3	2	341	A
3	2	344	A
3	2	345	U
3	2	352	A
3	2	359	A
3	2	360	A
3	2	361	C
3	2	380	U
3	2	390	G
3	2	399	A
3	2	400	A
3	2	401	A
3	2	402	C
3	2	404	G
3	2	416	A
3	2	417	A
3	2	419	G

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Mol	Chain	Res	Type
3	2	423	G
3	2	424	C
3	2	425	A
3	2	426	G
3	2	434	G
3	2	439	U
3	2	444	C
3	2	447	U
3	2	448	C
3	2	454	U
3	2	459	G
3	2	460	A
3	2	468	A
3	2	469	C
3	2	477	A
3	2	480	G
3	2	481	A
3	2	482	U
3	2	483	A
3	2	484	C
3	2	486	G
3	2	487	G
3	2	490	C
3	2	492	A
3	2	493	U
3	2	494	U
3	2	495	C
3	2	496	G
3	2	497	G
3	2	498	G
3	2	499	U
3	2	500	C
3	2	501	U
3	2	503	G
3	2	504	U
3	2	505	A
3	2	506	A
3	2	507	U
3	2	511	A
3	2	515	A
3	2	519	C
3	2	520	A

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Mol	Chain	Res	Type
3	2	527	A
3	2	534	A
3	2	538	A
3	2	541	A
3	2	543	C
3	2	544	A
3	2	548	G
3	2	549	G
3	2	551	G
3	2	555	A
3	2	558	U
3	2	559	C
3	2	563	U
3	2	564	G
3	2	565	C
3	2	566	C
3	2	567	A
3	2	568	G
3	2	574	G
3	2	575	C
3	2	576	G
3	2	577	G
3	2	578	U
3	2	579	A
3	2	580	A
3	2	581	U
3	2	582	U
3	2	583	C
3	2	594	A
3	2	595	G
3	2	606	A
3	2	611	U
3	2	613	G
3	2	619	A
3	2	620	A
3	2	622	A
3	2	623	A
3	2	624	G
3	2	634	G
3	2	635	A
3	2	639	U
3	2	640	U

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Mol	Chain	Res	Type
3	2	648	G
3	2	649	U
3	2	650	U
3	2	652	G
3	2	653	C
3	2	654	C
3	2	655	G
3	2	656	G
3	2	658	C
3	2	677	G
3	2	679	U
3	2	684	A
3	2	685	A
3	2	687	G
3	2	691	C
3	2	696	C
3	2	697	C
3	2	698	U
3	2	708	C
3	2	709	C
3	2	712	G
3	2	714	G
3	2	715	U
3	2	717	C
3	2	718	U
3	2	719	U
3	2	720	G
3	2	721	U
3	2	722	G
3	2	723	G
3	2	728	U
3	2	738	G
3	2	739	G
3	2	740	A
3	2	741	C
3	2	742	U
3	2	743	U
3	2	754	A
3	2	761	G
3	2	762	A
3	2	765	G
3	2	766	U

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Mol	Chain	Res	Type
3	2	774	A
3	2	775	G
3	2	779	U
3	2	780	A
3	2	781	U
3	2	782	U
3	2	783	G
3	2	786	C
3	2	787	G
3	2	789	A
3	2	793	A
3	2	795	U
3	2	811	A
3	2	813	U
3	2	815	G
3	2	816	G
3	2	818	C
3	2	820	U
3	2	821	U
3	2	824	G
3	2	826	U
3	2	827	C
3	2	829	A
3	2	830	U
3	2	832	U
3	2	834	G
3	2	835	U
3	2	839	U
3	2	840	U
3	2	841	U
3	2	844	A
3	2	846	G
3	2	848	C
3	2	849	C
3	2	850	A
3	2	851	U
3	2	852	C
3	2	854	U
3	2	855	A
3	2	856	A
3	2	857	U
3	2	863	A

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Mol	Chain	Res	Type
3	2	876	G
3	2	881	A
3	2	886	U
3	2	887	A
3	2	893	U
3	2	898	A
3	2	900	A
3	2	904	G
3	2	905	A
3	2	906	A
3	2	908	U
3	2	909	U
3	2	910	C
3	2	911	U
3	2	913	G
3	2	914	G
3	2	921	U
3	2	931	C
3	2	933	A
3	2	935	U
3	2	940	A
3	2	942	G
3	2	945	U
3	2	960	U
3	2	966	A
3	2	988	A
3	2	992	A
3	2	993	A
3	2	997	G
3	2	998	A
3	2	999	U
3	2	1000	C
3	2	1002	G
3	2	1003	A
3	2	1004	U
3	2	1005	A
3	2	1006	C
3	2	1011	G
3	2	1026	A
3	2	1028	C
3	2	1029	U
3	2	1030	A

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Mol	Chain	Res	Type
3	2	1031	U
3	2	1040	G
3	2	1044	U
3	2	1051	G
3	2	1053	G
3	2	1057	U
3	2	1058	U
3	2	1059	U
3	2	1061	A
3	2	1063	U
3	2	1064	G
3	2	1072	C
3	2	1078	C
3	2	1080	U
3	2	1081	A
3	2	1082	C
3	2	1092	A
3	2	1096	C
3	2	1097	U
3	2	1098	U
3	2	1100	G
3	2	1111	G
3	2	1137	A
3	2	1138	A
3	2	1140	G
3	2	1143	A
3	2	1145	U
3	2	1146	G
3	2	1147	A
3	2	1148	C
3	2	1149	G
3	2	1151	A
3	2	1154	G
3	2	1155	G
3	2	1156	C
3	2	1157	A
3	2	1158	C
3	2	1160	A
3	2	1164	G
3	2	1165	G
3	2	1167	G
3	2	1183	A

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Mol	Chain	Res	Type
3	2	1185	U
3	2	1186	U
3	2	1189	A
3	2	1198	G
3	2	1200	G
3	2	1201	G
3	2	1203	A
3	2	1207	C
3	2	1212	G
3	2	1215	C
3	2	1216	C
3	2	1218	G
3	2	1219	A
3	2	1220	C
3	2	1227	A
3	2	1228	G
3	2	1229	G
3	2	1230	A
3	2	1232	U
3	2	1233	G
3	2	1234	A
3	2	1235	C
3	2	1239	U
3	2	1240	U
3	2	1242	A
3	2	1249	U
3	2	1252	C
3	2	1254	U
3	2	1256	A
3	2	1257	U
3	2	1258	U
3	2	1264	G
3	2	1267	G
3	2	1268	G
3	2	1269	U
3	2	1270	G
3	2	1272	U
3	2	1273	G
3	2	1275	A
3	2	1276	U
3	2	1277	G
3	2	1278	G

