



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 04:58 AM UTC

PDB ID : 9L5S / pdb_00009l5s
EMDB ID : EMD-62842
Title : Cryo-EM structure of the thermophile spliceosome (state B*Q1)
Authors : Li, Y.; Fischer, P.; Wang, M.; Yuan, R.; Meng, W.; Luehrmann, R.; Lau, B.; Hurt, E.; Cheng, J.
Deposited on : 2024-12-23
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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

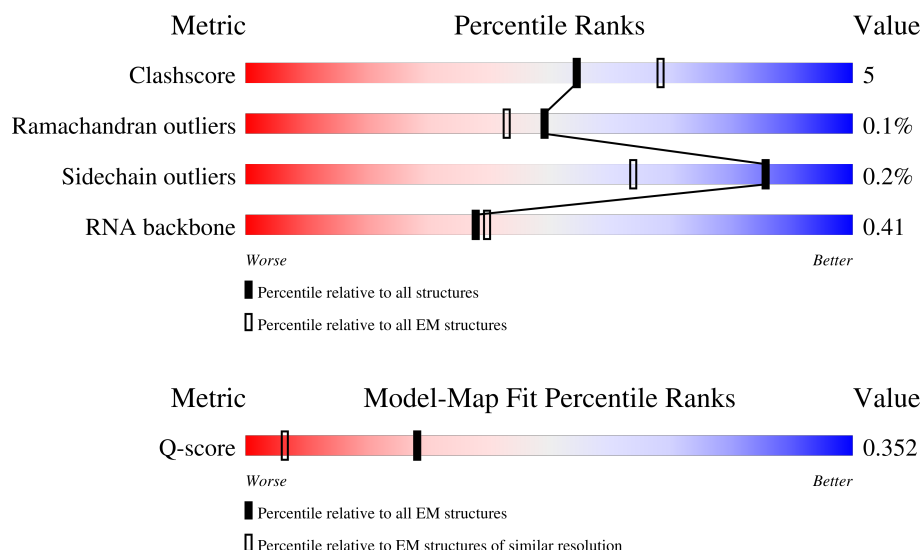
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	193	
2	5	116	
3	6	101	

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Mol	Chain	Length	Quality of chain
4	A	2463	
5	B	326	
6	C	1011	
7	E	352	
8	F	233	
9	I	839	
10	J	687	
11	L	768	
12	K	231	
13	q	480	
13	r	480	
13	s	480	
13	t	480	
14	N	148	
15	S	167	
16	T	496	
17	M	395	
18	O	408	
19	R	578	
20	W	547	
21	P	260	
22	Y	1416	
23	1	698	
24	z	672	
25	j	98	

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Mol	Chain	Length	Quality of chain
26	k	82	
27	l	94	
28	m	592	
29	o	118	
30	p	211	
31	u	114	
32	V	223	
33	Z	678	
34	CY	510	
35	Ck	66	
36	Cb	700	
37	8	25	
38	CV	246	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	P5P	8	3	-	-	X	-
37	Y5P	8	4	-	-	X	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 87114 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 U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	37	Total	C	N	O	P	0	0
			778	348	126	267	37		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	111	Total	C	N	O	P	0	0
			2343	1048	398	786	111		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	92	Total	C	N	O	P	0	0
			1966	879	359	636	92		

- Molecule 4 is a protein called PRP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1988	Total	C	N	O	S	0	0
			16398	10544	2851	2941	62		

- Molecule 5 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	258	Total	C	N	O	S	0	0
			1874	1152	351	366	5		

- Molecule 6 is a protein called SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	922	Total	C	N	O	S	0	0
			7301	4668	1229	1368	36		

- Molecule 7 is a protein called Anaphase-promoting complex subunit 4-like WD40 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	310	Total	C	N	O	S	0	0
			2379	1493	414	462	10		

- Molecule 8 is a protein called CCDC12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	110	Total	C	N	O		0	0
			547	327	110	110			

- Molecule 9 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	724	Total	C	N	O		0	0
			3596	2148	724	724			

- Molecule 10 is a protein called Suppressor of forked domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	608	Total	C	N	O	S	0	0
			4043	2510	769	759	5		

- Molecule 11 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	611	Total	C	N	O	S	0	0
			4034	2465	772	789	8		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	231	Total	C	N	O		0	0
			1148	685	231	232			

- Molecule 13 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	q	139	Total	C	N	O		0	0
			691	413	139	139			
13	t	141	Total	C	N	O		0	0
			701	419	141	141			

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Mol	Chain	Residues	Atoms				AltConf	Trace
13	r	143	Total	C	N	O	0	0
			711	425	143	143		
13	s	140	Total	C	N	O	0	0
			696	416	140	140		

- Molecule 14 is a protein called Putative bud site selection protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	148	Total	C	N	O	S	0	0
			1200	755	213	220	12		

- Molecule 15 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	157	Total	C	N	O	S	0	0
			1209	763	217	223	6		

- Molecule 16 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	339	Total	C	N	O	S	0	0
			2653	1675	479	485	14		

- Molecule 17 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	248	Total	C	N	O	S	0	0
			1964	1238	355	354	17		

- Molecule 18 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	0	277	Total	C	N	O	S	0	0
			2235	1387	428	413	7		

- Molecule 19 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	339	Total	C	N	O	S	0	0
			2670	1659	508	496	7		

- Molecule 20 is a protein called PRP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	94	Total	C	N	O	S	0	0
			738	456	141	137	4		

- Molecule 21 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	94	Total	C	N	O	S	0	0
			772	483	150	138	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	1333	Total	C	N	O		0	0
			6601	3935	1333	1333			

- Molecule 23 is a protein called GPATCH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	325	Total	C	N	O	S	0	0
			2514	1582	443	484	5		

- Molecule 24 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	z	655	Total	C	N	O	S	0	0
			5149	3270	878	983	18		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	88	Total	C	N	O	S	0	0
			704	456	121	126	1		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	k	73	Total	C	N	O	S	0	0
			577	369	101	105	2		

- Molecule 27 is a protein called Sm protein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	l	81	Total	C	N	O	S	0	0
			649	412	114	120	3		

- Molecule 28 is a protein called Delta(14)-sterol reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	m	86	Total	C	N	O	S	0	0
			678	427	129	118	4		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	o	87	Total	C	N	O	S	0	0
			679	433	114	128	4		

- Molecule 30 is a protein called Sm protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	p	103	Total	C	N	O	S	0	0
			788	490	148	145	5		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	u	90	Total	C	N	O	S	0	0
			716	449	132	131	4		

- Molecule 32 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	V	82	Total	C	N	O	0	0
			478	287	99	92		

- Molecule 33 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	211	Total	C	N	O	S	0	0
			1729	1104	304	313	8		

- Molecule 34 is a protein called Nineteen complex-related protein 2-domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	CY	25	Total	C	N	O	S	0	0
			190	110	35	44	1		

- Molecule 35 is a protein called GCFC2.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Ck	42	Total	C	N	O	0	0
			205	121	42	42		

- Molecule 36 is a protein called TFIP11.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Cb	391	Total	C	N	O	0	0
			1938	1156	391	391		

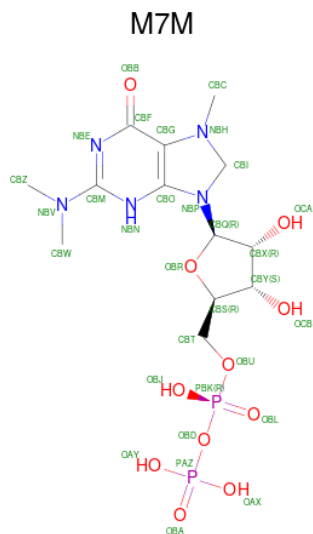
- Molecule 37 is a RNA chain called Unknown mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	8	24	Total	C	N	O	P	0	0
			468	228	72	144	24		

- Molecule 38 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	CV	68	Total	C	N	O	0	0
			337	201	68	68		

- Molecule 39 is N,N,7-trimethylguanosine 5'-(trihydrogen diphosphate) (CCD ID: M7M) (formula: C₁₃H₂₃N₅O₁₁P₂).

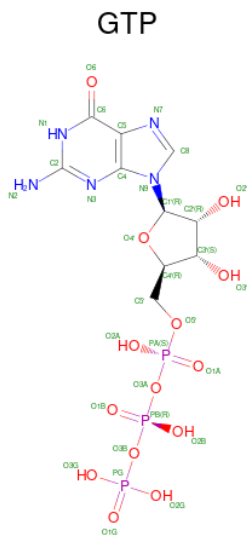


Mol	Chain	Residues	Atoms					AltConf
39	B	1	Total 30	C 13	N 5	O 10	P 2	0

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
40	C	1	Total Mg 1 1	0

- Molecule 41 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



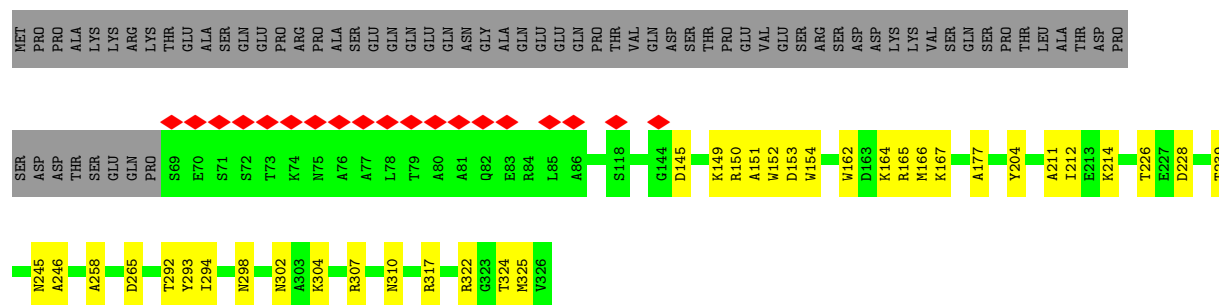
Mol	Chain	Residues	Atoms					AltConf
41	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 42 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
42	N	3	Total	Zn	0
			3	3	
42	M	1	Total	Zn	0
			1	1	

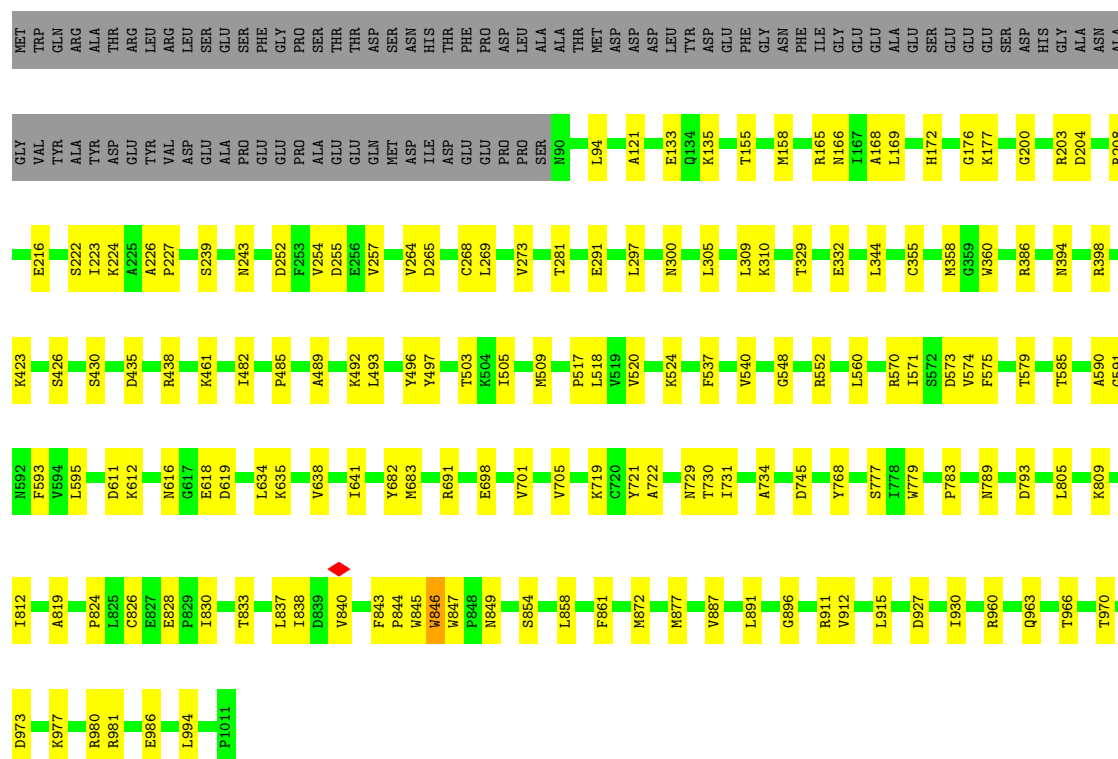
- Molecule 5: Pre-mRNA-splicing factor SYF2





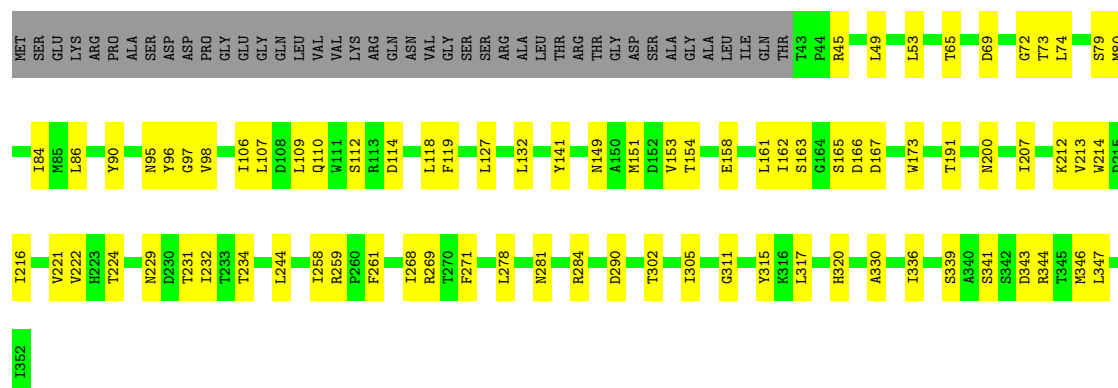
• Molecule 6: SNU114

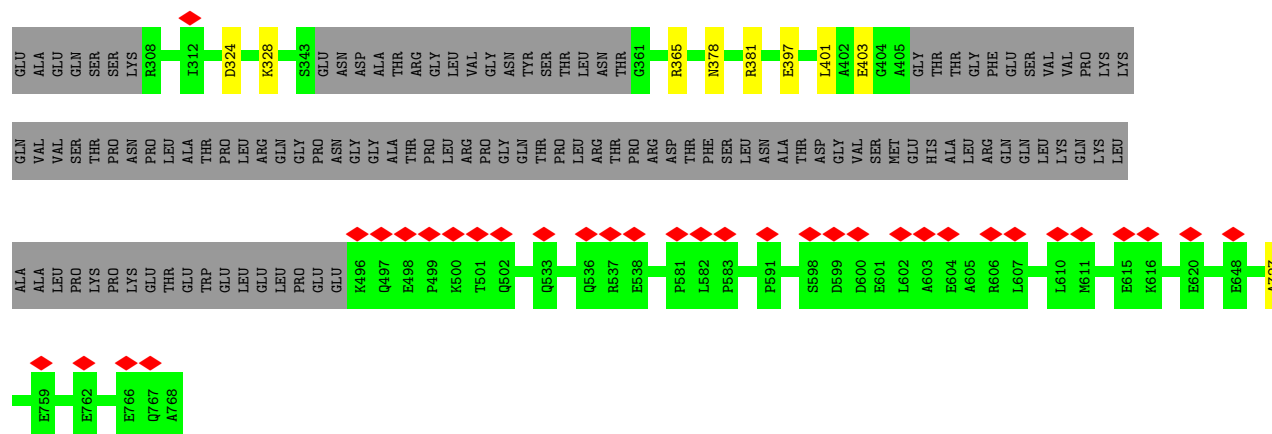
Chain C: 76% 15% 9%



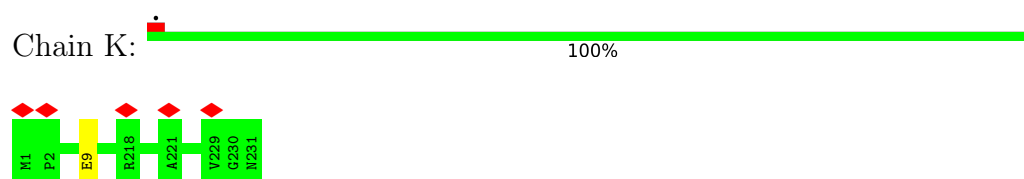
• Molecule 7: Anaphase-promoting complex subunit 4-like WD40 domain-containing protein

Chain E: 66% 22% 12%

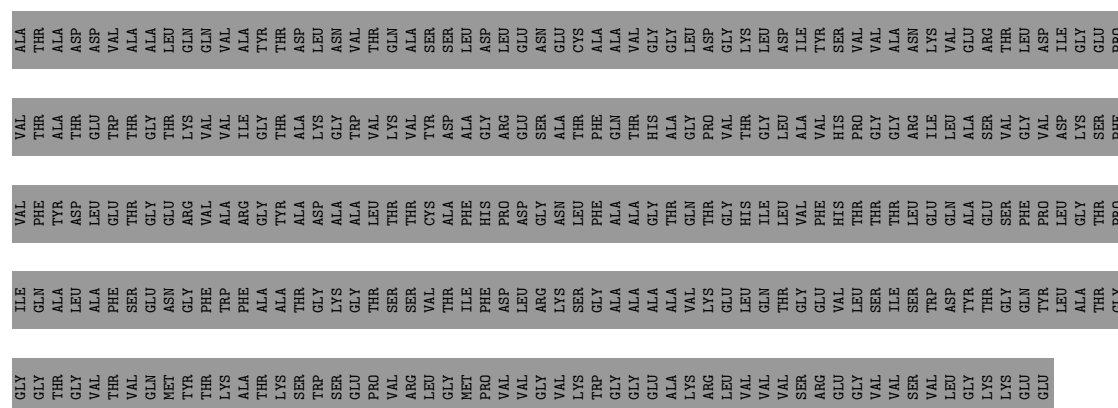
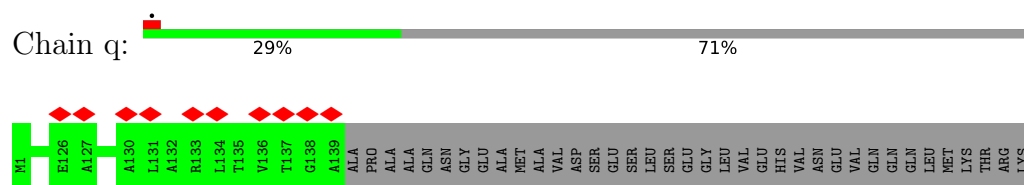




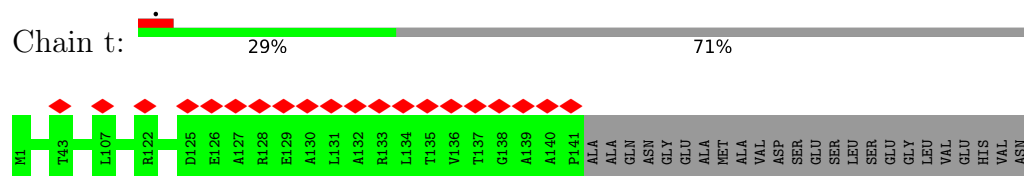
- Molecule 12: Pre-mRNA-splicing factor SPF27



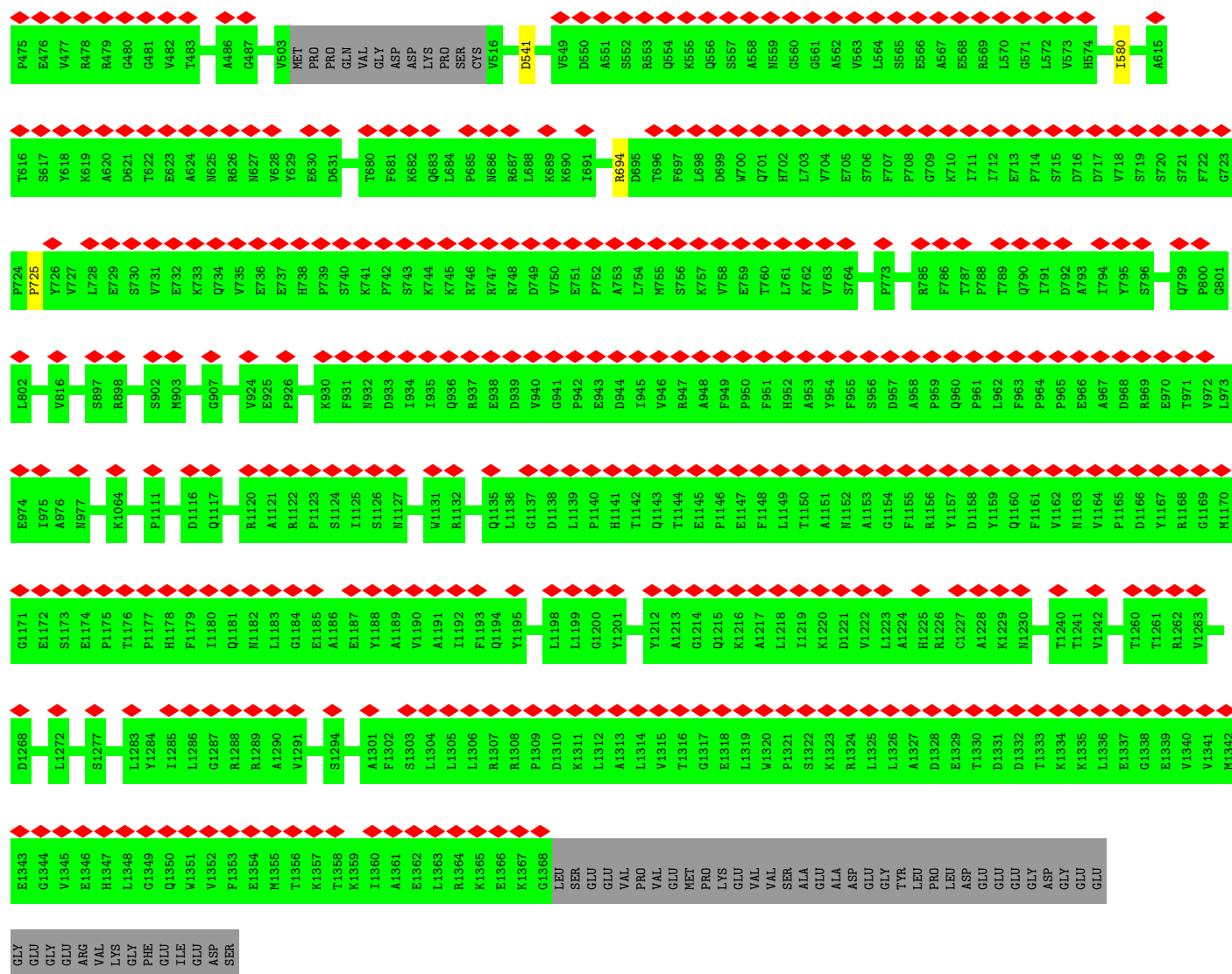
- Molecule 13: Pre-mRNA-processing factor 19



