



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 03:57 AM UTC

PDB ID : 6ZVH / pdb_00006zvh
EMDB ID : EMD-11456
Title : EDF1-ribosome complex
Authors : Best, K.M.; Denk, T.; Cheng, J.; Thoms, M.; Berninghausen, O.; Beckmann, R.
Deposited on : 2020-07-24
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

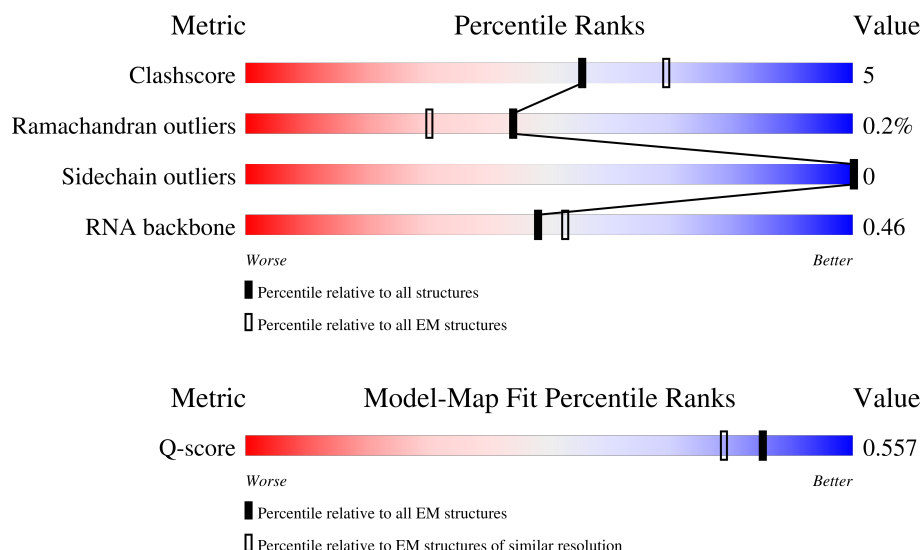
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	2	1740	
2	A	221	
3	B	264	

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Mol	Chain	Length	Quality of chain
4	D	227	
5	E	262	
6	F	189	
7	H	189	
8	I	206	
9	K	98	
10	L	153	
11	P	129	
12	Q	144	
13	R	135	
14	S	145	
15	T	143	
16	U	104	
17	V	83	
18	X	141	
19	a	102	
20	c	64	
21	d	55	
22	g	313	
23	C	222	
24	G	237	
25	J	185	
26	M	122	
27	N	150	
28	O	140	

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Mol	Chain	Length	Quality of chain
29	W	129	
30	Y	131	
31	Z	75	
32	b	83	
33	e	42	
34	f	67	
35	x	75	
36	y	72	
37	i	110	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 79014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1740	Total	C	N	O	P	0	0
			36896	16458	6597	12102	1739		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 9 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	129	Total	C	N	O	S	0	0
			1061	672	202	180	7		

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 15 is a protein called 40S ribosomal protein S19.

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

- Molecule 16 is a protein called 40S ribosomal protein S20.

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

- Molecule 17 is a protein called 40S ribosomal protein S21.

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

- Molecule 18 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 19 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 20 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 21 is a protein called 40S ribosomal protein S29.

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

- Molecule 22 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 23 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	C	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 24 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	G	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 25 is a protein called 40S ribosomal protein S9.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	122	Total	C	N	O	S	0	0
			942	590	165	179	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	52	GLN	LEU	conflict	UNP P25398
M	69	LEU	CYS	conflict	UNP P25398
M	99	ASN	LYS	conflict	UNP P25398

- Molecule 27 is a protein called 40S ribosomal protein S13.

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

- Molecule 28 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 29 is a protein called 40S ribosomal protein S15a.

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

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	42	Total	C	N	O	S	0	0
			342	211	78	52	1		

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 35 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	x	75	Total	C	N	O	P	0	0
			1589	710	279	525	75		

- Molecule 36 is a protein called Cell growth-regulating nucleolar protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	y	72	Total	C	N	O	0	0
			603	395	105	103		

- Molecule 37 is a protein called Endothelial differentiation-related factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	i	110	Total	C	N	O	0	0
			865	530	169	166		

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	2	28	Total	Mg	0
			28	28	
38	G	1	Total	Mg	0
			1	1	
38	O	1	Total	Mg	0
			1	1	

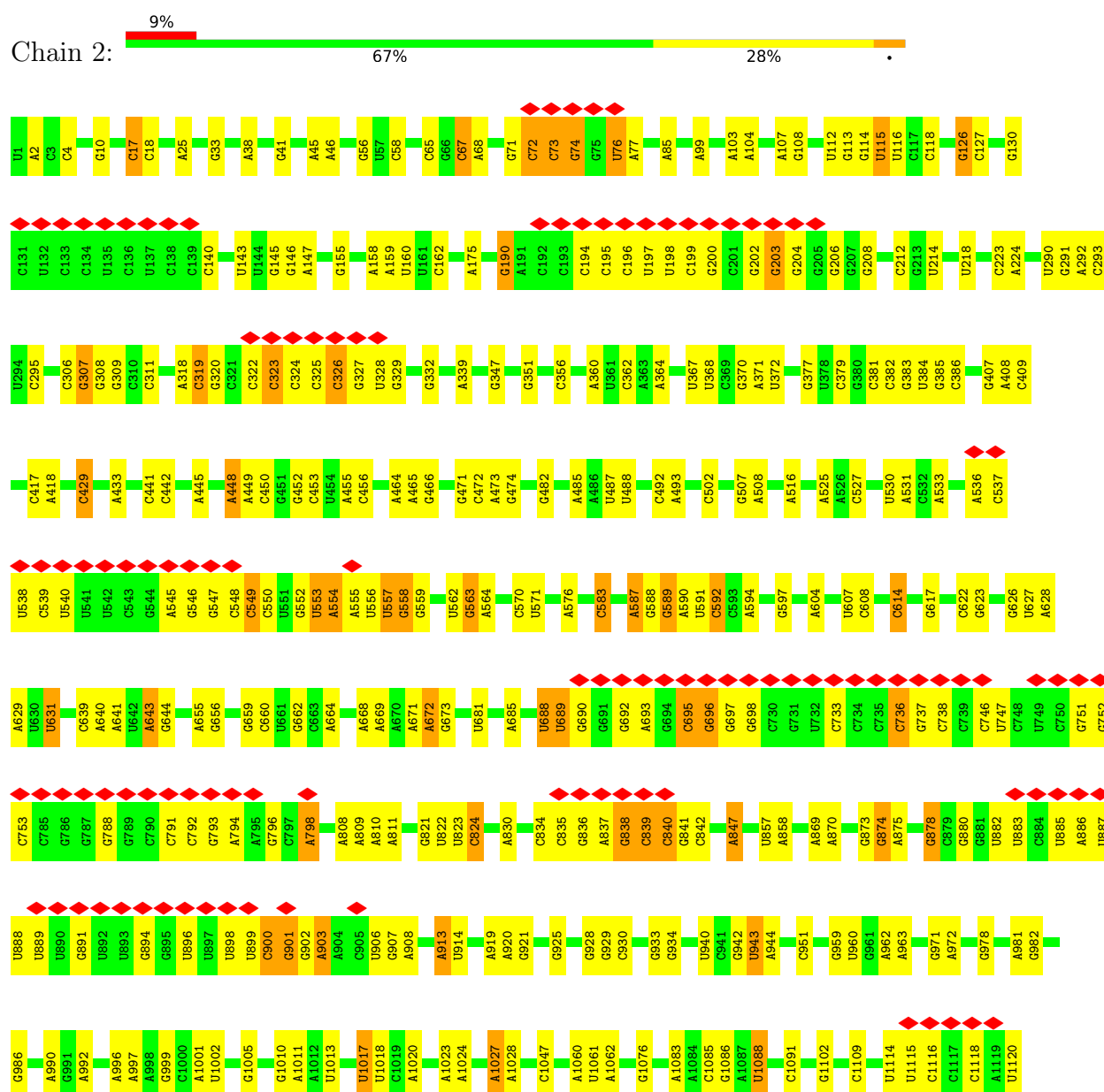
- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

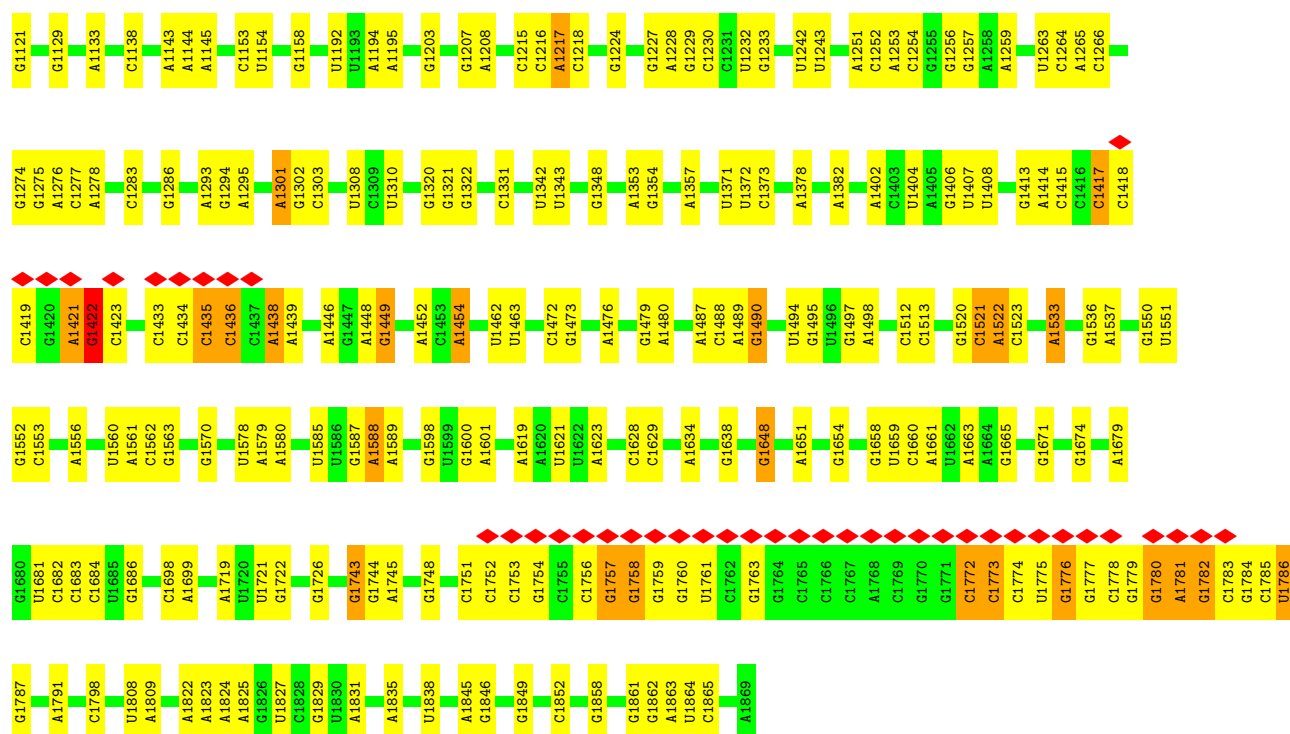
Mol	Chain	Residues	Atoms		AltConf
39	a	1	Total	Zn	0
			1	1	
39	d	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

3 Residue-property plots

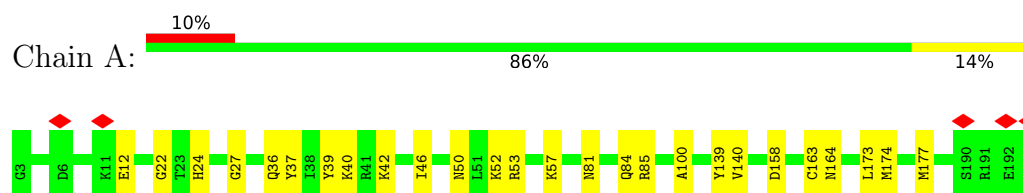
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 18S rRNA

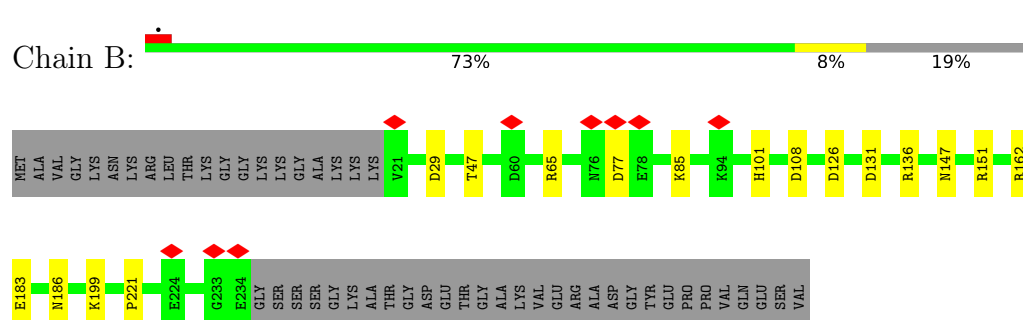




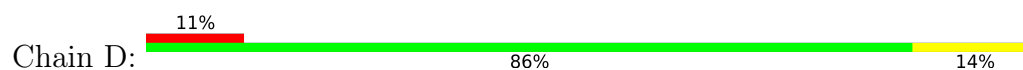
• Molecule 2: 40S ribosomal protein SA

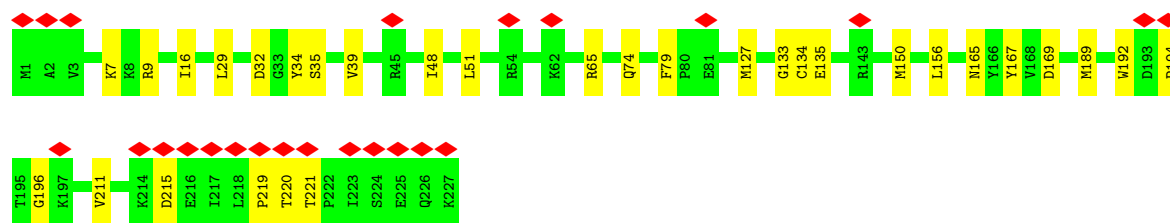


• Molecule 3: 40S ribosomal protein S3a



• Molecule 4: 40S ribosomal protein S3

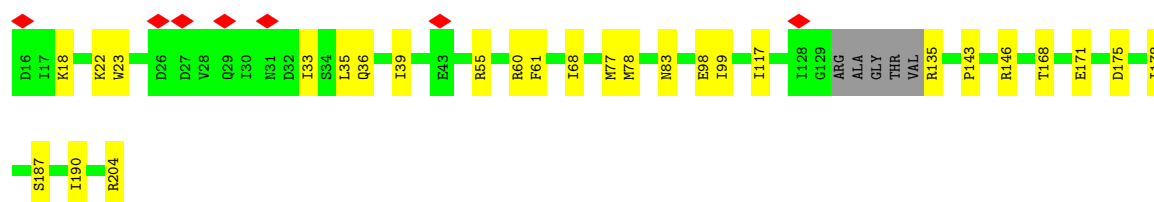
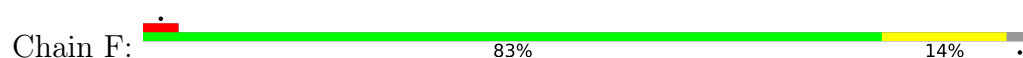




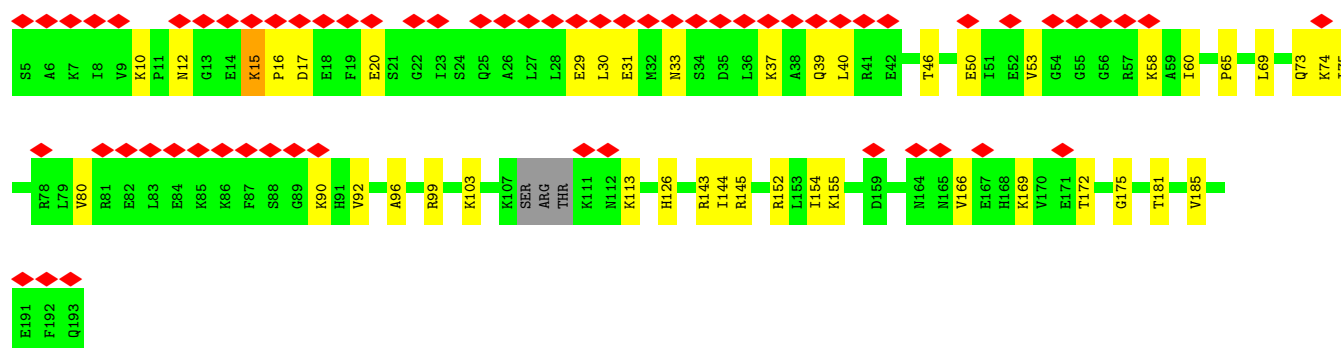
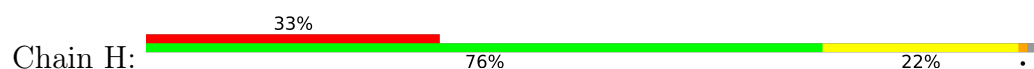
- Molecule 5: 40S ribosomal protein S4, X isoform



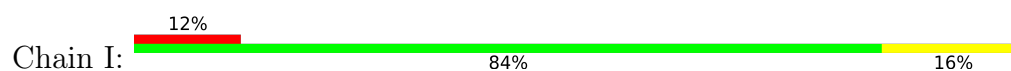
- Molecule 6: 40S ribosomal protein S5



- Molecule 7: 40S ribosomal protein S7

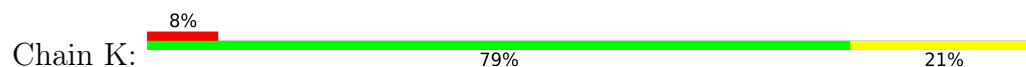


- Molecule 8: 40S ribosomal protein S8





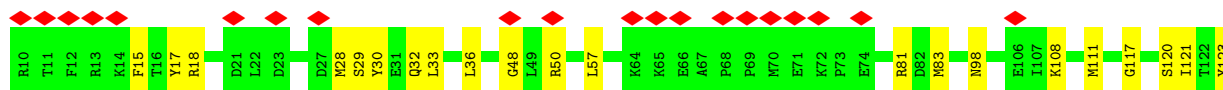
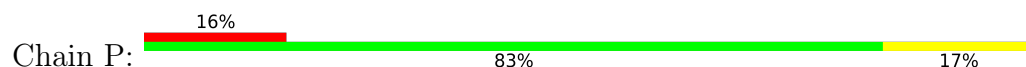
- Molecule 9: 40S ribosomal protein S10



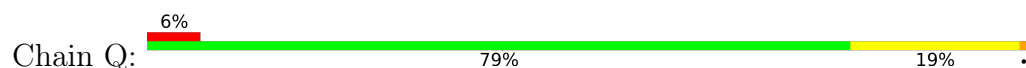
- Molecule 10: 40S ribosomal protein S11



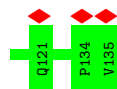
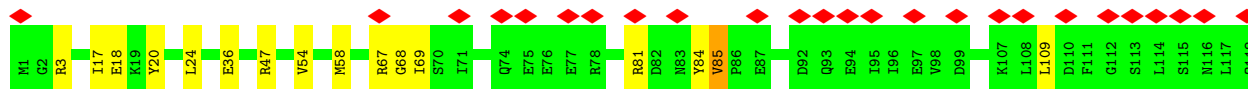
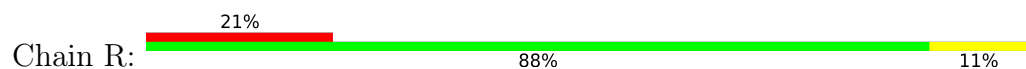
- Molecule 11: 40S ribosomal protein S15



