



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:17 PM UTC

PDB ID : 9L5T / pdb_00009l5t
EMDB ID : EMD-62843
Title : Cryo-EM structure of the thermophile spliceosome (state B*Q2)
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 : 3.50 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

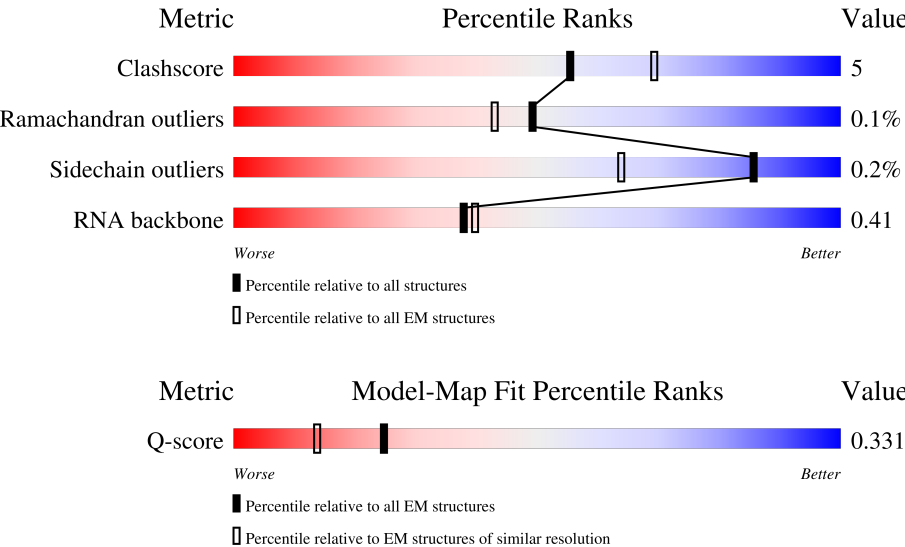
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



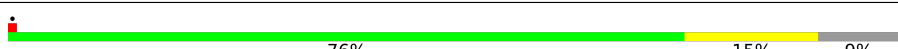
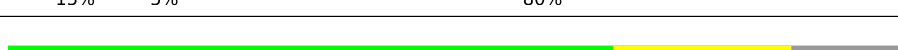
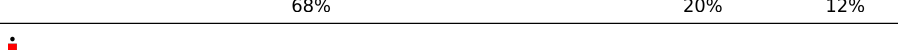
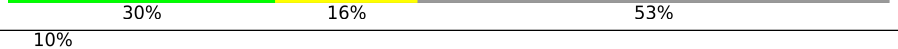
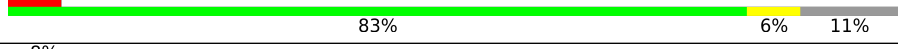
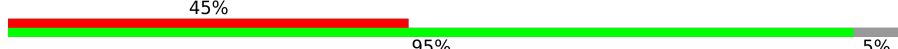
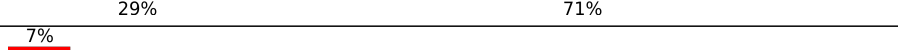
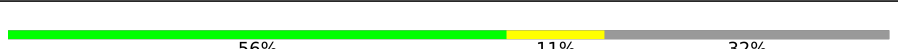
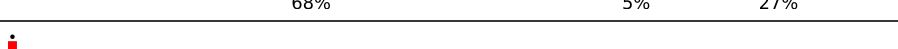
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	D	325	
8	E	352	
9	F	233	
10	I	839	
11	J	687	
12	L	768	
13	K	231	
14	Y	1416	
15	q	480	
15	r	480	
15	s	480	
15	t	480	
16	N	148	
17	S	167	
18	T	496	
19	M	395	
20	o	408	
21	R	578	
22	W	547	
23	P	260	
24	j	98	
25	k	82	

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Mol	Chain	Length	Quality of chain
26	l	94	
27	m	592	
28	o	118	
29	p	211	
30	u	114	
31	1	698	
32	z	672	
33	V	223	
34	Z	678	
35	CY	510	
36	Ck	42	
37	Cb	391	
38	8	22	
39	Cc	764	

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 92448 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	90	Total	C	N	O	P	0	0
			1924	860	352	622	90		

- Molecule 4 is a protein called PRP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1991	Total	C	N	O	S	0	0
			16416	10555	2854	2945	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
			1941	1198	362	376	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 SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	64	Total	C	N	O	S	0	0
			532	322	103	105	2		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4-like WD40 domain-containing protein.

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

- Molecule 9 is a protein called CCDC12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	110	Total	C	N	O	S	0	0
			879	544	166	167	2		

- Molecule 10 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	731	Total	C	N	O	S	0	0
			4879	3044	893	928	14		

- Molecule 11 is a protein called Suppressor of forked domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	608	Total	C	N	O	S	0	0
			4047	2513	770	759	5		

- Molecule 12 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	637	Total	C	N	O	S	0	0
			4222	2578	808	827	9		

- Molecule 13 is a protein called Pre-mRNA-splicing factor SPF27.

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

- Molecule 14 is a protein called Pre-mRNA-splicing factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Y	1345	Total	C	N	O	0	0
			6660	3970	1345	1345		

- Molecule 15 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	q	139	Total	C	N	O	0	0
			691	413	139	139		
15	t	141	Total	C	N	O	0	0
			701	419	141	141		
15	r	143	Total	C	N	O	0	0
			711	425	143	143		
15	s	140	Total	C	N	O	0	0
			696	416	140	140		

- Molecule 16 is a protein called Putative bud site selection protein.

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

- Molecule 17 is a protein called Peptidyl-prolyl cis-trans isomerase.

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

- Molecule 18 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	322	Total	C	N	O	S	0	0
			2507	1583	448	462	14		

- Molecule 19 is a protein called Putative pre-mRNA splicing protein.

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

- Molecule 20 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	0	276	Total	C	N	O	S	0	0
			2224	1381	424	412	7		

- Molecule 21 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	340	Total	C	N	O	S	0	0
			2678	1664	509	497	8		

- Molecule 22 is a protein called PRP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	401	Total	C	N	O	S	0	0
			2244	1348	448	444	4		

- Molecule 23 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	114	Total	C	N	O	S	0	0
			925	577	182	165	1		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	j	88	Total	C	N	O	0	0
			436	259	88	89		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
25	k	73	Total	C	N	O	0	0
			359	213	73	73		

- Molecule 26 is a protein called Sm protein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	l	81	Total	C	N	O	0	0
			400	238	81	81		

- Molecule 27 is a protein called Delta(14)-sterol reductase.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	m	86	Total	C	N	O	0	0
			426	253	86	87		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	o	87	Total	C	N	O	0	0
			431	257	87	87		

- Molecule 29 is a protein called Sm protein B.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	p	103	Total	C	N	O	0	0
			537	323	109	105		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	u	90	Total	C	N	O	0	0
			444	264	90	90		

- Molecule 31 is a protein called GPATCH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1	325	Total	C	N	O	S	0	0
			2514	1582	443	484	5		

- Molecule 32 is a protein called RNA helicase.

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

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

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

- Molecule 34 is a protein called Putative pre-mRNA splicing protein.

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

- Molecule 35 is a protein called Nineteen complex-related protein 2-domain-containing protein.

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

- Molecule 36 is a protein called GCFC2.

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

- Molecule 37 is a protein called TFIP11.

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

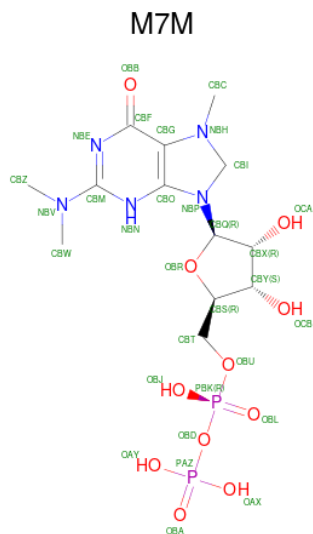
- Molecule 38 is a RNA chain called Unknown mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	8	21	Total	C	N	O	P	0	0
			405	198	60	126	21		

- Molecule 39 is a protein called RNA helicase.

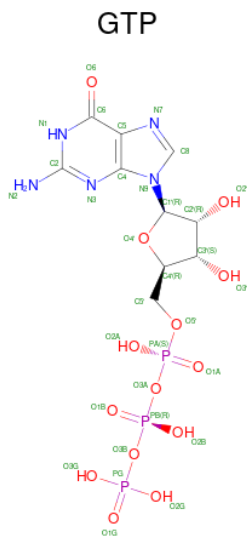
Mol	Chain	Residues	Atoms				AltConf	Trace
39	Cc	714	Total	C	N	O	0	0
			3541	2112	714	715		

- Molecule 40 is N,N,7-trimethylguanosine 5'-(trihydrogen diphosphate) (CCD ID: M7M) (formula: C₁₃H₂₃N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
40	2	1	Total	C	N	O	P	0
			30	13	5	10	2	

- 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	

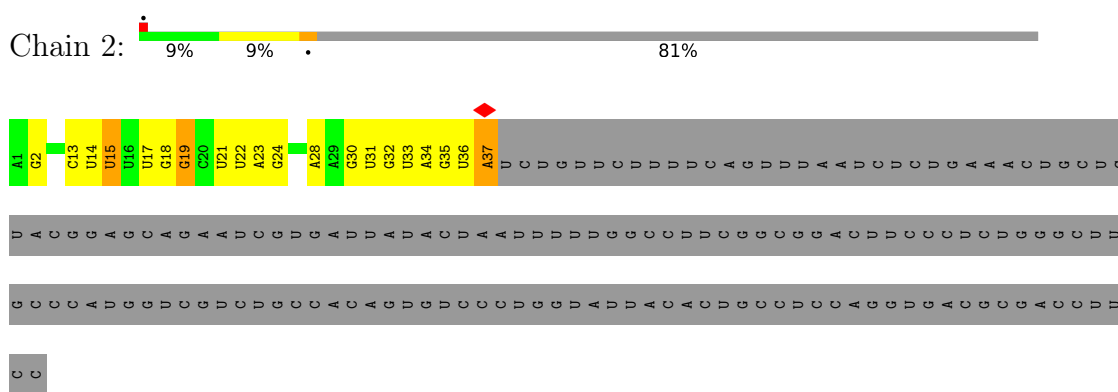
- Molecule 42 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
42	N	3	Total 3	Zn 3	0
42	M	2	Total 2	Zn 2	0

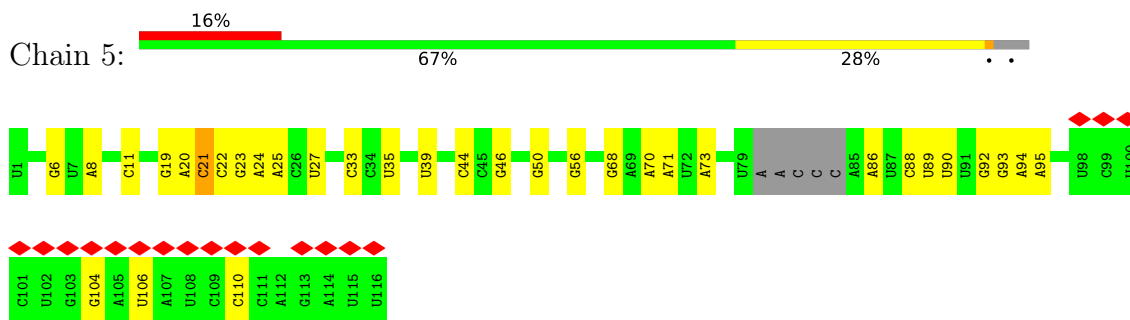
3 Residue-property plots [i](#)

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

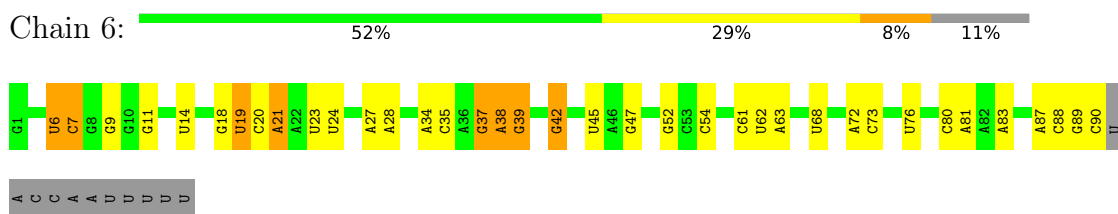
• Molecule 1: U2 snRNA



• Molecule 2: U5 snRNA



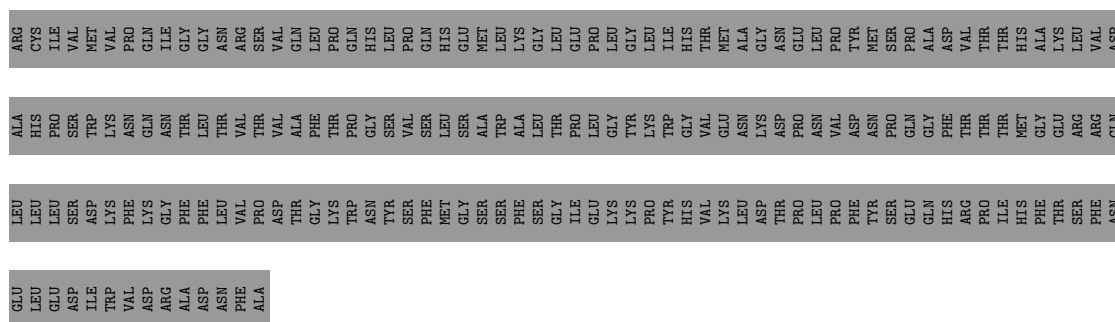
• Molecule 3: U6 snRNA



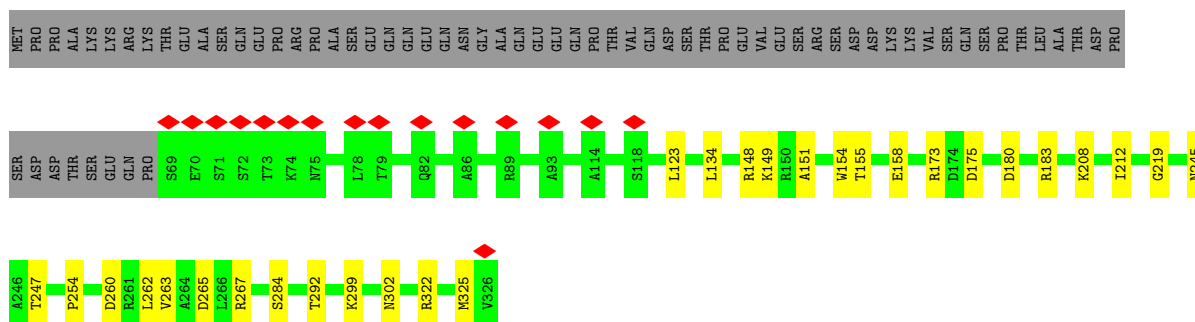
• Molecule 4: PRP8



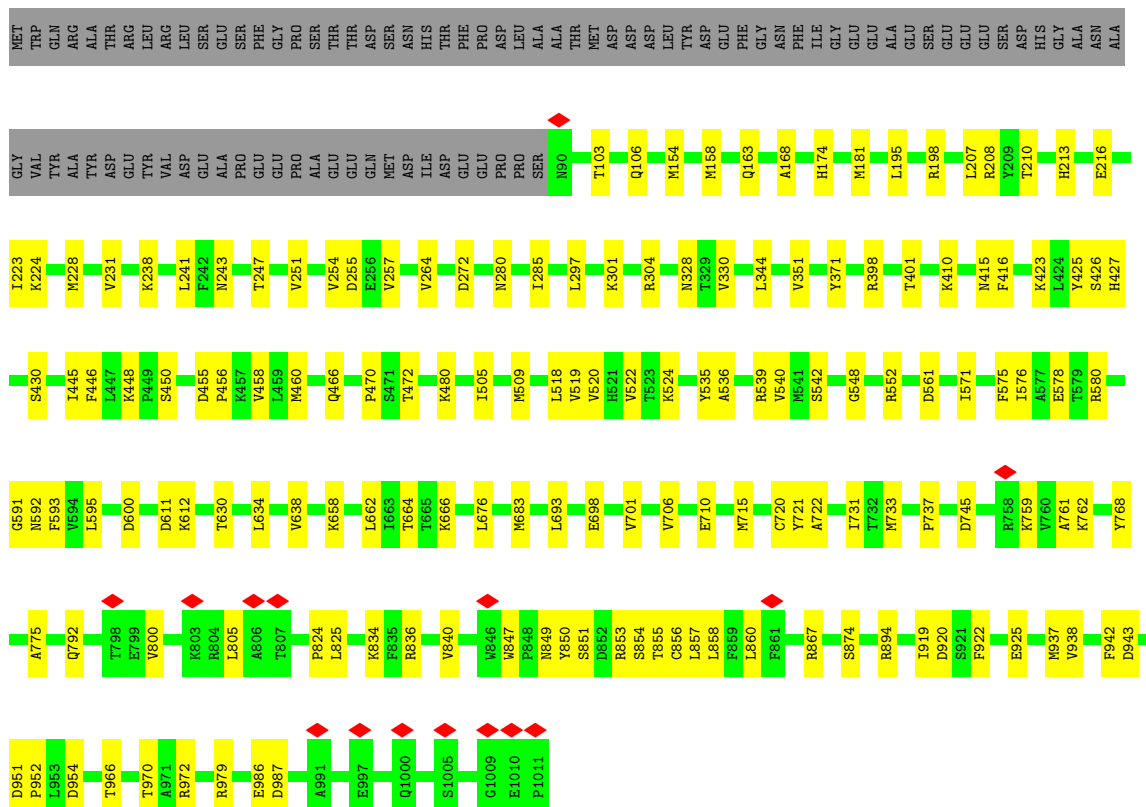
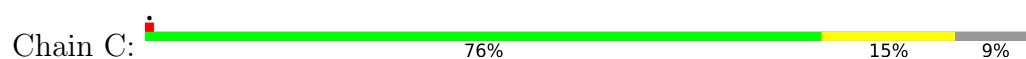