- Molecule 13: Pre-mRNA-processing factor 19

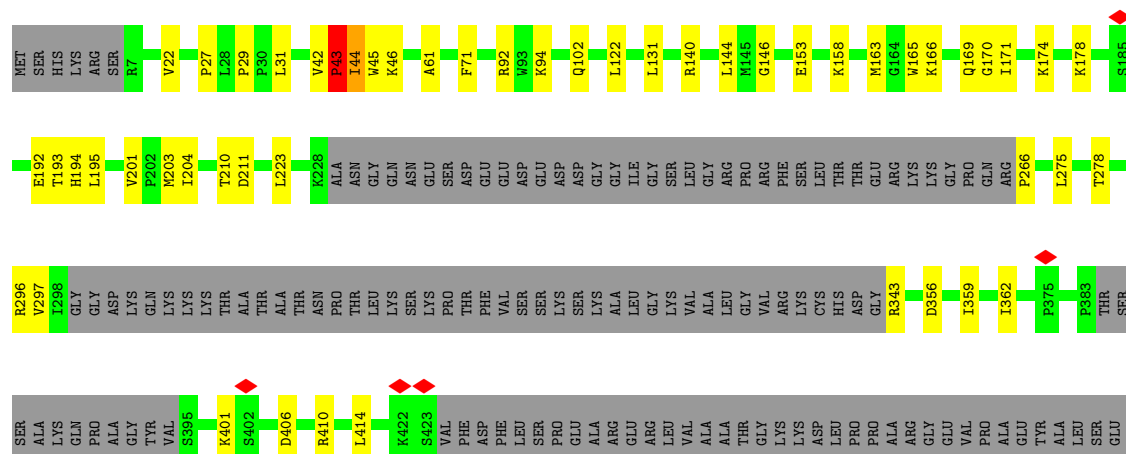




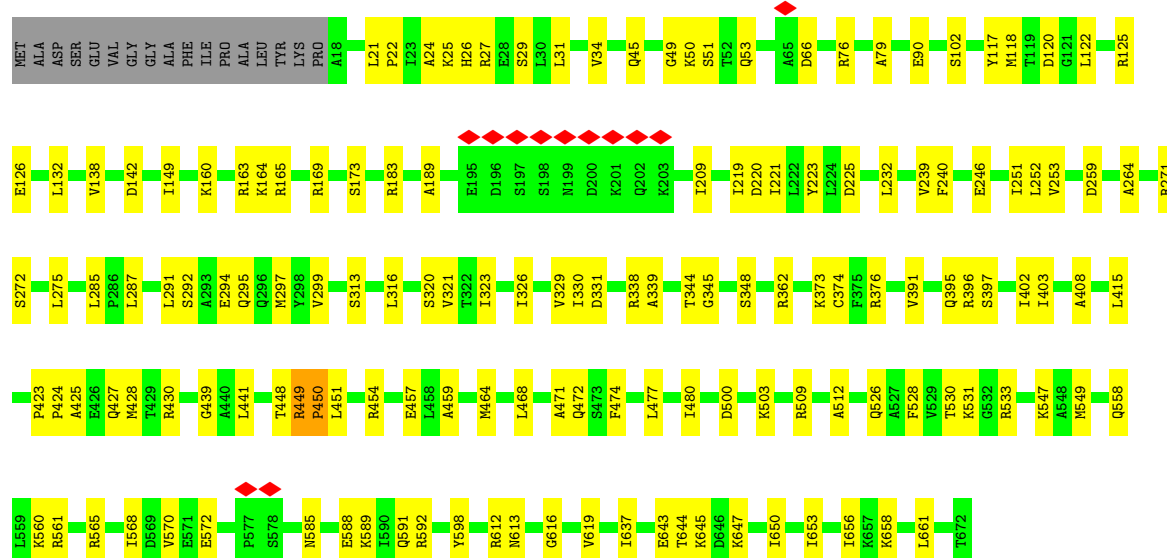


• Molecule 23: GPATCH1

Chain 1: 39% 7% 53%



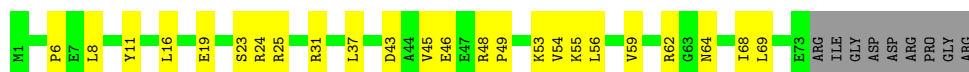
- Molecule 24: RNA helicase



- Molecule 25: Small nuclear ribonucleoprotein E



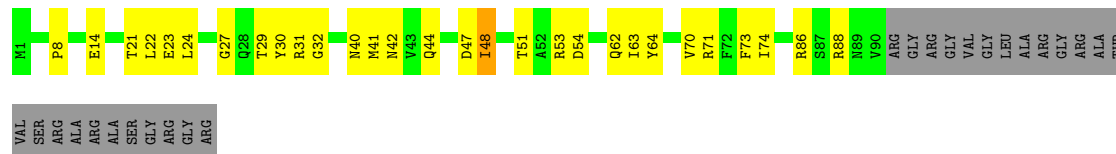
- Molecule 26: Small nuclear ribonucleoprotein G



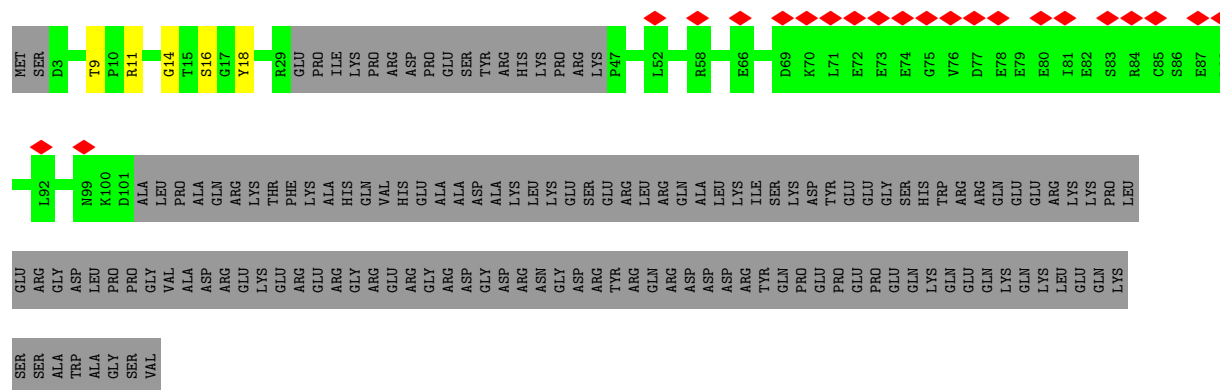
- Molecule 27: Sm protein F



- Molecule 31: Small nuclear ribonucleoprotein Sm D3

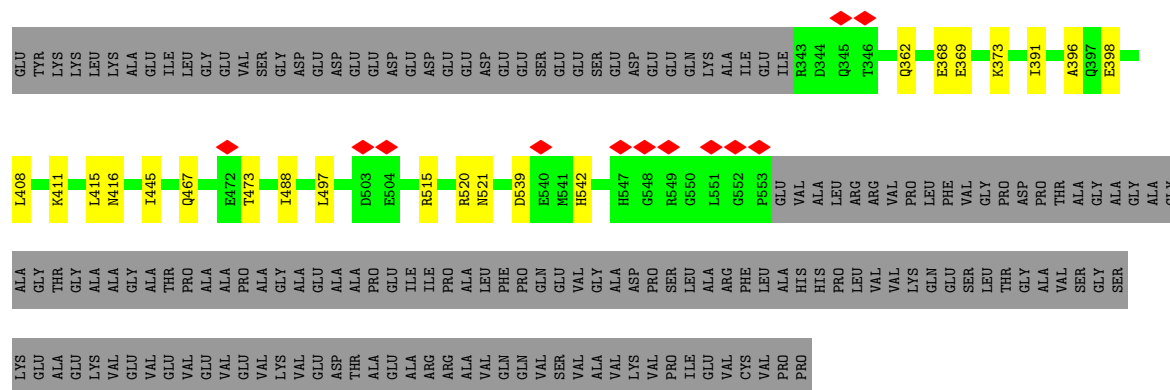


- Molecule 32: Putative pre-mRNA splicing protein



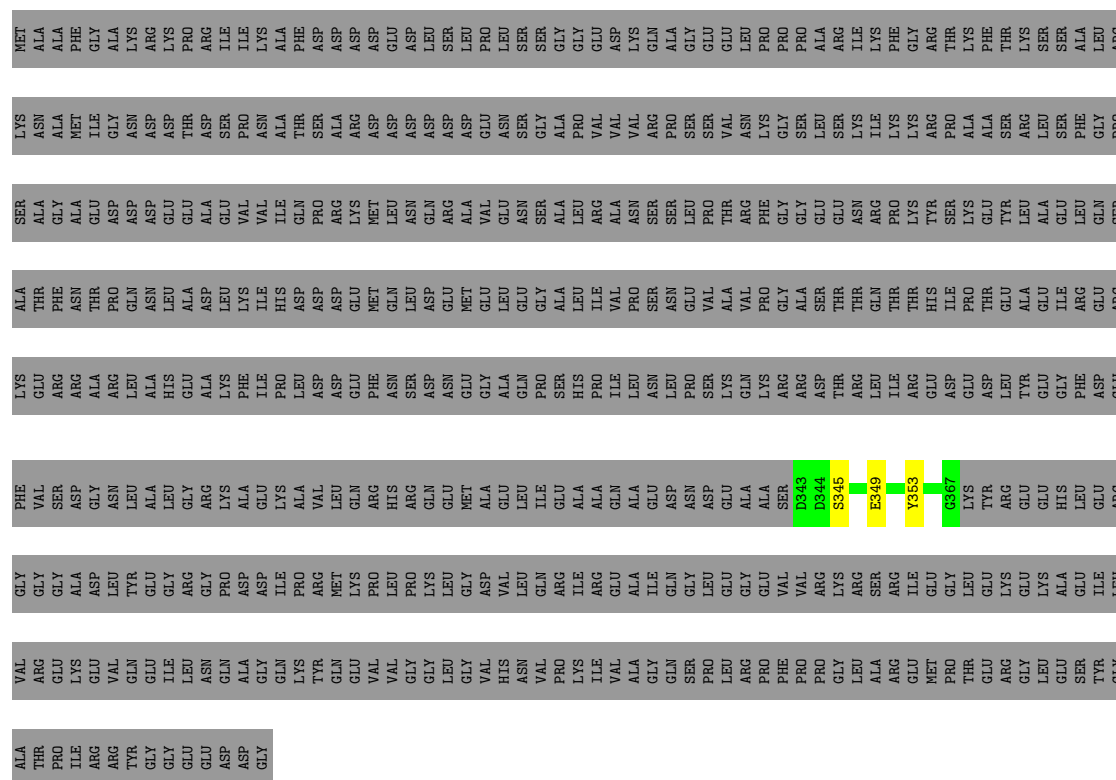
- Molecule 33: Putative pre-mRNA splicing protein





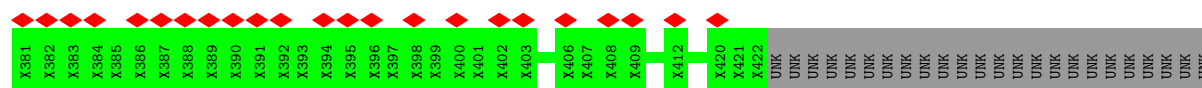
- Molecule 34: Nineteen complex-related protein 2-domain-containing protein

Chain CY: 95%



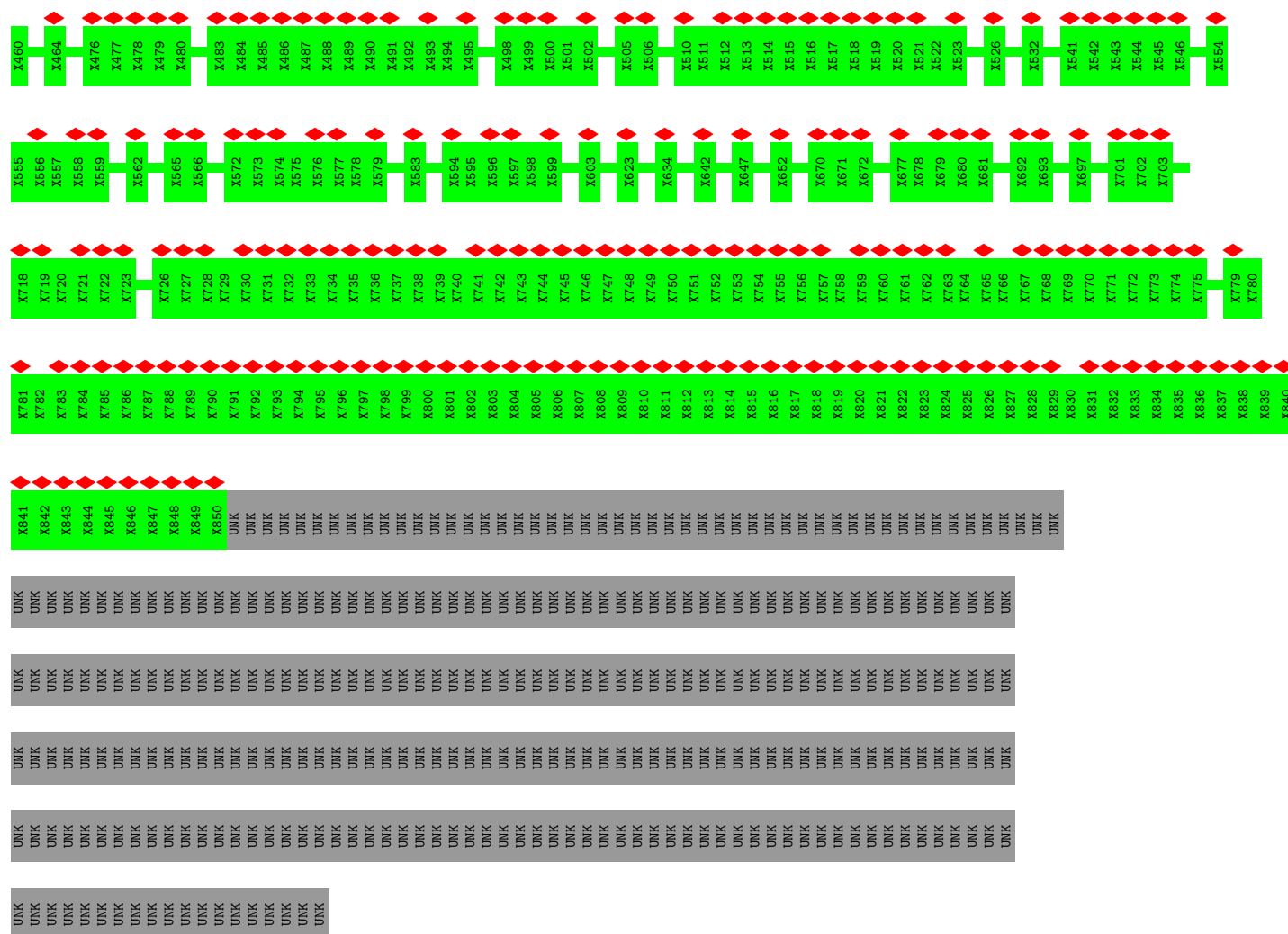
- Molecule 35: GCFC2

Chain Ck: 35%
64% 36%



- Molecule 36: TFIP11

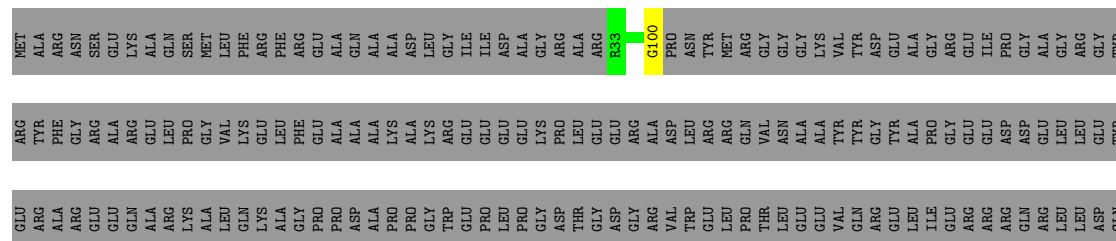
Chain Cb: 28%
56% 44%



- Molecule 37: Unknown mRNA



- Molecule 38: Putative pre-mRNA splicing protein



LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66478	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0035	Depositor
Map size ($\text{\AA}$)	447.36, 447.36, 447.36	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.932, 0.932, 0.932	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, M7M, P5P, MG, GTP, Y5P

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	0.19	0/866	0.33	0/1345
2	5	0.12	0/2612	0.26	0/4059
3	6	0.10	0/2200	0.24	0/3425
4	A	0.18	0/16823	0.45	2/22806 (0.0%)
5	B	0.17	0/1898	0.45	0/2558
6	C	0.17	0/7464	0.43	0/10117
7	E	0.17	0/2428	0.49	0/3295
8	F	0.10	0/546	0.30	0/761
9	I	0.10	0/3595	0.28	0/5017
10	J	0.15	0/4103	0.36	0/5609
11	L	0.14	0/4076	0.34	0/5552
12	K	0.12	0/1147	0.25	0/1598
13	q	0.11	0/690	0.25	0/962
13	r	0.12	0/710	0.24	0/990
13	s	0.11	0/695	0.25	0/969
13	t	0.11	0/700	0.25	0/976
14	N	0.25	0/1227	0.49	0/1655
15	S	0.20	0/1235	0.59	0/1671
16	T	0.21	0/2723	0.57	2/3701 (0.1%)
17	M	0.16	0/2006	0.44	0/2703
18	0	0.29	0/2289	0.55	2/3095 (0.1%)
19	R	0.16	0/2730	0.43	0/3689
20	W	0.18	0/752	0.48	0/1008
21	P	0.12	0/787	0.33	0/1049
22	Y	0.09	0/6599	0.25	0/9197
23	1	0.21	0/2573	0.51	1/3473 (0.0%)
24	z	0.17	0/5245	0.47	2/7100 (0.0%)
25	j	0.17	0/716	0.50	0/969
26	k	0.18	0/584	0.58	0/787
27	l	0.18	0/661	0.60	1/898 (0.1%)
28	m	0.15	0/687	0.47	0/922
29	o	0.17	0/691	0.50	0/940

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	p	0.19	0/799	0.56	0/1079
31	u	0.21	0/726	0.55	0/979
32	V	0.17	0/481	0.38	0/661
33	Z	0.17	0/1768	0.42	0/2384
34	CY	0.23	0/190	0.63	0/253
38	CV	0.14	0/336	0.35	0/467
All	All	0.17	0/86358	0.42	10/118719 (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
16	T	0	1
19	R	0	1
24	z	0	1
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	43	PRO	N-CA-CB	-8.93	93.88	103.25
24	z	448	THR	CA-C-N	5.85	128.52	120.39
24	z	448	THR	C-N-CA	5.85	128.52	120.39
27	l	61	GLY	N-CA-C	5.83	118.03	111.85
16	T	181	ARG	CA-C-N	5.20	131.33	121.97
16	T	181	ARG	C-N-CA	5.20	131.33	121.97
4	A	1353	ALA	CA-C-N	5.19	129.29	121.40
4	A	1353	ALA	C-N-CA	5.19	129.29	121.40
18	0	308	GLU	CA-C-N	5.00	127.76	120.51
18	0	308	GLU	C-N-CA	5.00	127.76	120.51