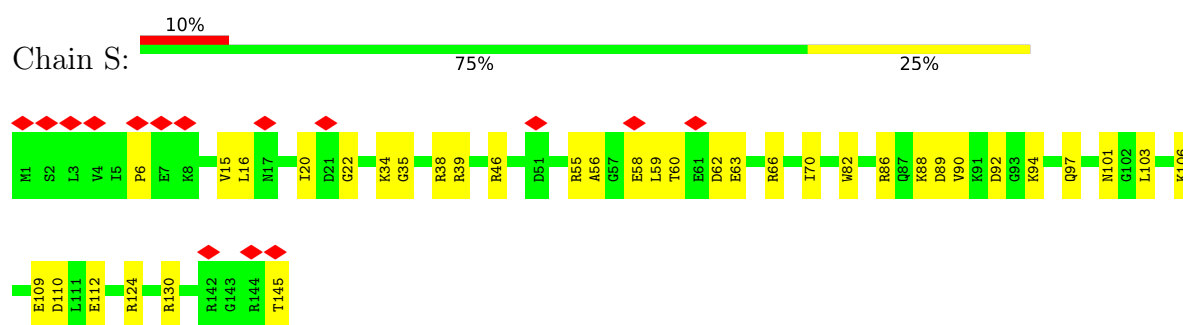
- Molecule 12: 40S ribosomal protein S16



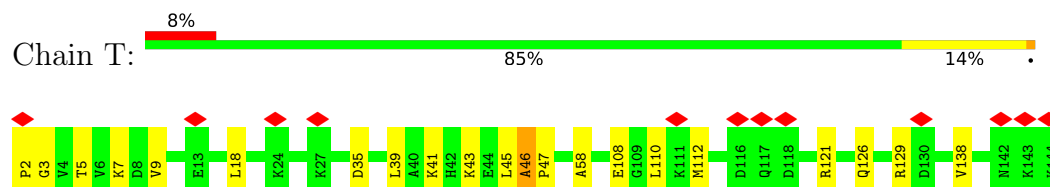
- Molecule 13: 40S ribosomal protein S17



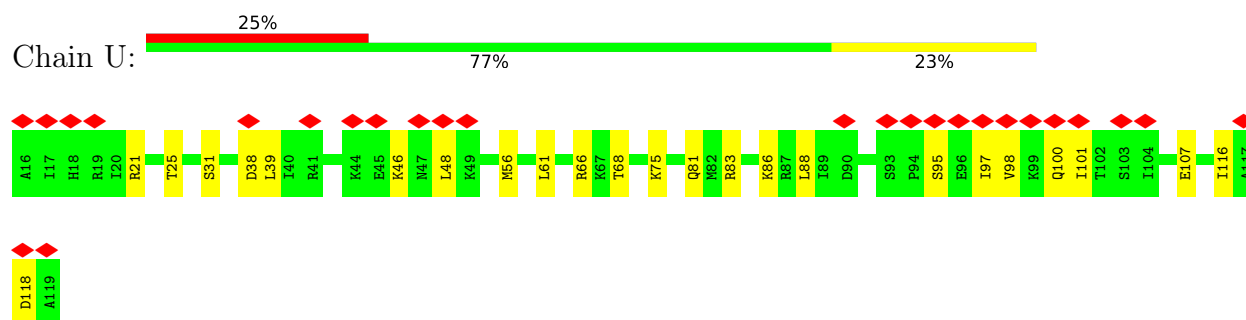
- Molecule 14: 40S ribosomal protein S18



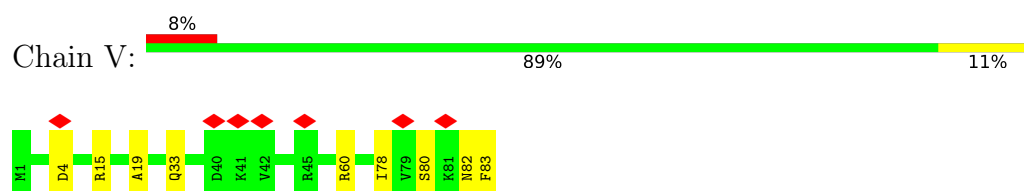
- Molecule 15: 40S ribosomal protein S19



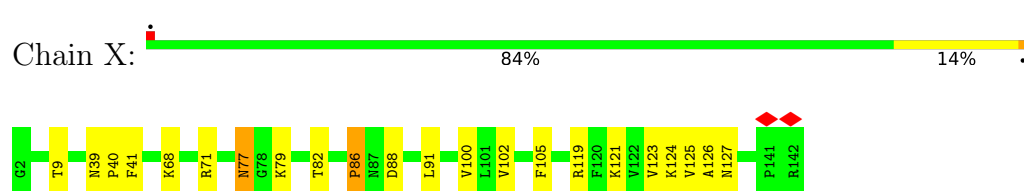
- Molecule 16: 40S ribosomal protein S20



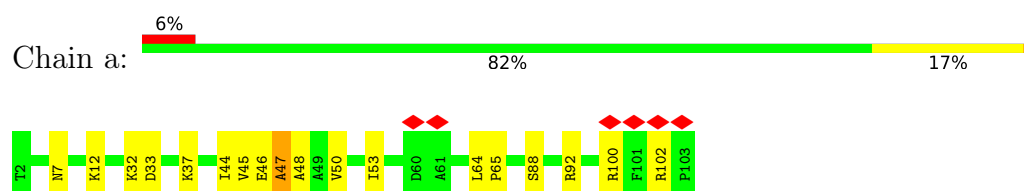
- Molecule 17: 40S ribosomal protein S21



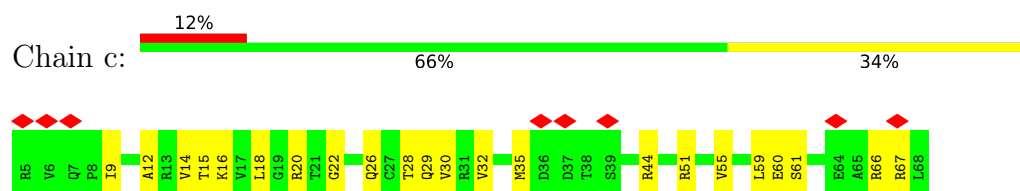
- Molecule 18: 40S ribosomal protein S23



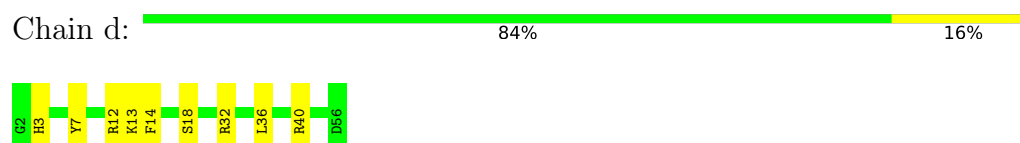
- Molecule 19: 40S ribosomal protein S26



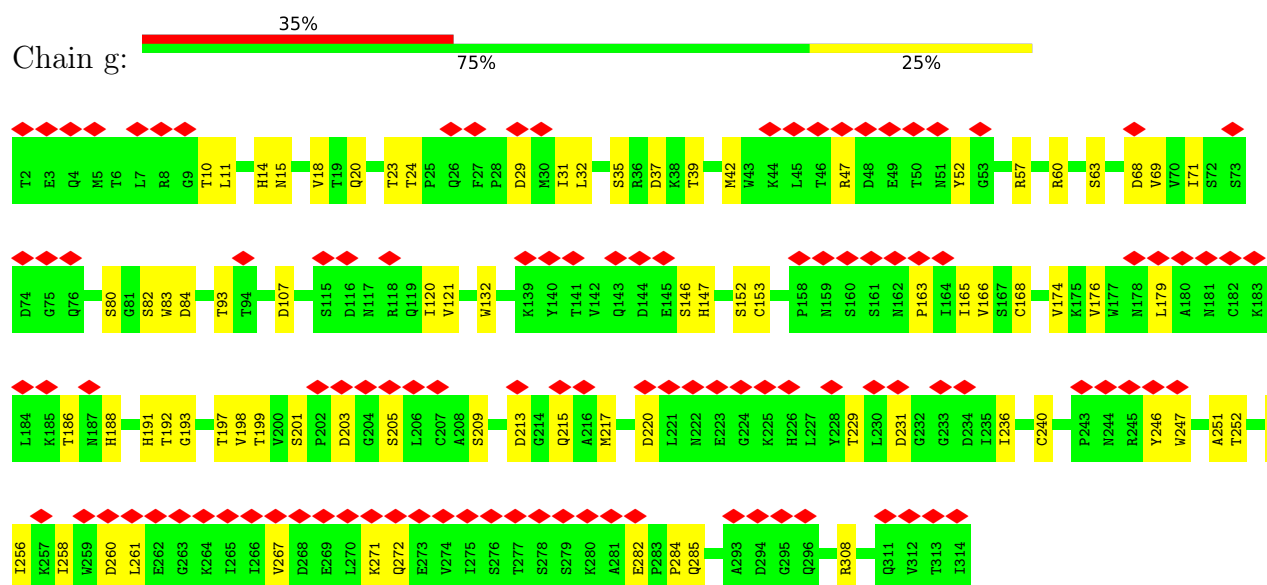
- Molecule 20: 40S ribosomal protein S28



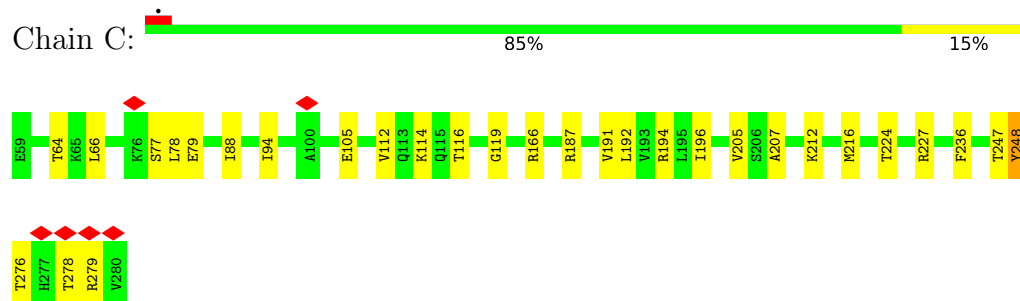
- Molecule 21: 40S ribosomal protein S29



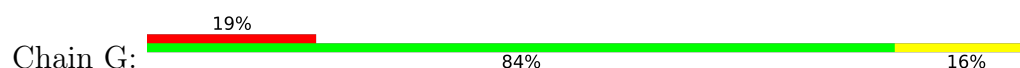
- Molecule 22: Receptor of activated protein C kinase 1

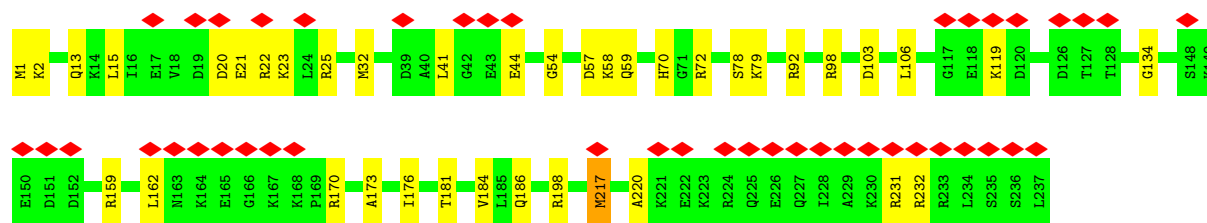


- Molecule 23: 40S ribosomal protein S2

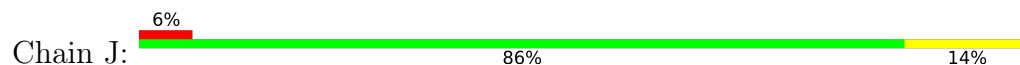


- Molecule 24: 40S ribosomal protein S6

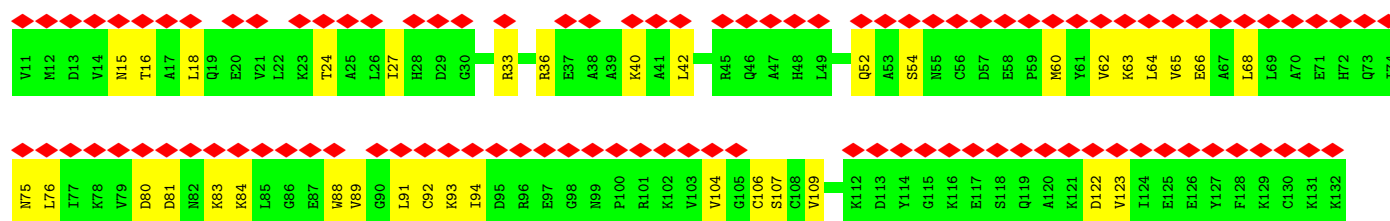
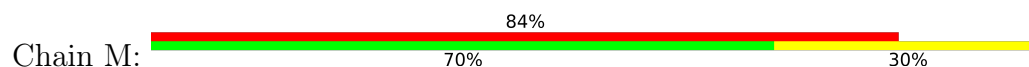




- Molecule 25: 40S ribosomal protein S9



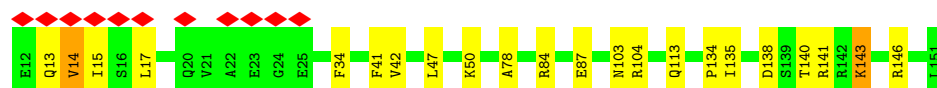
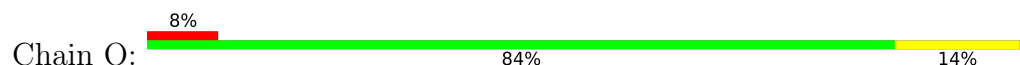
- Molecule 26: 40S ribosomal protein S12



- Molecule 27: 40S ribosomal protein S13



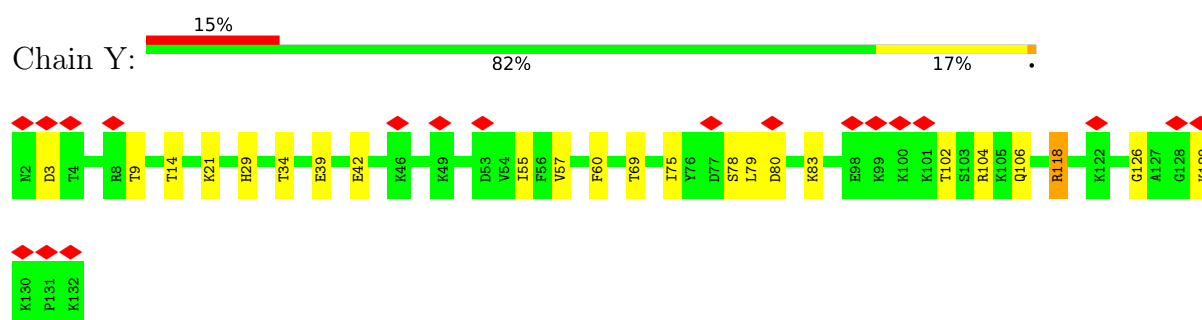
- Molecule 28: 40S ribosomal protein S14



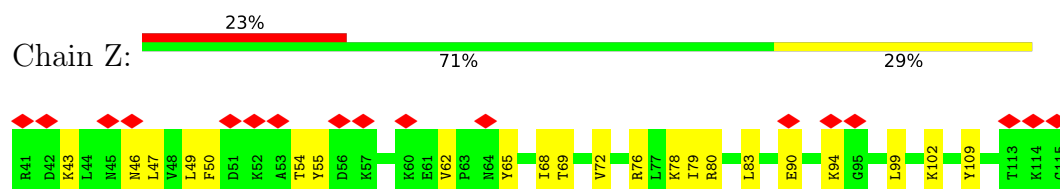
- Molecule 29: 40S ribosomal protein S15a



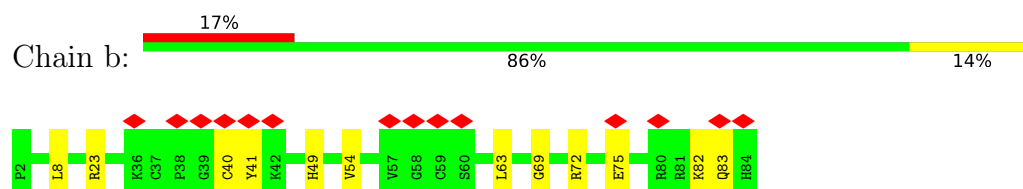
- Molecule 30: 40S ribosomal protein S24



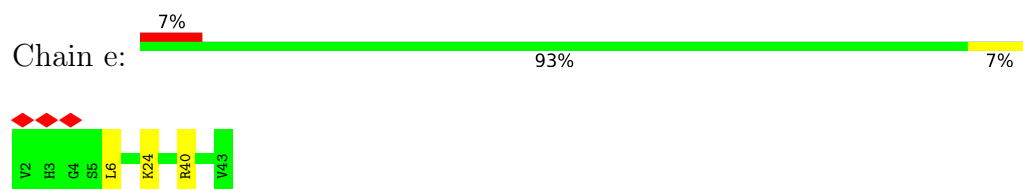
- Molecule 31: 40S ribosomal protein S25



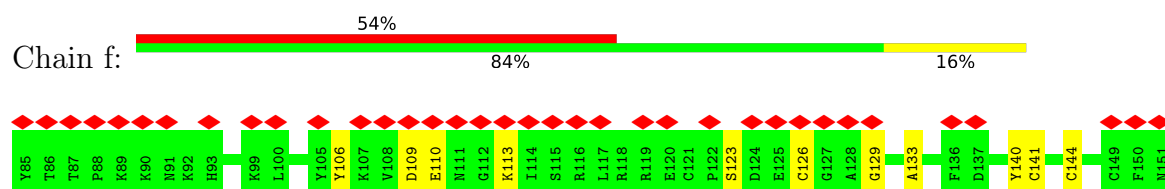
- Molecule 32: 40S ribosomal protein S27



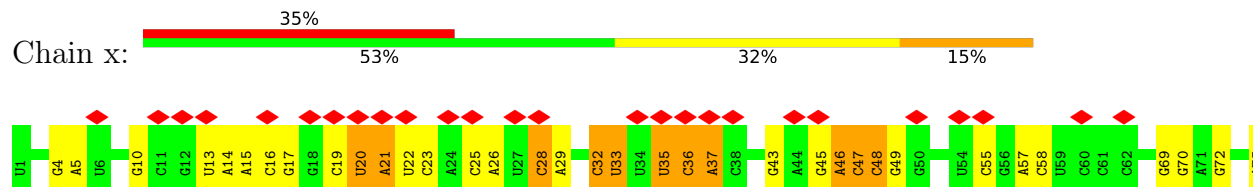
- Molecule 33: 40S ribosomal protein S30



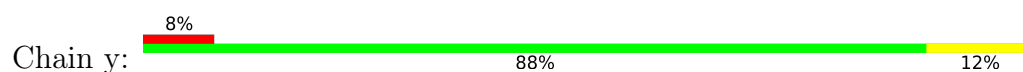
- Molecule 34: Ubiquitin-40S ribosomal protein S27a

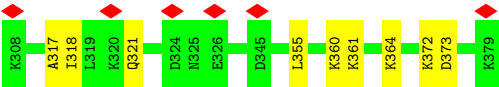


- Molecule 35: E-site tRNA

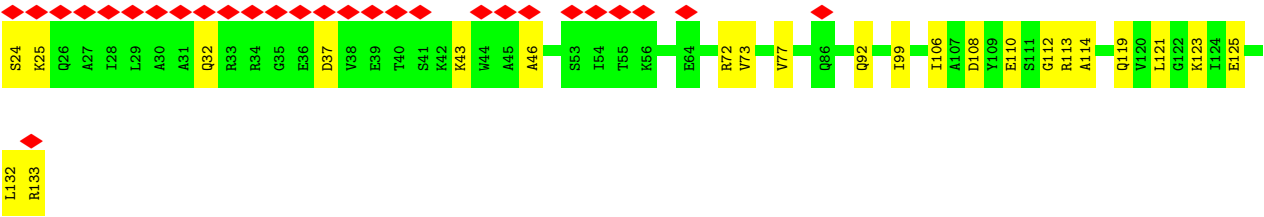
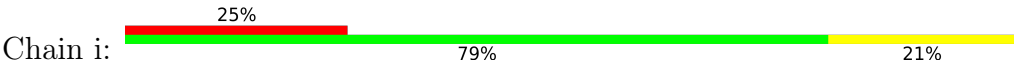


