



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 11:51 pm GMT

PDB ID : 6YBW
EMDB ID : EMD-10775
Title : Structure of a human 48S translational initiation complex - 40S body
Authors : Brito Querido, J.; Sokabe, M.; Kraatz, S.; Gordiyenko, Y.; Skehel, M.; Fraser, C.; Ramakrishnan, V.
Deposited on : 2020-03-18
Resolution : 3.10 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

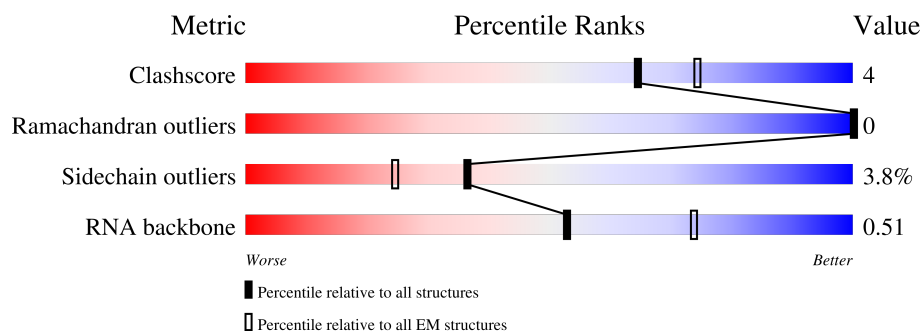
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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













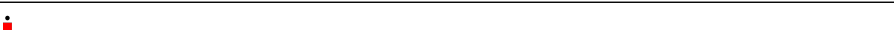

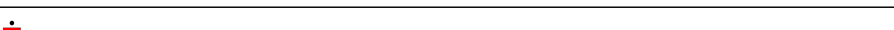
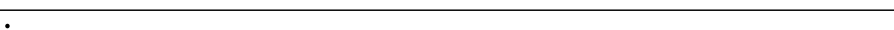



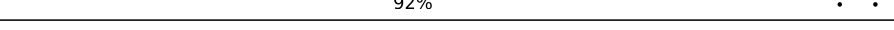
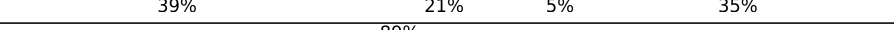
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	C	263	86% 10% . .
2	B	157	78% 12% . 10%
3	E	143	85% 13% .
4	D	194	79% 12% 9%
5	G	194	75% 16% 9%
6	F	59	78% . 20%
7	H	84	88% 8% .

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Mol	Chain	Length	Quality of chain
8	K	83	 92% 6% .
9	J	130	 92% 6% ..
10	M	135	 34% 6% 60%
11	L	293	 64% 10% . 25%
12	O	264	 66% 12% . 20%
13	N	295	 55% 15% 30%
14	Q	115	 80% 6% 14%
15	P	151	 68% 18% . 13%
16	S	249	 72% 19% . 8%
17	R	208	 82% 12% 5%
18	T	133	 81% 12% . 6%
19	q	144	 25% 53% 8% 39%
20	p	113	 70% 5% 25%
21	I	151	 85% 15% .
22	z	258	 62% 62% 38%
23	y	913	 15% 17% . 82%
24	9	25	 8% 92% . .
25	A	1869	 39% 21% 5% 35%
26	7	28	 25% 89% 71% .

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 52840 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 S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 2 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 3 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 4 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 6 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	47	Total	C	N	O	S	0	0
			378	231	85	61	1		

- Molecule 7 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 8 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 9 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 10 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	54	Total	C	N	O	S	0	0
			432	270	72	88	2		

- Molecule 11 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 12 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 14 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	131	Total	C	N	O	S	0	0
			982	600	193	183	6		

- Molecule 16 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 17 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 18 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 19 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	q	88	Total	C	N	O	S	0	0
			714	451	129	130	4		

- Molecule 20 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	p	85	Total	C	N	O	S	0	0
			691	438	125	126	2		

- Molecule 21 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 22 is a protein called Eukaryotic translation initiation factor 3 subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	z	160	Total	C	N	O		0	0
			795	475	160	160			

- Molecule 23 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	162	Total	C	N	O	S	0	0
			1145	714	212	217	2		

- Molecule 24 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 25 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	1220	Total	C	N	O	P	0	0
			26040	11635	4689	8497	1219		

- Molecule 26 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	7	28	Total	C	O	P	0	0
			336	140	168	28		

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	L	1	Total	Mg	0
			1	1	
27	S	1	Total	Mg	0
			1	1	
27	A	58	Total	Mg	0
			58	58	

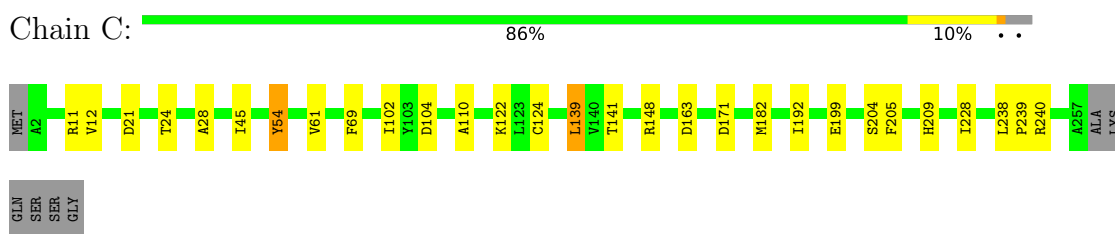
- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
28	Q	1	Total 1	Zn 1	0

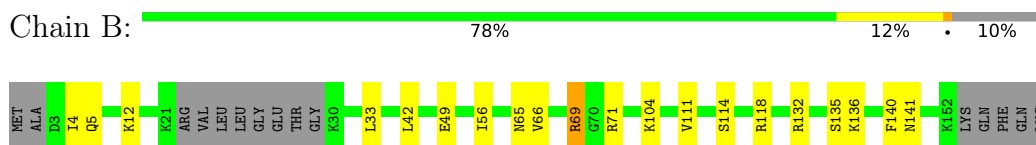
3 Residue-property plots [i](#)

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

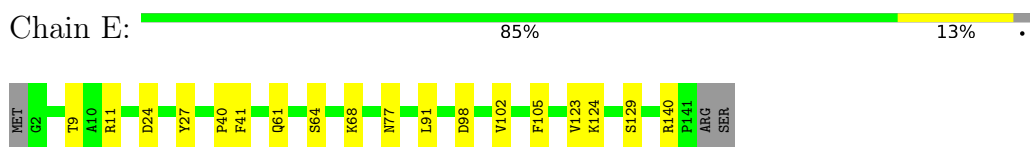
- Molecule 1: 40S ribosomal protein S4, X isoform



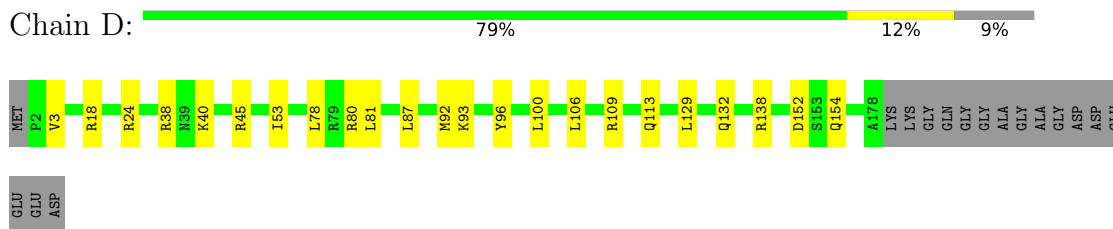
- Molecule 2: 40S ribosomal protein S11



- Molecule 3: 40S ribosomal protein S23



- Molecule 4: 40S ribosomal protein S9

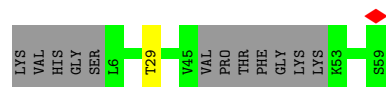
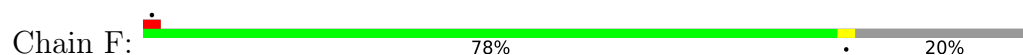


- Molecule 5: 40S ribosomal protein S7

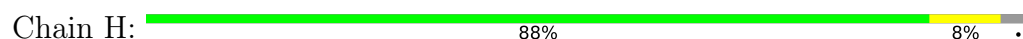




- Molecule 6: 40S ribosomal protein S30



- Molecule 7: 40S ribosomal protein S27



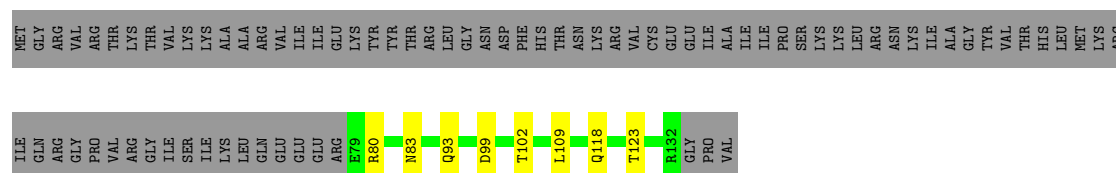
- Molecule 8: 40S ribosomal protein S21



- Molecule 9: 40S ribosomal protein S15a



- Molecule 10: 40S ribosomal protein S17



- Molecule 11: 40S ribosomal protein S2




- Molecule 16: 40S ribosomal protein S6

Chain S: 72% 19% 8%

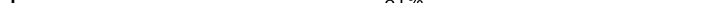


- Molecule 17: 40S ribosomal protein S8

Chain R:  82% 12% 5%



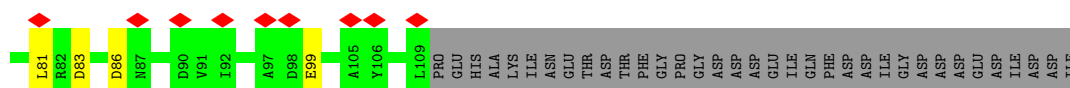
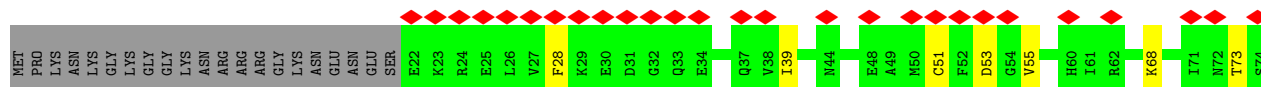
- Molecule 18: 40S ribosomal protein S24

Chain T:  81% 12% • 6%



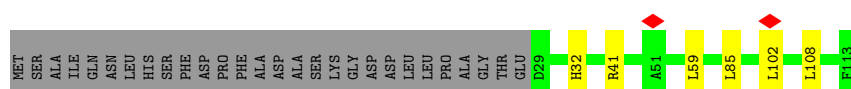
- Molecule 19: Eukaryotic translation initiation factor 1A, X-chromosomal

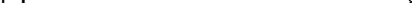
Chain q: 



- Molecule 20: Eukaryotic translation initiation factor 1

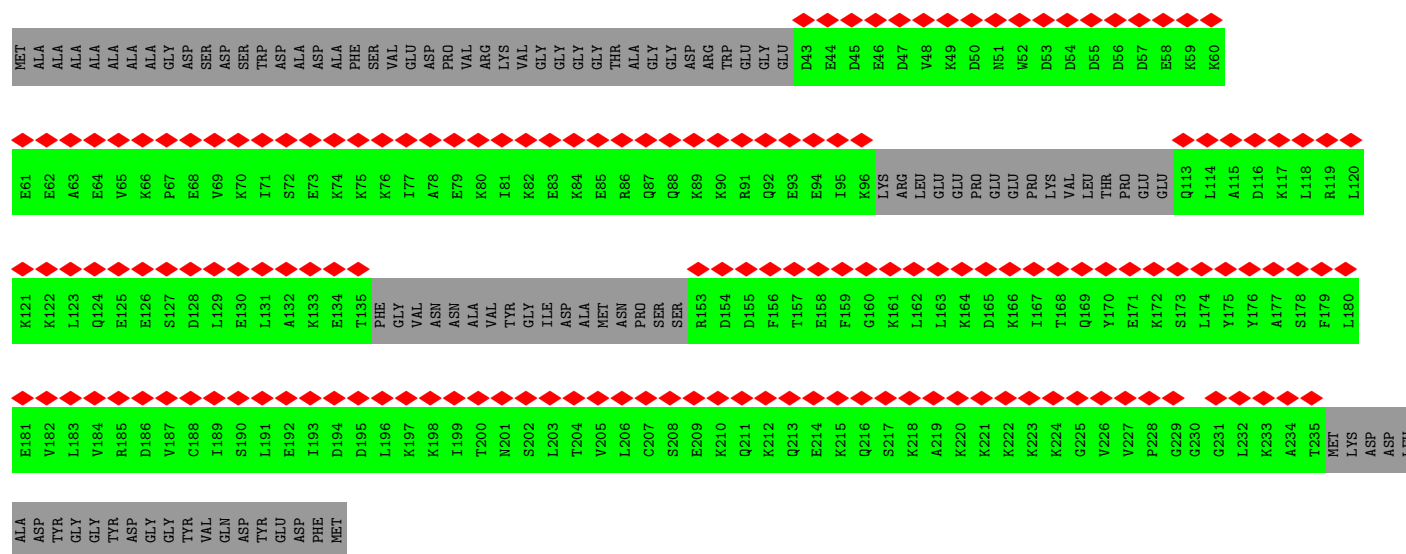
Chain p:  70% 5% 25%



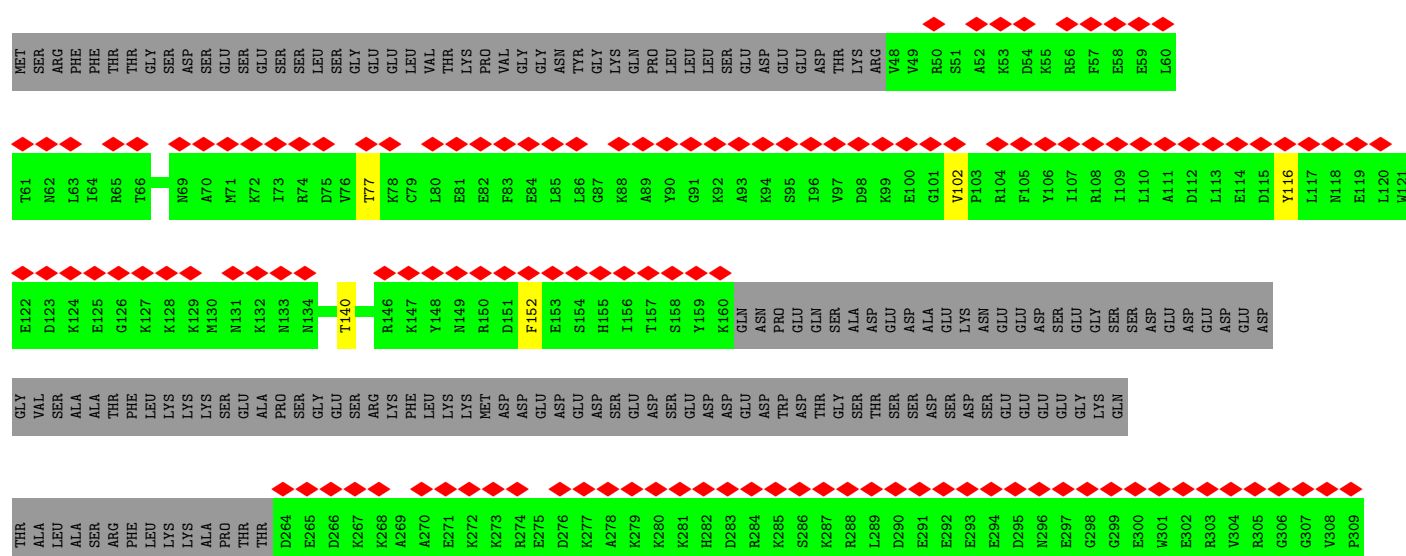
- Chain I:  85% 15%



- Chain z:  62% 38%

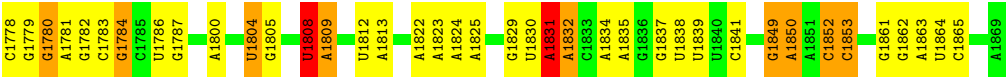
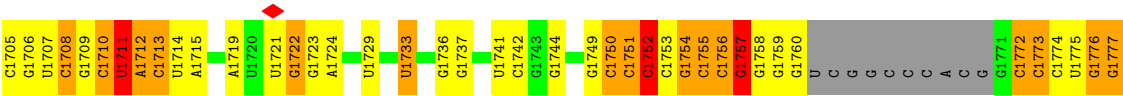