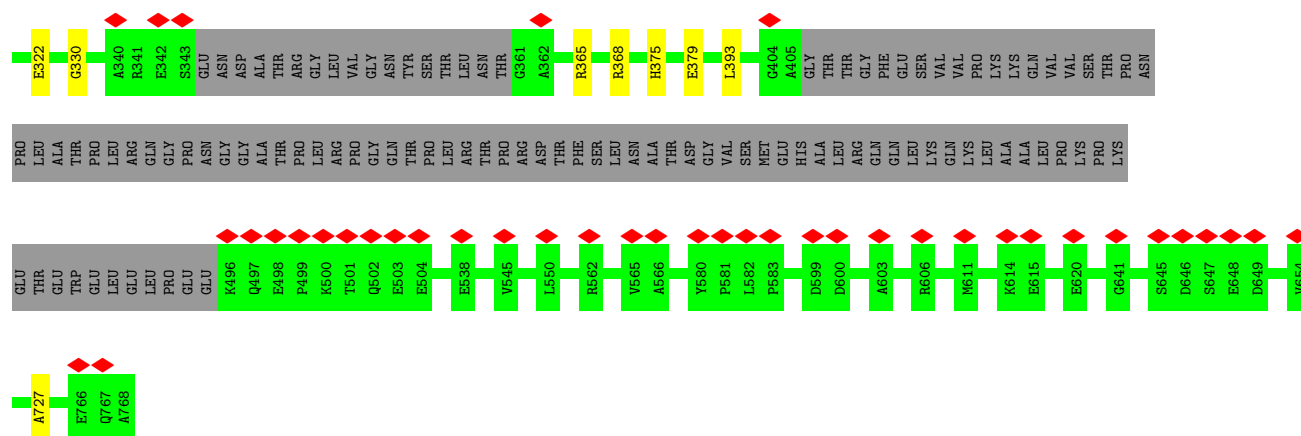


- Molecule 5: Pre-mRNA-splicing factor SYF2

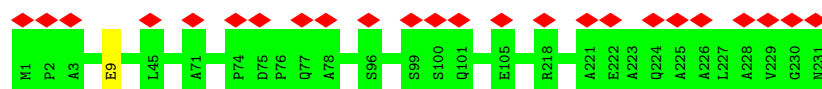


- Molecule 6: SNU114

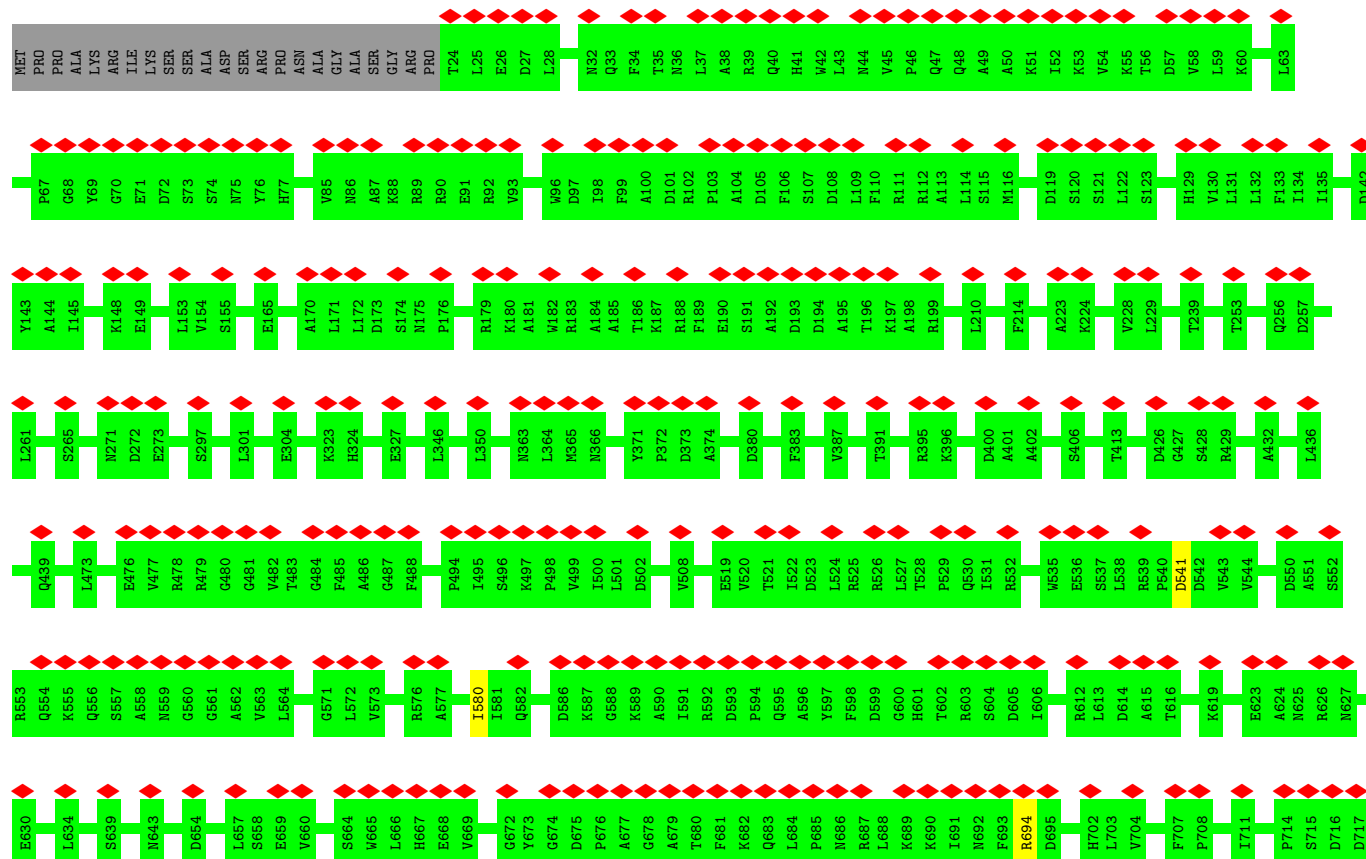


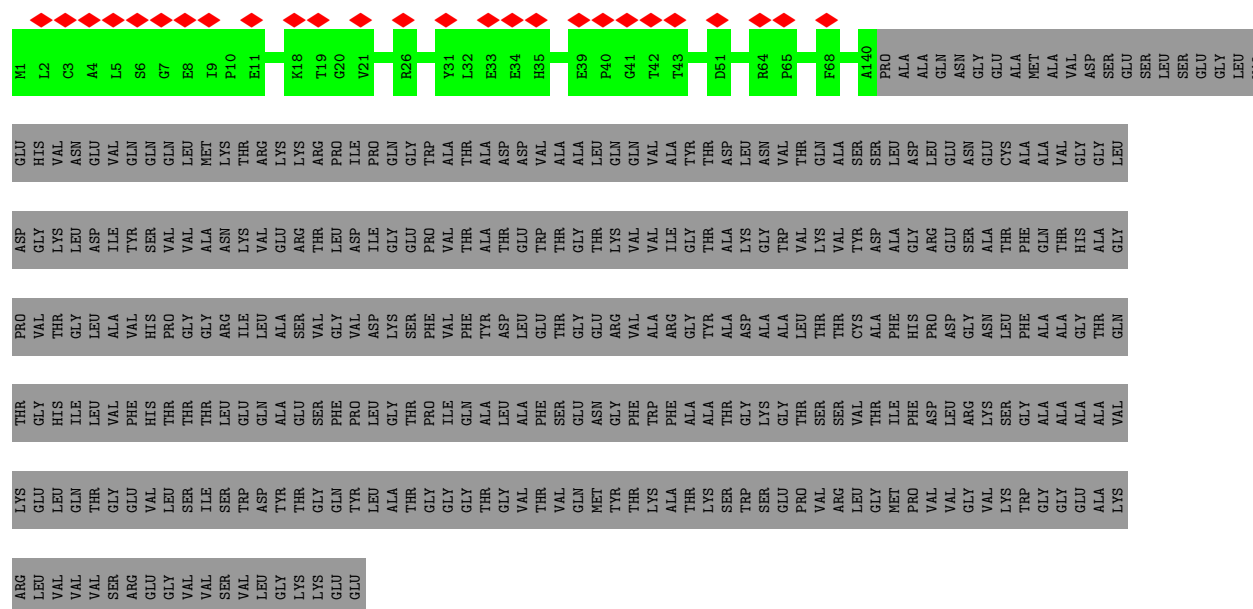


• Molecule 13: Pre-mRNA-splicing factor SPF27

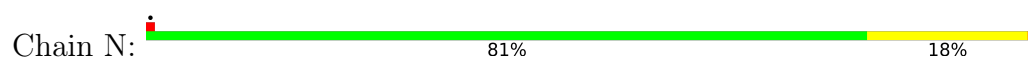


• Molecule 14: Pre-mRNA-splicing factor

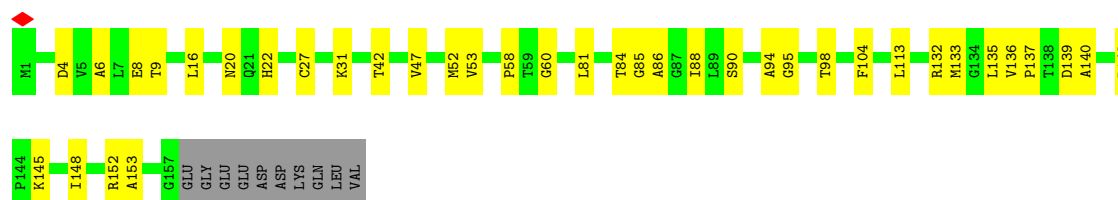




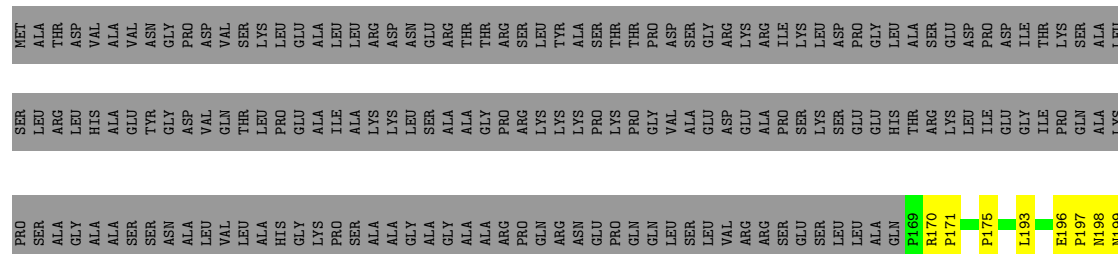
• Molecule 16: Putative bud site selection protein

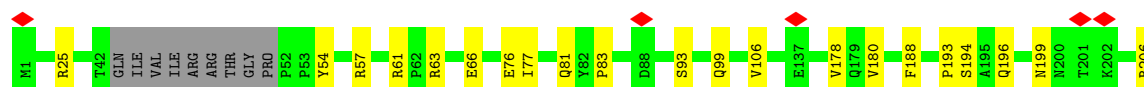


• Molecule 17: Peptidyl-prolyl cis-trans isomerase

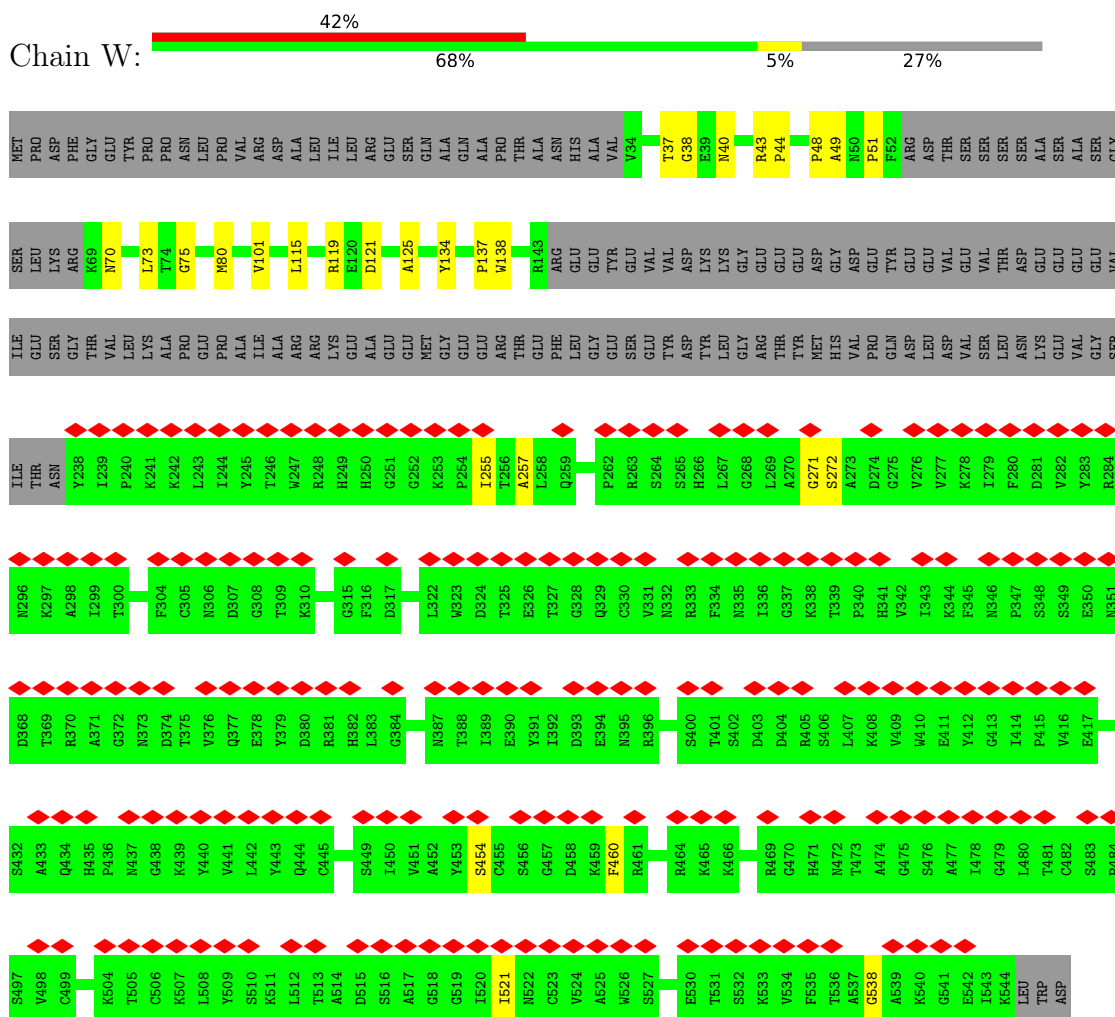


• Molecule 18: Pre-mRNA-splicing factor PRP46

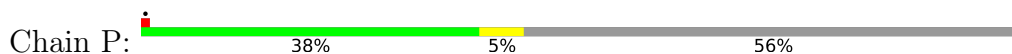


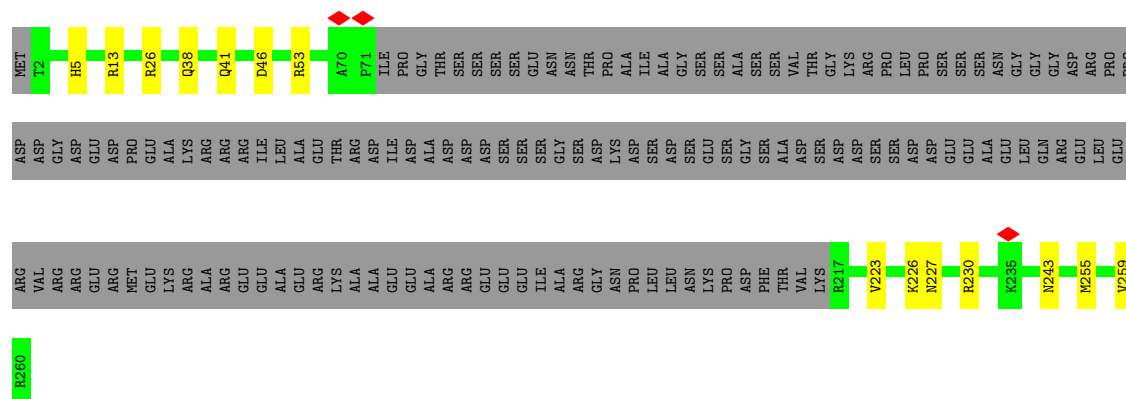


- Molecule 22: PRP17



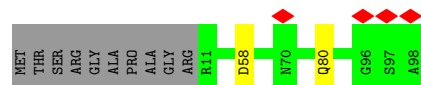
- Molecule 23: Putative pre-mRNA splicing protein





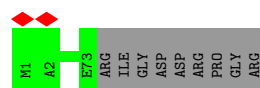
- Molecule 24: Small nuclear ribonucleoprotein E

Chain j: 88% 10%



- Molecule 25: Small nuclear ribonucleoprotein G

Chain k: 89% 11%



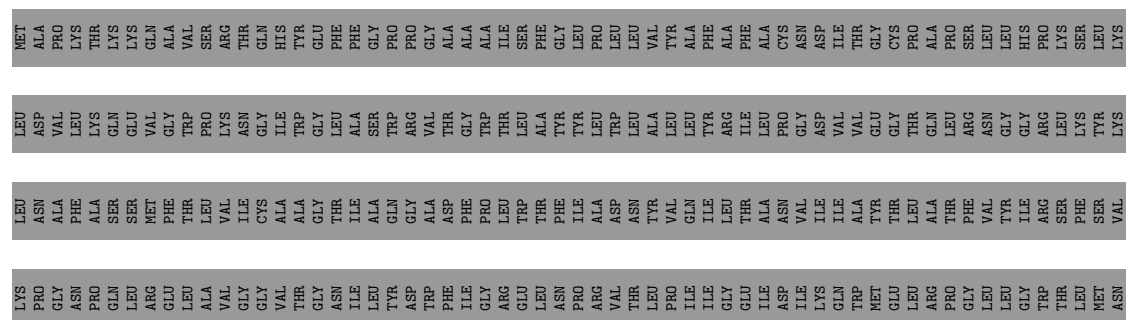
- Molecule 26: Sm protein F

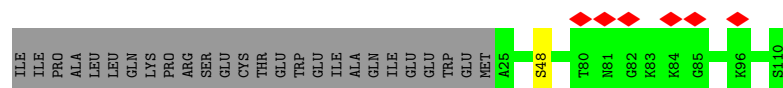
Chain l: 10% 83% 14%



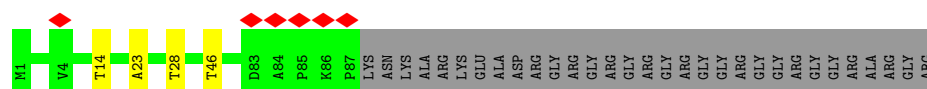
- Molecule 27: Delta(14)-sterol reductase

