



Full wwPDB EM Validation Report ⓘ

Sep 21, 2025 – 10:34 AM EDT

PDB ID : 9ED0 / pdb_00009ed0
EMDB ID : EMD-47929
Title : Human LARP1 bound to the 40S small ribosomal subunit
Authors : Dong, W.; Kaufhold, R.; Brito Querido, J.
Deposited on : 2024-11-15
Resolution : 2.80 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.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

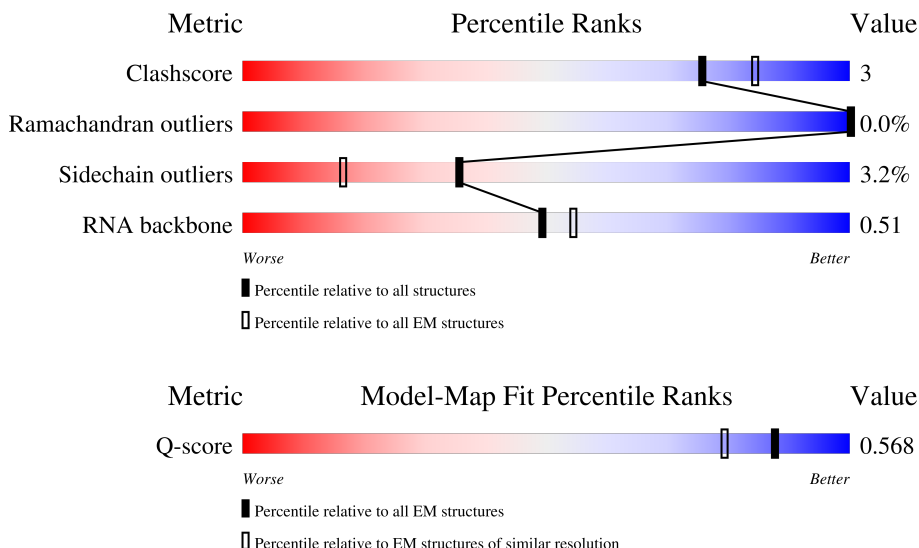
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	2	1869	
2	A	295	
3	B	264	

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Mol	Chain	Length	Quality of chain
4	C	293	
5	D	243	
6	E	263	
7	F	204	
8	G	249	
9	H	194	
10	I	208	
11	J	194	
12	K	165	
13	L	158	
14	M	132	
15	N	151	
16	O	151	
17	P	145	
18	Q	146	
19	R	135	
20	S	152	
21	T	145	
22	U	119	
23	V	83	
24	W	130	
25	X	143	
26	Y	133	
27	Z	125	
28	a	115	

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Mol	Chain	Length	Quality of chain
29	b	84	<div><div><div></div><div></div><div></div></div><div>21%77%18%...</div></div>
30	c	69	<div><div><div></div><div></div><div></div></div><div>29%65%14%.•14%</div></div>
31	d	56	<div><div><div></div><div></div><div></div></div><div>•88%11%.</div></div>
32	e	59	<div><div><div></div><div></div><div></div></div><div>15%78%15%7%</div></div>
33	f	156	<div><div><div></div><div></div><div></div></div><div>41%36%5%59%</div></div>
34	g	317	<div><div><div></div><div></div><div></div></div><div>79%76%21%..</div></div>
35	h	1096	<div><div><div></div><div></div><div></div></div><div>•96%</div></div>
36	n	25	<div><div><div></div><div></div><div></div></div><div>8%72%8%20%</div></div>

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 73475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1617	Total	C	N	O	P	6	0
			34700	15519	6236	11323	1622		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	206	Total	C	N	O	S	1	0
			1625	1040	287	290	8		

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	210	Total	C	N	O	S	0	0
			1711	1086	306	305	14		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	219	Total	C	N	O	S	1	0
			1708	1105	295	298	10		

- Molecule 5 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 6 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	257	Total	C	N	O	S	0	0
			2041	1305	379	349	8		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	182	Total	C	N	O	S	0	0
			1445	906	271	261	7		

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	227	Total	C	N	O	S	0	0
			1840	1149	367	317	7		

- Molecule 9 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	184	Total	C	N	O	S	0	0
			1477	942	271	263	1		

- Molecule 10 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 11 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 12 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 13 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	141	Total	C	N	O	S	0	0
			1157	737	217	197	6		

- Molecule 14 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	104	Total	C	N	O	S	0	0
			790	494	138	151	7		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	127	Total	C	N	O	S	0	0
			957	585	189	177	6		

- Molecule 17 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	123	Total	C	N	O	S	0	0
			998	635	188	169	6		

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	139	Total	C	N	O	S	0	0
			1105	704	207	191	3		

- Molecule 19 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 20 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	143	Total	C	N	O	S	1	0
			1192	751	240	200	1		

- Molecule 21 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 22 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 23 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 25 is a protein called 40S ribosomal protein S23.

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

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 27 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	72	Total	C	N	O	S	0	0
			570	366	104	99	1		

- Molecule 28 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 29 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 30 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	59	Total	C	N	O	S	0	0
			464	281	93	88	2		

- Molecule 31 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 32 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	55	Total	C	N	O	S	0	0
			438	271	95	71	1		

- Molecule 33 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	64	Total	C	N	O	S	0	0
			522	329	99	87	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	312	Total	C	N	O	S	0	0
			2408	1518	420	458	12		

- Molecule 35 is a protein called La-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	46	Total	C	N	O	S	0	0
			345	214	63	67	1		

- Molecule 36 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	20	Total	C	N	O	S	0	0
			193	119	51	20	3		

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

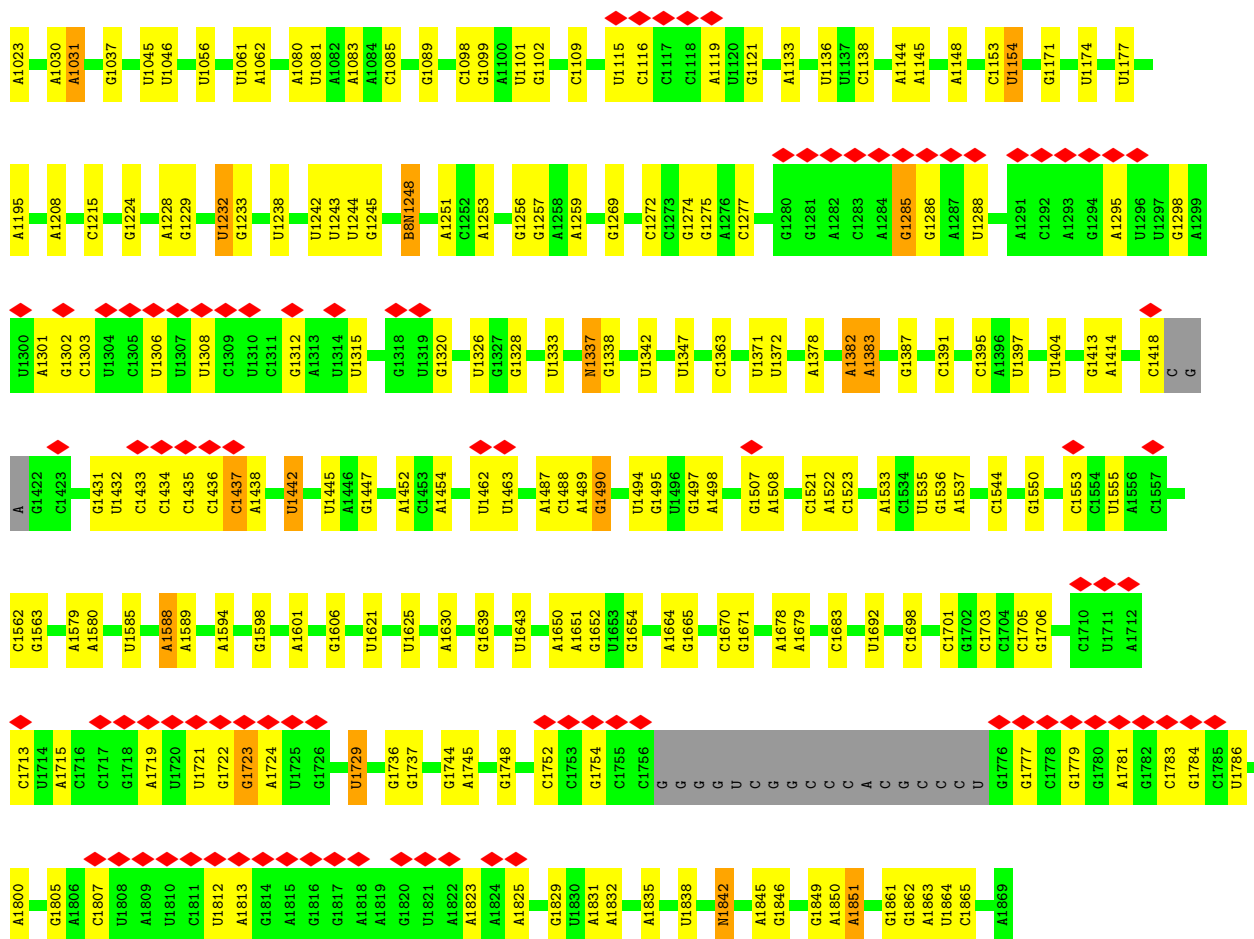
Mol	Chain	Residues	Atoms		AltConf
37	2	68	Total	K	0
			68	68	
37	S	1	Total	K	0
			1	1	
37	X	1	Total	K	0
			1	1	
37	d	1	Total	K	0
			1	1	

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

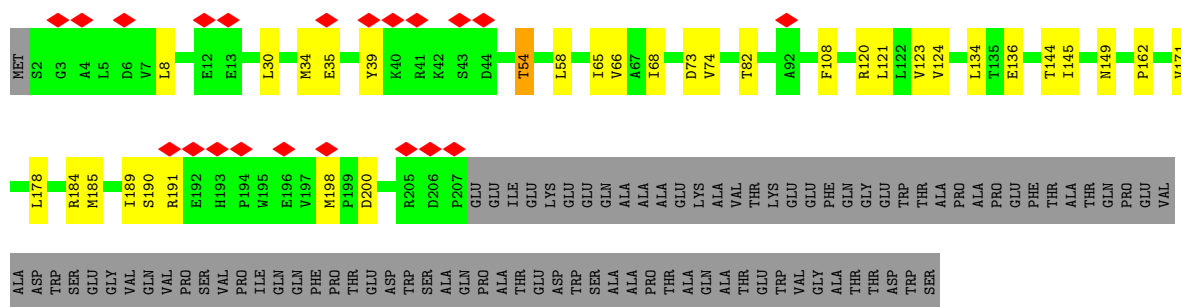
Mol	Chain	Residues	Atoms		AltConf
38	2	91	Total	Mg	0
			91	91	
38	G	1	Total	Mg	0
			1	1	

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

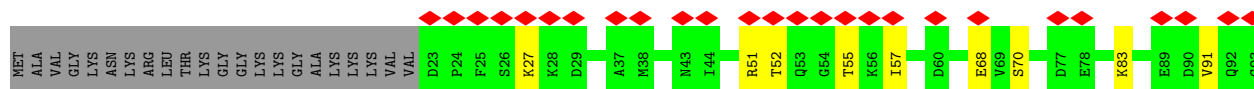
Mol	Chain	Residues	Atoms		AltConf
39	a	1	Total	Zn	0
			1	1	
39	d	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	



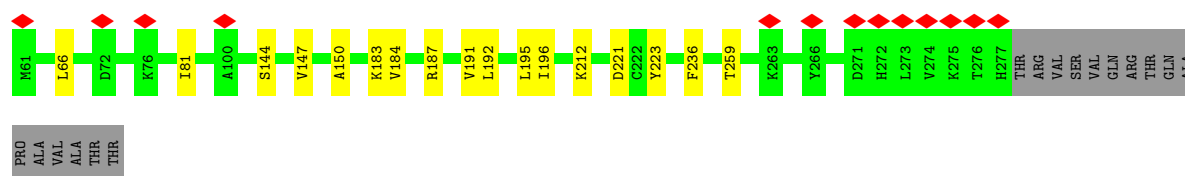
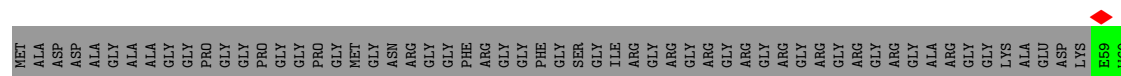
• Molecule 2: Small ribosomal subunit protein uS2



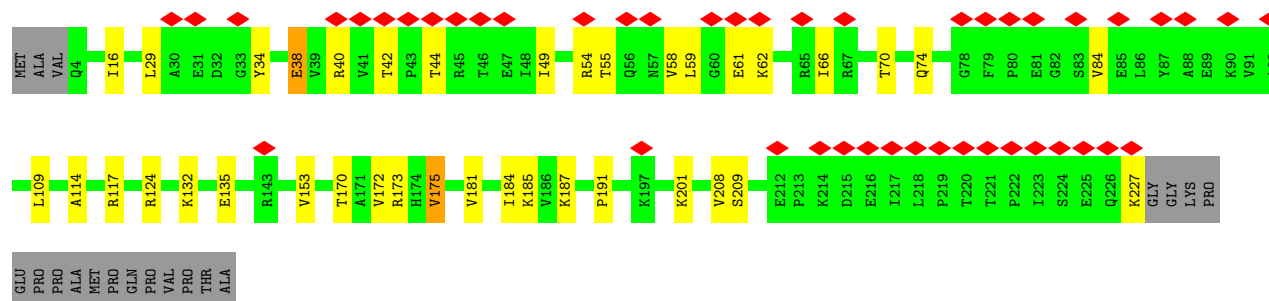
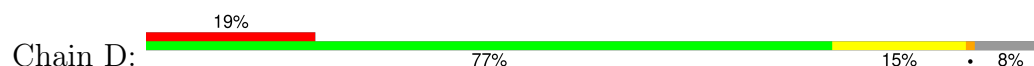
• Molecule 3: Small ribosomal subunit protein eS1



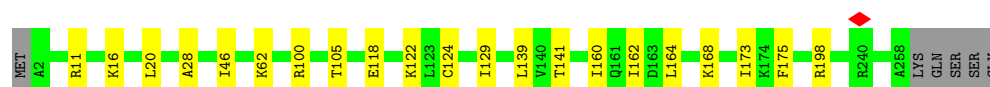
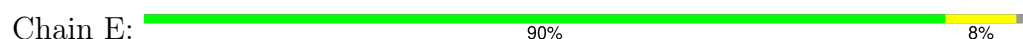
- Molecule 4: Small ribosomal subunit protein uS5



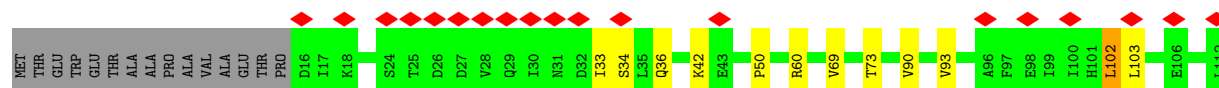
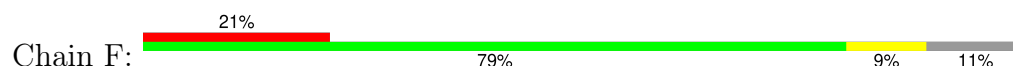
- Molecule 5: Small ribosomal subunit protein uS3

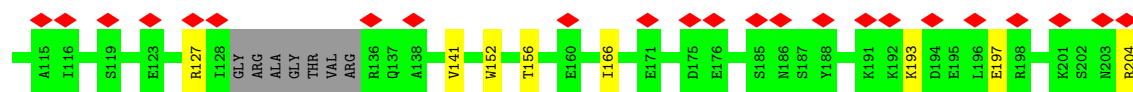


- Molecule 6: Small ribosomal subunit protein eS4, X isoform

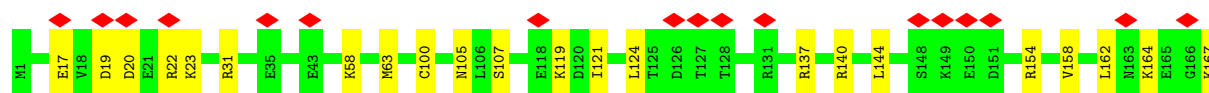
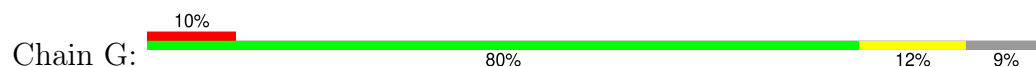


- Molecule 7: Small ribosomal subunit protein uS7

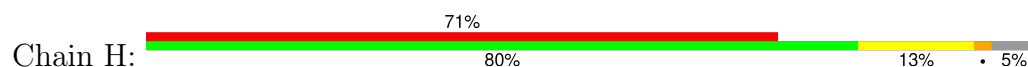




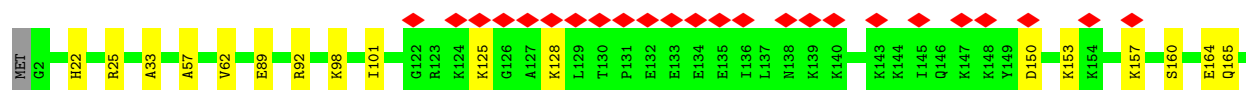
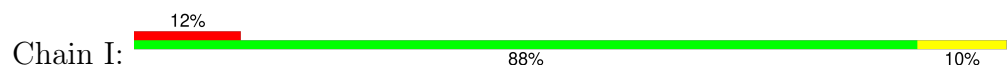
- Molecule 8: Small ribosomal subunit protein eS6



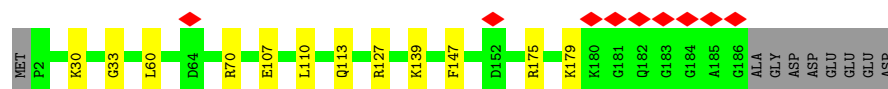
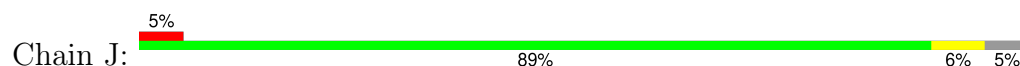
- Molecule 9: Small ribosomal subunit protein eS7



- Molecule 10: Small ribosomal subunit protein eS8



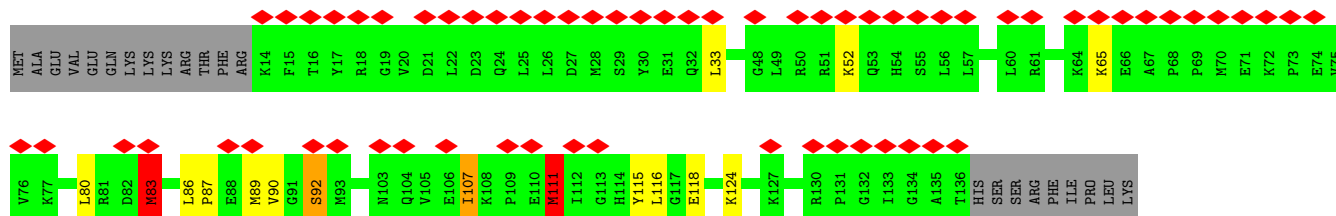
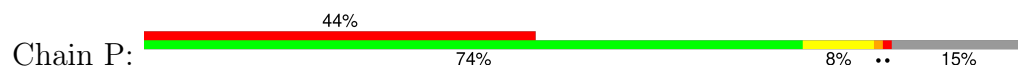
- Molecule 11: Small ribosomal subunit protein uS4



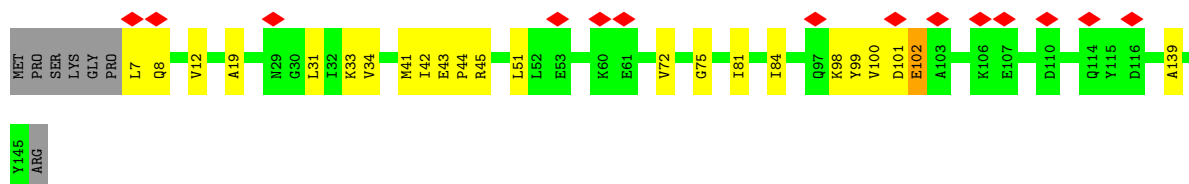
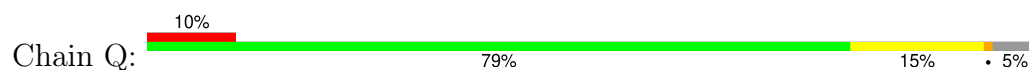
- Molecule 12: Small ribosomal subunit protein eS10



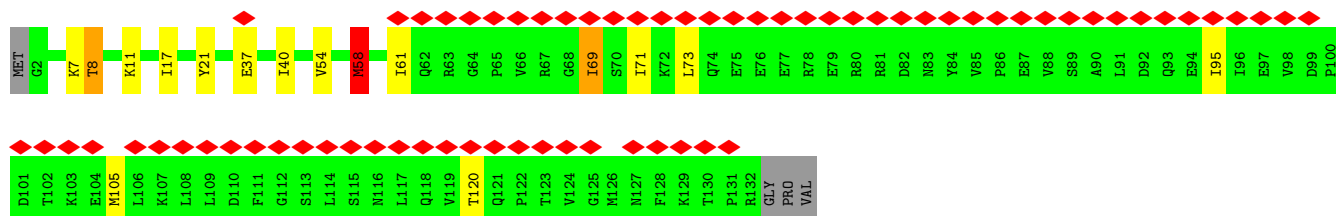
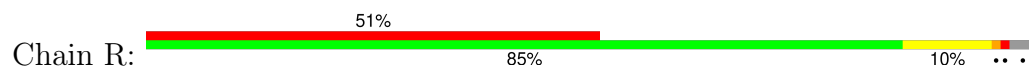
- Molecule 17: Small ribosomal subunit protein uS19



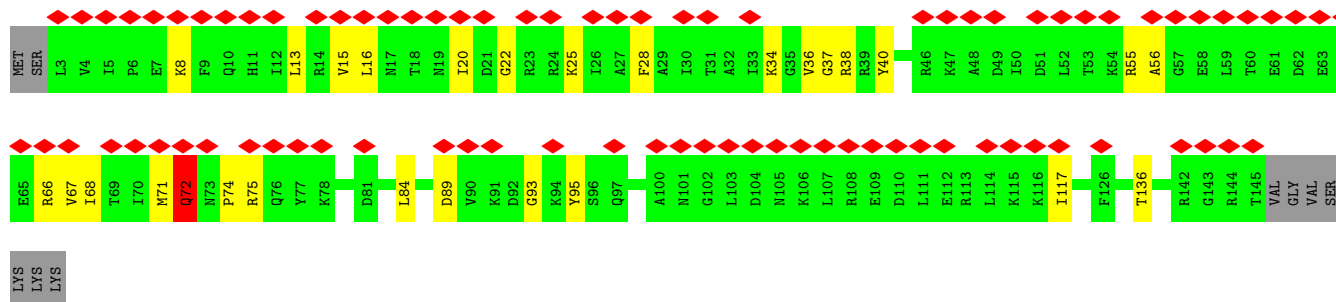
- Molecule 18: Small ribosomal subunit protein uS9



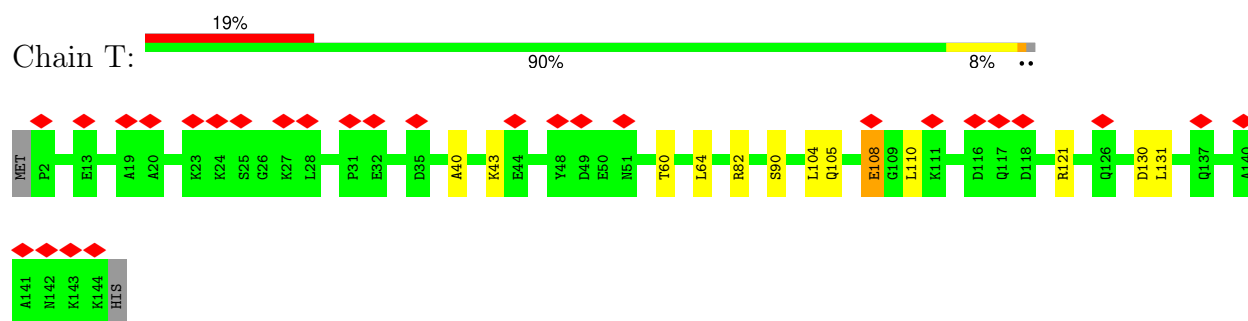
- Molecule 19: Small ribosomal subunit protein eS17