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	R	54	TYR	Peptide
16	T	318	ASP	Peptide
24	z	449	ARG	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	778	0	393	7	0
2	5	2343	0	1190	20	0
3	6	1966	0	994	39	0
4	A	16398	0	16409	159	0
5	B	1874	0	1664	27	0
6	C	7301	0	7338	102	0
7	E	2379	0	2343	48	0
8	F	547	0	260	0	0
9	I	3596	0	1641	3	0
10	J	4043	0	3105	23	0
11	L	4034	0	3376	29	0
12	K	1148	0	566	1	0
13	q	691	0	314	0	0
13	r	711	0	330	0	0
13	s	696	0	319	0	0
13	t	701	0	320	0	0
14	N	1200	0	1184	5	0
15	S	1209	0	1207	27	0
16	T	2653	0	2612	56	0
17	M	1964	0	1973	29	0
18	O	2235	0	2144	30	0
19	R	2670	0	2676	40	0
20	W	738	0	721	7	0
21	P	772	0	766	5	0
22	Y	6601	0	2980	2	0
23	l	2514	0	2473	48	0
24	z	5149	0	5221	103	0
25	j	704	0	743	18	0
26	k	577	0	611	19	0
27	l	649	0	652	17	0
28	m	678	0	723	14	0
29	o	679	0	711	16	0
30	p	788	0	816	24	0
31	u	716	0	738	20	0
32	V	478	0	317	7	0
33	Z	1729	0	1717	13	0
34	CY	190	0	167	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	Ck	205	0	39	0	0
36	Cb	1938	0	379	0	0
37	8	468	0	266	39	0
38	CV	337	0	141	1	0
39	B	30	0	19	1	0
40	C	1	0	0	0	0
41	C	32	0	12	0	0
42	M	1	0	0	0	0
42	N	3	0	0	0	0
All	All	87114	0	72570	818	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 (818) 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)
7:E:109:LEU:HA	7:E:119:PHE:O	1.23	1.30
16:T:404:VAL:HA	16:T:409:VAL:O	1.35	1.25
15:S:6:ALA:O	15:S:153:ALA:HA	1.37	1.22
3:6:32:A:H61	37:8:8:Y5P:H2	1.12	1.10
7:E:151:MET:HA	7:E:162:ILE:O	1.51	1.10
37:8:1:P5P:H4'	37:8:2:Y5P:OP2	1.36	1.09
32:V:16:SER:HB2	37:8:-8:P5P:C8	1.92	1.00
3:6:37:G:N2	37:8:4:Y5P:H4	1.80	0.96
4:A:1341:TRP:O	4:A:1354:HIS:HA	1.66	0.95
7:E:109:LEU:CA	7:E:119:PHE:O	2.16	0.91
24:z:252:LEU:O	24:z:329:VAL:HA	1.71	0.90
4:A:1948:ILE:O	4:A:2039:PRO:HA	1.75	0.86
3:6:32:A:H61	37:8:8:Y5P:C2	1.89	0.85
3:6:32:A:N6	37:8:8:Y5P:H2	1.94	0.82
3:6:38:A:C8	37:8:3:P5P:C4	2.63	0.82
17:M:241:SER:HB2	17:M:311:SER:O	1.81	0.81
16:T:319:LEU:HA	16:T:329:ILE:O	1.83	0.79
30:p:18:ARG:HB3	30:p:93:SER:O	1.83	0.79
6:C:721:TYR:HA	6:C:731:ILE:O	1.81	0.79
16:T:378:ILE:HB	16:T:392:PHE:HB2	1.66	0.78
3:6:38:A:C8	37:8:3:P5P:C2	2.68	0.77
37:8:1:P5P:C4'	37:8:2:Y5P:OP2	2.28	0.76
3:6:38:A:C8	37:8:3:P5P:N3	2.54	0.75
16:T:402:LEU:HA	16:T:411:PHE:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:824:PRO:HB3	6:C:858:LEU:HB3	1.68	0.73
23:1:71:PHE:CE1	37:8:2:Y5P:H4A	2.22	0.73
16:T:404:VAL:CA	16:T:409:VAL:O	2.27	0.73
3:6:36:A:C2	37:8:5:P5P:C6	2.73	0.71
24:z:102:SER:HB3	24:z:118:MET:HG3	1.72	0.71
4:A:835:THR:HG23	19:R:260:PRO:HD3	1.73	0.70
17:M:242:LEU:HB3	17:M:308:ILE:HD11	1.73	0.70
30:p:54:LYS:HG2	30:p:69:ILE:HG12	1.72	0.69
4:A:1026:ASN:HD22	4:A:1033:ASN:HD21	1.41	0.68
24:z:637:ILE:HG23	24:z:656:ILE:HD13	1.75	0.68
4:A:1558:SER:HB3	34:CY:353:TYR:HB2	1.76	0.67
4:A:285:ASP:HB3	4:A:288:GLU:HG2	1.75	0.67
32:V:16:SER:HB2	37:8:-8:P5P:N7	2.10	0.67
11:L:109:GLU:O	11:L:113:LEU:HB2	1.94	0.67
30:p:53:THR:OG1	30:p:70:GLN:NE2	2.25	0.67
5:B:310:ASN:HA	5:B:317:ARG:HH12	1.60	0.67
31:u:29:THR:HB	31:u:51:THR:O	1.94	0.67
15:S:87:GLY:N	15:S:106:THR:O	2.27	0.66
3:6:37:G:H21	37:8:4:Y5P:H4	1.59	0.66
16:T:182:VAL:HA	16:T:469:ILE:O	1.95	0.66
4:A:643:LEU:HD11	4:A:665:SER:HB2	1.78	0.65
25:j:62:GLU:HB3	25:j:76:ARG:HB3	1.78	0.65
7:E:244:LEU:HB2	7:E:258:ILE:HD12	1.78	0.64
23:1:170:GLY:HA2	24:z:425:ALA:HB2	1.78	0.64
7:E:151:MET:CA	7:E:162:ILE:O	2.38	0.64
6:C:505:ILE:HG13	6:C:509:MET:HE2	1.80	0.64
32:V:14:GLY:HA2	37:8:-8:P5P:C2	2.28	0.64
16:T:297:VAL:HB	16:T:307:HIS:HB2	1.79	0.64
23:1:122:LEU:HB2	24:z:658:LYS:HE3	1.80	0.64
4:A:1908:ASP:HB3	4:A:1935:PHE:HB2	1.80	0.63
17:M:88:ASP:OD1	17:M:98:ARG:NH1	2.31	0.63
23:1:171:ILE:HD11	24:z:423:PRO:HD2	1.80	0.63
4:A:1341:TRP:HB2	4:A:1355:ALA:HB3	1.79	0.63
31:u:32:GLY:HA2	31:u:47:ASP:HB2	1.81	0.63
30:p:28:GLN:HB2	30:p:50:PHE:HB2	1.79	0.63
6:C:208:ARG:NH2	6:C:216:GLU:O	2.31	0.63
16:T:296:ARG:HD2	16:T:305:ASN:HD21	1.63	0.63
3:6:17:G:H22	17:M:63:HIS:HA	1.64	0.62
6:C:777:SER:HB3	6:C:793:ASP:HB3	1.81	0.62
6:C:634:LEU:HD22	6:C:683:MET:HG3	1.81	0.62
16:T:318:ASP:HB3	16:T:361:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:36:A:N3	37:8:5:P5P:C2	2.62	0.62
3:6:36:A:C2	37:8:5:P5P:N1	2.67	0.62
6:C:252:ASP:HB3	6:C:682:TYR:HB2	1.82	0.62
15:S:6:ALA:O	15:S:153:ALA:CA	2.31	0.62
29:o:40:LEU:HD23	29:o:43:VAL:HG22	1.81	0.62
23:1:178:LYS:HD3	23:1:193:THR:H	1.65	0.62
19:R:313:ARG:HG2	19:R:317:MET:HE2	1.81	0.61
6:C:574:VAL:HB	6:C:585:THR:O	2.00	0.61
10:J:265:ARG:HE	19:R:12:LEU:HD12	1.65	0.61
29:o:3:LEU:HA	29:o:6:PHE:HD2	1.65	0.61
2:5:40:U:H3	37:8:-2:P5P:C2	2.13	0.61
4:A:1090:ASP:HB2	4:A:1204:ARG:HD2	1.80	0.61
5:B:298:ASN:HD21	19:R:271:THR:H	1.48	0.61
17:M:82:CYS:HB3	17:M:85:CYS:SG	2.40	0.61
7:E:149:ASN:ND2	7:E:166:ASP:OD1	2.34	0.61
16:T:255:CYS:HB3	16:T:265:ARG:HB2	1.82	0.61
16:T:364:HIS:O	19:R:145:ARG:NH2	2.33	0.61
23:1:204:ILE:HD13	24:z:391:VAL:HG11	1.81	0.61
27:l:23:ILE:HG13	27:l:79:ALA:HB2	1.83	0.61
16:T:182:VAL:HG22	16:T:470:LYS:HG2	1.83	0.61
24:z:612:ARG:HH21	24:z:619:VAL:HG22	1.65	0.61
4:A:972:ARG:NH2	4:A:1560:ASP:OD2	2.34	0.60
16:T:295:ALA:HB3	16:T:309:LEU:HB2	1.82	0.60
4:A:1341:TRP:O	4:A:1354:HIS:CA	2.47	0.60
4:A:432:TYR:O	6:C:691:ARG:NH1	2.34	0.60
4:A:679:ARG:HD2	4:A:716:THR:HG22	1.84	0.60
33:Z:488:ILE:HG22	33:Z:497:LEU:HD21	1.83	0.60
6:C:805:LEU:O	6:C:809:LYS:HB2	2.02	0.60
7:E:259:ARG:HD3	7:E:261:PHE:H	1.67	0.59
24:z:125:ARG:HH12	24:z:459:ALA:HA	1.67	0.59
24:z:560:LYS:HE3	24:z:570:VAL:HG11	1.82	0.59
25:j:76:ARG:NH1	25:j:77:PRO:O	2.34	0.59
6:C:485:PRO:O	6:C:489:ALA:HB2	2.02	0.59
16:T:277:LEU:HA	16:T:287:VAL:O	2.02	0.59
4:A:491:LEU:HD22	6:C:386:ARG:HE	1.67	0.59
6:C:297:LEU:HB2	6:C:344:LEU:HD13	1.84	0.59
24:z:285:LEU:HD13	24:z:299:VAL:HA	1.85	0.59
27:l:67:LEU:HB3	28:m:107:VAL:HB	1.84	0.59
5:B:150:ARG:HH22	39:B:401:M7M:HBT	1.67	0.59
30:p:82:ARG:NH1	31:u:41:MET:SD	2.75	0.59
2:5:92:G:OP2	27:l:71:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:67:A:OP2	37:8:4:Y5P:HA1	2.03	0.59
4:A:1722:GLN:O	4:A:1726:GLN:NE2	2.36	0.59
7:E:127:LEU:HB2	7:E:141:TYR:HB2	1.83	0.59
29:o:9:LYS:HB3	29:o:79:LEU:HD22	1.85	0.58
16:T:360:ALA:HB3	16:T:373:ALA:HB3	1.85	0.58
24:z:348:SER:HA	24:z:643:GLU:HB3	1.85	0.58
4:A:1767:THR:HG22	4:A:1779:ILE:HG12	1.85	0.58
18:0:120:CYS:HB3	18:0:123:PHE:HB3	1.83	0.58
6:C:548:GLY:N	6:C:571:ILE:O	2.37	0.58
7:E:302:THR:HA	7:E:317:LEU:O	2.04	0.58
11:L:20:ALA:HB2	11:L:35:LEU:HD22	1.85	0.58
19:R:14:LYS:HD2	19:R:15:PRO:HD2	1.85	0.58
24:z:397:SER:O	24:z:427:GLN:NE2	2.37	0.58
4:A:1864:ASN:HB3	4:A:1867:LEU:HB2	1.85	0.58
4:A:1402:ARG:NH1	4:A:1500:ILE:O	2.33	0.58
27:l:27:LYS:HA	27:l:74:LEU:HG	1.84	0.58
6:C:540:VAL:O	6:C:591:GLY:N	2.36	0.58
16:T:328:VAL:HB	16:T:340:TRP:HB2	1.85	0.58
18:0:207:ILE:HG12	18:0:218:ILE:HG23	1.85	0.58
29:o:46:THR:HG22	29:o:52:PRO:HB3	1.86	0.58
33:Z:396:ALA:HB2	33:Z:445:ILE:HD11	1.85	0.58
1:2:23:A:H5"	4:A:908:ARG:HH21	1.69	0.57
31:u:23:GLU:OE1	31:u:29:THR:OG1	2.22	0.57
24:z:449:ARG:O	24:z:451:LEU:N	2.37	0.57
24:z:531:LYS:O	24:z:533:ARG:NH1	2.37	0.57
27:l:26:LEU:HD12	27:l:31:THR:HB	1.86	0.57
28:m:70:VAL:HG21	28:m:97:MET:HB2	1.85	0.57
23:1:203:MET:HE1	24:z:427:GLN:HB2	1.87	0.57
24:z:472:GLN:HG2	24:z:568:ILE:HG21	1.86	0.57
6:C:503:THR:OG1	6:C:618:GLU:OE2	2.23	0.57
16:T:361:LEU:HG	16:T:372:THR:HG22	1.86	0.57
33:Z:467:GLN:OE1	33:Z:515:ARG:NH2	2.35	0.57
4:A:1810:LYS:O	4:A:1814:TYR:HB2	2.04	0.57
6:C:121:ALA:HB2	16:T:220:GLN:HE22	1.69	0.57
10:J:138:ARG:NH2	16:T:496:TYR:O	2.37	0.57
20:W:125:ALA:HA	20:W:134:TYR:HB2	1.85	0.57
11:L:75:LEU:HD22	19:R:295:ALA:HA	1.87	0.57
16:T:193:LEU:HA	16:T:203:ALA:O	2.05	0.57
26:k:69:LEU:HB2	31:u:64:TYR:HB3	1.85	0.57
31:u:86:ARG:HH12	31:u:88:ARG:HG2	1.69	0.57
15:S:1:MET:HG3	15:S:21:GLN:HE22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:112:A:O2'	30:p:55:ARG:NH2	2.38	0.57
4:A:552:PRO:HB2	4:A:555:LYS:HB2	1.87	0.57
3:6:67:A:C4	37:8:3:P5P:H2	2.40	0.56
7:E:191:THR:OG1	7:E:232:ILE:O	2.22	0.56
16:T:343:ALA:HB2	19:R:158:THR:HG22	1.86	0.56
3:6:34:A:C2	37:8:7:P5P:C2	2.88	0.56
4:A:824:MET:O	16:T:356:LYS:NZ	2.35	0.56
5:B:324:THR:OG1	5:B:325:MET:SD	2.62	0.56
17:M:244:ILE:HB	17:M:278:ALA:HB3	1.87	0.56
24:z:122:LEU:O	24:z:126:GLU:HB2	2.05	0.56
2:5:91:U:O2	28:m:100:ARG:NH1	2.35	0.56
18:0:160:ALA:O	18:0:173:ASN:ND2	2.38	0.56
7:E:149:ASN:O	7:E:284:ARG:NH2	2.39	0.56
10:J:24:GLN:HG2	10:J:27:ARG:HH21	1.69	0.56
18:0:274:ARG:HG2	18:0:282:VAL:HG21	1.87	0.56
1:2:18:G:H22	3:6:49:A:H2	1.53	0.56
6:C:133:GLU:HG3	6:C:135:LYS:HG2	1.87	0.56
26:k:6:PRO:HB2	26:k:8:LEU:HD23	1.88	0.56
29:o:20:LYS:HA	29:o:66:ARG:HG3	1.88	0.56
2:5:88:C:H5''	2:5:89:U:H5'	1.87	0.56
4:A:188:ILE:HG12	4:A:191:VAL:HG22	1.88	0.56
4:A:415:ARG:NH2	6:C:981:ARG:O	2.39	0.56
18:0:314:HIS:O	18:0:323:ASN:ND2	2.39	0.56
24:z:612:ARG:HG2	24:z:616:GLY:HA2	1.88	0.56
16:T:197:PRO:HG3	16:T:239:PRO:HA	1.86	0.56
15:S:43:ILE:HG22	15:S:149:LYS:HD3	1.86	0.56
4:A:1118:THR:HG22	11:L:77:PRO:HD2	1.88	0.55
4:A:423:ARG:NH1	6:C:927:ASP:OD1	2.37	0.55
4:A:1719:ASP:OD1	23:1:102:GLN:NE2	2.39	0.55
30:p:16:ASN:O	30:p:32:GLN:NE2	2.36	0.55
4:A:1904:GLN:NE2	4:A:1987:GLN:OE1	2.40	0.55
19:R:61:ARG:O	19:R:63:ARG:NH1	2.40	0.55
4:A:1912:VAL:HG22	4:A:1934:ILE:HG12	1.89	0.55
6:C:394:ASN:O	6:C:398:ARG:N	2.39	0.55
11:L:378:ASN:OD1	11:L:381:ARG:NH2	2.36	0.55
15:S:74:GLU:HA	15:S:97:ASN:HB3	1.89	0.55
24:z:220:ASP:HB3	24:z:373:LYS:HG3	1.88	0.55
4:A:983:LEU:O	4:A:988:ARG:NH1	2.40	0.55
24:z:403:ILE:HD11	24:z:428:MET:HB2	1.89	0.55
23:1:29:PRO:O	24:z:509:ARG:NH1	2.38	0.55
3:6:26:G:H4'	3:6:27:A:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1329:ASN:ND2	4:A:1331:ASN:O	2.40	0.55
1:2:17:U:OP2	5:B:304:LYS:NZ	2.39	0.55
21:P:37:ARG:HD3	21:P:43:GLY:HA3	1.89	0.55
22:Y:541:ASP:N	22:Y:580:ILE:O	2.41	0.55
4:A:967:ILE:HD11	23:1:223:LEU:HD22	1.88	0.54
17:M:47:CYS:HA	17:M:115:ARG:HD2	1.87	0.54
24:z:183:ARG:HB2	24:z:209:ILE:HD11	1.88	0.54
4:A:1343:LEU:HB2	4:A:1353:ALA:HB3	1.89	0.54
26:k:23:SER:O	26:k:25:ARG:NH1	2.41	0.54
4:A:847:TRP:O	4:A:912:LYS:NZ	2.36	0.54
24:z:253:VAL:HG13	24:z:330:ILE:HB	1.89	0.54
26:k:62:ARG:NH1	26:k:64:ASN:OD1	2.40	0.54
3:6:57:U:OP2	4:A:790:ARG:NH2	2.41	0.54
15:S:3:THR:HG21	15:S:31:LYS:HD2	1.89	0.54
18:0:187:THR:H	18:0:190:ILE:HD11	1.72	0.54
4:A:1934:ILE:HB	4:A:1947:LYS:HB3	1.88	0.54
19:R:320:GLN:NE2	19:R:324:GLU:OE2	2.39	0.54
24:z:471:ALA:HB2	24:z:480:ILE:HD11	1.89	0.54
16:T:235:LEU:HA	16:T:245:PHE:O	2.07	0.54
28:m:67:LEU:HB2	28:m:97:MET:HB3	1.90	0.54
10:J:554:ILE:HA	10:J:577:ALA:HB1	1.89	0.54
24:z:21:LEU:HD13	24:z:49:GLY:HA3	1.90	0.54
3:6:14:U:OP2	4:A:164:ARG:NH2	2.41	0.54
4:A:346:LEU:HD11	4:A:528:ALA:HB2	1.89	0.54
4:A:357:GLU:HA	4:A:360:VAL:HG12	1.90	0.54
4:A:2019:PRO:HD3	4:A:2068:ARG:HH21	1.73	0.53
10:J:265:ARG:HD2	19:R:13:PRO:HD2	1.91	0.53
17:M:81:ALA:HB2	17:M:95:ILE:HD11	1.90	0.53
32:V:18:TYR:HE1	37:8:-10:P5P:H1'	1.72	0.53
2:5:90:U:OP1	29:o:63:ASN:ND2	2.41	0.53
4:A:1419:GLU:OE2	4:A:1444:TYR:OH	2.26	0.53
5:B:245:ASN:ND2	19:R:104:GLY:O	2.41	0.53
6:C:809:LYS:HA	6:C:812:ILE:HB	1.90	0.53
7:E:341:SER:OG	7:E:343:ASP:OD1	2.26	0.53
24:z:22:PRO:HA	24:z:25:LYS:HD3	1.88	0.53
32:V:14:GLY:HA2	37:8:-8:P5P:H2	1.89	0.53
11:L:57:LYS:O	11:L:89:ARG:NH1	2.42	0.53
4:A:1702:GLN:O	4:A:1705:ARG:NH1	2.41	0.53
7:E:161:LEU:HB2	7:E:173:TRP:HB2	1.91	0.53
23:1:204:ILE:HD11	24:z:396:ARG:HB3	1.91	0.53
4:A:371:LEU:HD11	4:A:429:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:0:110:ARG:NH2	18:0:133:ASP:O	2.41	0.53
3:6:67:A:C5	37:8:3:P5P:H2	2.44	0.53
4:A:1864:ASN:HD22	4:A:1867:LEU:HG	1.73	0.53
24:z:500:ASP:HB3	24:z:503:LYS:HB3	1.91	0.53
31:u:24:LEU:HG	31:u:70:VAL:HG12	1.90	0.53
2:5:87:U:O2	26:k:62:ARG:NH1	2.42	0.53
3:6:32:A:N6	37:8:8:Y5P:C2	2.64	0.53
15:S:89:LEU:HD23	15:S:121:GLY:HA3	1.91	0.53
29:o:59:THR:HB	30:p:89:LEU:HB3	1.91	0.53
3:6:38:A:N7	37:8:3:P5P:C4	2.72	0.52
4:A:191:VAL:HG11	4:A:633:LEU:HD11	1.90	0.52
7:E:234:THR:HB	7:E:284:ARG:HA	1.91	0.52
7:E:305:ILE:HB	7:E:315:TYR:HB2	1.91	0.52
17:M:25:ASN:HB2	19:R:197:MET:HE1	1.92	0.52
27:l:46:ILE:HB	27:l:68:ILE:HB	1.91	0.52
3:6:73:C:H42	11:L:177:LYS:HD3	1.74	0.52
4:A:415:ARG:HE	6:C:981:ARG:HA	1.75	0.52
5:B:239:THR:HB	5:B:246:ALA:HB2	1.92	0.52
5:B:265:ASP:OD2	10:J:148:TYR:OH	2.28	0.52
6:C:616:ASN:ND2	6:C:618:GLU:OE1	2.43	0.52
16:T:421:PHE:HB2	16:T:431:GLN:HB3	1.90	0.52
6:C:731:ILE:HG12	6:C:843:PHE:HE1	1.74	0.52
15:S:88:ILE:HD11	19:R:73:ALA:HB3	1.90	0.52
15:S:111:PRO:HB3	18:0:304:LEU:HD23	1.92	0.52
17:M:46:LEU:HD12	17:M:75:CYS:HB3	1.92	0.52
4:A:1176:ASP:OD1	4:A:1215:TYR:OH	2.23	0.52
7:E:268:ILE:HG22	7:E:269:ARG:HB2	1.92	0.52
16:T:403:ALA:HB3	16:T:411:PHE:HB3	1.92	0.52
28:m:45:SER:HB3	28:m:106:ILE:HG22	1.92	0.52
3:6:21:A:H4'	4:A:195:LYS:HG3	1.91	0.52
15:S:15:ILE:HB	15:S:125:LYS:HB2	1.91	0.52
24:z:509:ARG:HA	24:z:512:ALA:HB2	1.92	0.52
2:5:19:G:H2'	4:A:590:ARG:HB2	1.92	0.52
4:A:1659:ARG:HG2	4:A:1695:THR:HG23	1.92	0.52
6:C:877:MET:O	6:C:911:ARG:HA	2.10	0.52
23:1:414:LEU:HD13	24:z:160:LYS:HZ3	1.75	0.52
28:m:54:ALA:HB2	28:m:70:VAL:HG13	1.91	0.52
1:2:11:G:H4'	5:B:177:ALA:HA	1.91	0.52
23:1:192:GLU:OE2	23:1:194:HIS:NE2	2.43	0.52
24:z:149:ILE:HG21	24:z:402:ILE:HG12	1.91	0.52
5:B:212:ILE:HD11	19:R:33:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:227:PRO:O	6:C:579:THR:OG1	2.27	0.52
7:E:320:HIS:CG	7:E:341:SER:HG	2.27	0.52
17:M:250:ASP:OD1	18:O:260:ARG:NH1	2.43	0.52
23:1:174:LYS:HE3	23:1:195:LEU:HB3	1.92	0.51
7:E:213:VAL:O	7:E:222:VAL:N	2.42	0.51
15:S:90:SER:HB2	15:S:104:PHE:HD2	1.75	0.51
16:T:183:ILE:HB	16:T:469:ILE:HB	1.91	0.51
19:R:88:ASP:N	19:R:88:ASP:OD1	2.44	0.51
7:E:79:SER:OG	7:E:80:MET:N	2.43	0.51
29:o:6:PHE:HE1	29:o:80:LEU:HA	1.74	0.51
2:5:91:U:O2'	27:l:69:ARG:NH2	2.38	0.51
4:A:267:ARG:NH2	4:A:745:THR:OG1	2.43	0.51
23:1:166:LYS:O	23:1:169:GLN:NE2	2.43	0.51
24:z:253:VAL:HG22	24:z:330:ILE:HD13	1.92	0.51
6:C:520:VAL:HG22	6:C:540:VAL:HA	1.91	0.51
4:A:1621:GLY:HA3	4:A:1871:ARG:HD3	1.93	0.51
4:A:921:HIS:NE2	4:A:1116:GLU:OE2	2.38	0.51
5:B:149:LYS:HA	5:B:152:TRP:HD1	1.76	0.51
6:C:638:VAL:HG12	6:C:701:VAL:HG22	1.92	0.51
24:z:331:ASP:OD1	24:z:362:ARG:NH1	2.40	0.51
33:Z:391:ILE:HD11	33:Z:408:LEU:HG	1.91	0.51
6:C:493:LEU:HD21	6:C:509:MET:HB3	1.91	0.51
11:L:166:ALA:O	11:L:170:LEU:HB2	2.10	0.51
24:z:468:LEU:O	24:z:472:GLN:NE2	2.44	0.51
17:M:84:CYS:O	18:O:150:ASN:ND2	2.43	0.51
17:M:247:ILE:O	17:M:276:HIS:ND1	2.44	0.51
18:O:317:ARG:NH1	19:R:200:ASN:OD1	2.44	0.51
26:k:19:GLU:HB3	26:k:68:ILE:HB	1.93	0.51
5:B:258:ALA:HB1	10:J:153:LEU:HA	1.93	0.51
6:C:216:GLU:HG3	6:C:223:ILE:HG12	1.92	0.51
18:O:119:PHE:HD2	18:O:153:CYS:HB2	1.76	0.51
25:j:43:THR:O	25:j:60:ALA:HA	2.10	0.51
3:6:21:A:H61	18:O:129:PRO:HD2	1.75	0.50
24:z:76:ARG:HB2	24:z:79:ALA:HB3	1.93	0.50
24:z:528:PHE:CG	24:z:549:MET:HE1	2.46	0.50
24:z:558:GLN:HG2	24:z:561:ARG:HH21	1.75	0.50
6:C:223:ILE:HG13	6:C:224:LYS:HG2	1.93	0.50
16:T:297:VAL:HG11	16:T:342:LEU:HD11	1.93	0.50
25:j:70:ASN:OD1	26:k:48:ARG:NH1	2.45	0.50
4:A:1069:PRO:HG3	4:A:1218:TYR:CZ	2.47	0.50
6:C:966:THR:O	6:C:970:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:246:GLU:OE1	11:L:249:ARG:NH2	2.45	0.50
11:L:397:GLU:HA	19:R:313:ARG:HH22	1.77	0.50
23:1:140:ARG:NH2	23:1:146:GLY:O	2.45	0.50
24:z:395:GLN:HG2	24:z:424:PRO:HD3	1.93	0.50
3:6:58:G:N1	3:6:61:C:OP1	2.44	0.50
4:A:824:MET:HB3	4:A:830:GLN:HE21	1.76	0.50
4:A:820:LEU:HD21	4:A:836:VAL:HG11	1.93	0.50
4:A:1728:LEU:HB2	23:1:92:ARG:HH12	1.76	0.50
5:B:292:THR:HA	10:J:26:LEU:HD13	1.93	0.50
6:C:524:LYS:HB3	6:C:537:PHE:HB3	1.93	0.50
33:Z:539:ASP:O	33:Z:542:HIS:NE2	2.44	0.50
24:z:51:SER:O	24:z:117:TYR:OH	2.29	0.50
25:j:12:VAL:O	26:k:31:ARG:NH1	2.45	0.50
25:j:57:ILE:O	25:j:80:GLN:HA	2.11	0.50
4:A:1617:PHE:O	4:A:1620:THR:OG1	2.29	0.50
7:E:165:SER:OG	7:E:167:ASP:OD1	2.23	0.50
10:J:50:LEU:HD22	11:L:254:PRO:HG3	1.93	0.49
17:M:101:ALA:HB2	18:O:265:ILE:HG22	1.93	0.49
33:Z:467:GLN:O	33:Z:473:THR:OG1	2.30	0.49
4:A:768:MET:HA	4:A:771:ILE:HG22	1.94	0.49
6:C:980:ARG:HD3	6:C:986:GLU:HG2	1.93	0.49
6:C:722:ALA:O	6:C:730:THR:HA	2.11	0.49
6:C:789:ASN:OD1	6:C:833:THR:OG1	2.29	0.49
4:A:555:LYS:HG2	4:A:559:LEU:HD23	1.94	0.49
34:CY:345:SER:O	34:CY:349:GLU:HG2	2.13	0.49
4:A:267:ARG:NH2	4:A:745:THR:O	2.46	0.49
4:A:825:PRO:HD2	4:A:828:ILE:HG13	1.93	0.49
30:p:17:TRP:HE1	30:p:91:VAL:HG13	1.77	0.49
33:Z:520:ARG:NH2	33:Z:521:ASN:OD1	2.46	0.49
28:m:39:HIS:O	28:m:55:ARG:NH1	2.46	0.49
4:A:159:ARG:NH2	7:E:281:ASN:OD1	2.44	0.49
24:z:450:PRO:O	24:z:454:ARG:N	2.44	0.49
30:p:53:THR:HG1	30:p:70:GLN:HE21	1.57	0.49
4:A:572:VAL:HG12	4:A:576:LYS:HE2	1.93	0.49
4:A:1616:LEU:HG	4:A:1667:PRO:HD3	1.94	0.49
6:C:485:PRO:O	6:C:489:ALA:CB	2.61	0.49
24:z:24:ALA:HA	24:z:27:ARG:HB2	1.95	0.49
4:A:1788:TRP:HD1	4:A:1824:SER:HB3	1.77	0.49
11:L:727:ALA:HB1	12:K:9:GLU:HA	1.93	0.49
19:R:180:VAL:HG11	19:R:217:PRO:HG3	1.95	0.49
23:1:92:ARG:HD3	23:1:94:LYS:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:m:91:ASP:OD1	28:m:91:ASP:N	2.44	0.49
7:E:110:GLN:HG2	7:E:153:VAL:HG22	1.95	0.49
16:T:287:VAL:HG12	16:T:319:LEU:HD11	1.94	0.49
23:1:343:ARG:NH2	24:z:246:GLU:OE2	2.39	0.49
24:z:464:MET:HB2	24:z:598:TYR:HE1	1.78	0.49
33:Z:368:GLU:HG2	33:Z:411:LYS:HE2	1.94	0.49
4:A:342:TRP:HB3	4:A:545:MET:HE3	1.93	0.48
4:A:409:GLU:OE2	4:A:415:ARG:NH1	2.45	0.48
4:A:1345:ASP:O	4:A:1349:LYS:N	2.46	0.48
6:C:269:LEU:HD11	6:C:281:THR:HG23	1.94	0.48
10:J:236:ILE:HD12	10:J:249:LEU:HD11	1.95	0.48
23:1:43:PRO:HB3	23:1:45:TRP:CE2	2.47	0.48
4:A:1098:GLY:HA2	4:A:1307:LYS:HD2	1.94	0.48
4:A:1448:GLU:HB3	23:1:266:PRO:HB2	1.95	0.48
24:z:287:LEU:HB3	24:z:313:SER:HA	1.95	0.48
27:l:67:LEU:HB2	28:m:31:LEU:HD11	1.95	0.48
33:Z:515:ARG:HD2	33:Z:521:ASN:HB3	1.94	0.48
6:C:719:LYS:HD3	6:C:838:ILE:HG21	1.96	0.48
1:2:16:U:O4	5:B:307:ARG:NH2	2.44	0.48
23:1:171:ILE:HD13	24:z:428:MET:HE2	1.95	0.48
24:z:76:ARG:NH1	24:z:320:SER:OG	2.46	0.48
25:j:75:LYS:O	27:l:87:THR:OG1	2.30	0.48
4:A:461:LEU:O	4:A:526:ARG:NH1	2.45	0.48
7:E:271:PHE:HE1	7:E:311:GLY:HA2	1.78	0.48
9:I:721:GLY:O	11:L:365:ARG:NH1	2.46	0.48
10:J:193:ARG:NH2	10:J:219:PHE:O	2.47	0.48
19:R:84:TRP:CD1	19:R:87:ASN:HD21	2.32	0.48
24:z:232:LEU:HD11	24:z:264:ALA:HB2	1.95	0.48
24:z:344:THR:O	24:z:430:ARG:NH2	2.46	0.48
30:p:14:TYR:HD2	30:p:19:MET:HE1	1.79	0.48
3:6:38:A:C8	37:8:3:P5P:C5	2.97	0.48
11:L:324:ASP:O	11:L:328:LYS:HG2	2.13	0.48
23:1:410:ARG:NH1	24:z:408:ALA:O	2.46	0.48
4:A:1318:GLY:HA2	4:A:1363:ASP:OD2	2.14	0.48
26:k:45:VAL:HG11	26:k:53:LYS:HD3	1.96	0.48
26:k:46:GLU:HB2	26:k:56:LEU:HD21	1.95	0.48
4:A:871:LYS:NZ	16:T:445:GLU:OE1	2.36	0.48
4:A:1255:PHE:HA	4:A:1297:TRP:HZ2	1.79	0.48
6:C:734:ALA:HB2	6:C:838:ILE:HD11	1.94	0.48
2:5:40:U:H3	37:8:-2:P5P:H2	1.78	0.47
4:A:990:GLU:HG3	4:A:1040:PRO:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1718:MET:O	4:A:1722:GLN:OE1	2.32	0.47
23:1:153:GLU:O	23:1:158:LYS:NZ	2.46	0.47
30:p:79:THR:HG22	31:u:74:ILE:HG13	1.96	0.47
4:A:1306:SER:O	4:A:1328:ARG:NH1	2.47	0.47
7:E:278:LEU:HB3	20:W:90:LYS:HE3	1.95	0.47
24:z:294:GLU:HA	24:z:297:MET:HE2	1.95	0.47
3:6:38:A:H8	37:8:3:P5P:C5	2.26	0.47
4:A:719:TYR:CE1	37:8:-5:Y5P:HA	2.50	0.47
4:A:1236:LEU:HG	4:A:1279:ALA:HB1	1.96	0.47
10:J:262:GLU:HB3	10:J:265:ARG:HG3	1.95	0.47
16:T:494:ARG:NH1	16:T:495:LYS:O	2.47	0.47
3:6:34:A:C2	37:8:7:P5P:N3	2.83	0.47
3:6:37:G:H22	37:8:4:Y5P:H4	1.75	0.47
5:B:162:TRP:HA	5:B:165:ARG:HE	1.78	0.47
6:C:518:LEU:N	6:C:611:ASP:OD2	2.43	0.47
7:E:212:LYS:HG2	7:E:224:THR:HG22	1.97	0.47
7:E:207:ILE:HA	7:E:231:THR:HG22	1.96	0.47
24:z:22:PRO:O	24:z:25:LYS:HB2	2.15	0.47
25:j:54:ASN:OD1	25:j:85:GLY:N	2.47	0.47
26:k:25:ARG:HH22	26:k:49:PRO:HA	1.78	0.47
3:6:37:G:H21	37:8:4:Y5P:C4	2.26	0.47
4:A:1320:GLU:HB2	4:A:1360:THR:HG22	1.96	0.47
4:A:2025:LYS:O	4:A:2074:GLN:NE2	2.48	0.47