Chain m: 14% 85%

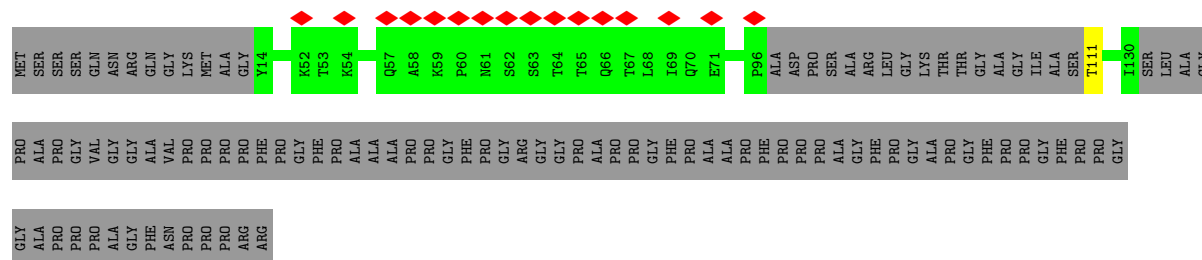




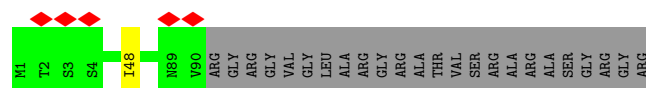
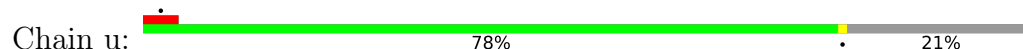
- Molecule 28: Small nuclear ribonucleoprotein Sm D1



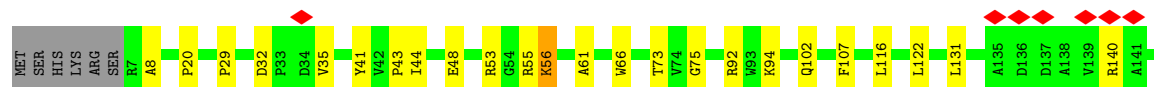
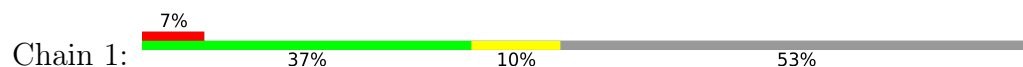
- Molecule 29: Sm protein B



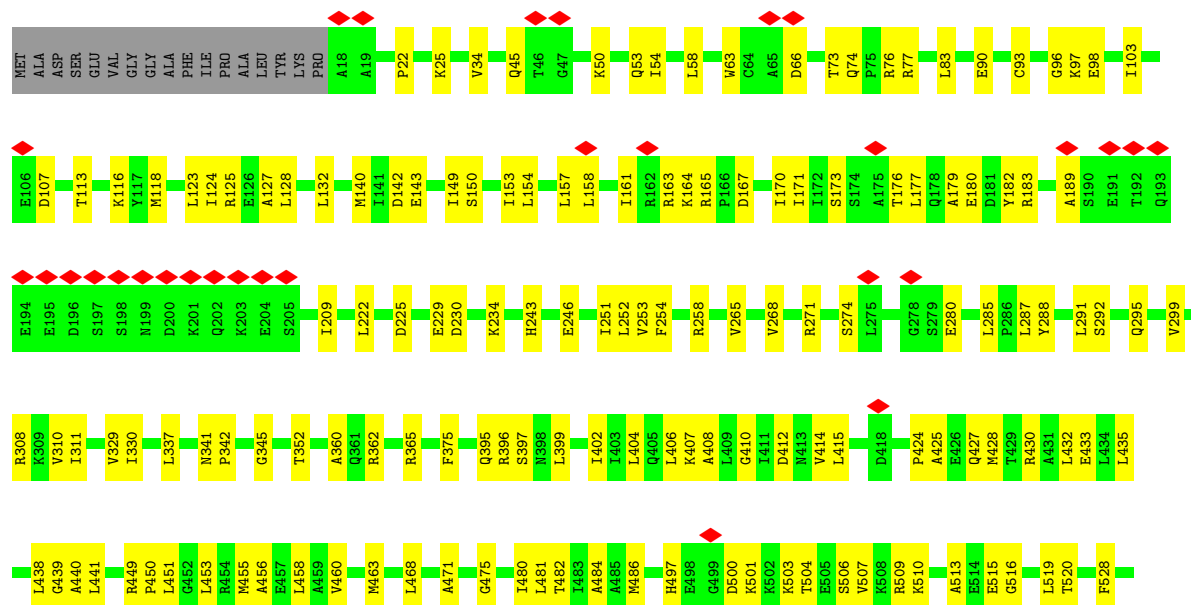
- Molecule 30: Small nuclear ribonucleoprotein Sm D3

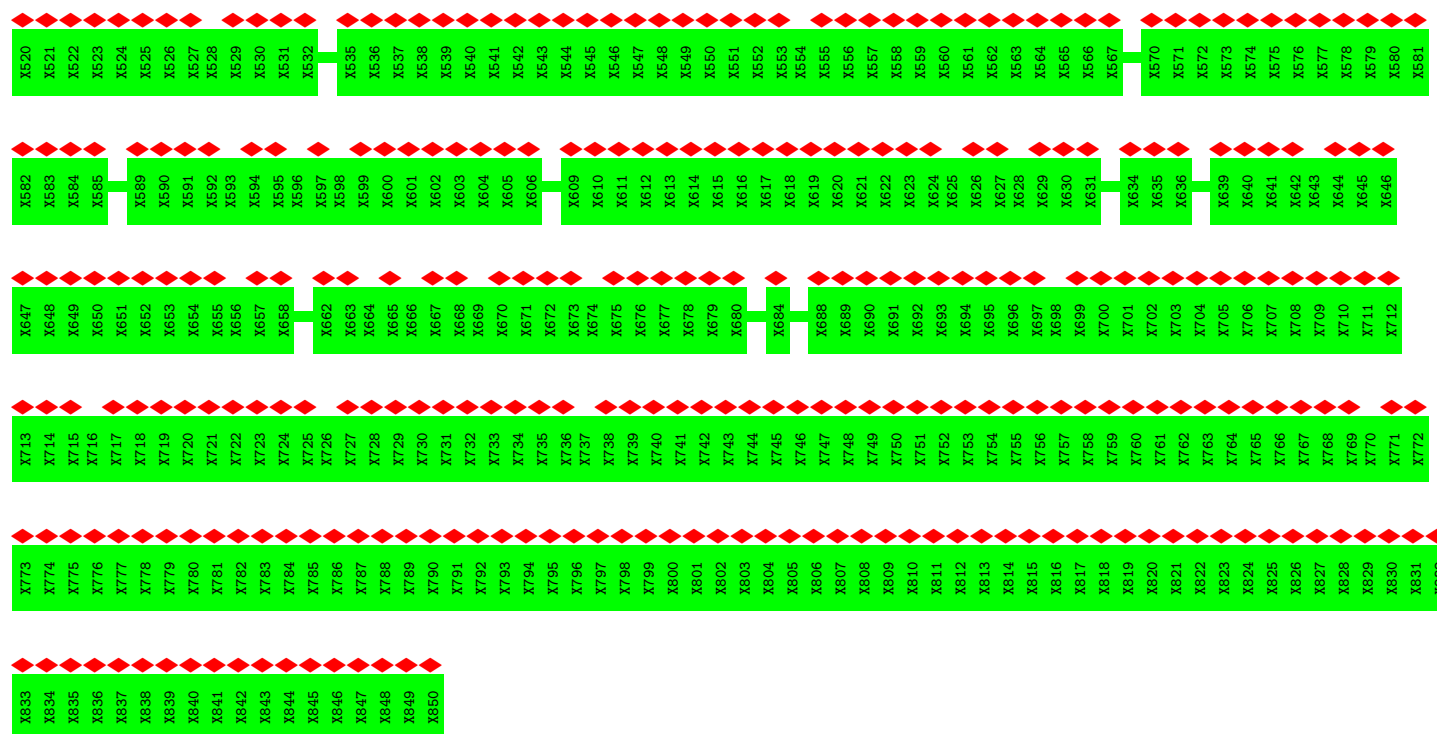


- Molecule 31: GPATCH1



- Molecule 32: RNA helicase





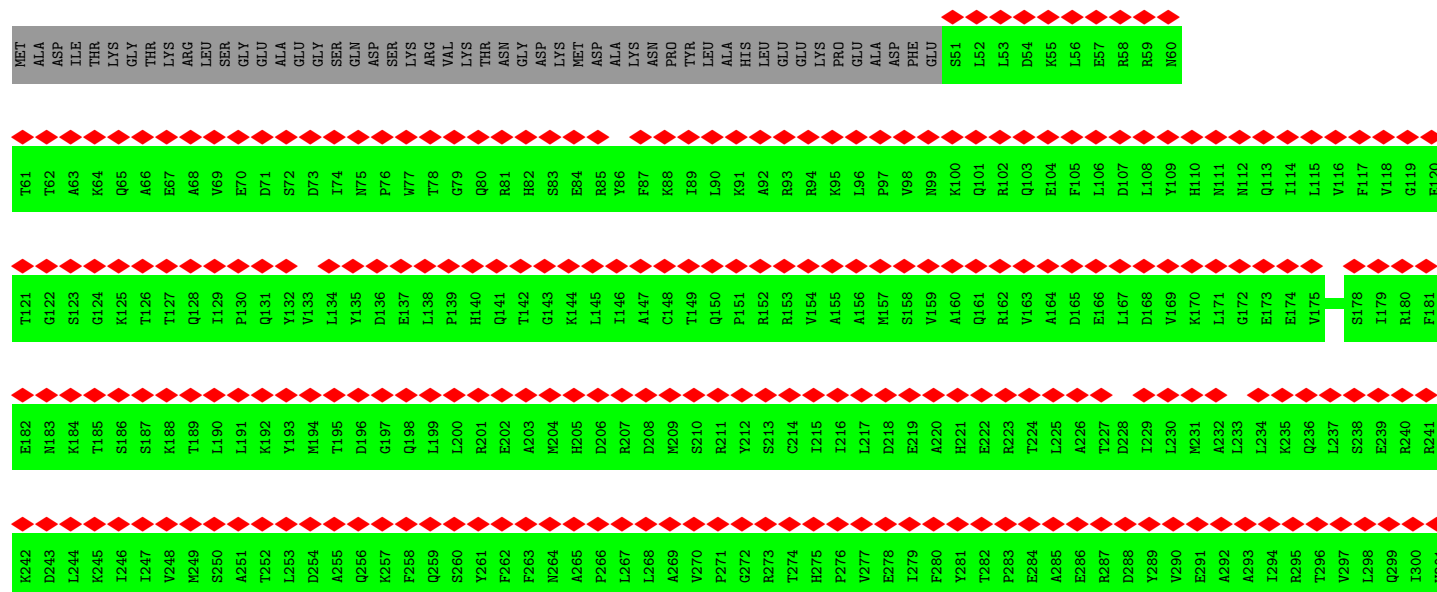
• Molecule 38: Unknown mRNA

Chain 8: 36% 45% 14% 5%



• Molecule 39: RNA helicase

Chain Cc: 89% 93% 7%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16442	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	0.045	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	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: GTP, Y5P, M7M, ZN, P5P

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	0.32	0/866	0.38	0/1345
2	5	0.34	0/2612	0.35	0/4059
3	6	0.38	0/2153	0.40	0/3352
4	A	0.35	0/16842	0.50	1/22833 (0.0%)
5	B	0.22	0/1968	0.43	0/2646
6	C	0.27	0/7464	0.46	0/10117
7	D	0.26	0/536	0.66	0/711
8	E	0.28	0/2428	0.58	0/3295
9	F	0.29	0/891	0.84	5/1201 (0.4%)
10	I	0.20	0/4952	0.46	3/6765 (0.0%)
11	J	0.26	0/4107	0.38	0/5613
12	L	0.26	0/4265	0.43	0/5803
13	K	0.13	0/1147	0.24	0/1598
14	Y	0.09	0/6659	0.25	0/9282
15	q	0.10	0/690	0.26	0/962
15	r	0.11	0/710	0.25	0/990
15	s	0.10	0/695	0.32	0/969
15	t	0.11	0/700	0.27	0/976
16	N	0.37	0/1227	0.55	1/1655 (0.1%)
17	S	0.21	0/1235	0.57	1/1671 (0.1%)
18	T	0.46	0/2576	0.71	2/3504 (0.1%)
19	M	0.25	0/2006	0.51	2/2703 (0.1%)
20	0	0.31	0/2278	0.57	0/3081
21	R	0.31	0/2738	0.48	0/3699
22	W	0.18	0/2257	0.46	0/3096
23	P	0.32	0/945	0.43	0/1264
24	j	0.11	0/435	0.31	0/603
25	k	0.13	0/358	0.36	0/496
26	l	0.11	0/399	0.35	0/554
27	m	0.11	0/425	0.35	0/589
28	o	0.10	0/430	0.28	0/598
29	p	0.13	0/538	0.34	0/745

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	u	0.12	0/443	0.45	0/615
31	1	0.25	0/2573	0.56	1/3473 (0.0%)
32	z	0.19	0/5245	0.50	0/7100
33	V	0.18	0/481	0.44	0/661
34	Z	0.21	0/1768	0.52	0/2384
35	CY	0.19	0/190	0.46	0/253
39	Cc	0.10	0/3540	0.28	0/4935
All	All	0.27	0/91772	0.46	16/126196 (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
4	A	0	2
19	M	0	1
All	All	0	3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	1	44	ILE	N-CA-C	-6.49	107.55	113.71
9	F	161	GLU	N-CA-CB	6.15	119.77	110.30
4	A	203	TYR	N-CA-C	-6.06	104.01	111.40
16	N	38	PRO	CA-N-CD	-5.90	103.75	112.00
10	I	604	MET	CB-CG-SD	-5.70	95.61	112.70
19	M	29	GLU	CA-C-N	5.69	128.38	120.65
19	M	29	GLU	C-N-CA	5.69	128.38	120.65
18	T	206	ALA	CA-C-N	5.32	131.84	121.41
18	T	206	ALA	C-N-CA	5.32	131.84	121.41
10	I	549	TYR	CA-C-N	-5.30	111.87	121.14
10	I	549	TYR	C-N-CA	-5.30	111.87	121.14
17	S	31	LYS	CA-CB-CG	5.16	124.42	114.10
9	F	97	LYS	CA-C-N	5.16	131.40	121.54
9	F	97	LYS	C-N-CA	5.16	131.40	121.54
9	F	112	GLU	N-CA-CB	5.14	118.25	110.28
9	F	165	GLU	N-CA-CB	5.04	118.05	110.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1430	LEU	Peptide
4	A	885	ARG	Sidechain
19	M	27	LEU	Peptide