- Chain γ : 

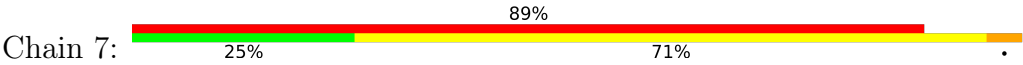








• Molecule 26: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144882	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 ($e^-/\text{\AA}^2$)	107	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.410	Depositor
Minimum map value	-0.228	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	537.0, 537.0, 537.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.074, 1.074, 1.074	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, PSU, ZN, OMC, 5MU, A2M, OMU, OMG, UR3, 6MZ, 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	C	0.31	0/2077	0.58	2/2796 (0.1%)
2	B	0.34	0/1186	0.56	0/1585
3	E	0.32	0/1105	0.58	0/1476
4	D	0.29	0/1502	0.51	0/2008
5	G	0.34	0/1451	0.60	1/1942 (0.1%)
6	F	0.26	0/380	0.47	0/496
7	H	0.30	0/644	0.52	0/864
8	K	0.30	0/623	0.48	0/833
9	J	0.32	0/1051	0.54	0/1406
10	M	0.31	0/438	0.66	0/593
11	L	0.33	0/1743	0.53	0/2354
12	O	0.30	0/1742	0.59	1/2330 (0.0%)
13	N	0.31	0/1670	0.54	0/2271
14	Q	0.32	0/805	0.53	0/1079
15	P	0.30	0/994	0.61	0/1332
16	S	0.31	0/1885	0.57	0/2510
17	R	0.33	0/1654	0.58	1/2203 (0.0%)
18	T	0.30	0/1032	0.49	0/1371
19	q	0.32	0/722	0.71	2/963 (0.2%)
20	p	0.30	0/701	0.74	1/936 (0.1%)
21	I	0.31	0/1232	0.63	1/1656 (0.1%)
22	z	0.27	0/792	0.46	0/1101
23	y	0.32	0/1156	0.56	0/1561
24	9	0.27	0/231	0.55	0/294
25	A	0.48	0/28528	1.15	201/44454 (0.5%)
26	7	0.31	0/363	1.07	0/556
All	All	0.41	0/55707	0.93	210/80970 (0.3%)

There are no bond length outliers.

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1756	C	N1-C2-O2	12.89	126.64	118.90
25	A	501	C	N1-C2-O2	12.43	126.36	118.90
25	A	537	C	N1-C2-O2	11.66	125.90	118.90
25	A	537	C	N3-C2-O2	-11.51	113.84	121.90
25	A	501	C	C2-N1-C1'	11.00	130.90	118.80
25	A	1756	C	N3-C2-O2	-10.73	114.39	121.90
25	A	1752	C	N1-C2-O2	10.67	125.30	118.90
25	A	537	C	C6-N1-C2	-10.32	116.17	120.30
25	A	501	C	N3-C2-O2	-9.89	114.98	121.90
25	A	1115	U	C2-N1-C1'	9.70	129.34	117.70
25	A	1756	C	C2-N1-C1'	9.49	129.24	118.80
25	A	1115	U	N1-C2-O2	9.11	129.18	122.80
25	A	882	U	N1-C2-O2	9.09	129.16	122.80
25	A	882	U	N3-C2-O2	-8.86	116.00	122.20
25	A	1115	U	N3-C2-O2	-8.84	116.01	122.20
25	A	1139	C	N1-C2-O2	8.81	124.19	118.90
25	A	537	C	C2-N1-C1'	8.77	128.45	118.80
25	A	1752	C	N3-C2-O2	-8.74	115.78	121.90
25	A	1752	C	C2-N1-C1'	8.74	128.41	118.80
25	A	1139	C	N3-C2-O2	-8.45	115.99	121.90
25	A	965	U	N3-C2-O2	-8.29	116.39	122.20
25	A	1773	C	N1-C2-O2	8.26	123.86	118.90
25	A	965	U	N1-C2-O2	8.13	128.49	122.80
25	A	1139	C	C2-N1-C1'	8.08	127.68	118.80
25	A	996	A	O4'-C1'-N9	8.02	114.61	108.20
25	A	501	C	C6-N1-C2	-7.97	117.11	120.30
25	A	1756	C	C6-N1-C2	-7.83	117.17	120.30
25	A	494	C	N1-C2-O2	7.77	123.56	118.90
25	A	1772	C	N1-C2-O2	7.71	123.53	118.90
25	A	1078	C	C6-N1-C2	-7.69	117.22	120.30
25	A	1776	G	N3-C4-C5	-7.62	124.79	128.60
25	A	879	C	C2-N1-C1'	7.61	127.17	118.80
25	A	1776	G	C4-N9-C1'	7.54	136.30	126.50
25	A	1710	C	O4'-C1'-N1	7.51	114.21	108.20
21	I	11	LEU	CA-CB-CG	7.39	132.29	115.30
25	A	501	C	C6-N1-C1'	-7.36	111.97	120.80
25	A	1751	C	O4'-C1'-N1	7.29	114.03	108.20
25	A	1776	G	N3-C4-N9	7.24	130.34	126.00
25	A	201	C	N1-C2-O2	7.23	123.24	118.90
25	A	118	C	N1-C2-O2	7.22	123.23	118.90
25	A	1804	U	C5-C6-N1	7.22	126.31	122.70
25	A	168	C	N1-C2-O2	7.14	123.18	118.90
20	p	59	LEU	CA-CB-CG	7.13	131.70	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1772	C	C6-N1-C2	-7.13	117.45	120.30
25	A	1078	C	C2-N1-C1'	7.12	126.63	118.80
25	A	556	U	N3-C2-O2	-7.12	117.22	122.20
25	A	1804	U	C6-N1-C2	-7.12	116.73	121.00
25	A	1078	C	N1-C2-O2	7.11	123.17	118.90
25	A	556	U	C2-N1-C1'	7.10	126.22	117.70
25	A	318	A	C2-N3-C4	7.09	114.14	110.60
25	A	882	U	C2-N1-C1'	7.06	126.17	117.70
25	A	556	U	N1-C2-O2	7.05	127.74	122.80
25	A	130	G	N3-C4-C5	-7.05	125.08	128.60
25	A	579	C	N1-C2-O2	6.98	123.09	118.90
25	A	566	U	N1-C2-O2	6.97	127.68	122.80
25	A	688	U	P-O3'-C3'	6.95	128.04	119.70
25	A	836	G	C4-N9-C1'	6.94	135.52	126.50
25	A	310	C	N1-C2-O2	6.89	123.03	118.90
25	A	834	C	C6-N1-C2	-6.86	117.56	120.30
25	A	1078	C	N3-C2-O2	-6.83	117.12	121.90
25	A	402	C	C6-N1-C2	-6.73	117.61	120.30
25	A	1773	C	N3-C2-O2	-6.72	117.20	121.90
25	A	310	C	N3-C2-O2	-6.71	117.20	121.90
25	A	632	C	C2-N1-C1'	6.68	126.14	118.80
25	A	402	C	C5-C6-N1	6.68	124.34	121.00
25	A	1	U	OP1-P-O3'	6.66	119.85	105.20
25	A	1022	U	C2-N1-C1'	6.66	125.69	117.70
25	A	1710	C	N1-C2-O2	6.65	122.89	118.90
25	A	1772	C	N3-C2-O2	-6.59	117.29	121.90
25	A	1710	C	N3-C2-O2	-6.55	117.32	121.90
25	A	566	U	N3-C2-O2	-6.52	117.64	122.20
25	A	1713	C	O4'-C1'-N1	6.51	113.41	108.20
25	A	1804	U	N3-C2-O2	-6.50	117.65	122.20
25	A	178	C	N1-C2-O2	6.46	122.78	118.90
25	A	1742	C	N1-C2-O2	6.45	122.77	118.90
25	A	1752	C	C6-N1-C2	-6.45	117.72	120.30
25	A	130	G	C4-N9-C1'	6.43	134.86	126.50
12	O	191	ASP	CB-CG-OD1	6.42	124.08	118.30
25	A	1115	U	C6-N1-C1'	-6.39	112.26	121.20
25	A	501	C	C5-C6-N1	6.38	124.19	121.00
25	A	1111	U	N3-C2-O2	-6.36	117.75	122.20
25	A	1852	C	N1-C2-O2	6.29	122.67	118.90
25	A	836	G	N3-C4-N9	6.28	129.76	126.00
25	A	1773	C	C2-N1-C1'	6.26	125.69	118.80
25	A	201	C	C6-N1-C2	-6.21	117.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1139	C	C6-N1-C2	-6.21	117.81	120.30
25	A	201	C	N3-C2-O2	-6.18	117.58	121.90
25	A	879	C	C6-N1-C2	-6.17	117.83	120.30
25	A	1776	G	C8-N9-C1'	-6.17	118.98	127.00
25	A	879	C	N1-C2-O2	6.14	122.58	118.90
25	A	834	C	N3-C2-O2	-6.13	117.61	121.90
25	A	188	C	C2-N1-C1'	6.12	125.53	118.80
25	A	1752	C	C6-N1-C1'	-6.12	113.46	120.80
25	A	566	U	C2-N1-C1'	6.12	125.04	117.70
25	A	1116	C	N1-C2-O2	6.10	122.56	118.90
25	A	494	C	N3-C2-O2	-6.08	117.65	121.90
25	A	130	G	C2-N3-C4	6.05	114.93	111.90
25	A	836	G	N3-C4-C5	-6.05	125.57	128.60
25	A	130	G	N3-C4-N9	6.04	129.62	126.00
25	A	118	C	N3-C2-O2	-6.03	117.68	121.90
25	A	1123	C	C6-N1-C2	-6.03	117.89	120.30
25	A	1756	C	C6-N1-C1'	-6.02	113.58	120.80
25	A	632	C	C6-N1-C2	-6.02	117.89	120.30
25	A	552	G	C8-N9-C4	-5.99	104.00	106.40
25	A	1123	C	C2-N1-C1'	5.93	125.32	118.80
25	A	632	C	C5-C6-N1	5.93	123.96	121.00
25	A	585	C	O4'-C1'-N1	5.90	112.92	108.20
25	A	624	C	N1-C2-O2	5.84	122.40	118.90
25	A	1708	C	C6-N1-C2	-5.83	117.97	120.30
25	A	836	G	C8-N9-C1'	-5.82	119.43	127.00
25	A	973	C	N1-C2-O2	5.80	122.38	118.90
25	A	624	C	C2-N1-C1'	5.80	125.18	118.80
25	A	833	C	N1-C2-O2	5.76	122.36	118.90
25	A	752	G	C4-N9-C1'	5.75	133.97	126.50
25	A	291	G	P-O3'-C3'	5.74	126.59	119.70
25	A	550	C	C6-N1-C1'	5.73	127.68	120.80
25	A	579	C	N3-C2-O2	-5.73	117.89	121.90
25	A	1729	U	N1-C2-O2	5.73	126.81	122.80
25	A	1772	C	C2-N1-C1'	5.66	125.02	118.80
25	A	1831	A	N9-C1'-C2'	-5.65	105.79	112.00
25	A	324	C	C2-N1-C1'	5.63	125.00	118.80
25	A	1111	U	N1-C2-O2	5.62	126.73	122.80
25	A	996	A	P-O3'-C3'	5.61	126.44	119.70
25	A	537	C	C5-C6-N1	5.58	123.79	121.00
25	A	1756	C	C5-C6-N1	5.55	123.77	121.00
1	C	139	LEU	CA-CB-CG	5.54	128.05	115.30
25	A	1808	U	C2-N1-C1'	5.54	124.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	588	G	N3-C4-N9	5.53	129.32	126.00
25	A	81	U	N3-C2-O2	-5.53	118.33	122.20
25	A	1742	C	N3-C2-O2	-5.50	118.05	121.90
25	A	4	C	C2-N1-C1'	5.50	124.85	118.80
25	A	1742	C	C2-N1-C1'	5.50	124.85	118.80
25	A	659	G	C4-N9-C1'	5.50	133.65	126.50
25	A	1022	U	N1-C2-O2	5.50	126.65	122.80
25	A	1784	G	N3-C4-N9	5.50	129.30	126.00
25	A	853	C	C6-N1-C2	-5.50	118.10	120.30
25	A	1172	U	N1-C2-O2	5.49	126.64	122.80
19	q	81	LEU	CA-CB-CG	5.47	127.89	115.30
25	A	1804	U	N1-C2-O2	5.47	126.63	122.80
25	A	494	C	C2-N1-C1'	5.46	124.81	118.80
25	A	168	C	N3-C2-O2	-5.46	118.08	121.90
25	A	1808	U	N3-C2-O2	-5.46	118.38	122.20
25	A	473	A	OP2-P-O3'	5.43	117.15	105.20
5	G	28	LEU	CA-CB-CG	5.43	127.79	115.30
25	A	753	C	N1-C2-O2	5.43	122.16	118.90
25	A	1776	G	C2-N3-C4	5.42	114.61	111.90
25	A	188	C	C6-N1-C2	-5.42	118.13	120.30
17	R	119	LEU	CA-CB-CG	5.42	127.75	115.30
25	A	593	C	N1-C2-O2	5.41	122.14	118.90
25	A	53	C	C6-N1-C2	-5.39	118.14	120.30
25	A	1772	C	C5-C6-N1	5.38	123.69	121.00
25	A	1090	C	C6-N1-C2	-5.37	118.15	120.30
25	A	965	U	C2-N1-C1'	5.37	124.14	117.70
25	A	1808	U	N1-C2-O2	5.37	126.56	122.80
25	A	1757	G	N3-C4-C5	-5.37	125.92	128.60
25	A	459	C	C2-N1-C1'	5.36	124.70	118.80
25	A	735	C	N1-C2-O2	5.35	122.11	118.90
25	A	1109	C	N1-C2-O2	5.33	122.10	118.90
25	A	179	C	N1-C2-O2	5.33	122.10	118.90
25	A	1751	C	C5-C6-N1	5.32	123.66	121.00
25	A	1733	U	C2-N1-C1'	5.32	124.08	117.70
25	A	216	C	C6-N1-C2	-5.32	118.17	120.30
25	A	1757	G	C4-N9-C1'	5.30	133.39	126.50
25	A	1852	C	C2-N1-C1'	5.30	124.63	118.80
25	A	178	C	N3-C2-O2	-5.29	118.19	121.90
25	A	882	U	C5-C6-N1	5.29	125.35	122.70
25	A	1773	C	C6-N1-C2	-5.29	118.19	120.30
25	A	752	G	N3-C4-C5	-5.28	125.96	128.60
25	A	663	C	C6-N1-C2	-5.27	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1139	C	C6-N1-C1'	-5.26	114.49	120.80
25	A	1115	U	C5-C6-N1	5.24	125.32	122.70
25	A	666	U	C2-N1-C1'	5.23	123.97	117.70
25	A	402	C	N1-C2-O2	5.22	122.03	118.90
25	A	324	C	N1-C2-O2	5.22	122.03	118.90
25	A	1711	U	O4'-C1'-N1	5.21	112.37	108.20
25	A	140	U	C2-N1-C1'	5.20	123.94	117.70
25	A	1852	C	N3-C2-O2	-5.20	118.26	121.90
25	A	30	C	C5-C6-N1	5.19	123.59	121.00
25	A	1784	G	N3-C4-C5	-5.17	126.01	128.60
25	A	663	C	C5-C6-N1	5.16	123.58	121.00
25	A	1067	C	N1-C2-O2	5.14	121.98	118.90
1	C	163	ASP	CB-CG-OD1	5.14	122.92	118.30
25	A	1757	G	N3-C4-N9	5.13	129.08	126.00
25	A	178	C	C2-N1-C1'	5.13	124.44	118.80
25	A	459	C	C6-N1-C2	-5.13	118.25	120.30
25	A	87	U	N3-C2-O2	-5.12	118.61	122.20
25	A	1751	C	N1-C2-O2	5.12	121.97	118.90
25	A	1804	U	O4'-C1'-N1	5.12	112.30	108.20
25	A	1022	U	N3-C2-O2	-5.12	118.62	122.20
25	A	571	U	N3-C2-O2	-5.11	118.62	122.20
25	A	409	C	C6-N1-C2	-5.11	118.26	120.30
25	A	4	C	C6-N1-C2	-5.10	118.26	120.30
25	A	168	C	C2-N1-C1'	5.09	124.41	118.80
25	A	86	C	C6-N1-C2	-5.09	118.26	120.30
25	A	930	C	N1-C2-O2	5.09	121.96	118.90
25	A	570	C	N1-C2-O2	5.08	121.95	118.90
25	A	1714	U	C5-C6-N1	5.08	125.24	122.70
25	A	578	C	N1-C2-O2	5.08	121.94	118.90
25	A	1109	C	C6-N1-C2	-5.07	118.27	120.30
19	q	83	ASP	CB-CG-OD2	5.07	122.86	118.30
25	A	188	C	N1-C2-O2	5.06	121.94	118.90
25	A	571	U	N1-C2-O2	5.06	126.34	122.80
25	A	1123	C	N1-C2-O2	5.06	121.93	118.90
25	A	626	G	C4-N9-C1'	5.04	133.05	126.50
25	A	1733	U	N1-C2-O2	5.03	126.32	122.80
25	A	1729	U	N3-C2-O2	-5.03	118.68	122.20
25	A	178	C	C6-N1-C2	-5.02	118.29	120.30
25	A	578	C	C6-N1-C2	-5.01	118.30	120.30
25	A	1784	G	N3-C2-N2	5.01	123.41	119.90
25	A	850	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