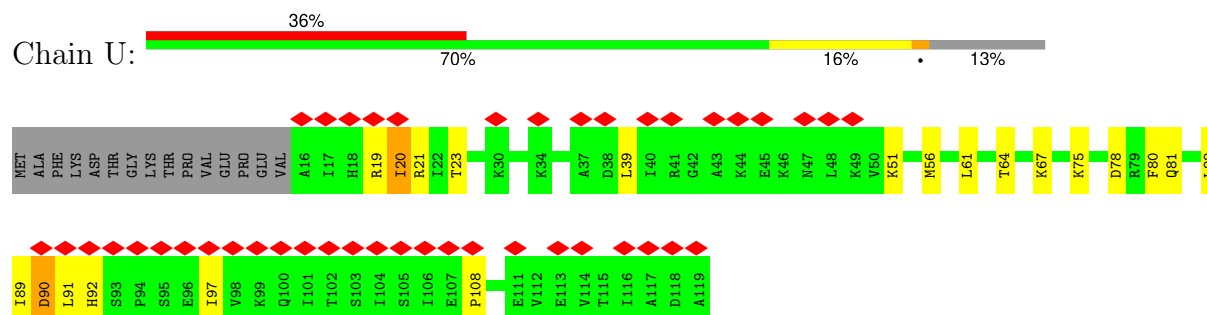
- Molecule 20: Small ribosomal subunit protein uS13



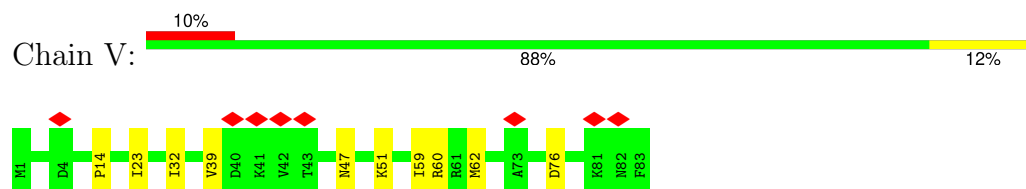
- Molecule 21: Small ribosomal subunit protein eS19



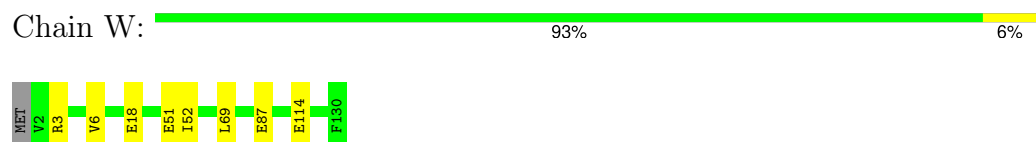
- Molecule 22: Small ribosomal subunit protein uS10



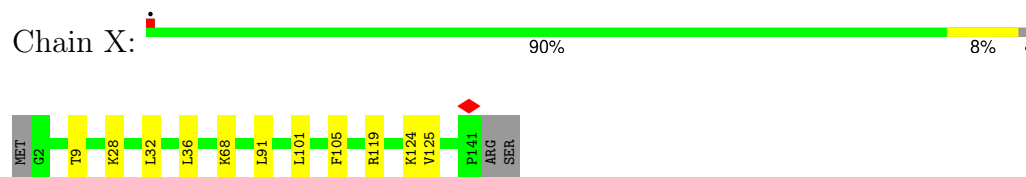
- Molecule 23: Small ribosomal subunit protein eS21



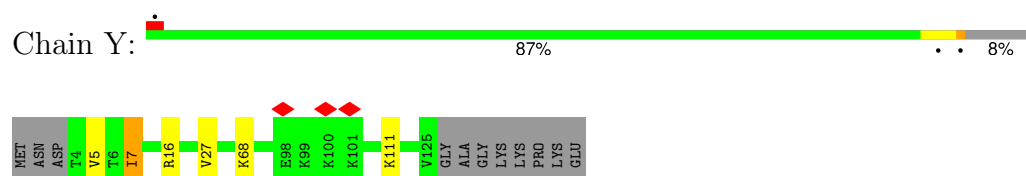
- Molecule 24: Small ribosomal subunit protein uS8

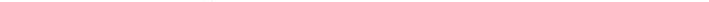


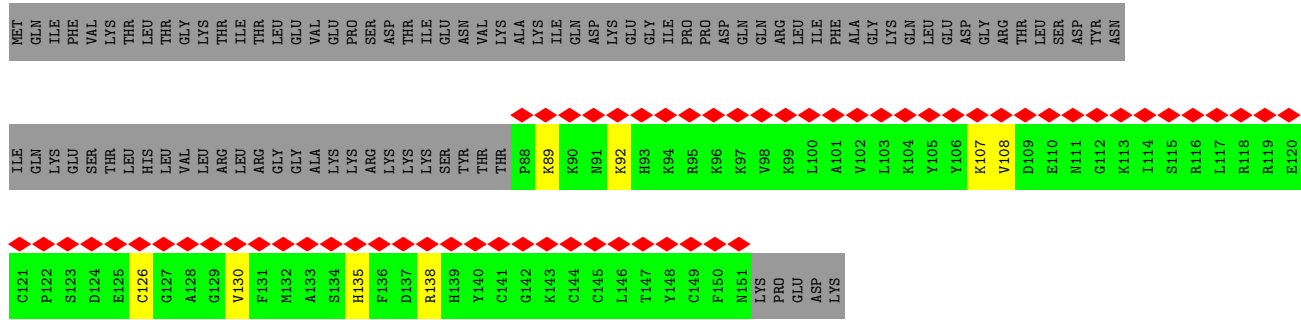
- Molecule 25: 40S ribosomal protein S23



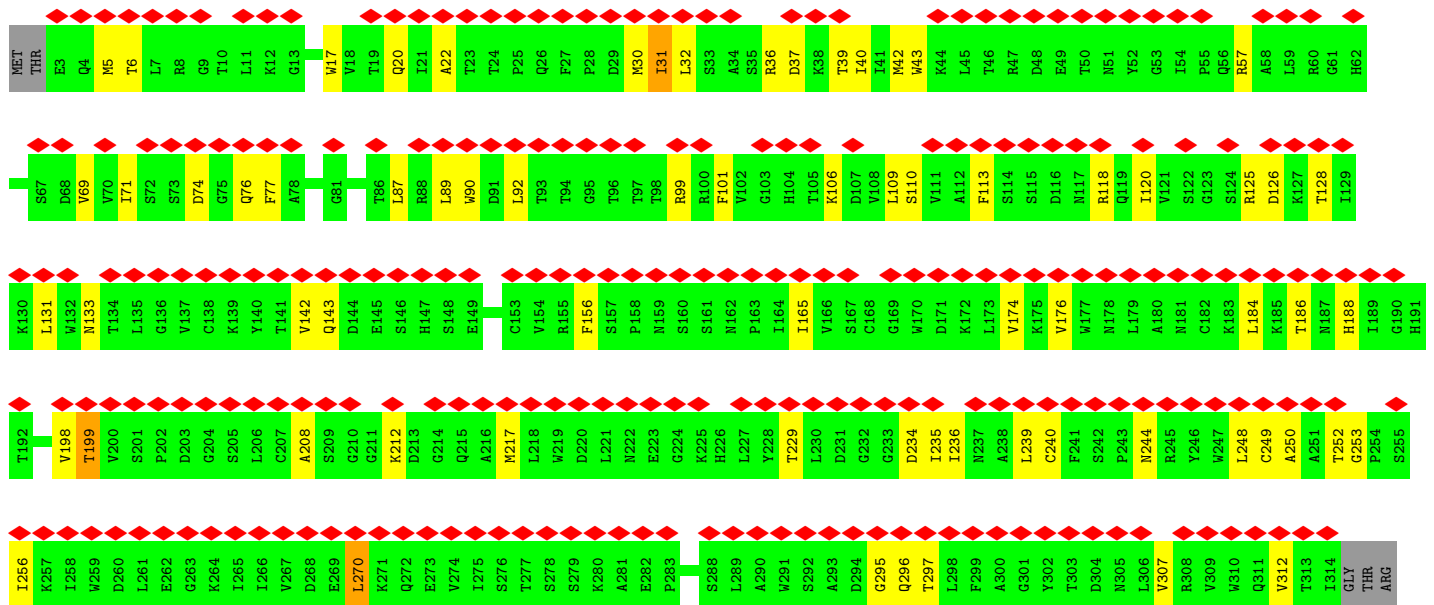
- Molecule 26: 40S ribosomal protein S24



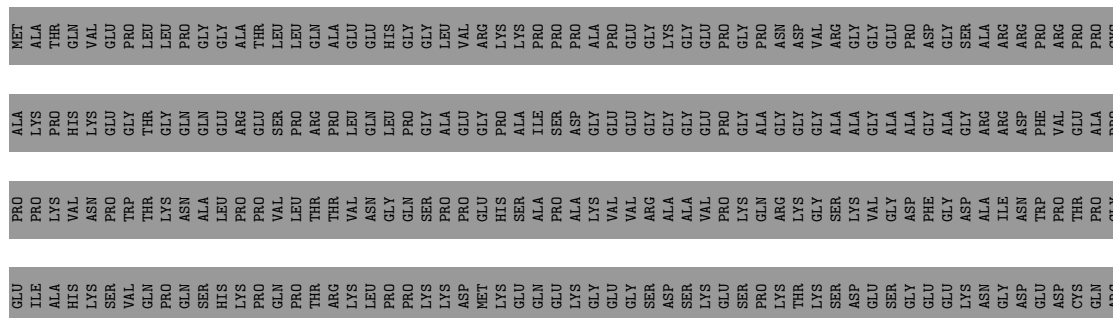
Chain f: 



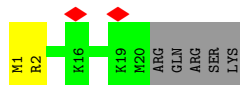
Chain g:  79% 76% 21%



Chain h: 96%



- Molecule 36: Small ribosomal subunit protein eS32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124913	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (\AA)	411.5, 411.5, 411.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.823, 0.823, 0.823	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, OMG, MG, MA6, ZN, OMU, PSU, B8N, 6MZ, OMC, 4AC, 7MG, A2M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.27	1/37048 (0.0%)	0.39	1/57731 (0.0%)
2	A	0.33	0/1665	0.56	0/2262
3	B	0.25	0/1738	0.50	1/2325 (0.0%)
4	C	0.28	0/1748	0.49	0/2361
5	D	0.25	0/1773	0.48	0/2387
6	E	0.28	0/2083	0.50	0/2805
7	F	0.37	1/1465 (0.1%)	0.58	0/1969
8	G	0.39	2/1863 (0.1%)	0.57	1/2481 (0.0%)
9	H	0.27	0/1498	0.63	0/2005
10	I	0.36	1/1711 (0.1%)	0.52	0/2282
11	J	0.29	0/1550	0.45	0/2069
12	K	0.60	0/840	0.71	0/1133
13	L	0.31	0/1177	0.47	0/1574
14	M	0.63	1/796 (0.1%)	0.66	0/1072
15	N	0.23	0/1232	0.45	0/1656
16	O	0.32	0/969	0.51	0/1298
17	P	0.39	2/1017 (0.2%)	0.61	1/1361 (0.1%)
18	Q	0.65	6/1122 (0.5%)	0.62	2/1503 (0.1%)
19	R	0.43	1/1078 (0.1%)	0.55	1/1447 (0.1%)
20	S	0.65	3/1214 (0.2%)	1.22	4/1626 (0.2%)
21	T	0.33	1/1131 (0.1%)	0.56	1/1515 (0.1%)
22	U	0.29	0/831	0.60	0/1115
23	V	0.46	1/643 (0.2%)	0.49	0/860
24	W	0.30	0/1051	0.51	0/1406
25	X	0.26	0/1105	0.52	0/1476
26	Y	0.26	0/1019	0.42	0/1354
27	Z	0.36	1/576 (0.2%)	0.54	0/774
28	a	0.32	0/805	0.53	1/1079 (0.1%)
29	b	0.45	2/653 (0.3%)	0.54	1/876 (0.1%)
30	c	0.85	3/465 (0.6%)	0.81	1/621 (0.2%)
31	d	0.27	0/470	0.48	0/623
32	e	0.19	0/443	0.46	0/582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.18	0/533	0.47	0/706
34	g	0.43	2/2465 (0.1%)	0.66	1/3359 (0.0%)
35	h	0.45	1/352 (0.3%)	0.70	0/475
36	n	0.30	0/194	0.57	0/246
All	All	0.33	29/76323 (0.0%)	0.49	16/110414 (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
9	H	0	1
20	S	0	1
All	All	0	2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S	72	GLN	CD-NE2	14.96	1.64	1.33
14	M	110	VAL	CB-CG1	-11.73	1.13	1.52
30	c	58	LEU	CG-CD2	-11.33	1.15	1.52
18	Q	102	GLU	CD-OE1	-10.08	1.06	1.25
23	V	47	ASN	CG-OD1	-8.91	1.06	1.23
20	S	72	GLN	CD-OE1	-8.91	1.06	1.23
18	Q	102	GLU	CA-C	-8.84	1.41	1.52
30	c	14	VAL	CB-CG1	-8.70	1.23	1.52
20	S	72	GLN	CA-CB	-8.66	1.40	1.53
7	F	36	GLN	CD-OE1	-8.58	1.07	1.23
8	G	17	GLU	CD-OE1	-7.69	1.10	1.25
29	b	57	VAL	CB-CG1	-7.39	1.28	1.52
34	g	76	GLN	CD-OE1	-7.38	1.09	1.23
18	Q	102	GLU	CG-CD	-6.96	1.34	1.52
18	Q	102	GLU	CA-CB	6.68	1.64	1.54
10	I	168	GLN	CD-OE1	-6.41	1.11	1.23
18	Q	102	GLU	CD-OE2	-6.28	1.13	1.25
19	R	58	MET	SD-CE	-6.12	1.64	1.79
8	G	19	ASP	CG-OD2	-5.89	1.14	1.25
17	P	83	MET	SD-CE	-5.86	1.65	1.79
34	g	253	GLY	CA-C	-5.85	1.43	1.51
30	c	44	ARG	CG-CD	-5.41	1.36	1.52
27	Z	62	VAL	C-N	5.37	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	T	130	ASP	CG-OD2	-5.35	1.15	1.25
17	P	111	MET	SD-CE	-5.24	1.66	1.79
18	Q	101	ASP	C-O	-5.11	1.18	1.23
35	h	666	THR	CB-CG2	-5.09	1.35	1.52
29	b	42	LYS	CD-CE	-5.08	1.37	1.52
1	2	484	A2M	O3'-P	5.05	1.61	1.56

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S	72	GLN	CA-CB-CG	32.95	179.99	114.10
20	S	72	GLN	OE1-CD-NE2	-25.78	96.82	122.60
20	S	72	GLN	N-CA-CB	-6.61	100.49	110.73
20	S	72	GLN	N-CA-C	6.40	121.14	112.88
30	c	44	ARG	CG-CD-NE	6.16	125.54	112.00
1	2	627	U	P-O3'-C3'	5.90	129.05	120.20
17	P	83	MET	CG-SD-CE	5.79	113.63	100.90
18	Q	102	GLU	OE1-CD-OE2	-5.72	109.16	122.90
8	G	17	GLU	CG-CD-OE1	-5.71	105.26	118.40
34	g	253	GLY	CA-C-O	-5.65	113.43	121.52
29	b	42	LYS	CD-CE-NZ	5.65	129.98	111.90
3	B	172	MET	CG-SD-CE	-5.57	88.64	100.90
21	T	108	GLU	CA-CB-CG	5.51	125.11	114.10
19	R	37	GLU	OE1-CD-OE2	-5.50	109.69	122.90
18	Q	102	GLU	N-CA-C	-5.44	106.64	113.72
28	a	98	PRO	O-C-N	5.12	123.56	121.15

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	H	15	LYS	Peptide
20	S	72	GLN	Sidechain

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	2	34700	0	17574	84	0
2	A	1625	0	1645	19	0
3	B	1711	0	1782	9	0
4	C	1708	0	1797	7	0
5	D	1745	0	1839	18	0
6	E	2041	0	2143	10	0
7	F	1445	0	1495	11	0
8	G	1840	0	1989	14	0
9	H	1477	0	1573	16	0
10	I	1682	0	1769	11	0
11	J	1525	0	1640	9	0
12	K	816	0	841	20	0
13	L	1157	0	1222	5	0
14	M	790	0	808	12	0
15	N	1208	0	1293	5	0
16	O	957	0	982	8	0
17	P	998	0	1041	11	0
18	Q	1105	0	1172	11	0
19	R	1064	0	1118	8	0
20	S	1192	0	1253	18	0
21	T	1112	0	1146	4	0
22	U	821	0	883	10	0
23	V	636	0	637	5	0
24	W	1034	0	1080	5	0
25	X	1087	0	1154	6	0
26	Y	1002	0	1075	2	0
27	Z	570	0	626	6	0
28	a	792	0	841	4	0
29	b	640	0	665	9	0
30	c	464	0	488	7	0
31	d	459	0	448	3	0
32	e	438	0	484	5	0
33	f	522	0	529	6	0
34	g	2408	0	2339	36	0
35	h	345	0	303	1	0
36	n	193	0	237	2	0
37	2	68	0	0	0	0
37	S	1	0	0	0	0
37	X	1	0	0	0	0
37	d	1	0	0	0	0
38	2	91	0	0	0	0
38	G	1	0	0	0	0
39	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	d	1	0	0	0	0
39	f	1	0	0	0	0
All	All	73475	0	57911	372	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 3.