5:B:151:ALA:HA	5:B:154:TRP:CD1	2.50	0.47
6:C:819:ALA:HB2	6:C:854:SER:HB3	1.97	0.47
6:C:845:TRP:HB2	6:C:846:TRP:HE3	1.80	0.47
16:T:253:VAL:HB	16:T:267:TYR:HB2	1.97	0.47
24:z:526:GLN:O	24:z:530:THR:OG1	2.29	0.47
1:2:31:U:O3'	24:z:647:LYS:NZ	2.47	0.47
4:A:788:GLU:HA	19:R:224:LYS:HA	1.97	0.47
4:A:914:GLU:OE2	4:A:917:ARG:NH2	2.40	0.47
4:A:1290:ARG:HG3	6:C:94:LEU:HD11	1.95	0.47
6:C:155:THR:HA	6:C:158:MET:HE2	1.95	0.47
6:C:826:CYS:HB2	6:C:828:GLU:HG2	1.95	0.47
7:E:65:THR:OG1	7:E:107:LEU:O	2.29	0.47
7:E:339:SER:O	7:E:346:MET:HA	2.15	0.47
15:S:138:THR:HA	15:S:144:PRO:HA	1.95	0.47
23:1:178:LYS:HA	23:1:193:THR:HA	1.96	0.47
23:1:210:THR:HG22	24:z:645:LYS:HB2	1.96	0.47
23:1:211:ASP:OD1	23:1:211:ASP:N	2.48	0.47
4:A:283:PRO:HB3	4:A:690:GLN:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:619:ASP:OD1	6:C:619:ASP:N	2.44	0.47
7:E:214:TRP:HA	7:E:221:VAL:HA	1.96	0.47
16:T:402:LEU:CA	16:T:411:PHE:O	2.60	0.47
4:A:1243:GLU:OE2	21:P:230:ARG:NH2	2.47	0.47
4:A:2090:GLN:HB2	4:A:2093:HIS:HB2	1.96	0.47
6:C:200:GLY:O	6:C:203:ARG:HG2	2.15	0.47
18:O:235:HIS:HA	18:O:243:ILE:HG23	1.97	0.47
2:5:24:A:N6	6:C:204:ASP:OD2	2.48	0.46
10:J:26:LEU:HD21	19:R:271:THR:HG21	1.97	0.46
23:1:359:ILE:HD11	24:z:219:ILE:HD12	1.97	0.46
24:z:53:GLN:NE2	24:z:90:GLU:OE1	2.48	0.46
24:z:132:LEU:O	24:z:165:ARG:NH1	2.47	0.46
29:o:39:ALA:HA	29:o:59:THR:HA	1.97	0.46
30:p:20:ARG:HH21	30:p:28:GLN:HG3	1.80	0.46
6:C:779:TRP:CD2	6:C:809:LYS:HD2	2.50	0.46
19:R:199:ASN:N	19:R:199:ASN:OD1	2.48	0.46
24:z:66:ASP:OD1	24:z:66:ASP:N	2.42	0.46
4:A:427:ARG:NH1	4:A:434:TYR:O	2.40	0.46
10:J:239:THR:HG23	10:J:240:LEU:HD12	1.97	0.46
16:T:181:ARG:NH2	21:P:60:GLU:OE2	2.48	0.46
29:o:30:ALA:HB2	29:o:41:ARG:HG3	1.96	0.46
4:A:1519:LYS:NZ	4:A:1534:ASP:O	2.44	0.46
7:E:73:THR:HG22	7:E:90:TYR:HD2	1.81	0.46
7:E:86:LEU:HD12	7:E:97:GLY:HA3	1.97	0.46
18:O:280:GLU:OE2	18:O:295:ARG:NH2	2.48	0.46
3:6:14:U:O2'	20:W:92:ARG:NH1	2.40	0.46
7:E:84:ILE:HG13	7:E:106:ILE:HD13	1.97	0.46
24:z:142:ASP:HA	24:z:173:SER:HB3	1.97	0.46
24:z:259:ASP:N	24:z:259:ASP:OD1	2.48	0.46
4:A:330:ASP:OD1	4:A:330:ASP:N	2.44	0.46
9:I:595:PRO:HA	9:I:598:ALA:HB3	1.98	0.46
11:L:10:THR:HG22	11:L:149:ARG:HE	1.81	0.46
15:S:66:ARG:H	15:S:101:SER:HB3	1.80	0.46
23:1:178:LYS:HE2	23:1:192:GLU:HG3	1.96	0.46
26:k:45:VAL:HA	26:k:54:VAL:O	2.16	0.46
24:z:120:ASP:OD1	24:z:120:ASP:N	2.47	0.46
29:o:19:LEU:HA	29:o:65:ILE:HA	1.97	0.46
30:p:49:GLU:OE1	30:p:74:ARG:NH2	2.43	0.46
4:A:670:ALA:HB2	4:A:778:TRP:HB3	1.98	0.46
4:A:1497:ARG:NH2	33:Z:398:GLU:OE2	2.49	0.46
6:C:783:PRO:HD3	6:C:789:ASN:HD22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:p:33:MET:HA	30:p:44:LEU:HA	1.97	0.46
6:C:641:ILE:HD12	6:C:698:GLU:HB3	1.96	0.46
10:J:58:ARG:NH1	11:L:222:ASN:OD1	2.48	0.46
4:A:395:PRO:HD3	32:V:9:THR:HG23	1.98	0.45
4:A:2129:LEU:O	23:1:296:ARG:NH1	2.49	0.45
6:C:745:ASP:OD2	6:C:768:TYR:OH	2.34	0.45
10:J:46:ASP:OD1	10:J:46:ASP:N	2.48	0.45
18:0:58:ASP:OD1	18:0:58:ASP:N	2.50	0.45
5:B:153:ASP:OD1	5:B:153:ASP:N	2.47	0.45
6:C:358:MET:HA	6:C:461:LYS:HG3	1.98	0.45
17:M:23:CYS:HB2	19:R:197:MET:HE2	1.99	0.45
17:M:150:LEU:HD11	18:0:266:GLU:HB3	1.99	0.45
24:z:252:LEU:O	24:z:329:VAL:CA	2.53	0.45
30:p:23:LEU:HD21	31:u:71:ARG:HD3	1.98	0.45
4:A:302:PRO:HG3	14:N:4:ILE:HG23	1.99	0.45
4:A:2068:ARG:NH1	4:A:2137:ILE:O	2.49	0.45
5:B:226:THR:HG23	5:B:228:ASP:H	1.80	0.45
6:C:255:ASP:OD1	6:C:255:ASP:N	2.49	0.45
11:L:210:LYS:H	11:L:210:LYS:HG3	1.51	0.45
16:T:408:ASN:HB3	16:T:424:TRP:HB3	1.98	0.45
16:T:448:ILE:HA	16:T:464:GLU:HG3	1.98	0.45
2:5:45:C:O2	32:V:11:ARG:NH1	2.49	0.45
4:A:520:LEU:HA	6:C:423:LYS:HG2	1.99	0.45
11:L:215:LYS:N	11:L:218:GLN:OE1	2.48	0.45
17:M:291:ALA:O	17:M:295:LEU:HB2	2.17	0.45
24:z:472:GLN:HG3	24:z:477:LEU:HD13	1.99	0.45
1:2:35:G:O6	24:z:338:ARG:NH1	2.50	0.45
11:L:155:LEU:O	11:L:160:LYS:NZ	2.49	0.45
14:N:60:ARG:HH12	14:N:101:LYS:HA	1.82	0.45
14:N:101:LYS:NZ	14:N:148:ASP:O	2.43	0.45
16:T:197:PRO:HA	16:T:455:MET:HE2	1.98	0.45
17:M:298:ARG:HB3	17:M:335:PHE:HE1	1.81	0.45
18:0:181:VAL:HG23	18:0:246:VAL:HG22	1.99	0.45
26:k:11:TYR:HB3	26:k:16:LEU:HD11	1.98	0.45
29:o:14:THR:HA	29:o:28:THR:HA	1.99	0.45
15:S:2:ALA:HB1	15:S:17:GLU:HB2	1.99	0.45
27:l:26:LEU:HD11	27:l:33:TYR:HE1	1.81	0.45
31:u:44:GLN:HA	31:u:63:ILE:O	2.17	0.45
9:I:472:ARG:O	19:R:25:ARG:NH2	2.49	0.45
11:L:401:LEU:HB3	11:L:403:GLU:HG3	1.99	0.45
19:R:178:VAL:HG22	19:R:180:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:z:138:VAL:HG12	24:z:169:ARG:HB2	1.99	0.45
25:j:31:GLN:HB3	25:j:92:GLN:HB3	1.98	0.45
2:5:93:G:H4'	28:m:47:ARG:HH22	1.82	0.45
4:A:1789:ILE:HD13	4:A:1828:LEU:HB3	1.98	0.45
6:C:166:ASN:O	6:C:265:ASP:N	2.49	0.45
7:E:45:ARG:NH1	7:E:49:LEU:O	2.50	0.45
7:E:330:ALA:HB2	7:E:336:ILE:HB	1.99	0.45
17:M:23:CYS:HB3	17:M:89:LEU:HD21	1.99	0.45
24:z:239:VAL:HG22	24:z:251:ILE:HG21	1.99	0.45
27:l:25:ARG:HG2	27:l:75:TRP:CE2	2.51	0.45
2:5:93:G:N2	2:5:94:A:N7	2.57	0.45
4:A:1857:MET:HA	4:A:1860:ILE:HG22	1.99	0.45
5:B:204:TYR:OH	10:J:160:ARG:NH2	2.49	0.45
5:B:294:ILE:HG12	5:B:298:ASN:HD22	1.81	0.45
6:C:973:ASP:OD1	6:C:977:LYS:NZ	2.37	0.45
37:8:-4:Y5P:H2'	37:8:-3:P5P:H8	1.98	0.45
4:A:817:MET:HE1	4:A:833:VAL:HB	1.99	0.45
6:C:548:GLY:C	6:C:570:ARG:HE	2.24	0.45
7:E:112:SER:OG	7:E:114:ASP:OD1	2.31	0.45
24:z:31:LEU:HA	24:z:34:VAL:HG12	1.98	0.45
24:z:285:LEU:HB3	24:z:299:VAL:HG22	1.99	0.45
3:6:37:G:N2	37:8:4:Y5P:C4	2.67	0.44
4:A:501:GLU:HA	4:A:504:ALA:HB2	2.00	0.44
4:A:1371:ILE:HG21	4:A:1418:CYS:HB3	1.98	0.44
6:C:994:LEU:HD23	6:C:994:LEU:HA	1.88	0.44
16:T:401:THR:OG1	16:T:451:SER:OG	2.27	0.44
22:Y:694:ARG:O	22:Y:725:PRO:HA	2.17	0.44
23:1:43:PRO:HB3	23:1:45:TRP:CZ2	2.52	0.44
24:z:45:GLN:O	24:z:50:LYS:NZ	2.50	0.44
24:z:323:ILE:HG23	24:z:326:ILE:HG13	1.99	0.44
25:j:92:GLN:HA	26:k:59:VAL:HG12	1.98	0.44
2:5:91:U:H3	28:m:64:ASN:HD21	1.64	0.44
4:A:481:LYS:HE3	6:C:329:THR:HG23	1.97	0.44
6:C:505:ILE:HD13	6:C:517:PRO:HG2	1.98	0.44
31:u:22:LEU:HD13	31:u:73:PHE:CD2	2.53	0.44
6:C:226:ALA:HB1	6:C:579:THR:HG21	1.99	0.44
6:C:426:SER:O	6:C:430:SER:OG	2.34	0.44
14:N:65:LEU:HD23	14:N:65:LEU:HA	1.86	0.44
30:p:95:PRO:HA	30:p:96:PRO:HD3	1.86	0.44
4:A:1170:TYR:CZ	4:A:1174:ILE:HD11	2.52	0.44
7:E:69:ASP:HB2	7:E:74:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:47:ARG:HA	11:L:144:GLU:HB2	1.99	0.44
17:M:251:LEU:HD12	17:M:252:PRO:HD2	1.98	0.44
2:5:85:A:N1	27:l:45:ASN:ND2	2.65	0.44
4:A:894:VAL:HA	4:A:1376:MET:HE2	2.00	0.44
4:A:2016:LEU:HD23	4:A:2141:MET:HB3	2.00	0.44
6:C:165:ARG:NE	6:C:482:ILE:O	2.51	0.44
6:C:273:VAL:HG21	6:C:305:LEU:HD11	1.99	0.44
6:C:305:LEU:HD23	6:C:309:LEU:HD12	1.99	0.44
7:E:69:ASP:HB3	7:E:72:GLY:H	1.82	0.44
15:S:136:VAL:HG23	19:R:97:VAL:HG21	1.99	0.44
3:6:18:G:O3'	17:M:65:ARG:NH2	2.50	0.44
3:6:52:G:O2'	3:6:54:C:OP1	2.26	0.44
4:A:663:LYS:NZ	37:8:4:Y5P:OP1	2.35	0.44
24:z:644:THR:OG1	24:z:647:LYS:O	2.32	0.44
27:l:67:LEU:HB2	28:m:31:LEU:HD21	2.00	0.44
4:A:306:ILE:HD11	4:A:699:PHE:HA	2.00	0.44
17:M:139:THR:O	17:M:141:GLU:N	2.51	0.44
19:R:291:ASN:OD1	19:R:292:ASP:N	2.50	0.44
24:z:650:ILE:HG13	24:z:653:ILE:HD11	1.99	0.44
3:6:79:U:OP2	10:J:107:GLN:NE2	2.50	0.44
4:A:1766:VAL:HB	4:A:1844:GLN:HB3	2.00	0.44
6:C:960:ARG:HB2	6:C:963:GLN:HG3	2.00	0.44
11:L:397:GLU:OE1	19:R:313:ARG:NH2	2.51	0.44
15:S:54:GLN:NE2	15:S:102:GLN:OE1	2.51	0.44
16:T:181:ARG:O	16:T:470:LYS:HA	2.18	0.44
30:p:34:LEU:HB2	30:p:43:VAL:HG12	1.99	0.44
4:A:1237:ILE:HD11	4:A:1276:LEU:HB2	2.00	0.43
24:z:26:HIS:O	24:z:29:SER:HB2	2.17	0.43
5:B:145:ASP:OD1	5:B:145:ASP:N	2.48	0.43
7:E:200:ASN:HA	7:E:216:ILE:HD12	2.00	0.43
23:1:44:ILE:C	23:1:46:LYS:H	2.26	0.43
26:k:43:ASP:OD1	26:k:55:LYS:NZ	2.50	0.43
4:A:617:VAL:HG21	4:A:692:ARG:HG3	2.00	0.43
2:5:23:G:OP1	2:5:57:U:O2'	2.33	0.43
4:A:915:GLN:HG2	4:A:1151:HIS:HB3	2.00	0.43
4:A:1268:ARG:NH2	4:A:1308:ASP:HB2	2.33	0.43
16:T:235:LEU:HA	16:T:235:LEU:HD23	1.89	0.43
16:T:353:HIS:CG	16:T:381:TRP:HH2	2.37	0.43
18:0:140:LEU:HD11	18:0:201:TRP:HA	2.00	0.43
24:z:287:LEU:HA	24:z:291:LEU:HD11	2.00	0.43
23:1:22:VAL:HG21	23:1:27:PRO:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:p:43:VAL:HG23	31:u:8:PRO:HG3	2.00	0.43
4:A:1698:ILE:HG12	23:1:61:ALA:HB2	1.99	0.43
6:C:552:ARG:NH1	6:C:611:ASP:O	2.52	0.43
6:C:891:LEU:HD22	6:C:896:GLY:HA3	2.00	0.43
15:S:113:LEU:HD23	15:S:117:HIS:CD2	2.53	0.43
18:0:320:ASN:HD22	20:W:49:ALA:HB1	1.84	0.43
19:R:101:ASP:OD1	19:R:105:LYS:N	2.50	0.43
23:1:414:LEU:O	24:z:164:LYS:NZ	2.48	0.43
4:A:1239:ARG:HG2	4:A:1282:TRP:HH2	1.83	0.43
4:A:1282:TRP:O	4:A:1286:ASN:ND2	2.51	0.43
15:S:139:ASP:OD1	15:S:140:ALA:N	2.48	0.43
28:m:56:VAL:HA	28:m:67:LEU:HD23	2.01	0.43
30:p:35:ALA:HB3	30:p:43:VAL:HB	1.99	0.43
4:A:970:LEU:HD22	4:A:994:ILE:HG23	2.01	0.43
6:C:573:ASP:OD1	6:C:573:ASP:N	2.49	0.43
15:S:60:GLY:O	15:S:143:ARG:NH1	2.44	0.43
18:0:186:VAL:HG23	38:CV:100:GLY:H	1.84	0.43
24:z:163:ARG:NH2	24:z:189:ALA:O	2.52	0.43
24:z:439:GLY:O	24:z:441:LEU:N	2.51	0.43
24:z:464:MET:HB2	24:z:598:TYR:CE1	2.54	0.43
27:l:51:THR:HG21	27:l:66:VAL:HB	2.01	0.43
29:o:74:LEU:HD12	29:o:75:PRO:HD2	2.01	0.43
4:A:252:GLU:HG2	4:A:537:PRO:HG3	2.01	0.43
10:J:240:LEU:HB3	10:J:244:ALA:HB3	1.99	0.43
30:p:41:ASN:OD1	30:p:83:GLY:N	2.43	0.43
5:B:164:LYS:HA	5:B:167:LYS:HG2	2.00	0.43
7:E:154:THR:OG1	7:E:158:GLU:O	2.29	0.43
31:u:31:ARG:O	31:u:48:ILE:HA	2.19	0.43
4:A:1522:GLU:OE2	4:A:1528:ARG:NH2	2.47	0.42
5:B:322:ARG:HG3	5:B:324:THR:H	1.84	0.42
7:E:127:LEU:HD21	7:E:163:SER:HB3	2.01	0.42
11:L:195:ALA:HA	11:L:198:LYS:HG2	2.01	0.42
15:S:32:THR:HB	15:S:68:ILE:HG21	2.01	0.42
16:T:196:GLU:HG2	16:T:201:TRP:CE2	2.54	0.42
31:u:29:THR:CB	31:u:51:THR:O	2.65	0.42
4:A:427:ARG:HD3	4:A:434:TYR:HB3	2.02	0.42
4:A:1497:ARG:HG2	33:Z:362:GLN:HA	2.01	0.42
4:A:1654:ASN:N	4:A:1654:ASN:HD22	2.16	0.42
4:A:1756:ILE:HB	4:A:1789:ILE:HB	2.01	0.42
6:C:168:ALA:HB2	6:C:264:VAL:HG11	2.02	0.42
6:C:552:ARG:HG3	6:C:612:LYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:847:TRP:HD1	6:C:849:ASN:H	1.65	0.42
10:J:106:THR:HG22	10:J:136:LEU:HD13	2.01	0.42
16:T:355:LYS:HA	19:R:241:HIS:CE1	2.53	0.42
24:z:125:ARG:NH2	24:z:457:GLU:O	2.52	0.42
24:z:613:ASN:OD1	24:z:613:ASN:N	2.52	0.42
26:k:6:PRO:HG2	26:k:37:LEU:HB2	2.00	0.42
30:p:32:GLN:O	30:p:45:ALA:N	2.45	0.42
4:A:962:ASP:OD1	4:A:1048:TYR:OH	2.37	0.42
6:C:239:SER:N	31:u:14:GLU:OE2	2.46	0.42
7:E:84:ILE:O	7:E:98:VAL:HA	2.20	0.42
7:E:344:ARG:NH2	19:R:185:GLU:OE2	2.52	0.42
19:R:129:LEU:HD21	19:R:240:MET:HB3	2.02	0.42
19:R:226:LYS:HB2	19:R:226:LYS:HE2	1.84	0.42
2:5:41:U:O4	37:8:-2:P5P:N1	2.52	0.42
4:A:796:ALA:HB2	16:T:271:LEU:HD23	2.01	0.42
16:T:411:PHE:CE1	16:T:419:MET:HG2	2.55	0.42
18:0:152:ASP:OD1	18:0:156:ARG:N	2.53	0.42
4:A:1385:LYS:HE2	4:A:1389:LYS:HE3	2.01	0.42
10:J:288:GLN:HA	10:J:291:THR:HG22	2.01	0.42
3:6:10:G:O6	20:W:109:LYS:NZ	2.40	0.42
4:A:967:ILE:HG13	23:1:223:LEU:HD13	2.01	0.42
4:A:1555:SER:HB2	34:CY:349:GLU:OE2	2.20	0.42
7:E:290:ASP:OD1	7:E:290:ASP:N	2.52	0.42
11:L:20:ALA:HB3	11:L:32:VAL:HG13	2.00	0.42
16:T:364:HIS:NE2	16:T:408:ASN:OD1	2.47	0.42
18:0:282:VAL:HA	18:0:285:ILE:HB	2.01	0.42
23:1:359:ILE:HG13	23:1:362:ILE:HD12	2.02	0.42
4:A:1199:LEU:HD22	4:A:1214:LEU:HD22	2.01	0.42
6:C:243:ASN:HB3	6:C:593:PHE:CD2	2.55	0.42
6:C:977:LYS:O	6:C:981:ARG:HB2	2.19	0.42
15:S:11:MET:HE3	15:S:11:MET:HB3	1.87	0.42
23:1:131:LEU:O	24:z:613:ASN:ND2	2.38	0.42
24:z:272:SER:HA	24:z:275:LEU:HG	2.01	0.42
24:z:316:LEU:HB3	24:z:321:VAL:HG22	2.01	0.42
24:z:339:ALA:HA	24:z:396:ARG:HB2	2.02	0.42
31:u:40:ASN:OD1	31:u:42:ASN:ND2	2.53	0.42
4:A:371:LEU:HD12	6:C:930:ILE:HD11	2.02	0.42
6:C:635:LYS:HB3	6:C:705:VAL:HG13	2.01	0.42
6:C:830:ILE:HD13	6:C:861:PHE:CZ	2.54	0.42
11:L:210:LYS:HB2	11:L:210:LYS:HE3	1.73	0.42
17:M:24:GLU:H	19:R:196:GLN:HE21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:212:HIS:ND1	4:A:776:GLU:OE2	2.53	0.42
17:M:20:PRO:HB2	17:M:22:VAL:HG23	2.01	0.42
25:j:50:ASP:OD1	25:j:54:ASN:N	2.52	0.42
25:j:92:GLN:HB2	26:k:56:LEU:HD12	2.02	0.42
30:p:52:LYS:HE2	30:p:52:LYS:HB2	1.90	0.42
4:A:2021:GLN:H	4:A:2021:GLN:HG2	1.69	0.42
4:A:2054:ILE:HD12	4:A:2058:THR:HB	2.02	0.42
6:C:176:GLY:HA3	6:C:300:ASN:HD22	1.85	0.42
6:C:426:SER:O	6:C:430:SER:CB	2.68	0.42
26:k:46:GLU:HB3	26:k:54:VAL:HB	2.00	0.42
4:A:482:ASN:ND2	6:C:332:GLU:OE2	2.52	0.41
4:A:1960:LEU:O	4:A:1964:ALA:HB2	2.20	0.41
6:C:310:LYS:HB2	6:C:310:LYS:HE3	1.91	0.41
16:T:459:ARG:HG2	21:P:56:LEU:HD21	2.02	0.41
19:R:29:ARG:HA	19:R:29:ARG:HD3	1.95	0.41
27:l:48:LEU:HD22	27:l:51:THR:HG22	2.02	0.41
29:o:25:VAL:HG22	29:o:45:TYR:HD1	1.85	0.41
3:6:14:U:H5"	14:N:118:THR:HG21	2.02	0.41
4:A:960:LYS:HG3	4:A:961:HIS:CD2	2.55	0.41
4:A:1203:ASP:N	4:A:1203:ASP:OD1	2.52	0.41
6:C:435:ASP:OD1	6:C:438:ARG:NH2	2.54	0.41
6:C:887:VAL:HG11	6:C:912:VAL:HG11	2.02	0.41
7:E:229:ASN:N	7:E:229:ASN:OD1	2.52	0.41
16:T:280:HIS:HE2	16:T:327:GLN:HE21	1.66	0.41
19:R:301:LEU:HD23	19:R:301:LEU:HA	1.93	0.41
33:Z:415:LEU:HG	33:Z:416:ASN:H	1.85	0.41
6:C:793:ASP:HA	6:C:837:LEU:HB2	2.03	0.41
10:J:190:GLU:OE2	10:J:194:GLN:NE2	2.45	0.41
24:z:240:PHE:CZ	24:z:271:ARG:HB3	2.56	0.41
24:z:292:SER:OG	24:z:295:GLN:OE1	2.39	0.41
24:z:588:GLU:HA	24:z:591:GLN:HG2	2.00	0.41
28:m:98:PHE:HB3	29:o:68:TYR:HB2	2.03	0.41
4:A:1903:THR:HB	4:A:1985:PRO:HA	2.03	0.41
10:J:173:GLU:OE2	10:J:207:ARG:NH2	2.53	0.41
11:L:51:TRP:CE2	11:L:147:PRO:HA	2.55	0.41
18:0:193:ILE:HG22	18:0:196:ARG:HH22	1.85	0.41
4:A:1225:PHE:HE1	4:A:1312:LEU:HD21	1.85	0.41
4:A:1481:ARG:HH12	4:A:1485:SER:H	1.69	0.41
6:C:216:GLU:HG2	6:C:222:SER:HA	2.02	0.41
6:C:492:LYS:HB2	6:C:492:LYS:HE2	1.86	0.41
6:C:540:VAL:HG12	6:C:590:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:575:PHE:HB2	6:C:595:LEU:HB3	2.02	0.41
11:L:47:ARG:NH2	11:L:147:PRO:O	2.53	0.41
16:T:245:PHE:CZ	16:T:300:MET:HE3	2.56	0.41
31:u:22:LEU:HD11	31:u:70:VAL:HB	2.02	0.41
31:u:27:GLY:HA2	31:u:53:ARG:NH1	2.35	0.41
4:A:399:ASP:OD1	4:A:400:ILE:N	2.53	0.41
4:A:718:MET:HG2	4:A:725:LEU:HD11	2.02	0.41
5:B:211:ALA:HA	5:B:214:LYS:HG2	2.03	0.41
15:S:46:ARG:HG2	15:S:142:ASP:HB2	2.03	0.41
16:T:339:MET:O	16:T:348:MET:N	2.52	0.41
18:0:194:VAL:HG13	18:0:198:PHE:HD2	1.85	0.41
23:1:401:LYS:HG2	24:z:565:ARG:HD2	2.03	0.41
25:j:54:ASN:HB3	25:j:82:LEU:HD11	2.02	0.41
2:5:111:C:H2'	2:5:112:A:C8	2.55	0.41
4:A:974:ARG:HD3	4:A:994:ILE:HG21	2.01	0.41
4:A:1217:ARG:HG3	4:A:1222:ILE:HG22	2.02	0.41
7:E:118:LEU:HB2	7:E:132:LEU:HD11	2.02	0.41
23:1:356:ASP:HB3	23:1:359:ILE:HG22	2.02	0.41
24:z:223:TYR:OH	24:z:376:ARG:NH1	2.48	0.41
24:z:474:PHE:CE2	24:z:592:ARG:HD2	2.56	0.41
24:z:570:VAL:HG12	24:z:572:GLU:HG2	2.03	0.41
5:B:325:MET:HG3	11:L:57:LYS:HD3	2.03	0.41
6:C:172:HIS:O	6:C:177:LYS:NZ	2.54	0.41
6:C:254:VAL:O	6:C:257:VAL:HB	2.20	0.41
7:E:95:ASN:HD22	7:E:96:TYR:N	2.19	0.41
17:M:139:THR:OG1	17:M:140:ASP:N	2.54	0.41
17:M:269:LEU:HD13	17:M:280:VAL:HG22	2.02	0.41
23:1:201:VAL:HG13	24:z:424:PRO:HG3	2.02	0.41
4:A:190:ASP:OD1	4:A:190:ASP:N	2.50	0.41
4:A:540:ARG:HA	4:A:540:ARG:HD3	1.96	0.41
6:C:291:GLU:OE1	6:C:496:TYR:OH	2.31	0.41
11:L:179:LYS:HB3	11:L:183:ARG:HH12	1.86	0.41
15:S:75:ASP:HB3	15:S:77:ILE:HD12	2.02	0.41
15:S:92:ALA:HB1	20:W:47:GLY:HA2	2.03	0.41
16:T:301:ARG:HG3	21:P:34:LEU:HG	2.03	0.41
18:0:192:GLU:OE1	18:0:196:ARG:NH2	2.54	0.41
19:R:176:LYS:O	19:R:178:VAL:N	2.54	0.41
19:R:291:ASN:HD21	19:R:293:LYS:HD3	1.86	0.41
23:1:406:ASP:OD1	23:1:406:ASP:N	2.52	0.41
24:z:221:ILE:HA	24:z:374:CYS:HB3	2.03	0.41
25:j:46:ILE:HA	25:j:57:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:j:47:ARG:HB3	25:j:56:VAL:HG12	2.02	0.41
4:A:451:ILE:HD13	4:A:451:ILE:HA	1.94	0.41
7:E:53:LEU:HD21	7:E:347:LEU:HD22	2.02	0.41
16:T:278:LYS:HA	16:T:278:LYS:HD3	1.91	0.41
18:0:91:LEU:HB3	18:0:92:SER:H	1.69	0.41
23:1:163:MET:HE1	24:z:415:LEU:HB3	2.03	0.41
25:j:50:ASP:OD1	25:j:50:ASP:N	2.54	0.41
25:j:84:LYS:HZ2	27:l:73:VAL:HB	1.84	0.41
2:5:104:G:H1	2:5:110:C:H42	1.68	0.40
4:A:281:PHE:HD1	4:A:683:LEU:HD22	1.86	0.40
4:A:549:GLN:O	4:A:762:ARG:NE	2.54	0.40
4:A:605:GLN:HB3	19:R:182:THR:HG21	2.03	0.40
5:B:166:MET:HE3	5:B:166:MET:HB3	1.83	0.40
16:T:320:VAL:HG22	16:T:329:ILE:HB	2.03	0.40
17:M:31:PRO:HD2	20:W:94:VAL:HG11	2.04	0.40
17:M:242:LEU:HB2	17:M:280:VAL:HB	2.03	0.40
17:M:323:GLU:O	17:M:327:MET:HG2	2.21	0.40
24:z:225:ASP:OD1	24:z:225:ASP:N	2.54	0.40
24:z:344:THR:OG1	24:z:345:GLY:N	2.54	0.40
24:z:656:ILE:HD12	24:z:661:LEU:HD21	2.03	0.40
30:p:56:MET:HE1	30:p:67:THR:HG23	2.03	0.40
4:A:1654:ASN:HD21	23:1:275:LEU:HD12	1.87	0.40
6:C:169:LEU:HD23	6:C:268:CYS:HB2	2.02	0.40
6:C:872:MET:HB3	6:C:915:LEU:HD12	2.02	0.40
15:S:77:ILE:HG12	15:S:115:GLY:HA2	2.03	0.40
18:0:86:ARG:HD2	37:8:8:Y5P:H2'	2.02	0.40
23:1:195:LEU:HD23	23:1:195:LEU:HA	1.93	0.40
27:l:21:ASP:HA	27:l:36:ARG:HE	1.85	0.40
33:Z:369:GLU:HG2	33:Z:373:LYS:HE2	2.01	0.40
4:A:279:MET:HE1	4:A:687:ALA:HA	2.04	0.40
5:B:293:TYR:HB3	5:B:302:ASN:HD22	1.86	0.40
6:C:497:TYR:CZ	6:C:509:MET:HE1	2.57	0.40
24:z:509:ARG:HE	24:z:509:ARG:HB3	1.66	0.40
25:j:38:LEU:HD22	26:k:24:ARG:HD2	2.03	0.40
3:6:36:A:C2	37:8:5:P5P:C2	3.04	0.40
4:A:1023:ILE:HG23	4:A:1146:TYR:HB2	2.03	0.40
6:C:355:CYS:HB3	6:C:360:TRP:CE2	2.57	0.40
6:C:560:LEU:HD23	6:C:560:LEU:HA	1.91	0.40
7:E:107:LEU:O	7:E:284:ARG:NH1	2.50	0.40
15:S:111:PRO:HG2	18:0:302:TYR:HB2	2.03	0.40
16:T:454:ASP:OD1	16:T:457:GLY:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1:31:LEU:HG	24:z:509:ARG:HH11	1.85	0.40
24:z:585:ASN:O	24:z:589:LYS:HB2	2.21	0.40
29:o:19:LEU:O	29:o:66:ARG:NH1	2.55	0.40
31:u:54:ASP:OD1	31:u:54:ASP:N	2.50	0.40
4:A:1065:ASN:OD1	4:A:1065:ASN:N	2.55	0.40
4:A:1904:GLN:HG2	4:A:1987:GLN:HB3	2.03	0.40
4:A:1988:LEU:N	4:A:2010:SER:O	2.48	0.40
4:A:2139:LEU:HD11	23:1:144:LEU:HD22	2.04	0.40
6:C:729:ASN:HA	6:C:844:PRO:HD2	2.04	0.40
6:C:779:TRP:NE1	6:C:793:ASP:HB2	2.36	0.40
16:T:182:VAL:CA	16:T:469:ILE:O	2.66	0.40
16:T:442:LEU:HB2	16:T:445:GLU:HG3	2.04	0.40
23:1:165:TRP:HB2	24:z:415:LEU:HD22	2.03	0.40
24:z:547:LYS:HB2	24:z:547:LYS:HE2	1.90	0.40
31:u:21:THR:HA	31:u:30:TYR:O	2.21	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	
4	A	1984/2463 (81%)	1915 (96%)	67 (3%)	2 (0%)	48	77
5	B	256/326 (78%)	247 (96%)	9 (4%)	0	100	100
6	C	920/1011 (91%)	891 (97%)	27 (3%)	2 (0%)	43	72
7	E	308/352 (88%)	292 (95%)	16 (5%)	0	100	100
8	F	108/233 (46%)	105 (97%)	3 (3%)	0	100	100
9	I	722/839 (86%)	712 (99%)	10 (1%)	0	100	100
10	J	604/687 (88%)	595 (98%)	9 (2%)	0	100	100
11	L	603/768 (78%)	593 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	229/231 (99%)	229 (100%)	0	0	100	100
13	q	137/480 (28%)	136 (99%)	1 (1%)	0	100	100
13	r	141/480 (29%)	141 (100%)	0	0	100	100
13	s	138/480 (29%)	137 (99%)	1 (1%)	0	100	100
13	t	139/480 (29%)	139 (100%)	0	0	100	100
14	N	146/148 (99%)	141 (97%)	4 (3%)	1 (1%)	18	48
15	S	155/167 (93%)	141 (91%)	13 (8%)	1 (1%)	21	51
16	T	337/496 (68%)	323 (96%)	14 (4%)	0	100	100
17	M	242/395 (61%)	232 (96%)	9 (4%)	1 (0%)	30	59
18	0	275/408 (67%)	251 (91%)	24 (9%)	0	100	100
19	R	335/578 (58%)	318 (95%)	17 (5%)	0	100	100
20	W	90/547 (16%)	86 (96%)	3 (3%)	1 (1%)	11	36
21	P	90/260 (35%)	89 (99%)	1 (1%)	0	100	100
22	Y	1329/1416 (94%)	1320 (99%)	9 (1%)	0	100	100
23	1	317/698 (45%)	300 (95%)	14 (4%)	3 (1%)	14	41
24	z	653/672 (97%)	619 (95%)	33 (5%)	1 (0%)	43	72
25	j	86/98 (88%)	85 (99%)	1 (1%)	0	100	100
26	k	71/82 (87%)	70 (99%)	1 (1%)	0	100	100
27	l	79/94 (84%)	79 (100%)	0	0	100	100
28	m	84/592 (14%)	83 (99%)	1 (1%)	0	100	100
29	o	85/118 (72%)	80 (94%)	5 (6%)	0	100	100
30	p	99/211 (47%)	94 (95%)	5 (5%)	0	100	100
31	u	88/114 (77%)	83 (94%)	3 (3%)	2 (2%)	5	19
32	V	78/223 (35%)	72 (92%)	6 (8%)	0	100	100
33	Z	209/678 (31%)	200 (96%)	9 (4%)	0	100	100
34	CY	23/510 (4%)	23 (100%)	0	0	100	100
38	CV	66/246 (27%)	66 (100%)	0	0	100	100
All	All	11226/17581 (64%)	10887 (97%)	325 (3%)	14 (0%)	49	77