There are no planarity outliers.

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	C	2035	0	2138	15	0
2	B	1166	0	1233	11	0
3	E	1087	0	1154	10	0
4	D	1477	0	1589	14	0
5	G	1430	0	1520	14	0
6	F	378	0	417	0	0
7	H	631	0	657	4	0
8	K	617	0	622	1	0
9	J	1034	0	1080	10	0
10	M	432	0	429	5	0
11	L	1707	0	1794	12	0
12	O	1715	0	1785	24	0
13	N	1633	0	1640	25	0
14	Q	792	0	843	3	0
15	P	982	0	1005	18	0
16	S	1862	0	2018	37	0
17	R	1627	0	1706	17	0
18	T	1015	0	1086	11	0
19	q	714	0	735	0	0
20	p	691	0	706	0	0
21	I	1208	0	1294	10	0
22	z	795	0	341	0	0
23	y	1145	0	1000	0	0
24	9	230	0	276	1	0
25	A	26040	0	13175	157	0
26	7	336	0	169	1	0
27	A	58	0	0	0	0
27	L	1	0	0	0	0
27	S	1	0	0	0	0
28	Q	1	0	0	0	0
All	All	52840	0	40412	332	0

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

All (332) 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)
25:A:885:U:H3	25:A:901:G:H1	1.07	0.97
25:A:1722:G:H1	25:A:1812:U:H3	1.07	0.93
25:A:1033:G:H1	25:A:1080:A:HO2'	1.28	0.81
12:O:52:THR:HG22	12:O:58:ALA:H	1.55	0.71
2:B:4:ILE:HG13	2:B:5:GLN:HE21	1.57	0.69
16:S:135:PRO:HB2	16:S:141:ILE:HG12	1.73	0.69
25:A:751:G:H22	25:A:789:G:H5''	1.58	0.68
9:J:2:VAL:N	25:A:1091:C:HO2'	1.91	0.67
25:A:693:A:N1	25:A:737:G:O6	2.29	0.66
25:A:925:G:H1	25:A:1017:U:H3	1.45	0.64
2:B:104:LYS:O	3:E:11:ARG:NH2	2.31	0.63
25:A:928:G:H1	25:A:1013:U:H3	1.46	0.63
25:A:1708:C:H2'	25:A:1709:G:H8	1.66	0.61
16:S:142:ARG:HA	16:S:147:LEU:HB2	1.83	0.61
16:S:78:SER:HB3	16:S:92:ARG:HG2	1.82	0.60
25:A:1831:A:H2'	25:A:1832:6MZ:H8	1.82	0.60
9:J:71:LYS:NZ	25:A:1156:U:OP1	2.33	0.60
14:Q:32:LYS:NZ	25:A:987:A:OP1	2.34	0.60
17:R:87:ASN:HB3	17:R:90:LEU:HG	1.84	0.59
16:S:49:VAL:HB	16:S:115:LYS:HB3	1.85	0.59
26:7:7:A:H5''	26:7:8:A:H5'	1.85	0.59
12:O:108:ASP:OD1	12:O:108:ASP:N	2.37	0.58
13:N:177:MET:SD	13:N:180:ARG:NH2	2.77	0.58
25:A:72:C:O2'	25:A:74:G:N2	2.37	0.58
9:J:80:ASP:N	9:J:80:ASP:OD1	2.36	0.58
25:A:887:U:H2'	25:A:888:U:H2'	1.84	0.58
16:S:63:MET:HG2	16:S:98:ARG:HD2	1.85	0.58
1:C:204:SER:OG	1:C:205:PHE:N	2.37	0.57
16:S:23:LYS:HD3	16:S:41:LEU:HA	1.87	0.57
25:A:948:C:H2'	25:A:949:G:H8	1.69	0.57
16:S:58:LYS:HA	16:S:107:SER:HB2	1.86	0.57
21:I:107:LYS:NZ	25:A:1075:C:OP1	2.37	0.57
13:N:80:ARG:NH2	13:N:126:ASP:OD1	2.38	0.56
25:A:835:C:H5''	25:A:836:G:H5'	1.87	0.56
4:D:80:ARG:NH2	25:A:818:A:OP1	2.38	0.56
16:S:188:LYS:NZ	25:A:142:C:OP2	2.38	0.56
3:E:40:PRO:O	3:E:77:ASN:ND2	2.39	0.56
12:O:171:ILE:HG12	12:O:174:ARG:HH22	1.69	0.56
13:N:37:TYR:HA	13:N:53:ARG:HD3	1.88	0.56
16:S:2:LYS:HB2	16:S:108:VAL:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:92:ARG:O	25:A:453:C:O2'	2.23	0.56
4:D:18:ARG:O	4:D:24:ARG:NH1	2.39	0.56
18:T:80:ASP:OD1	18:T:80:ASP:N	2.39	0.55
15:P:55:ARG:NH1	25:A:973:C:N3	2.52	0.55
25:A:476:A:N3	25:A:488:U:O2'	2.35	0.55
5:G:39:GLN:HG3	5:G:75:ILE:HG21	1.88	0.55
2:B:69:ARG:NH2	25:A:114:G:N7	2.54	0.55
16:S:168:LYS:O	25:A:67:C:N4	2.39	0.55
2:B:66:VAL:HG11	2:B:141:ASN:HD22	1.71	0.55
16:S:170:ARG:NH1	25:A:71:G:N7	2.54	0.55
18:T:108:LYS:NZ	25:A:507:G:OP1	2.38	0.54
15:P:151:LEU:HB2	25:A:1064:C:H5'	1.89	0.54
25:A:752:G:N2	25:A:793:G:O2'	2.40	0.54
5:G:154:ILE:HB	5:G:185:VAL:HG12	1.88	0.54
1:C:54:TYR:O	18:T:15:ASN:ND2	2.41	0.54
4:D:113:GLN:OE1	4:D:154:GLN:NE2	2.41	0.54
25:A:834:C:O2'	25:A:836:G:N1	2.40	0.54
16:S:167:LYS:NZ	25:A:70:G:OP2	2.36	0.54
13:N:104:THR:O	13:N:107:THR:OG1	2.25	0.54
17:R:101:ILE:HD12	17:R:190:LEU:HD11	1.90	0.54
25:A:1750:C:N4	25:A:1751:C:N4	2.56	0.53
12:O:137:LEU:HG	12:O:215:VAL:HG22	1.90	0.53
25:A:84:A:N3	25:A:150:A:O2'	2.36	0.53
12:O:162:ARG:NH1	25:A:1005:G:OP2	2.42	0.53
17:R:184:ARG:NH2	25:A:218:U:O2	2.41	0.53
1:C:199:GLU:OE2	1:C:209:HIS:NE2	2.42	0.53
12:O:47:THR:OG1	12:O:65:ARG:NH1	2.42	0.53
25:A:75:G:N2	25:A:76:U:O4	2.42	0.53
25:A:198:U:H1'	25:A:202:G:H1	1.74	0.53
25:A:588:G:H4'	25:A:589:G:H5'	1.90	0.53
7:H:7:LEU:HD12	9:J:24:GLN:HB3	1.91	0.52
4:D:38:ARG:NH1	25:A:643:A:OP1	2.43	0.52
5:G:184:ASP:OD2	5:G:184:ASP:N	2.42	0.52
17:R:41:ARG:HA	17:R:59:ARG:O	2.09	0.52
1:C:102:ILE:HD12	1:C:239:PRO:HD3	1.90	0.52
25:A:878:G:H1	25:A:908:A:H61	1.56	0.52
7:H:34:ASP:O	7:H:79:PHE:HA	2.10	0.52
13:N:125:THR:HG23	13:N:175:TRP:HE1	1.74	0.52
25:A:43:U:OP2	25:A:485:A:N6	2.43	0.52
25:A:848:U:H2'	25:A:849:A:H8	1.74	0.52
2:B:49:GLU:HG2	2:B:118:ARG:HH12	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:874:G:H2'	25:A:875:A:H8	1.74	0.51
25:A:1010:G:H2'	25:A:1011:A:H8	1.74	0.51
25:A:1114:U:O2'	25:A:1119:A:N6	2.43	0.51
13:N:145:ILE:HG12	13:N:159:ILE:HB	1.93	0.51
3:E:98:ASP:OD1	3:E:140:ARG:NH2	2.43	0.51
16:S:132:ARG:NH1	25:A:151:C:O2'	2.43	0.51
5:G:44:ASN:OD1	5:G:44:ASN:N	2.43	0.51
9:J:28:ARG:HH22	25:A:1093:A:H5''	1.75	0.51
12:O:188:LEU:HD11	12:O:215:VAL:HG21	1.92	0.51
1:C:45:ILE:HA	1:C:61:VAL:HG11	1.92	0.51
12:O:146:ARG:NH1	25:A:1122:A:N3	2.58	0.51
11:L:125:LYS:HG2	11:L:143:CYS:HB2	1.93	0.51
16:S:74:ARG:NH1	16:S:96:SER:OG	2.44	0.51
21:I:55:ARG:HD3	25:A:1017:U:H5'	1.92	0.51
21:I:4:MET:HE3	25:A:924:G:H5'	1.94	0.50
25:A:585:C:H2'	25:A:586:G:C8	2.46	0.50
25:A:1722:G:N2	25:A:1812:U:O2	2.36	0.50
16:S:12:CYS:SG	16:S:13:GLN:N	2.83	0.50
25:A:579:C:H2'	25:A:580:U:H6	1.77	0.50
25:A:1707:U:H2'	25:A:1708:C:H6	1.76	0.50
25:A:583:A:H2'	25:A:584:A:H8	1.76	0.50
12:O:144:LYS:HE2	12:O:208:HIS:HB3	1.94	0.49
1:C:11:ARG:HA	1:C:28:ALA:HB2	1.93	0.49
25:A:920:A:O2'	25:A:922:A:OP1	2.30	0.49
25:A:980:A:H2'	25:A:981:A:C8	2.47	0.49
25:A:981:A:H2'	25:A:982:G:C8	2.47	0.49
4:D:40:LYS:NZ	25:A:641:A:OP1	2.42	0.49
9:J:28:ARG:NH1	25:A:922:A:OP2	2.45	0.49
12:O:73:ASP:OD1	15:P:128:ARG:NE	2.44	0.49
1:C:104:ASP:HB3	1:C:110:ALA:HB2	1.95	0.49
17:R:49:ARG:NH1	25:A:447:A:OP1	2.44	0.49
11:L:167:ARG:HB3	11:L:177:PRO:HB2	1.95	0.49
16:S:136:LYS:HG3	16:S:174:PRO:HB2	1.93	0.49
18:T:5:VAL:O	18:T:43:LYS:NZ	2.44	0.49
18:T:117:VAL:HG21	18:T:125:VAL:HG21	1.95	0.49
25:A:323:C:O2'	25:A:326:C:N3	2.41	0.49
14:Q:74:CYS:SG	14:Q:75:VAL:N	2.85	0.49
16:S:15:LEU:HD13	25:A:155:G:H4'	1.93	0.49
25:A:838:G:O2'	25:A:840:C:OP2	2.30	0.48
13:N:69:GLU:N	13:N:69:GLU:OE1	2.45	0.48
13:N:76:VAL:HG12	13:N:123:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:583:A:H2'	25:A:584:A:C8	2.48	0.48
25:A:1757:G:H8	25:A:1777:G:H1	1.61	0.48
25:A:882:U:N3	25:A:883:U:O2	2.46	0.48
25:A:1786:U:H2'	25:A:1787:G:H8	1.79	0.48
3:E:9:THR:HG22	25:A:681:U:H4'	1.95	0.48
13:N:128:ARG:NH2	13:N:151:ASP:O	2.46	0.48
16:S:186:GLN:NE2	25:A:333:G:O6	2.45	0.48
8:K:15:ARG:NH1	8:K:33:GLN:OE1	2.46	0.48
2:B:135:SER:OG	2:B:136:LYS:N	2.44	0.48
15:P:98:ARG:HB3	15:P:132:VAL:HG23	1.95	0.48
10:M:123:THR:OG1	13:N:44:ASP:OD1	2.31	0.48
11:L:262:THR:OG1	11:L:263:LYS:N	2.45	0.48
17:R:31:ARG:NH1	25:A:380:G:OP1	2.40	0.47
4:D:93:LYS:HB2	4:D:96:TYR:HD2	1.79	0.47
21:I:37:ILE:HD11	21:I:63:VAL:HG21	1.95	0.47
21:I:3:ARG:HB2	21:I:6:ALA:HB3	1.96	0.47
16:S:186:GLN:OE1	25:A:319:C:N4	2.47	0.47
5:G:46:THR:HG21	5:G:97:GLN:HG2	1.95	0.47
2:B:71:ARG:NH2	25:A:109:U:O2	2.47	0.47
12:O:48:LEU:HG	15:P:51:GLU:HG2	1.97	0.47
16:S:72:ARG:NH2	25:A:467:G:O5'	2.48	0.47
25:A:533:A:H2'	25:A:534:G:C8	2.50	0.47
25:A:1705:C:H2'	25:A:1706:G:C8	2.50	0.47
11:L:144:SER:OG	11:L:145:LYS:N	2.47	0.47
16:S:134:GLY:HA3	16:S:158:VAL:HG11	1.96	0.47
5:G:20:GLU:OE2	5:G:48:ALA:N	2.48	0.47
10:M:109:LEU:HD22	13:N:52:LYS:HE2	1.96	0.47
13:N:134:LEU:HD22	13:N:144:THR:HG21	1.97	0.47
25:A:1722:G:O6	25:A:1812:U:O4	2.33	0.47
25:A:877:C:H2'	25:A:878:G:C8	2.51	0.46
15:P:30:VAL:HG23	15:P:47:LEU:HA	1.96	0.46
16:S:53:SER:O	16:S:53:SER:OG	2.34	0.46
25:A:1707:U:H2'	25:A:1708:C:C6	2.51	0.46
3:E:123:VAL:HG12	3:E:124:LYS:HG3	1.97	0.46
13:N:44:ASP:OD1	13:N:44:ASP:N	2.48	0.46
25:A:191:A:H62	25:A:208:G:H21	1.62	0.46
25:A:604:A:N3	25:A:639:C:O2'	2.42	0.46
25:A:928:G:H2'	25:A:929:G:C8	2.51	0.46
25:A:940:U:H3	25:A:1002:U:H3	1.62	0.46
12:O:56:LYS:HB2	12:O:56:LYS:HE3	1.78	0.46
15:P:40:THR:O	15:P:58:GLY:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:96:LYS:HD3	15:P:132:VAL:HG11	1.98	0.46
25:A:1712:A:H2'	25:A:1713:C:C6	2.50	0.46
25:A:527:C:H2'	25:A:528:A:H8	1.79	0.46
5:G:69:LEU:HD22	5:G:96:ALA:HB2	1.97	0.46
16:S:57:ASP:OD1	16:S:58:LYS:N	2.49	0.46
17:R:201:LYS:HA	17:R:201:LYS:HD2	1.76	0.46
1:C:148:ARG:NH2	16:S:202:ASN:OD1	2.37	0.46
12:O:185:VAL:HA	12:O:188:LEU:HB2	1.98	0.46
25:A:532:C:H2'	25:A:533:A:C8	2.51	0.46
25:A:545:A:O2'	25:A:546:G:O4'	2.27	0.45
2:B:65:ASN:O	2:B:132:ARG:NH2	2.49	0.45
13:N:54:THR:HA	13:N:162:PRO:HD2	1.98	0.45
13:N:77:ILE:HG12	13:N:99:ILE:HB	1.98	0.45
25:A:1013:U:OP1	25:A:1129:G:O2'	2.32	0.45
10:M:93:GLN:HE21	13:N:20:ALA:HB1	1.80	0.45
25:A:1708:C:H2'	25:A:1709:G:C8	2.49	0.45
25:A:1722:G:H2'	25:A:1723:G:H8	1.82	0.45
5:G:87:PHE:HB3	5:G:90:LYS:HD2	1.98	0.45
4:D:138:ARG:NH2	4:D:152:ASP:O	2.50	0.45
9:J:55:ASP:OD1	9:J:55:ASP:N	2.46	0.45
15:P:65:ASP:OD1	15:P:65:ASP:N	2.48	0.45
18:T:86:GLU:OE2	18:T:90:ARG:NH1	2.40	0.45