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Mol	Chain	Res	Type
3	2	1279	C
3	2	1280	C
3	2	1281	G
3	2	1282	U
3	2	1283	U
3	2	1284	C
3	2	1285	U
3	2	1286	U
3	2	1287	A
3	2	1288	G
3	2	1293	U
3	2	1294	G
3	2	1295	G
3	2	1296	A
3	2	1297	G
3	2	1314	U
3	2	1315	U
3	2	1321	A
3	2	1324	G
3	2	1327	C
3	2	1328	G
3	2	1330	G
3	2	1332	C
3	2	1335	U
3	2	1336	A
3	2	1337	A
3	2	1338	C
3	2	1340	U
3	2	1343	U
3	2	1344	A
3	2	1345	A
3	2	1346	A
3	2	1347	U
3	2	1354	G
3	2	1360	A
3	2	1361	U
3	2	1362	U
3	2	1363	U
3	2	1364	G
3	2	1367	G
3	2	1370	U
3	2	1371	A

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Mol	Chain	Res	Type
3	2	1373	C
3	2	1378	U
3	2	1385	G
3	2	1388	A
3	2	1390	U
3	2	1391	A
3	2	1398	U
3	2	1399	C
3	2	1400	A
3	2	1413	U
3	2	1415	U
3	2	1418	G
3	2	1419	G
3	2	1420	C
3	2	1421	A
3	2	1422	A
3	2	1426	C
3	2	1427	A
3	2	1429	G
3	2	1431	C
3	2	1432	U
3	2	1435	G
3	2	1436	A
3	2	1437	U
3	2	1438	G
3	2	1439	C
3	2	1440	C
3	2	1441	C
3	2	1442	U
3	2	1443	U
3	2	1444	A
3	2	1446	A
3	2	1447	C
3	2	1448	G
3	2	1449	U
3	2	1450	U
3	2	1451	C
3	2	1455	G
3	2	1457	C
3	2	1459	C
3	2	1460	A
3	2	1471	A

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Mol	Chain	Res	Type
3	2	1473	U
3	2	1474	G
3	2	1475	A
3	2	1478	G
3	2	1479	A
3	2	1483	A
3	2	1486	G
3	2	1490	C
3	2	1491	U
3	2	1493	A
3	2	1494	C
3	2	1496	U
3	2	1500	C
3	2	1506	G
3	2	1510	U
3	2	1515	A
3	2	1516	A
3	2	1520	U
3	2	1521	G
3	2	1523	G
3	2	1524	A
3	2	1535	U
3	2	1536	G
3	2	1537	C
3	2	1538	U
3	2	1540	G
3	2	1542	G
3	2	1543	A
3	2	1557	U
3	2	1559	A
3	2	1568	C
3	2	1569	A
3	2	1571	C
3	2	1573	A
3	2	1574	G
3	2	1583	A
3	2	1584	G
3	2	1595	U
3	2	1596	C
3	2	1597	A
3	2	1598	U
3	2	1601	G

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Mol	Chain	Res	Type
3	2	1607	G
3	2	1618	C
3	2	1619	C
3	2	1622	G
3	2	1624	C
3	2	1626	U
3	2	1630	U
3	2	1631	A
3	2	1633	A
3	2	1634	C
3	2	1635	A
3	2	1636	C
3	2	1637	C
3	2	1638	G
3	2	1639	C
3	2	1640	C
3	2	1641	C
3	2	1642	G
3	2	1648	A
3	2	1649	G
3	2	1651	A
3	2	1652	C
3	2	1653	C
3	2	1654	G
3	2	1655	A
3	2	1657	U
3	2	1658	G
3	2	1659	A
3	2	1664	C
3	2	1683	C
3	2	1687	U
3	2	1688	U
3	2	1689	A
3	2	1690	G
3	2	1693	A
3	2	1698	G
3	2	1701	A
3	2	1702	A
3	2	1703	C
3	2	1707	A
3	2	1712	A
3	2	1714	A

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Mol	Chain	Res	Type
3	2	1715	G
3	2	1717	G
3	2	1732	A
3	2	1736	G
3	2	1737	G
3	2	1739	C
3	2	1741	U
3	2	1742	U
3	2	1743	U
3	2	1744	A
3	2	1745	G
3	2	1748	G
3	2	1749	A
3	2	1750	A
3	2	1751	C
3	2	1752	U
3	2	1753	A
3	2	1754	A
3	2	1755	A
3	2	1757	G
3	2	1758	U
3	2	1759	C
3	2	1760	G
3	2	1761	U
3	2	1763	A
3	2	1764	C
3	2	1766	A
3	2	1768	G
3	2	1769	U
3	2	1770	U
3	2	1782	A
3	2	1783	C
3	2	1791	A
3	2	1792	G
3	2	1793	G
3	2	1795	U
3	2	1799	U

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	2	155	U

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Mol	Chain	Res	Type
3	2	216	U
3	2	278	U
3	2	418	G
3	2	567	A
3	2	782	U
3	2	912	U
3	2	1150	G
3	2	1156	C
3	2	1229	G
3	2	1231	U
3	2	1343	U
3	2	1442	U
3	2	1458	G
3	2	1570	A
3	2	1573	A
3	2	1652	C

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](#)

There are no ligands in this entry.

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
34	D	2

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Mol	Chain	Number of breaks
3	2	2
22	k	1
19	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	52:ALA	C	53:THR	N	3.81
1	2	1377:U	O3'	1378:U	P	3.34
1	2	1219:A	O3'	1220:C	P	3.23
1	k	80:ASN	C	81:GLY	N	3.23
1	d	31:ILE	C	32:ARG	N	3.21
1	D	63:GLY	C	64:ARG	N	3.19

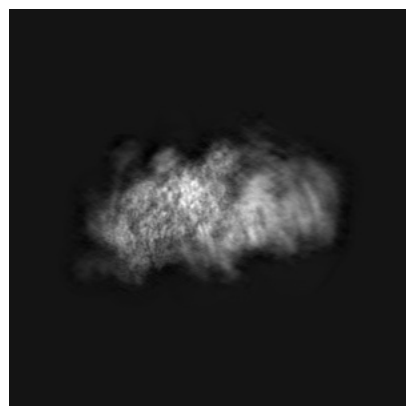
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4792. These allow visual inspection of the internal detail of the map and identification of artifacts.