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	C	840	VAL

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Mol	Chain	Res	Type
17	M	140	ASP
20	W	101	VAL
23	1	43	PRO
23	1	297	VAL
4	A	1219	ILE
15	S	156	VAL
23	1	278	THR
4	A	1402	ARG
6	C	846	TRP
14	N	6	PRO
24	z	450	PRO
31	u	62	GLN
31	u	48	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1796/2212 (81%)	1796 (100%)	0	100	100
5	B	150/270 (56%)	150 (100%)	0	100	100
6	C	809/884 (92%)	809 (100%)	0	100	100
7	E	254/287 (88%)	254 (100%)	0	100	100
10	J	244/592 (41%)	244 (100%)	0	100	100
11	L	281/635 (44%)	280 (100%)	1 (0%)	84	94
14	N	131/131 (100%)	129 (98%)	2 (2%)	57	84
15	S	126/135 (93%)	125 (99%)	1 (1%)	73	90
16	T	286/408 (70%)	286 (100%)	0	100	100
17	M	210/293 (72%)	210 (100%)	0	100	100
18	0	228/335 (68%)	224 (98%)	4 (2%)	51	80
19	R	279/478 (58%)	279 (100%)	0	100	100
20	W	73/459 (16%)	73 (100%)	0	100	100
21	P	76/213 (36%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	1	266/564 (47%)	263 (99%)	3 (1%)	65	88
24	z	559/571 (98%)	559 (100%)	0	100	100
25	j	79/85 (93%)	79 (100%)	0	100	100
26	k	64/71 (90%)	64 (100%)	0	100	100
27	l	72/84 (86%)	72 (100%)	0	100	100
28	m	77/497 (16%)	77 (100%)	0	100	100
29	o	78/95 (82%)	78 (100%)	0	100	100
30	p	84/152 (55%)	84 (100%)	0	100	100
31	u	80/94 (85%)	80 (100%)	0	100	100
32	V	22/197 (11%)	22 (100%)	0	100	100
33	Z	182/575 (32%)	182 (100%)	0	100	100
34	CY	17/418 (4%)	17 (100%)	0	100	100
All	All	6523/10735 (61%)	6512 (100%)	11 (0%)	85	96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	L	210	LYS
14	N	40	ASP
14	N	41	ASN
15	S	78	HIS
18	0	210	LEU
18	0	212	ASN
18	0	213	ARG
18	0	250	THR
23	1	42	VAL
23	1	43	PRO
23	1	44	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	147	GLN
4	A	156	GLN
4	A	296	ASN
4	A	343	ASN
4	A	420	ASN