25:A:116:OMU:HM23	25:A:116:OMU:H1'	1.80	0.45
25:A:982:G:H2'	25:A:983:A:H8	1.82	0.45
17:R:98:LYS:HD3	25:A:377:G:H5'	1.99	0.45
21:I:75:LEU:HD22	21:I:80:LEU:HB2	1.98	0.45
25:A:1722:G:H2'	25:A:1723:G:C8	2.52	0.45
12:O:168:MET:HG2	12:O:197:ILE:HG21	1.98	0.45
17:R:10:LYS:HE3	17:R:10:LYS:HB3	1.84	0.45
11:L:207:ALA:HB2	25:A:4:C:H4'	1.98	0.44
12:O:33:VAL:HG13	12:O:44:ILE:HG12	1.97	0.44
16:S:4:ASN:HB3	16:S:110:ASN:HD22	1.82	0.44
16:S:131:ARG:NE	25:A:167:G:O2'	2.50	0.44
25:A:28:U:H2'	25:A:29:G:H8	1.82	0.44
25:A:692:G:H2'	25:A:693:A:C8	2.53	0.44
5:G:145:ARG:NH1	9:J:51:GLU:OE1	2.51	0.44
16:S:195:LYS:NZ	25:A:126:G:OP2	2.39	0.44
11:L:204:ILE:HD12	11:L:215:MET:HG3	1.98	0.44
25:A:1010:G:H2'	25:A:1011:A:C8	2.51	0.44
15:P:36:SER:OG	15:P:37:PHE:N	2.50	0.44
3:E:41:PHE:HZ	3:E:102:VAL:HG12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:LEU:HD22	4:D:92:MET:HA	2.00	0.44
11:L:187:ARG:HH21	11:L:190:SER:HA	1.82	0.44
25:A:1849:G:H2'	25:A:1850:MA6:C8	2.48	0.44
13:N:38:ILE:HD12	13:N:47:TYR:HB3	2.00	0.44
13:N:154:LEU:HD23	13:N:154:LEU:HA	1.85	0.44
11:L:70:VAL:HG21	11:L:93:ILE:HG23	1.98	0.44
16:S:132:ARG:H	16:S:132:ARG:HG2	1.66	0.43
25:A:223:C:H2'	25:A:224:A:H8	1.83	0.43
25:A:562:U:H2'	25:A:563:G:C8	2.53	0.43
11:L:207:ALA:HB3	11:L:210:PRO:HD2	2.00	0.43
18:T:34:THR:O	25:A:570:C:O2'	2.31	0.43
21:I:16:LEU:HD22	25:A:919:A:H5''	2.01	0.43
13:N:137:ALA:HB1	13:N:142:LEU:HB3	1.99	0.43
21:I:94:LYS:HG2	21:I:118:ILE:HD13	2.00	0.43
25:A:640:A:H2'	25:A:641:A:C8	2.53	0.43
16:S:98:ARG:NH1	16:S:101:ILE:O	2.51	0.43
25:A:145:G:H2'	25:A:146:G:C8	2.53	0.43
25:A:1710:C:O2'	25:A:1711:U:H5'	2.18	0.43
4:D:106:LEU:HD23	4:D:109:ARG:HD2	1.99	0.43
18:T:116:LYS:HB3	25:A:161:U:H5'	1.99	0.43
25:A:747:U:H3	25:A:795:A:H61	1.66	0.43
7:H:62:VAL:O	7:H:74:THR:OG1	2.32	0.43
10:M:118:GLN:HE21	10:M:118:GLN:HB2	1.62	0.43
13:N:147:LEU:O	13:N:165:ASN:ND2	2.51	0.43
4:D:45:ARG:NH1	25:A:521:A:OP1	2.50	0.43
13:N:66:VAL:HG21	13:N:185:MET:HB2	2.00	0.43
25:A:691:G:O6	25:A:740:C:N4	2.52	0.43
16:S:186:GLN:HE22	25:A:318:A:N6	2.17	0.43
5:G:17:ASP:OD1	5:G:17:ASP:N	2.50	0.43
25:A:106:C:H2'	25:A:107:A:H8	1.84	0.43
25:A:527:C:H2'	25:A:528:A:C8	2.53	0.43
10:M:83:ASN:OD1	13:N:89:LYS:NZ	2.49	0.42
11:L:145:LYS:HE2	11:L:145:LYS:HB2	1.82	0.42
15:P:84:ARG:HD2	15:P:84:ARG:HA	1.71	0.42
1:C:21:ASP:OD1	1:C:21:ASP:N	2.47	0.42
1:C:240:ARG:NH2	25:A:844:U:OP1	2.52	0.42
5:G:138:GLU:OE1	21:I:19:ARG:NE	2.39	0.42
12:O:73:ASP:OD1	12:O:73:ASP:N	2.53	0.42
12:O:167:LYS:HE2	12:O:167:LYS:HB2	1.87	0.42
16:S:159:ARG:NH2	16:S:171:THR:O	2.53	0.42
25:A:1754:G:H2'	25:A:1755:C:H4'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1754:G:OP1	25:A:1780:G:N1	2.52	0.42
1:C:182:MET:HB2	1:C:228:ILE:HD13	2.00	0.42
9:J:30:CYS:HB2	9:J:61:ILE:HG13	2.00	0.42
11:L:109:ILE:HD11	11:L:151:ILE:HD11	2.01	0.42
12:O:34:LYS:HB3	12:O:34:LYS:HE2	1.81	0.42
25:A:367:U:H4'	25:A:371:A:C8	2.53	0.42
2:B:12:LYS:HA	2:B:56:ILE:HD13	2.02	0.42
2:B:42:LEU:HD23	2:B:42:LEU:HA	1.86	0.42
2:B:111:VAL:HG12	2:B:140:PHE:HB2	2.02	0.42
15:P:50:LYS:HE3	25:A:976:G:H21	1.85	0.42
25:A:1736:G:H2'	25:A:1737:G:C8	2.54	0.42
1:C:124:CYS:HB3	1:C:141:THR:HB	2.00	0.42
15:P:86:LYS:HB3	15:P:86:LYS:HE2	1.83	0.42
16:S:44:GLU:HG3	16:S:45:TRP:HD1	1.85	0.42
18:T:21:LYS:NZ	25:A:838:G:O6	2.52	0.42
25:A:72:C:O2	25:A:74:G:N2	2.52	0.42
25:A:186:C:H2'	25:A:187:G:H8	1.84	0.42
1:C:192:ILE:HD13	1:C:238:LEU:HD22	2.01	0.42
15:P:34:PHE:HB3	15:P:41:PHE:HB2	2.01	0.42
9:J:43:LYS:HA	9:J:43:LYS:HD2	1.93	0.42
11:L:65:LYS:HG3	11:L:68:ARG:HH21	1.85	0.42
25:A:107:A:H2'	25:A:108:G:C8	2.55	0.42
17:R:158:ILE:HD12	17:R:158:ILE:HA	1.86	0.42
25:A:472:C:O2'	25:A:474:G:OP1	2.33	0.42
25:A:1752:C:H41	25:A:1754:G:H3'	1.84	0.42
5:G:40:LEU:HD12	5:G:40:LEU:HA	1.91	0.42
12:O:65:ARG:HB3	15:P:48:SER:HB2	2.02	0.42
15:P:100:THR:HG22	15:P:105:THR:HG22	2.01	0.42
16:S:203:LYS:HE3	16:S:203:LYS:HB2	1.79	0.42
25:A:1852:C:H2'	25:A:1853:C:C6	2.54	0.42
4:D:87:LEU:HD13	4:D:100:LEU:HD21	2.02	0.41
5:G:183:LYS:H	5:G:183:LYS:HG2	1.67	0.41
14:Q:4:LYS:NZ	25:A:1864:U:OP2	2.47	0.41
25:A:674:C:H2'	25:A:675:U:C6	2.55	0.41
13:N:155:ARG:NH2	25:A:1137:U:O2'	2.53	0.41
1:C:21:ASP:OD2	1:C:24:THR:OG1	2.37	0.41
17:R:119:LEU:HD21	17:R:153:LYS:HG2	2.01	0.41
25:A:174:OMC:HM23	25:A:174:OMC:H1'	1.81	0.41
25:A:1751:C:H6	25:A:1751:C:H2'	1.65	0.41
4:D:129:LEU:HD23	4:D:129:LEU:HA	1.93	0.41
12:O:136:ARG:HE	12:O:218:LEU:HD11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:103:ASN:OD1	15:P:103:ASN:N	2.42	0.41
18:T:8:ARG:HD3	25:A:837:A:H62	1.84	0.41
25:A:851:C:H5''	25:A:852:G:H5'	2.01	0.41
13:N:110:ASN:HD22	13:N:113:GLN:HE21	1.69	0.41
15:P:28:PHE:HB3	15:P:47:LEU:HD21	2.01	0.41
21:I:102:LEU:HD12	21:I:102:LEU:HA	1.92	0.41
4:D:132:GLN:HB3	25:A:562:U:H4'	2.02	0.41
17:R:43:ILE:HG12	17:R:57:ALA:HA	2.02	0.41
25:A:1101:U:H2'	25:A:1102:G:C8	2.56	0.41
16:S:5:ILE:HG21	16:S:45:TRP:HH2	1.86	0.41
17:R:124:LYS:HA	17:R:124:LYS:HD2	1.73	0.41
17:R:203:LYS:HB2	17:R:203:LYS:HE3	1.85	0.41
25:A:116:OMU:H6	25:A:116:OMU:O5'	2.20	0.41
25:A:879:C:H2'	25:A:880:G:H5''	2.03	0.41
25:A:223:C:H2'	25:A:224:A:C8	2.56	0.41
25:A:579:C:H2'	25:A:580:U:C6	2.55	0.41
25:A:683:OMG:H1'	25:A:683:OMG:HM23	1.83	0.41
12:O:50:THR:OG1	12:O:51:ARG:N	2.53	0.41
16:S:46:LYS:HB3	16:S:46:LYS:HE3	1.84	0.41
25:A:557:U:H2'	25:A:558:G:C8	2.56	0.41
25:A:582:U:O2'	25:A:583:A:H5'	2.20	0.41
25:A:692:G:O6	25:A:739:C:N4	2.53	0.41
25:A:1723:G:H2'	25:A:1724:A:C8	2.56	0.41
17:R:103:LEU:HA	17:R:171:LEU:O	2.21	0.41
18:T:32:LYS:HE2	18:T:32:LYS:HB3	1.90	0.41
1:C:122:LYS:HE3	1:C:122:LYS:HB2	1.87	0.40
3:E:24:ASP:HB3	3:E:27:TYR:HB3	2.03	0.40
3:E:68:LYS:HB3	3:E:91:LEU:HD22	2.03	0.40
7:H:30:SER:OG	25:A:1016:U:OP1	2.27	0.40
24:9:1:MET:HB2	25:A:1706:G:H5'	2.01	0.40
4:D:53:ILE:HD13	4:D:81:LEU:HD21	2.04	0.40
5:G:53:VAL:HG21	5:G:172:THR:HA	2.03	0.40
16:S:2:LYS:NZ	25:A:156:G:OP1	2.40	0.40
3:E:124:LYS:HG2	3:E:129:SER:HA	2.04	0.40
13:N:33:GLN:HB3	13:N:154:LEU:HD12	2.03	0.40
17:R:42:ARG:NH1	25:A:1741:U:OP1	2.48	0.40
25:A:186:C:H2'	25:A:187:G:C8	2.56	0.40
12:O:62:LEU:HD13	12:O:91:VAL:HG11	2.03	0.40
25:A:121:OMU:H1'	25:A:121:OMU:HM23	1.82	0.40
25:A:1703:OMC:HM23	25:A:1703:OMC:H1'	1.81	0.40
3:E:64:SER:OG	25:A:615:C:OP2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:32:ASP:OD1	12:O:32:ASP:N	2.54	0.40
12:O:202:GLN:HG2	25:A:1113:A:H4'	2.04	0.40
17:R:25:ARG:HA	25:A:448:A:H5''	2.02	0.40
25:A:952:G:H2'	25:A:953:C:C6	2.57	0.40
25:A:1808:U:H2'	25:A:1809:A:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	254/263 (97%)	251 (99%)	3 (1%)	0	100	100
2	B	138/157 (88%)	136 (99%)	2 (1%)	0	100	100
3	E	138/143 (96%)	133 (96%)	5 (4%)	0	100	100
4	D	175/194 (90%)	173 (99%)	2 (1%)	0	100	100
5	G	171/194 (88%)	165 (96%)	6 (4%)	0	100	100
6	F	43/59 (73%)	43 (100%)	0	0	100	100
7	H	79/84 (94%)	77 (98%)	2 (2%)	0	100	100
8	K	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
9	J	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
10	M	52/135 (38%)	51 (98%)	1 (2%)	0	100	100
11	L	218/293 (74%)	211 (97%)	7 (3%)	0	100	100
12	O	209/264 (79%)	200 (96%)	9 (4%)	0	100	100
13	N	205/295 (70%)	195 (95%)	10 (5%)	0	100	100
14	Q	97/115 (84%)	93 (96%)	4 (4%)	0	100	100
15	P	129/151 (85%)	125 (97%)	4 (3%)	0	100	100
16	S	228/249 (92%)	222 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	194/208 (93%)	186 (96%)	8 (4%)	0	100	100
18	T	123/133 (92%)	122 (99%)	1 (1%)	0	100	100
19	q	86/144 (60%)	75 (87%)	11 (13%)	0	100	100
20	p	83/113 (74%)	80 (96%)	3 (4%)	0	100	100
21	I	148/151 (98%)	135 (91%)	13 (9%)	0	100	100
22	z	154/258 (60%)	139 (90%)	15 (10%)	0	100	100
23	y	158/913 (17%)	152 (96%)	6 (4%)	0	100	100
24	9	22/25 (88%)	22 (100%)	0	0	100	100
All	All	3310/4754 (70%)	3186 (96%)	124 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	220/225 (98%)	215 (98%)	5 (2%)	50	77
2	B	129/141 (92%)	126 (98%)	3 (2%)	50	77
3	E	112/115 (97%)	110 (98%)	2 (2%)	59	82
4	D	158/168 (94%)	157 (99%)	1 (1%)	86	94
5	G	159/174 (91%)	150 (94%)	9 (6%)	20	52
6	F	38/48 (79%)	37 (97%)	1 (3%)	46	74
7	H	73/76 (96%)	72 (99%)	1 (1%)	67	86
8	K	65/67 (97%)	62 (95%)	3 (5%)	27	59
9	J	112/113 (99%)	110 (98%)	2 (2%)	59	82
10	M	51/122 (42%)	48 (94%)	3 (6%)	19	50
11	L	186/225 (83%)	172 (92%)	14 (8%)	13	42
12	O	192/231 (83%)	186 (97%)	6 (3%)	40	70
13	N	173/243 (71%)	168 (97%)	5 (3%)	42	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	Q	86/98 (88%)	83 (96%)	3 (4%)	36	68
15	P	102/119 (86%)	97 (95%)	5 (5%)	25	57
16	S	200/218 (92%)	194 (97%)	6 (3%)	41	71
17	R	172/180 (96%)	168 (98%)	4 (2%)	50	77
18	T	107/115 (93%)	103 (96%)	4 (4%)	34	66
19	q	75/123 (61%)	66 (88%)	9 (12%)	5	20
20	p	74/96 (77%)	69 (93%)	5 (7%)	16	45
21	I	130/131 (99%)	123 (95%)	7 (5%)	22	53
23	y	91/811 (11%)	86 (94%)	5 (6%)	21	53
24	9	23/24 (96%)	23 (100%)	0	100	100
All	All	2728/3863 (71%)	2625 (96%)	103 (4%)	36	66