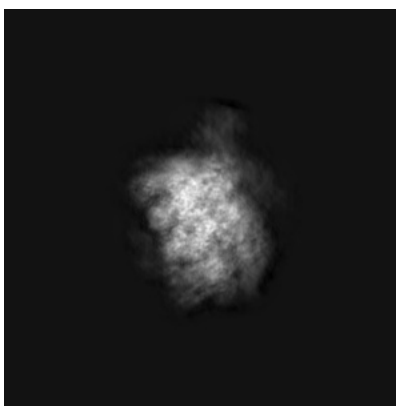
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

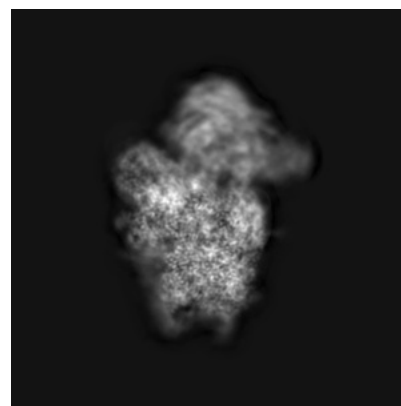
6.1.1 Primary map



X

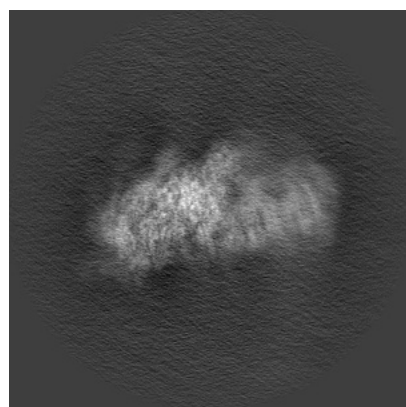


Y

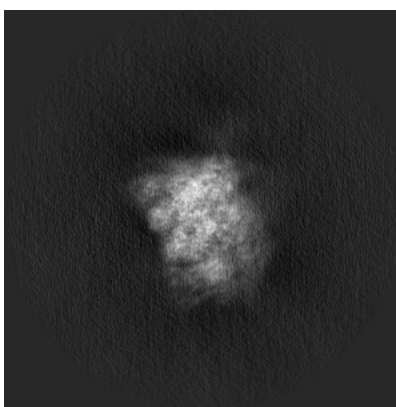


Z

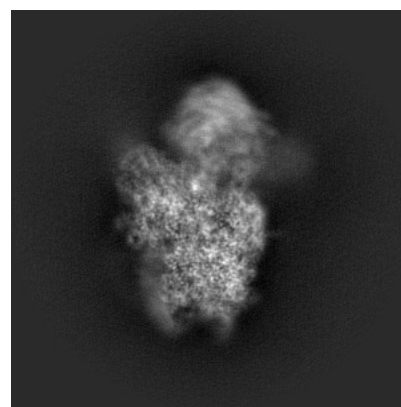
6.1.2 Raw map



X



Y

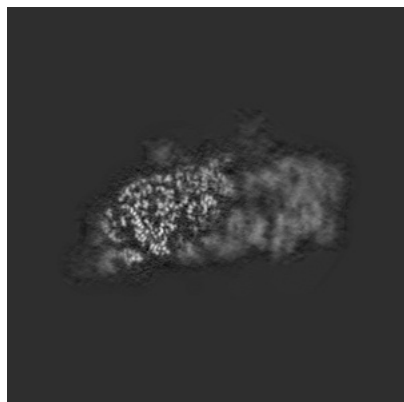


Z

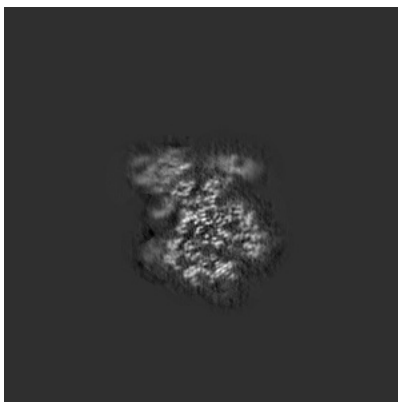
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

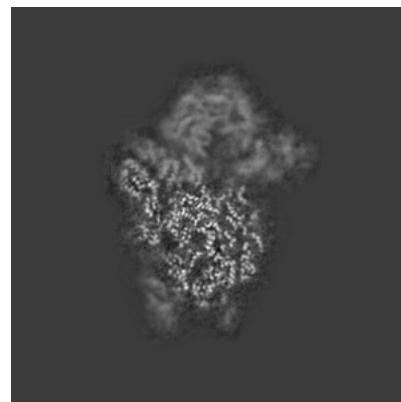
6.2.1 Primary map



X Index: 192

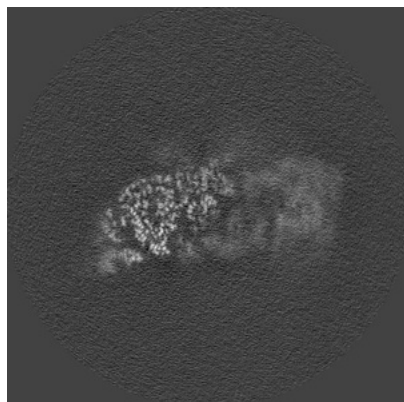


Y Index: 192

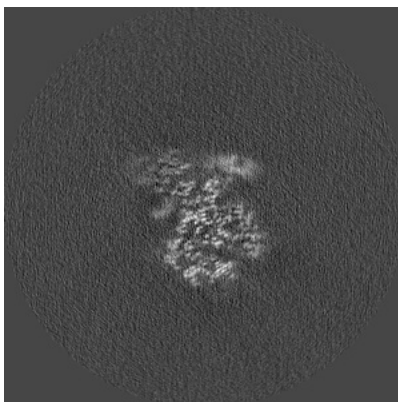


Z Index: 192

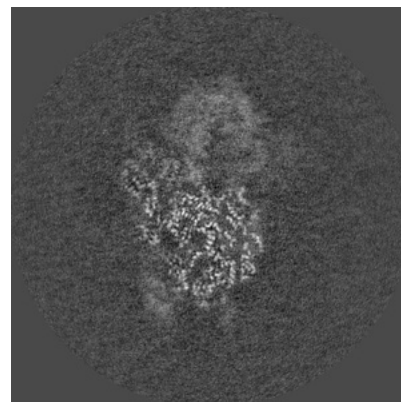
6.2.2 Raw map



X Index: 192



Y Index: 192

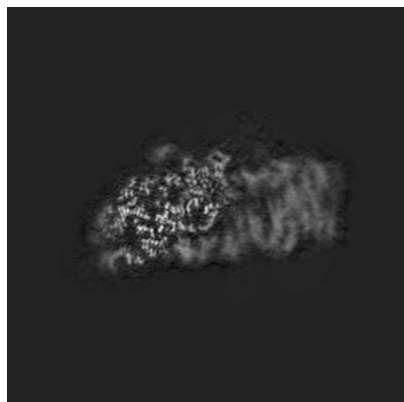


Z Index: 192

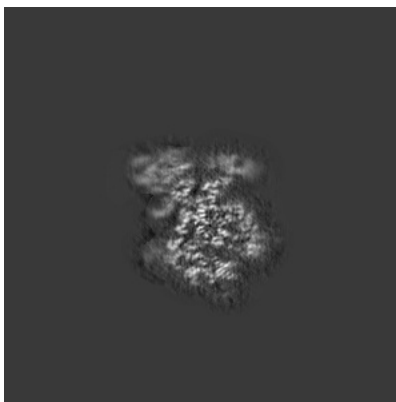
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