5.2 Too-close contacts [i](#)

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	6	0
2	5	2343	0	1190	10	0
3	6	1924	0	973	20	0
4	A	16416	0	16426	190	0
5	B	1941	0	1805	23	0
6	C	7301	0	7339	97	0
7	D	532	0	534	12	0
8	E	2379	0	2343	49	0
9	F	879	0	899	26	0
10	I	4879	0	3846	48	0
11	J	4047	0	3116	32	0
12	L	4222	0	3572	39	0
13	K	1148	0	566	1	0
14	Y	6660	0	3003	2	0
15	q	691	0	314	1	0
15	r	711	0	330	0	0
15	s	696	0	319	0	0
15	t	701	0	320	0	0
16	N	1200	0	1184	22	0
17	S	1209	0	1207	25	0
18	T	2507	0	2448	37	0
19	M	1964	0	1969	33	0
20	0	2224	0	2131	35	0
21	R	2678	0	2688	32	0
22	W	2244	0	1407	22	0
23	P	925	0	918	13	0
24	j	436	0	186	1	0
25	k	359	0	159	0	0
26	l	400	0	175	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	m	426	0	185	1	0
28	o	431	0	188	2	0
29	p	537	0	313	1	0
30	u	444	0	197	0	0
31	l	2514	0	2473	55	0
32	z	5149	0	5221	124	0
33	V	478	0	317	3	0
34	Z	1729	0	1717	33	0
35	CY	190	0	167	5	0
36	Ck	205	0	39	0	0
37	Cb	1938	0	378	0	0
38	8	405	0	236	10	0
39	Cc	3541	0	1590	2	0
40	2	30	0	19	0	0
41	C	32	0	12	0	0
42	M	2	0	0	0	0
42	N	3	0	0	0	0
All	All	92448	0	74812	835	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 (835) 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)
8:E:109:LEU:HA	8:E:119:PHE:O	1.35	1.21
8:E:151:MET:HA	8:E:162:ILE:O	1.40	1.21
18:T:404:VAL:HA	18:T:409:VAL:O	1.41	1.16
17:S:6:ALA:O	17:S:153:ALA:HA	1.57	1.04
32:z:252:LEU:O	32:z:329:VAL:HA	1.70	0.91
8:E:151:MET:CA	8:E:162:ILE:O	2.27	0.77
4:A:888:ILE:HD12	4:A:902:ASN:HD22	1.50	0.77
10:I:615:ALA:HB1	10:I:648:ASN:HD21	1.52	0.74
16:N:107:CYS:HB3	16:N:119:CYS:SG	2.28	0.73
31:1:358:LEU:HD11	32:z:360:ALA:HB1	1.71	0.72
10:I:449:MET:SD	10:I:452:ARG:NH2	2.63	0.70
4:A:1864:ASN:HB3	4:A:1867:LEU:HB2	1.73	0.70
19:M:148:ARG:HH22	20:0:286:GLU:HA	1.57	0.70
31:1:122:LEU:HD11	32:z:669:TYR:HB3	1.73	0.70
4:A:1946:LEU:HB3	4:A:2042:VAL:HB	1.73	0.70
12:L:12:ILE:HD12	12:L:163:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:230:ASP:HB3	8:E:249:MET:HB2	1.74	0.69
4:A:2010:SER:HA	31:1:166:LYS:HE3	1.74	0.68
32:z:639:HIS:HB2	32:z:652:ASP:HB2	1.75	0.68
20:0:205:GLU:OE2	20:0:260:ARG:NH2	2.26	0.68
4:A:1342:SER:HB2	4:A:1351:ARG:HE	1.56	0.68
8:E:244:LEU:HB2	8:E:258:ILE:HD11	1.75	0.68
8:E:109:LEU:CA	8:E:119:PHE:O	2.29	0.67
10:I:721:GLY:H	12:L:365:ARG:HH22	1.40	0.67
6:C:208:ARG:NH2	6:C:216:GLU:O	2.28	0.67
7:D:165:ILE:HG23	7:D:169:MET:HE2	1.77	0.66
32:z:438:LEU:HD11	32:z:463:MET:HG2	1.77	0.66
6:C:163:GLN:HE21	6:C:238:LYS:HE2	1.59	0.66
4:A:1908:ASP:HB3	4:A:1935:PHE:HB2	1.78	0.66
16:N:5:ARG:HB2	16:N:10:ARG:HG2	1.76	0.66
19:M:244:ILE:HB	19:M:278:ALA:HB3	1.78	0.66
18:T:378:ILE:HB	18:T:392:PHE:HB2	1.78	0.65
4:A:450:GLN:O	6:C:304:ARG:NH2	2.29	0.65
31:1:73:THR:HG22	31:1:75:GLY:H	1.60	0.65
4:A:359:LEU:O	4:A:556:HIS:NE2	2.29	0.65
7:D:178:ARG:HG3	7:D:182:GLN:HE22	1.62	0.65
8:E:234:THR:HG21	8:E:285:GLY:H	1.61	0.65
2:5:6:G:O6	2:5:73:A:N6	2.30	0.65
6:C:448:LYS:NZ	6:C:450:SER:OG	2.28	0.65
4:A:1364:ILE:HG12	4:A:1411:LEU:HD13	1.80	0.64
3:6:20:C:N4	20:0:134:CYS:SG	2.70	0.64
9:F:98:ALA:HB2	10:I:604:MET:HE2	1.78	0.64
18:T:341:ASP:HB2	18:T:348:MET:HE3	1.80	0.64
8:E:127:LEU:HB2	8:E:141:TYR:HB2	1.80	0.63
6:C:634:LEU:HD22	6:C:683:MET:HG3	1.80	0.63
16:N:125:ARG:HD2	22:W:115:LEU:HD23	1.79	0.63
6:C:371:TYR:OH	6:C:416:PHE:O	2.16	0.63
3:6:14:U:OP2	4:A:164:ARG:NH2	2.32	0.63
4:A:1772:LEU:HD21	4:A:1854:GLN:HB3	1.80	0.63
6:C:548:GLY:N	6:C:571:ILE:O	2.32	0.62
18:T:255:CYS:HB3	18:T:265:ARG:HB2	1.80	0.62
32:z:637:ILE:HG23	32:z:656:ILE:HD13	1.82	0.62
31:1:410:ARG:NH2	32:z:127:ALA:O	2.32	0.62
34:Z:433:THR:HB	34:Z:436:ARG:HH12	1.63	0.62
6:C:925:GLU:HG3	6:C:938:VAL:HB	1.80	0.62
11:J:236:ILE:HD12	11:J:249:LEU:HD11	1.81	0.62
18:T:402:LEU:HA	18:T:411:PHE:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:111:SER:O	19:M:115:ARG:NH1	2.33	0.62
31:1:204:ILE:HD11	32:z:396:ARG:HB3	1.81	0.62
34:Z:488:ILE:HG22	34:Z:497:LEU:HD11	1.81	0.62
4:A:959:TYR:OH	4:A:1056:GLN:NE2	2.33	0.62
4:A:871:LYS:NZ	18:T:445:GLU:OE2	2.32	0.61
9:F:107:ARG:HA	9:F:110:GLN:HG3	1.83	0.61
11:J:251:ILE:HD11	11:J:285:LEU:HA	1.82	0.61
22:W:454:SER:O	22:W:460:PHE:HA	1.99	0.61
4:A:1722:GLN:HB2	31:1:94:LYS:HZ2	1.63	0.61
22:W:125:ALA:HA	22:W:134:TYR:HB2	1.81	0.61
6:C:540:VAL:O	6:C:591:GLY:N	2.33	0.61
4:A:258:GLN:NE2	4:A:322:PHE:O	2.34	0.61
4:A:520:LEU:HA	6:C:423:LYS:HG2	1.82	0.61
4:A:2019:PRO:HD3	4:A:2068:ARG:HH21	1.65	0.61
6:C:720:CYS:HB2	6:C:860:LEU:HD11	1.82	0.61
6:C:721:TYR:HA	6:C:731:ILE:O	2.01	0.61
9:F:130:LYS:NZ	10:I:647:SER:O	2.33	0.61
19:M:150:LEU:HD11	20:O:266:GLU:HB3	1.83	0.60
4:A:1659:ARG:NH1	31:1:61:ALA:O	2.33	0.60
8:E:193:VAL:HA	8:E:203:TYR:O	2.00	0.60
10:I:582:LEU:HD13	10:I:608:LEU:HD11	1.82	0.60
19:M:30:ASN:O	21:R:206:ARG:NH1	2.34	0.60
9:F:157:ARG:HA	9:F:160:ARG:HE	1.66	0.60
21:R:193:PRO:HA	22:W:75:GLY:HA3	1.83	0.60
3:6:39:G:OP1	12:L:180:ARG:NH2	2.31	0.60
31:1:131:LEU:O	32:z:613:ASN:ND2	2.34	0.60
31:1:208:ARG:HH12	32:z:646:ASP:HA	1.66	0.60
3:6:42:G:OP1	12:L:31:ARG:NH1	2.35	0.60
4:A:1403:GLU:OE2	4:A:1502:TRP:N	2.35	0.60
6:C:792:GLN:O	6:C:836:ARG:HA	2.02	0.60
16:N:101:LYS:NZ	16:N:148:ASP:OXT	2.33	0.60
31:1:20:PRO:HD2	32:z:510:LYS:HZ3	1.67	0.60
4:A:1056:GLN:OE1	4:A:1060:ARG:NH1	2.35	0.60
4:A:2068:ARG:NH1	4:A:2137:ILE:O	2.35	0.59
21:R:207:ILE:HD12	22:W:80:MET:HE1	1.82	0.59
31:1:356:ASP:HB3	31:1:359:ILE:HG12	1.83	0.59
18:T:196:GLU:HG2	18:T:198:ASN:H	1.67	0.59
4:A:409:GLU:O	4:A:415:ARG:NH1	2.34	0.59
20:O:245:ASN:OD1	20:O:247:ARG:NH1	2.35	0.59
31:1:358:LEU:HA	31:1:361:GLU:HG3	1.84	0.59
6:C:854:SER:HA	6:C:857:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:133:ASN:OD1	10:I:616:ARG:NH2	2.36	0.59
19:M:247:ILE:O	19:M:276:HIS:ND1	2.35	0.59
19:M:101:ALA:HB2	20:0:265:ILE:HG22	1.84	0.59
4:A:823:MET:HE2	4:A:861:PRO:HB3	1.85	0.59
20:0:320:ASN:OD1	20:0:321:ALA:N	2.35	0.59
1:2:36:U:O2	1:2:37:A:N6	2.36	0.59
5:B:134:LEU:HD21	7:D:181:TRP:HB3	1.85	0.58
16:N:103:CYS:HB3	16:N:144:CYS:SG	2.43	0.58
21:R:196:GLN:NE2	21:R:199:ASN:O	2.36	0.58
9:F:69:ASN:OD1	10:I:531:ASN:ND2	2.36	0.58
4:A:1256:LYS:NZ	4:A:1297:TRP:O	2.37	0.58
18:T:408:ASN:HB3	18:T:424:TRP:HB3	1.84	0.58
19:M:257:ARG:HH12	20:0:203:GLN:HA	1.67	0.58
31:1:29:PRO:O	32:z:509:ARG:NH2	2.37	0.58
32:z:451:LEU:HB3	32:z:455:MET:HE1	1.86	0.58
6:C:867:ARG:NH2	6:C:951:ASP:OD1	2.37	0.58
3:6:34:A:C2	38:8:7:P5P:C2	2.87	0.58
4:A:1912:VAL:HG22	4:A:1934:ILE:HG12	1.86	0.58
12:L:74:LYS:NZ	21:R:299:GLU:OE2	2.36	0.58
18:T:361:LEU:HG	18:T:372:THR:HG22	1.86	0.58
20:0:101:ASN:HD22	20:0:104:ARG:HE	1.52	0.57
1:2:31:U:O4	32:z:630:ASN:ND2	2.38	0.57
6:C:664:THR:HB	6:C:676:LEU:HB2	1.86	0.57
4:A:1265:SER:O	4:A:1311:ASN:ND2	2.36	0.57
4:A:1832:ILE:HD12	4:A:1861:MET:HE1	1.85	0.57
6:C:894:ARG:NH1	6:C:920:ASP:O	2.38	0.57
22:W:40:ASN:HA	22:W:43:ARG:HD2	1.86	0.57
4:A:2025:LYS:O	4:A:2074:GLN:NE2	2.38	0.57
4:A:649:PHE:O	4:A:675:ARG:NH1	2.36	0.57
32:z:140:MET:HA	32:z:171:ILE:O	2.04	0.57
4:A:725:LEU:HD11	4:A:764:TRP:HZ3	1.70	0.57
20:0:286:GLU:HG2	20:0:288:LYS:HG2	1.87	0.57
22:W:257:ALA:HB3	22:W:271:GLY:H	1.70	0.57
32:z:77:ARG:HD3	32:z:103:ILE:HB	1.85	0.57
9:F:150:ARG:NH1	9:F:151:THR:OG1	2.38	0.57
11:J:43:ARG:NH2	12:L:257:GLN:O	2.38	0.57
32:z:531:LYS:O	32:z:533:ARG:NH1	2.38	0.57
1:2:19:G:N7	23:P:5:HIS:HB3	2.20	0.56
32:z:397:SER:O	32:z:427:GLN:NE2	2.37	0.56
11:J:52:GLU:OE1	12:L:192:ARG:NH2	2.37	0.56
32:z:132:LEU:O	32:z:165:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1637:GLU:OE2	4:A:1660:ARG:NH2	2.38	0.56
10:I:557:SER:OG	10:I:558:TYR:N	2.37	0.56
4:A:823:MET:HB2	18:T:398:ILE:HD11	1.88	0.56
21:R:194:SER:OG	22:W:70:ASN:OD1	2.24	0.56
32:z:254:PHE:CD2	32:z:362:ARG:HD2	2.40	0.56
4:A:1757:GLN:HE21	4:A:1786:LYS:HD3	1.69	0.56
8:E:192:ALA:HB1	8:E:235:LEU:HG	1.87	0.56
8:E:294:ILE:O	8:E:305:ILE:HA	2.04	0.56
34:Z:460:TRP:CD1	34:Z:500:ARG:HH21	2.24	0.56
18:T:360:ALA:HB3	18:T:373:ALA:HB3	1.86	0.56
19:M:269:LEU:HD13	19:M:280:VAL:HG22	1.86	0.56
11:J:244:ALA:HA	11:J:281:ARG:HH12	1.69	0.56
32:z:644:THR:HG22	32:z:645:LYS:H	1.71	0.56
32:z:661:LEU:HD12	32:z:669:TYR:HE2	1.71	0.56
4:A:799:VAL:HB	18:T:229:ILE:HD11	1.88	0.55
11:J:115:ALA:O	11:J:119:ASN:ND2	2.39	0.55
18:T:170:ARG:HD2	18:T:171:PRO:HD2	1.88	0.55
32:z:158:LEU:HD13	32:z:170:ILE:HG13	1.88	0.55
34:Z:351:VAL:HG12	34:Z:354:ARG:HH21	1.70	0.55
4:A:1470:CYS:SG	4:A:1479:HIS:ND1	2.80	0.55
4:A:1725:ASP:O	31:1:92:ARG:NH2	2.39	0.55
10:I:426:GLU:OE2	10:I:430:LYS:NZ	2.38	0.55
8:E:267:HIS:NE2	8:E:270:THR:OG1	2.34	0.55
18:T:193:LEU:HA	18:T:203:ALA:O	2.06	0.55
20:O:196:ARG:NH2	20:O:239:ASP:OD2	2.39	0.55
4:A:588:ARG:HH21	4:A:590:ARG:HD2	1.72	0.55
4:A:509:ALA:HA	6:C:398:ARG:HH12	1.72	0.55
17:S:139:ASP:OD1	17:S:140:ALA:N	2.39	0.55
6:C:445:ILE:HG23	6:C:466:GLN:HE21	1.71	0.55
7:D:178:ARG:O	7:D:182:GLN:NE2	2.40	0.55
17:S:60:GLY:O	17:S:143:ARG:NH2	2.40	0.55
32:z:271:ARG:NH1	32:z:274:SER:OG	2.39	0.55
5:B:155:THR:OG1	5:B:158:GLU:OE1	2.20	0.55
11:J:58:ARG:NH1	12:L:222:ASN:OD1	2.40	0.55
16:N:133:ASP:OD2	20:O:110:ARG:NH1	2.40	0.55
32:z:163:ARG:NH1	32:z:189:ALA:O	2.39	0.55
32:z:365:ARG:O	32:z:365:ARG:NH1	2.40	0.55
6:C:737:PRO:O	6:C:834:LYS:NZ	2.38	0.55
31:1:178:LYS:HD3	31:1:193:THR:H	1.71	0.55
2:5:35:U:O2	33:V:11:ARG:NH2	2.40	0.55
4:A:315:ASP:OD1	4:A:354:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1341:TRP:HB2	4:A:1355:ALA:HB3	1.89	0.54
8:E:321:LYS:N	8:E:343:ASP:OD2	2.32	0.54
12:L:157:GLU:HG3	32:z:501:LYS:HD3	1.87	0.54
20:0:320:ASN:O	20:0:325:ARG:NE	2.38	0.54
8:E:154:THR:HG22	8:E:195:VAL:HG21	1.89	0.54
18:T:407:GLN:OE1	23:P:53:ARG:NH1	2.41	0.54
6:C:255:ASP:HB3	6:C:662:LEU:HD12	1.89	0.54
10:I:627:ARG:HH22	10:I:660:ARG:HH21	1.55	0.54
31:1:140:ARG:NH2	31:1:149:ARG:O	2.41	0.54
4:A:1903:THR:HB	4:A:1985:PRO:HA	1.89	0.54
18:T:297:VAL:HB	18:T:307:HIS:HB2	1.90	0.54
1:2:34:A:OP1	32:z:645:LYS:NZ	2.41	0.54
32:z:116:LYS:HB3	32:z:118:MET:HE3	1.89	0.54
4:A:795:VAL:HG11	23:P:26:ARG:HH21	1.73	0.54
9:F:152:GLU:HA	9:F:155:ILE:HG22	1.89	0.54
16:N:125:ARG:NH2	22:W:115:LEU:O	2.40	0.54
17:S:84:THR:HA	20:0:304:LEU:HD21	1.90	0.54
4:A:384:ASN:HD21	33:V:8:PRO:HB3	1.72	0.54
4:A:1628:LEU:HD23	4:A:1880:LEU:HD11	1.90	0.54
10:I:610:GLU:OE1	10:I:644:LYS:NZ	2.41	0.54
4:A:1361:GLU:OE2	4:A:1410:ASN:ND2	2.40	0.54
9:F:107:ARG:HH12	9:F:108:LYS:HE3	1.73	0.54
12:L:133:LYS:O	12:L:135:ARG:NH1	2.41	0.54
14:Y:541:ASP:N	14:Y:580:ILE:O	2.40	0.54
8:E:231:THR:HB	8:E:249:MET:HG2	1.89	0.54
17:S:113:LEU:HD11	22:W:48:PRO:HG3	1.89	0.54
32:z:639:HIS:N	32:z:651:ARG:O	2.40	0.54
4:A:1767:THR:HA	4:A:1779:ILE:HA	1.88	0.53
18:T:338:ARG:HH21	18:T:347:THR:HG21	1.72	0.53
18:T:405:ASN:HB2	18:T:409:VAL:HB	1.90	0.53
32:z:243:HIS:HE1	32:z:280:GLU:HB3	1.72	0.53
4:A:2082:ARG:NH2	4:A:2089:THR:OG1	2.41	0.53
6:C:722:ALA:HB2	6:C:856:CYS:HB3	1.91	0.53
8:E:119:PHE:HB3	8:E:151:MET:HE1	1.89	0.53
32:z:161:ILE:O	32:z:165:ARG:N	2.31	0.53
4:A:1128:MET:HE1	4:A:1136:ILE:HD12	1.90	0.53
6:C:297:LEU:HB3	6:C:351:VAL:HG22	1.90	0.53
11:J:92:ARG:NE	11:J:116:GLU:OE2	2.39	0.53
17:S:137:PRO:HD3	21:R:99:GLN:HB3	1.90	0.53
16:N:103:CYS:SG	16:N:104:CYS:N	2.81	0.53
18:T:390:GLN:NE2	18:T:425:LYS:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:4:ASP:HA	17:S:16:LEU:O	2.09	0.53
9:F:139:GLU:OE2	9:F:143:ARG:NH2	2.42	0.53
6:C:522:VAL:HG11	6:C:536:ALA:HB1	1.91	0.52
6:C:966:THR:O	6:C:970:THR:OG1	2.26	0.52
10:I:422:ARG:NH1	10:I:450:GLU:OE2	2.42	0.52
34:Z:506:LEU:HG	34:Z:510:LEU:HD23	1.92	0.52
6:C:847:TRP:HD1	6:C:849:ASN:H	1.56	0.52
19:M:270:VAL:HG21	20:O:191:GLU:HB3	1.91	0.52
4:A:449:PRO:HG3	6:C:174:HIS:HB3	1.92	0.52
5:B:245:ASN:OD1	17:S:132:ARG:NH1	2.43	0.52
34:Z:541:MET:HE1	34:Z:543:PRO:HG3	1.90	0.52
6:C:285:ILE:HG21	6:C:330:VAL:HG13	1.91	0.52
17:S:94:ALA:HB1	22:W:44:PRO:HG2	1.90	0.52
31:1:48:GLU:HB3	31:1:56:LYS:HD2	1.91	0.52
32:z:149:ILE:HG21	32:z:402:ILE:HG21	1.90	0.52
4:A:210:MET:HG3	4:A:674:MET:HE2	1.92	0.52
4:A:835:THR:HG23	21:R:260:PRO:HD3	1.91	0.52
4:A:1767:THR:HG22	4:A:1779:ILE:HG12	1.91	0.52
5:B:148:ARG:NH2	9:F:95:GLU:OE1	2.35	0.52
6:C:410:LYS:HG3	6:C:415:ASN:HB2	1.92	0.52
32:z:179:ALA:O	32:z:182:TYR:HB2	2.09	0.52
3:6:6:U:OP2	3:6:7:C:N4	2.43	0.52
7:D:170:GLU:HA	7:D:173:GLU:HG3	1.92	0.52
22:W:521:ILE:HA	22:W:538:GLY:HA2	1.92	0.52
32:z:253:VAL:HG22	32:z:330:ILE:HD13	1.92	0.52
4:A:195:LYS:O	16:N:44:LYS:NZ	2.42	0.52
11:J:217:GLU:O	21:R:25:ARG:NH1	2.42	0.52
32:z:395:GLN:HG2	32:z:424:PRO:HD3	1.91	0.52
3:6:83:A:O2'	5:B:173:ARG:NH1	2.40	0.52
5:B:149:LYS:NZ	9:F:81:PHE:O	2.42	0.52
6:C:600:ASP:O	6:C:658:LYS:NZ	2.40	0.52
12:L:38:ARG:NH2	12:L:159:GLU:OE2	2.43	0.52
4:A:148:LYS:HG2	8:E:207:ILE:HD12	1.92	0.52
10:I:629:VAL:O	10:I:634:ARG:NH2	2.44	0.51
4:A:647:TYR:O	4:A:682:LYS:NZ	2.41	0.51
6:C:519:VAL:HG12	6:C:542:SER:HB3	1.93	0.51
16:N:125:ARG:NH2	22:W:119:ARG:HB2	2.25	0.51
18:T:171:PRO:HG2	18:T:485:ILE:HG21	1.93	0.51
6:C:715:MET:SD	6:C:715:MET:N	2.80	0.51
6:C:850:TYR:HD1	6:C:853:ARG:HH22	1.58	0.51
12:L:283:PRO:HB2	12:L:287:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1432:SER:HB2	38:8:-5:Y5P:OP1	2.10	0.51
4:A:1803:ILE:HD13	4:A:1833:ASP:HB2	1.92	0.51
11:J:554:ILE:HA	11:J:577:ALA:HB1	1.92	0.51
19:M:20:PRO:HB2	19:M:22:VAL:HG23	1.92	0.51
4:A:1582:TRP:H	4:A:1582:TRP:CD1	2.29	0.51
5:B:322:ARG:NH1	5:B:325:MET:SD	2.84	0.51
8:E:320:HIS:CG	8:E:341:SER:HG	2.29	0.51
31:1:178:LYS:HE2	31:1:192:GLU:HG3	1.92	0.51
23:P:223:VAL:O	23:P:226:LYS:NZ	2.38	0.51
6:C:867:ARG:HE	6:C:952:PRO:HD2	1.75	0.51
8:E:79:SER:OG	8:E:81:ASP:OD1	2.28	0.51
9:F:158:MET:HG3	9:F:162:ARG:HH21	1.74	0.51
10:I:476:ASP:HB3	10:I:479:ASP:HB2	1.92	0.51