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	12	VAL
1	C	54	TYR
1	C	69	PHE
1	C	139	LEU
1	C	171	ASP
2	B	33	LEU
2	B	69	ARG
2	B	114	SER
3	E	61	GLN
3	E	105	PHE
4	D	3	VAL
5	G	10	LYS
5	G	30	LEU
5	G	33	ASN
5	G	57	ARG
5	G	72	PHE
5	G	105	THR
5	G	160	LYS
5	G	171	GLU
5	G	188	GLU
6	F	29	THR
7	H	75	GLU
8	K	50	PHE

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Mol	Chain	Res	Type
8	K	52	THR
8	K	81	LYS
9	J	30	CYS
9	J	80	ASP
10	M	80	ARG
10	M	99	ASP
10	M	102	THR
11	L	57	ASP
11	L	77	SER
11	L	167	ARG
11	L	180	VAL
11	L	182	CYS
11	L	192	LEU
11	L	200	ARG
11	L	225	SER
11	L	236	PHE
11	L	248	TYR
11	L	250	TYR
11	L	259	THR
11	L	262	THR
11	L	264	SER
12	O	44	ILE
12	O	48	LEU
12	O	55	THR
12	O	73	ASP
12	O	98	THR
12	O	213	ARG
13	N	15	VAL
13	N	58	LEU
13	N	73	ASP
13	N	80	ARG
13	N	188	THR
14	Q	29	CYS
14	Q	60	ASP
14	Q	67	LEU
15	P	46	ASP
15	P	65	ASP
15	P	69	SER
15	P	81	VAL
15	P	130	GLU
16	S	15	LEU
16	S	43	GLU

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Mol	Chain	Res	Type
16	S	53	SER
16	S	98	ARG
16	S	120	ASP
16	S	221	LYS
17	R	72	CYS
17	R	135	GLU
17	R	155	ASN
17	R	182	CYS
18	T	23	MET
18	T	80	ASP
18	T	100	LYS
18	T	113	ARG
19	q	28	PHE
19	q	39	ILE
19	q	51	CYS
19	q	53	ASP
19	q	55	VAL
19	q	68	LYS
19	q	73	THR
19	q	86	ASP
19	q	99	GLU
20	p	32	HIS
20	p	41	ARG
20	p	85	LEU
20	p	102	LEU
20	p	108	LEU
21	I	13	GLN
21	I	24	THR
21	I	29	THR
21	I	30	SER
21	I	35	GLU
21	I	87	ASP
21	I	93	LYS
23	y	77	THR
23	y	102	VAL
23	y	116	TYR
23	y	140	THR
23	y	152	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	50	ASN
2	B	5	GLN
2	B	112	HIS
2	B	121	GLN
3	E	20	GLN
3	E	46	HIS
3	E	77	ASN
3	E	110	HIS
4	D	134	HIS
4	D	140	GLN
5	G	114	GLN
6	F	15	GLN
7	H	26	GLN
9	J	56	HIS
10	M	93	GLN
10	M	116	ASN
10	M	118	GLN
11	L	178	HIS
11	L	235	ASN
12	O	40	ASN
12	O	186	ASN
12	O	232	HIS
13	N	29	ASN
13	N	110	ASN
14	Q	17	HIS
16	S	110	ASN
16	S	197	GLN
17	R	165	GLN
17	R	168	GLN
19	q	87	ASN
20	p	32	HIS
20	p	76	HIS
20	p	89	GLN
21	I	90	HIS
23	y	118	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	A	1207/1869 (64%)	301 (24%)	13 (1%)
26	7	27/28 (96%)	20 (74%)	0
All	All	1234/1897 (65%)	321 (26%)	13 (1%)

All (321) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	A	2	A
25	A	4	C
25	A	17	C
25	A	23	G
25	A	33	G
25	A	41	G
25	A	42	A
25	A	44	U
25	A	46	A
25	A	56	G
25	A	58	C
25	A	59	U
25	A	62	G
25	A	64	A
25	A	65	C
25	A	67	C
25	A	68	A
25	A	72	C
25	A	73	C
25	A	74	G
25	A	78	C
25	A	82	G
25	A	103	A
25	A	110	U
25	A	114	G
25	A	115	U
25	A	126	G
25	A	129	C
25	A	130	G
25	A	140	U
25	A	142	C
25	A	143	U
25	A	147	A
25	A	155	G
25	A	158	A
25	A	160	U
25	A	163	U
25	A	168	C
25	A	173	A
25	A	180	G
25	A	182	C
25	A	184	G

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Mol	Chain	Res	Type
25	A	190	G
25	A	198	U
25	A	200	G
25	A	202	G
25	A	203	G
25	A	204	G
25	A	206	G
25	A	208	G
25	A	288	G
25	A	291	G
25	A	292	A
25	A	294	U
25	A	295	C
25	A	306	C
25	A	307	G
25	A	308	G
25	A	309	G
25	A	314	U
25	A	318	A
25	A	319	C
25	A	320	G
25	A	321	C
25	A	323	C
25	A	324	C
25	A	325	C
25	A	326	C
25	A	327	G
25	A	328	U
25	A	329	G
25	A	332	G
25	A	347	G
25	A	362	C
25	A	363	A
25	A	364	A
25	A	368	U
25	A	369	C
25	A	370	G
25	A	382	C
25	A	385	G
25	A	386	C
25	A	409	C
25	A	418	A

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Mol	Chain	Res	Type
25	A	421	G
25	A	447	A
25	A	448	A
25	A	449	A
25	A	450	C
25	A	452	G
25	A	465	A
25	A	471	G
25	A	472	C
25	A	473	A
25	A	474	G
25	A	476	A
25	A	482	G
25	A	487	U
25	A	492	C
25	A	508	A
25	A	512	A
25	A	516	A
25	A	525	A
25	A	533	A
25	A	534	G
25	A	536	A
25	A	537	C
25	A	538	U
25	A	539	C
25	A	540	U
25	A	541	U
25	A	542	U
25	A	543	C
25	A	544	G
25	A	545	A
25	A	546	G
25	A	547	G
25	A	550	C
25	A	553	U
25	A	554	A
25	A	556	U
25	A	557	U
25	A	558	G
25	A	559	G
25	A	563	G
25	A	564	A

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Mol	Chain	Res	Type
25	A	566	U
25	A	568	C
25	A	576	A
25	A	583	A
25	A	589	G
25	A	590	A
25	A	591	U
25	A	598	G
25	A	604	A
25	A	606	G
25	A	607	U
25	A	608	C
25	A	614	C
25	A	624	C
25	A	626	G
25	A	627	U
25	A	628	A
25	A	629	A
25	A	631	U
25	A	643	A
25	A	655	A
25	A	659	G
25	A	660	C
25	A	662	G
25	A	664	A
25	A	668	A2M
25	A	669	A
25	A	671	A
25	A	672	A
25	A	673	G
25	A	688	U
25	A	689	U
25	A	691	G
25	A	693	A
25	A	694	G
25	A	734	C
25	A	736	C
25	A	748	C
25	A	749	U
25	A	751	G
25	A	752	G
25	A	753	C

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Mol	Chain	Res	Type
25	A	790	C
25	A	791	C
25	A	797	C
25	A	798	G
25	A	799	U
25	A	801	U
25	A	810	A
25	A	811	A
25	A	821	G
25	A	827	A
25	A	830	A
25	A	836	G
25	A	837	A
25	A	838	G
25	A	839	C
25	A	840	C
25	A	841	G
25	A	845	G
25	A	869	A
25	A	870	A
25	A	872	A
25	A	873	G
25	A	878	G
25	A	880	G
25	A	886	A
25	A	888	U
25	A	889	U
25	A	890	U
25	A	891	G
25	A	892	U
25	A	894	G
25	A	895	G
25	A	896	U
25	A	897	U
25	A	898	U
25	A	899	U
25	A	900	C
25	A	903	A
25	A	904	A
25	A	909	G
25	A	913	A
25	A	920	A

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Mol	Chain	Res	Type
25	A	922	A
25	A	930	C
25	A	933	G
25	A	943	U
25	A	950	C
25	A	963	A
25	A	965	U
25	A	969	U
25	A	970	G
25	A	972	A
25	A	990	A
25	A	992	A
25	A	999	G
25	A	1002	U
25	A	1017	U
25	A	1023	A
25	A	1045	U
25	A	1061	U
25	A	1062	A
25	A	1083	A
25	A	1085	C
25	A	1109	C
25	A	1112	U
25	A	1113	A
25	A	1114	U
25	A	1115	U
25	A	1116	C
25	A	1117	C
25	A	1120	U
25	A	1138	C
25	A	1153	C
25	A	1154	U
25	A	1170	A
25	A	1195	A
25	A	1701	C
25	A	1711	U
25	A	1712	A
25	A	1715	A
25	A	1719	A
25	A	1721	U
25	A	1722	G
25	A	1733	U

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Mol	Chain	Res	Type
25	A	1744	G
25	A	1749	G
25	A	1750	C
25	A	1752	C
25	A	1753	C
25	A	1754	G
25	A	1755	C
25	A	1756	C
25	A	1757	G
25	A	1758	G
25	A	1759	G
25	A	1760	G
25	A	1772	C
25	A	1773	C
25	A	1774	C
25	A	1775	U
25	A	1776	G
25	A	1777	G
25	A	1778	C
25	A	1779	G
25	A	1780	G
25	A	1781	A
25	A	1782	G
25	A	1783	C
25	A	1784	G
25	A	1800	A
25	A	1804	U
25	A	1805	G
25	A	1808	U
25	A	1809	A
25	A	1813	A
25	A	1822	A
25	A	1823	A
25	A	1824	A
25	A	1825	A
25	A	1829	G
25	A	1831	A
25	A	1834	A
25	A	1835	A
25	A	1837	G
25	A	1838	U
25	A	1839	U

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Mol	Chain	Res	Type
25	A	1841	C
25	A	1849	G
25	A	1853	C
25	A	1861	G
25	A	1862	G
25	A	1863	A
25	A	1865	C
26	7	4	A
26	7	5	A
26	7	7	A
26	7	9	A
26	7	10	A
26	7	11	A
26	7	12	A
26	7	13	A
26	7	14	A
26	7	15	A
26	7	16	A
26	7	17	A
26	7	18	A
26	7	20	A
26	7	21	A
26	7	22	A
26	7	24	A
26	7	25	A
26	7	26	A
26	7	27	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	1	U
25	A	291	G
25	A	368	U
25	A	370	G
25	A	688	U
25	A	797	C
25	A	798	G
25	A	1753	C
25	A	1757	G
25	A	1759	G
25	A	1775	U

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Mol	Chain	Res	Type
25	A	1781	A
25	A	1834	A