All (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:67:VAL:O	20:S:71:MET:HB2	1.62	1.00
1:2:538:U:H3	1:2:549:C:H42	1.11	0.97
2:A:58:LEU:HD12	2:A:178:LEU:HD23	1.74	0.68
14:M:44:LYS:HG2	14:M:46:GLN:HG3	1.75	0.68
34:g:87:LEU:HB2	34:g:101:PHE:HB2	1.76	0.67
20:S:75:ARG:HE	20:S:95:TYR:HB2	1.60	0.66
19:R:21:TYR:HD1	19:R:73:LEU:HD13	1.61	0.66
34:g:212:LYS:HA	34:g:235:ILE:HG22	1.75	0.66
17:P:115:TYR:H	17:P:118:GLU:HG3	1.61	0.66
18:Q:102:GLU:OE2	34:g:57:ARG:HA	1.96	0.65
1:2:538:U:O2	1:2:549:C:N3	2.29	0.65
12:K:5:LYS:HE2	12:K:5:LYS:H	1.62	0.65
20:S:16:LEU:HD11	20:S:72:GLN:NE2	2.12	0.65
18:Q:51:LEU:HD21	18:Q:81:ILE:HG12	1.79	0.65
1:2:940:U:H3	1:2:1002:U:H3	1.43	0.64
34:g:106:LYS:HB2	34:g:126:ASP:HB3	1.80	0.64
12:K:55:ARG:HE	12:K:57:TYR:HE1	1.45	0.64
5:D:135:GLU:HG3	5:D:153:VAL:HG12	1.79	0.64
2:A:66:VAL:HG21	2:A:185:MET:HB2	1.81	0.63
1:2:1550:G:H3'	1:2:1579:A:H61	1.64	0.61
34:g:234:ASP:HB3	34:g:252:THR:HG23	1.81	0.61
22:U:80:PHE:HB3	31:d:52:PHE:HB3	1.83	0.61
16:O:30:VAL:HG12	16:O:94:HIS:HB2	1.83	0.61
34:g:128:THR:HA	34:g:142:VAL:O	2.01	0.61
4:C:183:LYS:HA	4:C:195:LEU:O	2.01	0.60
1:2:1729:U:H3	1:2:1805:G:H1	1.47	0.60
21:T:105:GLN:HA	21:T:108:GLU:OE1	2.02	0.59
5:D:124:ARG:HH21	35:h:685:TYR:HB3	1.66	0.59
30:c:14:VAL:HG11	30:c:51:ARG:O	2.03	0.59
34:g:198:VAL:HA	34:g:208:ALA:O	2.02	0.58
2:A:198:MET:HG2	2:A:200:ASP:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:41:MET:HA	18:Q:45:ARG:HH21	1.67	0.58
1:2:536:A:H61	1:2:546:G:H1	1.50	0.58
1:2:928:G:H1	1:2:1013:U:H3	1.51	0.58
1:2:77:A:H5'	8:G:154:ARG:HB3	1.85	0.58
11:J:127:ARG:HD3	32:e:31:ARG:HD3	1.85	0.58
24:W:51:GLU:HG2	29:b:8:LEU:HD11	1.85	0.58
24:W:3:ARG:HD3	24:W:6:VAL:HG12	1.86	0.57
34:g:128:THR:HG22	34:g:143:GLN:HB3	1.87	0.57
22:U:67:LYS:HG2	22:U:78:ASP:OD2	2.05	0.57
18:Q:31:LEU:HD11	18:Q:33:LYS:HE3	1.87	0.57
34:g:156:PHE:HA	34:g:165:ILE:HG22	1.86	0.57
3:B:27:LYS:HA	3:B:51:ARG:HE	1.69	0.57
1:2:1228:A:H2'	1:2:1229:G:C8	2.41	0.56
9:H:69:LEU:HD13	9:H:96:ALA:HB2	1.86	0.56
7:F:50:PRO:HG2	7:F:90:VAL:HG22	1.87	0.56
20:S:16:LEU:HD21	20:S:72:GLN:HE22	1.70	0.56
34:g:174:VAL:HB	34:g:188:HIS:HB2	1.87	0.56
1:2:433:A:H5''	10:I:22:HIS:HB3	1.87	0.56
1:2:1228:A:H2'	1:2:1229:G:H8	1.71	0.56
2:A:184:ARG:HD2	2:A:191:ARG:HG2	1.86	0.56
20:S:13:LEU:HB2	20:S:20:ILE:HB	1.87	0.56
13:L:75:GLY:HA3	13:L:88:ILE:HD12	1.87	0.56
8:G:181:THR:HG22	8:G:183:ARG:H	1.69	0.55
6:E:11:ARG:HA	6:E:28:ALA:HB2	1.87	0.55
17:P:52:LYS:HB3	17:P:80:LEU:HD11	1.89	0.55
25:X:68:LYS:HB3	25:X:91:LEU:HD22	1.89	0.55
3:B:146:ARG:HE	3:B:206:PRO:HG2	1.73	0.54
23:V:32:ILE:HG12	23:V:60:ARG:HD2	1.89	0.54
5:D:114:ALA:HB3	5:D:117:ARG:HG3	1.90	0.54
17:P:86:LEU:H	17:P:89:MET:HE2	1.72	0.54
2:A:68:ILE:HD11	2:A:74:VAL:HG23	1.88	0.54
7:F:204:ARG:HG2	30:c:63:ARG:HH22	1.71	0.54
7:F:73:THR:HG22	7:F:93:VAL:HG21	1.90	0.54
34:g:199:THR:HG21	34:g:240:CYS:HA	1.89	0.54
1:2:1017:U:H5'	15:N:55:ARG:HD3	1.90	0.53
22:U:21:ARG:HD2	22:U:88:LEU:HD22	1.91	0.53
1:2:874:G:H2'	1:2:875:A:H8	1.73	0.53
2:A:54:THR:HG22	2:A:162:PRO:HG2	1.90	0.53
5:D:16:ILE:HD11	31:d:36:LEU:HD23	1.89	0.53
15:N:100:LYS:HE2	15:N:104:ARG:HH22	1.72	0.53
29:b:34:ASP:O	29:b:79:PHE:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:851:C:H5''	1:2:852:G:H5'	1.91	0.53
3:B:52:THR:HG22	3:B:57:ILE:HA	1.90	0.53
7:F:152:TRP:O	7:F:156:THR:HG23	2.08	0.53
14:M:84:LYS:HA	14:M:87:GLU:HB2	1.91	0.53
1:2:587:A:H5'	1:2:592:C:H41	1.74	0.53
1:2:1748:G:H1	1:2:1786:U:H3	1.57	0.53
12:K:71:LEU:HD11	12:K:79:LEU:HD12	1.91	0.53
8:G:164:LYS:HD3	8:G:167:LYS:HG3	1.91	0.52
27:Z:73:VAL:HG21	27:Z:88:LEU:HD11	1.91	0.52
23:V:14:PRO:HG2	23:V:23:ILE:HD12	1.91	0.52
5:D:172:VAL:HG22	5:D:185:LYS:HG2	1.91	0.52
6:E:122:LYS:HD2	6:E:164:LEU:HD21	1.92	0.52
22:U:39:LEU:HD13	22:U:89:ILE:HD12	1.90	0.52
13:L:126:VAL:HG12	13:L:145:VAL:HG22	1.92	0.52
10:I:89:GLU:CD	10:I:92:ARG:HE	2.18	0.51
23:V:59:ILE:HD13	23:V:62:MET:HE3	1.91	0.51
18:Q:19:ALA:HB2	18:Q:75:GLY:HA3	1.92	0.51
34:g:239:LEU:HA	34:g:249:CYS:O	2.11	0.51
9:H:74:LYS:HG3	9:H:75:ILE:HD13	1.91	0.51
34:g:256:ILE:HB	34:g:270:LEU:HB2	1.92	0.51
24:W:18:GLU:HG3	24:W:69:LEU:HB3	1.92	0.51
8:G:20:ASP:HB3	8:G:23:LYS:HG3	1.92	0.51
20:S:22:GLY:HA2	20:S:56:ALA:HB3	1.92	0.51
1:2:377:G:H5'	10:I:98:LYS:HB3	1.92	0.51
1:2:921:G:H5'	29:b:21:LYS:HE3	1.93	0.51
15:N:67:THR:HG21	15:N:74:ILE:HD11	1.92	0.51
9:H:30:LEU:HD22	9:H:82:GLU:HB3	1.92	0.50
1:2:379:C:H5'	10:I:33:ALA:HA	1.93	0.50
14:M:31:LEU:HD23	14:M:109:VAL:HG21	1.92	0.50
22:U:20:ILE:HG12	22:U:91:LEU:HB2	1.93	0.50
4:C:66:LEU:HD21	4:C:81:ILE:HG12	1.92	0.50
11:J:30:LYS:HE2	32:e:42:PHE:CE1	2.46	0.50
34:g:176:VAL:HB	34:g:186:THR:HG22	1.93	0.50
6:E:100:ARG:HH21	6:E:118:GLU:HG2	1.75	0.50
1:2:616:A:H1'	32:e:12:VAL:HG13	1.93	0.50
3:B:124:HIS:HA	3:B:137:LEU:O	2.12	0.50
1:2:1315:U:H4'	12:K:2:LEU:HD22	1.93	0.50
5:D:61:GLU:HG2	5:D:62:LYS:HG3	1.93	0.50
30:c:60:GLU:OE1	30:c:63:ARG:HG3	2.12	0.50
11:J:175:ARG:O	11:J:179:LYS:HG3	2.11	0.49
14:M:63:LYS:NZ	33:f:108:VAL:HG12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:23:THR:HG22	22:U:88:LEU:HD23	1.95	0.49
14:M:110:VAL:O	14:M:110:VAL:HG13	2.11	0.49
1:2:1337:4AC:H2'	1:2:1338:G:H8	1.78	0.49
8:G:58:LYS:HE2	8:G:105:ASN:HA	1.94	0.49
26:Y:7:ILE:HG22	26:Y:27:VAL:HG13	1.94	0.49
10:I:101:ILE:HD12	10:I:190:LEU:HD11	1.93	0.49
13:L:33:LEU:HD12	13:L:34:PRO:HD2	1.94	0.49
28:a:11:ALA:HB3	28:a:33:ASP:HB2	1.94	0.49
1:2:1723:G:H2'	1:2:1724:A:C8	2.47	0.49
1:2:1706:G:H5'	36:n:1:MET:HB2	1.94	0.49
9:H:144:ILE:HB	24:W:52:ILE:HB	1.93	0.49
18:Q:34:VAL:HB	18:Q:42:ILE:HD11	1.93	0.49
1:2:1650:A:H5''	18:Q:139:ALA:HB2	1.94	0.49
12:K:59:LYS:HG3	12:K:70:TYR:HB2	1.93	0.49
2:A:73:ASP:HB3	2:A:120:ARG:HB2	1.94	0.49
22:U:64:THR:HA	22:U:78:ASP:O	2.13	0.49
30:c:32:VAL:O	30:c:41:SER:HA	2.12	0.48
34:g:20:GLN:HG2	34:g:69:VAL:H	1.77	0.48
10:I:125:LYS:HE3	10:I:128:LYS:HD2	1.96	0.48
1:2:1435:C:H4'	1:2:1437:C:H41	1.78	0.48
17:P:111:MET:HG2	20:S:117:ILE:HB	1.95	0.48
9:H:51:ILE:HD11	9:H:176:VAL:HG22	1.95	0.48
20:S:28[A]:PHE:HE2	20:S:38:ARG:HE	1.61	0.48
1:2:925:G:H1	1:2:1017:U:H3	1.60	0.48
1:2:385:G:H3'	13:L:136:LYS:HB2	1.96	0.48
1:2:535:G:H2'	1:2:536:A:C8	2.48	0.48
16:O:40:THR:HG21	16:O:74:ALA:HB2	1.96	0.48
17:P:33:LEU:HD21	17:P:87:PRO:HG2	1.95	0.48
5:D:38:GLU:HG3	5:D:49:ILE:HB	1.96	0.48
11:J:107:GLU:O	11:J:113:GLN:NE2	2.43	0.48
15:N:72:LEU:HD13	15:N:76:LYS:HD2	1.96	0.48
14:M:22:LEU:HD13	14:M:88:TRP:HB3	1.95	0.48
18:Q:43:GLU:HG2	18:Q:44:PRO:HA	1.95	0.48
1:2:543:C:H3'	1:2:544:G:H8	1.79	0.47
4:C:187:ARG:HD3	4:C:192:LEU:HD12	1.96	0.47
5:D:59:LEU:HD23	5:D:66:ILE:HG21	1.96	0.47
19:R:17:ILE:HG22	19:R:69:ILE:HG21	1.95	0.47
2:A:65:ILE:HG23	2:A:74:VAL:HG21	1.96	0.47
2:A:108:PHE:HB2	2:A:136:GLU:HG2	1.95	0.47
12:K:83:LEU:HB3	12:K:85:LEU:HG	1.97	0.47
17:P:111:MET:HE2	20:S:117:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:196:ILE:HB	4:C:223:TYR:HB2	1.97	0.47
6:E:20:LEU:HD21	6:E:46:ILE:HD12	1.97	0.47
18:Q:72:VAL:HG11	18:Q:84:ILE:HD11	1.95	0.47
1:2:1723:G:H2'	1:2:1724:A:H8	1.79	0.47
34:g:31:ILE:HG13	34:g:43:TRP:HB2	1.96	0.47
34:g:42:MET:HE3	34:g:57:ARG:HD2	1.96	0.47
12:K:20:VAL:HG12	12:K:70:TYR:HA	1.96	0.47
16:O:34:PHE:HB3	16:O:41:PHE:HB2	1.96	0.47
5:D:227:LYS:HD2	34:g:184:LEU:HD11	1.97	0.47
34:g:236:ILE:HG13	34:g:250:ALA:HB1	1.97	0.47
7:F:34:SER:HB3	30:c:55:VAL:HG12	1.96	0.46
20:S:36:VAL:HG22	20:S:40:TYR:HD2	1.79	0.46
29:b:19:HIS:HB3	29:b:22:LYS:HG3	1.97	0.46
1:2:1030:A:H2'	1:2:1031:A2M:H8	1.97	0.46
14:M:52:LEU:HD21	14:M:62:VAL:HG13	1.97	0.46
3:B:181:LEU:O	3:B:185:VAL:HG12	2.16	0.46
2:A:30:LEU:HD21	2:A:35:GLU:HG2	1.97	0.46
33:f:126:CYS:HB3	33:f:130:VAL:HG21	1.97	0.46
11:J:60:LEU:HD22	11:J:70:ARG:HA	1.98	0.46
25:X:28:LYS:HE2	25:X:32:LEU:HD11	1.98	0.46
1:2:1630:A:H5''	20:S:37:GLY:H	1.81	0.46
8:G:193:ALA:HA	8:G:196:LYS:HE3	1.98	0.46
2:A:121[B]:LEU:HD11	2:A:145:ILE:HD12	1.98	0.46
9:H:73:GLN:HA	9:H:76:GLN:HB2	1.98	0.46
14:M:44:LYS:HB2	14:M:44:LYS:HE3	1.71	0.46
1:2:165:G:H2'	1:2:166:A2M:H8	1.97	0.46
1:2:1382:A:H2'	1:2:1383:A2M:H8	1.98	0.46
1:2:1842:4AC:HM73	36:n:2:ARG:HH22	1.81	0.46
5:D:170:THR:HG23	5:D:187:LYS:HG3	1.97	0.46
9:H:58:LYS:HB2	9:H:90:LYS:HG3	1.98	0.46
17:P:83:MET:HE2	17:P:83:MET:HA	1.97	0.46
1:2:1037:G:H4'	1:2:1845:A:H4'	1.98	0.45
5:D:132:LYS:HG3	5:D:191:PRO:HA	1.97	0.45
12:K:16:PHE:CD2	12:K:79:LEU:HB3	2.50	0.45
34:g:89:LEU:HB3	34:g:99:ARG:HB3	1.98	0.45
3:B:139:CYS:HB2	3:B:172:MET:HE1	1.97	0.45
8:G:31:ARG:HE	8:G:31:ARG:HB2	1.57	0.45
21:T:104:LEU:HD13	21:T:121:ARG:HD3	1.98	0.45
34:g:5:MET:HB2	34:g:270:LEU:HD11	1.96	0.45
17:P:52:LYS:HD2	17:P:80:LEU:HD21	1.98	0.45
1:2:382:C:H2'	1:2:383:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:157:LYS:HD2	10:I:157:LYS:HA	1.65	0.45
14:M:61:TYR:O	14:M:65:VAL:HG12	2.17	0.45
16:O:98:ARG:HG3	16:O:132:VAL:HG23	1.98	0.45
20:S:15:VAL:HG13	20:S:68:ILE:HD11	1.97	0.45
2:A:8:LEU:HD11	23:V:39:VAL:HG21	1.98	0.45
1:2:640:A:H2'	1:2:641:A:C8	2.52	0.45
1:2:1845:A:H2'	1:2:1846:G:C8	2.52	0.45
33:f:135:HIS:HB2	33:f:138:ARG:HG2	1.97	0.45
9:H:10:LYS:HZ3	9:H:20:GLU:HG3	1.82	0.45
34:g:40:ILE:HG21	34:g:69:VAL:HG21	1.99	0.45
2:A:39:TYR:CG	19:R:105:MET:HG3	2.52	0.45
7:F:193:LYS:O	7:F:197:GLU:HG2	2.17	0.45
9:H:30:LEU:HD12	9:H:33:ASN:HD21	1.81	0.45
16:O:75:MET:HG3	16:O:118:ALA:HB2	1.98	0.45
34:g:42:MET:HE2	34:g:92:LEU:HB3	1.99	0.45
1:2:28:U:H2'	1:2:29:G:H8	1.83	0.44
12:K:31:LYS:HD2	12:K:36:ALA:HA	1.99	0.44
22:U:61:LEU:O	22:U:81:GLN:HA	2.17	0.44
1:2:448:A:H5''	10:I:25:ARG:HA	1.98	0.44
1:2:484:A2M:H8	1:2:484:A2M:O5'	2.17	0.44
1:2:1588:A:H2'	1:2:1589:A:C8	2.51	0.44
20:S:25:LYS:HA	20:S:55:ARG:HA	1.99	0.44
25:X:68:LYS:HE2	32:e:9:ALA:HB2	1.99	0.44
27:Z:73:VAL:HG12	27:Z:79:ILE:HD11	2.00	0.44
29:b:42:LYS:HE2	29:b:57:VAL:HG12	1.98	0.44
1:2:5:U:H2'	1:2:6:G:H8	1.82	0.44
8:G:137:ARG:HB3	8:G:140:ARG:HG3	2.00	0.44
4:C:191:VAL:HG11	4:C:236:PHE:HA	1.98	0.44
12:K:3:MET:HE3	12:K:3:MET:HB2	1.69	0.44
28:a:64:LEU:HD12	28:a:64:LEU:HA	1.85	0.44
34:g:120:ILE:O	34:g:131:LEU:HA	2.18	0.44
34:g:296:GLN:HG2	34:g:312:VAL:HG12	1.98	0.44
17:P:65:LYS:HE3	17:P:65:LYS:HB3	1.78	0.44
1:2:1387:G:H21	19:R:8:THR:HG21	1.82	0.44
1:2:1413:G:H2'	1:2:1414:A:H8	1.82	0.44
12:K:52:LEU:HD22	12:K:57:TYR:HD1	1.83	0.44
1:2:1562:C:H2'	1:2:1563:G:H8	1.83	0.44
5:D:109:LEU:HD12	5:D:184:ILE:HD11	2.00	0.44
20:S:36:VAL:HG22	20:S:40:TYR:CD2	2.53	0.44
1:2:1010:G:H2'	1:2:1011:A:C8	2.53	0.44
1:2:1679:A:H2'	7:F:60:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:201:LYS:HB2	5:D:201:LYS:HE3	1.73	0.44
7:F:50:PRO:HB3	7:F:69:VAL:HG23	2.00	0.44
29:b:34:ASP:HB3	29:b:43:ILE:HD11	1.99	0.44
34:g:30:MET:HE2	34:g:30:MET:HB3	1.80	0.44
12:K:49:MET:HE3	12:K:49:MET:HB3	1.83	0.43
1:2:601:OMG:HM23	1:2:601:OMG:H1'	1.64	0.43
1:2:981:A:H2'	1:2:982:G:C8	2.53	0.43
1:2:1232:PSU:H2'	1:2:1233:G:H8	1.83	0.43
7:F:69:VAL:O	7:F:73:THR:HG23	2.19	0.43
9:H:135:PHE:CD2	9:H:136:PRO:HA	2.52	0.43
14:M:63:LYS:HZ3	33:f:108:VAL:HG12	1.83	0.43
34:g:37:ASP:OD1	34:g:39:THR:HG22	2.18	0.43
2:A:34:MET:HE3	2:A:34:MET:HB3	1.63	0.43
11:J:33:GLY:HA3	32:e:38:TYR:CG	2.53	0.43
16:O:30:VAL:O	16:O:44:VAL:HA	2.19	0.43
17:P:92:SER:O	17:P:107:ILE:HG12	2.18	0.43
20:S:89:ASP:HB3	20:S:93:GLY:H	1.82	0.43
1:2:681:PSU:H4'	25:X:9:THR:HG22	2.01	0.43
8:G:58:LYS:HA	8:G:107:SER:HB3	1.99	0.43
9:H:15:LYS:HA	9:H:15:LYS:HD2	1.92	0.43
1:2:874:G:H2'	1:2:875:A:C8	2.53	0.43
1:2:928:G:H2'	1:2:929:G:C8	2.52	0.43
6:E:124:CYS:HB3	6:E:141:THR:HB	2.01	0.43
14:M:84:LYS:HE2	14:M:88:TRP:CH2	2.54	0.43
20:S:74:PRO:HG2	20:S:84:LEU:HD11	2.01	0.43
25:X:101:LEU:HB3	25:X:124:LYS:HB2	2.01	0.43
30:c:14:VAL:HG23	30:c:30:VAL:HB	1.99	0.43
34:g:77:PHE:HA	34:g:90:TRP:O	2.18	0.43
15:N:25:TRP:H	15:N:25:TRP:CD1	2.36	0.43
17:P:83:MET:HB3	17:P:116:LEU:HD13	2.01	0.43
27:Z:96:LEU:HD12	27:Z:97:ILE:HG23	2.01	0.43
31:d:3:HIS:CE1	31:d:5:GLN:HB2	2.54	0.43
34:g:244:ASN:HD21	34:g:295:GLY:HA3	1.83	0.43
5:D:70:THR:HG23	5:D:84:VAL:HG12	2.00	0.43
12:K:71:LEU:HD13	12:K:76:ILE:HG22	2.01	0.43
29:b:33:MET:HE2	29:b:48:SER:HA	2.00	0.43
25:X:28:LYS:HG2	25:X:32:LEU:HD12	2.01	0.43
1:2:857:U:H2'	1:2:858:A:C8	2.54	0.42
8:G:119:LYS:HE2	8:G:119:LYS:HB2	1.78	0.42
33:f:107:LYS:HA	33:f:107:LYS:HD2	1.73	0.42
11:J:30:LYS:HB2	11:J:30:LYS:HE3	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:67:THR:HG22	29:b:69:GLY:H	1.84	0.42
1:2:528:A:H2'	1:2:529:A:H8	1.84	0.42
1:2:1101:U:H2'	1:2:1102:G:C8	2.54	0.42
1:2:1337:4AC:H2'	1:2:1338:G:C8	2.54	0.42
19:R:54:VAL:O	19:R:58:MET:HB2	2.19	0.42
34:g:109:LEU:HD11	34:g:125:ARG:HG2	2.00	0.42
1:2:858:A:H2'	1:2:859:G:H8	1.84	0.42
3:B:136:ARG:HB3	3:B:216:LYS:HB2	2.02	0.42
6:E:129:ILE:HD13	6:E:139:LEU:HB3	2.02	0.42
1:2:5:U:H2'	1:2:6:G:C8	2.54	0.42
1:2:186:C:H2'	1:2:187:G:H8	1.84	0.42
1:2:812:A:H5''	6:E:16:LYS:HD2	2.00	0.42
13:L:79:LYS:HE3	13:L:79:LYS:HB2	1.74	0.42
23:V:51:LYS:HZ3	23:V:76:ASP:CG	2.28	0.42
12:K:16:PHE:CE2	12:K:79:LEU:HB3	2.55	0.42
1:2:609:U:H2'	1:2:610:G:H8	1.85	0.42
8:G:162:LEU:HD11	8:G:172:LYS:HD2	2.02	0.42
19:R:7:LYS:HG3	19:R:11:LYS:HE2	2.01	0.42
1:2:1154:U:H2'	4:C:192:LEU:HD11	2.02	0.42
12:K:9:ILE:HD12	12:K:9:ILE:HA	1.82	0.42
1:2:494:C:N4	1:2:509:OMG:HN22	2.17	0.42
1:2:1098:C:H2'	1:2:1099:G:C8	2.55	0.42
1:2:1705:C:H2'	1:2:1706:G:C8	2.55	0.42
8:G:221:LYS:HE3	8:G:222:GLU:HG2	2.01	0.42
7:F:102:LEU:HD11	27:Z:110:THR:HB	2.02	0.41
12:K:14:LEU:HD12	12:K:14:LEU:HA	1.87	0.41
20:S:8:LYS:HD2	20:S:8:LYS:HA	1.91	0.41
24:W:87:GLU:OE2	24:W:87:GLU:HA	2.20	0.41
34:g:22:ALA:HB3	34:g:32:LEU:HB2	2.02	0.41
1:2:1277:C:H5''	12:K:55:ARG:HH11	1.85	0.41
8:G:121:ILE:HG21	8:G:124:LEU:HD12	2.02	0.41
30:c:44:ARG:HH11	30:c:58:LEU:HD23	1.85	0.41
2:A:124:VAL:HG21	2:A:134:LEU:HD21	2.02	0.41
5:D:173:ARG:HD3	5:D:173:ARG:HA	1.94	0.41
20:S:34:LYS:HB2	20:S:34:LYS:HE2	1.65	0.41
22:U:51:LYS:HB2	22:U:90:ASP:HB2	2.00	0.41
28:a:18:VAL:HG21	28:a:33:ASP:OD1	2.20	0.41
1:2:1736:G:H2'	1:2:1737:G:C8	2.56	0.41
19:R:58:MET:HE3	19:R:58:MET:HA	2.02	0.41
34:g:118:ARG:HH12	34:g:133:ASN:HB2	1.85	0.41
34:g:217:MET:HB2	34:g:217:MET:HE3	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1598:G:H3'	27:Z:80:ARG:HD2	2.01	0.41
5:D:40:ARG:HD3	22:U:108:PRO:HG3	2.02	0.41
6:E:175:PHE:HE2	6:E:198:ARG:HD2	1.84	0.41
9:H:10:LYS:NZ	9:H:20:GLU:HG3	2.36	0.41
11:J:110:LEU:HB2	11:J:147:PHE:HB3	2.02	0.41
12:K:6:LYS:HB2	12:K:6:LYS:HE3	1.79	0.41
1:2:944:A:H5''	16:O:134:PRO:HB3	2.02	0.41
1:2:955:A:H4'	16:O:60:MET:HE3	2.01	0.41
2:A:82:THR:HG22	2:A:171:VAL:HG11	2.03	0.41
3:B:166:LYS:O	3:B:170:GLU:HG3	2.21	0.41
4:C:144:SER:HB2	4:C:150:ALA:HB2	2.01	0.41
9:H:30:LEU:HD21	9:H:83:LEU:HD22	2.02	0.41
9:H:32:MET:HE2	9:H:32:MET:HB3	1.85	0.41
10:I:57:ALA:HB2	10:I:183:GLY:HA2	2.03	0.41
10:I:150:ASP:HA	10:I:153:LYS:HG2	2.02	0.41
12:K:29:MET:HB3	12:K:42:ASN:HB2	2.02	0.41
21:T:60:THR:O	21:T:64:LEU:HD22	2.21	0.41
27:Z:72:VAL:O	27:Z:76:ARG:HB2	2.21	0.41
5:D:29:LEU:HB2	5:D:34:TYR:HB2	2.01	0.41
8:G:63:MET:HE3	8:G:100:CYS:HA	2.01	0.41
28:a:70:LYS:HB3	28:a:70:LYS:HE3	1.85	0.41
29:b:63:LEU:HD12	29:b:63:LEU:HA	1.95	0.41
1:2:1285:G:H5'	14:M:35:ILE:HG13	2.02	0.41
1:2:1651:A:H2'	1:2:1652:G:H8	1.86	0.41
12:K:57:TYR:HB3	12:K:75:GLY:HA2	2.02	0.41
1:2:35:C:H5''	1:2:579:C:H5''	2.03	0.41
1:2:509:OMG:H1'	1:2:509:OMG:HM23	1.77	0.41
2:A:134:LEU:HD22	2:A:144:THR:HG21	2.03	0.41
9:H:7:LYS:HD3	9:H:7:LYS:HA	1.79	0.41
9:H:63:PHE:HB3	9:H:97:GLN:HG2	2.03	0.41
34:g:17:TRP:H	34:g:36:ARG:HB2	1.86	0.41
1:2:1536:G:H2'	1:2:1537:A:C8	2.56	0.41
2:A:184:ARG:HG2	2:A:189:ILE:HG13	2.02	0.41
6:E:62:LYS:HE3	6:E:62:LYS:HB3	1.72	0.41
2:A:34:MET:HE2	2:A:149:ASN:O	2.21	0.40
18:Q:8:GLN:HG2	18:Q:99:TYR:CE1	2.56	0.40
21:T:40:ALA:HB3	21:T:43:LYS:HG2	2.02	0.40
26:Y:111:LYS:HE2	26:Y:111:LYS:HB3	1.97	0.40
7:F:127:ARG:HA	7:F:127:ARG:HD2	1.83	0.40
18:Q:98:LYS:HD3	18:Q:99:TYR:CE2	2.56	0.40
1:2:1144:A:H2'	1:2:1145:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:68:GLU:HB3	3:B:83:LYS:HD2	2.02	0.40
6:E:160:ILE:HD12	6:E:162:ILE:HD11	2.03	0.40
34:g:234:ASP:HB3	34:g:252:THR:CG2	2.49	0.40
1:2:15:U:H2'	1:2:16:G:O4'	2.22	0.40
1:2:191:A:H62	1:2:208:G:H21	1.70	0.40
11:J:139:LYS:HB3	11:J:139:LYS:HE3	1.93	0.40
19:R:95:ILE:HD13	19:R:95:ILE:HA	1.97	0.40
34:g:22:ALA:HB1	34:g:71:ILE:HG22	2.03	0.40
1:2:544:G:H3'	1:2:545:A:H8	1.85	0.40
1:2:1670:C:H2'	1:2:1671:G:C8	2.56	0.40
5:D:175:VAL:O	5:D:181:VAL:HA	2.21	0.40
10:I:160:SER:O	10:I:164:GLU:HG2	2.20	0.40
33:f:92:LYS:HD2	33:f:92:LYS:HA	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	
2	A	205/295 (70%)	199 (97%)	6 (3%)	0	100	100
3	B	208/264 (79%)	207 (100%)	1 (0%)	0	100	100
4	C	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
5	D	222/243 (91%)	222 (100%)	0	0	100	100
6	E	255/263 (97%)	251 (98%)	4 (2%)	0	100	100
7	F	178/204 (87%)	171 (96%)	7 (4%)	0	100	100
8	G	225/249 (90%)	221 (98%)	4 (2%)	0	100	100
9	H	180/194 (93%)	166 (92%)	14 (8%)	0	100	100
10	I	203/208 (98%)	194 (96%)	9 (4%)	0	100	100
11	J	183/194 (94%)	179 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	95/165 (58%)	94 (99%)	1 (1%)	0	100	100
13	L	137/158 (87%)	132 (96%)	5 (4%)	0	100	100
14	M	100/132 (76%)	92 (92%)	8 (8%)	0	100	100
15	N	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
16	O	125/151 (83%)	119 (95%)	5 (4%)	1 (1%)	16	44
17	P	121/145 (83%)	120 (99%)	1 (1%)	0	100	100
18	Q	137/146 (94%)	134 (98%)	3 (2%)	0	100	100
19	R	129/135 (96%)	125 (97%)	4 (3%)	0	100	100
20	S	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
21	T	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
22	U	102/119 (86%)	96 (94%)	6 (6%)	0	100	100
23	V	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
24	W	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
25	X	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
26	Y	120/133 (90%)	119 (99%)	1 (1%)	0	100	100
27	Z	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
28	a	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
29	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
30	c	57/69 (83%)	55 (96%)	2 (4%)	0	100	100
31	d	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
32	e	53/59 (90%)	52 (98%)	1 (2%)	0	100	100
33	f	62/156 (40%)	56 (90%)	6 (10%)	0	100	100
34	g	310/317 (98%)	297 (96%)	13 (4%)	0	100	100
35	h	44/1096 (4%)	41 (93%)	3 (7%)	0	100	100
36	n	18/25 (72%)	18 (100%)	0	0	100	100
All	All	4764/6597 (72%)	4626 (97%)	137 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	O	138	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	173/243 (71%)	170 (98%)	3 (2%)	56	84
3	B	192/231 (83%)	187 (97%)	5 (3%)	41	75
4	C	186/225 (83%)	181 (97%)	5 (3%)	40	74
5	D	188/202 (93%)	178 (95%)	10 (5%)	19	49
6	E	220/225 (98%)	217 (99%)	3 (1%)	62	87
7	F	155/170 (91%)	149 (96%)	6 (4%)	27	61
8	G	198/218 (91%)	195 (98%)	3 (2%)	60	86
9	H	164/174 (94%)	157 (96%)	7 (4%)	25	57
10	I	178/180 (99%)	175 (98%)	3 (2%)	56	84
11	J	161/168 (96%)	161 (100%)	0	100	100
12	K	88/136 (65%)	82 (93%)	6 (7%)	13	38
13	L	128/142 (90%)	126 (98%)	2 (2%)	58	85
14	M	86/108 (80%)	83 (96%)	3 (4%)	31	65
15	N	130/131 (99%)	128 (98%)	2 (2%)	60	86
16	O	100/119 (84%)	96 (96%)	4 (4%)	27	60
17	P	106/130 (82%)	100 (94%)	6 (6%)	17	46
18	Q	115/121 (95%)	112 (97%)	3 (3%)	41	75
19	R	119/122 (98%)	112 (94%)	7 (6%)	16	44
20	S	125/132 (95%)	123 (98%)	2 (2%)	58	85
21	T	113/115 (98%)	109 (96%)	4 (4%)	31	65
22	U	94/107 (88%)	87 (93%)	7 (7%)	11	33
23	V	67/67 (100%)	67 (100%)	0	100	100
24	W	112/113 (99%)	111 (99%)	1 (1%)	75	92
25	X	112/115 (97%)	108 (96%)	4 (4%)	30	64
26	Y	107/115 (93%)	103 (96%)	4 (4%)	29	63
27	Z	63/103 (61%)	62 (98%)	1 (2%)	58	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	a	86/98 (88%)	85 (99%)	1 (1%)	67	89
29	b	74/76 (97%)	70 (95%)	4 (5%)	18	48
30	c	52/62 (84%)	45 (86%)	7 (14%)	3	10
31	d	48/49 (98%)	46 (96%)	2 (4%)	25	58
32	e	45/48 (94%)	41 (91%)	4 (9%)	8	25
33	f	57/140 (41%)	56 (98%)	1 (2%)	54	83
34	g	264/275 (96%)	253 (96%)	11 (4%)	25	58
35	h	31/948 (3%)	30 (97%)	1 (3%)	34	68
36	n	19/24 (79%)	19 (100%)	0	100	100
All	All	4156/5632 (74%)	4024 (97%)	132 (3%)	36	68