18:T:313:THR:OG1	18:T:334:ASP:OD2	2.28	0.51
31:1:171:ILE:HG23	32:z:415:LEU:HA	1.93	0.51
32:z:96:GLY:O	32:z:113:THR:OG1	2.29	0.51
20:0:206:ARG:HB2	20:0:219:THR:HB	1.92	0.51
4:A:148:LYS:HE3	8:E:207:ILE:HB	1.93	0.50
10:I:365:ALA:H	10:I:399:GLY:HA3	1.75	0.50
11:J:246:ASP:OD2	11:J:248:ARG:NH1	2.44	0.50
31:1:178:LYS:HA	31:1:193:THR:HA	1.92	0.50
18:T:438:GLN:HE21	23:P:243:ASN:HB2	1.76	0.50
19:M:80:ASN:HD21	19:M:90:GLN:HE22	1.60	0.50
34:Z:367:PRO:HB2	34:Z:407:LEU:HD23	1.93	0.50
32:z:475:GLY:HA3	32:z:589:LYS:HE2	1.93	0.50
32:z:504:THR:HA	32:z:507:VAL:HG22	1.93	0.50
32:z:594:LEU:O	32:z:598:TYR:N	2.44	0.50
8:E:240:ASP:OD1	8:E:240:ASP:N	2.44	0.50
32:z:229:GLU:HB3	32:z:234:LYS:HZ1	1.77	0.50
4:A:251:ILE:HG22	4:A:253:PRO:HD2	1.94	0.50
4:A:1101:ASN:HB2	4:A:1305:TYR:HB3	1.93	0.50
4:A:1497:ARG:NH2	34:Z:398:GLU:OE2	2.44	0.50
4:A:1537:ASP:OD1	4:A:1537:ASP:N	2.40	0.50
8:E:165:SER:OG	8:E:167:ASP:OD1	2.25	0.50
10:I:722:ASN:HD22	12:L:368:ARG:HE	1.58	0.50
32:z:150:SER:HA	32:z:153:ILE:HG22	1.93	0.50
32:z:285:LEU:HD13	32:z:299:VAL:HA	1.93	0.50
34:Z:467:GLN:OE1	34:Z:469:THR:OG1	2.25	0.50
3:6:52:G:O2'	3:6:54:C:OP1	2.24	0.50
19:M:242:LEU:HB2	19:M:280:VAL:HB	1.94	0.50
32:z:342:PRO:O	32:z:430:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:8:4:Y5P:H2'	38:8:5:P5P:O4'	2.12	0.50
4:A:914:GLU:OE2	4:A:917:ARG:NH2	2.42	0.50
4:A:1494:ASN:H	34:Z:363:SER:HA	1.76	0.50
32:z:142:ASP:HA	32:z:173:SER:HB3	1.93	0.50
32:z:176:THR:OG1	32:z:177:LEU:N	2.45	0.50
4:A:1510:GLN:HG3	35:CY:365:LEU:HD22	1.94	0.49
4:A:2003:LEU:HD12	4:A:2011:ILE:HD11	1.94	0.49
5:B:292:THR:HG23	5:B:302:ASN:HD22	1.77	0.49
10:I:587:GLU:OE2	10:I:624:ARG:NH2	2.42	0.49
21:R:76:GLU:HG2	21:R:77:ILE:HD12	1.94	0.49
22:W:121:ASP:N	22:W:121:ASP:OD1	2.42	0.49
4:A:249:ARG:NH1	4:A:338:SER:O	2.45	0.49
5:B:180:ASP:OD1	5:B:180:ASP:N	2.44	0.49
17:S:6:ALA:O	17:S:153:ALA:CA	2.46	0.49
4:A:1071:ASP:OD2	4:A:1562:GLY:N	2.44	0.49
19:M:103:GLU:HG3	19:M:104:LEU:HG	1.94	0.49
31:1:155:MET:HA	31:1:158:LYS:HG2	1.93	0.49
31:1:362:ILE:HG23	31:1:363:ILE:HD12	1.94	0.49
4:A:1913:TYR:HE1	4:A:1929:PRO:HB3	1.76	0.49
11:J:192:ALA:HA	11:J:195:ILE:HD12	1.95	0.49
31:1:415:GLY:HA3	32:z:164:LYS:HE2	1.94	0.49
4:A:1326:LYS:O	4:A:1330:GLN:NE2	2.46	0.49
8:E:259:ARG:O	8:E:266:ARG:NH2	2.44	0.49
16:N:18:SER:HA	16:N:21:GLU:HG2	1.93	0.49
32:z:140:MET:HE1	32:z:142:ASP:HB3	1.94	0.49
32:z:258:ARG:HG3	32:z:288:TYR:CE1	2.48	0.49
32:z:500:ASP:HB3	32:z:503:LYS:HB2	1.94	0.49
4:A:552:PRO:HB2	4:A:555:LYS:HB2	1.94	0.49
4:A:1973:ALA:HB2	4:A:2002:ASN:HB3	1.95	0.49
21:R:180:VAL:HG11	21:R:217:PRO:HG3	1.95	0.49
4:A:1214:LEU:HB2	4:A:1225:PHE:HB3	1.93	0.49
34:Z:367:PRO:HG3	34:Z:404:PHE:HA	1.95	0.49
34:Z:523:THR:HA	34:Z:526:ILE:HD12	1.94	0.49
4:A:1199:LEU:HD22	4:A:1214:LEU:HD22	1.94	0.49
10:I:482:LEU:HD23	10:I:486:GLN:HE21	1.78	0.49
19:M:77:ARG:HA	22:W:73:LEU:HD11	1.94	0.49
34:Z:504:GLU:HA	34:Z:507:GLN:HG2	1.94	0.49
6:C:509:MET:HE2	6:C:519:VAL:HG21	1.93	0.49
10:I:532:TYR:CG	10:I:548:ILE:HG12	2.48	0.49
32:z:183:ARG:HG3	32:z:209:ILE:HD11	1.95	0.49
16:N:125:ARG:HH22	22:W:119:ARG:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:z:73:THR:HG22	32:z:123:LEU:HD12	1.95	0.49
32:z:439:GLY:O	32:z:441:LEU:N	2.46	0.49
3:6:14:U:H3	16:N:127:GLN:HE22	1.61	0.48
4:A:1534:ASP:OD1	4:A:1534:ASP:N	2.42	0.48
6:C:154:MET:HE1	6:C:576:ILE:HD13	1.94	0.48
20:0:187:THR:H	20:0:190:ILE:HD11	1.78	0.48
21:R:230:ARG:HH12	23:P:13:ARG:HB2	1.77	0.48
32:z:22:PRO:HA	32:z:25:LYS:HE2	1.94	0.48
10:I:550:GLU:OE1	11:J:294:LYS:HG3	2.13	0.48
17:S:42:THR:HG22	17:S:58:PRO:HA	1.95	0.48
23:P:255:MET:HE3	23:P:255:MET:HB3	1.73	0.48
31:1:361:GLU:HA	31:1:364:ALA:HB3	1.95	0.48
32:z:252:LEU:O	32:z:329:VAL:CA	2.53	0.48
1:2:33:U:O2	32:z:623:HIS:NE2	2.46	0.48
4:A:1176:ASP:OD1	4:A:1215:TYR:OH	2.26	0.48
4:A:1445:THR:HB	4:A:1451:GLY:HA3	1.94	0.48
4:A:2090:GLN:HB2	4:A:2093:HIS:HB2	1.94	0.48
32:z:45:GLN:O	32:z:50:LYS:NZ	2.42	0.48
4:A:932:GLU:OE1	4:A:1291:SER:OG	2.31	0.48
6:C:154:MET:HE3	6:C:158:MET:HE3	1.94	0.48
9:F:110:GLN:HA	9:F:113:GLN:HG3	1.95	0.48
18:T:336:THR:HG22	18:T:352:THR:HG22	1.95	0.48
32:z:497:HIS:ND1	32:z:543:MET:SD	2.86	0.48
2:5:92:G:N2	2:5:94:A:O3'	2.46	0.48
6:C:328:ASN:ND2	6:C:344:LEU:O	2.38	0.48
6:C:456:PRO:O	6:C:460:MET:HB2	2.12	0.48
19:M:312:ILE:O	19:M:314:ARG:NH1	2.46	0.48
31:1:159:LEU:HD11	32:z:432:LEU:HD13	1.95	0.48
34:Z:506:LEU:HD12	34:Z:509:TYR:HB2	1.95	0.48
5:B:265:ASP:OD2	11:J:148:TYR:OH	2.29	0.48
11:J:138:ARG:NH1	21:R:241:HIS:O	2.46	0.48
6:C:919:ILE:HD12	6:C:922:PHE:HE2	1.77	0.48
8:E:210:ASP:OD1	8:E:210:ASP:N	2.44	0.48
18:T:425:LYS:HE3	18:T:425:LYS:HB2	1.70	0.48
32:z:404:LEU:HD21	32:z:456:ALA:HA	1.96	0.48
4:A:984:ASN:N	4:A:987:GLN:OE1	2.46	0.48
9:F:94:LEU:HD11	10:I:604:MET:HG3	1.95	0.48
10:I:558:TYR:HA	10:I:561:ALA:HB3	1.96	0.48
18:T:290:GLY:O	18:T:293:GLY:N	2.43	0.48
20:0:110:ARG:NH2	20:0:135:ASP:OD1	2.45	0.48
32:z:435:LEU:HB3	32:z:441:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:19:U:H5''	19:M:65:ARG:HH11	1.79	0.48
4:A:519:GLU:O	6:C:427:HIS:NE2	2.46	0.48
4:A:1934:ILE:HB	4:A:1947:LYS:HB3	1.96	0.48
6:C:195:LEU:HD11	6:C:207:LEU:HD13	1.95	0.48
21:R:61:ARG:O	21:R:63:ARG:NE	2.47	0.48
4:A:1106:THR:HB	4:A:1300:THR:HG22	1.96	0.48
4:A:1405:ALA:HA	4:A:1411:LEU:HD23	1.95	0.48
3:6:42:G:H1'	12:L:169:ARG:HH11	1.79	0.47
4:A:1200:GLN:NE2	35:CY:367:GLY:O	2.42	0.47
6:C:630:THR:HB	6:C:942:PHE:HB3	1.95	0.47
10:I:434:LYS:NZ	10:I:438:GLU:OE2	2.38	0.47
6:C:509:MET:HE2	6:C:519:VAL:HG11	1.96	0.47
6:C:552:ARG:HG3	6:C:612:LYS:HA	1.95	0.47
8:E:254:ARG:HG2	8:E:270:THR:HG23	1.96	0.47
11:J:32:ARG:NH2	12:L:167:ARG:HG2	2.29	0.47
15:q:31:TYR:O	15:q:35:HIS:N	2.43	0.47
19:M:234:PRO:HG2	19:M:239:ILE:HD12	1.96	0.47
32:z:97:LYS:HD2	32:z:98:GLU:HG3	1.97	0.47
4:A:1907:ILE:HD11	4:A:1988:LEU:HD22	1.96	0.47
6:C:874:SER:HB3	6:C:943:ASP:HB2	1.97	0.47
8:E:245:LEU:HD22	8:E:294:ILE:HD12	1.96	0.47
19:M:251:LEU:HD12	19:M:252:PRO:HD2	1.96	0.47
31:1:41:TYR:OH	32:z:607:PRO:O	2.32	0.47
2:5:86:A:N6	26:l:42:SER:O	2.44	0.47
3:6:39:G:H4'	12:L:177:LYS:HG3	1.96	0.47
4:A:1203:ASP:OD1	4:A:1203:ASP:N	2.47	0.47
4:A:1473:THR:OG1	4:A:1476:GLY:O	2.32	0.47
6:C:247:THR:HB	6:C:257:VAL:HG22	1.96	0.47
4:A:944:LEU:HD13	12:L:393:LEU:HD11	1.96	0.47
4:A:1551:GLN:O	4:A:1554:ARG:NH1	2.47	0.47
6:C:745:ASP:OD2	6:C:768:TYR:OH	2.33	0.47
32:z:93:CYS:HB2	32:z:97:LYS:HE3	1.96	0.47
34:Z:359:LEU:O	34:Z:363:SER:OG	2.26	0.47
32:z:251:ILE:HB	32:z:310:VAL:HG12	1.96	0.47
4:A:518:GLU:HB3	6:C:427:HIS:CE1	2.50	0.47
4:A:679:ARG:HD2	4:A:716:THR:HG22	1.96	0.47
4:A:847:TRP:O	4:A:912:LYS:NZ	2.40	0.47
4:A:1341:TRP:CD1	4:A:1503:GLU:HB2	2.49	0.47
4:A:1465:SER:O	4:A:1798:TYR:OH	2.30	0.47
4:A:1618:LYS:O	4:A:1837:ASN:ND2	2.47	0.47
4:A:1711:LYS:HD2	31:1:107:PHE:HD1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1788:TRP:NE1	4:A:1824:SER:O	2.38	0.47
6:C:223:ILE:HG13	6:C:224:LYS:HG2	1.97	0.47
9:F:122:LEU:HA	10:I:683:ARG:HH22	1.80	0.47
20:O:140:LEU:HD12	20:O:141:PRO:HD2	1.97	0.47
20:O:190:ILE:HD12	20:O:211:ASN:HB3	1.97	0.47
21:R:54:TYR:HA	21:R:57:ARG:HH12	1.80	0.47
32:z:74:GLN:HE22	32:z:83:LEU:HD12	1.79	0.47
32:z:125:ARG:NH1	32:z:458:LEU:O	2.47	0.47
31:1:145:MET:HE2	31:1:145:MET:HB3	1.84	0.47
32:z:513:ALA:H	32:z:520:THR:HG22	1.80	0.47
5:B:123:LEU:HB3	7:D:191:LYS:HE2	1.97	0.47
5:B:263:VAL:O	5:B:267:ARG:HG2	2.15	0.47
6:C:561:ASP:N	6:C:561:ASP:OD1	2.44	0.47
6:C:851:SER:O	6:C:855:THR:OG1	2.29	0.47
12:L:214:ARG:NH1	12:L:218:GLN:O	2.36	0.47
20:O:181:VAL:HG12	20:O:184:ILE:HD11	1.96	0.47
6:C:535:TYR:HB3	6:C:595:LEU:HG	1.97	0.47
9:F:137:LYS:HB3	9:F:141:LYS:NZ	2.30	0.47
17:S:136:VAL:HG11	17:S:148:ILE:HD11	1.95	0.47
31:1:209:LYS:NZ	31:1:211:ASP:O	2.47	0.47
32:z:225:ASP:OD1	32:z:225:ASP:N	2.47	0.47
32:z:229:GLU:HB3	32:z:234:LYS:NZ	2.30	0.47
6:C:520:VAL:HG22	6:C:540:VAL:HA	1.97	0.46
19:M:47:CYS:HB3	19:M:75:CYS:SG	2.55	0.46
4:A:712:VAL:O	4:A:716:THR:OG1	2.32	0.46
6:C:446:PHE:O	6:C:466:GLN:NE2	2.37	0.46
4:A:1722:GLN:HB2	31:1:94:LYS:NZ	2.30	0.46
4:A:1766:VAL:HG21	4:A:1826:THR:HG21	1.96	0.46
6:C:951:ASP:HB3	6:C:954:ASP:HB2	1.97	0.46
8:E:257:ASP:HB2	8:E:266:ARG:HB3	1.97	0.46
16:N:50:PRO:O	16:N:53:GLN:HB2	2.15	0.46
34:Z:385:PRO:HG3	34:Z:422:LEU:HD21	1.97	0.46
11:J:92:ARG:NH2	12:L:245:ASN:OD1	2.34	0.46
17:S:8:GLU:N	17:S:152:ARG:O	2.40	0.46
18:T:279:LEU:HD22	18:T:300:MET:HE2	1.97	0.46
21:R:310:GLU:OE1	21:R:313:ARG:NH2	2.48	0.46
22:W:255:ILE:HA	22:W:272:SER:HA	1.97	0.46
32:z:592:ARG:HA	32:z:595:THR:HG22	1.98	0.46
4:A:308:MET:HE1	4:A:355:LEU:HD22	1.98	0.46
4:A:1558:SER:HB3	35:CY:353:TYR:HB2	1.96	0.46
8:E:247:TYR:CD2	8:E:296:VAL:HG11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Z:344:ASP:HB3	34:Z:347:ASN:HA	1.97	0.46
4:A:660:LYS:HE2	38:8:5:P5P:OP2	2.15	0.46
6:C:638:VAL:HG12	6:C:701:VAL:HG22	1.96	0.46
32:z:561:ARG:HB3	32:z:565:ARG:HH12	1.81	0.46
4:A:273:ARG:NH2	4:A:275:LEU:O	2.42	0.46
4:A:719:TYR:HA	4:A:725:LEU:HD23	1.97	0.46
4:A:1351:ARG:NH1	34:Z:490:GLU:O	2.48	0.46
6:C:213:HIS:HE2	6:C:693:LEU:HD11	1.79	0.46
6:C:518:LEU:N	6:C:611:ASP:OD2	2.49	0.46
17:S:90:SER:HB2	17:S:104:PHE:HB3	1.96	0.46
19:M:112:GLU:HB3	19:M:113:ILE:HD12	1.97	0.46
38:8:12:Y5P:H6	38:8:12:Y5P:H2'	1.68	0.46
3:6:37:G:H1	31:1:55:ARG:HG3	1.81	0.46
7:D:185:ILE:HA	7:D:188:THR:HG22	1.97	0.46
8:E:65:THR:HG21	8:E:108:ASP:HA	1.98	0.46
10:I:745:ASN:OD1	12:L:300:ARG:NH1	2.47	0.46
20:0:313:VAL:HG13	22:W:51:PRO:HB2	1.98	0.46
34:Z:526:ILE:HD11	34:Z:541:MET:HE3	1.98	0.46
4:A:964:LYS:HD2	4:A:1559:PHE:HE2	1.81	0.46
10:I:674:CYS:SG	10:I:697:ALA:HB2	2.56	0.46
11:J:265:ARG:O	11:J:269:ILE:HG12	2.16	0.46
16:N:120:ILE:HD12	19:M:61:ARG:HD2	1.98	0.46
20:0:233:MET:HE2	20:0:233:MET:HB3	1.83	0.46
39:Cc:739:LYS:HA	39:Cc:740:GLY:HA2	1.75	0.46
4:A:351:ASN:C	4:A:351:ASN:HD22	2.24	0.46
19:M:63:HIS:CE1	19:M:65:ARG:HB2	2.51	0.46
19:M:80:ASN:ND2	19:M:90:GLN:HE22	2.14	0.46
6:C:254:VAL:O	6:C:257:VAL:HB	2.16	0.45
7:D:168:GLU:HA	7:D:171:LYS:HG2	1.98	0.45
17:S:9:THR:HG21	17:S:133:MET:HE1	1.97	0.45
18:T:197:PRO:HG3	18:T:239:PRO:HA	1.98	0.45
18:T:199:ASN:O	18:T:199:ASN:ND2	2.48	0.45
21:R:213:ARG:NH1	21:R:214:GLN:O	2.49	0.45
32:z:154:LEU:HA	32:z:157:LEU:HG	1.99	0.45
2:5:104:G:H1	2:5:110:C:H42	1.64	0.45
4:A:1488:GLU:OE2	34:Z:378:LYS:N	2.49	0.45
6:C:154:MET:HG3	6:C:231:VAL:HG23	1.98	0.45
32:z:341:ASN:O	32:z:345:GLY:CA	2.64	0.45
32:z:458:LEU:HB3	32:z:460:VAL:HG12	1.98	0.45
4:A:1936:ILE:HD11	4:A:1972:VAL:HG22	1.99	0.45
6:C:181:MET:HG2	6:C:210:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:251:VAL:HG12	6:C:280:ASN:HB2	1.98	0.45
6:C:575:PHE:HB2	6:C:595:LEU:HB3	1.98	0.45
6:C:759:LYS:HA	6:C:762:LYS:HE3	1.97	0.45
10:I:619:MET:HE3	10:I:648:ASN:HD22	1.80	0.45
11:J:22:ALA:HB1	12:L:19:ALA:HB2	1.98	0.45
12:L:22:SER:OG	21:R:272:ILE:O	2.32	0.45
32:z:449:ARG:HH21	32:z:453:LEU:HD21	1.80	0.45
4:A:980:LYS:HB2	31:1:279:GLY:HA2	1.97	0.45
31:1:406:ASP:OD1	31:1:406:ASP:N	2.47	0.45
32:z:50:LYS:O	32:z:54:ILE:HB	2.17	0.45
32:z:515:GLU:HB2	32:z:519:LEU:HD12	1.98	0.45
4:A:387:LEU:HD21	4:A:428:VAL:HG21	1.99	0.45
4:A:1716:VAL:HG23	4:A:1860:ILE:HD12	1.98	0.45
17:S:84:THR:HG22	21:R:81:GLN:HB2	1.97	0.45
4:A:910:TRP:CD1	23:P:259:VAL:HG11	2.52	0.45
6:C:524:LYS:HD2	6:C:524:LYS:HA	1.79	0.45
32:z:253:VAL:HG13	32:z:330:ILE:HB	1.98	0.45
4:A:976:ALA:HB1	4:A:1574:LEU:HD21	1.97	0.45
4:A:1018:PHE:O	12:L:81:ARG:NH2	2.50	0.45
4:A:1072:SER:OG	4:A:1073:GLU:OE2	2.35	0.45
4:A:1374:ILE:O	4:A:1378:SER:OG	2.24	0.45
8:E:156:ARG:HH22	8:E:197:GLU:HB3	1.82	0.45
9:F:124:ILE:HG12	12:L:330:GLY:HA3	1.98	0.45
19:M:244:ILE:HG12	19:M:308:ILE:HG12	1.97	0.45
32:z:34:VAL:HG11	32:z:58:LEU:HD11	1.99	0.45
4:A:276:PHE:HB3	4:A:752:PRO:HG2	1.99	0.45
6:C:761:ALA:HA	6:C:775:ALA:HB1	1.99	0.45
7:D:189:GLU:HA	7:D:192:GLN:HG3	1.99	0.45
8:E:185:GLU:N	8:E:185:GLU:OE1	2.49	0.45
4:A:673:LEU:HD23	4:A:775:LEU:HD13	1.98	0.45
9:F:61:VAL:HG23	9:F:62:LEU:HD12	1.97	0.45
23:P:46:ASP:OD1	23:P:46:ASP:N	2.48	0.45
31:1:278:THR:OG1	31:1:279:GLY:N	2.50	0.45
4:A:728:GLN:HG2	4:A:767:PHE:HB2	1.98	0.45
4:A:1055:TYR:HE1	4:A:1059:GLN:HE21	1.64	0.45
4:A:1519:LYS:O	4:A:1523:ALA:HB2	2.17	0.45
4:A:1557:LEU:HD21	31:1:226:LEU:HD21	1.99	0.45
32:z:167:ASP:OD1	32:z:167:ASP:N	2.48	0.45
6:C:154:MET:HG2	6:C:241:LEU:HD12	1.99	0.44
11:J:16:ALA:HA	12:L:153:ILE:HD13	1.98	0.44
4:A:964:LYS:NZ	35:CY:349:GLU:OE2	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1486:HIS:HE1	34:Z:353:LEU:HD13	1.82	0.44
5:B:151:ALA:HA	5:B:154:TRP:CD1	2.52	0.44
8:E:214:TRP:HA	8:E:221:VAL:HA	1.99	0.44
12:L:35:LEU:HD23	12:L:35:LEU:HA	1.82	0.44
20:O:290:PRO:HA	20:O:293:ARG:HE	1.82	0.44
21:R:178:VAL:HB	21:R:180:VAL:HG22	1.99	0.44
32:z:230:ASP:H	32:z:234:LYS:HZ3	1.65	0.44
32:z:341:ASN:O	32:z:345:GLY:HA2	2.18	0.44
1:2:15:U:OP2	3:6:76:U:O2'	2.35	0.44
4:A:251:ILE:HG12	4:A:545:MET:SD	2.57	0.44
4:A:1719:ASP:OD1	31:1:102:GLN:NE2	2.42	0.44
6:C:470:PRO:HG2	6:C:472:THR:HG23	1.99	0.44
6:C:480:LYS:HB2	6:C:480:LYS:HE3	1.85	0.44
17:S:85:GLY:H	17:S:88:ILE:HD12	1.82	0.44
12:L:375:HIS:NE2	12:L:379:GLU:OE2	2.51	0.44
17:S:52:MET:HG3	17:S:104:PHE:CE2	2.52	0.44
17:S:86:ALA:HB3	21:R:83:PRO:HG2	2.00	0.44
32:z:337:LEU:HD23	32:z:352:THR:HB	2.00	0.44
34:Z:358:TYR:HB2	34:Z:390:MET:HE2	1.99	0.44
38:8:10:Y5P:H4A	38:8:11:Y5P:H4	1.98	0.44
2:5:95:A:H4'	27:m:48:SER:HA	1.99	0.44
4:A:1564:ARG:NH1	4:A:1582:TRP:O	2.51	0.44
11:J:43:ARG:HE	11:J:44:PHE:H	1.64	0.44
11:J:56:ARG:HD3	12:L:192:ARG:NH1	2.33	0.44
12:L:319:SER:OG	12:L:322:GLU:OE1	2.25	0.44
32:z:287:LEU:HA	32:z:291:LEU:HD11	1.99	0.44