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Mol	Chain	Res	Type
4	A	471	ASN
4	A	597	GLN
4	A	605	GLN
4	A	987	GLN
4	A	1033	ASN
4	A	1088	ASN
4	A	1121	ASN
4	A	1141	ASN
4	A	1183	GLN
4	A	1527	ASN
4	A	1654	ASN
4	A	1679	GLN
4	A	1713	HIS
4	A	1726	GLN
4	A	1864	ASN
4	A	1918	HIS
5	B	298	ASN
5	B	302	ASN
6	C	106	GLN
6	C	126	GLN
6	C	322	HIS
6	C	394	ASN
6	C	514	GLN
6	C	592	ASN
6	C	601	ASN
6	C	628	HIS
6	C	913	ASN
7	E	95	ASN
10	J	104	ASN
10	J	119	ASN
10	J	276	ASN
11	L	49	ASN
11	L	382	ASN
14	N	29	ASN
14	N	57	GLN
14	N	127	GLN
15	S	20	ASN
16	T	220	GLN
16	T	266	HIS
16	T	305	ASN
16	T	327	GLN
18	O	240	HIS

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Mol	Chain	Res	Type
18	0	245	ASN
18	0	254	ASN
19	R	28	GLN
19	R	196	GLN
19	R	314	GLN
21	P	25	GLN
21	P	228	GLN
23	1	47	GLN
23	1	276	ASN
24	z	53	GLN
24	z	56	GLN
24	z	178	GLN
24	z	193	GLN
24	z	263	GLN
24	z	405	GLN
24	z	427	GLN
25	j	92	GLN
28	m	62	HIS
28	m	64	ASN
30	p	39	HIS
31	u	18	HIS
33	Z	444	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	36/193 (18%)	11 (30%)	1 (2%)
2	5	109/116 (93%)	26 (23%)	1 (0%)
3	6	91/101 (90%)	30 (32%)	1 (1%)
37	8	22/25 (88%)	10 (45%)	0
All	All	258/435 (59%)	77 (29%)	3 (1%)

All (77) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	13	C
1	2	14	U
1	2	15	U
1	2	16	U
1	2	17	U
1	2	18	G

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Mol	Chain	Res	Type
1	2	23	A
1	2	28	A
1	2	30	G
1	2	35	G
1	2	37	A
2	5	2	U
2	5	6	G
2	5	8	A
2	5	19	G
2	5	20	A
2	5	21	C
2	5	22	C
2	5	23	G
2	5	24	A
2	5	33	C
2	5	39	U
2	5	41	U
2	5	42	U
2	5	44	C
2	5	50	G
2	5	52	G
2	5	53	A
2	5	56	G
2	5	70	A
2	5	71	A
2	5	87	U
2	5	88	C
2	5	92	G
2	5	93	G
2	5	94	A
2	5	106	U
3	6	6	U
3	6	7	C
3	6	9	G
3	6	18	G
3	6	20	C
3	6	21	A
3	6	23	U
3	6	24	U
3	6	26	G
3	6	28	A
3	6	32	A

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Mol	Chain	Res	Type
3	6	37	G
3	6	39	G
3	6	41	A
3	6	42	G
3	6	45	U
3	6	47	G
3	6	61	C
3	6	62	U
3	6	63	A
3	6	68	U
3	6	72	A
3	6	74	G
3	6	75	C
3	6	80	C
3	6	81	A
3	6	84	G
3	6	85	A
3	6	88	C
3	6	89	G
37	8	-6	P5P
37	8	-5	Y5P
37	8	0	P5P
37	8	1	P5P
37	8	2	Y5P
37	8	3	P5P
37	8	7	P5P
37	8	12	Y5P
37	8	13	Y5P
37	8	14	Y5P

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	13	C
2	5	70	A
3	6	83	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
37	Y5P	8	10	37	14,19,20	4.21	2 (14%)	18,26,29	1.03	1 (5%)
37	P5P	8	-8	37	20,23,24	0.42	0	27,33,36	0.69	1 (3%)
37	Y5P	8	-4	37	14,19,20	4.51	2 (14%)	18,26,29	1.39	2 (11%)
37	P5P	8	-10	37	20,23,24	0.43	0	27,33,36	0.78	1 (3%)
37	P5P	8	0	37	20,23,24	0.98	2 (10%)	27,33,36	1.95	4 (14%)
37	P5P	8	-9	37	20,23,24	0.42	0	27,33,36	0.76	1 (3%)
37	Y5P	8	8	37	14,19,20	4.52	2 (14%)	18,26,29	1.36	2 (11%)
37	Y5P	8	6	37	14,19,20	4.18	2 (14%)	18,26,29	1.05	1 (5%)
37	Y5P	8	13	37	14,19,20	4.22	2 (14%)	18,26,29	1.21	2 (11%)
37	P5P	8	5	37	20,23,24	0.96	2 (10%)	27,33,36	1.96	4 (14%)
37	Y5P	8	4	37	14,19,20	4.20	2 (14%)	18,26,29	1.12	1 (5%)
37	Y5P	8	14	37	14,19,20	4.17	2 (14%)	18,26,29	1.05	1 (5%)
37	P5P	8	-2	2,37	20,23,24	0.46	0	27,33,36	0.79	1 (3%)
37	Y5P	8	12	37	14,19,20	4.20	2 (14%)	18,26,29	1.08	1 (5%)
37	P5P	8	-1	2,37	20,23,24	0.98	2 (10%)	27,33,36	1.90	4 (14%)
37	Y5P	8	-7	37	14,19,20	4.50	2 (14%)	18,26,29	1.38	2 (11%)
37	P5P	8	-3	2,37	20,23,24	0.43	0	27,33,36	0.74	1 (3%)
37	Y5P	8	-5	37	14,19,20	4.54	2 (14%)	18,26,29	1.55	3 (16%)
37	P5P	8	1	37	20,23,24	0.97	2 (10%)	27,33,36	2.01	4 (14%)
37	P5P	8	7	37,3	20,23,24	0.94	2 (10%)	27,33,36	1.91	4 (14%)
37	P5P	8	3	37,3	20,23,24	0.44	0	27,33,36	0.71	1 (3%)
37	P5P	8	-6	37	20,23,24	0.95	2 (10%)	27,33,36	1.93	4 (14%)
37	Y5P	8	11	37	14,19,20	4.22	2 (14%)	18,26,29	1.05	1 (5%)
37	Y5P	8	2	37	14,19,20	4.19	2 (14%)	18,26,29	1.01	1 (5%)

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
37	Y5P	8	10	37	-	1/7/33/34	0/2/2/2
37	P5P	8	-8	37	-	0/7/25/26	0/3/3/3
37	Y5P	8	-4	37	-	3/7/33/34	0/2/2/2
37	P5P	8	-10	37	-	1/7/25/26	0/3/3/3
37	P5P	8	0	37	-	4/7/25/26	0/3/3/3
37	P5P	8	-9	37	-	0/7/25/26	0/3/3/3
37	Y5P	8	8	37	-	1/7/33/34	0/2/2/2
37	Y5P	8	6	37	-	1/7/33/34	0/2/2/2
37	Y5P	8	13	37	-	4/7/33/34	0/2/2/2
37	P5P	8	5	37	-	0/7/25/26	0/3/3/3
37	Y5P	8	4	37	-	1/7/33/34	0/2/2/2
37	Y5P	8	14	37	-	2/7/33/34	0/2/2/2
37	P5P	8	-2	2,37	-	0/7/25/26	0/3/3/3
37	Y5P	8	12	37	-	1/7/33/34	0/2/2/2
37	P5P	8	-1	2,37	-	2/7/25/26	0/3/3/3
37	Y5P	8	-7	37	-	1/7/33/34	0/2/2/2
37	P5P	8	-3	2,37	-	0/7/25/26	0/3/3/3
37	Y5P	8	-5	37	-	6/7/33/34	0/2/2/2
37	P5P	8	1	37	-	5/7/25/26	0/3/3/3
37	P5P	8	7	37,3	-	1/7/25/26	0/3/3/3
37	P5P	8	3	37,3	-	0/7/25/26	0/3/3/3
37	P5P	8	-6	37	-	2/7/25/26	0/3/3/3
37	Y5P	8	11	37	-	3/7/33/34	0/2/2/2
37	Y5P	8	2	37	-	4/7/33/34	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	8	-5	Y5P	C4-N3	-13.32	1.33	1.46
37	8	-4	Y5P	C4-N3	-13.23	1.33	1.46
37	8	11	Y5P	C2-N3	13.19	1.37	1.27
37	8	13	Y5P	C2-N3	13.17	1.37	1.27
37	8	2	Y5P	C2-N3	13.14	1.37	1.27
37	8	8	Y5P	C4-N3	-13.10	1.33	1.46
37	8	12	Y5P	C2-N3	13.10	1.37	1.27
37	8	10	Y5P	C2-N3	13.09	1.37	1.27
37	8	4	Y5P	C2-N3	13.07	1.37	1.27
37	8	14	Y5P	C2-N3	13.06	1.37	1.27
37	8	6	Y5P	C2-N3	13.04	1.37	1.27
37	8	-7	Y5P	C4-N3	-13.04	1.34	1.46
37	8	8	Y5P	C2-N3	10.63	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	8	-7	Y5P	C2-N3	10.61	1.35	1.27
37	8	-5	Y5P	C2-N3	10.46	1.35	1.27
37	8	-4	Y5P	C2-N3	10.39	1.35	1.27
37	8	10	Y5P	C4-N3	-8.71	1.38	1.46
37	8	12	Y5P	C4-N3	-8.63	1.38	1.46
37	8	4	Y5P	C4-N3	-8.62	1.38	1.46
37	8	13	Y5P	C4-N3	-8.61	1.38	1.46
37	8	11	Y5P	C4-N3	-8.61	1.38	1.46
37	8	6	Y5P	C4-N3	-8.60	1.38	1.46
37	8	2	Y5P	C4-N3	-8.51	1.38	1.46
37	8	14	Y5P	C4-N3	-8.46	1.38	1.46
37	8	-1	P5P	C6-N1	2.67	1.39	1.34
37	8	0	P5P	C6-N1	2.65	1.39	1.34
37	8	-6	P5P	C6-N1	2.62	1.39	1.34
37	8	1	P5P	C6-N1	2.61	1.39	1.34
37	8	7	P5P	C6-N1	2.61	1.39	1.34
37	8	5	P5P	C6-N1	2.58	1.39	1.34
37	8	5	P5P	C2-N1	2.17	1.37	1.33
37	8	0	P5P	C2-N1	2.17	1.37	1.33
37	8	-1	P5P	C2-N1	2.15	1.37	1.33
37	8	-6	P5P	C2-N1	2.13	1.37	1.33
37	8	1	P5P	C2-N1	2.12	1.37	1.33
37	8	7	P5P	C2-N1	2.09	1.37	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	8	5	P5P	C6-N1-C2	8.01	125.26	115.80
37	8	-6	P5P	C6-N1-C2	7.93	125.16	115.80
37	8	7	P5P	C6-N1-C2	7.88	125.10	115.80
37	8	1	P5P	C6-N1-C2	7.83	125.05	115.80
37	8	-1	P5P	C6-N1-C2	7.75	124.94	115.80
37	8	0	P5P	C6-N1-C2	7.73	124.92	115.80
37	8	-4	Y5P	C5-C4-N3	4.84	121.95	114.15
37	8	8	Y5P	C5-C4-N3	4.83	121.94	114.15
37	8	-5	Y5P	C5-C4-N3	4.82	121.93	114.15
37	8	-7	Y5P	C5-C4-N3	4.82	121.92	114.15
37	8	-6	P5P	C5-C6-N1	-4.24	111.33	121.90
37	8	5	P5P	C5-C6-N1	-4.20	111.43	121.90
37	8	1	P5P	C5-C6-N1	-4.16	111.54	121.90
37	8	7	P5P	C5-C6-N1	-4.15	111.57	121.90
37	8	-1	P5P	C5-C6-N1	-4.14	111.59	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	8	0	P5P	C5-C6-N1	-4.13	111.60	121.90
37	8	13	Y5P	N1-C2-N3	-3.84	114.73	125.39
37	8	11	Y5P	N1-C2-N3	-3.84	114.75	125.39
37	8	12	Y5P	N1-C2-N3	-3.84	114.75	125.39
37	8	4	Y5P	N1-C2-N3	-3.83	114.78	125.39
37	8	2	Y5P	N1-C2-N3	-3.82	114.79	125.39
37	8	10	Y5P	N1-C2-N3	-3.82	114.80	125.39
37	8	6	Y5P	N1-C2-N3	-3.82	114.81	125.39
37	8	14	Y5P	N1-C2-N3	-3.81	114.83	125.39
37	8	0	P5P	C6-C5-C4	3.26	119.80	116.24
37	8	1	P5P	C6-C5-C4	3.16	119.69	116.24
37	8	-6	P5P	C6-C5-C4	3.04	119.56	116.24
37	8	7	P5P	C6-C5-C4	2.98	119.50	116.24
37	8	5	P5P	C6-C5-C4	2.83	119.33	116.24
37	8	-1	P5P	C6-C5-C4	2.64	119.12	116.24
37	8	-3	P5P	C6-N1-C2	2.43	118.67	115.80
37	8	-2	P5P	C6-N1-C2	2.41	118.64	115.80
37	8	-8	P5P	C6-N1-C2	2.37	118.60	115.80
37	8	-10	P5P	C6-N1-C2	2.33	118.55	115.80
37	8	-9	P5P	C6-N1-C2	2.32	118.54	115.80
37	8	3	P5P	C6-N1-C2	2.30	118.52	115.80
37	8	-5	Y5P	O3'-C3'-C4'	-2.28	104.53	111.08
37	8	7	P5P	N1-C2-N3	-2.24	123.53	127.33
37	8	-7	Y5P	N1-C2-N3	-2.23	119.22	125.39
37	8	5	P5P	N1-C2-N3	-2.22	123.55	127.33
37	8	8	Y5P	N1-C2-N3	-2.21	119.27	125.39
37	8	-4	Y5P	N1-C2-N3	-2.20	119.29	125.39
37	8	-5	Y5P	N1-C2-N3	-2.19	119.31	125.39
37	8	0	P5P	N1-C2-N3	-2.17	123.64	127.33
37	8	1	P5P	N1-C2-N3	-2.17	123.64	127.33
37	8	-1	P5P	N1-C2-N3	-2.14	123.70	127.33
37	8	-6	P5P	N1-C2-N3	-2.11	123.75	127.33
37	8	13	Y5P	O3'-C3'-C4'	2.08	117.04	111.08

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	8	1	P5P	O4'-C4'-C5'-O5'
37	8	2	Y5P	C3'-C4'-C5'-O5'
37	8	6	Y5P	O4'-C1'-N1-C2
37	8	-7	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
37	8	-4	Y5P	O4'-C1'-N1-C2
37	8	4	Y5P	O4'-C1'-N1-C2
37	8	8	Y5P	O4'-C1'-N1-C2
37	8	10	Y5P	O4'-C1'-N1-C2
37	8	13	Y5P	O4'-C1'-N1-C2
37	8	-4	Y5P	C3'-C4'-C5'-O5'
37	8	2	Y5P	O4'-C4'-C5'-O5'
37	8	-6	P5P	O4'-C4'-C5'-O5'
37	8	-5	Y5P	O4'-C4'-C5'-O5'
37	8	11	Y5P	O4'-C4'-C5'-O5'
37	8	13	Y5P	C3'-C4'-C5'-O5'
37	8	0	P5P	O4'-C1'-N9-C4
37	8	-6	P5P	C3'-C4'-C5'-O5'
37	8	1	P5P	C3'-C4'-C5'-O5'
37	8	13	Y5P	O4'-C4'-C5'-O5'
37	8	-5	Y5P	C3'-C4'-C5'-O5'
37	8	11	Y5P	O4'-C1'-N1-C2
37	8	-4	Y5P	O4'-C4'-C5'-O5'
37	8	0	P5P	O4'-C4'-C5'-O5'
37	8	11	Y5P	C3'-C4'-C5'-O5'
37	8	2	Y5P	O4'-C1'-N1-C2
37	8	1	P5P	O4'-C1'-N9-C8
37	8	14	Y5P	O4'-C1'-N1-C2
37	8	-1	P5P	O4'-C4'-C5'-O5'
37	8	0	P5P	C3'-C4'-C5'-O5'
37	8	1	P5P	O4'-C1'-N9-C4
37	8	0	P5P	O4'-C1'-N9-C8
37	8	-5	Y5P	C2'-C1'-N1-C2
37	8	2	Y5P	C4'-C5'-O5'-P
37	8	-5	Y5P	O4'-C1'-N1-C2
37	8	12	Y5P	O4'-C1'-N1-C2
37	8	1	P5P	C4'-C5'-O5'-P
37	8	-10	P5P	C4'-C5'-O5'-P
37	8	-5	Y5P	C2'-C1'-N1-C6
37	8	-5	Y5P	O4'-C1'-N1-C6
37	8	7	P5P	C4'-C5'-O5'-P
37	8	14	Y5P	C4'-C5'-O5'-P
37	8	13	Y5P	C4'-C5'-O5'-P
37	8	-1	P5P	C3'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	8	-8	P5P	4	0
37	8	-4	Y5P	1	0
37	8	-10	P5P	1	0
37	8	8	Y5P	5	0
37	8	5	P5P	4	0
37	8	4	Y5P	7	0
37	8	-2	P5P	3	0
37	8	-3	P5P	1	0
37	8	-5	Y5P	1	0
37	8	1	P5P	2	0
37	8	7	P5P	2	0
37	8	3	P5P	8	0
37	8	2	Y5P	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	M7M	B	401	-	28,32,33	4.33	17 (60%)	31,49,52	1.23	3 (9%)
41	GTP	C	1102	40	33,34,34	0.96	1 (3%)	50,54,54	1.63	9 (18%)

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
39	M7M	B	401	-	-	3/17/47/48	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	C	1102	40	-	4/22/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	401	M7M	CBI-NBP	8.63	1.51	1.45
39	B	401	M7M	CBG-NBH	7.72	1.45	1.35
39	B	401	M7M	OBR-CBS	7.50	1.61	1.45
39	B	401	M7M	CBY-CBS	-7.04	1.35	1.53
39	B	401	M7M	CBO-NBP	6.71	1.46	1.35
39	B	401	M7M	CBM-NBV	6.41	1.46	1.35
39	B	401	M7M	CBO-NBN	6.26	1.48	1.37
39	B	401	M7M	CBM-NBE	5.98	1.46	1.32
39	B	401	M7M	CBM-NBN	5.39	1.49	1.36
39	B	401	M7M	OBR-CBQ	-5.03	1.30	1.42
39	B	401	M7M	CBF-NBE	3.80	1.44	1.38
39	B	401	M7M	CBG-CBO	3.25	1.44	1.36
39	B	401	M7M	OCB-CBY	3.19	1.50	1.43
39	B	401	M7M	OCA-CBX	-2.85	1.35	1.43
39	B	401	M7M	OBB-CBF	-2.52	1.19	1.23
39	B	401	M7M	PBK-OBV	2.23	1.68	1.59
39	B	401	M7M	CBI-NBH	2.17	1.52	1.42
41	C	1102	GTP	C2-N3	2.03	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	C	1102	GTP	C5-C4-N3	-4.89	120.61	128.39
41	C	1102	GTP	C2-N3-C4	4.61	120.24	112.30
39	B	401	M7M	CBO-CBG-NBH	3.89	109.72	106.86
41	C	1102	GTP	N9-C4-N3	3.04	132.03	125.95
41	C	1102	GTP	C2-N1-C6	-2.85	119.94	125.11
39	B	401	M7M	NBP-CBI-NBH	2.78	107.31	103.37
39	B	401	M7M	CBY-CBX-CBQ	2.72	106.61	101.46
41	C	1102	GTP	N9-C8-N7	-2.70	108.39	113.40
41	C	1102	GTP	C8-N7-C5	2.50	108.71	104.26
41	C	1102	GTP	C5-C6-N1	2.49	119.60	113.25
41	C	1102	GTP	O6-C6-C5	-2.39	120.21	126.53
41	C	1102	GTP	O2A-PA-O3A	2.09	112.93	107.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