- Molecule 36: Cell growth-regulating nucleolar protein





• Molecule 37: Endothelial differentiation-related factor 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81976	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.332	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.44	0/41241	0.42	3/64258 (0.0%)
2	A	0.40	0/1778	0.63	2/2416 (0.1%)
3	B	0.36	0/1765	0.49	0/2362
4	D	0.37	0/1793	0.64	1/2414 (0.0%)
5	E	0.38	0/2118	0.59	2/2849 (0.1%)
6	F	0.38	0/1481	0.63	0/1988
7	H	0.34	0/1519	0.67	0/2033
8	I	0.38	0/1715	0.57	2/2287 (0.1%)
9	K	0.38	0/851	0.62	0/1147
10	L	0.43	0/1268	0.59	0/1696
11	P	0.36	0/1082	0.65	0/1446
12	Q	0.39	0/1160	0.72	0/1553
13	R	0.33	0/1105	0.70	2/1484 (0.1%)
14	S	0.37	0/1216	0.66	0/1628
15	T	0.37	0/1131	0.65	0/1515
16	U	0.36	0/831	0.64	0/1115
17	V	0.39	0/643	0.64	0/860
18	X	0.43	0/1116	0.67	2/1490 (0.1%)
19	a	0.42	0/836	0.71	2/1121 (0.2%)
20	c	0.37	0/508	0.79	0/680
21	d	0.45	0/470	0.67	0/623
22	g	0.31	0/2493	0.61	2/3394 (0.1%)
23	C	0.43	0/1762	0.69	2/2381 (0.1%)
24	G	0.32	0/1946	0.59	0/2590
25	J	0.37	0/1550	0.60	0/2069
26	M	0.26	0/952	0.67	0/1279
27	N	0.40	0/1232	0.50	0/1656
28	O	0.40	0/1062	0.68	3/1425 (0.2%)
29	W	0.42	0/1051	0.56	0/1406
30	Y	0.37	0/1083	0.56	0/1438
31	Z	0.30	0/604	0.68	0/810
32	b	0.36	0/665	0.60	0/891

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.34	0/345	0.48	0/451
34	f	0.30	0/560	0.73	0/745
35	x	0.17	0/1773	0.35	0/2759
36	y	0.25	0/613	0.56	0/819
37	i	0.26	0/872	0.51	0/1167
All	All	0.40	0/84190	0.52	23/122245 (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
3	B	0	1
4	D	0	1
6	F	0	1
7	H	0	2
12	Q	0	1
13	R	0	1
15	T	0	1
16	U	0	1
17	V	0	1
18	X	0	3
24	G	0	1
25	J	0	1
28	O	0	1
29	W	0	1
30	Y	0	1
31	Z	0	1
32	b	0	1
All	All	0	20

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1417	C	N3-C4-N4	-6.90	97.29	118.00
22	g	93	THR	CA-C-N	6.30	134.83	124.31
22	g	93	THR	C-N-CA	6.30	134.83	124.31
13	R	85	VAL	N-CA-C	-6.26	101.44	107.76
13	R	85	VAL	CB-CA-C	6.23	117.37	110.71
5	E	92	ILE	CA-C-N	6.05	133.10	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	92	ILE	C-N-CA	6.05	133.10	121.54
4	D	165	ASN	N-CA-C	-5.95	107.84	114.62
28	O	14	VAL	CA-C-N	5.91	132.33	121.70
28	O	14	VAL	C-N-CA	5.91	132.33	121.70
23	C	248	TYR	CA-C-N	-5.82	109.65	121.18
23	C	248	TYR	C-N-CA	-5.82	109.65	121.18
1	2	1422	G	N1-C6-O6	-5.61	103.08	119.90
1	2	1417	C	C5-C4-N4	5.56	136.87	120.20
19	a	7	ASN	CA-C-N	-5.48	113.73	122.66
19	a	7	ASN	C-N-CA	-5.48	113.73	122.66
18	X	86	PRO	CA-C-N	5.22	131.51	121.54
18	X	86	PRO	C-N-CA	5.22	131.51	121.54
2	A	140	VAL	CA-C-N	5.18	130.17	122.82
2	A	140	VAL	C-N-CA	5.18	130.17	122.82
28	O	141	ARG	N-CA-C	5.15	117.94	110.42
8	I	129	LEU	CA-C-N	5.09	129.62	121.62
8	I	129	LEU	C-N-CA	5.09	129.62	121.62