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
25	OMU	A	121	25	19,22,23	0.37	0	26,31,34	0.47	0
25	6MZ	A	1832	25,27	18,25,26	0.77	0	16,36,39	0.85	2 (12%)
25	MA6	A	1851	25	19,26,27	0.77	0	18,38,41	0.54	0
25	OMC	A	174	25,27	19,22,23	0.37	0	26,31,34	0.43	0
25	OMG	A	644	25	18,26,27	1.03	2 (11%)	19,38,41	0.78	1 (5%)
25	A2M	A	166	25	18,25,26	0.60	0	18,36,39	0.99	1 (5%)
25	UR3	A	1830	25	19,22,23	0.38	0	26,32,35	1.03	2 (7%)
25	A2M	A	668	25,27	18,25,26	0.62	0	18,36,39	0.84	1 (5%)
25	5MU	A	814	25	19,22,23	0.39	0	28,32,35	0.56	0
25	OMG	A	509	25,27	18,26,27	1.03	2 (11%)	19,38,41	0.80	1 (5%)
25	PSU	A	822	25	18,21,22	1.00	1 (5%)	22,30,33	0.80	1 (4%)
25	PSU	A	612	25	18,21,22	1.04	2 (11%)	22,30,33	0.80	1 (4%)
25	A2M	A	484	25	18,25,26	0.59	0	18,36,39	0.78	1 (5%)
25	A2M	A	1031	25	18,25,26	0.60	0	18,36,39	0.86	1 (5%)
25	PSU	A	823	25	18,21,22	1.01	1 (5%)	22,30,33	0.68	0
25	OMU	A	116	25	19,22,23	0.33	0	26,31,34	0.48	0
25	A2M	A	27	25,27	18,25,26	0.59	0	18,36,39	0.79	1 (5%)
25	OMC	A	517	25	19,22,23	0.42	0	26,31,34	0.39	0
25	OMC	A	1703	25	19,22,23	0.37	0	26,31,34	0.38	0
25	OMG	A	683	25	18,26,27	1.05	2 (11%)	19,38,41	0.90	1 (5%)
25	MA6	A	1850	25	19,26,27	0.86	1 (5%)	18,38,41	0.55	0
25	A2M	A	159	25	18,25,26	0.58	0	18,36,39	0.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PSU	A	1081	25	18,21,22	1.02	2 (11%)	22,30,33	0.79	0
25	PSU	A	119	25	18,21,22	0.94	1 (5%)	22,30,33	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	OMU	A	121	25	-	0/9/27/28	0/2/2/2
25	6MZ	A	1832	25,27	-	2/5/27/28	0/3/3/3
25	MA6	A	1851	25	-	5/7/29/30	0/3/3/3
25	OMC	A	174	25,27	-	0/9/27/28	0/2/2/2
25	OMG	A	644	25	-	1/5/27/28	0/3/3/3
25	A2M	A	166	25	-	0/5/27/28	0/3/3/3
25	UR3	A	1830	25	-	2/7/25/26	0/2/2/2
25	A2M	A	668	25,27	-	2/5/27/28	0/3/3/3
25	5MU	A	814	25	-	0/7/25/26	0/2/2/2
25	OMG	A	509	25,27	-	0/5/27/28	0/3/3/3
25	PSU	A	822	25	-	0/7/25/26	0/2/2/2
25	PSU	A	612	25	-	0/7/25/26	0/2/2/2
25	A2M	A	484	25	-	0/5/27/28	0/3/3/3
25	A2M	A	1031	25	-	0/5/27/28	0/3/3/3
25	PSU	A	823	25	-	0/7/25/26	0/2/2/2
25	OMU	A	116	25	-	0/9/27/28	0/2/2/2
25	A2M	A	27	25,27	-	0/5/27/28	0/3/3/3
25	OMC	A	517	25	-	0/9/27/28	0/2/2/2
25	OMC	A	1703	25	-	0/9/27/28	0/2/2/2
25	OMG	A	683	25	-	0/5/27/28	0/3/3/3
25	MA6	A	1850	25	-	3/7/29/30	0/3/3/3
25	A2M	A	159	25	-	2/5/27/28	0/3/3/3
25	PSU	A	1081	25	-	1/7/25/26	0/2/2/2
25	PSU	A	119	25	-	0/7/25/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	823	PSU	C6-C5	3.48	1.39	1.35
25	A	1081	PSU	C6-C5	3.38	1.39	1.35
25	A	119	PSU	C6-C5	3.35	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	822	PSU	C6-C5	3.32	1.39	1.35
25	A	612	PSU	C6-C5	3.31	1.39	1.35
25	A	683	OMG	C5-C6	-2.71	1.41	1.47
25	A	509	OMG	C5-C6	-2.70	1.41	1.47
25	A	644	OMG	C5-C6	-2.67	1.42	1.47
25	A	612	PSU	O4'-C1'	-2.19	1.40	1.43
25	A	683	OMG	C8-N7	-2.15	1.31	1.35
25	A	644	OMG	C8-N7	-2.10	1.31	1.35
25	A	509	OMG	C8-N7	-2.06	1.31	1.35
25	A	1850	MA6	C8-N7	-2.03	1.31	1.34
25	A	1081	PSU	O4'-C1'	-2.02	1.41	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1830	UR3	C6-N1-C2	-2.42	119.62	121.79
25	A	612	PSU	O4'-C1'-C2'	2.35	108.46	105.14
25	A	668	A2M	C5-C6-N6	2.27	123.80	120.35
25	A	1830	UR3	C1'-N1-C2	2.26	120.81	116.99
25	A	822	PSU	O4'-C1'-C2'	2.24	108.30	105.14
25	A	1031	A2M	C5-C6-N6	2.24	123.75	120.35
25	A	1832	6MZ	C2-N1-C6	2.23	118.50	116.59
25	A	27	A2M	C5-C6-N6	2.22	123.73	120.35
25	A	159	A2M	C5-C6-N6	2.22	123.73	120.35
25	A	484	A2M	C5-C6-N6	2.20	123.69	120.35
25	A	166	A2M	C5-C6-N6	2.19	123.68	120.35
25	A	1832	6MZ	C9-N6-C6	2.03	124.62	122.87
25	A	644	OMG	O6-C6-C5	2.03	128.33	124.37
25	A	509	OMG	O6-C6-C5	2.01	128.30	124.37
25	A	683	OMG	O6-C6-C5	2.01	128.29	124.37

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1832	6MZ	N1-C6-N6-C9
25	A	1850	MA6	C5-C6-N6-C10
25	A	1851	MA6	O4'-C4'-C5'-O5'
25	A	1851	MA6	C5-C6-N6-C10
25	A	668	A2M	O4'-C4'-C5'-O5'
25	A	668	A2M	C3'-C4'-C5'-O5'
25	A	1851	MA6	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
25	A	1850	MA6	N1-C6-N6-C10
25	A	1851	MA6	N1-C6-N6-C10
25	A	159	A2M	C3'-C4'-C5'-O5'
25	A	1830	UR3	O4'-C1'-N1-C6
25	A	1830	UR3	O4'-C1'-N1-C2
25	A	159	A2M	O4'-C4'-C5'-O5'
25	A	1850	MA6	C5-C6-N6-C9
25	A	1851	MA6	C5-C6-N6-C9
25	A	1081	PSU	C4'-C5'-O5'-P
25	A	644	OMG	C4'-C5'-O5'-P
25	A	1832	6MZ	C5-C6-N6-C9

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	121	OMU	1	0
25	A	1832	6MZ	1	0
25	A	174	OMC	1	0
25	A	116	OMU	2	0
25	A	1703	OMC	1	0
25	A	683	OMG	1	0
25	A	1850	MA6	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 61 ligands modelled in this entry, 61 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

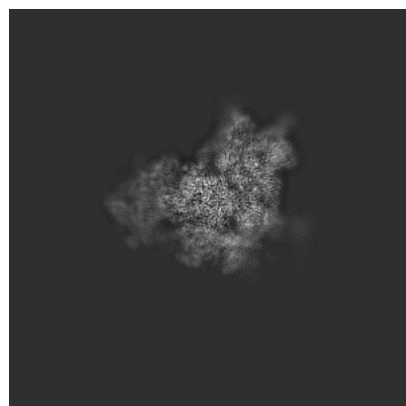
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10775. These allow visual inspection of the internal detail of the map and identification of artifacts.

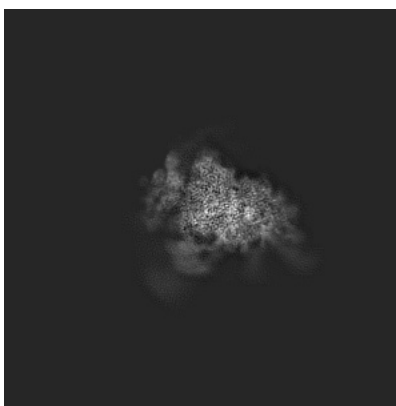
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

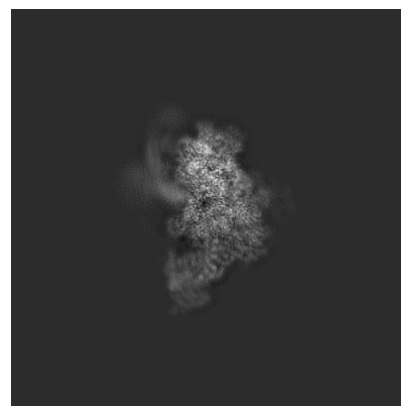
6.1.1 Primary map



X

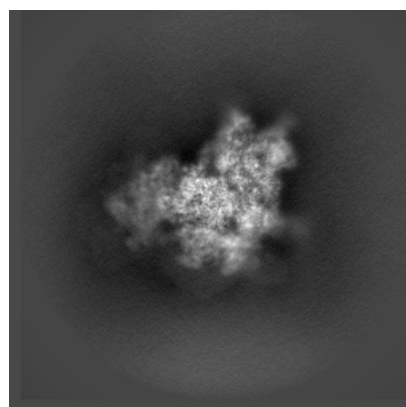


Y

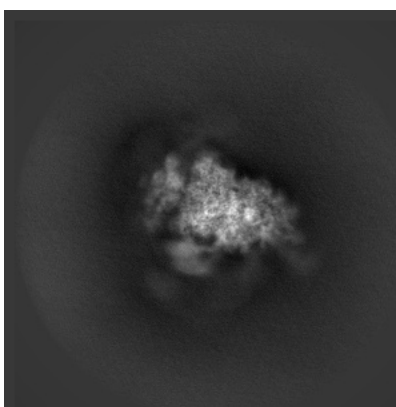


Z

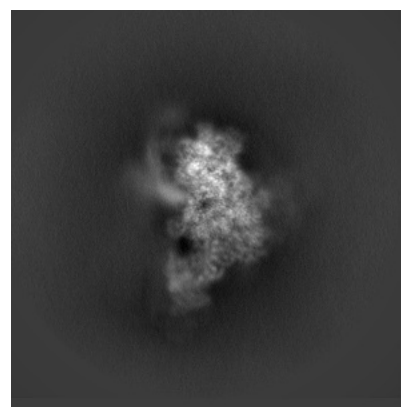
6.1.2 Raw map



X



Y

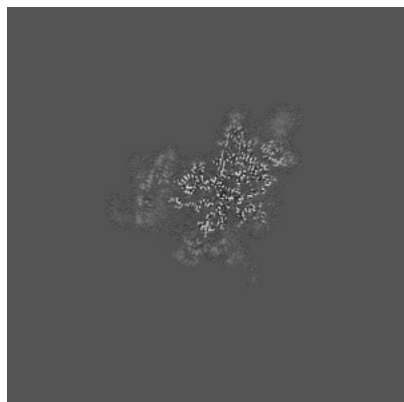


Z

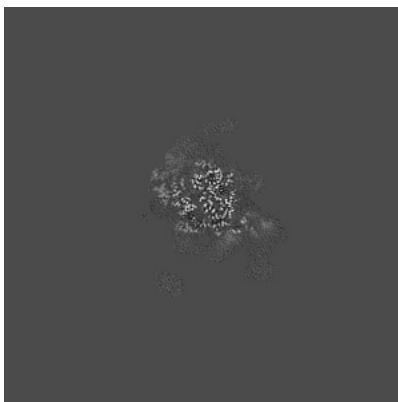
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

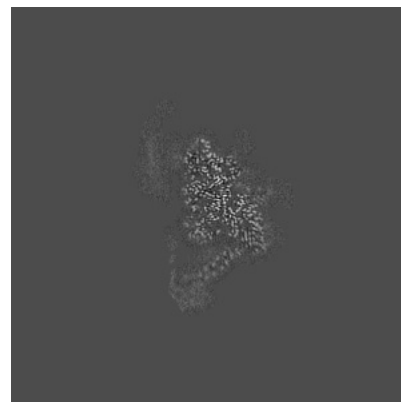
6.2.1 Primary map



X Index: 250

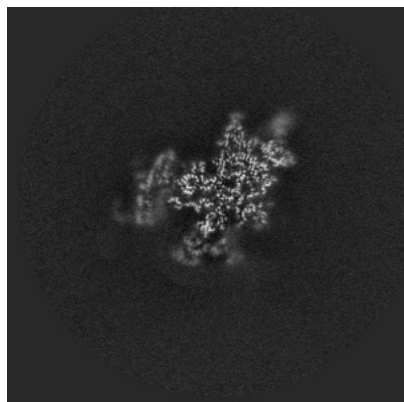


Y Index: 250

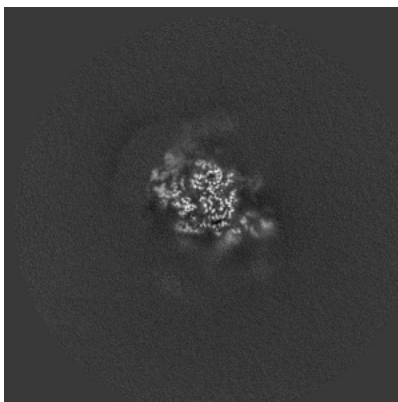


Z Index: 250

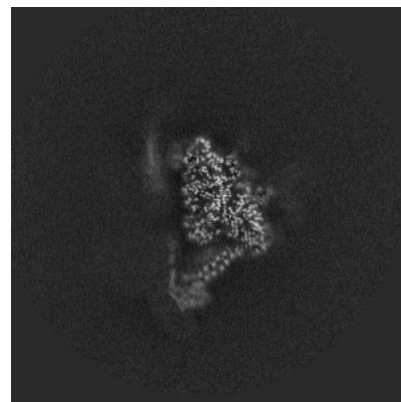
6.2.2 Raw map



X Index: 250



Y Index: 250

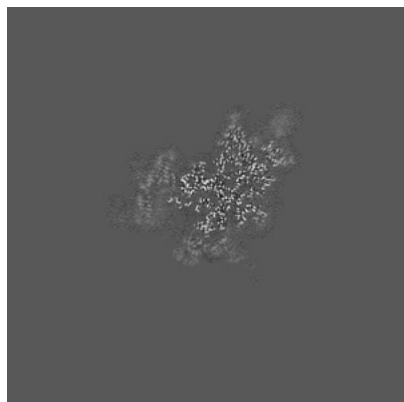


Z Index: 250

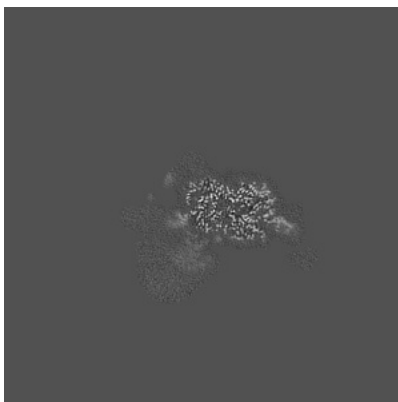
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