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	54	THR
2	A	123	VAL
2	A	190	SER
3	B	55	THR
3	B	70	SER
3	B	91	VAL
3	B	97	LEU
3	B	225	LEU
4	C	147	VAL
4	C	184	VAL
4	C	212	LYS
4	C	221	ASP
4	C	259	THR
5	D	38	GLU
5	D	42	THR
5	D	44	THR
5	D	54	ARG
5	D	55	THR
5	D	58	VAL
5	D	74	GLN
5	D	175	VAL
5	D	208	VAL
5	D	209	SER
6	E	105	THR
6	E	168	LYS

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Mol	Chain	Res	Type
6	E	173	ILE
7	F	33	ILE
7	F	42	LYS
7	F	102	LEU
7	F	103	LEU
7	F	141	VAL
7	F	166	ILE
8	G	22	ARG
8	G	144	LEU
8	G	158	VAL
9	H	10	LYS
9	H	23	ILE
9	H	50	GLU
9	H	75	ILE
9	H	77	VAL
9	H	92	VAL
9	H	93	VAL
10	I	62	VAL
10	I	165	GLN
10	I	193	LYS
12	K	3	MET
12	K	9	ILE
12	K	21	MET
12	K	79	LEU
12	K	83	LEU
12	K	90	VAL
13	L	83	GLN
13	L	120	VAL
14	M	16	THR
14	M	49	LEU
14	M	68	LEU
15	N	26	LEU
15	N	72	LEU
16	O	40	THR
16	O	56	VAL
16	O	107	THR
16	O	130	GLU
17	P	83	MET
17	P	90	VAL
17	P	92	SER
17	P	107	ILE
17	P	111	MET

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Mol	Chain	Res	Type
17	P	124	LYS
18	Q	7	LEU
18	Q	12	VAL
18	Q	100	VAL
19	R	8	THR
19	R	40	ILE
19	R	58	MET
19	R	61	ILE
19	R	69	ILE
19	R	71	ILE
19	R	120	THR
20	S	66	ARG
20	S	136	THR
21	T	82	ARG
21	T	90	SER
21	T	110	LEU
21	T	131	LEU
22	U	19	ARG
22	U	20	ILE
22	U	56	MET
22	U	75	LYS
22	U	90	ASP
22	U	92	HIS
22	U	97	ILE
24	W	114	GLU
25	X	36	LEU
25	X	105	PHE
25	X	119	ARG
25	X	125	VAL
26	Y	5	VAL
26	Y	7	ILE
26	Y	16	ARG
26	Y	68	LYS
27	Z	92	LEU
28	a	64	LEU
29	b	37	CYS
29	b	44	THR
29	b	57	VAL
29	b	81	ARG
30	c	14	VAL
30	c	17	VAL
30	c	27	CYS

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Mol	Chain	Res	Type
30	c	28	THR
30	c	41	SER
30	c	56	LEU
30	c	58	LEU
31	d	6	LEU
31	d	30	LEU
32	e	16	THR
32	e	21	LYS
32	e	29	THR
32	e	46	VAL
33	f	89	LYS
34	g	6	THR
34	g	31	ILE
34	g	74	ASP
34	g	110	SER
34	g	113	PHE
34	g	199	THR
34	g	229	THR
34	g	248	LEU
34	g	270	LEU
34	g	297	THR
34	g	307	VAL
35	h	677	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	GLN
3	B	149	GLN
6	E	50	ASN
9	H	12	ASN
9	H	163	GLN
10	I	165	GLN
12	K	28	HIS
12	K	61	GLN
13	L	19	ASN
15	N	13	GLN
17	P	53	GLN
18	Q	29	ASN
19	R	121	GLN
20	S	72	GLN
21	T	63	HIS

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Mol	Chain	Res	Type
21	T	117	GLN
23	V	35	ASN
24	W	24	GLN
24	W	64	ASN
28	a	86	ASN
30	c	45	ASN
31	d	26	ASN
31	d	37	ASN
32	e	44	ASN
34	g	15	ASN
34	g	178	ASN
34	g	188	HIS
34	g	215	GLN
34	g	226	HIS
34	g	285	GLN
34	g	305	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1601/1869 (85%)	261 (16%)	4 (0%)

All (261) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	17	C
1	2	25	A
1	2	33	G
1	2	41	G
1	2	45	A
1	2	46	A
1	2	56	G
1	2	65	C
1	2	67	C
1	2	68	A
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	77	A
1	2	99	A2M

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Mol	Chain	Res	Type
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G
1	2	130	G
1	2	142	C
1	2	143	U
1	2	155	G
1	2	160	U
1	2	168	C
1	2	175	A
1	2	178	C
1	2	182	C
1	2	191	A
1	2	212	C
1	2	302	A
1	2	306	C
1	2	309	G
1	2	319	C
1	2	320	G
1	2	330	G
1	2	332	G
1	2	339	A
1	2	340	C
1	2	362	C
1	2	364	A
1	2	369	C
1	2	370	G
1	2	385	G
1	2	386	C
1	2	400	C
1	2	409	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	464	A
1	2	465	A
1	2	471	G
1	2	472	C
1	2	474	G
1	2	482	G

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Mol	Chain	Res	Type
1	2	487	U
1	2	492	C
1	2	508	A
1	2	512	A2M
1	2	516	A
1	2	525	A
1	2	532	C
1	2	537	C
1	2	538	U
1	2	539	C
1	2	540	U
1	2	541	U
1	2	544	G
1	2	546	G
1	2	547	G
1	2	548	C
1	2	549	C
1	2	550	C
1	2	554	A
1	2	555	A
1	2	559	G
1	2	563	G
1	2	564	A
1	2	576	A2M
1	2	583	C
1	2	587	A
1	2	589	G
1	2	591	U
1	2	593	C
1	2	604	A
1	2	608	C
1	2	614	C
1	2	617	G
1	2	626	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	630	U
1	2	632	C
1	2	643	A
1	2	655	A
1	2	660	C

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Mol	Chain	Res	Type
1	2	663	C
1	2	668	A2M
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	687	C
1	2	688	U
1	2	689	U
1	2	821	G
1	2	822	PSU
1	2	834	C
1	2	847	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	913	A
1	2	914	U
1	2	920	A
1	2	922	A
1	2	933	G
1	2	943	U
1	2	950	C
1	2	955	A
1	2	970	G
1	2	971	G
1	2	990	A
1	2	992	A
1	2	1017	U
1	2	1023	A
1	2	1061	U
1	2	1062	A
1	2	1080	A
1	2	1083	A
1	2	1085	C
1	2	1089	G
1	2	1109	C
1	2	1115	U
1	2	1116	C
1	2	1119	A
1	2	1121	G
1	2	1133	A

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Mol	Chain	Res	Type
1	2	1138	C
1	2	1148	A
1	2	1153	C
1	2	1154	U
1	2	1171	G
1	2	1195	A
1	2	1208	A
1	2	1215	C
1	2	1224	G
1	2	1242	U
1	2	1243	U
1	2	1245	G
1	2	1248	B8N
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1269	G
1	2	1274	G
1	2	1275	G
1	2	1285	G
1	2	1286	G
1	2	1295	A
1	2	1298	G
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1306	U
1	2	1308	U
1	2	1312	G
1	2	1320	G
1	2	1333	U
1	2	1342	U
1	2	1363	C
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1382	A
1	2	1395	C
1	2	1397	U
1	2	1404	U

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Mol	Chain	Res	Type
1	2	1418	C
1	2	1431	G
1	2	1432	U
1	2	1433	C
1	2	1434	C
1	2	1436	C
1	2	1437	C
1	2	1438	A
1	2	1442	OMU
1	2	1452	A
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1487	A
1	2	1488	C
1	2	1489	A
1	2	1490	OMG
1	2	1494	U
1	2	1495	G
1	2	1497	G
1	2	1498	A
1	2	1507	G
1	2	1508	A
1	2	1521	C
1	2	1522	A
1	2	1523	C
1	2	1533	A
1	2	1535	U
1	2	1544	C
1	2	1553	C
1	2	1555	U
1	2	1580	A
1	2	1585	U
1	2	1588	A
1	2	1594	A
1	2	1601	A
1	2	1606	G
1	2	1621	U
1	2	1654	G
1	2	1664	A
1	2	1665	G
1	2	1683	C

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Mol	Chain	Res	Type
1	2	1698	C
1	2	1701	C
1	2	1713	C
1	2	1715	A
1	2	1719	A
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1729	U
1	2	1744	G
1	2	1745	A
1	2	1752	C
1	2	1754	G
1	2	1777	G
1	2	1779	G
1	2	1781	A
1	2	1783	C
1	2	1784	G
1	2	1800	A
1	2	1807	C
1	2	1812	U
1	2	1813	A
1	2	1823	A
1	2	1825	A
1	2	1829	G
1	2	1831	A
1	2	1835	A
1	2	1838	U
1	2	1849	G
1	2	1851	MA6
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1865	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	331	C
1	2	531	A
1	2	627	U

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Mol	Chain	Res	Type
1	2	871	U

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

73 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
1	PSU	2	649	1	18,21,22	2.50	7 (38%)	21,30,33	2.10	4 (19%)
1	OMC	2	1391	1	19,22,23	1.78	5 (26%)	25,31,34	1.03	1 (4%)
1	PSU	2	814	1	18,21,22	2.50	8 (44%)	21,30,33	2.02	3 (14%)
1	PSU	2	572	1,37	18,21,22	2.47	7 (38%)	21,30,33	2.08	4 (19%)
1	PSU	2	36	1	18,21,22	2.52	7 (38%)	21,30,33	1.93	4 (19%)
1	OMU	2	121	1	19,22,23	2.80	7 (36%)	25,31,34	1.75	5 (20%)
1	A2M	2	512	1	18,25,26	4.34	4 (22%)	20,36,39	1.45	1 (5%)
1	PSU	2	1045	1	18,21,22	2.42	7 (38%)	21,30,33	2.02	4 (19%)
1	PSU	2	863	1	18,21,22	2.50	7 (38%)	21,30,33	2.04	4 (19%)
1	OMG	2	509	1,38	19,26,27	2.65	5 (26%)	21,38,41	1.27	3 (14%)
1	OMG	2	644	1	19,26,27	2.69	4 (21%)	21,38,41	1.30	2 (9%)
1	PSU	2	681	1	18,21,22	2.47	8 (44%)	21,30,33	1.99	4 (19%)
1	4AC	2	1337	1	21,24,25	1.97	7 (33%)	28,34,37	1.76	5 (17%)
1	PSU	2	1347	1	18,21,22	2.47	7 (38%)	21,30,33	2.04	4 (19%)
1	PSU	2	1232	1	18,21,22	2.48	7 (38%)	21,30,33	2.17	4 (19%)
1	PSU	2	1692	1,37	18,21,22	2.47	7 (38%)	21,30,33	2.01	4 (19%)
1	OMU	2	1288	1	19,22,23	2.70	6 (31%)	25,31,34	1.91	7 (28%)
1	OMC	2	462	1	19,22,23	1.79	5 (26%)	25,31,34	1.06	1 (4%)
1	A2M	2	1383	1	18,25,26	4.38	4 (22%)	20,36,39	1.48	2 (10%)
1	MA6	2	1850	1	19,26,27	1.32	1 (5%)	18,38,41	2.06	3 (16%)
1	PSU	2	105	1,37	18,21,22	2.48	7 (38%)	21,30,33	2.11	4 (19%)
1	A2M	2	590	1	18,25,26	4.33	4 (22%)	20,36,39	2.30	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2	1177	1	18,21,22	2.45	7 (38%)	21,30,33	2.04	4 (19%)
1	OMG	2	1447	1	19,26,27	2.69	4 (21%)	21,38,41	1.26	2 (9%)
1	4AC	2	1842	1	21,24,25	1.92	7 (33%)	28,34,37	2.00	8 (28%)
1	OMC	2	517	1	19,22,23	1.76	5 (26%)	25,31,34	1.11	1 (4%)
1	OMC	2	1272	1	19,22,23	1.74	4 (21%)	25,31,34	1.08	1 (4%)
1	PSU	2	686	1	18,21,22	2.39	7 (38%)	21,30,33	2.05	4 (19%)
1	PSU	2	1056	1	18,21,22	2.41	7 (38%)	21,30,33	1.98	4 (19%)
1	A2M	2	159	1	18,25,26	4.33	4 (22%)	20,36,39	1.36	3 (15%)
1	OMU	2	354	1	19,22,23	2.76	7 (36%)	25,31,34	1.81	5 (20%)
1	OMU	2	116	1	19,22,23	2.76	8 (42%)	25,31,34	1.82	4 (16%)
1	OMG	2	601	1	19,26,27	2.68	4 (21%)	21,38,41	1.27	2 (9%)
1	6MZ	2	1832	1,37,38	17,25,26	0.89	0	15,36,39	2.81	4 (26%)
1	PSU	2	1244	1	18,21,22	2.42	7 (38%)	21,30,33	2.06	4 (19%)
1	PSU	2	1643	1,38	18,21,22	2.44	7 (38%)	21,30,33	2.07	5 (23%)
1	7MG	2	1639	1	23,26,27	3.55	6 (26%)	27,39,42	2.12	8 (29%)
1	PSU	2	1445	1	18,21,22	2.41	7 (38%)	21,30,33	2.08	5 (23%)
1	A2M	2	484	1	18,25,26	4.29	4 (22%)	20,36,39	1.41	3 (15%)
1	PSU	2	1174	1,37	18,21,22	2.47	7 (38%)	21,30,33	2.08	4 (19%)
1	PSU	2	815	1	18,21,22	2.45	7 (38%)	21,30,33	2.10	4 (19%)
1	A2M	2	576	1,37	18,25,26	4.25	5 (27%)	20,36,39	1.37	2 (10%)
1	PSU	2	93	1	18,21,22	2.48	7 (38%)	21,30,33	2.00	4 (19%)
1	OMG	2	1490	1,38	19,26,27	2.65	4 (21%)	21,38,41	1.25	2 (9%)
1	A2M	2	1031	1	18,25,26	4.33	4 (22%)	20,36,39	1.46	2 (10%)
1	OMG	2	1328	1,37	19,26,27	2.69	4 (21%)	21,38,41	1.30	2 (9%)
1	PSU	2	1046	1	18,21,22	2.48	8 (44%)	21,30,33	2.04	3 (14%)
1	PSU	2	1081	1	18,21,22	2.58	8 (44%)	21,30,33	2.06	5 (23%)
1	OMG	2	436	1	19,26,27	2.70	4 (21%)	21,38,41	1.31	2 (9%)
1	A2M	2	166	1	18,25,26	4.40	4 (22%)	20,36,39	1.57	3 (15%)
1	OMU	2	428	1	19,22,23	2.75	7 (36%)	25,31,34	1.96	6 (24%)
1	PSU	2	119	1	18,21,22	2.56	7 (38%)	21,30,33	2.03	4 (19%)
1	PSU	2	1136	1	18,21,22	2.46	7 (38%)	21,30,33	2.09	4 (19%)
1	OMG	2	683	1	19,26,27	2.71	4 (21%)	21,38,41	1.31	2 (9%)
1	PSU	2	651	1	18,21,22	2.48	7 (38%)	21,30,33	2.08	4 (19%)
1	B8N	2	1248	1	25,29,30	2.56	8 (32%)	28,42,45	1.54	5 (17%)
1	PSU	2	1625	1	18,21,22	2.43	7 (38%)	21,30,33	1.96	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	2	174	1,38	19,22,23	1.77	5 (26%)	25,31,34	1.01	1 (4%)
1	PSU	2	1238	1	18,21,22	2.42	7 (38%)	21,30,33	2.00	4 (19%)
1	A2M	2	1678	1	18,25,26	4.38	4 (22%)	20,36,39	1.64	3 (15%)
1	MA6	2	1851	1	19,26,27	1.29	1 (5%)	18,38,41	2.16	3 (16%)
1	PSU	2	406	1	18,21,22	2.49	7 (38%)	21,30,33	2.05	4 (19%)
1	A2M	2	468	1	18,25,26	4.29	4 (22%)	20,36,39	1.66	2 (10%)
1	A2M	2	668	1,38	18,25,26	4.21	5 (27%)	20,36,39	1.89	5 (25%)
1	OMU	2	1442	1,38	19,22,23	2.73	7 (36%)	25,31,34	1.90	5 (20%)
1	PSU	2	822	1	18,21,22	2.53	8 (44%)	21,30,33	2.11	5 (23%)
1	OMU	2	1326	1,38	19,22,23	2.74	7 (36%)	25,31,34	2.03	6 (24%)
1	PSU	2	296	1	18,21,22	2.46	7 (38%)	21,30,33	2.15	4 (19%)
1	A2M	2	27	1,38	18,25,26	4.29	4 (22%)	20,36,39	1.57	3 (15%)
1	OMU	2	172	1	19,22,23	2.77	7 (36%)	25,31,34	1.96	5 (20%)
1	A2M	2	99	1,38	18,25,26	4.36	4 (22%)	20,36,39	1.39	2 (10%)
1	PSU	2	109	1,37	18,21,22	2.46	7 (38%)	21,30,33	2.12	4 (19%)
1	OMC	2	1703	1	19,22,23	1.77	5 (26%)	25,31,34	1.04	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	649	1	-	0/7/25/26	0/2/2/2
1	OMC	2	1391	1	-	0/9/27/28	0/2/2/2
1	PSU	2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	2	572	1,37	-	0/7/25/26	0/2/2/2
1	PSU	2	36	1	-	0/7/25/26	0/2/2/2
1	OMU	2	121	1	-	0/9/27/28	0/2/2/2
1	A2M	2	512	1	-	2/5/27/28	0/3/3/3
1	PSU	2	1045	1	-	2/7/25/26	0/2/2/2
1	PSU	2	863	1	-	0/7/25/26	0/2/2/2
1	OMG	2	509	1,38	-	0/5/27/28	0/3/3/3
1	OMG	2	644	1	-	1/5/27/28	0/3/3/3
1	PSU	2	681	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1337	1	-	4/11/29/30	0/2/2/2
1	PSU	2	1347	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1232	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	1692	1,37	-	0/7/25/26	0/2/2/2
1	OMU	2	1288	1	-	0/9/27/28	0/2/2/2
1	OMC	2	462	1	-	0/9/27/28	0/2/2/2
1	A2M	2	1383	1	-	0/5/27/28	0/3/3/3
1	MA6	2	1850	1	-	2/7/29/30	0/3/3/3
1	PSU	2	105	1,37	-	0/7/25/26	0/2/2/2
1	A2M	2	590	1	-	0/5/27/28	0/3/3/3
1	PSU	2	1177	1	-	0/7/25/26	0/2/2/2
1	OMG	2	1447	1	-	2/5/27/28	0/3/3/3
1	4AC	2	1842	1	-	2/11/29/30	0/2/2/2
1	OMC	2	517	1	-	0/9/27/28	0/2/2/2
1	OMC	2	1272	1	-	0/9/27/28	0/2/2/2
1	PSU	2	686	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1056	1	-	0/7/25/26	0/2/2/2
1	A2M	2	159	1	-	0/5/27/28	0/3/3/3
1	OMU	2	354	1	-	0/9/27/28	0/2/2/2
1	OMU	2	116	1	-	0/9/27/28	0/2/2/2
1	OMG	2	601	1	-	1/5/27/28	0/3/3/3
1	6MZ	2	1832	1,37,38	-	0/5/27/28	0/3/3/3
1	PSU	2	1244	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1643	1,38	-	0/7/25/26	0/2/2/2
1	7MG	2	1639	1	-	1/7/37/38	0/3/3/3
1	PSU	2	1445	1	-	0/7/25/26	0/2/2/2
1	A2M	2	484	1	-	0/5/27/28	0/3/3/3
1	PSU	2	1174	1,37	-	0/7/25/26	0/2/2/2
1	PSU	2	815	1	-	0/7/25/26	0/2/2/2
1	A2M	2	576	1,37	-	2/5/27/28	0/3/3/3
1	PSU	2	93	1	-	0/7/25/26	0/2/2/2
1	OMG	2	1490	1,38	-	1/5/27/28	0/3/3/3
1	A2M	2	1031	1	-	0/5/27/28	0/3/3/3
1	OMG	2	1328	1,37	-	0/5/27/28	0/3/3/3
1	PSU	2	1046	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1081	1	-	1/7/25/26	0/2/2/2
1	OMG	2	436	1	-	0/5/27/28	0/3/3/3
1	A2M	2	166	1	-	0/5/27/28	0/3/3/3
1	OMU	2	428	1	-	4/9/27/28	0/2/2/2
1	PSU	2	119	1	-	1/7/25/26	0/2/2/2
1	PSU	2	1136	1	-	0/7/25/26	0/2/2/2
1	OMG	2	683	1	-	2/5/27/28	0/3/3/3
1	PSU	2	651	1	-	0/7/25/26	0/2/2/2
1	B8N	2	1248	1	-	6/16/34/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	1625	1	-	0/7/25/26	0/2/2/2
1	OMC	2	174	1,38	-	0/9/27/28	0/2/2/2
1	PSU	2	1238	1	-	0/7/25/26	0/2/2/2
1	A2M	2	1678	1	-	0/5/27/28	0/3/3/3
1	MA6	2	1851	1	-	3/7/29/30	0/3/3/3
1	PSU	2	406	1	-	0/7/25/26	0/2/2/2
1	A2M	2	468	1	-	0/5/27/28	0/3/3/3
1	A2M	2	668	1,38	-	2/5/27/28	0/3/3/3
1	OMU	2	1442	1,38	-	0/9/27/28	0/2/2/2
1	PSU	2	822	1	-	0/7/25/26	0/2/2/2
1	OMU	2	1326	1,38	-	0/9/27/28	0/2/2/2
1	PSU	2	296	1	-	0/7/25/26	0/2/2/2
1	A2M	2	27	1,38	-	0/5/27/28	0/3/3/3
1	OMU	2	172	1	-	0/9/27/28	0/2/2/2
1	A2M	2	99	1,38	-	2/5/27/28	0/3/3/3
1	PSU	2	109	1,37	-	0/7/25/26	0/2/2/2
1	OMC	2	1703	1	-	0/9/27/28	0/2/2/2