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	221	PRO	Peptide
4	D	192	TRP	Peptide
6	F	78	MET	Peptide
24	G	217	MET	Peptide
7	H	15	LYS	Peptide
7	H	29	GLU	Peptide
25	J	137	VAL	Peptide
28	O	143	LYS	Peptide
12	Q	43	GLU	Peptide
13	R	84	TYR	Peptide
15	T	46	ALA	Peptide
16	U	61	LEU	Peptide
17	V	78	ILE	Peptide
29	W	54	ASP	Peptide
18	X	126	ALA	Peptide
18	X	77	ASN	Peptide
18	X	86	PRO	Peptide
30	Y	118	ARG	Peptide
31	Z	46	ASN	Peptide
32	b	75	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	36896	0	18603	217	0
2	A	1741	0	1746	25	0
3	B	1738	0	1809	14	0
4	D	1765	0	1865	19	0
5	E	2076	0	2177	13	0
6	F	1461	0	1511	17	0
7	H	1497	0	1590	30	0
8	I	1686	0	1772	23	0
9	K	827	0	854	11	0
10	L	1247	0	1323	12	0
11	P	1061	0	1107	14	0
12	Q	1142	0	1213	24	0
13	R	1090	0	1149	10	0
14	S	1198	0	1261	27	0
15	T	1112	0	1146	14	0
16	U	821	0	883	15	0
17	V	636	0	637	6	0
18	X	1098	0	1167	13	0
19	a	821	0	870	10	0
20	c	506	0	536	14	0
21	d	459	0	452	7	0
22	g	2436	0	2393	48	0
23	C	1725	0	1813	20	0
24	G	1923	0	2089	27	0
25	J	1525	0	1640	17	0
26	M	942	0	961	24	0
27	N	1208	0	1294	12	0
28	O	1049	0	1073	16	0
29	W	1034	0	1080	11	0
30	Y	1065	0	1142	15	0
31	Z	598	0	656	15	0
32	b	651	0	672	8	0
33	e	342	0	382	3	0
34	f	548	0	552	8	0
35	x	1589	0	810	24	0
36	y	603	0	660	9	0
37	i	865	0	899	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	28	0	0	0	0
38	G	1	0	0	0	0
38	O	1	0	0	0	0
39	a	1	0	0	0	0
39	d	1	0	0	0	0
39	f	1	0	0	0	0
All	All	79014	0	61787	683	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (683) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:886:A:N6	1:2:901:G:C4	2.18	1.11
1:2:1756:C:N4	1:2:1776:G:H22	1.59	1.00
1:2:1756:C:H42	1:2:1776:G:N2	1.67	0.92
1:2:1756:C:H42	1:2:1776:G:H22	1.21	0.82
1:2:1047:C:H5'	28:O:143:LYS:HB3	1.65	0.77
1:2:1756:C:N4	1:2:1776:G:N2	2.30	0.77
35:x:15:A:N1	35:x:47:C:N3	2.33	0.75
1:2:925:G:H1	1:2:1017:U:H3	1.32	0.75
1:2:886:A:N6	1:2:901:G:C5	2.56	0.74
27:N:25:TRP:HE1	32:b:83:GLN:HG2	1.51	0.74
22:g:120:ILE:HB	22:g:132:TRP:HB2	1.68	0.73
1:2:878:G:H1	1:2:908:A:H2	1.36	0.72
12:Q:97:GLN:HB2	12:Q:105:LYS:HG3	1.74	0.70
12:Q:43:GLU:OE2	12:Q:77:HIS:ND1	2.21	0.69
24:G:1:MET:HE2	24:G:106:LEU:HB2	1.75	0.68
31:Z:90:GLU:OE2	31:Z:94:LYS:NZ	2.26	0.68
23:C:275:LYS:HG3	23:C:276:THR:HG23	1.76	0.68
1:2:1563:G:OP1	15:T:121:ARG:NH2	2.28	0.67
1:2:1488:C:O2'	1:2:1490:G:OP2	2.13	0.67
8:I:136:ILE:HD12	8:I:139:LYS:HZ1	1.60	0.67
1:2:835:C:N4	30:Y:9:THR:O	2.27	0.67
6:F:187:SER:HB2	6:F:190:ILE:HG12	1.76	0.66
13:R:24:LEU:HB2	13:R:58:MET:HE2	1.78	0.65
37:i:43:LYS:HB2	37:i:46:ALA:HB2	1.77	0.65
1:2:1513:C:OP1	21:d:12:ARG:NH1	2.28	0.64
1:2:1858:G:OP2	28:O:146:ARG:NH2	2.30	0.64
1:2:695:C:N4	1:2:736:C:O2'	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:y:317:ALA:O	36:y:321:GLN:NE2	2.31	0.64
7:H:154:ILE:HB	7:H:185:VAL:HG12	1.78	0.64
2:A:42:LYS:HD3	2:A:46:ILE:HB	1.79	0.64
26:M:36:ARG:HH21	26:M:40:LYS:HE3	1.63	0.64
34:f:141:CYS:CB	34:f:144:CYS:SG	2.84	0.64
1:2:1192:U:OP2	18:X:119:ARG:NH2	2.31	0.63
20:c:44:ARG:NH2	20:c:61:SER:O	2.30	0.63
22:g:35:SER:OG	22:g:37:ASP:OD1	2.16	0.63
1:2:656:G:O2'	23:C:227:ARG:NH2	2.31	0.63
1:2:928:G:H1	1:2:1013:U:H3	1.47	0.62
7:H:53:VAL:HG21	7:H:172:THR:HA	1.81	0.62
35:x:10:G:N7	35:x:45:G:N1	2.46	0.62
1:2:563:G:H1	1:2:592:C:H5	1.47	0.62
7:H:145:ARG:NH1	29:W:51:GLU:OE2	2.32	0.62
20:c:18:LEU:HB3	20:c:67:ARG:HH22	1.65	0.62
3:B:173:THR:O	3:B:177:GLN:HB2	1.99	0.62
4:D:32:ASP:OD2	4:D:65:ARG:NH1	2.32	0.62
8:I:73:THR:O	8:I:74:ARG:NH1	2.32	0.62
22:g:199:THR:HG21	22:g:240:CYS:HA	1.82	0.62
1:2:1228:A:H2'	1:2:1229:G:C8	2.35	0.62
22:g:247:TRP:HB3	22:g:258:ILE:HD11	1.82	0.62
22:g:82:SER:OG	22:g:84:ASP:OD1	2.18	0.61
1:2:326:C:O2	1:2:327:G:N2	2.33	0.61
1:2:885:U:H3	1:2:901:G:H1	1.48	0.61
1:2:878:G:O6	1:2:908:A:N1	2.33	0.61
31:Z:72:VAL:O	31:Z:76:ARG:HB2	2.01	0.61
7:H:12:ASN:HB3	7:H:16:PRO:HD2	1.82	0.61
6:F:55:ARG:HH11	12:Q:125:ARG:HD3	1.66	0.61
28:O:14:VAL:HG21	28:O:17:LEU:HB2	1.82	0.61
16:U:116:ILE:HG22	16:U:118:ASP:H	1.66	0.61
22:g:282:GLU:OE1	22:g:285:GLN:NE2	2.33	0.61
1:2:1658:G:OP2	1:2:1660:C:N4	2.34	0.61
1:2:1648:G:H5''	12:Q:125:ARG:HB2	1.83	0.60
34:f:110:GLU:OE2	34:f:113:LYS:NZ	2.34	0.60
37:i:77:VAL:HG13	37:i:132:LEU:HD12	1.82	0.60
1:2:1076:G:H5''	27:N:106:ARG:HH22	1.65	0.60
7:H:69:LEU:HD13	7:H:96:ALA:HB2	1.83	0.60
1:2:65:C:N4	24:G:134:GLY:O	2.35	0.60
1:2:696:G:H21	1:2:737:G:H1	1.48	0.60
26:M:60:MET:HA	26:M:63:LYS:HG2	1.84	0.60
7:H:74:LYS:HG3	7:H:75:ILE:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:M:83:LYS:HE2	26:M:104:VAL:HA	1.82	0.60
11:P:18:ARG:NH1	14:S:88:LYS:O	2.35	0.60
26:M:33:ARG:HE	26:M:91:LEU:HD12	1.67	0.60
2:A:163:CYS:HB3	2:A:174:MET:HE2	1.84	0.59
16:U:95:SER:HA	16:U:98:VAL:HG22	1.84	0.59
4:D:16:ILE:HD11	21:d:36:LEU:HD23	1.84	0.59
7:H:53:VAL:HG23	7:H:175:GLY:HA3	1.83	0.59
22:g:83:TRP:HA	22:g:107:ASP:HB2	1.85	0.59
30:Y:102:THR:OG1	30:Y:106:GLN:OE1	2.19	0.59
37:i:125:GLU:HG2	37:i:132:LEU:HD23	1.84	0.59
1:2:959:G:OP1	28:O:104:ARG:NH2	2.35	0.59
7:H:65:PRO:O	7:H:69:LEU:N	2.36	0.59
1:2:847:A:O2'	5:E:106:LYS:NZ	2.35	0.59
2:A:22:GLY:O	2:A:24:HIS:ND1	2.35	0.58
7:H:144:ILE:HG23	29:W:52:ILE:HB	1.84	0.58
31:Z:99:LEU:HD11	31:Z:102:LYS:HB2	1.84	0.58
24:G:59:GLN:OE1	24:G:72:ARG:NH2	2.37	0.58
26:M:40:LYS:NZ	34:f:129:GLY:O	2.32	0.58
1:2:834:C:H42	1:2:839:C:H42	1.51	0.58
28:O:84:ARG:NH1	28:O:87:GLU:OE2	2.36	0.58
12:Q:32:ILE:HG13	12:Q:68:ILE:HB	1.84	0.58
28:O:103:ASN:ND2	28:O:140:THR:O	2.36	0.58
11:P:123:TYR:OH	14:S:124:ARG:NH1	2.36	0.58
16:U:25:THR:HG22	16:U:86:LYS:HG2	1.85	0.58
31:Z:47:LEU:HD23	31:Z:79:ILE:HD13	1.86	0.58
1:2:587:A:H5'	1:2:592:C:H42	1.69	0.58
3:B:85:LYS:HB3	3:B:101:HIS:HB3	1.83	0.58
24:G:98:ARG:NH2	24:G:103:ASP:OD1	2.37	0.58
12:Q:116:ASP:OD1	12:Q:118:THR:OG1	2.21	0.58
35:x:10:G:O6	35:x:45:G:O6	2.22	0.58
7:H:30:LEU:O	7:H:33:ASN:ND2	2.36	0.57
8:I:11:ARG:NH1	8:I:15:GLY:O	2.37	0.57
1:2:1017:U:H5'	27:N:55:ARG:HD3	1.86	0.57
25:J:93:LYS:HE2	25:J:96:TYR:HE2	1.68	0.57
30:Y:39:GLU:HA	30:Y:42:GLU:HG3	1.86	0.57
24:G:32:MET:HE2	24:G:54:GLY:HA2	1.87	0.57
25:J:116:LYS:NZ	37:i:32:GLN:O	2.37	0.57
35:x:32:C:H41	35:x:35:U:H5''	1.69	0.57
1:2:1763:G:OP2	1:2:1772:C:N4	2.38	0.57
1:2:928:G:H2'	1:2:929:G:C8	2.40	0.57
8:I:133:GLU:HA	8:I:136:ILE:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:x:10:G:N7	35:x:45:G:C2	2.72	0.57
2:A:27:GLY:H	2:A:46:ILE:HG23	1.69	0.57
1:2:1005:G:OP2	3:B:162:ARG:NH1	2.38	0.57
7:H:144:ILE:HD11	7:H:152:ARG:HD3	1.85	0.57
1:2:1759:G:N2	1:2:1760:G:O6	2.37	0.57
2:A:52:LYS:HG2	13:R:109:LEU:HD22	1.87	0.57
9:K:80:ARG:NH2	9:K:89:ILE:O	2.35	0.56
1:2:1748:G:H1	1:2:1786:U:H3	1.52	0.56
14:S:46:ARG:HG2	15:T:35:ASP:HB2	1.87	0.56
35:x:13:U:H2'	35:x:14:A:H8	1.70	0.56
1:2:197:U:OP2	1:2:203:G:N2	2.32	0.56
1:2:1252:C:OP1	16:U:75:LYS:NZ	2.37	0.56
1:2:1254:C:O2'	16:U:66:ARG:NH2	2.38	0.56
22:g:236:ILE:HG12	22:g:252:THR:HG22	1.86	0.56
37:i:108:ASP:HB3	37:i:114:ALA:HB2	1.85	0.56
17:V:19:ALA:O	29:W:23:ARG:NH2	2.39	0.56
35:x:21:A:H61	35:x:46:A:H2'	1.70	0.56
22:g:24:THR:HB	22:g:71:ILE:HG21	1.87	0.56
6:F:35:LEU:HD12	6:F:117:ILE:HD13	1.87	0.56
13:R:36:GLU:OE1	13:R:47:ARG:NH1	2.36	0.56
24:G:23:LYS:HB3	24:G:41:LEU:HB3	1.88	0.56
26:M:122:ASP:OD1	26:M:123:VAL:N	2.38	0.56
1:2:550:C:H5'	37:i:25:LYS:HG3	1.88	0.56
1:2:629:A:O2'	1:2:631:U:OP1	2.24	0.56
1:2:1418:C:H1'	1:2:1421:A:H2	1.71	0.56
3:B:47:THR:OG1	3:B:65:ARG:NH1	2.39	0.56
12:Q:97:GLN:NE2	22:g:60:ARG:HH12	2.03	0.56
30:Y:126:GLY:HA2	30:Y:129:LYS:HD2	1.86	0.56
1:2:1679:A:H2'	6:F:60:ARG:HD2	1.87	0.55
15:T:9:VAL:HG21	15:T:138:VAL:HG13	1.87	0.55
1:2:85:A:H5''	30:Y:118:ARG:HH12	1.71	0.55
22:g:215:GLN:HG3	22:g:231:ASP:HB2	1.89	0.55
1:2:553:U:OP1	33:e:40:ARG:NH2	2.36	0.55
7:H:39:GLN:HG3	7:H:75:ILE:HG21	1.88	0.55
14:S:38:ARG:HB3	15:T:45:LEU:HD21	1.88	0.55
1:2:1536:G:H2'	1:2:1537:A:C8	2.41	0.55
1:2:1521:C:OP2	14:S:124:ARG:NH2	2.34	0.55
3:B:183:GLU:HA	3:B:186:ASN:HB2	1.87	0.55
22:g:166:VAL:HG12	22:g:176:VAL:HG22	1.88	0.55
1:2:1091:C:OP1	27:N:9:LYS:NZ	2.34	0.55
6:F:175:ASP:HA	6:F:178:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:15:THR:HG22	20:c:16:LYS:H	1.72	0.54
12:Q:139:ALA:O	12:Q:140:ARG:NH2	2.41	0.54
1:2:433:A:H5''	8:I:22:HIS:HB3	1.90	0.54
11:P:108:LYS:HB2	11:P:111:MET:HE3	1.89	0.54
32:b:49:HIS:ND1	32:b:69:GLY:O	2.40	0.54
1:2:643:A:OP1	25:J:41:ARG:NH2	2.41	0.54
16:U:21:ARG:HD3	16:U:88:LEU:HD22	1.89	0.54
29:W:60:LYS:NZ	32:b:23:ARG:O	2.40	0.54
1:2:1751:C:H42	1:2:1782:G:H21	1.56	0.54
12:Q:43:GLU:O	12:Q:45:ARG:N	2.41	0.54
16:U:97:ILE:O	16:U:100:GLN:NE2	2.41	0.54
22:g:272:GLN:HE21	22:g:284:PRO:HG2	1.72	0.54
1:2:919:A:OP2	27:N:64:ARG:NH2	2.38	0.53
18:X:123:VAL:HG12	18:X:124:LYS:HG3	1.89	0.53
1:2:126:G:OP2	24:G:198:ARG:NH1	2.38	0.53
1:2:1512:C:O2'	21:d:7:TYR:O	2.23	0.53
1:2:127:C:O2	5:E:134:LYS:NZ	2.41	0.53
16:U:98:VAL:HA	16:U:101:ILE:HG22	1.89	0.53
1:2:1230:C:OP1	14:S:130:ARG:NH2	2.41	0.53
12:Q:112:LEU:HD22	12:Q:119:LEU:HD13	1.89	0.53
22:g:146:SER:OG	22:g:147:HIS:N	2.40	0.53
1:2:940:U:H3	1:2:1002:U:H3	1.56	0.53
1:2:1417:C:H42	1:2:1422:G:H1	1.57	0.53
4:D:127:MET:HE1	4:D:133:GLY:HA2	1.88	0.53
1:2:886:A:C6	1:2:901:G:N3	2.76	0.53
22:g:193:GLY:N	22:g:213:ASP:OD1	2.42	0.53
6:F:39:ILE:HG23	6:F:68:ILE:HG13	1.90	0.53
12:Q:42:ILE:HG13	12:Q:43:GLU:H	1.73	0.53
35:x:22:U:OP2	35:x:46:A:N6	2.41	0.53
1:2:507:G:OP2	30:Y:104:ARG:NH2	2.41	0.53
26:M:89:VAL:HG21	26:M:109:VAL:HG11	1.88	0.53
30:Y:14:THR:HG22	30:Y:21:LYS:HG2	1.91	0.53
1:2:672:A:N6	1:2:1027:A:OP1	2.33	0.52
6:F:61:PHE:CZ	20:c:51:ARG:HB2	2.44	0.52
14:S:109:GLU:HA	14:S:112:GLU:HG3	1.91	0.52
18:X:91:LEU:HD21	33:e:6:LEU:HD12	1.91	0.52
1:2:10:G:H21	23:C:114:LYS:HA	1.74	0.52
14:S:15:VAL:HG12	14:S:16:LEU:HG	1.91	0.52
1:2:1598:G:O2'	31:Z:80:ARG:O	2.21	0.52
2:A:163:CYS:SG	2:A:164:ASN:N	2.82	0.52
14:S:55:ARG:N	14:S:58:GLU:OE2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:71:G:N2	1:2:73:C:OP1	2.43	0.52
20:c:22:GLY:O	20:c:26:GLN:NE2	2.39	0.52
11:P:98:ASN:ND2	11:P:121:ILE:O	2.42	0.52
1:2:1551:U:OP1	4:D:9:ARG:NH2	2.42	0.52
9:K:15:LEU:HD22	9:K:49:MET:HE1	1.92	0.52
1:2:145:G:H2'	1:2:146:G:C8	2.45	0.52
1:2:1020:A:OP2	27:N:70:LYS:NZ	2.42	0.52
1:2:1120:U:OP1	32:b:72:ARG:NH2	2.42	0.52
37:i:92:GLN:NE2	37:i:110:GLU:OE1	2.29	0.52
7:H:46:THR:HG23	7:H:65:PRO:HD3	1.92	0.52
18:X:77:ASN:O	18:X:79:LYS:N	2.38	0.52
22:g:39:THR:HG22	22:g:60:ARG:HG2	1.92	0.52
1:2:688:U:O2	1:2:689:U:N3	2.43	0.51
17:V:15:ARG:NH1	17:V:33:GLN:OE1	2.41	0.51
6:F:135:ARG:N	35:x:33:U:OP2	2.43	0.51
10:L:126:VAL:HG12	10:L:145:VAL:HG22	1.92	0.51
22:g:191:HIS:NE2	22:g:209:SER:OG	2.40	0.51
23:C:64:THR:HG22	23:C:66:LEU:H	1.75	0.51
19:a:32:LYS:O	19:a:37:LYS:NZ	2.43	0.51
35:x:33:U:N3	35:x:37:A:C8	2.78	0.51
1:2:878:G:C6	1:2:908:A:N1	2.79	0.51
8:I:203:LYS:HA	8:I:206:LYS:HZ3	1.75	0.51
14:S:89:ASP:OD1	14:S:90:VAL:N	2.43	0.51
30:Y:57:VAL:HB	30:Y:60:PHE:HE2	1.74	0.51
1:2:17:C:O2'	1:2:1194:A:N1	2.41	0.51
12:Q:85:ARG:NH2	12:Q:116:ASP:OD2	2.43	0.51
1:2:1779:G:H2'	1:2:1780:G:C8	2.46	0.51
31:Z:50:PHE:HB2	31:Z:54:THR:HB	1.93	0.51
31:Z:50:PHE:HD1	31:Z:83:LEU:HD21	1.76	0.51
27:N:99:ARG:NH2	27:N:119:GLU:OE2	2.38	0.50
2:A:27:GLY:HA3	2:A:46:ILE:HA	1.93	0.50
7:H:15:LYS:HD3	7:H:16:PRO:HA	1.92	0.50
1:2:197:U:N3	1:2:202:G:N7	2.60	0.50
6:F:168:THR:OG1	6:F:171:GLU:OE1	2.29	0.50
23:C:205:VAL:O	23:C:224:THR:OG1	2.29	0.50
1:2:71:G:O6	24:G:170:ARG:NH1	2.44	0.50
24:G:159:ARG:HD2	24:G:173:ALA:HB2	1.94	0.50
30:Y:78:SER:OG	30:Y:80:ASP:OD1	2.22	0.50
31:Z:50:PHE:HE2	31:Z:55:TYR:HD1	1.58	0.50
1:2:944:A:H5''	28:O:134:PRO:HB3	1.93	0.50
1:2:1785:C:O2'	1:2:1786:U:O4'	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:28:MET:HE3	11:P:32:GLN:HG2	1.94	0.50
37:i:37:ASP:N	37:i:37:ASP:OD1	2.44	0.50
23:C:77:SER:O	23:C:79:GLU:N	2.45	0.50
1:2:886:A:N6	1:2:901:G:N3	2.58	0.50
12:Q:19:ALA:HB2	12:Q:75:GLY:HA3	1.93	0.50
1:2:583:C:OP1	25:J:162:ARG:NH2	2.42	0.49
7:H:58:LYS:HB2	7:H:90:LYS:HG2	1.93	0.49
29:W:18:GLU:HG2	29:W:69:LEU:HB3	1.94	0.49
7:H:69:LEU:O	7:H:73:GLN:HG2	2.13	0.49
19:a:88:SER:O	19:a:92:ARG:N	2.45	0.49
1:2:1277:C:H2'	1:2:1278:A:H8	1.77	0.49
1:2:1827:U:OP1	36:y:361:LYS:NZ	2.43	0.49
35:x:48:C:H2'	35:x:49:G:H8	1.77	0.49
12:Q:51:LEU:HD13	12:Q:81:ILE:HG23	1.93	0.49
24:G:231:ARG:HD3	24:G:232:ARG:HH21	1.77	0.49
1:2:367:U:H4'	1:2:371:A:C8	2.47	0.49
25:J:158:ASP:OD1	25:J:159:PHE:N	2.46	0.49
1:2:1743:G:H21	1:2:1791:A:H62	1.61	0.49
22:g:69:VAL:HG23	22:g:80:SER:HB3	1.94	0.49
34:f:141:CYS:HB3	34:f:144:CYS:SG	2.51	0.49
4:D:29:LEU:HD12	4:D:34:TYR:HB2	1.94	0.49
9:K:41:PRO:HG2	9:K:44:HIS:ND1	2.28	0.49
22:g:220:ASP:OD1	22:g:220:ASP:N	2.44	0.49
28:O:13:GLN:HB3	28:O:15:ILE:HG22	1.95	0.49
32:b:40:CYS:SG	32:b:41:TYR:N	2.85	0.49
1:2:857:U:H2'	1:2:858:A:C8	2.47	0.48
2:A:81:ASN:HA	2:A:84:GLN:HB2	1.95	0.48
7:H:80:VAL:HG23	7:H:92:VAL:HB	1.95	0.48
14:S:86:ARG:NH2	14:S:110:ASP:OD2	2.42	0.48
16:U:68:THR:O	21:d:40:ARG:NH1	2.43	0.48
35:x:48:C:H2'	35:x:49:G:C8	2.47	0.48
8:I:57:ALA:HB2	8:I:183:GLY:HA2	1.94	0.48
8:I:105:ASP:OD2	8:I:107:THR:OG1	2.25	0.48
12:Q:43:GLU:HG2	12:Q:44:PRO:HD3	1.95	0.48
1:2:1024:A:OP2	27:N:124:ARG:NH2	2.46	0.48
7:H:12:ASN:ND2	7:H:17:ASP:OD1	2.38	0.48
11:P:48:GLY:O	11:P:50:ARG:NH1	2.46	0.48
26:M:52:GLN:NE2	26:M:66:GLU:OE2	2.46	0.48
1:2:527:C:H4'	25:J:121:LYS:HE2	1.94	0.48
1:2:617:G:H4'	18:X:88:ASP:HA	1.95	0.48
11:P:81:ARG:NH2	11:P:117:GLY:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:17:ILE:HD11	13:R:54:VAL:HG13	1.96	0.48
1:2:1473:G:N1	1:2:1476:A:OP2	2.44	0.48
1:2:1217:A:H2'	1:2:1218:C:H6	1.79	0.48
1:2:1522:A:O2'	14:S:145:THR:OG1	2.26	0.48
9:K:29:MET:HE1	9:K:33:PRO:HG3	1.96	0.48
15:T:108:GLU:OE2	15:T:121:ARG:NE	2.37	0.48
34:f:123:SER:OG	34:f:126:CYS:SG	2.72	0.48
37:i:121:LEU:O	37:i:125:GLU:HG3	2.14	0.48
2:A:84:GLN:HG2	2:A:100:ALA:HB1	1.96	0.48
29:W:113:HIS:NE2	29:W:114:GLU:OE2	2.46	0.48
1:2:190:G:H5''	8:I:145:ILE:HD13	1.95	0.48
1:2:223:C:H2'	1:2:224:A:C8	2.48	0.48
1:2:1217:A:H2'	1:2:1218:C:C6	2.48	0.48
1:2:1536:G:H2'	1:2:1537:A:H8	1.77	0.48
37:i:99:ILE:HD11	37:i:106:ILE:HD11	1.95	0.48
1:2:218:U:O2	8:I:184:ARG:NH2	2.45	0.48
1:2:1353:A:OP1	2:A:139:TYR:OH	2.26	0.48
1:2:1651:A:O2'	6:F:83:ASN:OD1	2.26	0.48
9:K:7:ASN:HD22	9:K:40:VAL:HG22	1.78	0.48
14:S:89:ASP:OD2	14:S:106:LYS:NZ	2.46	0.48
15:T:126:GLN:OE1	15:T:129:ARG:NH2	2.46	0.48
1:2:1421:A:H5''	1:2:1422:G:C8	2.49	0.47
7:H:50:GLU:HG2	7:H:60:ILE:HG22	1.96	0.47
12:Q:5:GLY:O	12:Q:27:ARG:NH2	2.47	0.47
14:S:39:ARG:HH22	15:T:46:ALA:HB2	1.79	0.47
22:g:29:ASP:OD1	22:g:47:ARG:NH1	2.46	0.47
22:g:152:SER:OG	22:g:153:CYS:N	2.46	0.47
35:x:15:A:N6	35:x:47:C:O2	2.32	0.47
1:2:746:C:O2'	1:2:798:A:N1	2.40	0.47
1:2:1756:C:N3	1:2:1776:G:N1	2.41	0.47
11:P:133:ILE:HG21	36:y:318:ILE:HD11	1.96	0.47
17:V:80:SER:OG	17:V:82:ASN:OD1	2.32	0.47
19:a:46:GLU:CD	28:O:113:GLN:HG3	2.39	0.47
1:2:530:U:H3	1:2:554:A:N6	2.13	0.47
3:B:131:ASP:OD1	3:B:131:ASP:N	2.41	0.47
14:S:66:ARG:O	14:S:70:ILE:HG23	2.14	0.47
22:g:176:VAL:HB	22:g:186:THR:HG22	1.97	0.47
22:g:11:LEU:HD21	22:g:52:TYR:HD2	1.79	0.47
22:g:201:SER:OG	22:g:203:ASP:O	2.24	0.47
1:2:71:G:H2'	1:2:72:C:H4'	1.97	0.47
1:2:793:G:H2'	1:2:794:A:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:2:PRO:HA	15:T:3:GLY:HA3	1.71	0.47
22:g:163:PRO:HB2	22:g:179:LEU:HB2	1.96	0.47
25:J:122:SER:O	25:J:125:HIS:N	2.40	0.47
26:M:15:ASN:OD1	26:M:16:THR:N	2.47	0.47
35:x:35:U:H1'	35:x:36:C:H5'	1.96	0.47
1:2:1102:G:OP2	3:B:151:ARG:NH2	2.47	0.47
8:I:11:ARG:O	10:L:136:LYS:NZ	2.47	0.47
22:g:10:THR:HG22	22:g:308:ARG:HD3	1.97	0.47
22:g:251:ALA:HA	22:g:256:ILE:HG22	1.95	0.47
1:2:696:G:N2	1:2:737:G:H1	2.12	0.47
1:2:1679:A:OP1	20:c:20:ARG:NH2	2.46	0.47
8:I:42:ARG:HH21	8:I:59:ARG:NH1	2.13	0.47
10:L:23:VAL:HG23	10:L:25:LEU:HG	1.96	0.47
11:P:98:ASN:OD1	11:P:120:SER:OG	2.29	0.47
1:2:1588:A:H2'	1:2:1589:A:C8	2.49	0.47
22:g:153:CYS:HB3	22:g:197:THR:HA	1.96	0.47
24:G:44:GLU:HA	24:G:119:LYS:HD2	1.97	0.47
24:G:181:THR:HB	24:G:184:VAL:HG23	1.97	0.47
35:x:25:C:H2'	35:x:26:A:H8	1.80	0.47
5:E:36:HIS:NE2	5:E:88:ASP:OD2	2.47	0.47
10:L:111:VAL:HG11	10:L:128:VAL:HG11	1.97	0.47
31:Z:68:ILE:HB	31:Z:109:TYR:HB2	1.97	0.46
1:2:1354:G:N2	1:2:1357:A:OP2	2.35	0.46
1:2:1454:A:H5''	13:R:3:ARG:HD2	1.96	0.46
15:T:43:LYS:HE2	15:T:43:LYS:HB3	1.72	0.46
20:c:35:MET:HE1	20:c:55:VAL:HG22	1.95	0.46
24:G:57:ASP:OD1	24:G:58:LYS:N	2.44	0.46
35:x:10:G:O6	35:x:26:A:N6	2.48	0.46
1:2:942:G:H2'	1:2:943:U:C6	2.51	0.46
1:2:1417:C:N3	1:2:1422:G:O6	2.48	0.46
5:E:124:CYS:HB3	5:E:141:THR:HB	1.97	0.46
15:T:18:LEU:HD22	15:T:58:ALA:HA	1.97	0.46
26:M:15:ASN:HA	26:M:18:LEU:HD23	1.97	0.46
1:2:1413:G:H2'	1:2:1414:A:H8	1.81	0.46
1:2:1674:G:H4'	6:F:77:MET:HE1	1.97	0.46
1:2:1780:G:N2	1:2:1782:G:OP1	2.48	0.46
5:E:114:ILE:HD12	5:E:118:GLU:HG2	1.97	0.46
1:2:886:A:C6	1:2:901:G:C4	2.99	0.46
10:L:21:LYS:HA	10:L:21:LYS:HD2	1.75	0.46
23:C:166:ARG:HB3	23:C:247:THR:HB	1.97	0.46
25:J:110:LEU:HB2	25:J:147:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:100:LYS:HD3	27:N:104:ARG:HH22	1.81	0.46
1:2:1472:C:O3'	22:g:15:ASN:ND2	2.48	0.46
1:2:681:U:H4'	18:X:9:THR:HG22	1.98	0.46
1:2:900:C:H5'	1:2:901:G:N7	2.31	0.46
10:L:111:VAL:HG12	10:L:140:PHE:HB2	1.97	0.46
24:G:70:HIS:HA	24:G:98:ARG:HH12	1.80	0.46
25:J:3:VAL:HG22	25:J:5:ARG:HD3	1.98	0.46
1:2:640:A:H2'	1:2:641:A:C8	2.51	0.46
7:H:10:LYS:NZ	7:H:20:GLU:O	2.49	0.46
20:c:20:ARG:HD3	20:c:28:THR:HG22	1.98	0.46
27:N:25:TRP:CD2	32:b:82:LYS:HE2	2.51	0.46
14:S:60:THR:OG1	14:S:62:ASP:OD1	2.28	0.46
20:c:66:ARG:NH1	20:c:67:ARG:O	2.50	0.46
30:Y:3:ASP:N	30:Y:3:ASP:OD1	2.49	0.46
1:2:838:G:O2'	1:2:840:C:OP2	2.30	0.45
1:2:906:U:H2'	1:2:907:G:H8	1.81	0.45
1:2:1845:A:H2'	1:2:1846:G:C8	2.51	0.45
14:S:101:ASN:OD1	14:S:101:ASN:N	2.49	0.45
26:M:92:CYS:SG	26:M:93:LYS:N	2.86	0.45
14:S:6:PRO:HG3	14:S:58:GLU:HB3	1.98	0.45
19:a:45:VAL:HG21	19:a:64:LEU:HD22	1.98	0.45
1:2:549:C:H4'	37:i:24:SER:HB3	1.98	0.45
3:B:199:LYS:HE2	3:B:199:LYS:HB3	1.75	0.45
12:Q:32:ILE:HG12	12:Q:39:LEU:HD21	1.98	0.45
18:X:100:VAL:HG12	18:X:125:VAL:HA	1.98	0.45
37:i:73:VAL:HG23	37:i:112:GLY:HA2	1.98	0.45
1:2:617:G:OP2	18:X:68:LYS:NZ	2.49	0.45
7:H:166:VAL:HG23	7:H:169:LYS:HG3	1.97	0.45
8:I:162:LEU:HD11	8:I:191:GLU:HG2	1.97	0.45
12:Q:109:LYS:O	12:Q:113:ILE:HG12	2.17	0.45
24:G:21:GLU:OE2	24:G:25:ARG:NH1	2.49	0.45
32:b:54:VAL:HG23	32:b:63:LEU:HB2	1.98	0.45
1:2:77:A:H1'	24:G:176:ILE:HG12	1.97	0.45
1:2:323:C:H2'	1:2:327:G:H22	1.81	0.45
1:2:874:G:H2'	1:2:875:A:H8	1.81	0.45
1:2:1435:C:O2'	1:2:1436:C:O4'	2.29	0.45
8:I:136:ILE:O	8:I:139:LYS:NZ	2.46	0.45
1:2:115:U:H2'	1:2:116:U:C6	2.52	0.45
3:B:29:ASP:OD1	3:B:29:ASP:N	2.45	0.45
1:2:902:G:O2'	1:2:903:A:O4'	2.34	0.45
2:A:173:LEU:HD11	2:A:177:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:126:HIS:CE1	7:H:181:THR:HG23	2.51	0.45
23:C:271:ASP:OD1	23:C:272:HIS:N	2.50	0.45
1:2:194:C:H2'	1:2:195:C:H6	1.81	0.45
1:2:570:C:O2'	30:Y:34:THR:O	2.32	0.45
5:E:45:ILE:HA	5:E:61:VAL:HG11	1.99	0.45
8:I:126:GLY:O	8:I:128:LYS:NZ	2.36	0.45
22:g:42:MET:HE3	22:g:57:ARG:HB3	1.99	0.45
1:2:943:U:O2'	28:O:135:ILE:O	2.34	0.45
1:2:1277:C:H2'	1:2:1278:A:C8	2.52	0.45
1:2:1560:U:H2'	1:2:1561:A:H8	1.81	0.45
1:2:1562:C:H2'	1:2:1563:G:H8	1.82	0.45
4:D:169:ASP:OD2	4:D:169:ASP:N	2.49	0.45
37:i:125:GLU:OE2	37:i:133:ARG:NE	2.49	0.45
5:E:45:ILE:HD12	5:E:80:ILE:HD12	1.98	0.45
5:E:164:LEU:O	5:E:165:GLU:HG3	2.17	0.45
9:K:24:LYS:O	9:K:42:ASN:ND2	2.48	0.45
4:D:215:ASP:OD1	4:D:215:ASP:N	2.49	0.44
19:a:100:ARG:HH21	19:a:102:ARG:HH22	1.66	0.44
22:g:20:GLN:NE2	22:g:68:ASP:OD1	2.50	0.44
22:g:217:MET:HG3	22:g:229:THR:HG22	1.99	0.44
23:C:187:ARG:HD3	23:C:192:LEU:HD12	1.99	0.44
27:N:87:ASP:OD1	27:N:87:ASP:N	2.41	0.44
1:2:382:C:H2'	1:2:383:G:H8	1.82	0.44
3:B:77:ASP:OD1	3:B:77:ASP:N	2.51	0.44
5:E:98:ASN:O	5:E:114:ILE:HG12	2.16	0.44
21:d:13:LYS:O	21:d:18:SER:HB2	2.16	0.44
1:2:307:G:O6	8:I:44:HIS:ND1	2.51	0.44
4:D:219:PRO:HB2	22:g:192:THR:HG22	1.99	0.44
22:g:174:VAL:HB	22:g:188:HIS:HB2	1.99	0.44
22:g:272:GLN:HB3	22:g:308:ARG:HH12	1.82	0.44
22:g:14:HIS:HE1	22:g:18:VAL:HB	1.82	0.44
23:C:166:ARG:HB2	23:C:248:TYR:CD1	2.53	0.44
26:M:54:SER:HB2	26:M:80:ASP:HA	2.00	0.44
26:M:106:CYS:SG	26:M:107:SER:N	2.90	0.44
28:O:34:PHE:HB3	28:O:41:PHE:HB2	1.99	0.44
10:L:29:GLY:HA3	10:L:30:LYS:HA	1.72	0.44
14:S:35:GLY:O	14:S:97:GLN:NE2	2.49	0.44
23:C:191:VAL:HG11	23:C:236:PHE:HA	1.97	0.44
24:G:2:LYS:HG2	24:G:15:LEU:HD21	2.00	0.44
1:2:118:C:H1'	1:2:445:A:C5	2.53	0.44
1:2:453:C:O2'	24:G:92:ARG:O	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:x:20:U:O2'	35:x:21:A:N7	2.42	0.44
7:H:143:ARG:HB2	7:H:155:LYS:HB2	1.99	0.44
12:Q:97:GLN:CD	12:Q:105:LYS:HE2	2.42	0.44
36:y:361:LYS:HA	36:y:361:LYS:HD3	1.81	0.44
1:2:372:U:O2'	10:L:82:MET:SD	2.76	0.44
1:2:981:A:H2'	1:2:982:G:C8	2.52	0.44
1:2:1010:G:H2'	1:2:1011:A:C8	2.53	0.44
1:2:1683:C:H2'	1:2:1684:C:H6	1.82	0.44
2:A:85:ARG:HG3	13:R:81:ARG:HD2	2.00	0.44
12:Q:31:LEU:HB3	12:Q:67:ASP:OD2	2.17	0.44
19:a:12:LYS:HB2	19:a:33:ASP:OD2	2.17	0.44
31:Z:49:LEU:H	31:Z:83:LEU:HD22	1.82	0.44
1:2:107:A:H2'	1:2:108:G:C8	2.52	0.44
1:2:1158:G:H5''	29:W:76:SER:HB3	1.99	0.44
4:D:35:SER:OG	4:D:51:LEU:O	2.35	0.44
22:g:121:VAL:HG11	22:g:165:ILE:HD11	2.00	0.44
1:2:1628:C:H2'	1:2:1629:C:C6	2.53	0.43
2:A:158:ASP:OD2	17:V:60:ARG:NH1	2.51	0.43
23:C:88:ILE:HD13	23:C:94:ILE:HD11	1.99	0.43
2:A:36:GLN:O	2:A:53:ARG:NH1	2.51	0.43
4:D:74:GLN:NE2	4:D:79:PHE:O	2.49	0.43
14:S:62:ASP:OD1	14:S:63:GLU:N	2.51	0.43
26:M:40:LYS:HA	26:M:40:LYS:HD3	1.74	0.43
37:i:119:GLN:NE2	37:i:123:LYS:HD2	2.32	0.43
1:2:1438:A:H2'	1:2:1439:A:C8	2.54	0.43
1:2:1533:A:H2	1:2:1536:G:N3	2.15	0.43
6:F:33:ILE:HA	6:F:36:GLN:HG2	2.00	0.43
24:G:20:ASP:OD1	24:G:22:ARG:NH1	2.51	0.43
31:Z:69:THR:H	31:Z:72:VAL:HG22	1.84	0.43
37:i:72:ARG:NH2	37:i:113:ARG:O	2.44	0.43
1:2:384:U:O4	8:I:5:ARG:NH2	2.45	0.43
1:2:907:G:H2'	1:2:908:A:C8	2.53	0.43
4:D:150:MET:HB3	4:D:150:MET:HE2	1.82	0.43
4:D:211:VAL:O	13:R:20:TYR:OH	2.34	0.43
7:H:31:GLU:HA	7:H:37:LYS:HZ1	1.83	0.43
14:S:59:LEU:HD23	14:S:59:LEU:HA	1.90	0.43
14:S:82:TRP:CD1	14:S:82:TRP:H	2.37	0.43
1:2:1013:U:OP1	1:2:1129:G:O2'	2.36	0.43
1:2:1232:U:H2'	1:2:1233:G:H8	1.84	0.43
14:S:34:LYS:HB3	14:S:103:LEU:HD23	2.01	0.43
20:c:12:ALA:HB1	20:c:32:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:g:23:THR:HG22	22:g:31:ILE:HG22	2.00	0.43
26:M:75:ASN:OD1	26:M:76:LEU:N	2.52	0.43
1:2:886:A:C5	1:2:901:G:C2	3.07	0.43
1:2:921:G:C6	29:W:28:ARG:HD2	2.53	0.43
4:D:194:PRO:HG2	4:D:196:GLY:H	1.83	0.43
10:L:82:MET:HE3	10:L:85:THR:HG22	2.01	0.43
12:Q:97:GLN:HE22	22:g:60:ARG:HH22	1.66	0.43
23:C:278:THR:HA	23:C:279:ARG:HA	1.62	0.43
1:2:656:G:H5'	1:2:662:G:N2	2.34	0.43
1:2:913:A:OP2	7:H:99:ARG:NH2	2.52	0.43
1:2:1600:G:H5'	31:Z:43:LYS:HE3	2.00	0.43
1:2:1759:G:N3	1:2:1773:C:O2'	2.50	0.43
20:c:18:LEU:HB2	20:c:29:GLN:HB2	2.01	0.43
24:G:217:MET:HA	24:G:220:ALA:HB3	2.01	0.43
26:M:84:LYS:NZ	26:M:88:TRP:HE1	2.16	0.43
28:O:47:LEU:HD23	28:O:47:LEU:HA	1.87	0.43
34:f:133:ALA:N	34:f:140:TYR:O	2.41	0.43
35:x:69:G:H2'	35:x:70:G:C8	2.54	0.43
1:2:747:U:N3	1:2:796:G:N1	2.67	0.43
4:D:220:THR:OG1	4:D:221:THR:N	2.47	0.43
6:F:18:LYS:HE2	6:F:22:LYS:HA	2.01	0.43
11:P:15:PHE:CE2	11:P:17:TYR:HB2	2.53	0.43
22:g:246:TYR:CD2	22:g:261:LEU:HB2	2.53	0.43
23:C:116:THR:OG1	23:C:119:GLY:O	2.31	0.43
25:J:131:ARG:NH2	25:J:143:ASN:O	2.51	0.43
26:M:64:LEU:HD11	34:f:106:TYR:HD2	1.83	0.43
1:2:4:C:H4'	23:C:207:ALA:HB2	1.99	0.43
23:C:271:ASP:HA	23:C:274:VAL:HG12	2.00	0.43
26:M:42:LEU:HD11	26:M:68:LEU:HD23	2.00	0.43
1:2:557:U:O2'	1:2:558:G:O5'	2.34	0.42
1:2:951:C:O2'	28:O:50:LYS:NZ	2.52	0.42
1:2:1448:A:H2'	1:2:1449:G:O4'	2.18	0.42
10:L:104:LYS:HE3	10:L:104:LYS:HB2	1.91	0.42
23:C:105:GLU:HG2	23:C:216:MET:HE1	2.01	0.42
1:2:372:U:OP1	10:L:136:LYS:NZ	2.39	0.42
1:2:1659:U:OP1	21:d:32:ARG:HG2	2.19	0.42
2:A:198:MET:HE2	13:R:85:VAL:HG22	2.01	0.42
11:P:29:SER:OG	11:P:30:TYR:N	2.52	0.42
14:S:15:VAL:HG21	14:S:20:ILE:HD12	1.99	0.42
16:U:31:SER:HB2	16:U:107:GLU:CD	2.43	0.42
1:2:104:A:H62	1:2:356:C:H5	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1086:G:O2'	1:2:1088:U:OP2	2.32	0.42
1:2:1144:A:H2'	1:2:1145:A:C8	2.54	0.42
2:A:37:TYR:OH	2:A:57:LYS:NZ	2.51	0.42
18:X:71:ARG:NH2	18:X:82:THR:OG1	2.46	0.42
26:M:24:THR:HA	26:M:27:ILE:HG12	2.01	0.42
1:2:377:G:H5'	8:I:98:LYS:HB3	2.00	0.42
1:2:1778:C:H2'	1:2:1779:G:C8	2.54	0.42
2:A:50:ASN:HD22	2:A:53:ARG:HE	1.67	0.42
25:J:152:ASP:OD1	25:J:153:SER:N	2.52	0.42
26:M:92:CYS:HB3	26:M:94:ILE:HG13	2.01	0.42
34:f:109:ASP:OD1	34:f:109:ASP:N	2.52	0.42
35:x:4:G:H2'	35:x:5:A:H8	1.84	0.42
1:2:74:G:H5''	1:2:76:U:C4	2.54	0.42
2:A:40:LYS:HB2	2:A:40:LYS:HE3	1.79	0.42
6:F:99:ILE:HD13	6:F:171:GLU:HB3	2.02	0.42
35:x:28:C:H2'	35:x:29:A:C8	2.54	0.42
1:2:455:A:H2'	1:2:456:C:C6	2.55	0.42
1:2:538:U:H2'	1:2:539:C:C6	2.54	0.42
1:2:614:C:H2'	1:2:626:G:C8	2.54	0.42
3:B:147:ASN:OD1	3:B:147:ASN:N	2.51	0.42
6:F:143:PRO:HA	6:F:146:ARG:HG2	2.02	0.42
16:U:81:GLN:OE1	16:U:83:ARG:NH2	2.52	0.42
18:X:100:VAL:HG12	18:X:125:VAL:HG23	2.02	0.42
19:a:44:ILE:HD12	19:a:65:PRO:HB2	2.00	0.42
22:g:258:ILE:HG23	22:g:267:VAL:HB	2.01	0.42
26:M:62:VAL:HA	26:M:65:VAL:HG12	2.01	0.42
1:2:448:A:H5''	8:I:25:ARG:HA	2.01	0.42
1:2:1808:U:H2'	1:2:1809:A:C8	2.55	0.42
25:J:42:GLU:HG2	25:J:45:ARG:NH2	2.34	0.42
31:Z:78:LYS:HD3	31:Z:78:LYS:HA	1.74	0.42
1:2:429:C:O2'	1:2:811:A:N1	2.46	0.42
2:A:205:ARG:NH2	2:A:213:GLU:OE1	2.53	0.42
4:D:134:CYS:SG	4:D:135:GLU:N	2.93	0.42
26:M:80:ASP:OD1	26:M:81:ASP:N	2.53	0.42
1:2:72:C:H42	24:G:170:ARG:HB3	1.85	0.42
1:2:571:U:O2'	30:Y:60:PHE:O	2.29	0.42
1:2:1301:A:H4'	21:d:3:HIS:NE2	2.35	0.42
1:2:1357:A:H5''	23:C:112:VAL:HG21	2.01	0.42
4:D:39:VAL:HG12	4:D:48:ILE:HG12	2.02	0.42
6:F:204:ARG:NH1	20:c:60:GLU:HB2	2.35	0.42
18:X:41:PHE:HZ	18:X:102:VAL:HG12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:g:168:CYS:HB3	22:g:198:VAL:HG13	2.01	0.42
1:2:530:U:H3	1:2:554:A:H61	1.68	0.42
1:2:588:G:H4'	1:2:589:G:H5'	2.02	0.42
2:A:53:ARG:HD2	17:V:83:PHE:CD2	2.55	0.42
2:A:211:GLU:HA	2:A:214:GLU:HG2	2.01	0.42
5:E:18:TRP:HH2	5:E:31:PRO:HD3	1.85	0.42
1:2:441:C:H2'	1:2:442:C:C6	2.55	0.41
1:2:688:U:H5	7:H:103:LYS:H	1.68	0.41
12:Q:73:LYS:HA	12:Q:73:LYS:HD3	1.83	0.41
22:g:260:ASP:OD1	22:g:260:ASP:N	2.53	0.41
25:J:111:GLN:NE2	25:J:127:ARG:HB2	2.35	0.41
27:N:83:ASP:OD1	27:N:84:LEU:N	2.53	0.41
1:2:685:A:H5''	29:W:31:SER:HB3	2.02	0.41
1:2:960:U:O2'	1:2:962:A:N7	2.43	0.41
1:2:1858:G:N7	28:O:146:ARG:NH1	2.66	0.41
3:B:180:ASP:OD1	3:B:180:ASP:N	2.51	0.41
10:L:90:ARG:HD3	10:L:109:MET:HE3	2.03	0.41
16:U:38:ASP:OD2	16:U:39:LEU:N	2.54	0.41
23:C:212:LYS:HD3	23:C:212:LYS:HA	1.84	0.41
30:Y:29:HIS:NE2	30:Y:69:THR:OG1	2.33	0.41
7:H:37:LYS:NZ	7:H:40:LEU:HD22	2.36	0.41
19:a:47:ALA:HA	19:a:50:VAL:HB	2.03	0.41
28:O:42:VAL:HG11	28:O:78:ALA:HA	2.02	0.41
31:Z:62:VAL:HA	31:Z:65:TYR:CE1	2.55	0.41
1:2:379:C:H5'	8:I:33:ALA:HA	2.03	0.41
1:2:562:U:H2'	1:2:563:G:C8	2.55	0.41
1:2:886:A:N6	1:2:901:G:N9	2.59	0.41
1:2:921:G:C5	29:W:28:ARG:HD2	2.56	0.41
2:A:50:ASN:ND2	2:A:53:ARG:HE	2.19	0.41
5:E:67:GLN:HB3	5:E:69:PHE:CE1	2.54	0.41
14:S:86:ARG:HD2	14:S:86:ARG:HA	1.83	0.41
16:U:46:LYS:HB3	16:U:48:LEU:HD23	2.02	0.41
20:c:9:ILE:HD13	20:c:59:LEU:HA	2.02	0.41
1:2:319:C:H2'	1:2:320:G:H8	1.86	0.41
1:2:1232:U:H2'	1:2:1233:G:C8	2.56	0.41
1:2:1310:U:OP1	26:M:36:ARG:NH2	2.35	0.41
1:2:1681:U:H2'	1:2:1682:C:C6	2.56	0.41
9:K:63:ALA:HB2	9:K:68:TYR:HE2	1.86	0.41
24:G:13:GLN:HE21	24:G:13:GLN:HB2	1.64	0.41
1:2:17:C:H2'	1:2:18:C:C6	2.56	0.41
1:2:996:A:H2'	1:2:997:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1550:G:H3'	1:2:1579:A:H61	1.86	0.41
8:I:107:THR:HA	8:I:110:ARG:HG2	2.02	0.41
9:K:23:ALA:HB3	9:K:69:TRP:HZ3	1.85	0.41
15:T:126:GLN:HE22	15:T:129:ARG:HH21	1.68	0.41
16:U:56:MET:HB2	16:U:86:LYS:HB2	2.03	0.41
22:g:120:ILE:O	22:g:132:TRP:N	2.40	0.41
1:2:202:G:OP2	1:2:202:G:N2	2.47	0.41
1:2:381:C:OP2	8:I:54:LYS:NZ	2.43	0.41
5:E:102:ILE:HD12	5:E:239:PRO:HD3	2.02	0.41
15:T:110:LEU:HB3	15:T:112:MET:HE3	2.03	0.41
33:e:24:LYS:HE3	33:e:24:LYS:HB3	1.92	0.41
4:D:167:TYR:HE2	4:D:189:MET:HE2	1.86	0.41
11:P:57:LEU:HD21	11:P:83:MET:HE2	2.02	0.41
15:T:5:THR:HG23	15:T:7:LYS:H	1.86	0.41
29:W:62:VAL:HG11	32:b:8:LEU:HD22	2.02	0.41
1:2:38:A:OP1	25:J:5:ARG:HG3	2.20	0.41
1:2:639:C:H2'	1:2:640:A:C8	2.56	0.41
1:2:986:G:O4'	28:O:138:ASP:HB2	2.20	0.41
1:2:1331:C:N4	36:y:372:LYS:O	2.53	0.41
1:2:1757:G:H8	1:2:1758:G:H1'	1.86	0.41
1:2:1780:G:H3'	1:2:1781:A:H8	1.86	0.41
2:A:39:TYR:CD2	2:A:40:LYS:HG2	2.56	0.41
3:B:108:ASP:OD1	3:B:108:ASP:N	2.54	0.41
4:D:7:LYS:HE3	16:U:25:THR:HG21	2.02	0.41
7:H:60:ILE:HD11	7:H:92:VAL:HG22	2.03	0.41
12:Q:40:GLU:OE1	12:Q:40:GLU:N	2.53	0.41
13:R:18:GLU:OE1	13:R:69:ILE:N	2.54	0.41
13:R:67:ARG:HA	13:R:68:GLY:HA3	1.57	0.41
22:g:203:ASP:OD1	22:g:205:SER:OG	2.34	0.41
24:G:2:LYS:HB3	24:G:15:LEU:HD11	2.03	0.41
30:Y:79:LEU:HG	30:Y:83:LYS:HE3	2.03	0.41
35:x:28:C:H2'	35:x:29:A:H8	1.85	0.41
36:y:355:LEU:HD23	36:y:355:LEU:HA	1.90	0.41
36:y:360:LYS:O	36:y:364:LYS:HB2	2.20	0.41
1:2:65:C:H6	1:2:65:C:H2'	1.67	0.41
2:A:81:ASN:OD1	2:A:81:ASN:N	2.53	0.41
2:A:85:ARG:NH1	2:A:203:PHE:O	2.45	0.41
3:B:126:ASP:OD1	3:B:136:ARG:NE	2.51	0.41
12:Q:51:LEU:HA	12:Q:51:LEU:HD12	1.87	0.41
15:T:39:LEU:HD12	15:T:47:PRO:HG3	2.02	0.41
36:y:372:LYS:HB2	36:y:372:LYS:HE3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1407:U:H2'	1:2:1408:U:C6	2.55	0.40
11:P:28:MET:HE2	11:P:33:LEU:HB3	2.04	0.40
19:a:45:VAL:HG13	19:a:53:ILE:HG13	2.02	0.40
20:c:14:VAL:HG13	20:c:30:VAL:HB	2.03	0.40
26:M:36:ARG:HA	26:M:36:ARG:HD2	1.85	0.40
30:Y:55:ILE:HG12	30:Y:75:ILE:HD12	2.03	0.40
35:x:15:A:H2	35:x:47:C:H42	1.68	0.40
1:2:67:C:C5	24:G:162:LEU:HB3	2.56	0.40
9:K:47:LYS:HD3	9:K:47:LYS:HA	1.81	0.40
17:V:4:ASP:N	17:V:4:ASP:OD2	2.52	0.40
22:g:32:LEU:HD23	22:g:32:LEU:HA	1.80	0.40
22:g:63:SER:HB2	22:g:84:ASP:HB3	2.03	0.40
22:g:255:SER:HB3	22:g:271:LYS:HG3	2.03	0.40
23:C:194:ARG:HD3	23:C:196:ILE:HD11	2.03	0.40
24:G:78:SER:OG	24:G:79:LYS:N	2.55	0.40
1:2:906:U:H2'	1:2:907:G:C8	2.56	0.40
1:2:1276:A:N7	1:2:1322:G:H1'	2.36	0.40
5:E:63:LYS:HE2	5:E:63:LYS:HB3	1.90	0.40
8:I:113:TYR:OH	8:I:156:ALA:O	2.39	0.40
11:P:18:ARG:HB2	11:P:36:LEU:HD11	2.03	0.40
18:X:105:PHE:CD1	18:X:121:LYS:HB3	2.55	0.40
25:J:131:ARG:HD2	25:J:131:ARG:HA	1.82	0.40
31:Z:47:LEU:HD12	31:Z:47:LEU:HA	1.91	0.40
36:y:373:ASP:N	36:y:373:ASP:OD1	2.53	0.40
4:D:133:GLY:HA3	4:D:156:LEU:H	1.87	0.40
7:H:113:LYS:HD2	7:H:113:LYS:HA	1.98	0.40
18:X:39:ASN:HA	18:X:40:PRO:HD3	1.92	0.40
19:a:46:GLU:O	19:a:48:ALA:N	2.54	0.40
35:x:4:G:H2'	35:x:5:A:C8	2.56	0.40
1:2:318:A:N6	24:G:186:GLN:OE1	2.55	0.40
1:2:824:C:H1'	25:J:144:ILE:HG21	2.03	0.40
1:2:1320:G:H2'	1:2:1321:G:O4'	2.22	0.40
6:F:23:TRP:HH2	6:F:98:GLU:HG2	1.87	0.40
7:H:74:LYS:HE2	7:H:74:LYS:HB2	1.94	0.40
9:K:46:MET:HE3	9:K:67:PHE:HE2	1.85	0.40
9:K:95:ARG:O	9:K:96:ARG:NE	2.54	0.40
14:S:22:GLY:HA2	14:S:56:ALA:HB3	2.04	0.40
14:S:92:ASP:OD2	14:S:94:LYS:NZ	2.49	0.40
24:G:162:LEU:HD23	24:G:162:LEU:HA	1.91	0.40
25:J:63:LEU:HD23	25:J:63:LEU:HA	1.95	0.40
35:x:28:C:N4	35:x:43:G:O6	2.54	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	219/221 (99%)	206 (94%)	12 (6%)	1 (0%)	24	54
3	B	212/264 (80%)	205 (97%)	7 (3%)	0	100	100
4	D	225/227 (99%)	209 (93%)	16 (7%)	0	100	100
5	E	260/262 (99%)	252 (97%)	7 (3%)	1 (0%)	30	59
6	F	180/189 (95%)	171 (95%)	9 (5%)	0	100	100
7	H	182/189 (96%)	171 (94%)	11 (6%)	0	100	100
8	I	204/206 (99%)	199 (98%)	5 (2%)	0	100	100
9	K	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
10	L	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
11	P	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
12	Q	142/144 (99%)	129 (91%)	12 (8%)	1 (1%)	18	48
13	R	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
14	S	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
15	T	141/143 (99%)	135 (96%)	5 (4%)	1 (1%)	18	48
16	U	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
17	V	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
18	X	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	48
19	a	100/102 (98%)	94 (94%)	5 (5%)	1 (1%)	12	39
20	c	62/64 (97%)	54 (87%)	8 (13%)	0	100	100
21	d	53/55 (96%)	51 (96%)	1 (2%)	1 (2%)	6	23
22	g	311/313 (99%)	292 (94%)	19 (6%)	0	100	100
23	C	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	G	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
25	J	183/185 (99%)	176 (96%)	6 (3%)	1 (0%)	24	54
26	M	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
27	N	148/150 (99%)	148 (100%)	0	0	100	100
28	O	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
29	W	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
30	Y	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
31	Z	73/75 (97%)	64 (88%)	9 (12%)	0	100	100
32	b	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
33	e	40/42 (95%)	40 (100%)	0	0	100	100
34	f	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
36	y	70/72 (97%)	68 (97%)	2 (3%)	0	100	100
37	i	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
All	All	5000/5132 (97%)	4747 (95%)	244 (5%)	9 (0%)	44	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	X	127	ASN
23	C	78	LEU
15	T	41	LYS
25	J	123	ILE
2	A	12	GLU
21	d	14	PHE
5	E	93	ASP
12	Q	44	PRO
19	a	47	ALA