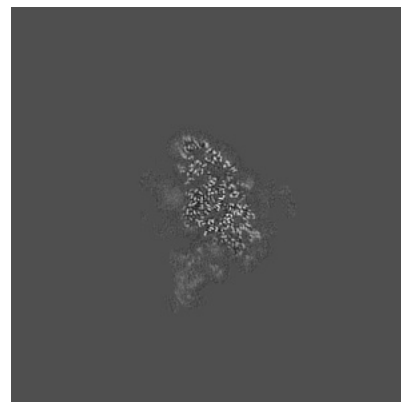
6.3.1 Primary map



X Index: 251

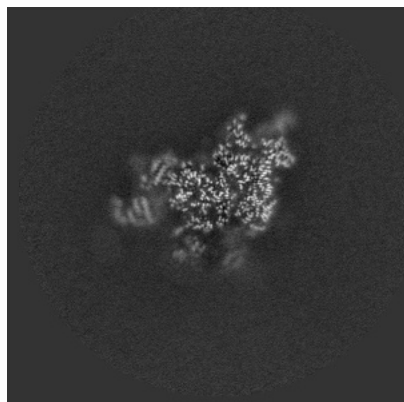


Y Index: 302

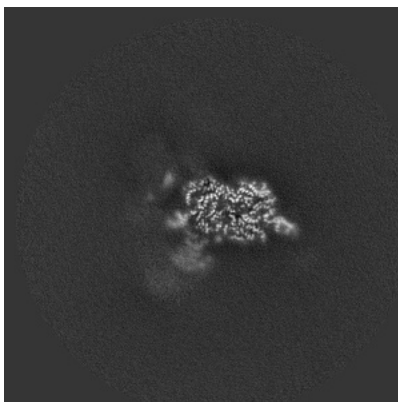


Z Index: 270

6.3.2 Raw map



X Index: 244



Y Index: 302

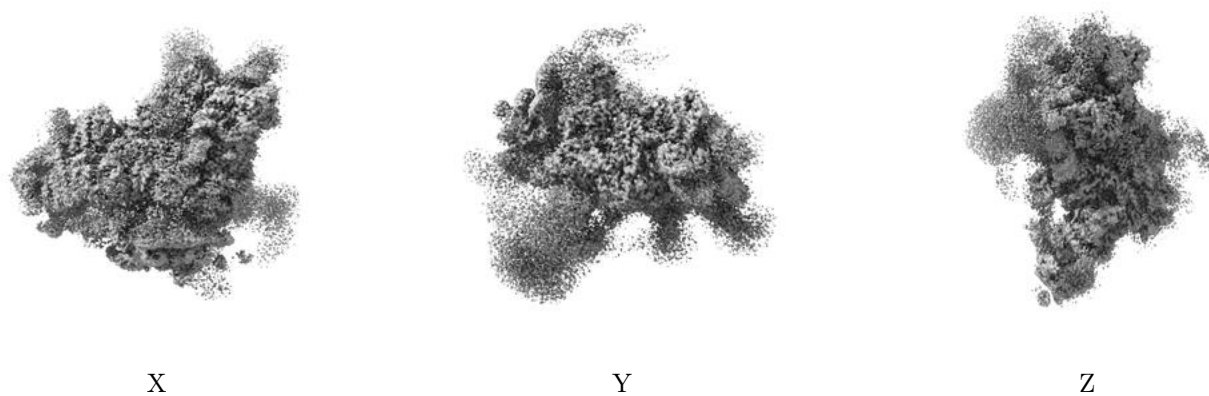


Z Index: 271

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

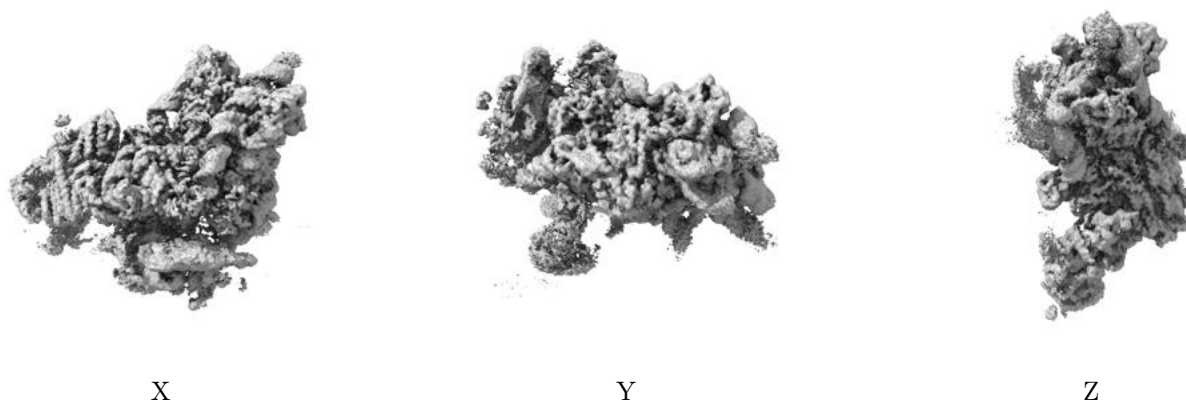
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

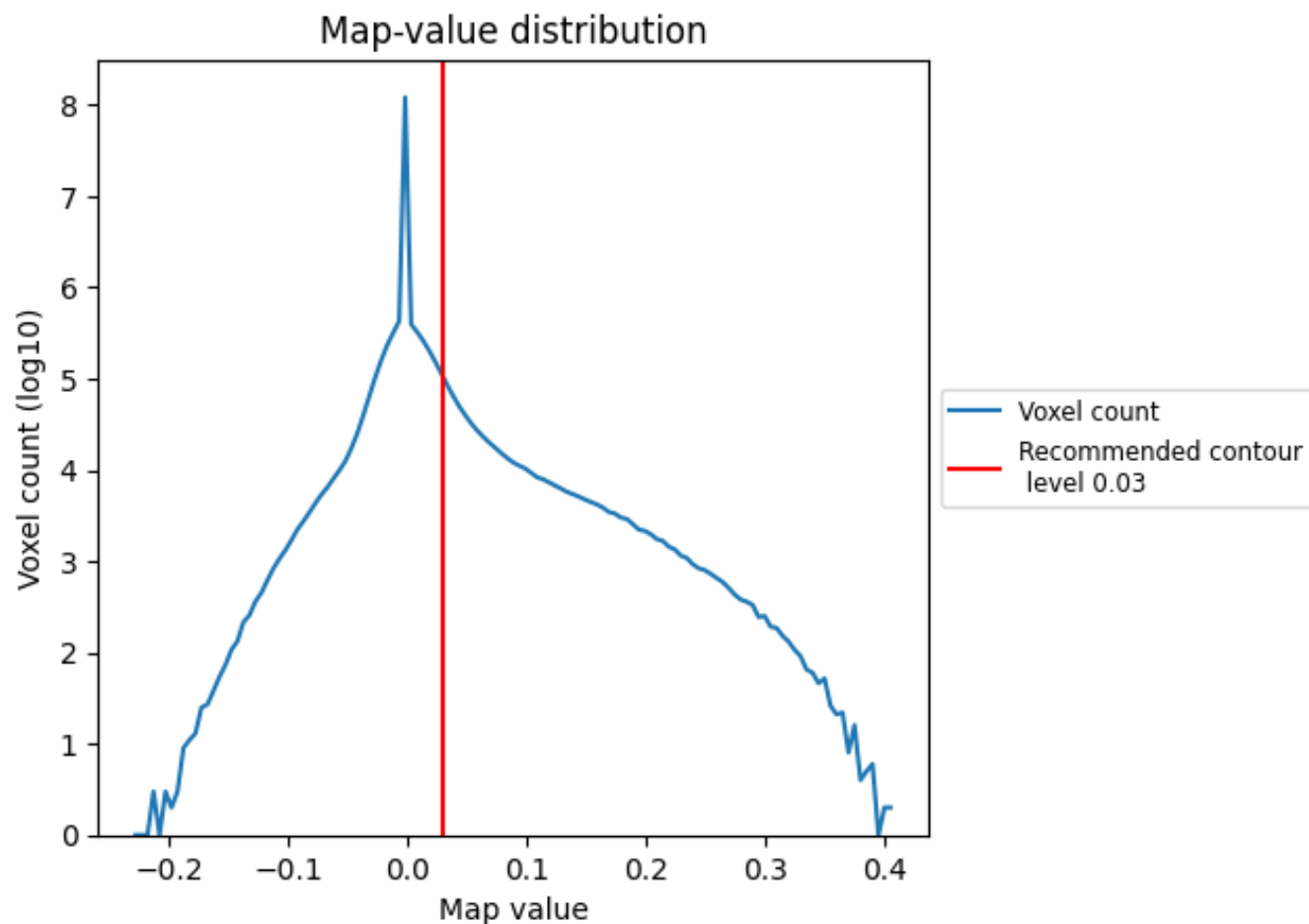
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

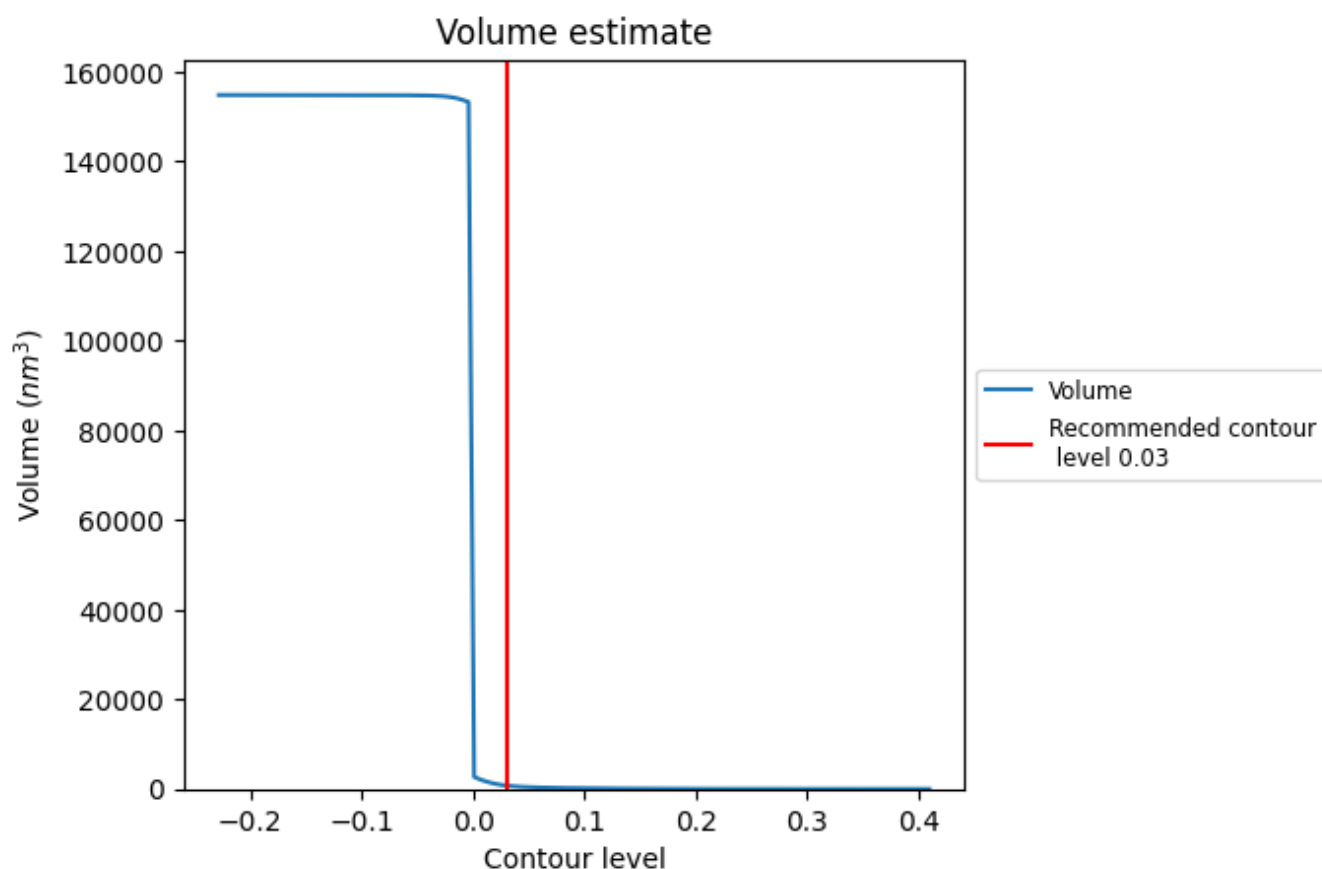
This section contains the results of statistical analysis of the map.

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.

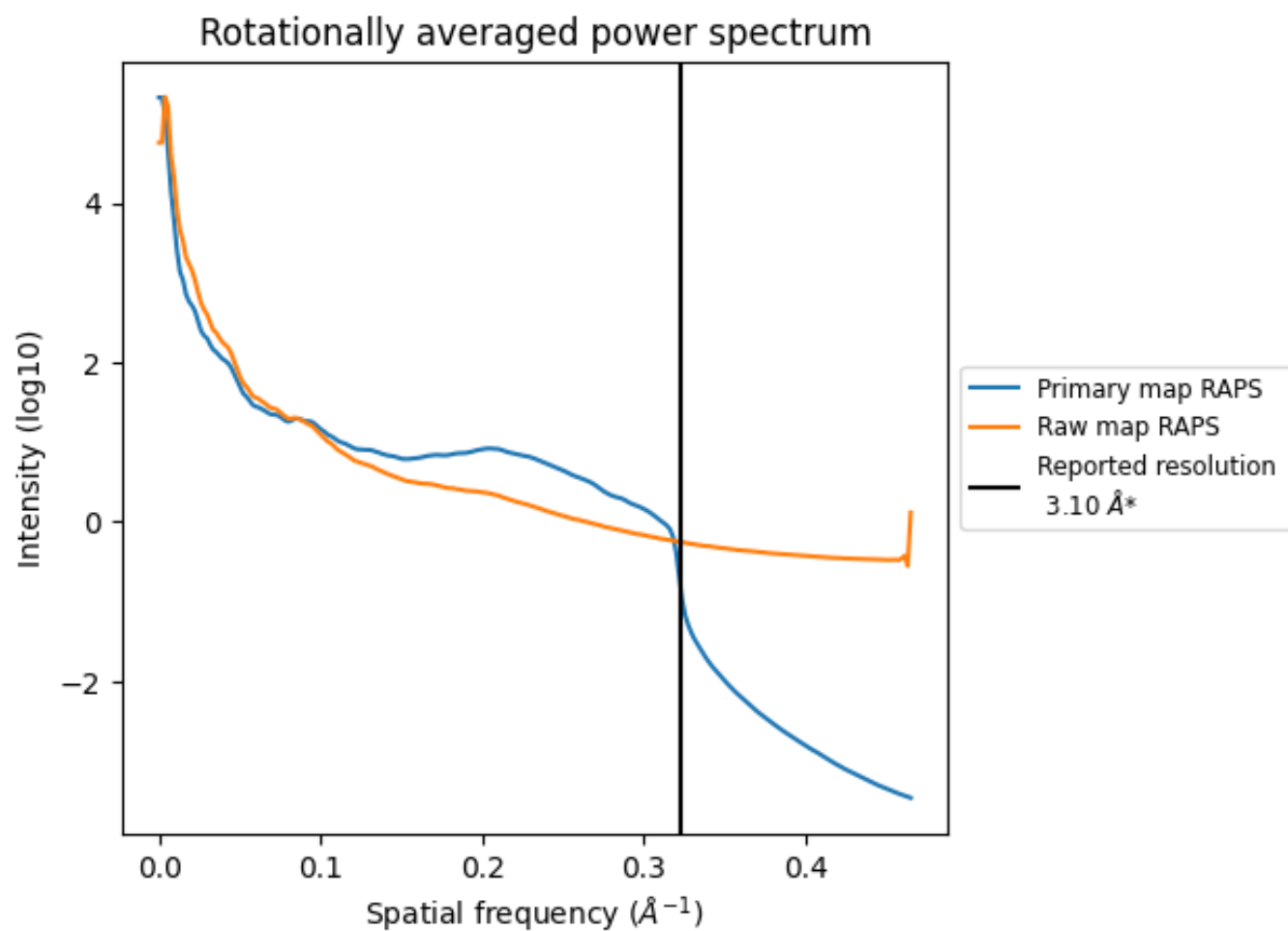
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 758 nm^3 ; this corresponds to an approximate mass of 685 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 ⓘ