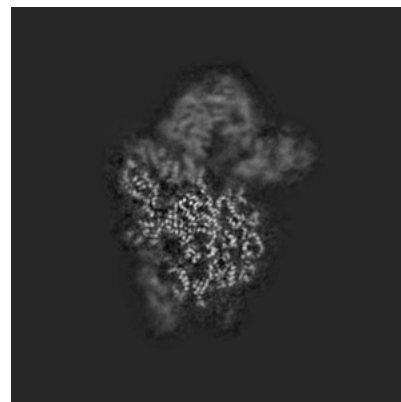
6.3.1 Primary map



X Index: 188

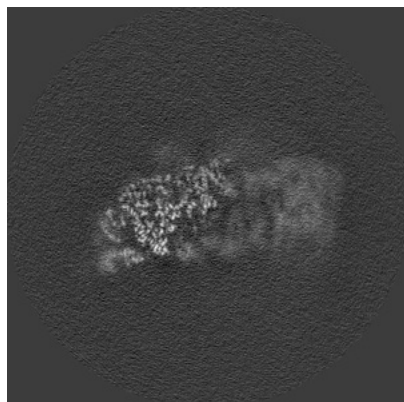


Y Index: 191

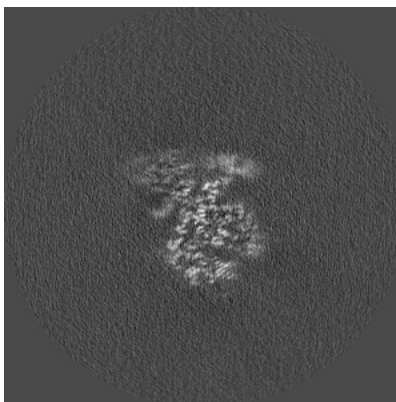


Z Index: 194

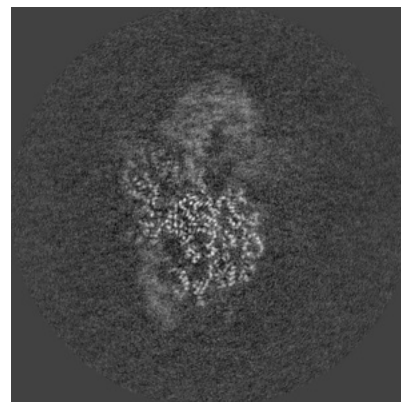
6.3.2 Raw map



X Index: 191



Y Index: 191

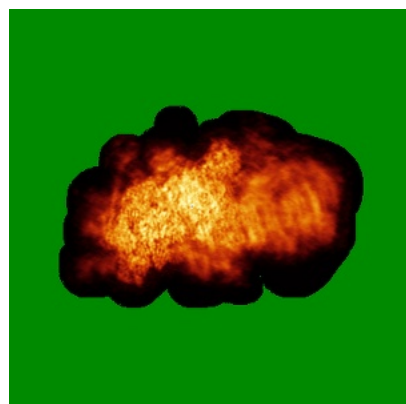


Z Index: 194

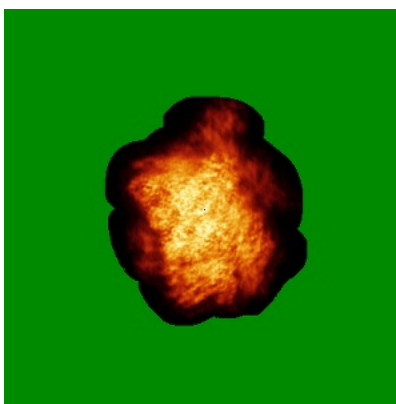
The images above show the largest variance slices of the map in three orthogonal directions.