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	183/183 (100%)	183 (100%)	0	100	100
3	B	195/231 (84%)	195 (100%)	0	100	100
4	D	190/190 (100%)	190 (100%)	0	100	100
5	E	224/224 (100%)	224 (100%)	0	100	100
6	F	156/159 (98%)	156 (100%)	0	100	100
7	H	166/169 (98%)	166 (100%)	0	100	100
8	I	178/178 (100%)	178 (100%)	0	100	100
9	K	89/89 (100%)	89 (100%)	0	100	100
10	L	137/137 (100%)	137 (100%)	0	100	100
11	P	115/115 (100%)	115 (100%)	0	100	100
12	Q	119/119 (100%)	119 (100%)	0	100	100
13	R	122/122 (100%)	122 (100%)	0	100	100
14	S	126/126 (100%)	126 (100%)	0	100	100
15	T	113/113 (100%)	113 (100%)	0	100	100
16	U	94/94 (100%)	94 (100%)	0	100	100
17	V	67/67 (100%)	67 (100%)	0	100	100
18	X	113/113 (100%)	113 (100%)	0	100	100
19	a	89/89 (100%)	89 (100%)	0	100	100
20	c	57/57 (100%)	57 (100%)	0	100	100
21	d	48/48 (100%)	48 (100%)	0	100	100
22	g	272/272 (100%)	272 (100%)	0	100	100
23	C	188/188 (100%)	188 (100%)	0	100	100
24	G	207/207 (100%)	207 (100%)	0	100	100
25	J	161/161 (100%)	161 (100%)	0	100	100
26	M	102/104 (98%)	102 (100%)	0	100	100
27	N	130/130 (100%)	130 (100%)	0	100	100
28	O	110/110 (100%)	110 (100%)	0	100	100
29	W	112/112 (100%)	112 (100%)	0	100	100
30	Y	113/113 (100%)	113 (100%)	0	100	100
31	Z	66/66 (100%)	66 (100%)	0	100	100
32	b	75/75 (100%)	75 (100%)	0	100	100
33	e	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	f	60/60 (100%)	60 (100%)	0	100	100
36	y	68/68 (100%)	68 (100%)	0	100	100
37	i	92/92 (100%)	92 (100%)	0	100	100
All	All	4371/4415 (99%)	4371 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	9	GLN
2	A	50	ASN
3	B	92	GLN
3	B	159	GLN
4	D	159	HIS
5	E	67	GLN
5	E	142	HIS
7	H	25	GLN
7	H	76	GLN
7	H	157	HIS
7	H	163	GLN
8	I	52	ASN
9	K	7	ASN
9	K	28	HIS
9	K	77	GLN
10	L	11	GLN
10	L	83	GLN
10	L	94	HIS
10	L	141	ASN
11	P	103	ASN
12	Q	97	GLN
13	R	74	GLN
13	R	83	ASN
14	S	72	GLN
18	X	23	HIS
22	g	4	GLN
22	g	20	GLN
22	g	196	ASN
22	g	237	ASN
22	g	311	GLN
23	C	136	HIS