All (424) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	166	A2M	O4'-C1'	16.36	1.62	1.40
1	2	1383	A2M	O4'-C1'	16.27	1.62	1.40
1	2	1678	A2M	O4'-C1'	16.18	1.62	1.40
1	2	99	A2M	O4'-C1'	16.11	1.62	1.40
1	2	512	A2M	O4'-C1'	16.08	1.62	1.40
1	2	1031	A2M	O4'-C1'	16.03	1.61	1.40
1	2	159	A2M	O4'-C1'	15.99	1.61	1.40
1	2	590	A2M	O4'-C1'	15.90	1.61	1.40
1	2	27	A2M	O4'-C1'	15.86	1.61	1.40
1	2	468	A2M	O4'-C1'	15.82	1.61	1.40
1	2	484	A2M	O4'-C1'	15.78	1.61	1.40
1	2	576	A2M	O4'-C1'	15.56	1.61	1.40
1	2	668	A2M	O4'-C1'	15.19	1.60	1.40
1	2	1288	OMU	O4-C4	9.92	1.43	1.24
1	2	172	OMU	O4-C4	9.79	1.43	1.24
1	2	116	OMU	O4-C4	9.76	1.43	1.24
1	2	121	OMU	O4-C4	9.73	1.43	1.24
1	2	428	OMU	O4-C4	9.66	1.43	1.24
1	2	1326	OMU	O4-C4	9.66	1.43	1.24
1	2	1442	OMU	O4-C4	9.62	1.43	1.24
1	2	354	OMU	O4-C4	9.56	1.43	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	7MG	C5-N7	9.11	1.47	1.35
1	2	1639	7MG	O6-C6	9.09	1.40	1.23
1	2	1248	B8N	O4-C4	8.40	1.40	1.23
1	2	1639	7MG	C4-N9	8.30	1.48	1.37
1	2	1447	OMG	C2-N2	8.17	1.53	1.34
1	2	683	OMG	C2-N2	8.12	1.53	1.34
1	2	1328	OMG	C2-N2	8.09	1.53	1.34
1	2	436	OMG	C2-N2	7.98	1.52	1.34
1	2	644	OMG	C2-N2	7.93	1.52	1.34
1	2	601	OMG	C2-N2	7.91	1.52	1.34
1	2	1490	OMG	C2-N2	7.71	1.52	1.34
1	2	509	OMG	C2-N2	7.59	1.51	1.34
1	2	668	A2M	O4'-C4'	-6.13	1.31	1.45
1	2	1328	OMG	O6-C6	6.12	1.37	1.23
1	2	1447	OMG	O6-C6	6.10	1.37	1.23
1	2	1490	OMG	O6-C6	6.08	1.37	1.23
1	2	683	OMG	O6-C6	6.08	1.37	1.23
1	2	644	OMG	O6-C6	6.06	1.37	1.23
1	2	601	OMG	O6-C6	6.05	1.37	1.23
1	2	436	OMG	O6-C6	6.00	1.37	1.23
1	2	509	OMG	O6-C6	5.88	1.37	1.23
1	2	590	A2M	O4'-C4'	-5.86	1.32	1.45
1	2	119	PSU	O4-C4	-5.85	1.12	1.23
1	2	1678	A2M	O4'-C4'	-5.67	1.32	1.45
1	2	863	PSU	O4-C4	-5.64	1.12	1.23
1	2	822	PSU	O4-C4	-5.62	1.12	1.23
1	2	1136	PSU	O4-C4	-5.62	1.12	1.23
1	2	576	A2M	O4'-C4'	-5.62	1.32	1.45
1	2	484	A2M	O4'-C4'	-5.61	1.32	1.45
1	2	468	A2M	O4'-C4'	-5.59	1.32	1.45
1	2	27	A2M	O4'-C4'	-5.58	1.32	1.45
1	2	572	PSU	O4-C4	-5.57	1.13	1.23
1	2	1177	PSU	O4-C4	-5.53	1.13	1.23
1	2	651	PSU	O4-C4	-5.53	1.13	1.23
1	2	99	A2M	O4'-C4'	-5.53	1.32	1.45
1	2	1081	PSU	O4-C4	-5.52	1.13	1.23
1	2	159	A2M	O4'-C4'	-5.51	1.32	1.45
1	2	36	PSU	O4-C4	-5.51	1.13	1.23
1	2	1031	A2M	O4'-C4'	-5.51	1.32	1.45
1	2	1232	PSU	O4-C4	-5.51	1.13	1.23
1	2	814	PSU	O4-C4	-5.50	1.13	1.23
1	2	681	PSU	O4-C4	-5.50	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1692	PSU	O4-C4	-5.49	1.13	1.23
1	2	1046	PSU	O4-C4	-5.47	1.13	1.23
1	2	109	PSU	O4-C4	-5.47	1.13	1.23
1	2	1383	A2M	O4'-C4'	-5.47	1.32	1.45
1	2	649	PSU	O4-C4	-5.47	1.13	1.23
1	2	815	PSU	O4-C4	-5.47	1.13	1.23
1	2	166	A2M	O4'-C4'	-5.46	1.32	1.45
1	2	686	PSU	O4-C4	-5.46	1.13	1.23
1	2	1347	PSU	O4-C4	-5.45	1.13	1.23
1	2	105	PSU	O4-C4	-5.42	1.13	1.23
1	2	406	PSU	O4-C4	-5.41	1.13	1.23
1	2	512	A2M	O4'-C4'	-5.41	1.33	1.45
1	2	296	PSU	O4-C4	-5.41	1.13	1.23
1	2	1643	PSU	O4-C4	-5.41	1.13	1.23
1	2	1174	PSU	O4-C4	-5.40	1.13	1.23
1	2	93	PSU	O4-C4	-5.40	1.13	1.23
1	2	1445	PSU	O4-C4	-5.40	1.13	1.23
1	2	1244	PSU	O4-C4	-5.38	1.13	1.23
1	2	1639	7MG	C2-N2	5.38	1.46	1.34
1	2	1056	PSU	O4-C4	-5.38	1.13	1.23
1	2	1045	PSU	O4-C4	-5.36	1.13	1.23
1	2	1238	PSU	O4-C4	-5.33	1.13	1.23
1	2	1625	PSU	O4-C4	-5.28	1.13	1.23
1	2	159	A2M	C6-N6	5.09	1.52	1.34
1	2	1081	PSU	C1'-C5	5.08	1.61	1.50
1	2	1678	A2M	C6-N6	5.08	1.52	1.34
1	2	576	A2M	C6-N6	5.08	1.52	1.34
1	2	166	A2M	C6-N6	5.07	1.52	1.34
1	2	468	A2M	C6-N6	5.06	1.52	1.34
1	2	484	A2M	C6-N6	5.05	1.52	1.34
1	2	512	A2M	C6-N6	5.04	1.52	1.34
1	2	1031	A2M	C6-N6	5.04	1.52	1.34
1	2	1383	A2M	C6-N6	5.03	1.52	1.34
1	2	27	A2M	C6-N6	5.02	1.52	1.34
1	2	590	A2M	C6-N6	5.02	1.52	1.34
1	2	668	A2M	C6-N6	5.01	1.52	1.34
1	2	99	A2M	C6-N6	4.96	1.51	1.34
1	2	119	PSU	C1'-C5	4.92	1.61	1.50
1	2	1850	MA6	C6-N6	4.87	1.48	1.37
1	2	1272	OMC	C4-N4	4.73	1.45	1.33
1	2	1046	PSU	C1'-C5	4.71	1.60	1.50
1	2	1045	PSU	C1'-C5	4.71	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1703	OMC	C4-N4	4.68	1.45	1.33
1	2	93	PSU	C1'-C5	4.67	1.60	1.50
1	2	462	OMC	C4-N4	4.66	1.45	1.33
1	2	436	OMG	C5-C6	-4.66	1.38	1.47
1	2	1625	PSU	C1'-C5	4.65	1.60	1.50
1	2	1490	OMG	C5-C6	-4.63	1.38	1.47
1	2	601	OMG	C5-C6	-4.62	1.38	1.47
1	2	174	OMC	C4-N4	4.62	1.45	1.33
1	2	644	OMG	C5-C6	-4.62	1.38	1.47
1	2	1391	OMC	C4-N4	4.61	1.45	1.33
1	2	683	OMG	C5-C6	-4.61	1.38	1.47
1	2	1851	MA6	C6-N6	4.60	1.48	1.37
1	2	822	PSU	C1'-C5	4.59	1.60	1.50
1	2	509	OMG	C5-C6	-4.58	1.38	1.47
1	2	1238	PSU	C1'-C5	4.55	1.60	1.50
1	2	1177	PSU	C1'-C5	4.55	1.60	1.50
1	2	1328	OMG	C5-C6	-4.55	1.38	1.47
1	2	863	PSU	C1'-C5	4.55	1.60	1.50
1	2	814	PSU	C1'-C5	4.54	1.60	1.50
1	2	1244	PSU	C1'-C5	4.54	1.60	1.50
1	2	1174	PSU	C1'-C5	4.54	1.60	1.50
1	2	649	PSU	C1'-C5	4.54	1.60	1.50
1	2	1447	OMG	C5-C6	-4.52	1.38	1.47
1	2	1056	PSU	C1'-C5	4.50	1.60	1.50
1	2	105	PSU	C1'-C5	4.46	1.60	1.50
1	2	517	OMC	C4-N4	4.45	1.44	1.33
1	2	1136	PSU	C1'-C5	4.44	1.60	1.50
1	2	1347	PSU	C1'-C5	4.43	1.60	1.50
1	2	1445	PSU	C1'-C5	4.41	1.60	1.50
1	2	815	PSU	C1'-C5	4.40	1.60	1.50
1	2	1232	PSU	C1'-C5	4.39	1.60	1.50
1	2	681	PSU	C1'-C5	4.39	1.60	1.50
1	2	572	PSU	C1'-C5	4.39	1.60	1.50
1	2	1692	PSU	C1'-C5	4.37	1.60	1.50
1	2	406	PSU	C1'-C5	4.37	1.60	1.50
1	2	1248	B8N	C4-N3	-4.36	1.32	1.40
1	2	109	PSU	C1'-C5	4.35	1.60	1.50
1	2	686	PSU	C1'-C5	4.35	1.60	1.50
1	2	1643	PSU	C1'-C5	4.35	1.60	1.50
1	2	36	PSU	C1'-C5	4.32	1.60	1.50
1	2	296	PSU	C1'-C5	4.31	1.60	1.50
1	2	651	PSU	C1'-C5	4.26	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1248	B8N	C1'-C5	-3.97	1.41	1.50
1	2	354	OMU	C4-N3	-3.85	1.32	1.38
1	2	1081	PSU	C2-N3	-3.84	1.31	1.37
1	2	36	PSU	C2-N3	-3.83	1.31	1.37
1	2	1248	B8N	C2-N3	-3.81	1.32	1.38
1	2	1337	4AC	C4-N4	3.81	1.45	1.39
1	2	1337	4AC	C2-N1	-3.79	1.32	1.40
1	2	119	PSU	C2-N3	-3.78	1.31	1.37
1	2	1842	4AC	C4-N4	3.76	1.45	1.39
1	2	296	PSU	C2-N1	-3.74	1.31	1.36
1	2	1337	4AC	C7-N4	3.74	1.44	1.37
1	2	1842	4AC	C7-N4	3.74	1.44	1.37
1	2	121	OMU	C4-N3	-3.73	1.32	1.38
1	2	406	PSU	C2-N3	-3.72	1.31	1.37
1	2	1842	4AC	C2-N1	-3.72	1.32	1.40
1	2	1347	PSU	C2-N3	-3.72	1.31	1.37
1	2	1248	B8N	C4-C5	-3.71	1.39	1.47
1	2	814	PSU	C2-N1	-3.71	1.31	1.36
1	2	651	PSU	C2-N3	-3.71	1.31	1.37
1	2	1692	PSU	C2-N3	-3.70	1.31	1.37
1	2	814	PSU	C2-N3	-3.69	1.31	1.37
1	2	93	PSU	C2-N3	-3.68	1.31	1.37
1	2	649	PSU	C2-N3	-3.67	1.31	1.37
1	2	681	PSU	C2-N3	-3.66	1.31	1.37
1	2	1081	PSU	C2-N1	-3.65	1.31	1.36
1	2	822	PSU	C2-N3	-3.64	1.31	1.37
1	2	406	PSU	C2-N1	-3.63	1.31	1.36
1	2	1046	PSU	C2-N1	-3.63	1.31	1.36
1	2	36	PSU	C2-N1	-3.62	1.31	1.36
1	2	36	PSU	C4-N3	-3.62	1.32	1.38
1	2	105	PSU	C2-N3	-3.61	1.31	1.37
1	2	572	PSU	C2-N3	-3.60	1.31	1.37
1	2	1136	PSU	C2-N3	-3.59	1.31	1.37
1	2	1174	PSU	C2-N1	-3.59	1.32	1.36
1	2	1232	PSU	C2-N3	-3.58	1.31	1.37
1	2	863	PSU	C2-N3	-3.57	1.31	1.37
1	2	109	PSU	C2-N3	-3.57	1.31	1.37
1	2	1174	PSU	C2-N3	-3.56	1.31	1.37
1	2	815	PSU	C2-N3	-3.56	1.31	1.37
1	2	1643	PSU	C2-N3	-3.54	1.31	1.37
1	2	119	PSU	C2-N1	-3.54	1.32	1.36
1	2	1442	OMU	C4-N3	-3.54	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	109	PSU	C2-N1	-3.53	1.32	1.36
1	2	1326	OMU	C2-N1	-3.53	1.32	1.38
1	2	822	PSU	C2-N1	-3.52	1.32	1.36
1	2	651	PSU	C4-N3	-3.52	1.32	1.38
1	2	1045	PSU	C2-N3	-3.51	1.31	1.37
1	2	1177	PSU	C2-N3	-3.51	1.31	1.37
1	2	649	PSU	C2-N1	-3.51	1.32	1.36
1	2	121	OMU	C2-N1	-3.51	1.33	1.38
1	2	105	PSU	C4-N3	-3.51	1.32	1.38
1	2	863	PSU	C2-N1	-3.50	1.32	1.36
1	2	1692	PSU	C4-N3	-3.50	1.32	1.38
1	2	651	PSU	C2-N1	-3.50	1.32	1.36
1	2	1347	PSU	C4-N3	-3.50	1.32	1.38
1	2	1244	PSU	C2-N3	-3.50	1.31	1.37
1	2	1238	PSU	C2-N3	-3.49	1.31	1.37
1	2	815	PSU	C2-N1	-3.49	1.32	1.36
1	2	1056	PSU	C2-N3	-3.48	1.31	1.37
1	2	406	PSU	C4-N3	-3.48	1.32	1.38
1	2	296	PSU	C2-N3	-3.48	1.31	1.37
1	2	681	PSU	C2-N1	-3.48	1.32	1.36
1	2	105	PSU	C2-N1	-3.46	1.32	1.36
1	2	822	PSU	C4-N3	-3.45	1.32	1.38
1	2	428	OMU	C4-N3	-3.45	1.32	1.38
1	2	1232	PSU	C4-N3	-3.45	1.32	1.38
1	2	93	PSU	C2-N1	-3.44	1.32	1.36
1	2	1625	PSU	C2-N3	-3.44	1.31	1.37
1	2	1347	PSU	C2-N1	-3.44	1.32	1.36
1	2	116	OMU	C4-N3	-3.43	1.32	1.38
1	2	172	OMU	C4-N3	-3.42	1.32	1.38
1	2	1288	OMU	C4-N3	-3.42	1.32	1.38
1	2	814	PSU	C4-N3	-3.42	1.32	1.38
1	2	119	PSU	C4-N3	-3.41	1.32	1.38
1	2	109	PSU	C4-N3	-3.41	1.32	1.38
1	2	462	OMC	C2-N1	-3.41	1.32	1.40
1	2	1692	PSU	C2-N1	-3.40	1.32	1.36
1	2	686	PSU	C2-N3	-3.40	1.31	1.37
1	2	1445	PSU	C2-N3	-3.40	1.31	1.37
1	2	572	PSU	C4-N3	-3.40	1.32	1.38
1	2	1391	OMC	C2-N1	-3.39	1.33	1.40
1	2	1136	PSU	C4-N3	-3.39	1.32	1.38
1	2	681	PSU	C4-N3	-3.39	1.32	1.38
1	2	649	PSU	C4-N3	-3.39	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	863	PSU	C4-N3	-3.39	1.32	1.38
1	2	1625	PSU	C2-N1	-3.39	1.32	1.36
1	2	172	OMU	C2-N1	-3.38	1.33	1.38
1	2	1046	PSU	C2-N3	-3.38	1.31	1.37
1	2	572	PSU	C2-N1	-3.37	1.32	1.36
1	2	174	OMC	C2-N1	-3.37	1.33	1.40
1	2	1643	PSU	C2-N1	-3.37	1.32	1.36
1	2	815	PSU	C4-N3	-3.37	1.32	1.38
1	2	1703	OMC	C2-N1	-3.36	1.33	1.40
1	2	428	OMU	C2-N1	-3.36	1.33	1.38
1	2	1081	PSU	C4-N3	-3.36	1.32	1.38
1	2	1326	OMU	C4-N3	-3.35	1.32	1.38
1	2	1056	PSU	C4-N3	-3.34	1.32	1.38
1	2	296	PSU	C4-N3	-3.34	1.32	1.38
1	2	93	PSU	C4-N3	-3.33	1.32	1.38
1	2	517	OMC	C2-N1	-3.33	1.33	1.40
1	2	1643	PSU	C4-N3	-3.33	1.32	1.38
1	2	1238	PSU	C2-N1	-3.32	1.32	1.36
1	2	1177	PSU	C2-N1	-3.32	1.32	1.36
1	2	1174	PSU	C4-N3	-3.31	1.32	1.38
1	2	1232	PSU	C2-N1	-3.29	1.32	1.36
1	2	1045	PSU	C2-N1	-3.29	1.32	1.36
1	2	116	OMU	C2-N1	-3.28	1.33	1.38
1	2	1056	PSU	C2-N1	-3.28	1.32	1.36
1	2	1136	PSU	C2-N1	-3.28	1.32	1.36
1	2	1177	PSU	C4-N3	-3.28	1.32	1.38
1	2	1244	PSU	C2-N1	-3.27	1.32	1.36
1	2	1272	OMC	C2-N1	-3.26	1.33	1.40
1	2	1244	PSU	C4-N3	-3.26	1.32	1.38
1	2	1445	PSU	C4-N3	-3.25	1.32	1.38
1	2	686	PSU	C4-N3	-3.25	1.32	1.38
1	2	1045	PSU	C4-N3	-3.25	1.32	1.38
1	2	1238	PSU	C4-N3	-3.24	1.32	1.38
1	2	1625	PSU	C4-N3	-3.23	1.32	1.38
1	2	1445	PSU	C2-N1	-3.22	1.32	1.36
1	2	686	PSU	C2-N1	-3.21	1.32	1.36
1	2	1639	7MG	C8-N9	3.20	1.47	1.45
1	2	1046	PSU	C4-N3	-3.20	1.32	1.38
1	2	1639	7MG	C6-N1	-3.11	1.33	1.38
1	2	159	A2M	O2'-C2'	3.09	1.50	1.42
1	2	354	OMU	C2-N1	-3.09	1.33	1.38
1	2	296	PSU	O2-C2	-3.07	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1678	A2M	O2'-C2'	3.05	1.50	1.42
1	2	354	OMU	C2-N3	-3.05	1.32	1.38
1	2	105	PSU	O2-C2	-3.02	1.16	1.23
1	2	166	A2M	O2'-C2'	3.00	1.50	1.42
1	2	1442	OMU	C2-N1	-3.00	1.33	1.38
1	2	1383	A2M	O2'-C2'	2.99	1.50	1.42
1	2	484	A2M	O2'-C2'	2.98	1.50	1.42
1	2	576	A2M	O2'-C2'	2.97	1.50	1.42
1	2	590	A2M	O2'-C2'	2.97	1.49	1.42
1	2	36	PSU	O2-C2	-2.95	1.17	1.23
1	2	121	OMU	C2-N3	-2.95	1.32	1.38
1	2	668	A2M	O2'-C2'	2.94	1.49	1.42
1	2	814	PSU	O2-C2	-2.93	1.17	1.23
1	2	406	PSU	O2-C2	-2.93	1.17	1.23
1	2	512	A2M	O2'-C2'	2.93	1.49	1.42
1	2	1643	PSU	O2-C2	-2.91	1.17	1.23
1	2	649	PSU	O2-C2	-2.91	1.17	1.23
1	2	1031	A2M	O2'-C2'	2.91	1.49	1.42
1	2	1692	PSU	O2-C2	-2.90	1.17	1.23
1	2	468	A2M	O2'-C2'	2.90	1.49	1.42
1	2	1232	PSU	O2-C2	-2.90	1.17	1.23
1	2	651	PSU	O2-C2	-2.90	1.17	1.23
1	2	99	A2M	O2'-C2'	2.90	1.49	1.42
1	2	815	PSU	O2-C2	-2.89	1.17	1.23
1	2	509	OMG	C6-N1	-2.89	1.33	1.37
1	2	572	PSU	O2-C2	-2.89	1.17	1.23
1	2	109	PSU	O2-C2	-2.89	1.17	1.23
1	2	681	PSU	O2-C2	-2.88	1.17	1.23
1	2	1347	PSU	O2-C2	-2.88	1.17	1.23
1	2	822	PSU	O2-C2	-2.88	1.17	1.23
1	2	1174	PSU	O2-C2	-2.87	1.17	1.23
1	2	1391	OMC	O2-C2	-2.87	1.18	1.23
1	2	1081	PSU	O2-C2	-2.86	1.17	1.23
1	2	1046	PSU	O2-C2	-2.86	1.17	1.23
1	2	93	PSU	O2-C2	-2.85	1.17	1.23
1	2	863	PSU	O2-C2	-2.84	1.17	1.23
1	2	1136	PSU	O2-C2	-2.84	1.17	1.23
1	2	1248	B8N	C6-C5	2.83	1.39	1.35
1	2	1244	PSU	O2-C2	-2.83	1.17	1.23
1	2	119	PSU	O2-C2	-2.83	1.17	1.23
1	2	1056	PSU	O2-C2	-2.82	1.17	1.23
1	2	1177	PSU	O2-C2	-2.81	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1445	PSU	O2-C2	-2.80	1.17	1.23
1	2	462	OMC	O2-C2	-2.80	1.18	1.23
1	2	1337	4AC	CM7-C7	2.80	1.56	1.50
1	2	1045	PSU	O2-C2	-2.77	1.17	1.23
1	2	1337	4AC	C6-N1	-2.76	1.31	1.38
1	2	174	OMC	O2-C2	-2.76	1.18	1.23
1	2	1703	OMC	O2-C2	-2.75	1.18	1.23
1	2	1238	PSU	O2-C2	-2.75	1.17	1.23
1	2	686	PSU	O2-C2	-2.74	1.17	1.23
1	2	517	OMC	O2-C2	-2.74	1.18	1.23
1	2	1625	PSU	O2-C2	-2.73	1.17	1.23
1	2	1337	4AC	O2-C2	-2.72	1.18	1.23
1	2	27	A2M	O2'-C2'	2.71	1.49	1.42
1	2	1232	PSU	C6-C5	2.69	1.38	1.35
1	2	1442	OMU	C2-N3	-2.69	1.33	1.38
1	2	1272	OMC	O2-C2	-2.68	1.18	1.23
1	2	428	OMU	C2-N3	-2.67	1.33	1.38
1	2	172	OMU	C2-N3	-2.65	1.33	1.38
1	2	1326	OMU	C2-N3	-2.63	1.33	1.38
1	2	1625	PSU	C6-C5	2.63	1.38	1.35
1	2	1238	PSU	C6-C5	2.62	1.38	1.35
1	2	1842	4AC	C6-N1	-2.60	1.31	1.38
1	2	116	OMU	C2-N3	-2.59	1.33	1.38
1	2	1842	4AC	O2-C2	-2.58	1.18	1.23
1	2	649	PSU	C6-C5	2.57	1.38	1.35
1	2	406	PSU	C6-C5	2.56	1.38	1.35
1	2	1174	PSU	C6-C5	2.54	1.38	1.35
1	2	601	OMG	C6-N1	-2.51	1.34	1.37
1	2	436	OMG	C6-N1	-2.48	1.34	1.37
1	2	1244	PSU	C6-C5	2.47	1.38	1.35
1	2	93	PSU	C6-C5	2.47	1.38	1.35
1	2	1490	OMG	C6-N1	-2.46	1.34	1.37
1	2	1081	PSU	C6-C5	2.45	1.38	1.35
1	2	644	OMG	C6-N1	-2.43	1.34	1.37
1	2	1442	OMU	O2-C2	-2.42	1.18	1.23
1	2	1045	PSU	C6-C5	2.41	1.38	1.35
1	2	815	PSU	C6-C5	2.41	1.38	1.35
1	2	863	PSU	C6-C5	2.41	1.38	1.35
1	2	686	PSU	C6-C5	2.40	1.38	1.35
1	2	1177	PSU	C6-C5	2.40	1.37	1.35
1	2	1288	OMU	C2-N3	-2.40	1.33	1.38
1	2	116	OMU	O2-C2	-2.39	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	121	OMU	O2-C2	-2.39	1.18	1.23
1	2	683	OMG	C6-N1	-2.39	1.34	1.37
1	2	517	OMC	C2-N3	-2.39	1.31	1.36
1	2	428	OMU	O2-C2	-2.39	1.18	1.23
1	2	172	OMU	O2-C2	-2.38	1.18	1.23
1	2	428	OMU	C6-C5	2.37	1.40	1.35
1	2	1326	OMU	O2-C2	-2.35	1.18	1.23
1	2	572	PSU	C6-C5	2.33	1.37	1.35
1	2	462	OMC	C6-N1	-2.33	1.32	1.38
1	2	651	PSU	C6-C5	2.32	1.37	1.35
1	2	1692	PSU	C6-C5	2.32	1.37	1.35
1	2	1288	OMU	C6-C5	2.32	1.40	1.35
1	2	1442	OMU	C6-C5	2.31	1.40	1.35
1	2	172	OMU	C6-C5	2.31	1.40	1.35
1	2	172	OMU	C6-N1	-2.30	1.32	1.38
1	2	354	OMU	O2-C2	-2.30	1.19	1.23
1	2	1391	OMC	C6-N1	-2.30	1.32	1.38
1	2	1445	PSU	C6-C5	2.30	1.37	1.35
1	2	1447	OMG	C6-N1	-2.29	1.34	1.37
1	2	36	PSU	C6-C5	2.29	1.37	1.35
1	2	1347	PSU	C6-C5	2.27	1.37	1.35
1	2	1248	B8N	C2-N1	-2.27	1.32	1.39
1	2	1326	OMU	C6-C5	2.26	1.40	1.35
1	2	1643	PSU	C6-C5	2.25	1.37	1.35
1	2	822	PSU	C6-C5	2.25	1.37	1.35
1	2	105	PSU	C6-C5	2.24	1.37	1.35
1	2	296	PSU	C6-N1	-2.23	1.32	1.36
1	2	1328	OMG	C6-N1	-2.22	1.34	1.37
1	2	174	OMC	C6-N1	-2.22	1.32	1.38
1	2	1136	PSU	C6-C5	2.22	1.37	1.35
1	2	121	OMU	C6-C5	2.22	1.40	1.35
1	2	1272	OMC	C6-N1	-2.21	1.32	1.38
1	2	354	OMU	C6-C5	2.21	1.40	1.35
1	2	668	A2M	C1'-N9	-2.20	1.44	1.49
1	2	1046	PSU	C6-C5	2.20	1.37	1.35
1	2	1842	4AC	CM7-C7	2.20	1.55	1.50
1	2	509	OMG	C2-N1	-2.20	1.32	1.37
1	2	1326	OMU	C6-N1	-2.19	1.32	1.38
1	2	1703	OMC	C6-N1	-2.18	1.32	1.38
1	2	428	OMU	C6-N1	-2.18	1.32	1.38
1	2	174	OMC	C2-N3	-2.17	1.32	1.36
1	2	116	OMU	C6-C5	2.17	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1288	OMU	C2-N1	-2.17	1.35	1.38
1	2	1391	OMC	C2-N3	-2.16	1.32	1.36
1	2	822	PSU	O4'-C1'	-2.15	1.40	1.43
1	2	462	OMC	C2-N3	-2.15	1.32	1.36
1	2	116	OMU	C6-N1	-2.14	1.33	1.38
1	2	1703	OMC	C2-N3	-2.14	1.32	1.36
1	2	1842	4AC	C2-N3	-2.13	1.32	1.36
1	2	109	PSU	C6-C5	2.12	1.37	1.35
1	2	1056	PSU	C6-C5	2.12	1.37	1.35
1	2	814	PSU	C6-C5	2.11	1.37	1.35
1	2	119	PSU	C6-C5	2.11	1.37	1.35
1	2	116	OMU	C5-C4	-2.10	1.39	1.43
1	2	517	OMC	C6-N1	-2.10	1.33	1.38
1	2	1337	4AC	C2-N3	-2.08	1.32	1.36
1	2	121	OMU	C5-C4	-2.07	1.39	1.43
1	2	681	PSU	C6-C5	2.06	1.37	1.35
1	2	576	A2M	C1'-N9	-2.06	1.44	1.49
1	2	1288	OMU	O2-C2	-2.05	1.19	1.23
1	2	814	PSU	C6-N1	-2.04	1.33	1.36
1	2	681	PSU	C6-N1	-2.04	1.33	1.36
1	2	1442	OMU	C6-N1	-2.04	1.33	1.38
1	2	1081	PSU	O4'-C1'	-2.03	1.41	1.43
1	2	354	OMU	C5-C4	-2.02	1.39	1.43
1	2	1046	PSU	C6-N1	-2.00	1.33	1.36
1	2	1248	B8N	C6-N1	-2.00	1.32	1.36