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

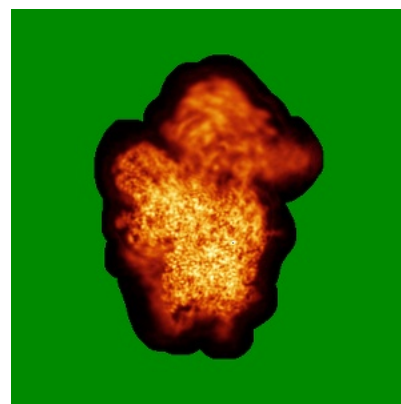
6.4.1 Primary map



X

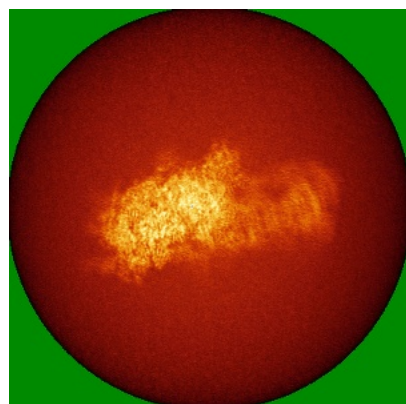


Y

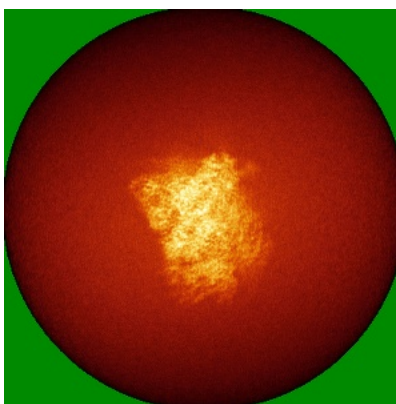


Z

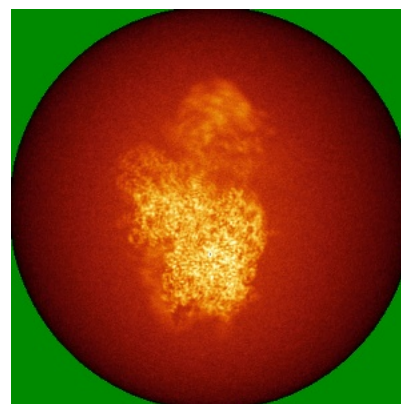
6.4.2 Raw map



X



Y



Z

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

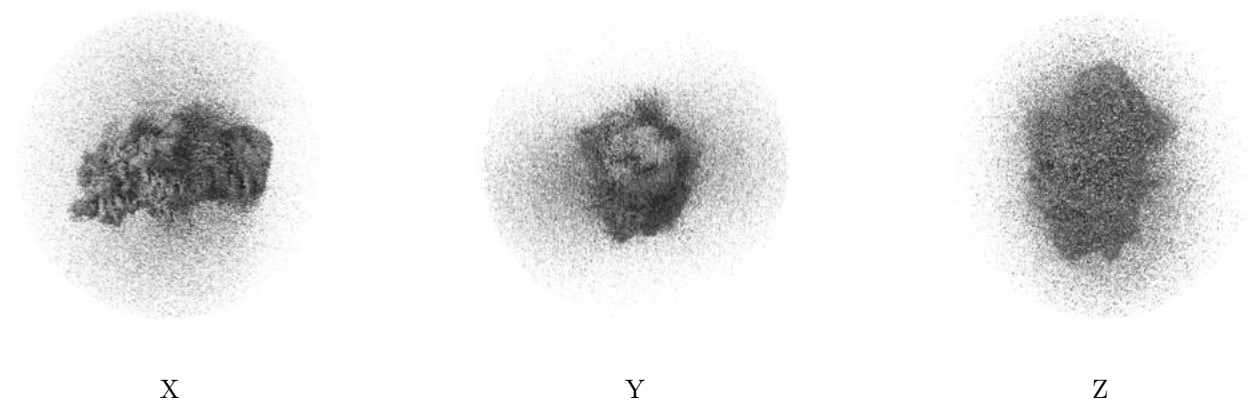
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

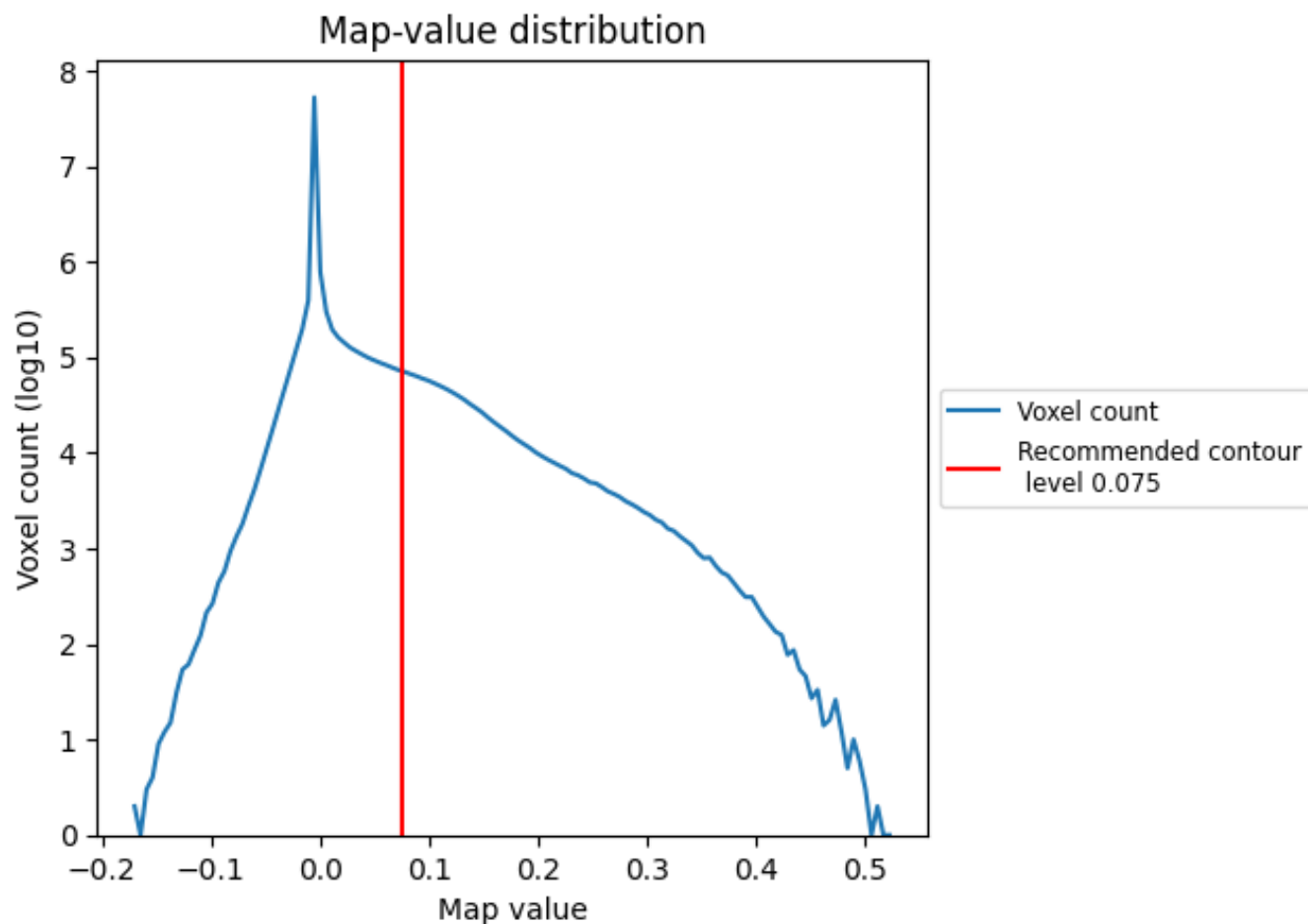
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

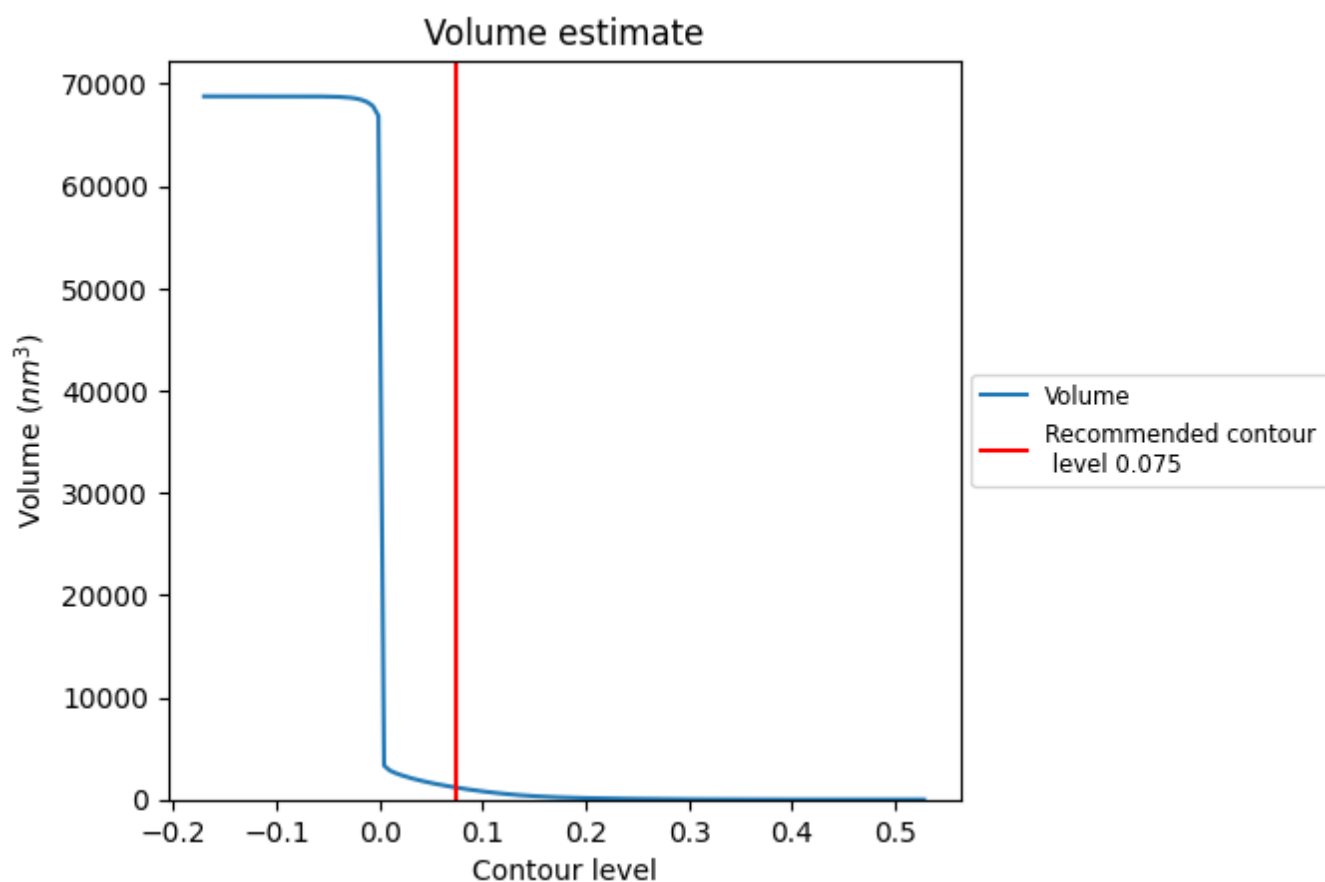
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