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Mol	Chain	Res	Type
23	C	272	HIS
25	J	75	ASN
26	M	52	GLN
26	M	99	ASN
27	N	58	HIS
29	W	82	GLN
29	W	90	GLN
30	Y	89	HIS
31	Z	112	ASN
36	y	321	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1715/1740 (98%)	375 (21%)	11 (0%)
35	x	74/75 (98%)	20 (27%)	0
All	All	1789/1815 (98%)	395 (22%)	11 (0%)

All (395) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
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	58	C
1	2	67	C
1	2	68	A
1	2	72	C
1	2	73	C
1	2	74	G
1	2	76	U
1	2	99	A
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U

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Mol	Chain	Res	Type
1	2	126	G
1	2	130	G
1	2	140	C
1	2	143	U
1	2	147	A
1	2	155	G
1	2	158	A
1	2	159	A
1	2	160	U
1	2	162	C
1	2	175	A
1	2	190	G
1	2	196	C
1	2	198	U
1	2	199	C
1	2	200	G
1	2	203	G
1	2	204	G
1	2	206	G
1	2	208	G
1	2	212	C
1	2	214	U
1	2	290	U
1	2	291	G
1	2	292	A
1	2	293	C
1	2	295	C
1	2	306	C
1	2	307	G
1	2	308	G
1	2	309	G
1	2	311	C
1	2	319	C
1	2	322	C
1	2	323	C
1	2	324	C
1	2	325	C
1	2	326	C
1	2	328	U
1	2	329	G
1	2	332	G
1	2	339	A

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Mol	Chain	Res	Type
1	2	347	G
1	2	351	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	368	U
1	2	370	G
1	2	385	G
1	2	386	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	417	C
1	2	418	A
1	2	429	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	452	G
1	2	464	A
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	482	G
1	2	485	A
1	2	487	U
1	2	488	U
1	2	492	C
1	2	493	A
1	2	502	C
1	2	508	A
1	2	516	A
1	2	525	A
1	2	531	A
1	2	533	A
1	2	536	A
1	2	537	C
1	2	540	U
1	2	545	A

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Mol	Chain	Res	Type
1	2	546	G
1	2	547	G
1	2	548	C
1	2	549	C
1	2	552	G
1	2	553	U
1	2	554	A
1	2	555	A
1	2	556	U
1	2	557	U
1	2	558	G
1	2	559	G
1	2	563	G
1	2	564	A
1	2	576	A
1	2	583	C
1	2	587	A
1	2	589	G
1	2	590	A
1	2	591	U
1	2	592	C
1	2	594	A
1	2	597	G
1	2	604	A
1	2	607	U
1	2	608	C
1	2	614	C
1	2	622	C
1	2	623	G
1	2	627	U
1	2	628	A
1	2	631	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	659	G
1	2	660	C
1	2	664	A
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A

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Mol	Chain	Res	Type
1	2	673	G
1	2	688	U
1	2	689	U
1	2	690	G
1	2	692	G
1	2	693	A
1	2	695	C
1	2	696	G
1	2	697	G
1	2	698	G
1	2	733	C
1	2	736	C
1	2	738	C
1	2	751	G
1	2	752	G
1	2	753	C
1	2	788	G
1	2	791	C
1	2	792	C
1	2	798	A
1	2	808	A
1	2	809	A
1	2	810	A
1	2	821	G
1	2	822	U
1	2	823	U
1	2	824	C
1	2	830	A
1	2	836	G
1	2	837	A
1	2	838	G
1	2	839	C
1	2	840	C
1	2	841	G
1	2	842	C
1	2	847	A
1	2	869	A
1	2	870	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	880	G

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Mol	Chain	Res	Type
1	2	882	U
1	2	883	U
1	2	887	U
1	2	888	U
1	2	889	U
1	2	891	G
1	2	894	G
1	2	896	U
1	2	898	U
1	2	899	U
1	2	900	C
1	2	901	G
1	2	903	A
1	2	913	A
1	2	914	U
1	2	920	A
1	2	930	C
1	2	933	G
1	2	934	G
1	2	943	U
1	2	963	A
1	2	971	G
1	2	972	A
1	2	978	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1001	A
1	2	1017	U
1	2	1018	U
1	2	1023	A
1	2	1027	A
1	2	1028	A
1	2	1060	A
1	2	1061	U
1	2	1062	A
1	2	1083	A
1	2	1085	C
1	2	1088	U
1	2	1109	C
1	2	1114	U
1	2	1115	U

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Mol	Chain	Res	Type
1	2	1116	C
1	2	1118	C
1	2	1121	G
1	2	1133	A
1	2	1138	C
1	2	1143	A
1	2	1153	C
1	2	1154	U
1	2	1195	A
1	2	1203	G
1	2	1207	G
1	2	1208	A
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1224	G
1	2	1227	G
1	2	1242	U
1	2	1243	U
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1263	U
1	2	1264	C
1	2	1265	A
1	2	1266	C
1	2	1274	G
1	2	1275	G
1	2	1283	C
1	2	1286	G
1	2	1293	A
1	2	1294	G
1	2	1295	A
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1308	U
1	2	1342	U
1	2	1343	U
1	2	1348	G

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Mol	Chain	Res	Type
1	2	1371	U
1	2	1372	U
1	2	1373	C
1	2	1378	A
1	2	1382	A
1	2	1402	A
1	2	1404	U
1	2	1406	G
1	2	1415	C
1	2	1419	C
1	2	1421	A
1	2	1422	G
1	2	1423	C
1	2	1433	C
1	2	1435	C
1	2	1436	C
1	2	1438	A
1	2	1446	A
1	2	1449	G
1	2	1452	A
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1479	G
1	2	1480	A
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1494	U
1	2	1495	G
1	2	1497	G
1	2	1498	A
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1523	C
1	2	1533	A
1	2	1552	G
1	2	1553	C
1	2	1556	A
1	2	1570	G
1	2	1578	U

Continued on next page...

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Mol	Chain	Res	Type
1	2	1580	A
1	2	1585	U
1	2	1587	G
1	2	1588	A
1	2	1601	A
1	2	1619	A
1	2	1621	U
1	2	1623	A
1	2	1634	A
1	2	1638	G
1	2	1648	G
1	2	1654	G
1	2	1661	A
1	2	1663	A
1	2	1665	G
1	2	1671	G
1	2	1686	G
1	2	1698	C
1	2	1699	A
1	2	1719	A
1	2	1721	U
1	2	1722	G
1	2	1726	G
1	2	1743	G
1	2	1744	G
1	2	1745	A
1	2	1752	C
1	2	1753	C
1	2	1754	G
1	2	1757	G
1	2	1758	G
1	2	1761	U
1	2	1772	C
1	2	1773	C
1	2	1774	C
1	2	1775	U
1	2	1776	G
1	2	1777	G
1	2	1780	G
1	2	1781	A
1	2	1782	G
1	2	1783	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1784	G
1	2	1786	U
1	2	1787	G
1	2	1798	C
1	2	1822	A
1	2	1823	A
1	2	1824	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	1852	C
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1865	C
35	x	16	C
35	x	17	G
35	x	19	C
35	x	20	U
35	x	21	A
35	x	23	C
35	x	28	C
35	x	32	C
35	x	33	U
35	x	35	U
35	x	36	C
35	x	37	A
35	x	46	A
35	x	47	C
35	x	48	C
35	x	55	C
35	x	57	A
35	x	58	C
35	x	72	G
35	x	75	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	112	U
1	2	158	A
1	2	291	G
1	2	417	C
1	2	552	G
1	2	563	G
1	2	668	A
1	2	688	U
1	2	1265	A
1	2	1434	C
1	2	1520	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 33 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	753:C	O3'	785:C	P	30.20
1	2	698:G	O3'	730:C	P	15.36
1	2	739:C	O3'	746:C	P	12.19
1	2	225:G	O3'	287:U	P	7.08

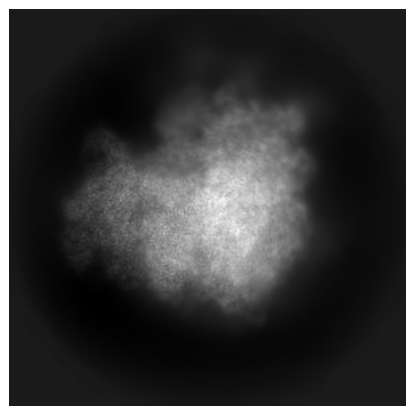
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11456. These allow visual inspection of the internal detail of the map and identification of artifacts.