4:A:496:ASN:O	4:A:498:GLU:N	2.51	0.44
4:A:1515:GLU:HB3	4:A:1519:LYS:NZ	2.33	0.44
32:z:83:LEU:HD23	32:z:83:LEU:HA	1.88	0.44
2:5:11:C:H5''	4:A:338:SER:HB3	1.99	0.44
19:M:307:ARG:HB2	19:M:334:ALA:HB2	1.98	0.44
34:Z:380:PRO:HB2	34:Z:383:GLN:HE22	1.83	0.44
6:C:539:ARG:HA	6:C:592:ASN:O	2.18	0.44
10:I:441:ASP:HA	10:I:444:ILE:HG12	1.98	0.44
20:O:110:ARG:HD3	20:O:133:ASP:HA	2.00	0.44
32:z:222:LEU:HD12	32:z:375:PHE:HE1	1.82	0.44
34:Z:372:HIS:HD2	34:Z:373:LYS:HD3	1.82	0.44
6:C:733:MET:HE1	6:C:857:LEU:HD23	2.00	0.44
19:M:311:SER:HB3	19:M:314:ARG:HH12	1.83	0.44
32:z:287:LEU:HB2	32:z:311:ILE:HD11	2.00	0.44
3:6:11:G:OP1	4:A:154:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1216:THR:HG22	4:A:1223:TRP:HB2	2.00	0.43
4:A:1564:ARG:HH22	4:A:1588:ASP:CG	2.26	0.43
4:A:1645:LEU:HD23	4:A:1650:ARG:HD3	1.99	0.43
6:C:455:ASP:HB2	6:C:458:VAL:HG22	2.00	0.43
9:F:154:ALA:O	9:F:157:ARG:HD3	2.18	0.43
10:I:489:HIS:O	10:I:495:TRP:NE1	2.45	0.43
16:N:22:GLU:O	16:N:26:ILE:HG13	2.17	0.43
28:o:14:THR:HA	28:o:28:THR:HA	2.00	0.43
31:1:157:VAL:O	31:1:161:LYS:HG2	2.16	0.43
32:z:468:LEU:HD21	32:z:484:ALA:HB2	2.00	0.43
32:z:506:SER:O	32:z:510:LYS:N	2.51	0.43
6:C:243:ASN:HB3	6:C:593:PHE:CD2	2.53	0.43
6:C:972:ARG:NH2	6:C:987:ASP:OD2	2.51	0.43
8:E:234:THR:O	8:E:235:LEU:HD23	2.18	0.43
8:E:289:LYS:NZ	8:E:331:PRO:O	2.45	0.43
9:F:70:TYR:N	10:I:500:ASP:OD2	2.51	0.43
20:0:114:ARG:HH21	20:0:115:PRO:HG2	1.83	0.43
20:0:206:ARG:HH21	20:0:260:ARG:HD3	1.83	0.43
31:1:418:GLN:NE2	32:z:410:GLY:O	2.46	0.43
34:Z:369:GLU:HB3	34:Z:373:LYS:NZ	2.33	0.43
5:B:260:ASP:OD1	11:J:120:ARG:NH1	2.36	0.43
10:I:472:ARG:HD2	10:I:472:ARG:HA	1.82	0.43
10:I:688:ASP:N	10:I:688:ASP:OD1	2.51	0.43
11:J:43:ARG:NH2	12:L:254:PRO:O	2.51	0.43
12:L:21:VAL:HG12	21:R:274:LEU:HD21	2.00	0.43
12:L:727:ALA:HB1	13:K:9:GLU:HA	2.00	0.43
14:Y:694:ARG:O	14:Y:725:PRO:HA	2.18	0.43
32:z:407:LYS:HD2	32:z:412:ASP:HA	2.01	0.43
4:A:1519:LYS:O	4:A:1523:ALA:CB	2.66	0.43
5:B:175:ASP:OD2	5:B:183:ARG:NH2	2.51	0.43
31:1:165:TRP:HD1	32:z:415:LEU:HD13	1.84	0.43
31:1:343:ARG:NH2	32:z:246:GLU:OE2	2.51	0.43
10:I:477:TYR:O	10:I:487:ARG:NH1	2.51	0.43
19:M:275:THR:HG23	19:M:319:MET:HG2	1.99	0.43
31:1:32:ASP:HB2	31:1:35:VAL:HG22	2.00	0.43
32:z:341:ASN:O	32:z:345:GLY:N	2.51	0.43
4:A:1531:THR:HA	31:1:297:VAL:HG12	2.00	0.43
6:C:710:GLU:HG2	6:C:825:LEU:HB3	2.01	0.43
18:T:291:ARG:HA	18:T:315:THR:HG23	2.01	0.43
19:M:88:ASP:OD2	19:M:98:ARG:HG3	2.19	0.43
31:1:282:ASP:OD1	31:1:282:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:z:107:ASP:OD1	32:z:107:ASP:N	2.52	0.43
32:z:128:LEU:HD11	32:z:408:ALA:HB1	2.00	0.43
4:A:650:ASN:OD1	4:A:679:ARG:NH2	2.51	0.43
6:C:666:LYS:HB3	6:C:666:LYS:HE2	1.73	0.43
6:C:979:ARG:NH1	6:C:986:GLU:O	2.52	0.43
11:J:32:ARG:HH22	12:L:167:ARG:HG2	1.84	0.43
11:J:291:THR:O	11:J:295:GLN:HB2	2.18	0.43
32:z:251:ILE:HD11	32:z:308:ARG:HH11	1.83	0.43
4:A:842:GLU:OE1	21:R:262:SER:OG	2.35	0.43
4:A:1493:PRO:HA	34:Z:363:SER:HB3	2.00	0.43
5:B:208:LYS:O	5:B:212:ILE:HG12	2.18	0.43
8:E:86:LEU:HB3	8:E:96:TYR:CZ	2.54	0.43
8:E:134:THR:O	29:p:111:THR:OG1	2.33	0.43
9:F:98:ALA:HA	9:F:101:LEU:HB2	2.01	0.43
12:L:160:LYS:HA	12:L:160:LYS:HD2	1.81	0.43
32:z:528:PHE:CD2	32:z:549:MET:HE1	2.53	0.43
4:A:1430:LEU:HA	4:A:1430:LEU:HD23	1.73	0.43
6:C:272:ASP:OD1	6:C:301:LYS:HD2	2.19	0.43
10:I:675:LEU:HD21	10:I:709:PHE:HD1	1.82	0.43
4:A:1547:ASN:HB2	31:1:294:TYR:CE1	2.54	0.43
4:A:1549:LEU:HD22	35:CY:354:GLU:HG2	2.01	0.43
6:C:168:ALA:HB2	6:C:264:VAL:HG11	2.01	0.43
7:D:155:GLU:OE2	12:L:292:LYS:NZ	2.40	0.43
8:E:288:SER:OG	8:E:289:LYS:N	2.52	0.43
10:I:603:LEU:HD23	10:I:603:LEU:HA	1.81	0.43
18:T:419:MET:HB2	18:T:433:LEU:HB2	2.01	0.43
34:Z:438:GLU:HB2	34:Z:441:LYS:HD3	2.00	0.43
4:A:1963:LEU:HA	4:A:1966:TRP:HB2	2.00	0.42
10:I:623:GLU:O	10:I:626:THR:OG1	2.28	0.42
18:T:175:PRO:HG2	18:T:474:GLU:HG2	2.01	0.42
22:W:119:ARG:NH2	22:W:137:PRO:O	2.52	0.42
17:S:22:HIS:ND1	17:S:81:LEU:HD11	2.34	0.42
21:R:243:PRO:HA	21:R:244:PRO:HD3	1.88	0.42
32:z:450:PRO:HB2	32:z:451:LEU:HD12	2.01	0.42
32:z:516:GLY:HA3	32:z:654:THR:HG23	2.00	0.42
32:z:667:ASP:N	32:z:667:ASP:OD1	2.45	0.42
5:B:284:SER:OG	5:B:299:LYS:NZ	2.50	0.42
8:E:294:ILE:HG12	8:E:308:SER:HB3	2.02	0.42
10:I:658:TYR:O	10:I:662:ILE:HG12	2.18	0.42
16:N:60:ARG:NH2	16:N:100:GLU:O	2.52	0.42
21:R:188:PHE:HA	21:R:208:ILE:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:o:23:ALA:HA	28:o:46:THR:O	2.19	0.42
32:z:535:GLU:OE1	32:z:538:TRP:N	2.44	0.42
4:A:1287:ARG:HG2	23:P:223:VAL:HG11	2.01	0.42
4:A:1395:ILE:O	4:A:1399:THR:OG1	2.29	0.42
4:A:1829:MET:O	4:A:1841:ALA:HA	2.18	0.42
16:N:17:PHE:O	16:N:21:GLU:HB3	2.19	0.42
31:1:174:LYS:HE3	31:1:195:LEU:HB3	2.00	0.42
4:A:188:ILE:HG12	4:A:191:VAL:HG22	2.02	0.42
4:A:302:PRO:HD2	16:N:6:PRO:HA	2.00	0.42
4:A:1612:LEU:HD12	4:A:1617:PHE:HB2	2.00	0.42
4:A:1749:MET:O	4:A:1814:TYR:OH	2.36	0.42
20:0:95:HIS:ND1	20:0:96:ALA:O	2.53	0.42
39:Cc:566:ALA:O	39:Cc:570:ALA:N	2.47	0.42
4:A:1336:VAL:HG22	4:A:1356:PHE:HZ	1.84	0.42
31:1:160:LEU:HA	31:1:163:MET:HG3	2.02	0.42
32:z:66:ASP:OD1	32:z:66:ASP:N	2.43	0.42
32:z:665:ALA:HB1	32:z:668:PHE:HB3	2.01	0.42
34:Z:416:ASN:OD1	34:Z:416:ASN:N	2.52	0.42
3:6:42:G:N7	12:L:31:ARG:HG2	2.34	0.42
4:A:1264:ASP:OD1	4:A:1264:ASP:N	2.52	0.42
6:C:425:TYR:HA	6:C:460:MET:HE1	2.01	0.42
18:T:414:GLY:O	18:T:417:GLY:N	2.41	0.42
20:0:314:HIS:O	20:0:323:ASN:ND2	2.31	0.42
20:0:320:ASN:HD21	22:W:49:ALA:HB3	1.84	0.42
22:W:37:THR:OG1	22:W:38:GLY:N	2.53	0.42
4:A:282:PRO:HA	4:A:283:PRO:HD3	1.92	0.42
4:A:670:ALA:HB2	4:A:778:TRP:HB3	2.02	0.42
4:A:1960:LEU:O	4:A:1964:ALA:HB2	2.20	0.42
6:C:824:PRO:HB3	6:C:858:LEU:HG	2.01	0.42
8:E:313:LEU:HD21	8:E:316:LYS:HB2	2.01	0.42
8:E:347:LEU:HD23	8:E:347:LEU:HA	1.90	0.42
9:F:144:MET:HA	9:F:147:LEU:HB2	2.01	0.42
19:M:148:ARG:NH2	20:0:286:GLU:HA	2.30	0.42
32:z:53:GLN:NE2	32:z:90:GLU:OE1	2.49	0.42
32:z:399:LEU:HD22	32:z:428:MET:HB3	2.01	0.42
32:z:406:LEU:HD23	32:z:414:VAL:HG12	2.01	0.42
4:A:1371:ILE:HG21	4:A:1418:CYS:HB3	2.00	0.42
4:A:1670:ASN:HB2	4:A:1696:LEU:HD21	2.01	0.42
7:D:182:GLN:HA	7:D:185:ILE:HG22	2.00	0.42
8:E:151:MET:HE3	8:E:151:MET:HB2	1.91	0.42
8:E:165:SER:OG	8:E:169:THR:OG1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:586:PHE:HE2	10:I:608:LEU:HD13	1.85	0.42
26:I:52:GLU:HA	26:I:62:HIS:HA	2.01	0.42
4:A:788:GLU:HA	21:R:224:LYS:HA	2.01	0.42
4:A:1605:LEU:HB2	4:A:1611:ILE:HD11	2.01	0.42
6:C:800:VAL:HG11	6:C:805:LEU:HD13	2.01	0.42
10:I:405:TRP:CE3	10:I:428:ALA:HB2	2.55	0.42
31:1:371:PRO:HG2	31:1:373:ILE:HD11	2.02	0.42
2:5:21:C:N4	6:C:198:ARG:HG2	2.35	0.41
4:A:384:ASN:ND2	4:A:395:PRO:HB3	2.35	0.41
7:D:162:TYR:HA	7:D:165:ILE:HG22	2.02	0.41
32:z:180:GLU:O	32:z:183:ARG:HB2	2.20	0.41
10:I:380:GLU:HA	10:I:383:LYS:HG2	2.01	0.41
11:J:132:ALA:HB1	11:J:142:LEU:HD13	2.02	0.41
32:z:482:THR:OG1	32:z:556:ARG:NE	2.43	0.41
4:A:772:ILE:O	4:A:776:GLU:HG3	2.19	0.41
4:A:1339:SER:O	4:A:1339:SER:OG	2.37	0.41
6:C:706:VAL:HG12	6:C:919:ILE:HD13	2.01	0.41
9:F:135:ASP:OD2	10:I:615:ALA:N	2.42	0.41
10:I:704:ARG:NH2	10:I:740:TYR:O	2.47	0.41
11:J:274:LEU:HD23	11:J:274:LEU:HA	1.89	0.41
18:T:332:SER:OG	18:T:333:LEU:N	2.53	0.41
20:O:193:ILE:HA	20:O:196:ARG:HG2	2.03	0.41
31:1:156:GLY:N	32:z:433:GLU:OE2	2.50	0.41
38:8:11:Y5P:H6	38:8:11:Y5P:O5'	2.20	0.41
4:A:1375:LEU:HD21	4:A:1422:ILE:HD13	2.02	0.41
9:F:139:GLU:HG2	9:F:142:GLN:HE21	1.84	0.41
10:I:533:ALA:HB1	10:I:545:SER:HB2	2.02	0.41
23:P:227:ASN:HB3	23:P:230:ARG:HD3	2.01	0.41
31:1:116:LEU:HD12	31:1:116:LEU:HA	1.88	0.41
32:z:292:SER:H	32:z:295:GLN:NE2	2.19	0.41
34:Z:478:ARG:HD2	34:Z:528:TYR:CE1	2.55	0.41
4:A:540:ARG:HA	4:A:540:ARG:HD3	1.90	0.41
5:B:219:GLY:N	21:R:66:GLU:OE2	2.52	0.41
6:C:228:MET:HE2	6:C:228:MET:HB3	1.79	0.41
4:A:279:MET:HE3	4:A:279:MET:HB2	1.91	0.41
4:A:1236:LEU:HG	4:A:1279:ALA:HB1	2.01	0.41
8:E:213:VAL:O	8:E:222:VAL:N	2.51	0.41
16:N:139:CYS:HB2	22:W:138:TRP:HZ2	1.85	0.41
17:S:20:ASN:HA	17:S:27:CYS:SG	2.61	0.41
17:S:47:VAL:HG12	17:S:53:VAL:HG13	2.03	0.41
32:z:606:GLN:HA	32:z:607:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:z:623:HIS:HA	32:z:624:PRO:HD3	1.94	0.41
3:6:38:A:H8	38:8:3:P5P:N3	2.18	0.41
6:C:937:MET:HE3	6:C:937:MET:HB3	1.67	0.41
9:F:149:VAL:O	9:F:152:GLU:HG3	2.21	0.41
17:S:145:LYS:HE3	17:S:145:LYS:HB3	1.86	0.41
18:T:292:ASP:OD1	18:T:292:ASP:N	2.53	0.41
32:z:482:THR:HG22	32:z:486:MET:HE2	2.01	0.41
38:8:10:Y5P:H2'	38:8:11:Y5P:O4'	2.21	0.41
3:6:21:A:H4'	4:A:195:LYS:HG2	2.02	0.41
4:A:515:PHE:HD1	4:A:518:GLU:HG3	1.84	0.41
4:A:1027:ASP:HA	4:A:1032:ILE:HG22	2.02	0.41
4:A:1251:ASN:O	4:A:1278:ARG:NH1	2.54	0.41
6:C:578:GLU:O	6:C:580:ARG:N	2.54	0.41
8:E:69:ASP:HB2	8:E:74:LEU:HB2	2.03	0.41
10:I:489:HIS:CD2	10:I:490:LYS:HG3	2.56	0.41
18:T:253:VAL:HB	18:T:267:TYR:HB2	2.03	0.41
31:1:381:LYS:HD2	32:z:63:TRP:HA	2.03	0.41
32:z:76:ARG:HH22	32:z:143:GLU:HG3	1.86	0.41
32:z:265:VAL:HA	32:z:268:VAL:HG22	2.02	0.41
32:z:471:ALA:HB2	32:z:480:ILE:HD11	2.02	0.41
34:Z:372:HIS:CD2	34:Z:373:LYS:HD3	2.56	0.41
2:5:25:A:H5''	4:A:552:PRO:HG3	2.03	0.41
3:6:11:G:N2	16:N:97:GLN:OE1	2.53	0.41
4:A:407:PHE:HA	4:A:411:ASN:HD21	1.85	0.41
4:A:498:GLU:HG3	6:C:401:THR:HG22	2.02	0.41
4:A:1193:GLN:OE1	4:A:1193:GLN:N	2.52	0.41
5:B:245:ASN:H	21:R:106:VAL:HG22	1.86	0.41
5:B:262:LEU:HA	11:J:152:MET:HE3	2.03	0.41
8:E:69:ASP:HB3	8:E:74:LEU:H	1.86	0.41
10:I:517:ARG:HA	10:I:517:ARG:HD2	1.81	0.41
10:I:730:LEU:HB3	10:I:734:ARG:HH12	1.86	0.41
12:L:177:LYS:O	12:L:181:LYS:HG2	2.21	0.41
16:N:60:ARG:O	16:N:64:GLU:HG2	2.20	0.41
17:S:95:GLY:N	17:S:98:THR:OG1	2.51	0.41
19:M:148:ARG:NH1	20:0:285:ILE:O	2.54	0.41
20:0:95:HIS:NE2	20:0:237:SER:HB2	2.36	0.41
21:R:54:TYR:HD1	21:R:57:ARG:HH12	1.68	0.41
24:j:58:ASP:HA	24:j:80:GLN:HA	2.03	0.41
31:1:199:ASP:OD1	31:1:199:ASP:N	2.54	0.41
34:Z:364:SER:HB2	34:Z:369:GLU:HB2	2.02	0.41
4:A:280:ARG:NH2	4:A:283:PRO:O	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:437:ARG:NE	6:C:698:GLU:OE1	2.51	0.41
4:A:859:PRO:HD2	4:A:862:ILE:HD12	2.03	0.41
5:B:151:ALA:HB1	10:I:560:VAL:HA	2.03	0.41
19:M:31:PRO:HA	21:R:206:ARG:HG2	2.03	0.41
21:R:337:LEU:HD12	21:R:337:LEU:HA	1.92	0.41
2:5:44:C:H4'	4:A:723:TYR:HB3	2.02	0.40
3:6:38:A:N7	38:8:3:P5P:H1'	2.36	0.40
4:A:463:ALA:N	4:A:521:GLU:OE1	2.52	0.40
5:B:254:PRO:HG3	11:J:122:ILE:HG21	2.03	0.40
6:C:426:SER:O	6:C:430:SER:OG	2.28	0.40
6:C:505:ILE:HD12	6:C:505:ILE:HA	1.99	0.40
8:E:290:ASP:OD1	8:E:290:ASP:N	2.47	0.40
31:1:200:ASN:OD1	32:z:425:ALA:N	2.50	0.40
32:z:481:LEU:HD11	32:z:559:LEU:HB3	2.03	0.40
4:A:447:SER:HB2	6:C:937:MET:HE1	2.03	0.40
4:A:941:VAL:HG22	4:A:1126:LEU:HD21	2.03	0.40
4:A:1505:GLU:OE2	4:A:1545:ARG:NH1	2.53	0.40
4:A:1655:GLN:HG3	31:1:66:TRP:CH2	2.55	0.40
4:A:1566:ARG:O	4:A:1570:LYS:HG2	2.21	0.40
4:A:1951:THR:HA	4:A:1954:TRP:HD1	1.86	0.40
5:B:247:THR:HG21	17:S:135:LEU:HD13	2.04	0.40
6:C:103:THR:HG23	6:C:106:GLN:H	1.86	0.40
6:C:297:LEU:HB2	6:C:344:LEU:HD13	2.03	0.40
6:C:847:TRP:CD1	6:C:849:ASN:H	2.37	0.40
8:E:64:PHE:CE2	8:E:80:MET:HB2	2.56	0.40
8:E:269:ARG:NH1	8:E:309:ASP:O	2.54	0.40
18:T:313:THR:HG22	23:P:13:ARG:HH22	1.86	0.40
33:V:23:LEU:HD21	34:Z:376:LYS:HG3	2.04	0.40
8:E:196:SER:HB3	8:E:201:GLU:HB2	2.02	0.40
11:J:90:ARG:HG2	12:L:225:ILE:HG12	2.02	0.40
12:L:237:ASP:HB2	21:R:93:SER:HB2	2.03	0.40
18:T:419:MET:HG2	18:T:448:ILE:HD11	2.03	0.40
19:M:298:ARG:HH21	19:M:335:PHE:HD1	1.69	0.40
20:0:102:ILE:HD13	20:0:140:LEU:HB2	2.04	0.40
4:A:508:PRO:O	6:C:398:ARG:NH1	2.54	0.40
11:J:271:LYS:NZ	11:J:289:TYR:OH	2.49	0.40
23:P:38:GLN:HB2	23:P:41:GLN:HG3	2.04	0.40
31:1:201:VAL:HG21	32:z:395:GLN:HE22	1.86	0.40
32:z:124:ILE:HD11	32:z:153:ILE:HG23	2.03	0.40
34:Z:481:ILE:HD13	34:Z:481:ILE:HA	1.94	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	1987/2463 (81%)	1891 (95%)	93 (5%)	3 (0%)	43	74
5	B	256/326 (78%)	249 (97%)	7 (3%)	0	100	100
6	C	920/1011 (91%)	877 (95%)	42 (5%)	1 (0%)	48	79
7	D	62/325 (19%)	60 (97%)	2 (3%)	0	100	100
8	E	308/352 (88%)	285 (92%)	23 (8%)	0	100	100
9	F	108/233 (46%)	106 (98%)	2 (2%)	0	100	100
10	I	727/839 (87%)	706 (97%)	20 (3%)	1 (0%)	48	79
11	J	604/687 (88%)	597 (99%)	7 (1%)	0	100	100
12	L	629/768 (82%)	613 (98%)	16 (2%)	0	100	100
13	K	229/231 (99%)	228 (100%)	1 (0%)	0	100	100
14	Y	1343/1416 (95%)	1332 (99%)	11 (1%)	0	100	100
15	q	137/480 (28%)	137 (100%)	0	0	100	100
15	r	141/480 (29%)	141 (100%)	0	0	100	100
15	s	138/480 (29%)	137 (99%)	1 (1%)	0	100	100
15	t	139/480 (29%)	139 (100%)	0	0	100	100
16	N	146/148 (99%)	141 (97%)	4 (3%)	1 (1%)	18	51
17	S	155/167 (93%)	142 (92%)	13 (8%)	0	100	100
18	T	320/496 (64%)	303 (95%)	17 (5%)	0	100	100
19	M	242/395 (61%)	226 (93%)	14 (6%)	2 (1%)	16	49
20	0	274/408 (67%)	254 (93%)	20 (7%)	0	100	100
21	R	336/578 (58%)	318 (95%)	18 (5%)	0	100	100
22	W	395/547 (72%)	377 (95%)	17 (4%)	1 (0%)	36	67
23	P	110/260 (42%)	103 (94%)	7 (6%)	0	100	100
24	j	86/98 (88%)	86 (100%)	0	0	100	100
25	k	71/82 (87%)	70 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	l	79/94 (84%)	79 (100%)	0	0	100	100
27	m	84/592 (14%)	82 (98%)	2 (2%)	0	100	100
28	o	85/118 (72%)	82 (96%)	3 (4%)	0	100	100
29	p	99/211 (47%)	98 (99%)	1 (1%)	0	100	100
30	u	88/114 (77%)	85 (97%)	2 (2%)	1 (1%)	11	43
31	1	317/698 (45%)	296 (93%)	19 (6%)	2 (1%)	21	54
32	z	653/672 (97%)	614 (94%)	38 (6%)	1 (0%)	43	74
33	V	78/223 (35%)	71 (91%)	7 (9%)	0	100	100
34	Z	209/678 (31%)	200 (96%)	9 (4%)	0	100	100
35	CY	23/510 (4%)	22 (96%)	1 (4%)	0	100	100
39	Cc	712/764 (93%)	699 (98%)	13 (2%)	0	100	100
All	All	12290/18424 (67%)	11846 (96%)	431 (4%)	13 (0%)	49	79