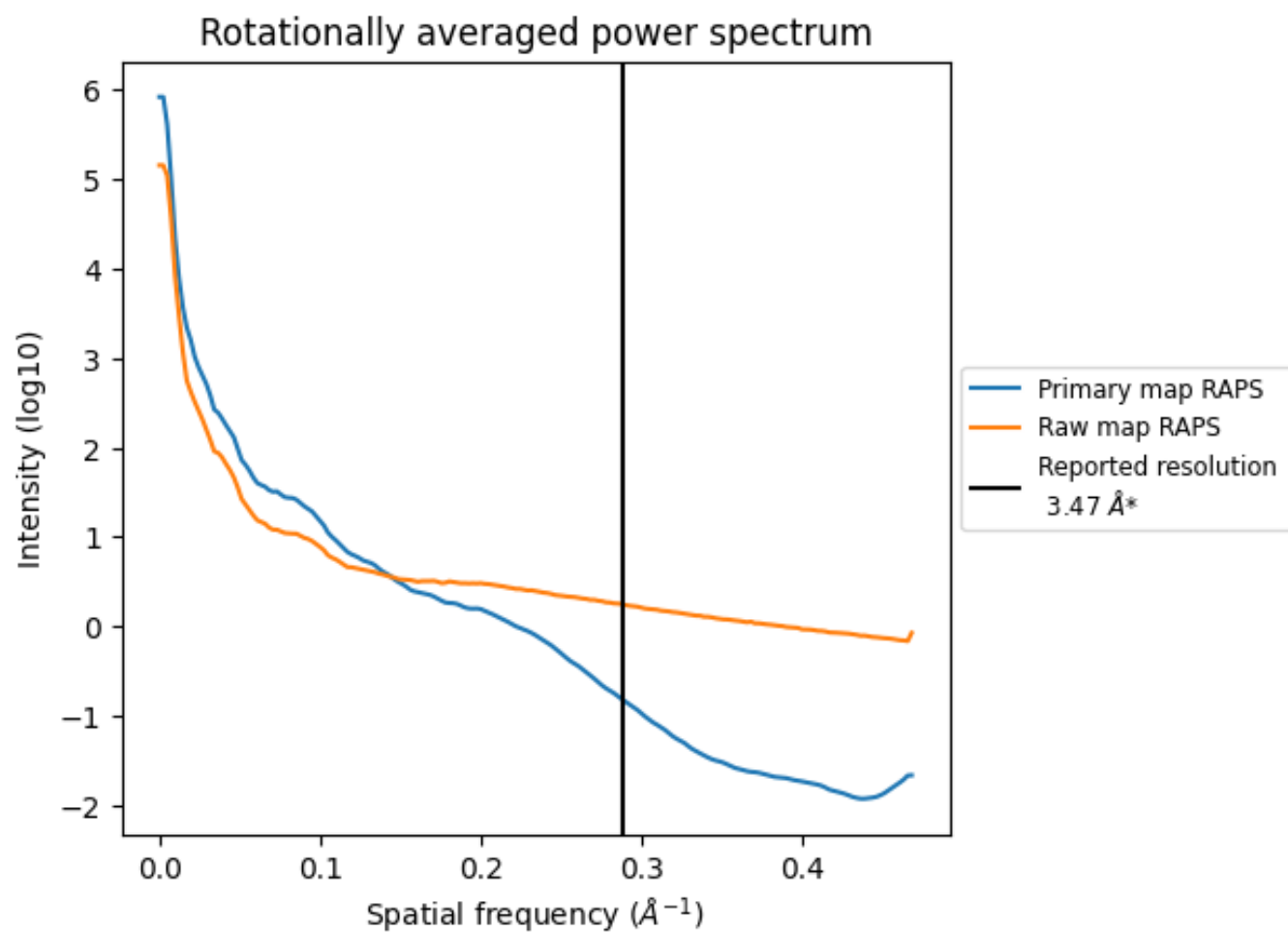
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1165 nm³; this corresponds to an approximate mass of 1053 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 ⓘ