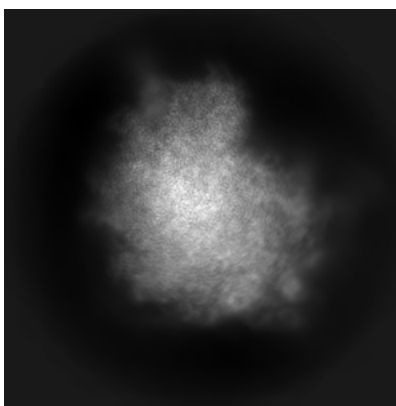
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

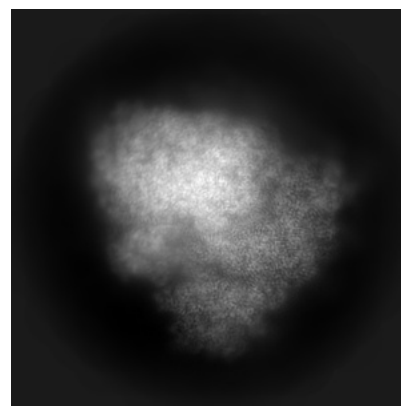
6.1.1 Primary map



X

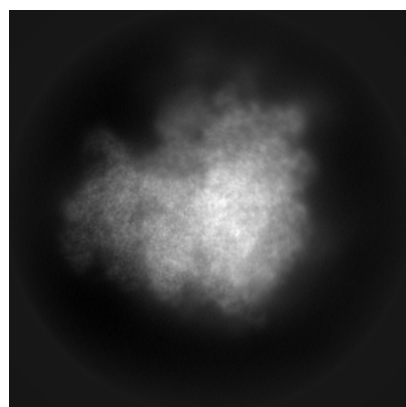


Y

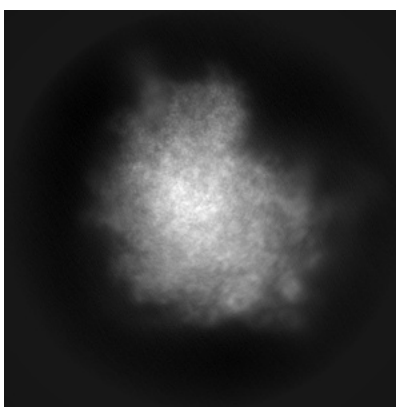


Z

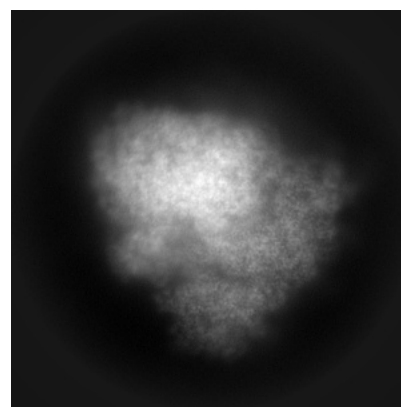
6.1.2 Raw map



X



Y

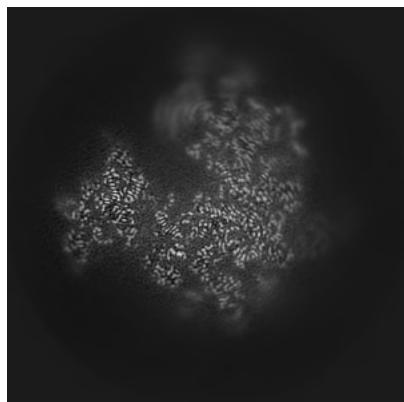


Z

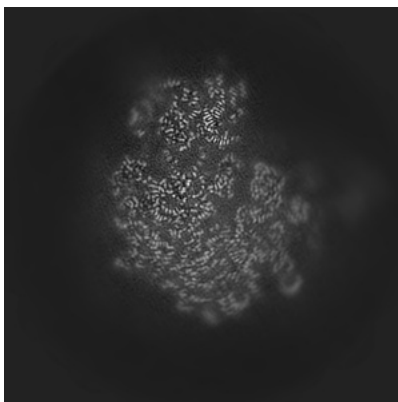
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

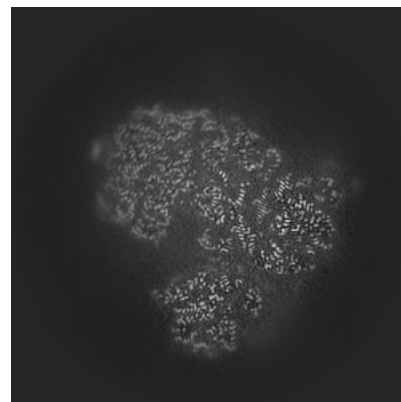
6.2.1 Primary map



X Index: 200

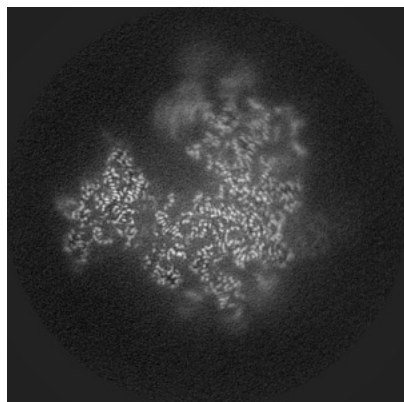


Y Index: 200

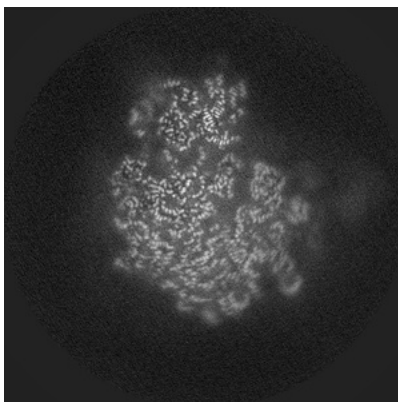


Z Index: 200

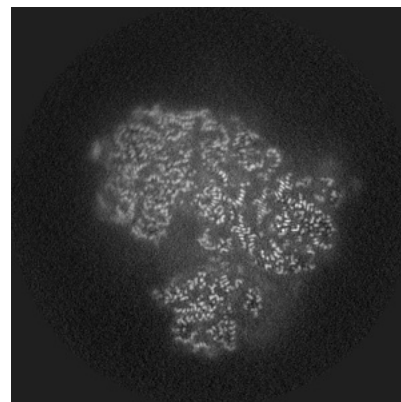
6.2.2 Raw map



X Index: 200



Y Index: 200

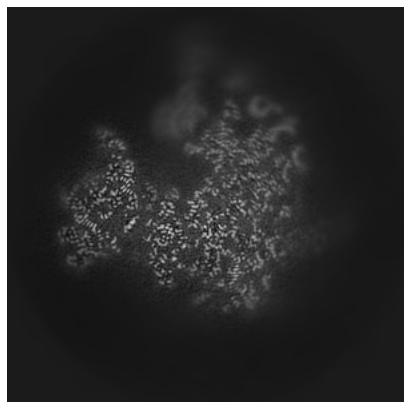


Z Index: 200

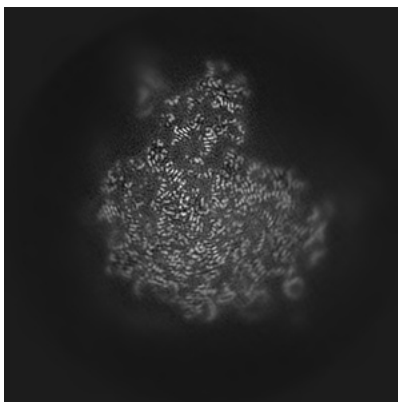
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

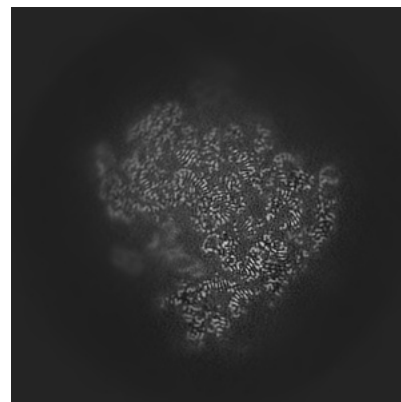
6.3.1 Primary map



X Index: 211

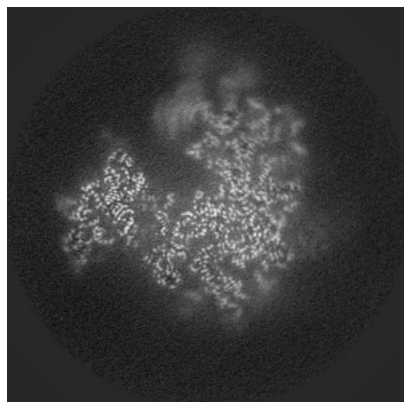


Y Index: 214

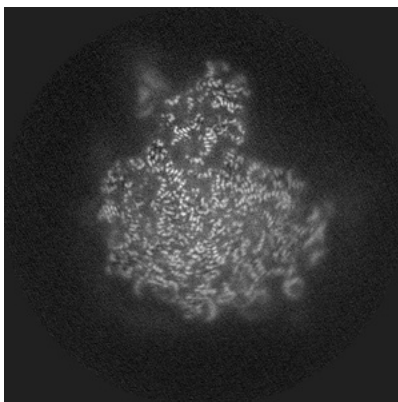


Z Index: 182

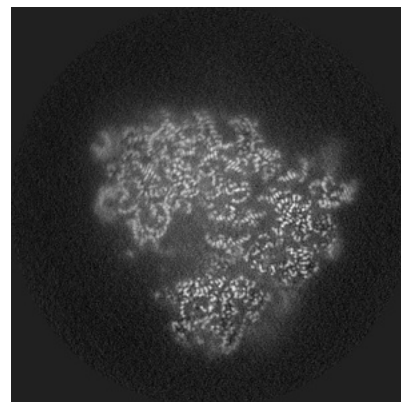
6.3.2 Raw map



X Index: 201



Y Index: 214

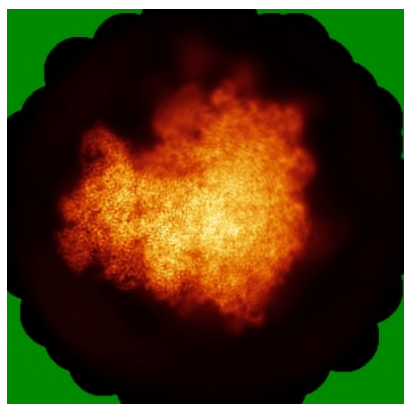


Z Index: 208

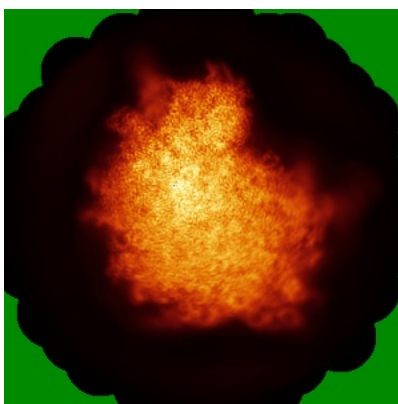
The images above show the largest variance slices of the map in three orthogonal directions.

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

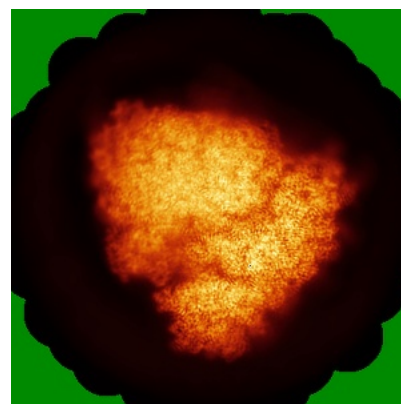
6.4.1 Primary map



X

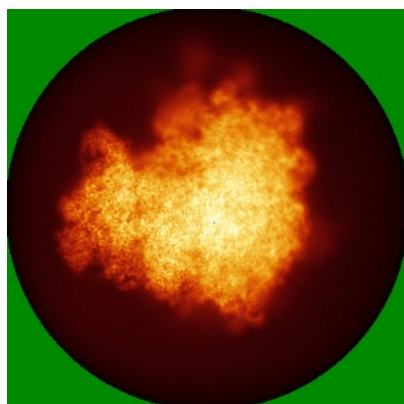


Y

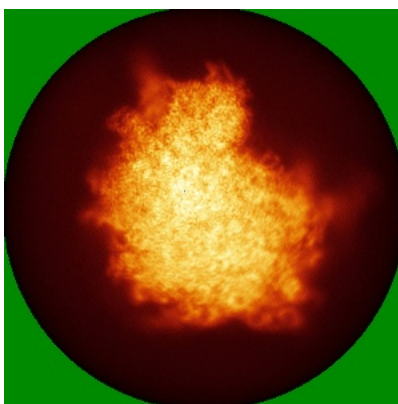


Z

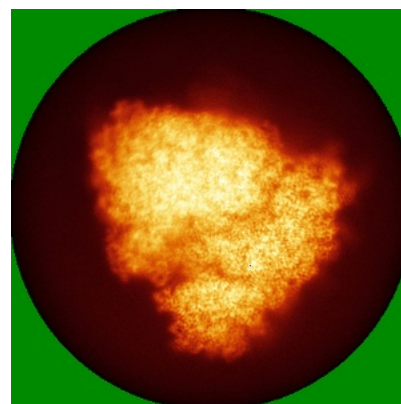
6.4.2 Raw map



X



Y

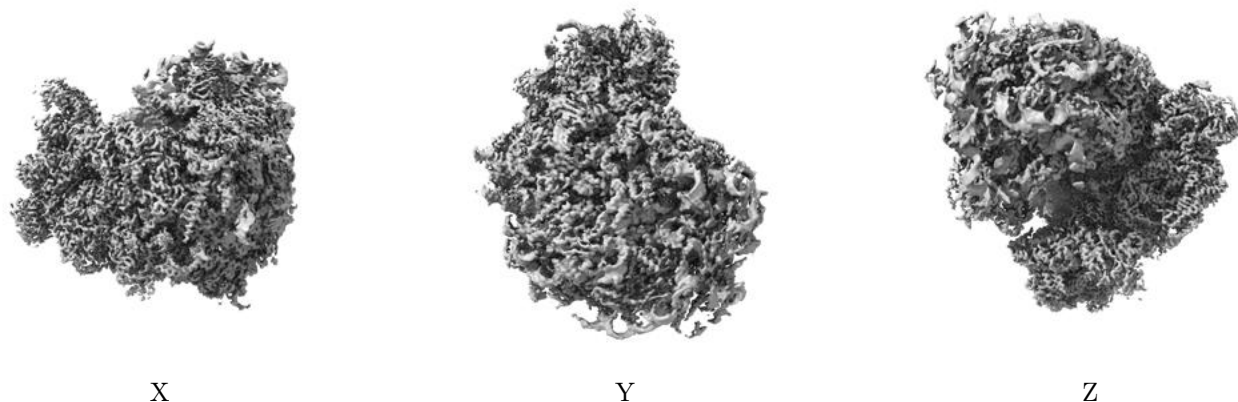


Z

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

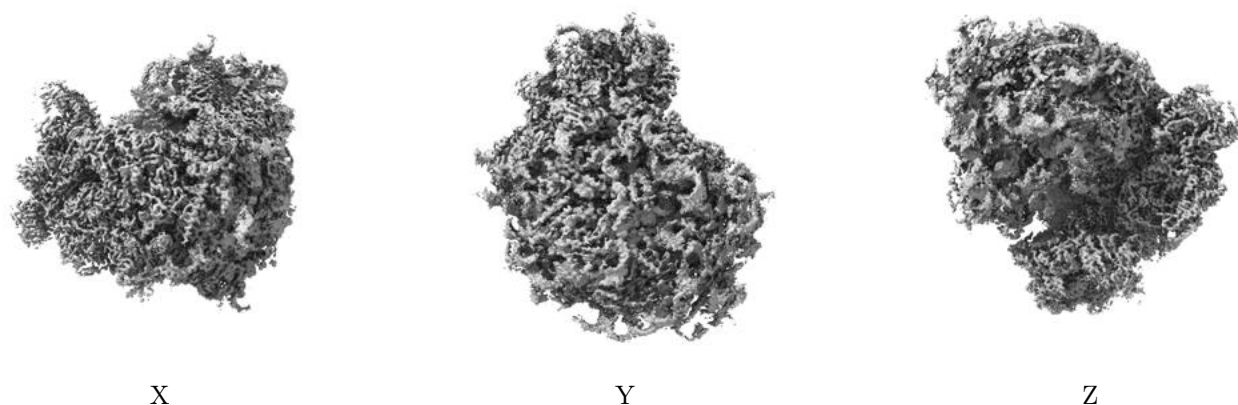
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

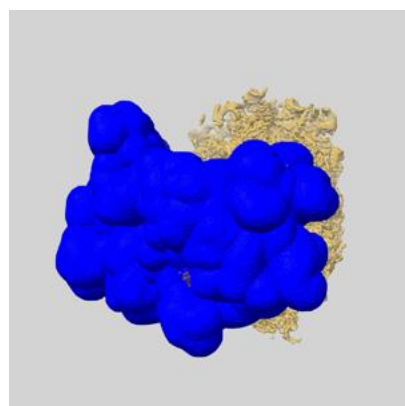
6.6 Mask visualisation [i](#)

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

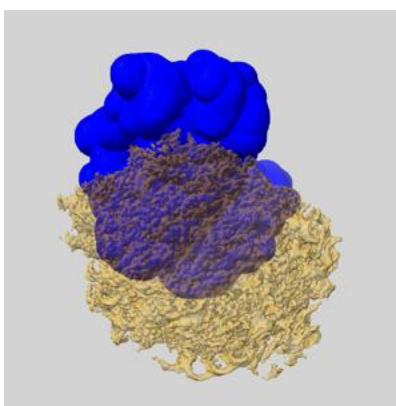
A mask typically either:

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

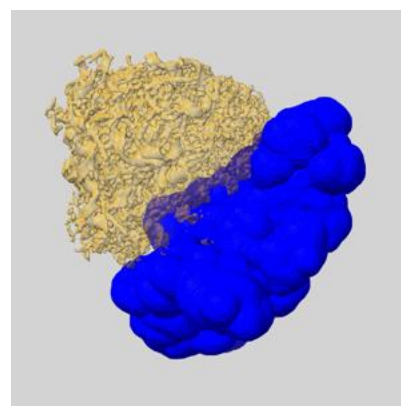
6.6.1 emd_11456_msk_1.map [i](#)