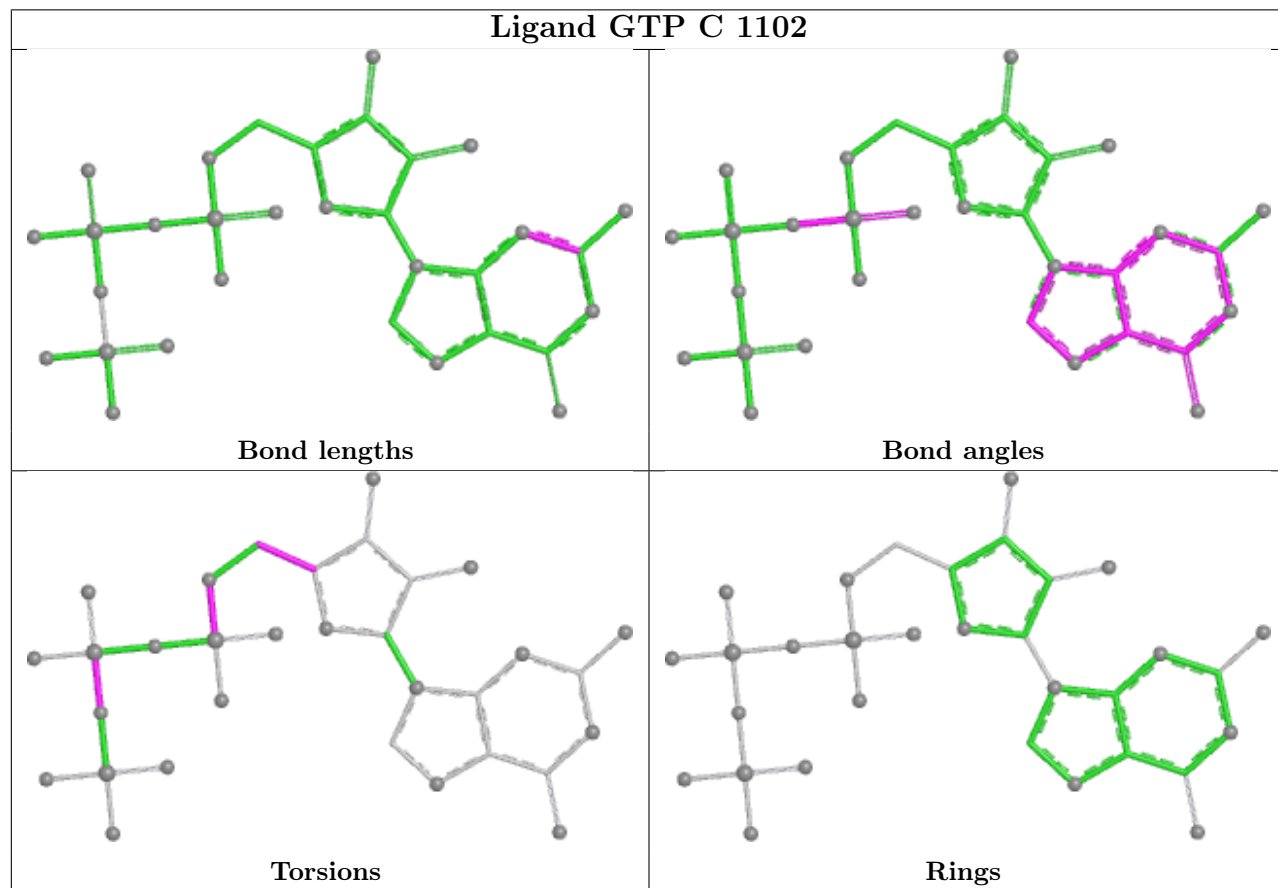
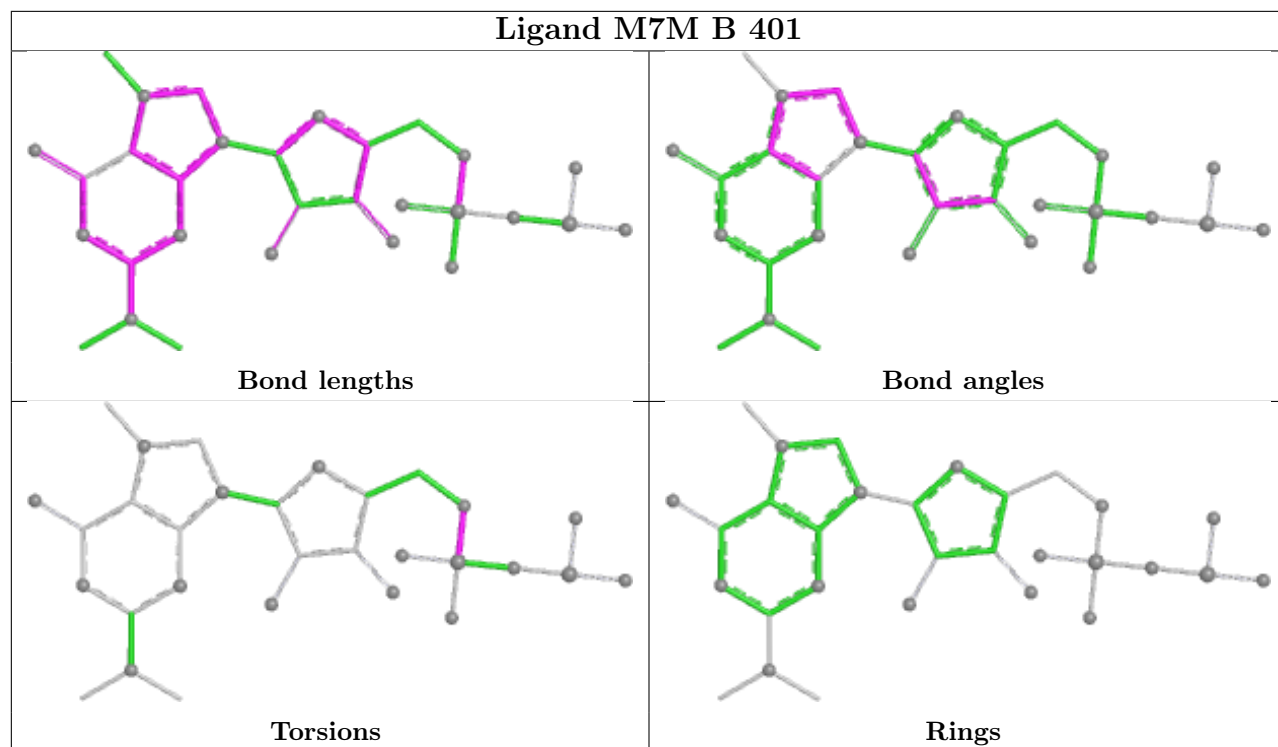
Mol	Chain	Res	Type	Atoms
39	B	401	M7M	CBT-OBU-PBK-OB
41	C	1102	GTP	C5'-O5'-PA-O1A
39	B	401	M7M	CBT-OBU-PBK-OB
39	B	401	M7M	CBT-OBU-PBK-OB
41	C	1102	GTP	PG-O3B-PB-O1B
41	C	1102	GTP	O4'-C4'-C5'-O5'
41	C	1102	GTP	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	B	401	M7M	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

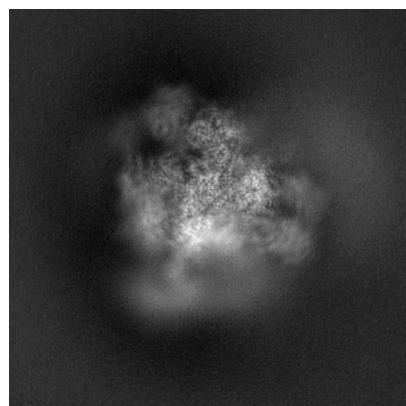
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62842. These allow visual inspection of the internal detail of the map and identification of artifacts.

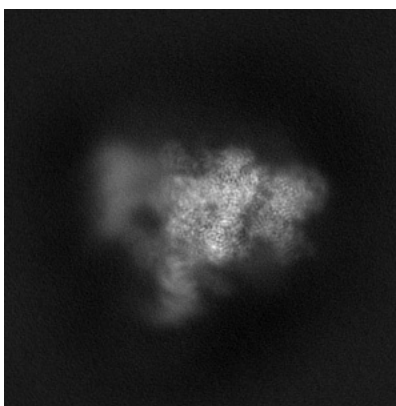
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

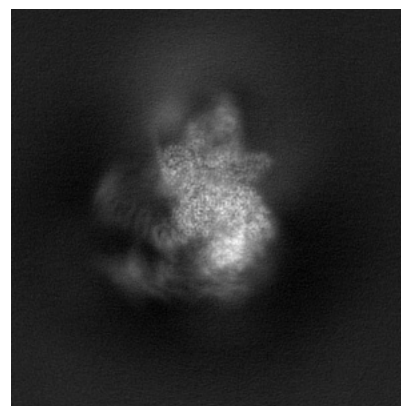
6.1.1 Primary map



X

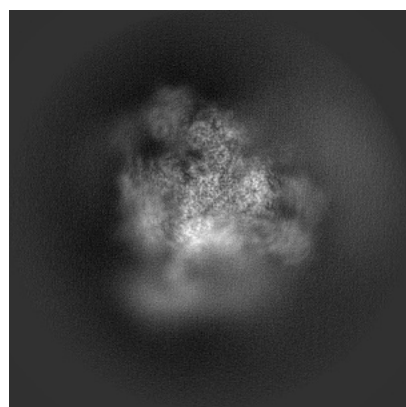


Y

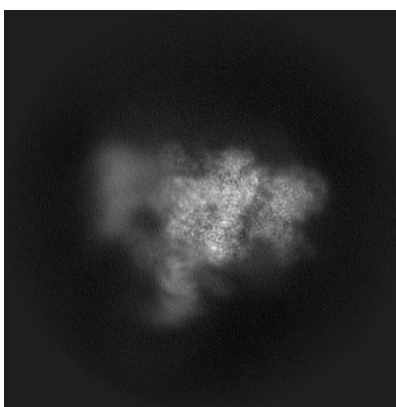


Z

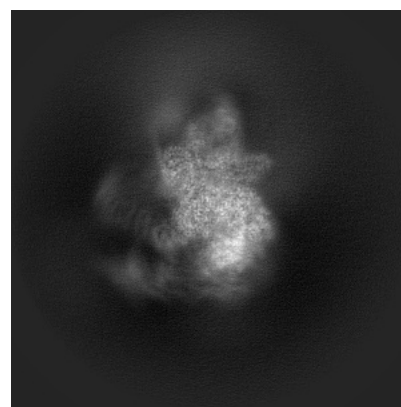
6.1.2 Raw map



X



Y

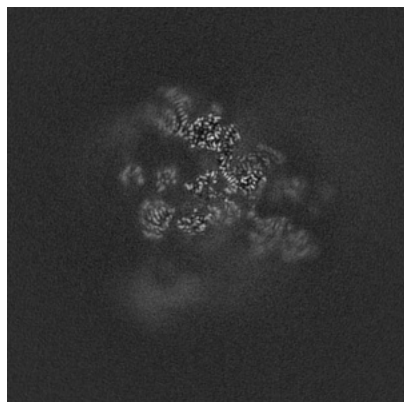


Z

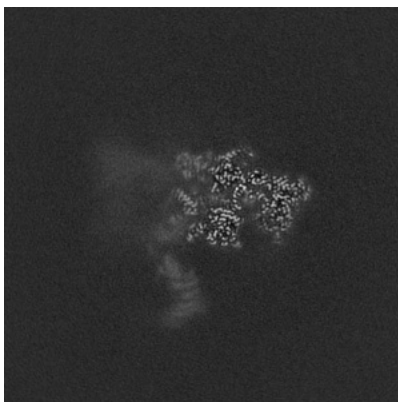
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

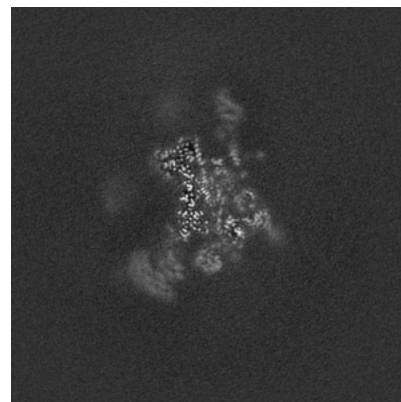
6.2.1 Primary map



X Index: 240

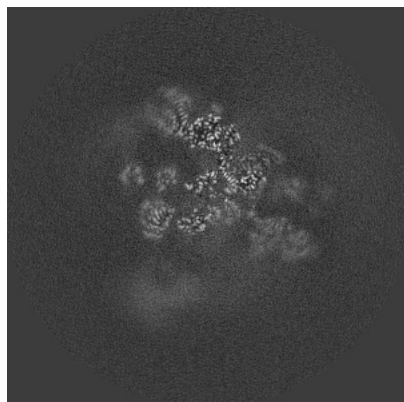


Y Index: 240

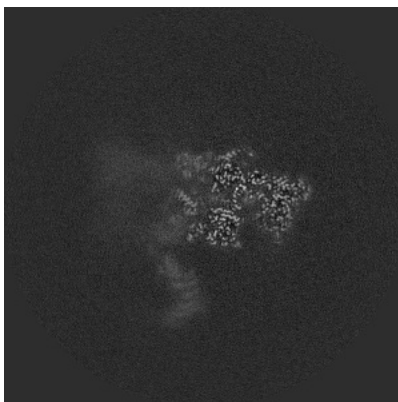


Z Index: 240

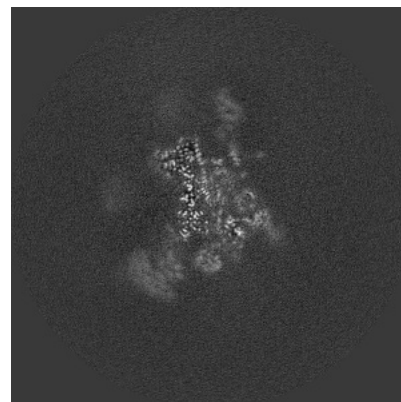
6.2.2 Raw map



X Index: 240



Y Index: 240

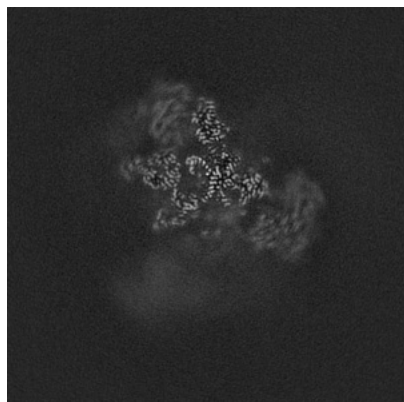


Z Index: 240

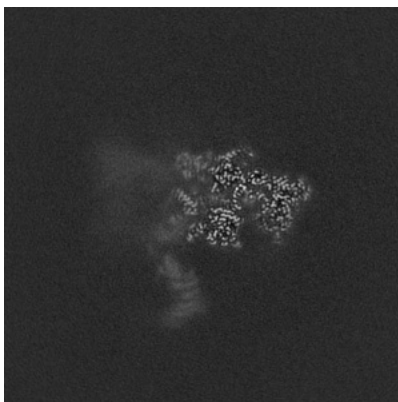
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

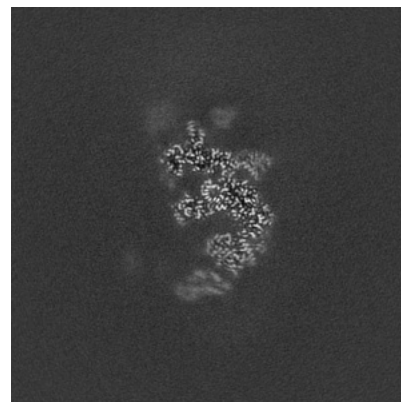
6.3.1 Primary map



X Index: 261

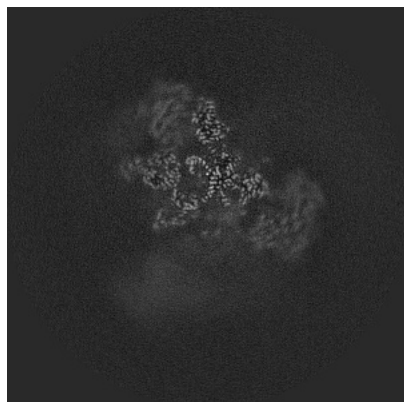


Y Index: 240

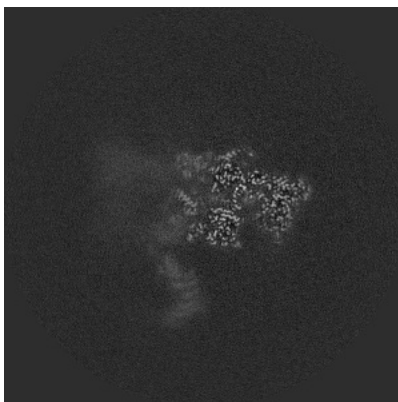


Z Index: 276

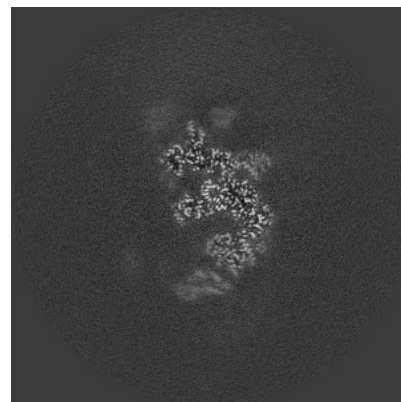
6.3.2 Raw map



X Index: 261



Y Index: 240

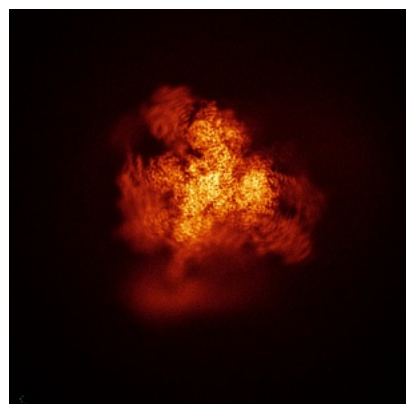


Z Index: 276

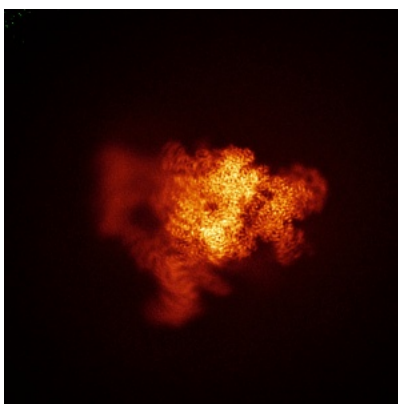
The images above show the largest variance slices of the map in three orthogonal directions.

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

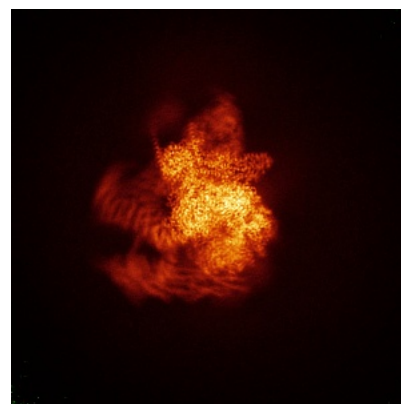
6.4.1 Primary map



X

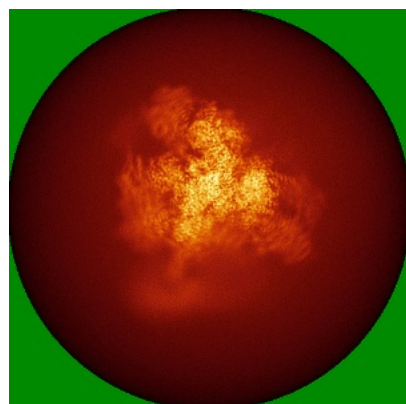


Y

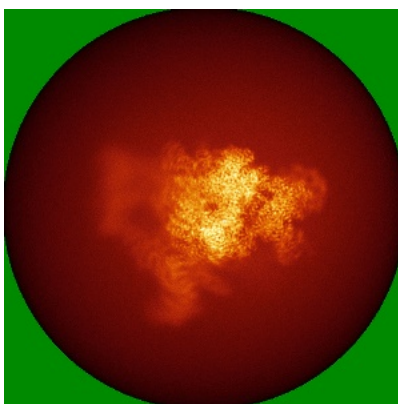


Z

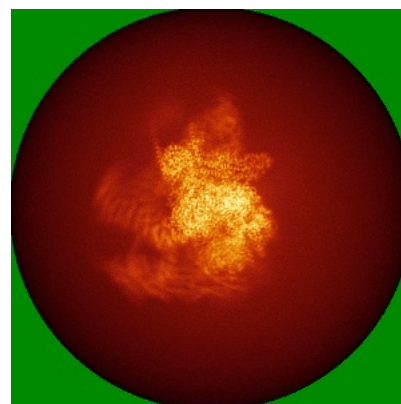
6.4.2 Raw map



X



Y

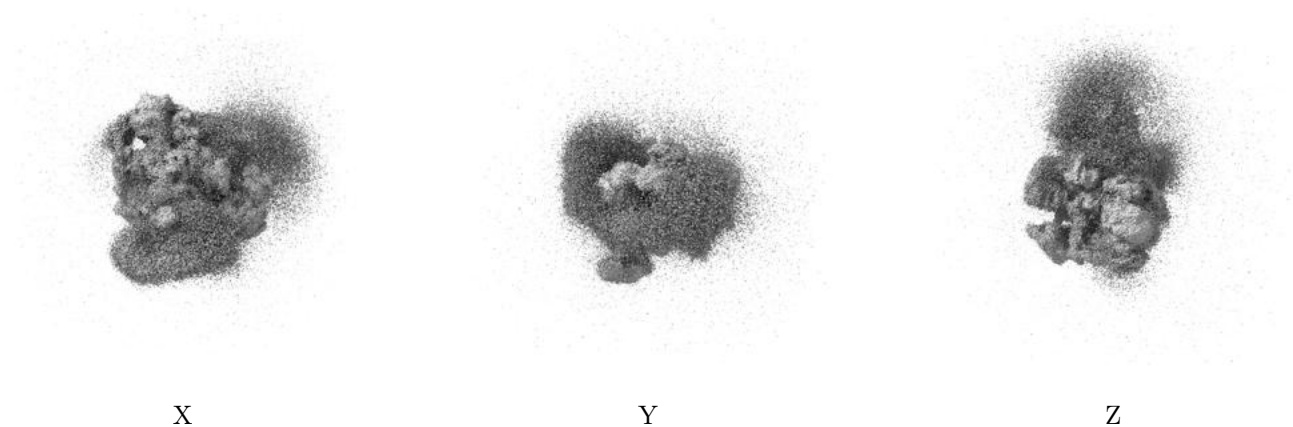


Z

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.

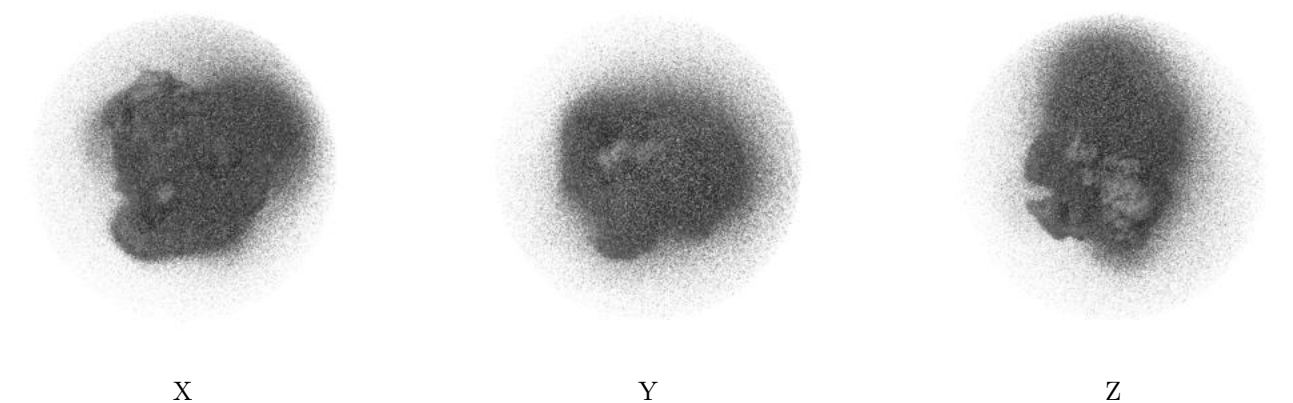
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

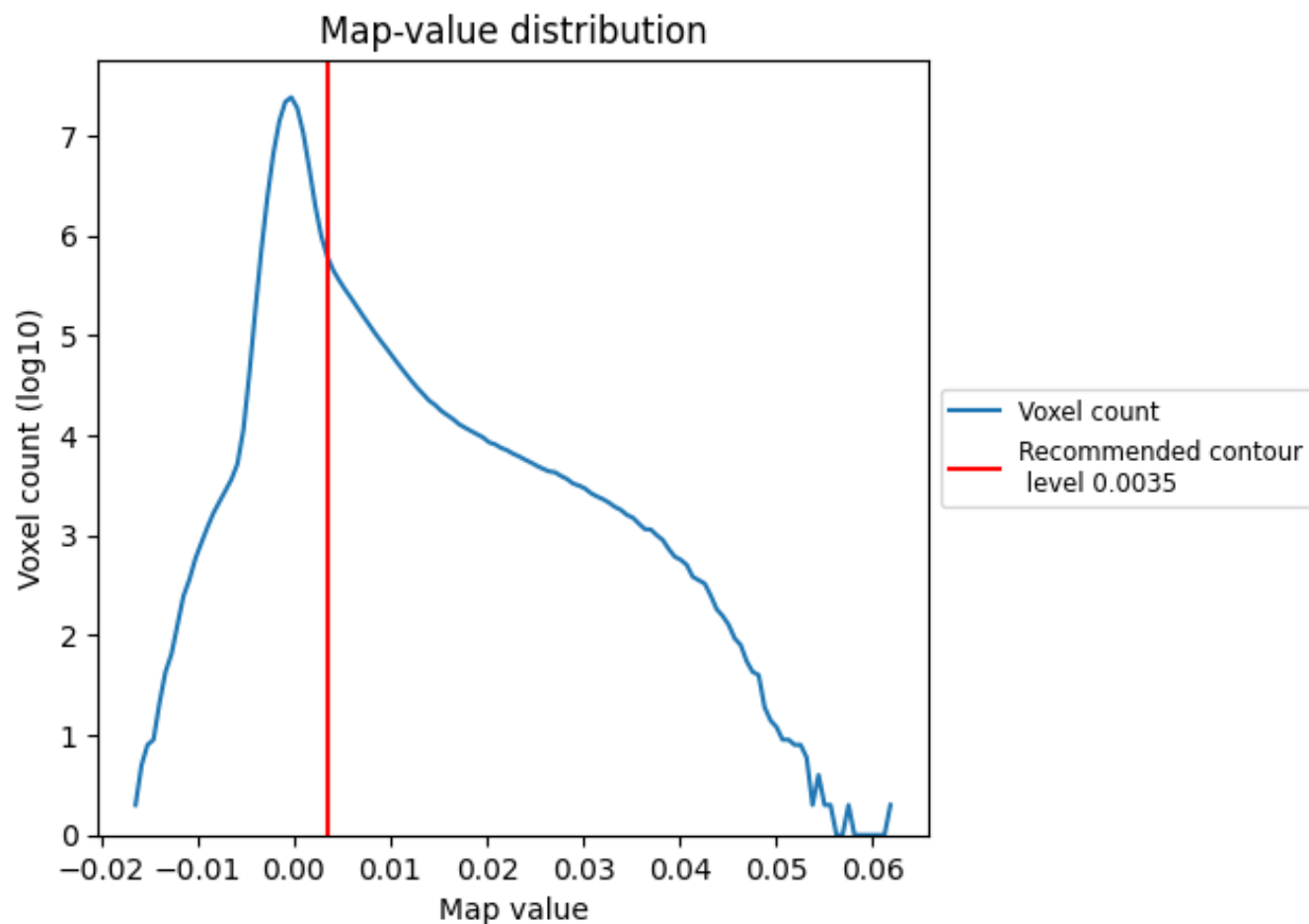
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