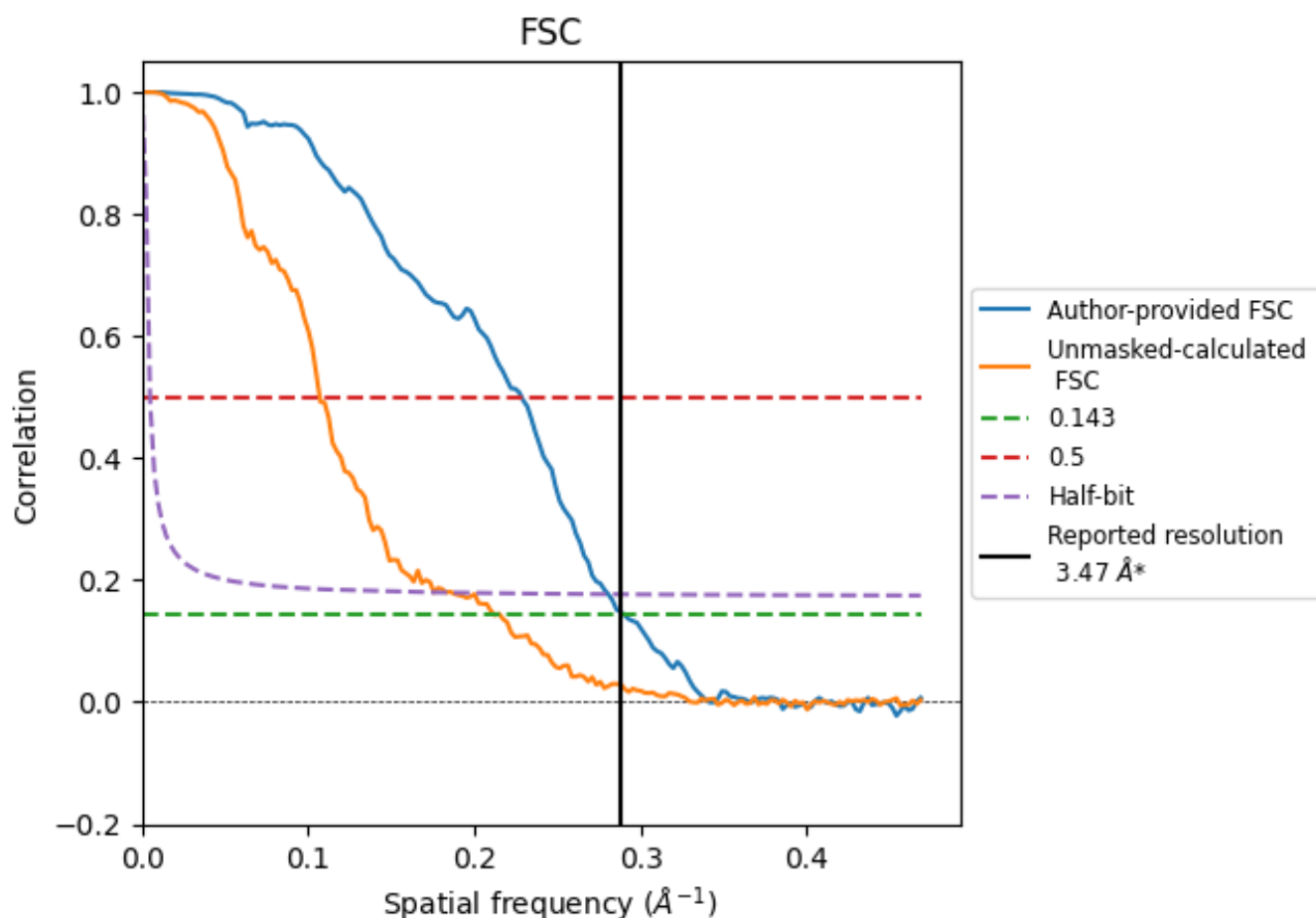


*Reported resolution corresponds to spatial frequency of $0.288 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.288 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

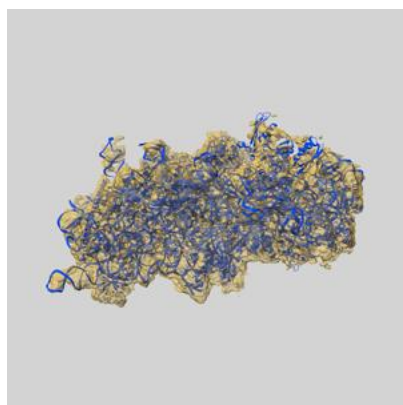
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.45	4.38	3.57
Unmasked-calculated*	4.71	9.35	5.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.71 differs from the reported value 3.47 by more than 10 %

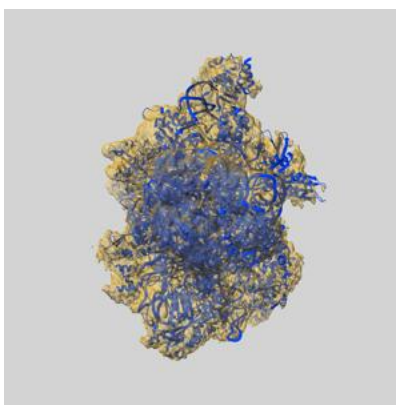
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4792 and PDB model 6RBD. Per-residue inclusion information can be found in section [3](#) on page [11](#).

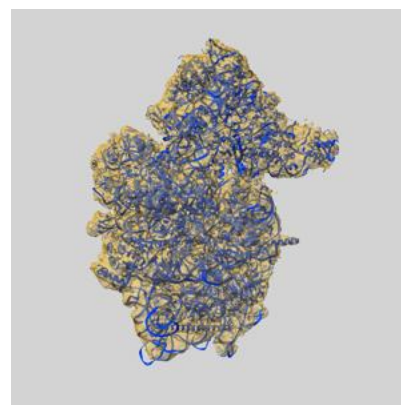
9.1 Map-model overlay [i](#)