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	590	A2M	C4'-O4'-C1'	-7.78	102.80	109.92
1	2	1842	4AC	CM7-C7-N4	7.29	127.03	115.27
1	2	1832	6MZ	C2-N1-C6	6.93	121.98	116.60
1	2	1232	PSU	N1-C2-N3	6.44	121.96	115.17
1	2	105	PSU	N1-C2-N3	6.35	121.87	115.17
1	2	1337	4AC	CM7-C7-N4	6.32	125.47	115.27
1	2	296	PSU	N1-C2-N3	6.31	121.83	115.17
1	2	815	PSU	N1-C2-N3	6.24	121.75	115.17
1	2	406	PSU	N1-C2-N3	6.20	121.71	115.17
1	2	651	PSU	N1-C2-N3	6.20	121.70	115.17
1	2	649	PSU	N1-C2-N3	6.19	121.69	115.17
1	2	109	PSU	N1-C2-N3	6.14	121.64	115.17
1	2	572	PSU	N1-C2-N3	6.10	121.60	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1643	PSU	N1-C2-N3	6.09	121.59	115.17
1	2	1445	PSU	N1-C2-N3	6.07	121.58	115.17
1	2	1174	PSU	N1-C2-N3	6.06	121.56	115.17
1	2	1347	PSU	N1-C2-N3	6.05	121.55	115.17
1	2	686	PSU	N1-C2-N3	6.04	121.54	115.17
1	2	1238	PSU	N1-C2-N3	6.03	121.53	115.17
1	2	1692	PSU	N1-C2-N3	6.02	121.51	115.17
1	2	822	PSU	N1-C2-N3	5.99	121.49	115.17
1	2	1244	PSU	N1-C2-N3	5.98	121.47	115.17
1	2	1046	PSU	N1-C2-N3	5.97	121.47	115.17
1	2	863	PSU	N1-C2-N3	5.96	121.45	115.17
1	2	814	PSU	N1-C2-N3	5.93	121.42	115.17
1	2	1136	PSU	N1-C2-N3	5.93	121.42	115.17
1	2	93	PSU	N1-C2-N3	5.89	121.39	115.17
1	2	1851	MA6	N3-C2-N1	-5.89	120.67	128.67
1	2	681	PSU	N1-C2-N3	5.87	121.36	115.17
1	2	1177	PSU	N1-C2-N3	5.86	121.35	115.17
1	2	1625	PSU	N1-C2-N3	5.86	121.35	115.17
1	2	1045	PSU	N1-C2-N3	5.84	121.33	115.17
1	2	1056	PSU	N1-C2-N3	5.84	121.33	115.17
1	2	36	PSU	N1-C2-N3	5.83	121.31	115.17
1	2	1081	PSU	N1-C2-N3	5.69	121.17	115.17
1	2	1850	MA6	N3-C2-N1	-5.65	121.00	128.67
1	2	1832	6MZ	N3-C2-N1	-5.64	121.02	128.67
1	2	119	PSU	N1-C2-N3	5.57	121.04	115.17
1	2	1442	OMU	N3-C2-N1	5.51	122.06	114.89
1	2	116	OMU	N3-C2-N1	5.35	121.85	114.89
1	2	172	OMU	N3-C2-N1	5.34	121.84	114.89
1	2	428	OMU	N3-C2-N1	5.32	121.81	114.89
1	2	512	A2M	N3-C2-N1	-5.31	121.46	128.67
1	2	354	OMU	N3-C2-N1	5.31	121.81	114.89
1	2	121	OMU	N3-C2-N1	5.31	121.80	114.89
1	2	1326	OMU	C4-N3-C2	-5.22	120.13	126.61
1	2	1326	OMU	N3-C2-N1	5.18	121.64	114.89
1	2	428	OMU	C4-N3-C2	-5.06	120.33	126.61
1	2	1639	7MG	C2-N3-C4	4.98	120.88	112.30
1	2	1639	7MG	N9-C4-N3	4.98	132.75	125.46
1	2	27	A2M	N3-C2-N1	-4.91	122.00	128.67
1	2	166	A2M	N3-C2-N1	-4.89	122.03	128.67
1	2	172	OMU	C4-N3-C2	-4.88	120.55	126.61
1	2	1288	OMU	N3-C2-N1	4.87	121.23	114.89
1	2	1639	7MG	C5-C4-N3	-4.85	119.02	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1851	MA6	C2-N1-C6	4.85	121.60	116.84
1	2	468	A2M	N3-C2-N1	-4.84	122.10	128.67
1	2	1031	A2M	N3-C2-N1	-4.83	122.12	128.67
1	2	1850	MA6	C2-N1-C6	4.82	121.57	116.84
1	2	590	A2M	N3-C2-N1	-4.81	122.14	128.67
1	2	668	A2M	C4'-O4'-C1'	-4.80	105.53	109.92
1	2	1383	A2M	N3-C2-N1	-4.80	122.16	128.67
1	2	668	A2M	N3-C2-N1	-4.79	122.17	128.67
1	2	1678	A2M	N3-C2-N1	-4.75	122.23	128.67
1	2	1232	PSU	C4-N3-C2	-4.73	119.85	126.37
1	2	1442	OMU	C4-N3-C2	-4.73	120.74	126.61
1	2	99	A2M	N3-C2-N1	-4.70	122.30	128.67
1	2	1136	PSU	C4-N3-C2	-4.69	119.91	126.37
1	2	109	PSU	C4-N3-C2	-4.59	120.05	126.37
1	2	484	A2M	N3-C2-N1	-4.57	122.47	128.67
1	2	1832	6MZ	C9-N6-C6	4.56	127.08	122.85
1	2	572	PSU	C4-N3-C2	-4.54	120.11	126.37
1	2	1445	PSU	C4-N3-C2	-4.54	120.12	126.37
1	2	822	PSU	C4-N3-C2	-4.53	120.13	126.37
1	2	1177	PSU	C4-N3-C2	-4.51	120.16	126.37
1	2	815	PSU	C4-N3-C2	-4.50	120.17	126.37
1	2	1244	PSU	C4-N3-C2	-4.50	120.17	126.37
1	2	105	PSU	C4-N3-C2	-4.47	120.21	126.37
1	2	576	A2M	N3-C2-N1	-4.45	122.63	128.67
1	2	651	PSU	C4-N3-C2	-4.44	120.25	126.37
1	2	686	PSU	C4-N3-C2	-4.44	120.25	126.37
1	2	649	PSU	C4-N3-C2	-4.43	120.26	126.37
1	2	1643	PSU	C4-N3-C2	-4.40	120.31	126.37
1	2	296	PSU	C4-N3-C2	-4.40	120.32	126.37
1	2	863	PSU	C4-N3-C2	-4.39	120.32	126.37
1	2	159	A2M	N3-C2-N1	-4.39	122.71	128.67
1	2	1045	PSU	C4-N3-C2	-4.39	120.33	126.37
1	2	1174	PSU	C4-N3-C2	-4.38	120.33	126.37
1	2	119	PSU	C4-N3-C2	-4.35	120.38	126.37
1	2	1347	PSU	C4-N3-C2	-4.34	120.39	126.37
1	2	296	PSU	O2-C2-N1	-4.30	118.35	122.79
1	2	1046	PSU	C4-N3-C2	-4.27	120.49	126.37
1	2	93	PSU	C4-N3-C2	-4.26	120.50	126.37
1	2	814	PSU	C4-N3-C2	-4.24	120.54	126.37
1	2	1639	7MG	C5-C6-N1	4.22	118.37	110.94
1	2	1692	PSU	C4-N3-C2	-4.22	120.56	126.37
1	2	1288	OMU	C1'-N1-C2	4.21	125.15	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	681	PSU	C4-N3-C2	-4.18	120.61	126.37
1	2	1056	PSU	C4-N3-C2	-4.17	120.63	126.37
1	2	1238	PSU	C4-N3-C2	-4.16	120.64	126.37
1	2	1248	B8N	C4-N3-C2	-4.15	120.52	125.62
1	2	354	OMU	C4-N3-C2	-4.13	121.49	126.61
1	2	406	PSU	C4-N3-C2	-4.11	120.70	126.37
1	2	1625	PSU	C4-N3-C2	-4.06	120.77	126.37
1	2	1081	PSU	C4-N3-C2	-4.06	120.78	126.37
1	2	1851	MA6	C4-C5-N7	-4.06	105.05	109.34
1	2	436	OMG	C8-N7-C5	3.95	109.28	102.55
1	2	683	OMG	C8-N7-C5	3.95	109.27	102.55
1	2	116	OMU	C4-N3-C2	-3.94	121.72	126.61
1	2	517	OMC	O2-C2-N3	-3.93	116.13	122.33
1	2	36	PSU	C4-N3-C2	-3.93	120.96	126.37
1	2	1832	6MZ	C4-C5-N7	-3.93	105.19	109.34
1	2	1678	A2M	C4'-O4'-C1'	-3.90	106.35	109.92
1	2	1328	OMG	C8-N7-C5	3.89	109.18	102.55
1	2	644	OMG	C8-N7-C5	3.89	109.17	102.55
1	2	601	OMG	C8-N7-C5	3.88	109.16	102.55
1	2	1490	OMG	C8-N7-C5	3.80	109.02	102.55
1	2	1447	OMG	C8-N7-C5	3.80	109.02	102.55
1	2	1248	B8N	N3-C2-N1	3.80	121.36	116.72
1	2	1046	PSU	O2-C2-N1	-3.79	118.88	122.79
1	2	1174	PSU	O2-C2-N1	-3.77	118.90	122.79
1	2	509	OMG	C8-N7-C5	3.76	108.95	102.55
1	2	109	PSU	O2-C2-N1	-3.71	118.96	122.79
1	2	121	OMU	C4-N3-C2	-3.71	122.00	126.61
1	2	468	A2M	C4'-O4'-C1'	-3.63	106.60	109.92
1	2	1850	MA6	C4-C5-N7	-3.61	105.52	109.34
1	2	1703	OMC	O2-C2-N3	-3.59	116.66	122.33
1	2	815	PSU	O2-C2-N1	-3.57	119.10	122.79
1	2	166	A2M	C4'-O4'-C1'	-3.55	106.67	109.92
1	2	1643	PSU	O2-C2-N1	-3.54	119.13	122.79
1	2	1326	OMU	C5-C4-N3	3.51	119.72	114.80
1	2	105	PSU	O2-C2-N1	-3.48	119.20	122.79
1	2	1288	OMU	C4-N3-C2	-3.46	122.32	126.61
1	2	649	PSU	O2-C2-N1	-3.46	119.22	122.79
1	2	1238	PSU	O2-C2-N1	-3.44	119.25	122.79
1	2	1445	PSU	O2-C2-N1	-3.43	119.25	122.79
1	2	462	OMC	O2-C2-N3	-3.41	116.96	122.33
1	2	1842	4AC	O7-C7-CM7	-3.40	116.00	122.05
1	2	428	OMU	C5-C4-N3	3.39	119.55	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	686	PSU	O2-C2-N1	-3.39	119.30	122.79
1	2	1391	OMC	O2-C2-N3	-3.38	117.00	122.33
1	2	822	PSU	O2-C2-N1	-3.38	119.30	122.79
1	2	572	PSU	O2-C2-N1	-3.37	119.31	122.79
1	2	1625	PSU	O2-C2-N1	-3.36	119.33	122.79
1	2	1045	PSU	O2-C2-N1	-3.35	119.33	122.79
1	2	1337	4AC	O7-C7-N4	-3.34	116.64	121.90
1	2	814	PSU	O2-C2-N1	-3.34	119.34	122.79
1	2	1244	PSU	O2-C2-N1	-3.34	119.35	122.79
1	2	406	PSU	O2-C2-N1	-3.32	119.36	122.79
1	2	1136	PSU	O2-C2-N1	-3.32	119.36	122.79
1	2	651	PSU	O2-C2-N1	-3.32	119.36	122.79
1	2	1056	PSU	O2-C2-N1	-3.32	119.36	122.79
1	2	174	OMC	O2-C2-N3	-3.32	117.10	122.33
1	2	1288	OMU	O2-C2-N3	-3.31	115.39	121.49
1	2	863	PSU	O2-C2-N1	-3.29	119.39	122.79
1	2	1177	PSU	O2-C2-N1	-3.28	119.40	122.79
1	2	1232	PSU	O2-C2-N1	-3.27	119.42	122.79
1	2	1347	PSU	O2-C2-N1	-3.26	119.42	122.79
1	2	1442	OMU	C5-C4-N3	3.25	119.35	114.80
1	2	354	OMU	C5-C4-N3	3.23	119.33	114.80
1	2	1272	OMC	O2-C2-N3	-3.21	117.26	122.33
1	2	1692	PSU	O2-C2-N1	-3.17	119.52	122.79
1	2	1383	A2M	C4'-O4'-C1'	-3.15	107.04	109.92
1	2	681	PSU	O2-C2-N1	-3.15	119.54	122.79
1	2	1842	4AC	O2-C2-N3	-3.14	117.37	122.33
1	2	1326	OMU	O4-C4-C5	-3.14	119.74	125.16
1	2	172	OMU	C5-C4-N3	3.14	119.20	114.80
1	2	1842	4AC	O7-C7-N4	-3.13	116.97	121.90
1	2	1081	PSU	O2-C2-N1	-3.13	119.56	122.79
1	2	93	PSU	O2-C2-N1	-3.09	119.60	122.79
1	2	1031	A2M	C4'-O4'-C1'	-2.99	107.18	109.92
1	2	119	PSU	C6-C5-C4	-2.99	116.16	118.17
1	2	119	PSU	O2-C2-N1	-2.98	119.72	122.79
1	2	428	OMU	O4-C4-C5	-2.97	120.04	125.16
1	2	116	OMU	O4-C4-C5	-2.91	120.14	125.16
1	2	1337	4AC	O2-C2-N3	-2.88	117.78	122.33
1	2	1639	7MG	C4-C5-N7	2.88	108.78	105.38
1	2	121	OMU	C5-C4-N3	2.88	118.83	114.80
1	2	36	PSU	O2-C2-N1	-2.87	119.83	122.79
1	2	1081	PSU	C6-C5-C4	-2.83	116.26	118.17
1	2	172	OMU	O4-C4-C5	-2.83	120.28	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	116	OMU	C5-C4-N3	2.82	118.75	114.80
1	2	27	A2M	O4'-C1'-N9	2.82	112.48	108.75
1	2	1326	OMU	O2-C2-N1	-2.75	119.21	122.80
1	2	121	OMU	O4-C4-C5	-2.68	120.53	125.16
1	2	1442	OMU	O4-C4-C5	-2.66	120.58	125.16
1	2	1136	PSU	C5-C6-N1	-2.64	118.48	122.14
1	2	1288	OMU	C5-C4-N3	2.61	118.46	114.80
1	2	1842	4AC	C5-C4-N3	-2.60	118.53	122.60
1	2	354	OMU	O4-C4-C5	-2.57	120.73	125.16
1	2	590	A2M	O4'-C4'-C3'	-2.57	100.06	105.15
1	2	1288	OMU	O4-C4-C5	-2.55	120.77	125.16
1	2	1232	PSU	C5-C6-N1	-2.54	118.61	122.14
1	2	354	OMU	O2-C2-N3	-2.53	116.83	121.49
1	2	1445	PSU	C5-C6-N1	-2.53	118.63	122.14
1	2	1639	7MG	O6-C6-C5	-2.53	121.42	127.62
1	2	109	PSU	C5-C6-N1	-2.52	118.64	122.14
1	2	1842	4AC	C4-N3-C2	2.52	123.44	120.11
1	2	651	PSU	C5-C6-N1	-2.50	118.67	122.14
1	2	1244	PSU	C5-C6-N1	-2.49	118.68	122.14
1	2	1643	PSU	C5-C6-N1	-2.48	118.70	122.14
1	2	428	OMU	O2-C2-N1	-2.48	119.57	122.80
1	2	99	A2M	C4'-O4'-C1'	-2.46	107.67	109.92
1	2	509	OMG	C5-C6-N1	2.45	118.75	114.07
1	2	572	PSU	C5-C6-N1	-2.45	118.74	122.14
1	2	1337	4AC	C5-C4-N3	-2.44	118.78	122.60
1	2	1347	PSU	C5-C6-N1	-2.42	118.79	122.14
1	2	686	PSU	C5-C6-N1	-2.41	118.79	122.14
1	2	1248	B8N	C1'-C5-C4	2.41	121.26	117.61
1	2	172	OMU	O2-C2-N1	-2.40	119.68	122.80
1	2	1692	PSU	C5-C6-N1	-2.39	118.82	122.14
1	2	644	OMG	C5-C6-N1	2.39	118.63	114.07
1	2	822	PSU	C5-C6-N1	-2.38	118.84	122.14
1	2	159	A2M	C4-C5-N7	-2.37	106.83	109.34
1	2	436	OMG	C5-C6-N1	2.37	118.58	114.07
1	2	1447	OMG	C5-C6-N1	2.36	118.57	114.07
1	2	601	OMG	C5-C6-N1	2.36	118.57	114.07
1	2	815	PSU	C5-C6-N1	-2.36	118.87	122.14
1	2	1288	OMU	C1'-N1-C6	-2.35	115.75	120.78
1	2	1326	OMU	C5-C6-N1	-2.35	118.03	121.84
1	2	1442	OMU	O2-C2-N3	-2.34	117.17	121.49
1	2	1337	4AC	O7-C7-CM7	-2.34	117.89	122.05
1	2	683	OMG	C5-C6-N1	2.33	118.52	114.07