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	C	840	VAL
30	u	48	ILE
31	1	43	PRO
4	A	1219	ILE
4	A	1526	GLN
10	I	558	TYR
16	N	6	PRO
19	M	28	PRO
19	M	105	ILE
31	1	8	ALA
32	z	440	ALA
4	A	497	ILE
22	W	101	VAL

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	1798/2212 (81%)	1798 (100%)	0	100	100
5	B	170/270 (63%)	170 (100%)	0	100	100
6	C	809/884 (92%)	809 (100%)	0	100	100
7	D	55/276 (20%)	55 (100%)	0	100	100
8	E	254/287 (88%)	254 (100%)	0	100	100
9	F	92/179 (51%)	91 (99%)	1 (1%)	65	74
10	I	327/729 (45%)	327 (100%)	0	100	100
11	J	245/592 (41%)	245 (100%)	0	100	100
12	L	300/635 (47%)	298 (99%)	2 (1%)	76	78
16	N	131/131 (100%)	131 (100%)	0	100	100
17	S	126/135 (93%)	126 (100%)	0	100	100
18	T	270/408 (66%)	269 (100%)	1 (0%)	84	81
19	M	210/293 (72%)	210 (100%)	0	100	100
20	0	227/335 (68%)	222 (98%)	5 (2%)	45	65
21	R	280/478 (59%)	280 (100%)	0	100	100
22	W	73/459 (16%)	73 (100%)	0	100	100
23	P	91/213 (43%)	91 (100%)	0	100	100
29	p	10/152 (7%)	10 (100%)	0	100	100
31	1	266/564 (47%)	264 (99%)	2 (1%)	73	77
32	z	559/571 (98%)	559 (100%)	0	100	100
33	V	22/197 (11%)	22 (100%)	0	100	100
34	Z	182/575 (32%)	182 (100%)	0	100	100
35	CY	17/418 (4%)	17 (100%)	0	100	100
All	All	6514/10993 (59%)	6503 (100%)	11 (0%)	85	85