X



Y

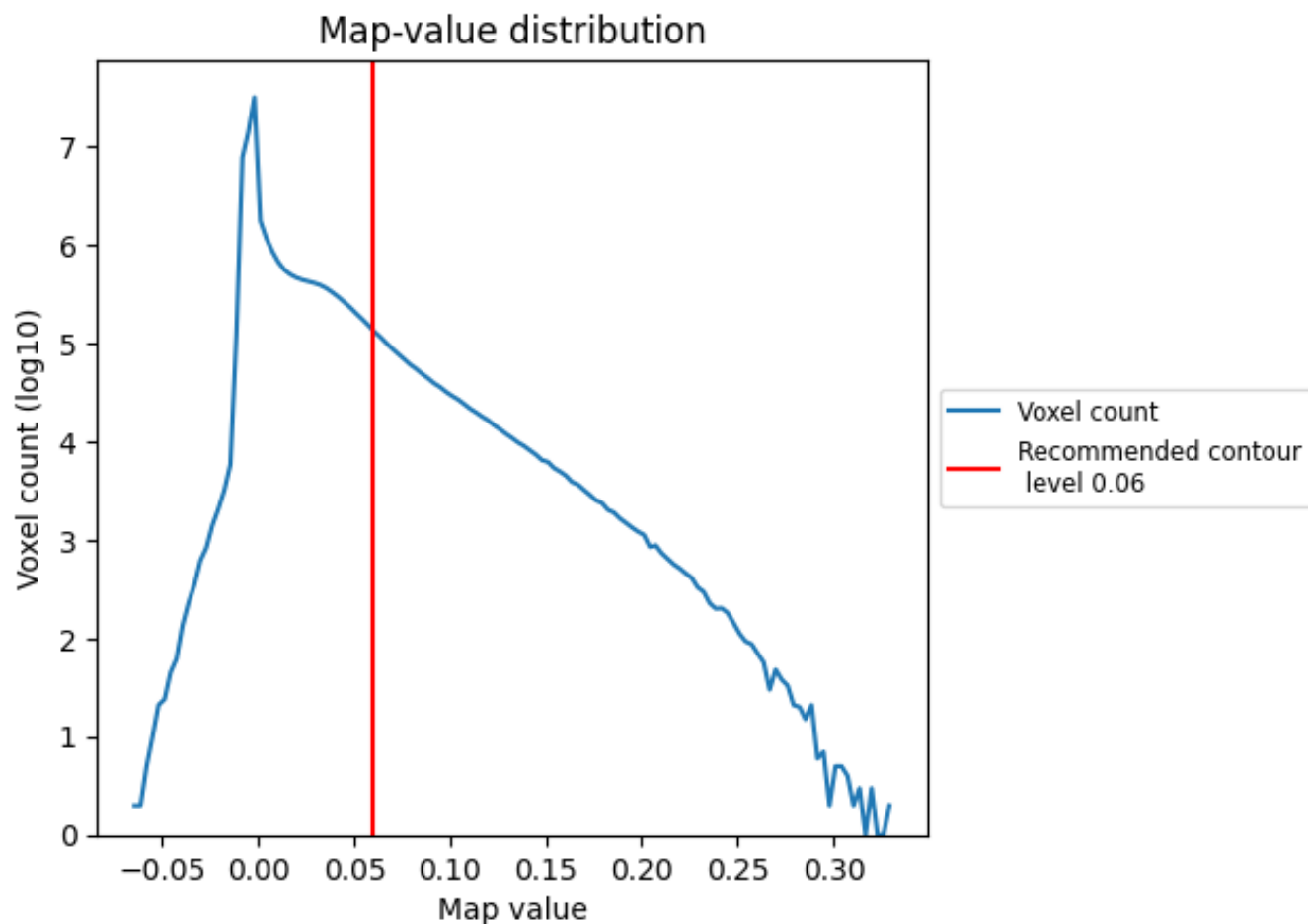


Z

7 Map analysis [i](#)

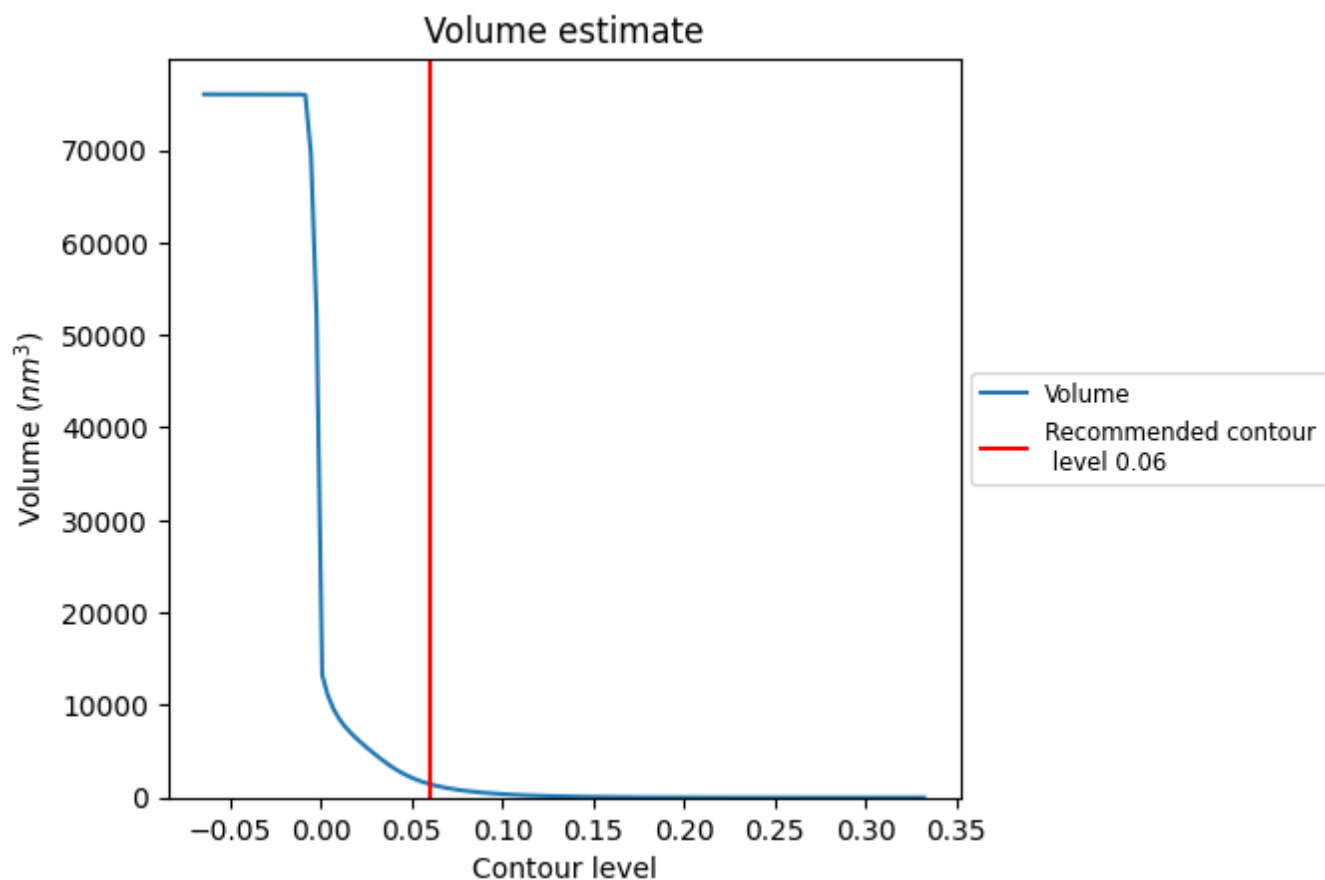
This section contains the results of statistical analysis of the map.

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.

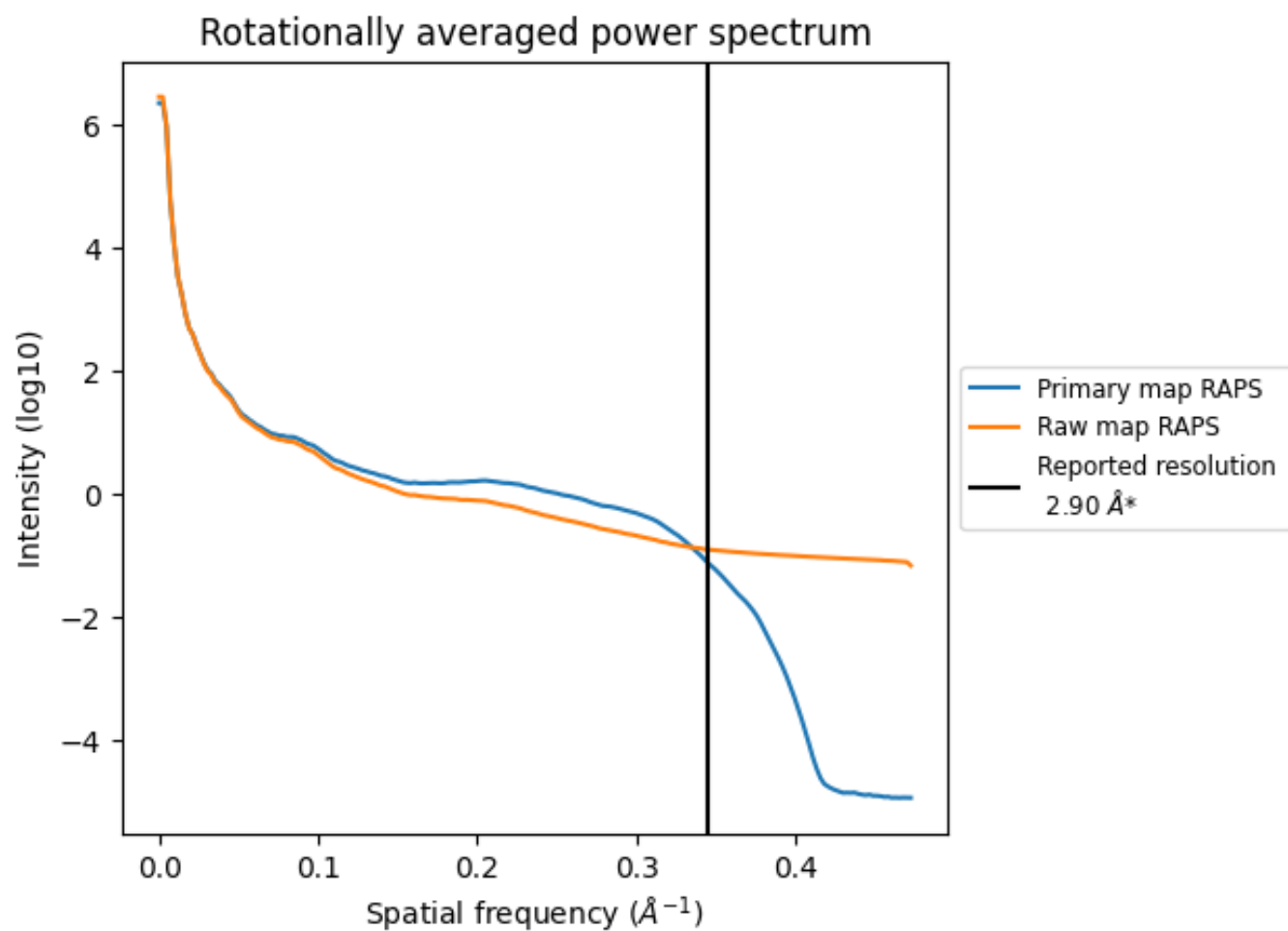
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1454 nm^3 ; this corresponds to an approximate mass of 1313 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 ⓘ

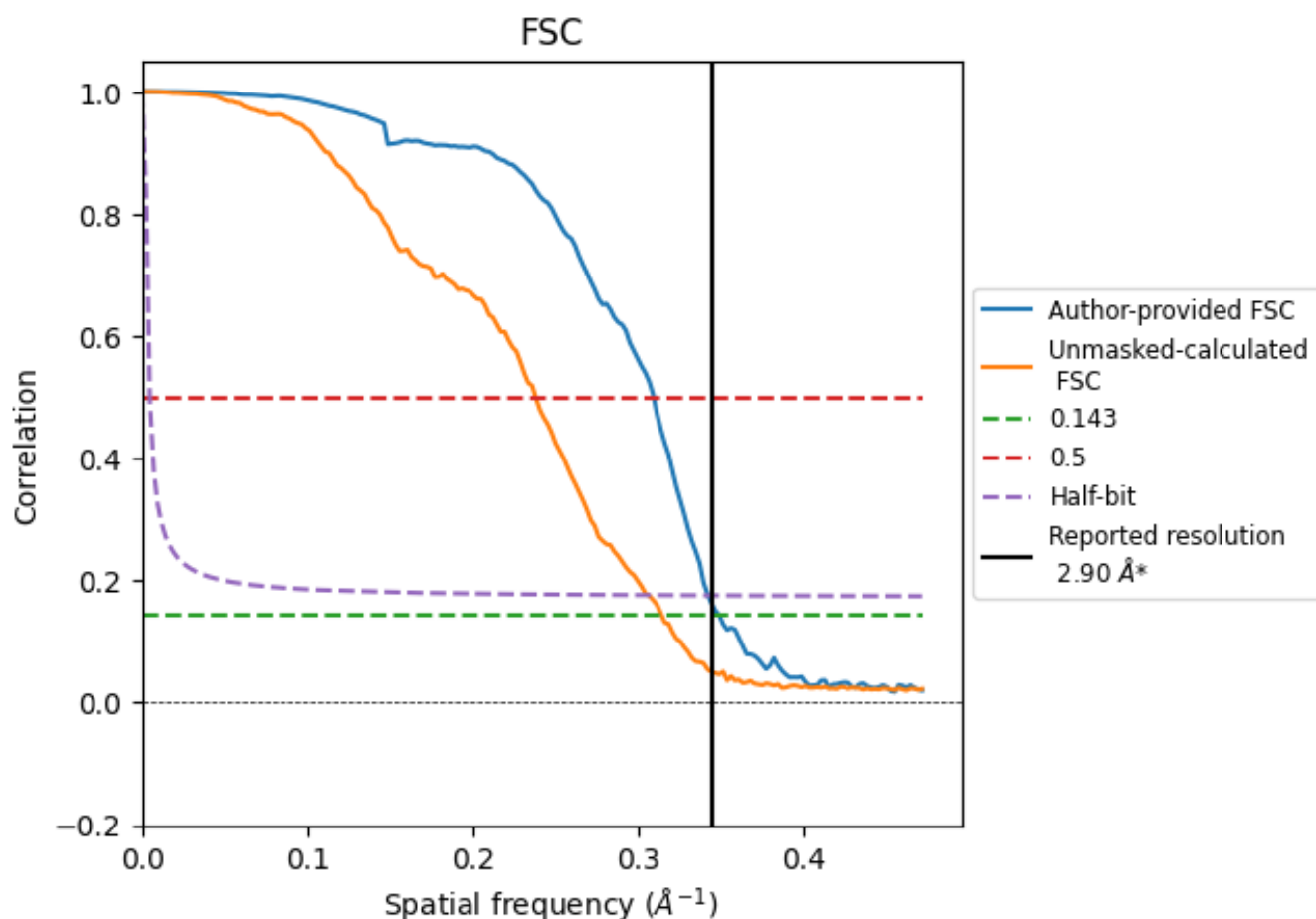


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

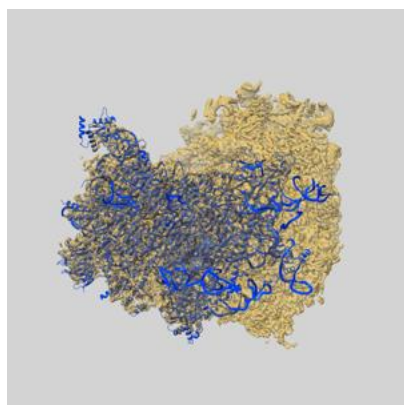
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.86	3.23	2.92
Unmasked-calculated*	3.18	4.20	3.27

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

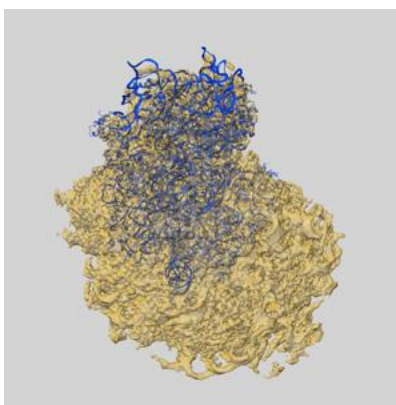
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11456 and PDB model 6ZVH. Per-residue inclusion information can be found in section 3 on page 11.

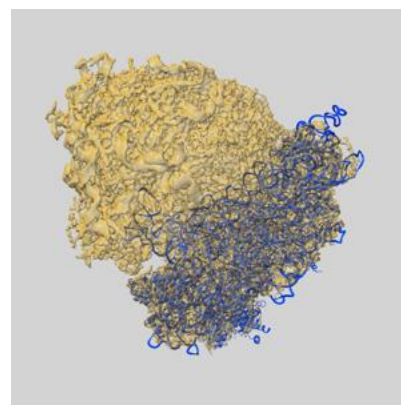
9.1 Map-model overlay [i](#)



X



Y



Z

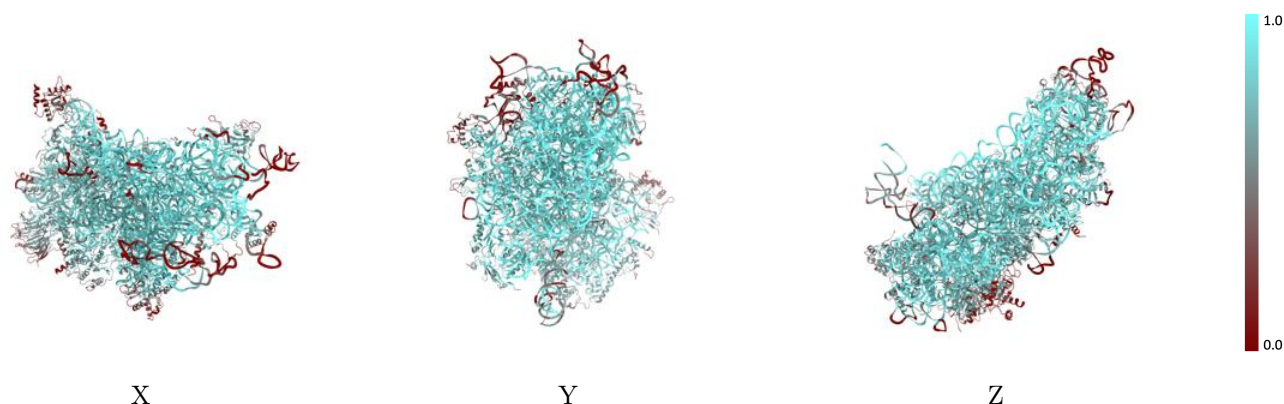
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



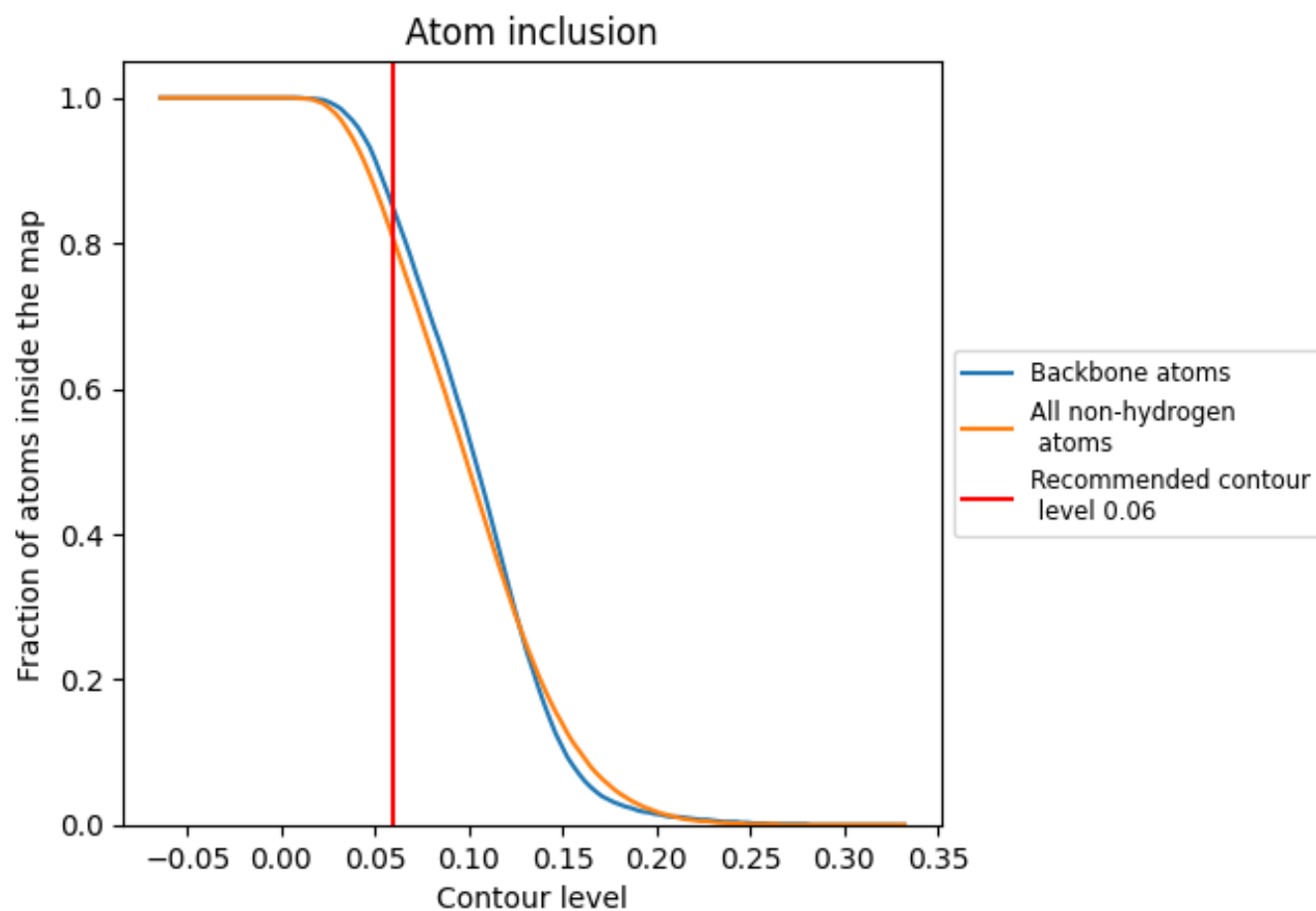
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8040	 0.5570
2	 0.8950	 0.5830
A	 0.7610	 0.5670
B	 0.8160	 0.5780
C	 0.8520	 0.5930
D	 0.7360	 0.5340
E	 0.8420	 0.5890
F	 0.8050	 0.5540
G	 0.6620	 0.5190
H	 0.5430	 0.4920
I	 0.8040	 0.5590
J	 0.8310	 0.5740
K	 0.7470	 0.5410
L	 0.8430	 0.5890
M	 0.1840	 0.3390
N	 0.8820	 0.6000
O	 0.8470	 0.5700
P	 0.6870	 0.5240
Q	 0.7870	 0.5680
R	 0.6600	 0.5180
S	 0.7230	 0.5280
T	 0.7380	 0.5470
U	 0.6550	 0.5060
V	 0.7600	 0.5680
W	 0.9250	 0.6180
X	 0.9250	 0.6110
Y	 0.7180	 0.5360
Z	 0.5820	 0.4910
a	 0.8720	 0.5860
b	 0.7110	 0.5550
c	 0.6960	 0.5220
d	 0.9390	 0.6100
e	 0.8140	 0.5780
f	 0.3410	 0.4070
g	 0.4880	 0.4870



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Chain	Atom inclusion	Q-score
i	 0.5750	 0.5310
x	 0.4910	 0.2680
y	 0.7420	 0.5410