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	105	PSU	C5-C6-N1	-2.32	118.92	122.14
1	2	1328	OMG	C5-C6-N1	2.31	118.48	114.07
1	2	668	A2M	C3'-C2'-C1'	2.31	107.22	102.81
1	2	1045	PSU	C5-C6-N1	-2.30	118.94	122.14
1	2	1678	A2M	C4-C5-N7	-2.30	106.90	109.34
1	2	822	PSU	O4'-C1'-C2'	2.30	108.33	105.15
1	2	1490	OMG	C5-C6-N1	2.26	118.39	114.07
1	2	1177	PSU	C5-C6-N1	-2.26	119.00	122.14
1	2	649	PSU	C5-C6-N1	-2.24	119.03	122.14
1	2	576	A2M	C4'-O4'-C1'	-2.24	107.88	109.92
1	2	406	PSU	C5-C6-N1	-2.23	119.05	122.14
1	2	484	A2M	C4-C5-N7	-2.22	106.99	109.34
1	2	428	OMU	C5-C6-N1	-2.21	118.24	121.84
1	2	1238	PSU	C5-C6-N1	-2.21	119.07	122.14
1	2	36	PSU	C5-C6-N1	-2.20	119.09	122.14
1	2	1174	PSU	C5-C6-N1	-2.20	119.09	122.14
1	2	668	A2M	C4-C5-N7	-2.19	107.02	109.34
1	2	590	A2M	O4'-C1'-N9	2.19	111.65	108.75
1	2	484	A2M	O4'-C1'-N9	2.18	111.64	108.75
1	2	1056	PSU	C5-C6-N1	-2.16	119.14	122.14
1	2	863	PSU	C5-C6-N1	-2.15	119.15	122.14
1	2	27	A2M	C4-C5-N7	-2.15	107.07	109.34
1	2	159	A2M	O4'-C1'-N9	2.15	111.59	108.75
1	2	1081	PSU	O4'-C1'-C2'	2.13	108.09	105.15
1	2	1842	4AC	C5-C4-N4	2.12	126.52	122.94
1	2	1639	7MG	C2-N1-C6	-2.09	121.32	125.11
1	2	668	A2M	O4'-C1'-N9	-2.09	105.97	108.75
1	2	166	A2M	C4-C5-N7	-2.09	107.13	109.34
1	2	509	OMG	C2-N1-C6	-2.08	121.30	125.11
1	2	1643	PSU	O4'-C1'-C2'	2.08	108.03	105.15
1	2	681	PSU	C5-C6-N1	-2.08	119.26	122.14
1	2	1639	7MG	C6-C5-C4	-2.07	118.76	122.40
1	2	1248	B8N	C5-C4-N3	2.05	119.88	116.15
1	2	1625	PSU	C5-C6-N1	-2.04	119.31	122.14
1	2	93	PSU	C5-C6-N1	-2.03	119.32	122.14
1	2	1842	4AC	O2-C2-N1	2.03	122.87	118.90
1	2	1445	PSU	O4'-C1'-C2'	2.02	107.94	105.15
1	2	1248	B8N	O4'-C1'-C2'	2.02	107.94	105.15
1	2	296	PSU	C5-C6-N1	-2.01	119.35	122.14
1	2	121	OMU	O2-C2-N3	-2.00	117.79	121.49

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	512	A2M	O4'-C4'-C5'-O5'
1	2	601	OMG	C1'-C2'-O2'-CM2
1	2	668	A2M	O4'-C4'-C5'-O5'
1	2	668	A2M	C3'-C4'-C5'-O5'
1	2	1248	B8N	O4'-C4'-C5'-O5'
1	2	1337	4AC	N3-C4-N4-C7
1	2	1337	4AC	C5-C4-N4-C7
1	2	1850	MA6	C5-C6-N6-C10
1	2	1851	MA6	O4'-C4'-C5'-O5'
1	2	99	A2M	O4'-C4'-C5'-O5'
1	2	576	A2M	C3'-C4'-C5'-O5'
1	2	1248	B8N	C3'-C4'-C5'-O5'
1	2	1850	MA6	N1-C6-N6-C10
1	2	1851	MA6	N1-C6-N6-C10
1	2	1447	OMG	C3'-C4'-C5'-O5'
1	2	1851	MA6	C3'-C4'-C5'-O5'
1	2	512	A2M	C3'-C4'-C5'-O5'
1	2	576	A2M	O4'-C4'-C5'-O5'
1	2	1045	PSU	O4'-C4'-C5'-O5'
1	2	428	OMU	O4'-C4'-C5'-O5'
1	2	1045	PSU	C3'-C4'-C5'-O5'
1	2	99	A2M	C3'-C4'-C5'-O5'
1	2	1447	OMG	O4'-C4'-C5'-O5'
1	2	1337	4AC	O7-C7-N4-C4
1	2	1337	4AC	CM7-C7-N4-C4
1	2	1842	4AC	O7-C7-N4-C4
1	2	1842	4AC	CM7-C7-N4-C4
1	2	428	OMU	C3'-C4'-C5'-O5'
1	2	683	OMG	O4'-C4'-C5'-O5'
1	2	1248	B8N	N3-C31-C32-C33
1	2	1248	B8N	O4'-C1'-C5-C4
1	2	1490	OMG	C4'-C5'-O5'-P
1	2	644	OMG	C4'-C5'-O5'-P
1	2	1081	PSU	C4'-C5'-O5'-P
1	2	119	PSU	O4'-C4'-C5'-O5'
1	2	1639	7MG	C2'-C1'-N9-C8
1	2	1248	B8N	C32-C33-C34-O36
1	2	428	OMU	C2'-C1'-N1-C6
1	2	1248	B8N	C32-C33-C34-O35
1	2	428	OMU	O4'-C1'-N1-C6
1	2	683	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	509	OMG	2	0
1	2	681	PSU	1	0
1	2	1337	4AC	2	0
1	2	1232	PSU	1	0
1	2	1383	A2M	1	0
1	2	1842	4AC	1	0
1	2	601	OMG	1	0
1	2	484	A2M	1	0
1	2	1031	A2M	1	0
1	2	166	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 166 ligands modelled in this entry, 166 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.

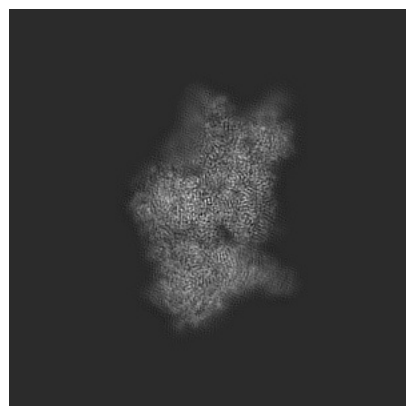
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47929. These allow visual inspection of the internal detail of the map and identification of artifacts.

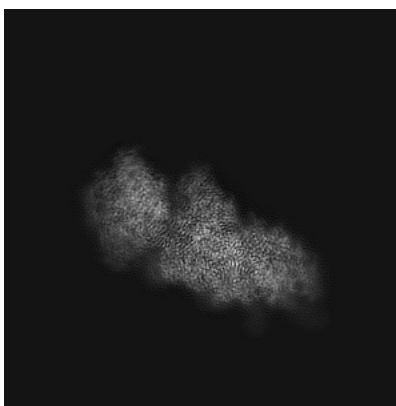
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

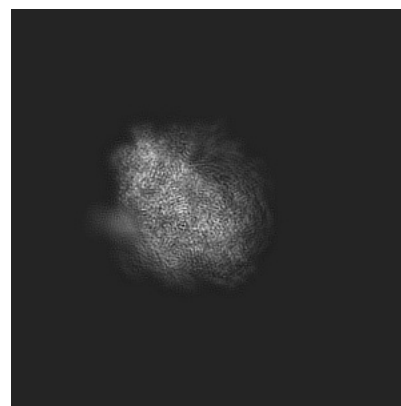
6.1.1 Primary map



X

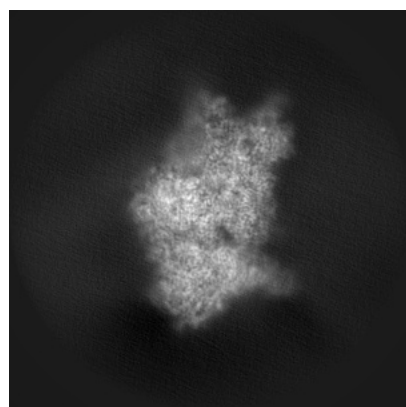


Y

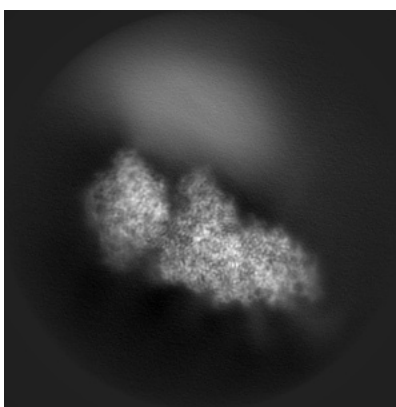


Z

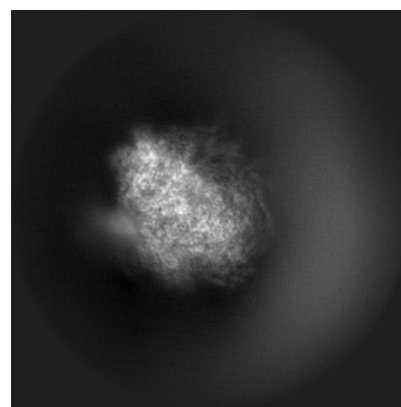
6.1.2 Raw map



X



Y



Z

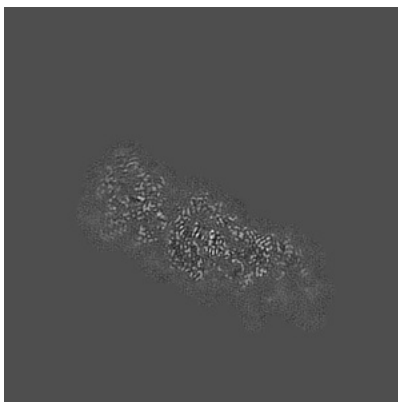
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

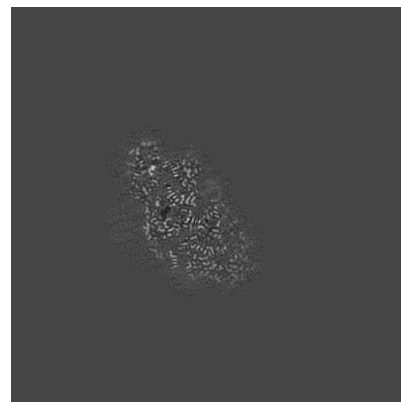
6.2.1 Primary map



X Index: 250

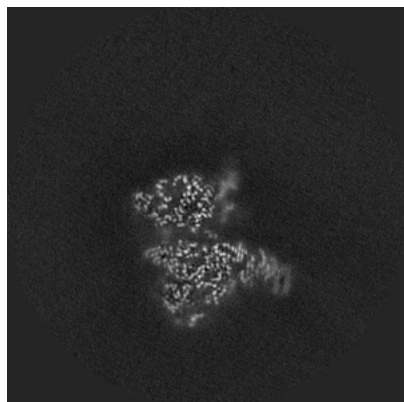


Y Index: 250

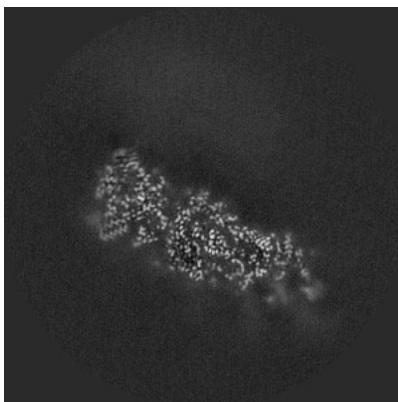


Z Index: 250

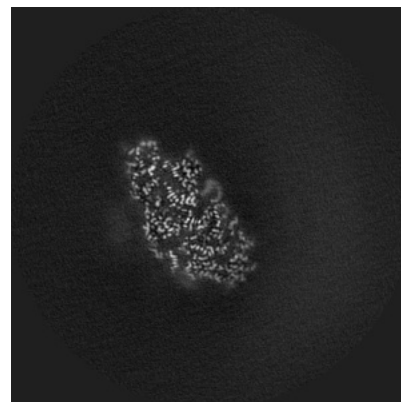
6.2.2 Raw map



X Index: 250



Y Index: 250

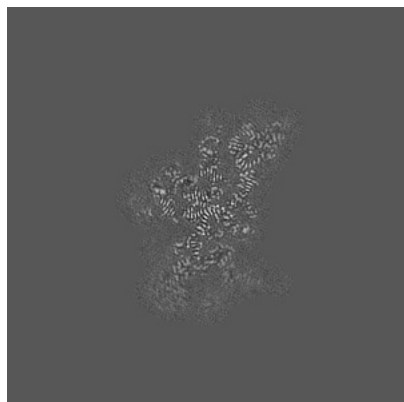


Z Index: 250

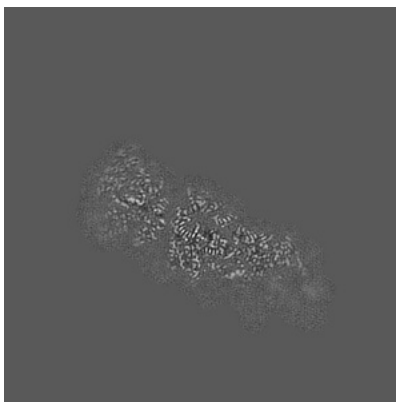
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

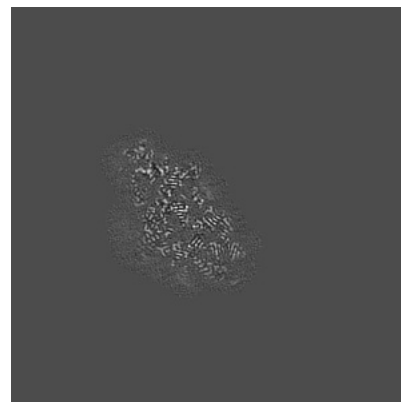
6.3.1 Primary map



X Index: 214

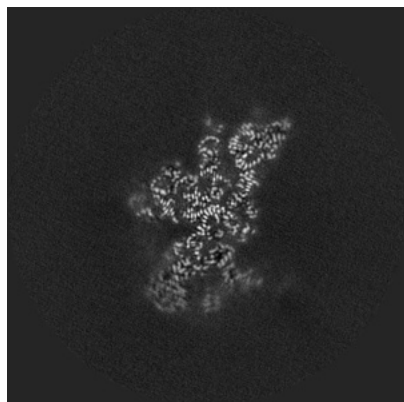


Y Index: 248

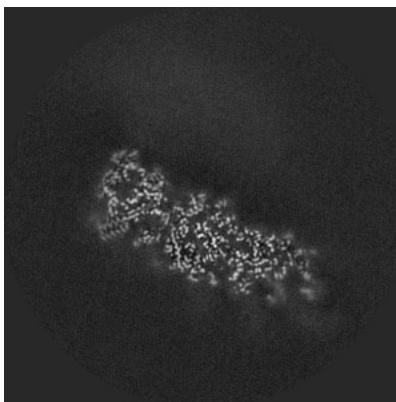


Z Index: 260

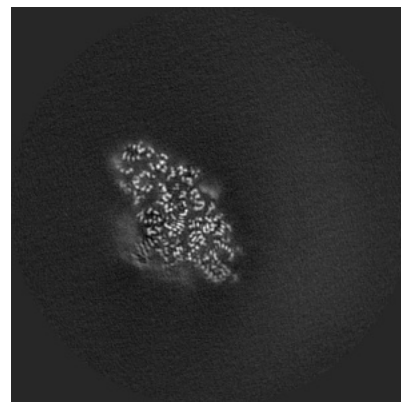
6.3.2 Raw map



X Index: 214



Y Index: 253

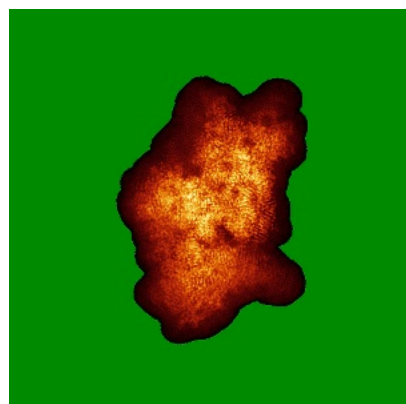


Z Index: 265

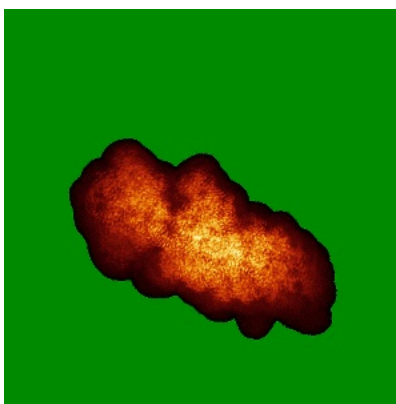
The images above show the largest variance slices of the map in three orthogonal directions.

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

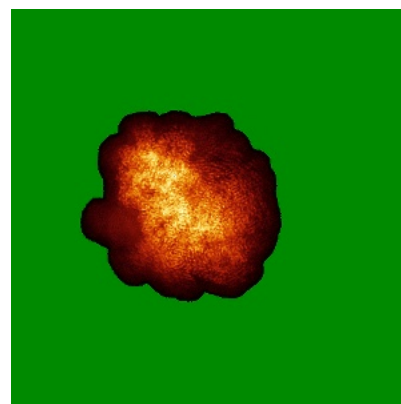
6.4.1 Primary map



X

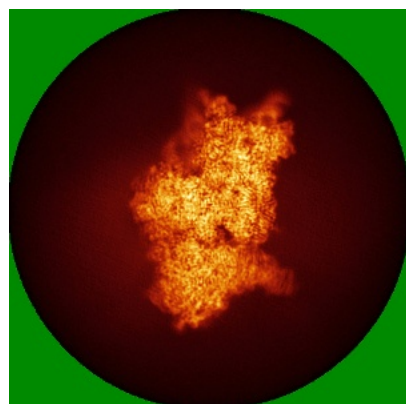


Y

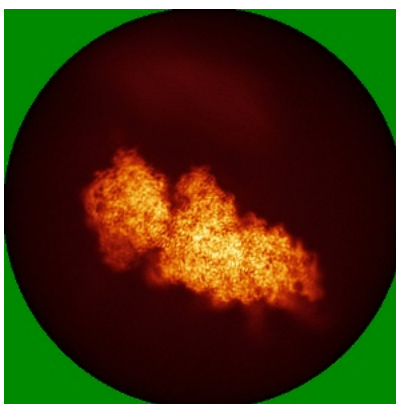


Z

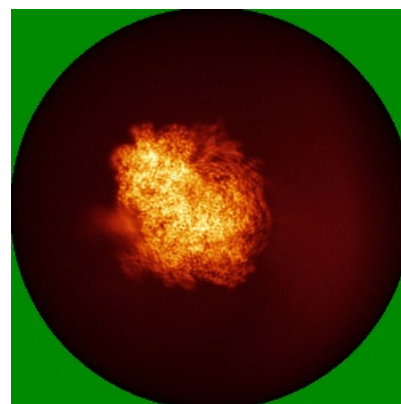
6.4.2 Raw map



X



Y

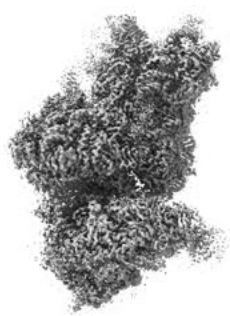


Z

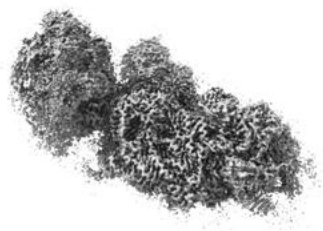
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



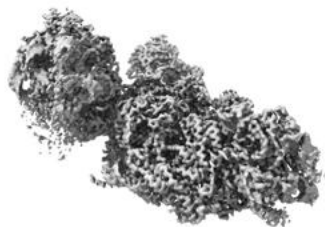
Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

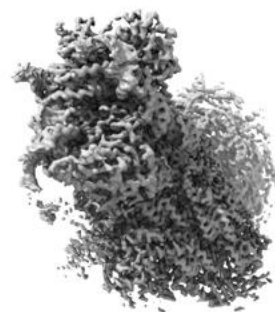
6.5.2 Raw map



X



Y



Z

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

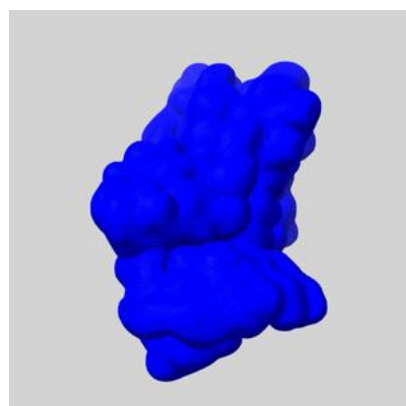
6.6 Mask visualisation [i](#)

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

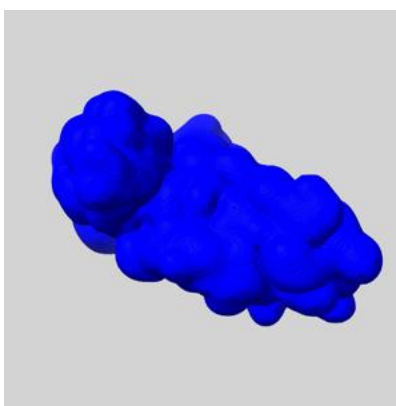
A mask typically either:

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

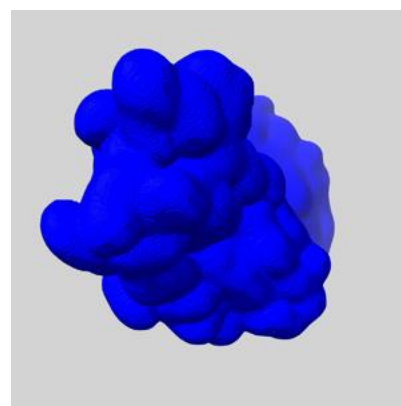
6.6.1 emd_47929_msk_1.map [i](#)