X



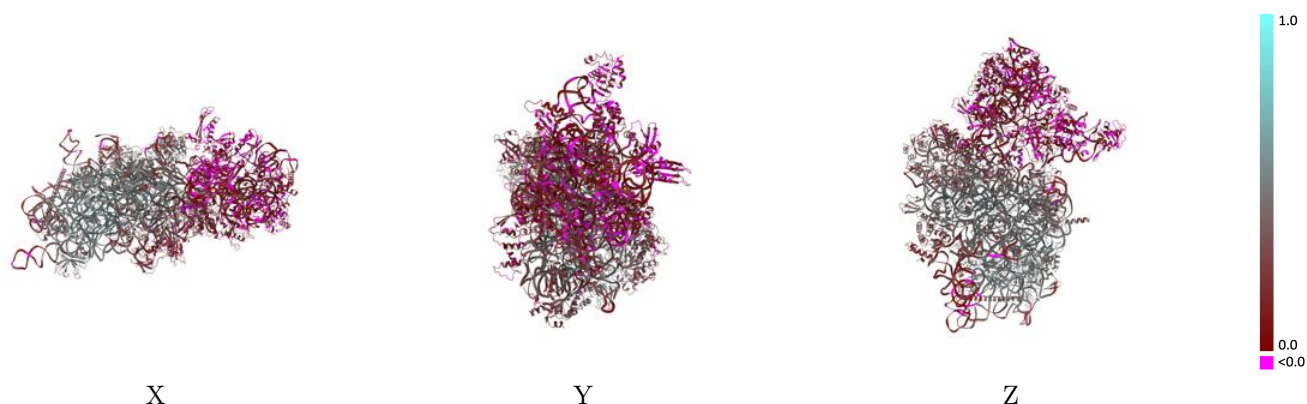
Y



Z

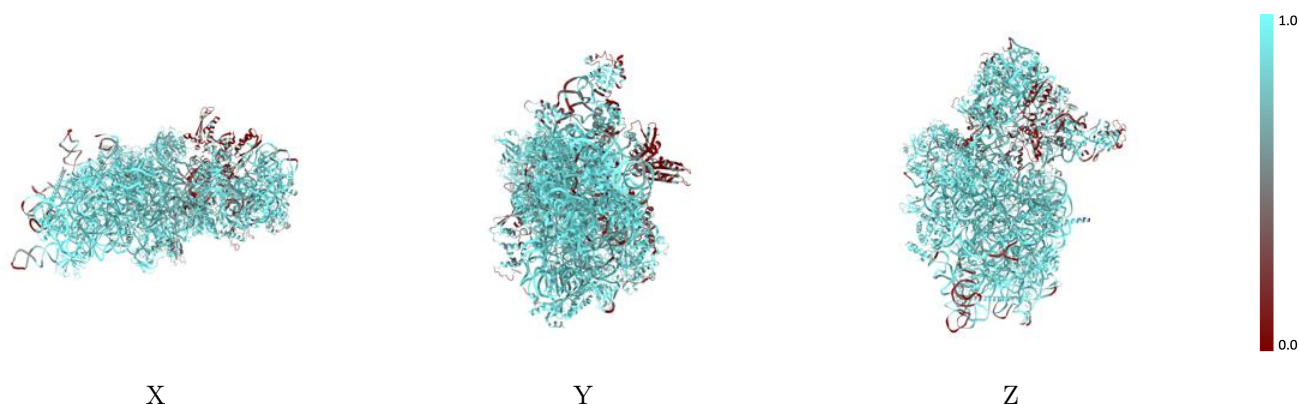
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



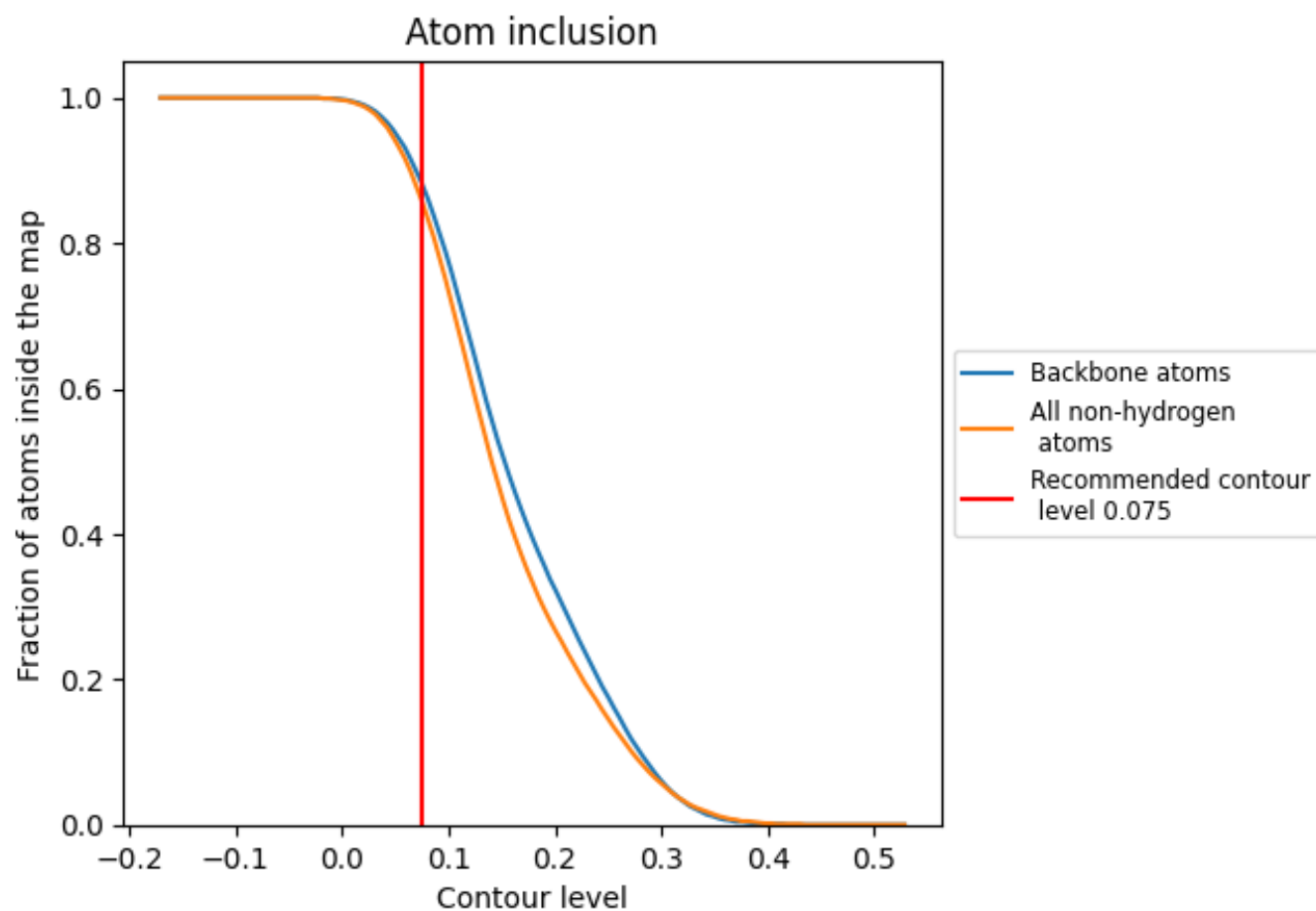
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.3010
2	 0.8910	 0.3250
A	 0.9620	 0.3880
B	 0.8830	 0.3430
C	 0.9370	 0.4320
D	 0.3210	 0.0700
E	 0.9580	 0.4940
F	 0.8760	 0.1080
G	 0.9110	 0.4150
H	 0.8770	 0.2990
I	 0.9230	 0.4640
J	 0.9330	 0.4440
L	 0.9540	 0.5010
M	 0.5690	 0.0680
N	 0.9210	 0.4260
O	 0.8820	 0.3060
P	 0.7980	 0.0860
Q	 0.8900	 0.1090
R	 0.5430	 0.1460
S	 0.7700	 0.0940
T	 0.9040	 0.0940
U	 0.2470	 0.0500
V	 0.9580	 0.4180
W	 0.9570	 0.4660
X	 0.9070	 0.4370
Y	 0.9360	 0.4610
Z	 0.8510	 0.1010
b	 0.9220	 0.4210
c	 0.7710	 0.1320
d	 0.5150	 0.0700
e	 0.7990	 0.3590
h	 0.8680	 0.2590
i	 0.6860	 0.0500
k	 0.8770	 0.2590
l	 0.7080	 0.1000
y	 0.6090	 0.1220