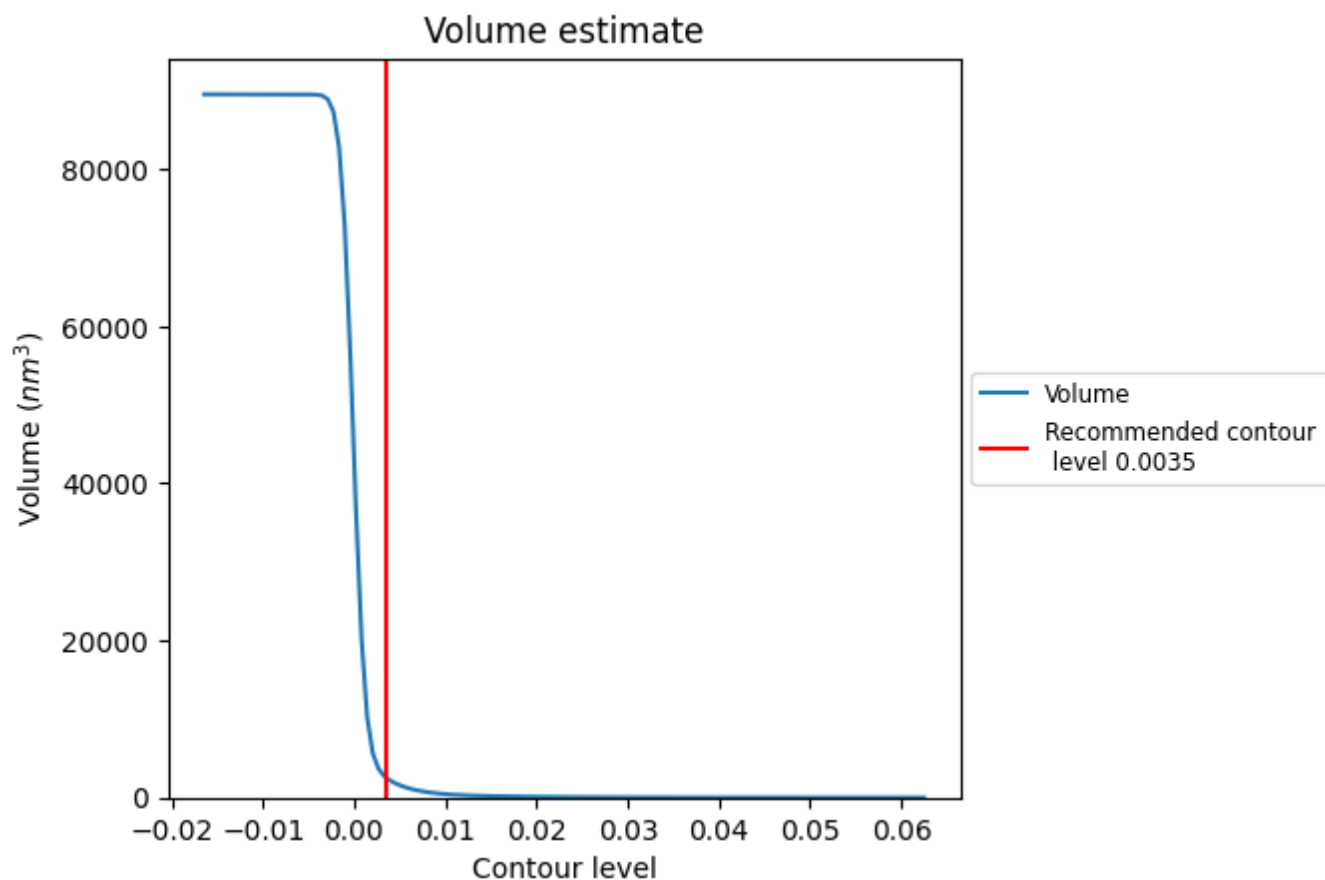
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

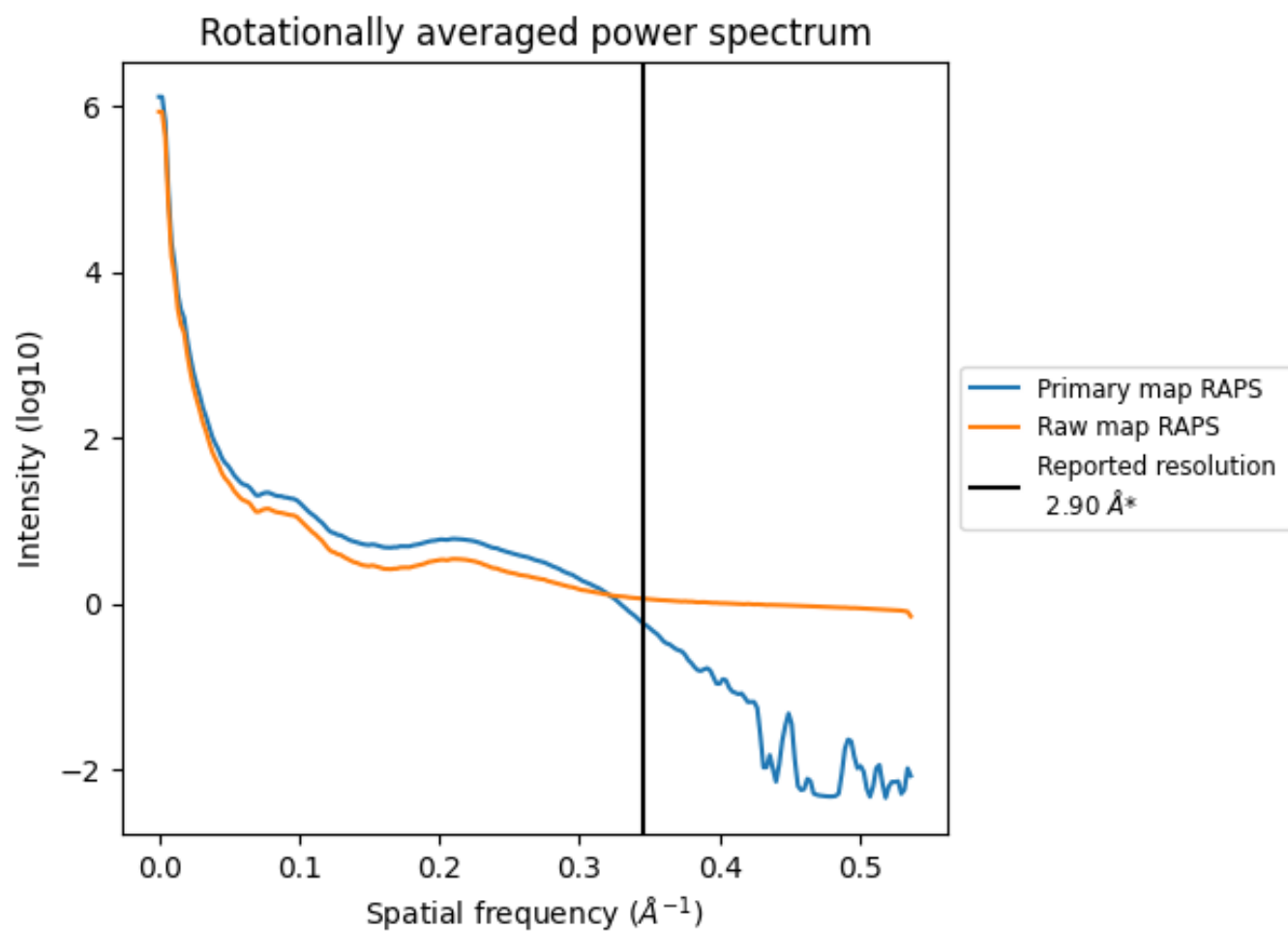
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2569 nm³; this corresponds to an approximate mass of 2320 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 ⓘ

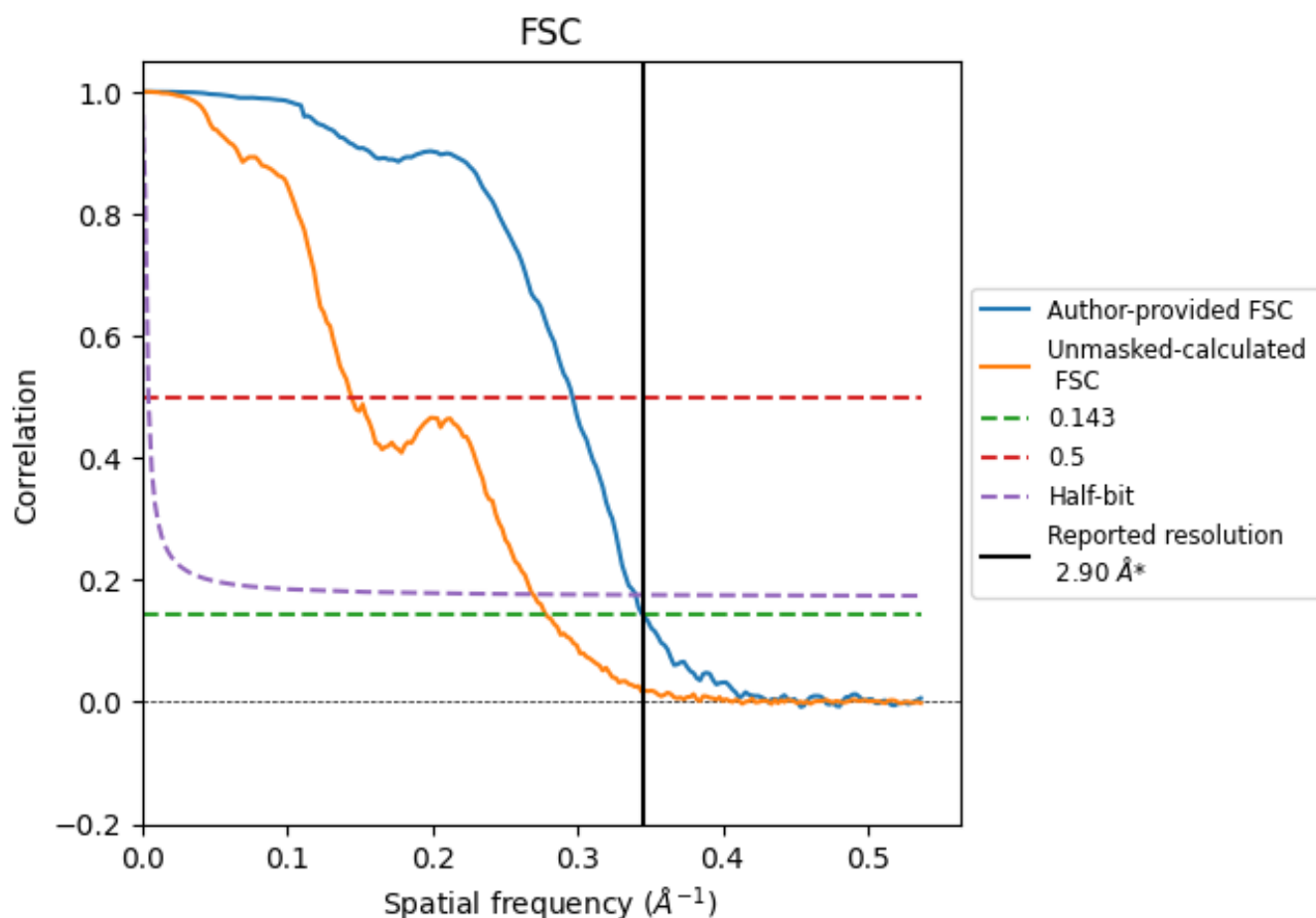


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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

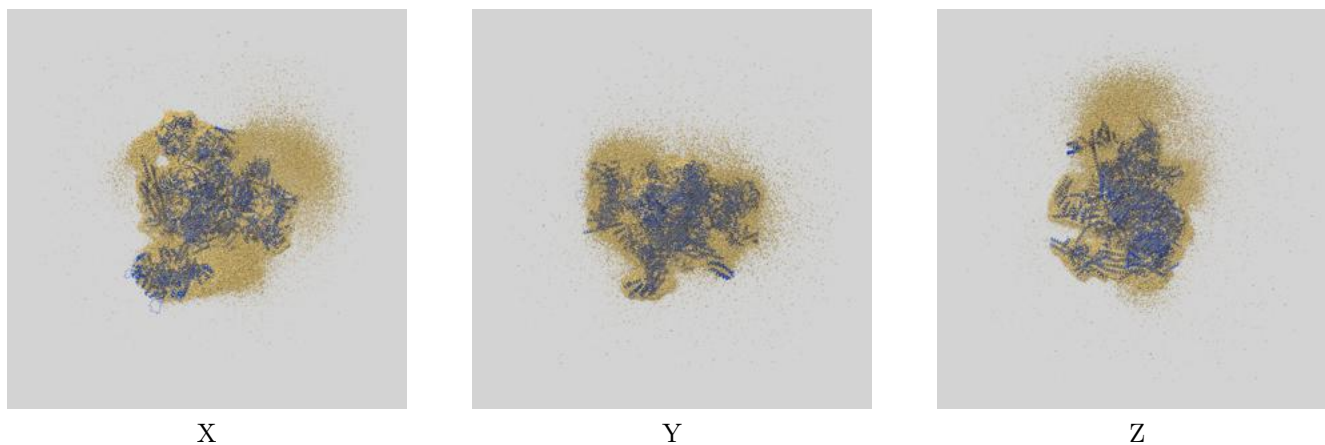
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.37	2.94
Unmasked-calculated*	3.59	6.93	3.71

*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 3.59 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

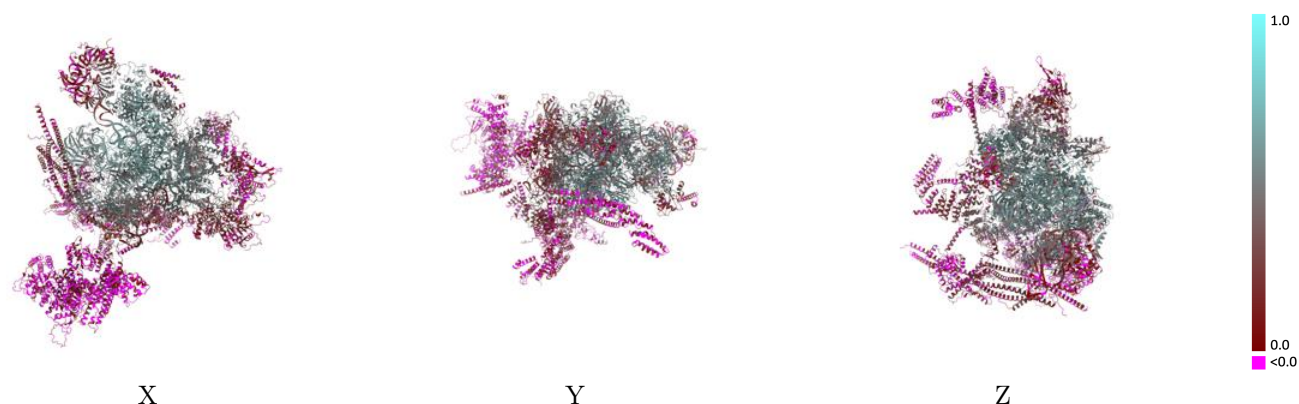
This section contains information regarding the fit between EMDB map EMD-62842 and PDB model 9L5S. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



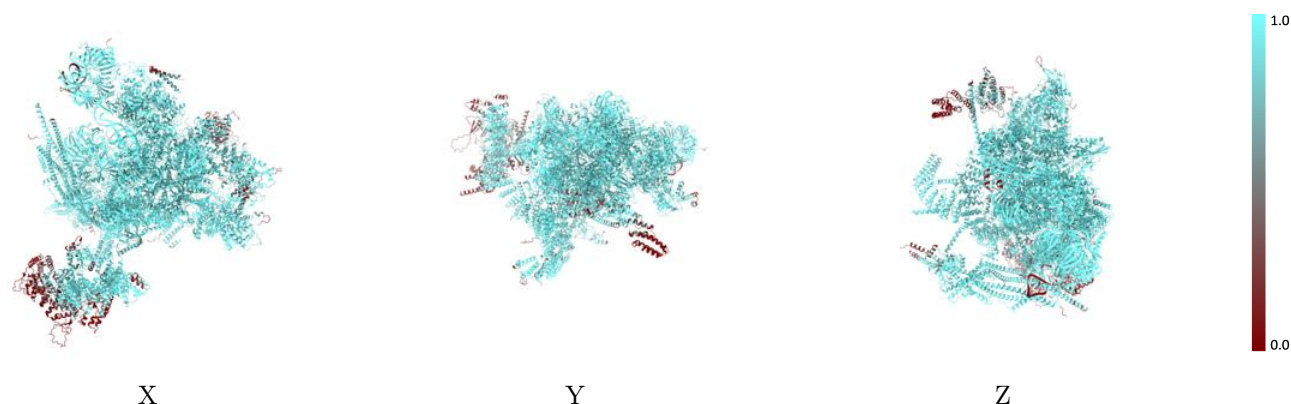
The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



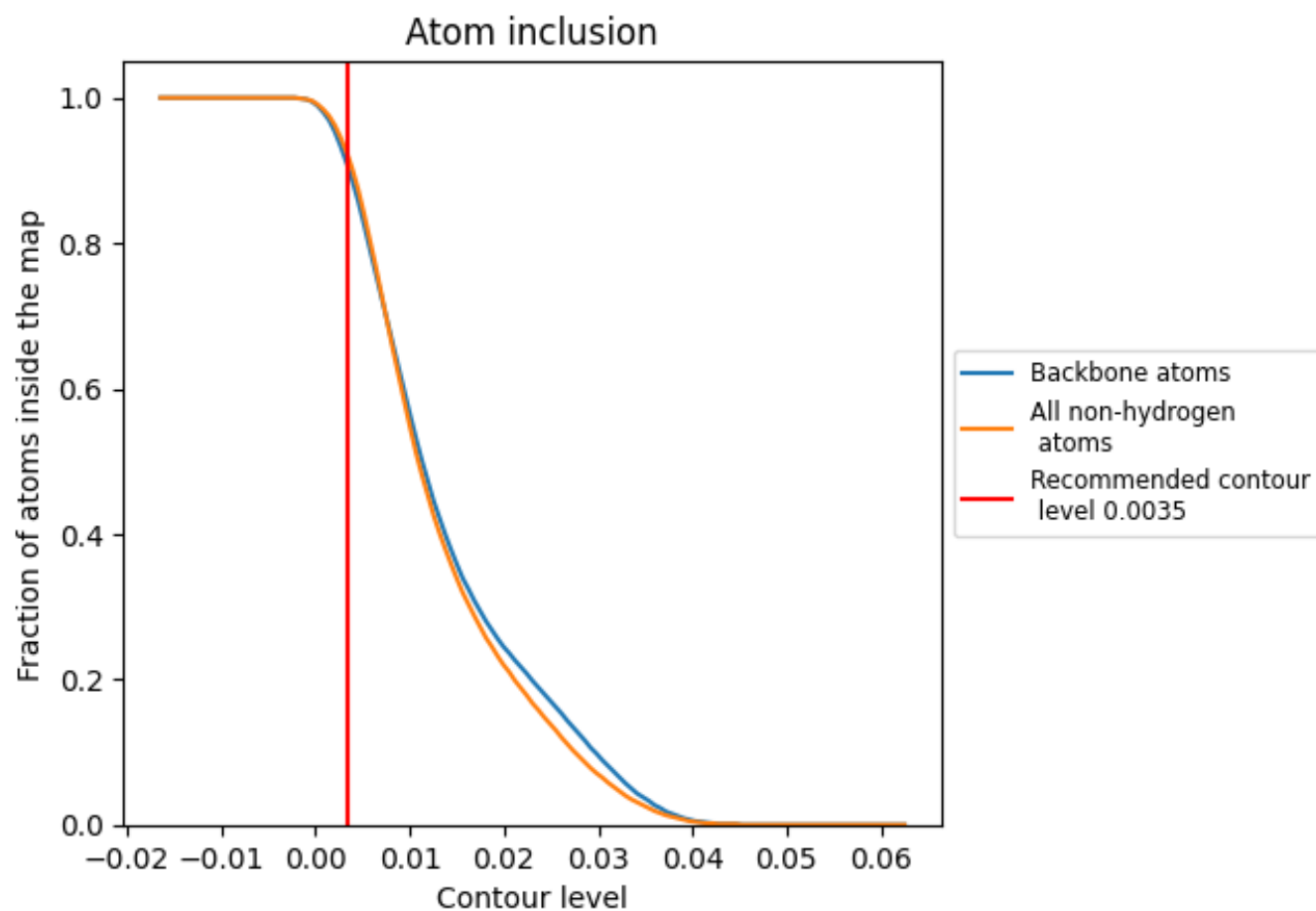
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 92% 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 (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.3520
0	 1.0000	 0.4640
1	 0.9510	 0.3210
2	 0.9990	 0.3860
5	 0.8770	 0.3950
6	 1.0000	 0.4680
8	 1.0000	 0.4340
A	 0.9830	 0.5070
B	 0.9240	 0.3120
C	 0.9920	 0.5070
CV	 0.9940	 0.2450
CY	 0.9400	 0.4510
Cb	 0.4860	 0.0450
Ck	 0.4190	 0.0390
E	 0.9990	 0.5360
F	 0.9600	 0.1030
I	 0.9390	 0.1030
J	 0.9760	 0.3400
K	 0.9620	 0.1710
L	 0.9210	 0.2890
M	 0.9900	 0.4020
N	 0.9940	 0.5760
P	 0.9760	 0.5130
R	 0.9740	 0.4580
S	 0.9990	 0.4680
T	 0.9980	 0.6050
V	 0.7120	 0.2720
W	 0.9990	 0.5300
Y	 0.5220	 0.0030
Z	 0.8310	 0.4110
j	 0.9740	 0.1830
k	 0.9960	 0.3150
l	 0.9720	 0.1030
m	 0.9730	 0.1080
o	 0.9790	 0.1620



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Chain	Atom inclusion	Q-score
p	 0.9010	 0.2850
q	 0.9250	 0.1590
r	 0.9690	 0.1510
s	 0.9470	 0.1030
t	 0.8390	 0.0530
u	 0.9930	 0.4130
z	 0.9590	 0.2330