X



Y

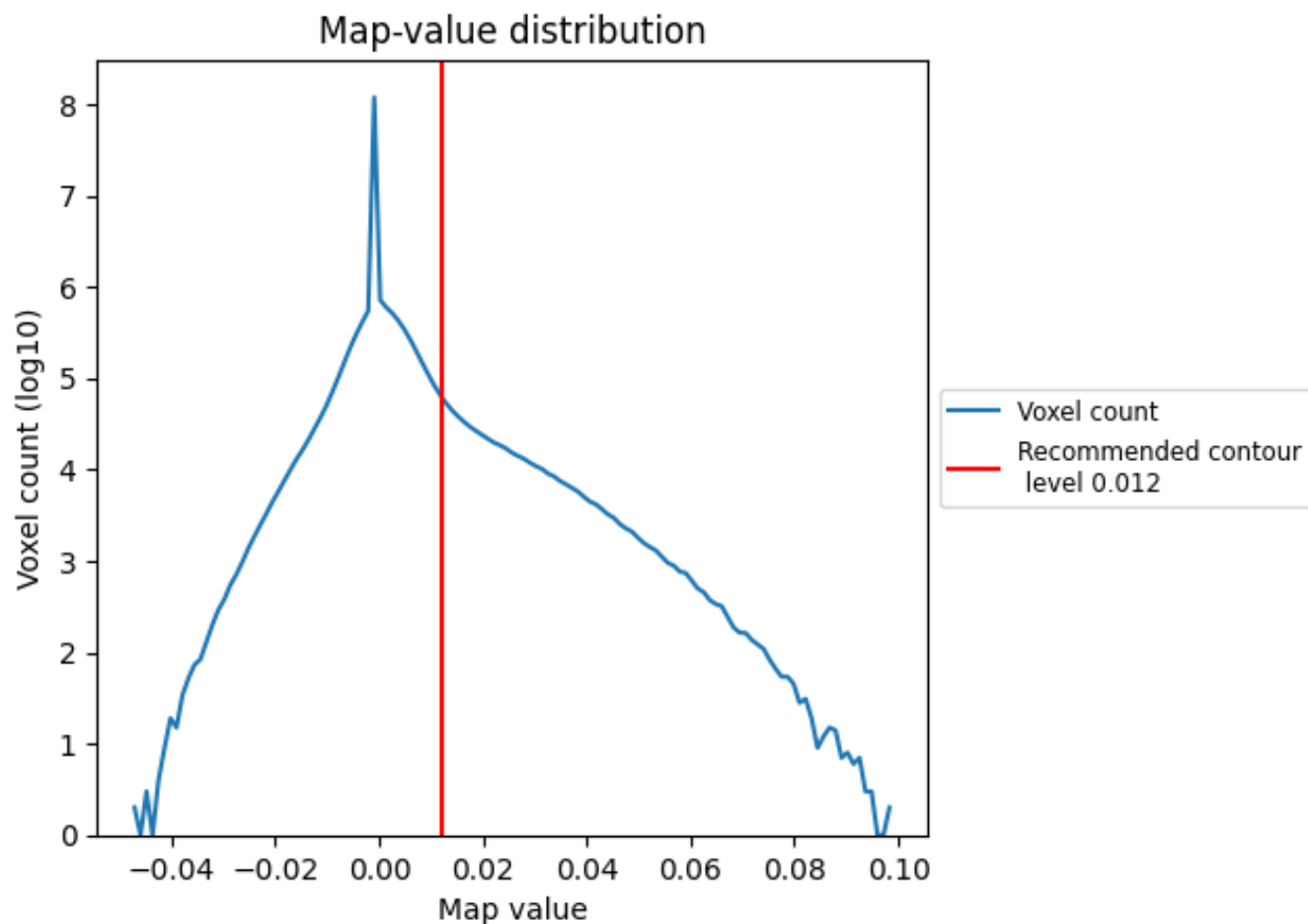


Z

7 Map analysis [i](#)

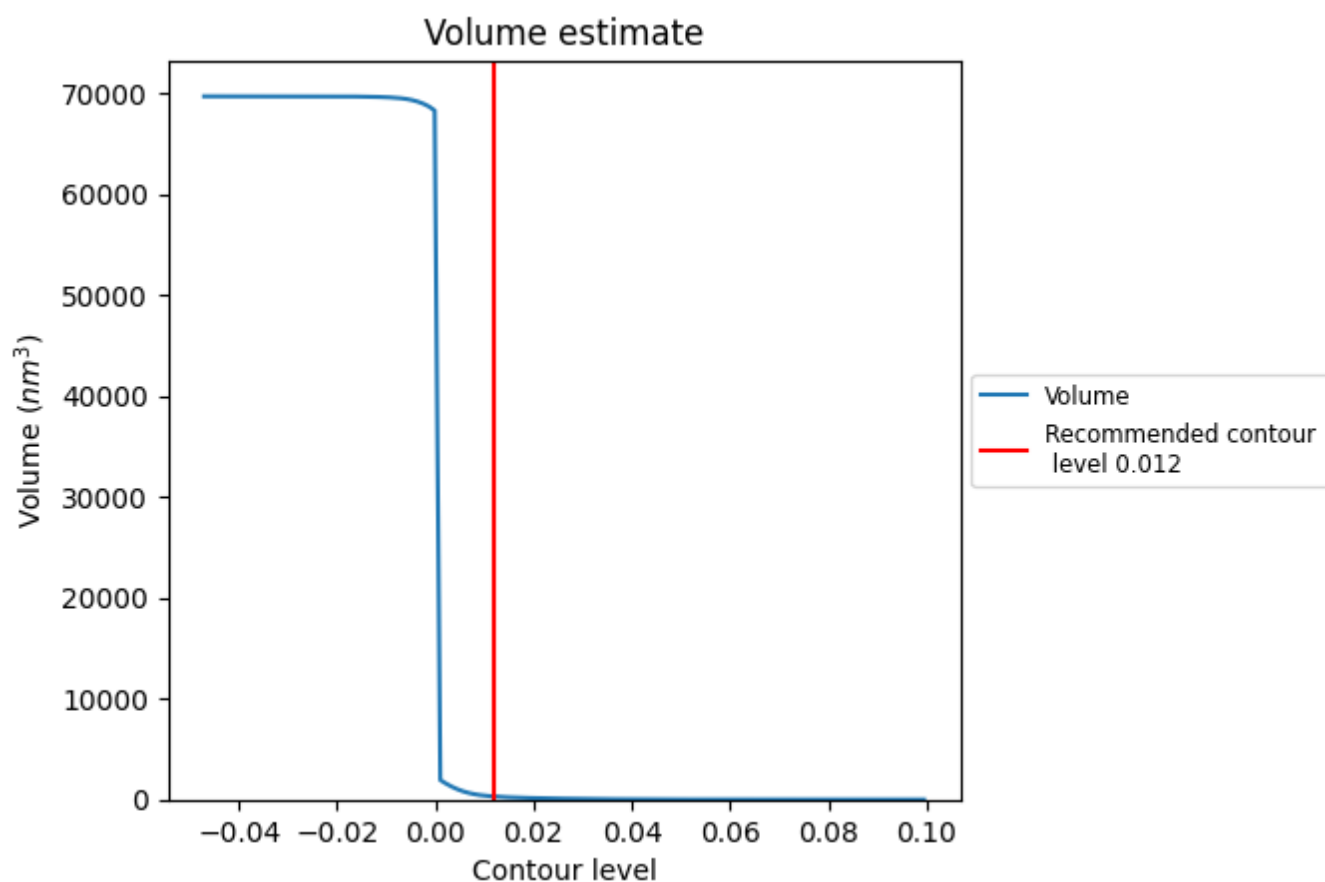
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

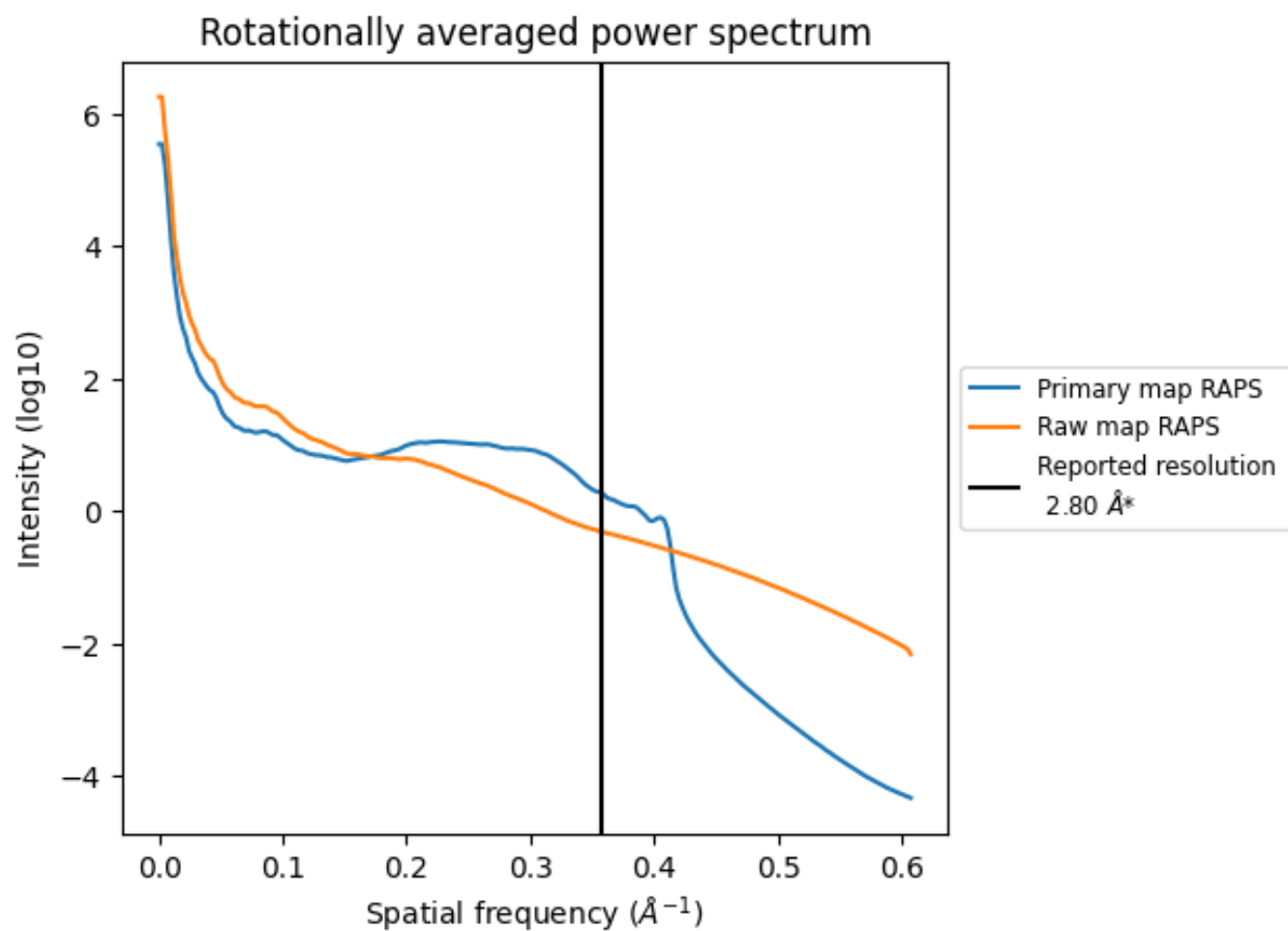
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm³; this corresponds to an approximate mass of 274 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 ⓘ

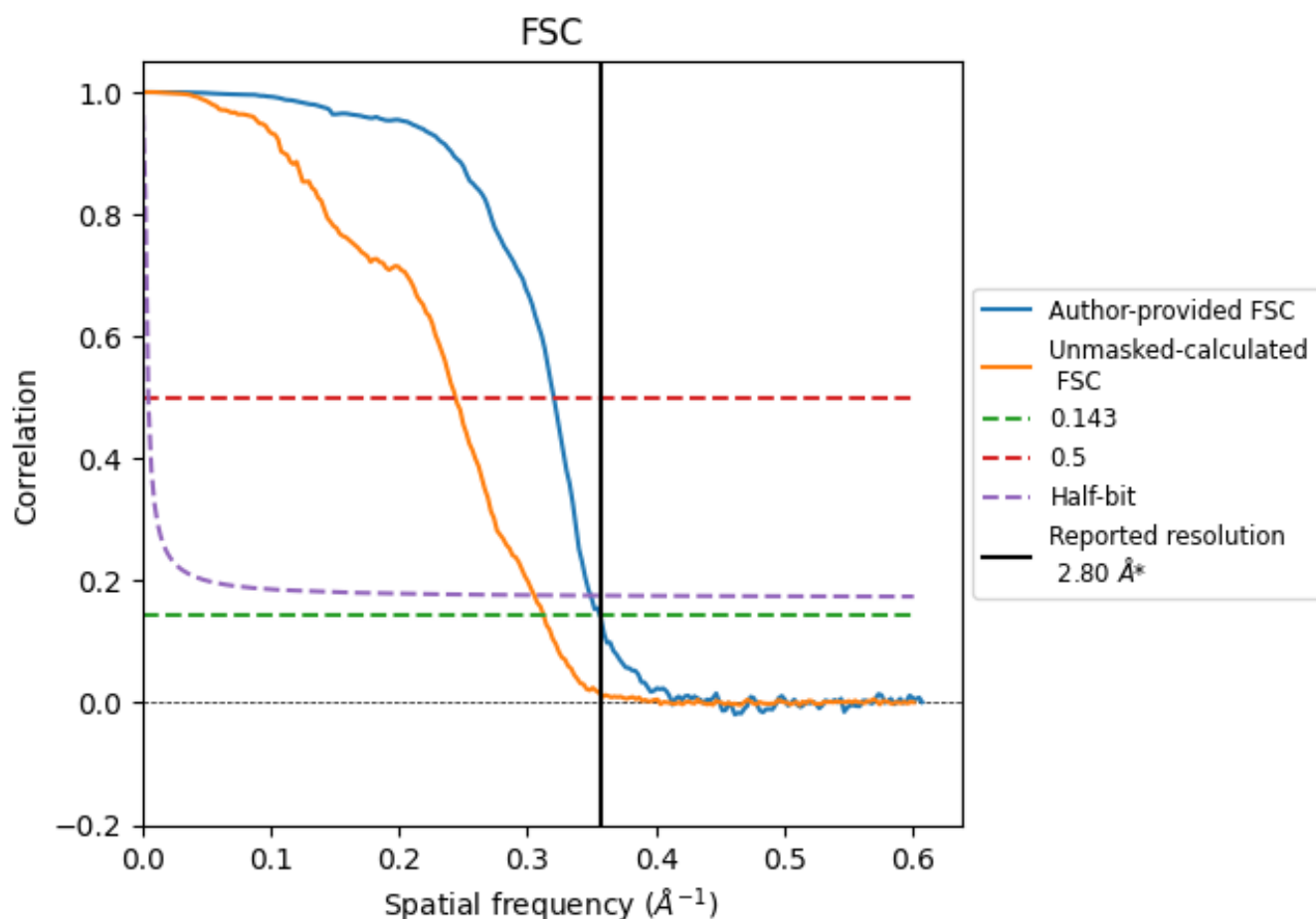


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

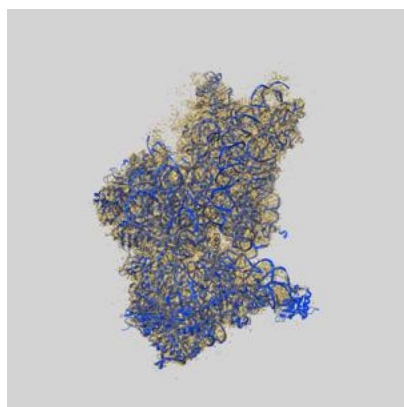
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.12	2.86
Unmasked-calculated*	3.20	4.10	3.28

*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 3.20 differs from the reported value 2.8 by more than 10 %

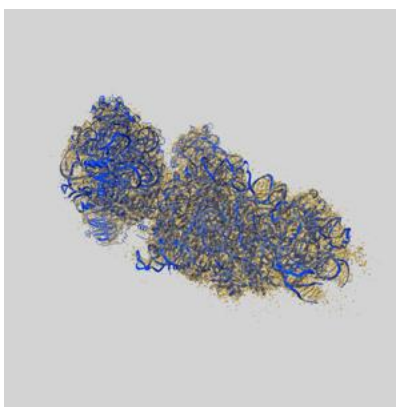
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47929 and PDB model 9ED0. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

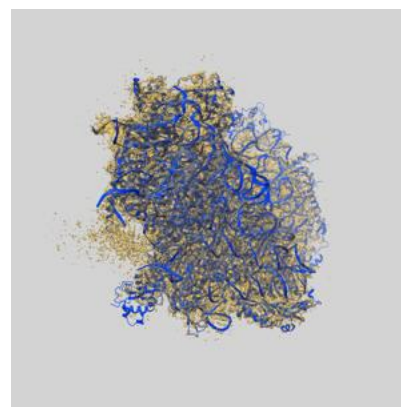
9.1 Map-model overlay [i](#)



X



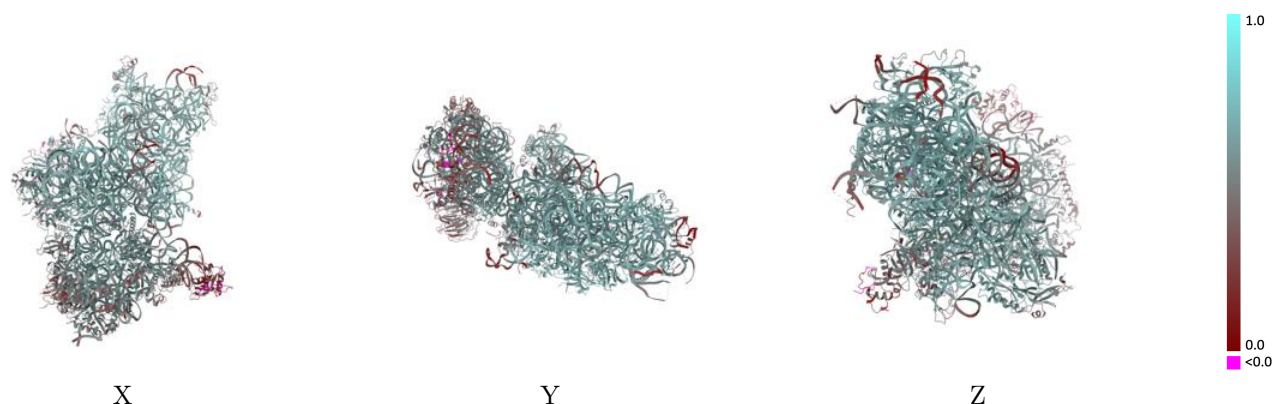
Y



Z

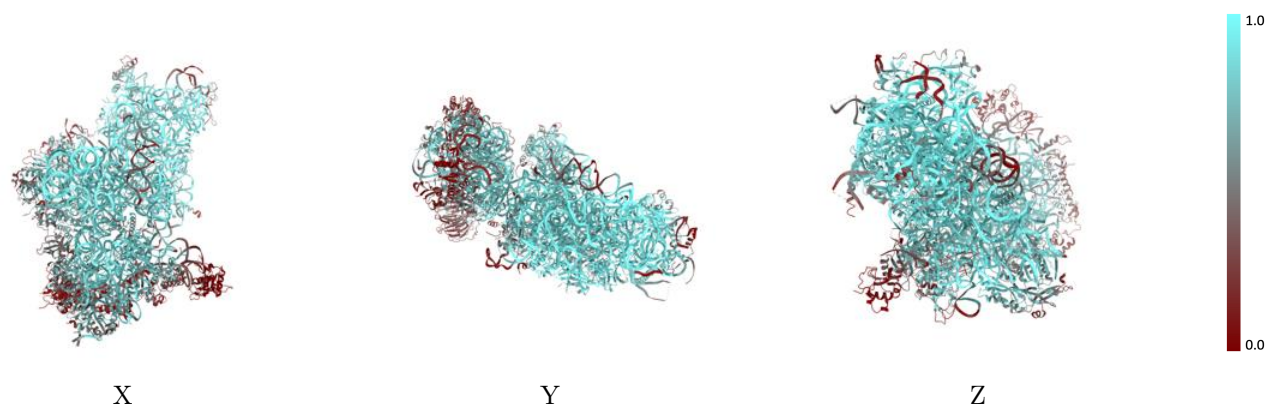
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



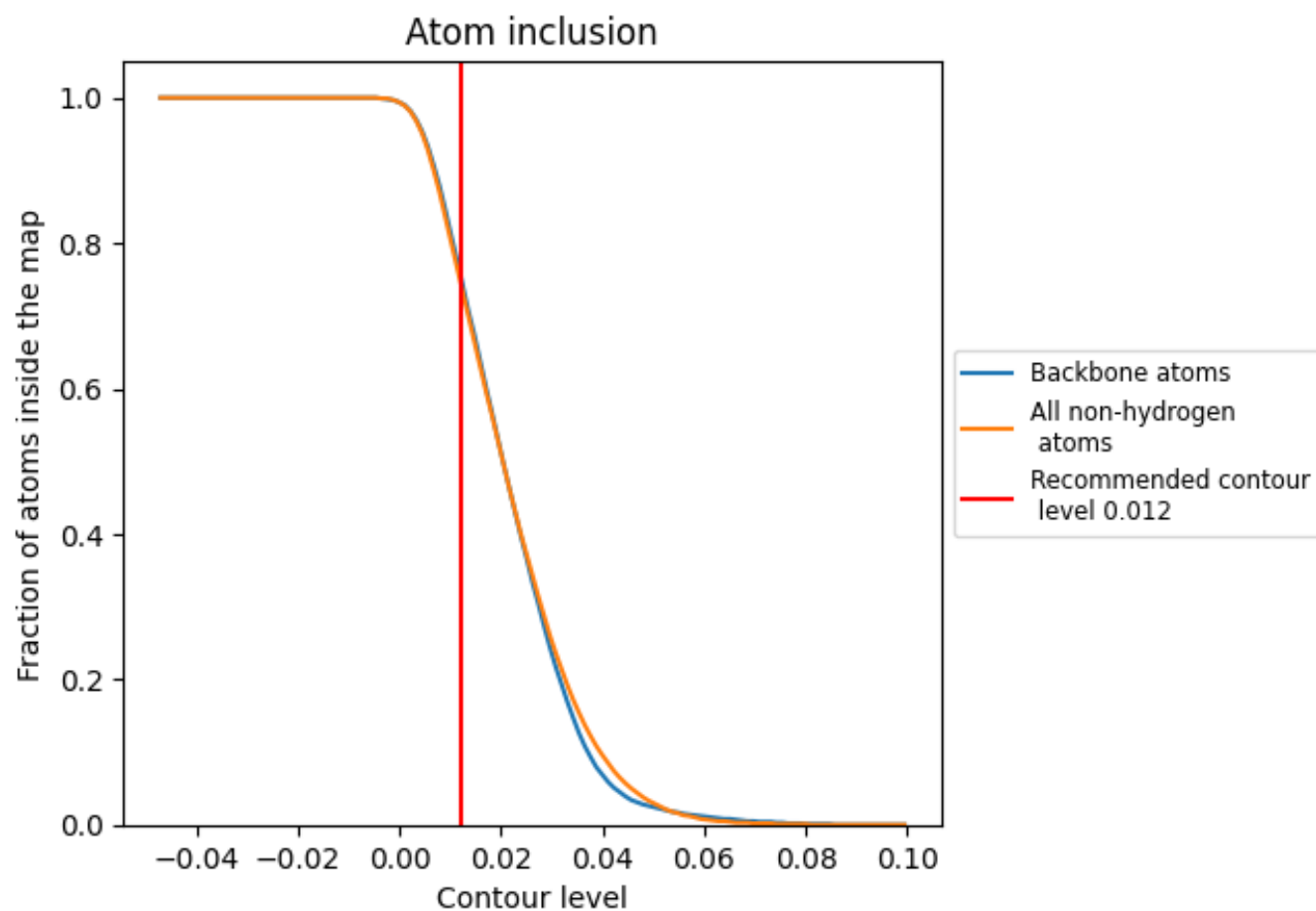
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 75% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7460	 0.5680
2	 0.8600	 0.5950
A	 0.7230	 0.5860
B	 0.6680	 0.5740
C	 0.8410	 0.6360
D	 0.6570	 0.5460
E	 0.9180	 0.6560
F	 0.6060	 0.5270
G	 0.7500	 0.5790
H	 0.2550	 0.3970
I	 0.7950	 0.6030
J	 0.8870	 0.6410
K	 0.5330	 0.5000
L	 0.8770	 0.6390
M	 0.0190	 0.2210
N	 0.7560	 0.6030
O	 0.7600	 0.5990
P	 0.4110	 0.4450
Q	 0.7390	 0.5770
R	 0.4100	 0.4580
S	 0.3830	 0.4280
T	 0.6550	 0.5410
U	 0.5270	 0.5000
V	 0.7440	 0.6010
W	 0.9260	 0.6570
X	 0.9150	 0.6560
Y	 0.8680	 0.6400
Z	 0.1940	 0.3970
a	 0.8280	 0.6190
b	 0.6160	 0.5500
c	 0.5020	 0.4980
d	 0.8530	 0.6280
e	 0.7260	 0.5900
f	 0.0250	 0.1880
g	 0.2270	 0.3680



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Chain	Atom inclusion	Q-score
h	 0.5560	 0.5080
n	 0.7900	 0.6090