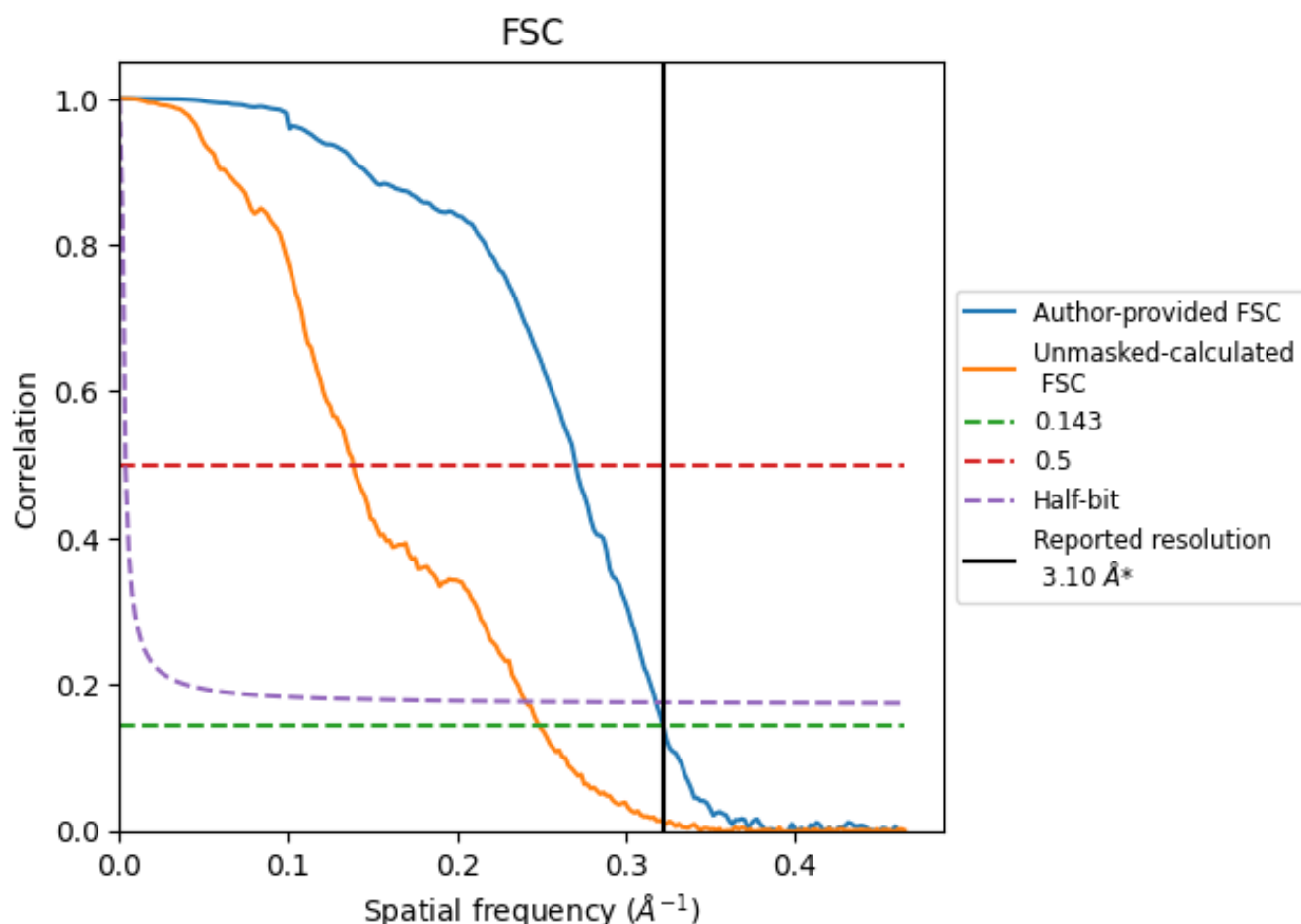


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

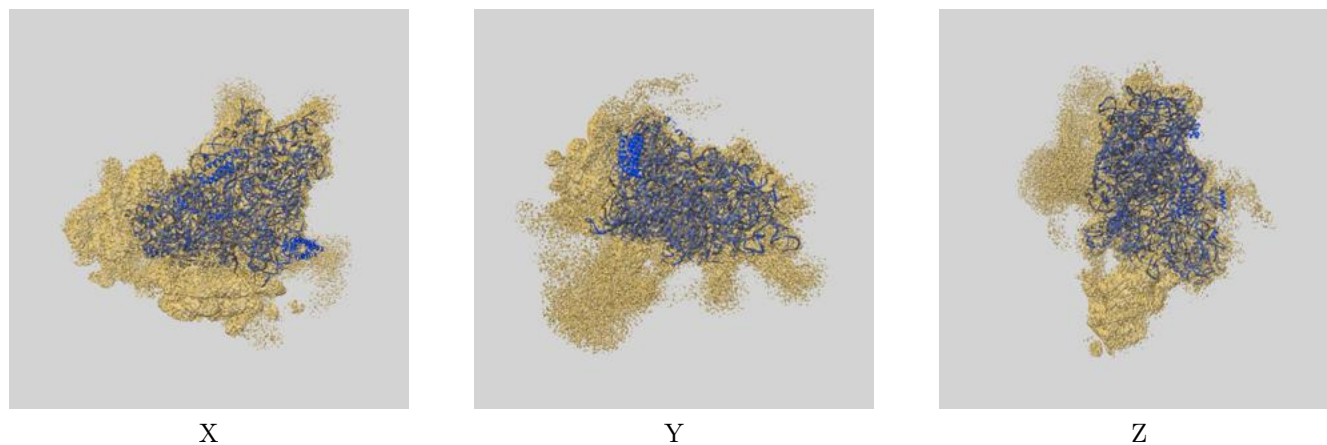
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.70	3.14
Unmasked-calculated*	4.02	7.22	4.15

*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 4.02 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

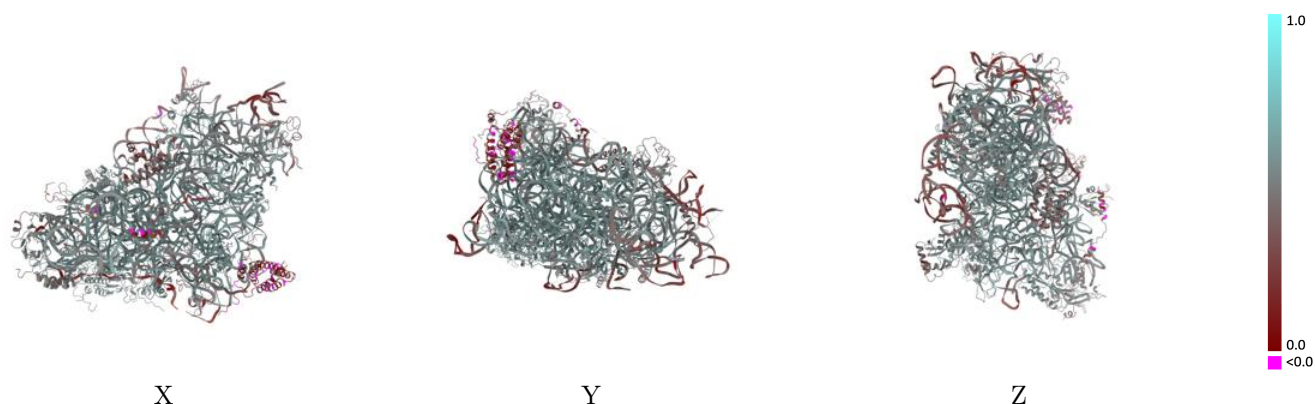
This section contains information regarding the fit between EMDB map EMD-10775 and PDB model 6YBW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



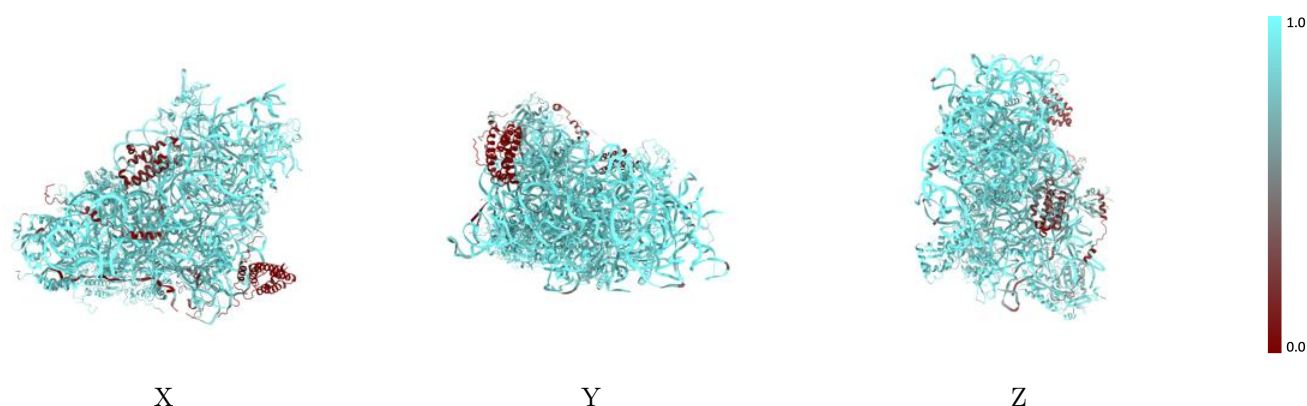
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



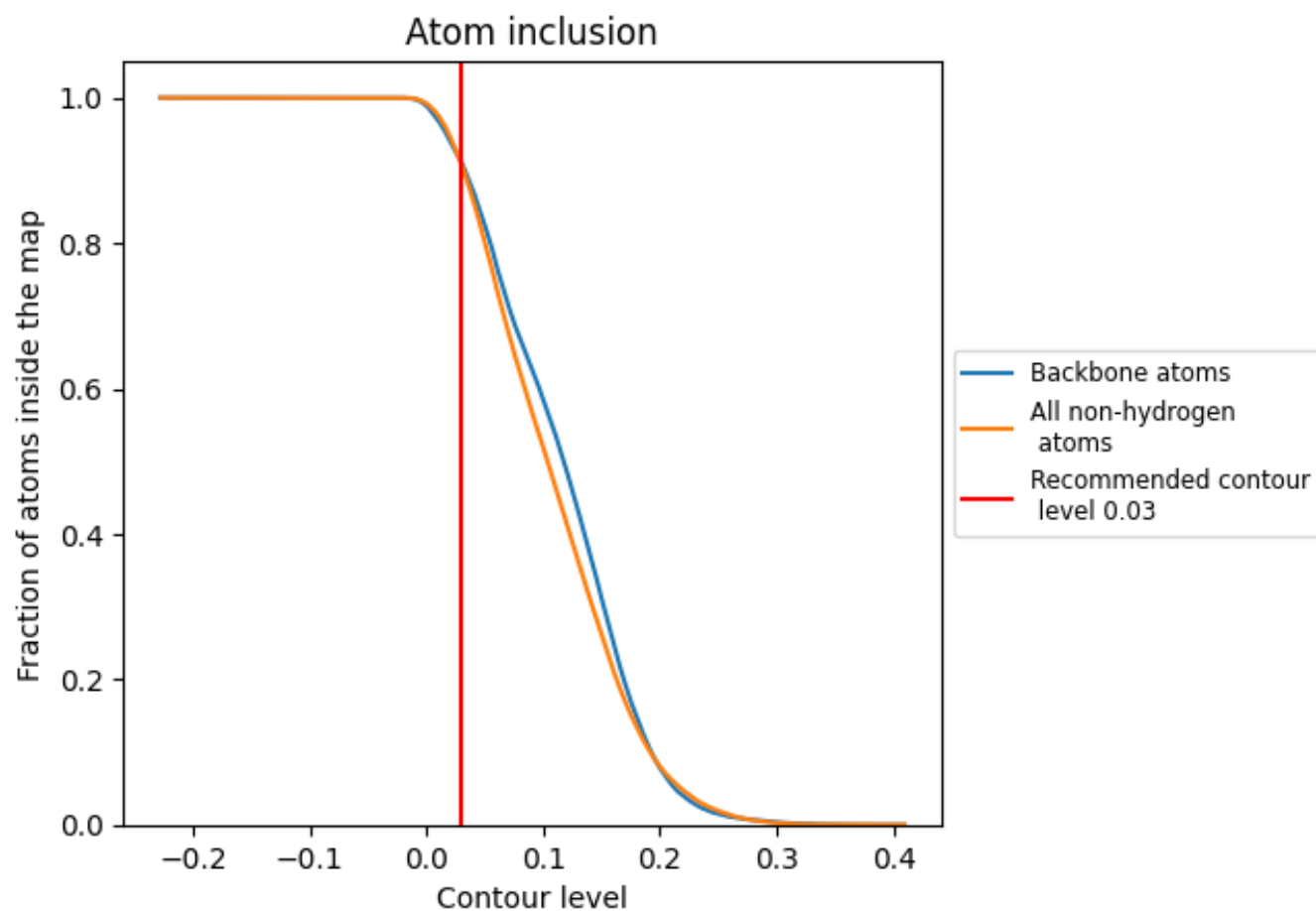
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9082	 0.5170
7	 0.1250	 0.2210
9	 0.7943	 0.5160
A	 0.9688	 0.5160
B	 0.9444	 0.5720
C	 0.9531	 0.5760
D	 0.9330	 0.5650
E	 0.9595	 0.5810
F	 0.9477	 0.5630
G	 0.9016	 0.5070
H	 0.9370	 0.5590
I	 0.9232	 0.5470
J	 0.9505	 0.5840
K	 0.9536	 0.5660
L	 0.9314	 0.5690
M	 0.8659	 0.5050
N	 0.9403	 0.5570
O	 0.9276	 0.5300
P	 0.9056	 0.5240
Q	 0.9331	 0.5590
R	 0.9420	 0.5270
S	 0.9328	 0.4950
T	 0.9503	 0.5460
p	 0.7618	 0.4760
q	 0.4590	 0.3740
y	 0.2243	 0.3430
z	 0.0189	 0.1780