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

Mol	Chain	Res	Type
9	F	110	GLN
12	L	207	ILE
12	L	211	ILE
18	T	391	ASN
20	0	180	TYR
20	0	184	ILE
20	0	207	ILE

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Mol	Chain	Res	Type
20	0	208	ARG
20	0	211	ASN
31	1	53	ARG
31	1	56	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	296	ASN
4	A	351	ASN
4	A	384	ASN
4	A	639	ASN
4	A	690	GLN
4	A	695	ASN
4	A	834	ASN
4	A	902	ASN
4	A	920	ASN
4	A	1026	ASN
4	A	1121	ASN
4	A	1388	ASN
4	A	1737	GLN
4	A	1911	ASN
4	A	2073	ASN
5	B	302	ASN
6	C	95	HIS
6	C	140	GLN
6	C	163	GLN
6	C	333	ASN
6	C	957	GLN
7	D	144	ASN
7	D	182	GLN
8	E	126	HIS
9	F	63	GLN
9	F	142	GLN
9	F	153	ASN
10	I	648	ASN
11	J	24	GLN
11	J	104	ASN
12	L	11	ASN
12	L	79	GLN
12	L	197	GLN
12	L	251	HIS

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Mol	Chain	Res	Type
16	N	29	ASN
16	N	35	GLN
16	N	116	ASN
18	T	391	ASN
19	M	90	GLN
20	0	56	GLN
20	0	197	HIS
20	0	262	GLN
21	R	28	GLN
22	W	76	HIS
32	z	26	HIS
32	z	74	GLN
32	z	361	GLN
32	z	427	GLN
32	z	472	GLN
32	z	591	GLN
32	z	606	GLN
34	Z	542	HIS
34	Z	547	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	36/193 (18%)	16 (44%)	1 (2%)
2	5	109/116 (93%)	20 (18%)	1 (0%)
3	6	89/101 (88%)	29 (32%)	1 (1%)
38	8	19/22 (86%)	8 (42%)	0
All	All	253/432 (58%)	73 (28%)	3 (1%)

All (73) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	G
1	2	13	C
1	2	14	U
1	2	15	U
1	2	17	U
1	2	18	G
1	2	19	G
1	2	21	U
1	2	22	U

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Mol	Chain	Res	Type
1	2	23	A
1	2	24	G
1	2	28	A
1	2	30	G
1	2	32	G
1	2	35	G
1	2	37	A
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	27	U
2	5	33	C
2	5	39	U
2	5	46	G
2	5	50	G
2	5	56	G
2	5	68	G
2	5	71	A
2	5	88	C
2	5	89	U
2	5	90	U
2	5	93	G
2	5	106	U
3	6	6	U
3	6	7	C
3	6	9	G
3	6	18	G
3	6	19	U
3	6	21	A
3	6	23	U
3	6	24	U
3	6	27	A
3	6	28	A
3	6	35	C
3	6	37	G
3	6	38	A
3	6	39	G
3	6	42	G

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Mol	Chain	Res	Type
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	73	C
3	6	80	C
3	6	81	A
3	6	87	A
3	6	88	C
3	6	89	G
3	6	90	C
38	8	-5	Y5P
38	8	0	P5P
38	8	1	P5P
38	8	2	Y5P
38	8	11	Y5P
38	8	12	Y5P
38	8	13	Y5P
38	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	37	G

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

21 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
38	Y5P	8	-7	38	14,19,20	4.50	2 (14%)	18,26,29	1.39	2 (11%)
38	P5P	8	-2	2,38	20,23,24	0.44	0	27,33,36	0.77	1 (3%)
38	P5P	8	7	3,38	20,23,24	0.93	2 (10%)	27,33,36	2.00	4 (14%)
38	P5P	8	-3	2,38	20,23,24	0.44	0	27,33,36	0.75	1 (3%)
38	Y5P	8	13	38	14,19,20	4.22	2 (14%)	18,26,29	1.13	1 (5%)
38	Y5P	8	11	38	14,19,20	4.21	2 (14%)	18,26,29	1.10	1 (5%)
38	Y5P	8	-4	38	14,19,20	4.53	2 (14%)	18,26,29	1.40	2 (11%)
38	P5P	8	-1	2,38	20,23,24	0.97	2 (10%)	27,33,36	1.89	4 (14%)
38	Y5P	8	6	38	14,19,20	4.18	2 (14%)	18,26,29	1.12	1 (5%)
38	Y5P	8	10	38	14,19,20	4.21	2 (14%)	18,26,29	1.04	1 (5%)
38	P5P	8	3	38	20,23,24	0.42	0	27,33,36	0.73	1 (3%)
38	Y5P	8	4	38	14,19,20	4.20	2 (14%)	18,26,29	1.18	1 (5%)
38	Y5P	8	-5	38	14,19,20	4.49	2 (14%)	18,26,29	1.54	3 (16%)
38	Y5P	8	12	38	14,19,20	4.17	2 (14%)	18,26,29	1.06	1 (5%)
38	P5P	8	5	38	20,23,24	0.96	2 (10%)	27,33,36	1.97	4 (14%)
38	Y5P	8	2	38	14,19,20	4.18	2 (14%)	18,26,29	1.06	1 (5%)
38	Y5P	8	8	38	14,19,20	4.52	2 (14%)	18,26,29	1.36	2 (11%)
38	P5P	8	-6	38	20,23,24	0.97	2 (10%)	27,33,36	1.93	4 (14%)
38	Y5P	8	14	38	14,19,20	4.20	2 (14%)	18,26,29	1.03	1 (5%)
38	P5P	8	1	38	20,23,24	0.98	2 (10%)	27,33,36	1.92	4 (14%)
38	P5P	8	0	38	20,23,24	0.43	0	27,33,36	0.88	2 (7%)

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
38	Y5P	8	-7	38	-	5/7/33/34	0/2/2/2
38	P5P	8	-2	2,38	-	0/7/25/26	0/3/3/3
38	P5P	8	7	3,38	-	0/7/25/26	0/3/3/3
38	P5P	8	-3	2,38	-	0/7/25/26	0/3/3/3
38	Y5P	8	13	38	-	6/7/33/34	0/2/2/2
38	Y5P	8	11	38	-	3/7/33/34	0/2/2/2
38	Y5P	8	-4	38	-	3/7/33/34	0/2/2/2
38	P5P	8	-1	2,38	-	2/7/25/26	0/3/3/3
38	Y5P	8	6	38	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	Y5P	8	10	38	-	4/7/33/34	0/2/2/2
38	P5P	8	3	38	-	1/7/25/26	0/3/3/3
38	Y5P	8	4	38	-	1/7/33/34	0/2/2/2
38	Y5P	8	-5	38	-	6/7/33/34	0/2/2/2
38	Y5P	8	12	38	-	4/7/33/34	0/2/2/2
38	P5P	8	5	38	-	0/7/25/26	0/3/3/3
38	Y5P	8	2	38	-	1/7/33/34	0/2/2/2
38	Y5P	8	8	38	-	1/7/33/34	0/2/2/2
38	P5P	8	-6	38	-	2/7/25/26	0/3/3/3
38	Y5P	8	14	38	-	3/7/33/34	0/2/2/2
38	P5P	8	1	38	-	4/7/25/26	0/3/3/3
38	P5P	8	0	38	-	4/7/25/26	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	11	Y5P	C2-N3	13.26	1.37	1.27
38	8	13	Y5P	C2-N3	13.20	1.37	1.27
38	8	-4	Y5P	C4-N3	-13.19	1.33	1.46
38	8	-5	Y5P	C4-N3	-13.14	1.33	1.46
38	8	10	Y5P	C2-N3	13.14	1.37	1.27
38	8	14	Y5P	C2-N3	13.12	1.37	1.27
38	8	8	Y5P	C4-N3	-13.08	1.33	1.46
38	8	4	Y5P	C2-N3	13.07	1.37	1.27
38	8	-7	Y5P	C4-N3	-13.04	1.34	1.46
38	8	2	Y5P	C2-N3	13.02	1.37	1.27
38	8	12	Y5P	C2-N3	13.01	1.37	1.27
38	8	6	Y5P	C2-N3	12.94	1.37	1.27
38	8	8	Y5P	C2-N3	10.69	1.35	1.27
38	8	-7	Y5P	C2-N3	10.61	1.35	1.27
38	8	-4	Y5P	C2-N3	10.56	1.35	1.27
38	8	-5	Y5P	C2-N3	10.43	1.35	1.27
38	8	6	Y5P	C4-N3	-8.76	1.38	1.46
38	8	4	Y5P	C4-N3	-8.63	1.38	1.46
38	8	13	Y5P	C4-N3	-8.62	1.38	1.46
38	8	10	Y5P	C4-N3	-8.62	1.38	1.46
38	8	14	Y5P	C4-N3	-8.59	1.38	1.46
38	8	2	Y5P	C4-N3	-8.56	1.38	1.46
38	8	12	Y5P	C4-N3	-8.54	1.38	1.46
38	8	11	Y5P	C4-N3	-8.44	1.38	1.46
38	8	1	P5P	C6-N1	2.68	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	-6	P5P	C6-N1	2.67	1.39	1.34
38	8	-1	P5P	C6-N1	2.67	1.39	1.34
38	8	5	P5P	C6-N1	2.62	1.39	1.34
38	8	7	P5P	C6-N1	2.56	1.39	1.34
38	8	-6	P5P	C2-N1	2.23	1.37	1.33
38	8	1	P5P	C2-N1	2.21	1.37	1.33
38	8	5	P5P	C2-N1	2.17	1.37	1.33
38	8	-1	P5P	C2-N1	2.15	1.37	1.33
38	8	7	P5P	C2-N1	2.05	1.37	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	7	P5P	C6-N1-C2	8.21	125.49	115.80
38	8	5	P5P	C6-N1-C2	8.16	125.44	115.80
38	8	1	P5P	C6-N1-C2	7.96	125.19	115.80
38	8	-6	P5P	C6-N1-C2	7.91	125.14	115.80
38	8	-1	P5P	C6-N1-C2	7.78	124.98	115.80
38	8	8	Y5P	C5-C4-N3	4.85	121.97	114.15
38	8	-5	Y5P	C5-C4-N3	4.84	121.95	114.15
38	8	-4	Y5P	C5-C4-N3	4.81	121.91	114.15
38	8	-7	Y5P	C5-C4-N3	4.81	121.91	114.15
38	8	5	P5P	C5-C6-N1	-4.26	111.30	121.90
38	8	7	P5P	C5-C6-N1	-4.23	111.37	121.90
38	8	-1	P5P	C5-C6-N1	-4.20	111.44	121.90
38	8	-6	P5P	C5-C6-N1	-4.20	111.45	121.90
38	8	1	P5P	C5-C6-N1	-4.18	111.48	121.90
38	8	13	Y5P	N1-C2-N3	-3.84	114.74	125.39
38	8	11	Y5P	N1-C2-N3	-3.84	114.75	125.39
38	8	10	Y5P	N1-C2-N3	-3.83	114.78	125.39
38	8	4	Y5P	N1-C2-N3	-3.83	114.78	125.39
38	8	2	Y5P	N1-C2-N3	-3.82	114.81	125.39
38	8	14	Y5P	N1-C2-N3	-3.81	114.81	125.39
38	8	6	Y5P	N1-C2-N3	-3.81	114.82	125.39
38	8	12	Y5P	N1-C2-N3	-3.81	114.83	125.39
38	8	-6	P5P	C6-C5-C4	2.91	119.42	116.24
38	8	1	P5P	C6-C5-C4	2.90	119.42	116.24
38	8	7	P5P	C6-C5-C4	2.89	119.40	116.24
38	8	5	P5P	C6-C5-C4	2.84	119.35	116.24
38	8	-1	P5P	C6-C5-C4	2.74	119.24	116.24
38	8	-2	P5P	C6-N1-C2	2.42	118.66	115.80
38	8	-3	P5P	C6-N1-C2	2.39	118.62	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	3	P5P	C6-N1-C2	2.35	118.57	115.80
38	8	7	P5P	N1-C2-N3	-2.29	123.43	127.33
38	8	0	P5P	C6-N1-C2	2.29	118.50	115.80
38	8	5	P5P	N1-C2-N3	-2.24	123.52	127.33
38	8	1	P5P	N1-C2-N3	-2.23	123.54	127.33
38	8	-7	Y5P	N1-C2-N3	-2.21	119.25	125.39
38	8	8	Y5P	N1-C2-N3	-2.21	119.26	125.39
38	8	-5	Y5P	N1-C2-N3	-2.21	119.27	125.39
38	8	-4	Y5P	N1-C2-N3	-2.19	119.32	125.39
38	8	-6	P5P	N1-C2-N3	-2.18	123.62	127.33
38	8	-5	Y5P	O3'-C3'-C4'	-2.17	104.84	111.08
38	8	-1	P5P	N1-C2-N3	-2.07	123.81	127.33
38	8	0	P5P	C2'-C1'-N9	2.01	118.30	113.30

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	8	1	P5P	O4'-C4'-C5'-O5'
38	8	10	Y5P	O4'-C4'-C5'-O5'
38	8	11	Y5P	O4'-C4'-C5'-O5'
38	8	11	Y5P	O4'-C1'-N1-C2
38	8	12	Y5P	C2'-C1'-N1-C6
38	8	13	Y5P	O4'-C4'-C5'-O5'
38	8	14	Y5P	O4'-C4'-C5'-O5'
38	8	14	Y5P	C3'-C4'-C5'-O5'
38	8	-4	Y5P	O4'-C1'-N1-C2
38	8	2	Y5P	O4'-C1'-N1-C2
38	8	4	Y5P	O4'-C1'-N1-C2
38	8	6	Y5P	O4'-C1'-N1-C2
38	8	8	Y5P	O4'-C1'-N1-C2
38	8	10	Y5P	O4'-C1'-N1-C2
38	8	-4	Y5P	C3'-C4'-C5'-O5'
38	8	0	P5P	O4'-C4'-C5'-O5'
38	8	10	Y5P	C3'-C4'-C5'-O5'
38	8	13	Y5P	C3'-C4'-C5'-O5'
38	8	12	Y5P	C2'-C1'-N1-C2
38	8	-5	Y5P	O4'-C4'-C5'-O5'
38	8	-5	Y5P	C3'-C4'-C5'-O5'
38	8	-1	P5P	O4'-C4'-C5'-O5'
38	8	13	Y5P	C2'-C1'-N1-C2
38	8	1	P5P	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
38	8	11	Y5P	C3'-C4'-C5'-O5'
38	8	13	Y5P	C2'-C1'-N1-C6
38	8	-4	Y5P	O4'-C4'-C5'-O5'
38	8	0	P5P	C3'-C4'-C5'-O5'
38	8	-7	Y5P	C2'-C1'-N1-C6
38	8	14	Y5P	O4'-C1'-N1-C2
38	8	-7	Y5P	C2'-C1'-N1-C2
38	8	0	P5P	O4'-C1'-N9-C4
38	8	-1	P5P	C3'-C4'-C5'-O5'
38	8	-6	P5P	C2'-C1'-N9-C8
38	8	13	Y5P	O4'-C1'-N1-C6
38	8	13	Y5P	O4'-C1'-N1-C2
38	8	-7	Y5P	O4'-C1'-N1-C2
38	8	-7	Y5P	O4'-C1'-N1-C6
38	8	1	P5P	C4'-C5'-O5'-P
38	8	-5	Y5P	C2'-C1'-N1-C2
38	8	-5	Y5P	O4'-C1'-N1-C2
38	8	-5	Y5P	C2'-C1'-N1-C6
38	8	0	P5P	O4'-C1'-N9-C8
38	8	12	Y5P	O4'-C1'-N1-C6
38	8	-7	Y5P	C4'-C5'-O5'-P
38	8	3	P5P	C4'-C5'-O5'-P
38	8	12	Y5P	C4'-C5'-O5'-P
38	8	-6	P5P	O4'-C1'-N9-C8
38	8	1	P5P	C2'-C1'-N9-C8
38	8	-5	Y5P	O4'-C1'-N1-C6
38	8	10	Y5P	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	8	7	P5P	1	0
38	8	11	Y5P	3	0
38	8	10	Y5P	2	0
38	8	3	P5P	2	0
38	8	4	Y5P	1	0
38	8	-5	Y5P	1	0
38	8	12	Y5P	1	0
38	8	5	P5P	2	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$
40	M7M	2	201	-	28,32,33	4.11	17 (60%)	31,49,52	1.21	3 (9%)
41	GTP	C	1101	-	33,34,34	0.95	2 (6%)	50,54,54	1.62	10 (20%)

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
40	M7M	2	201	-	-	3/17/47/48	0/3/3/3
41	GTP	C	1101	-	-	3/22/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	2	201	M7M	CBI-NBP	7.90	1.51	1.45
40	2	201	M7M	OBR-CBS	7.36	1.61	1.45
40	2	201	M7M	CBG-NBH	7.36	1.44	1.35
40	2	201	M7M	CBY-CBS	-7.31	1.34	1.53
40	2	201	M7M	CBO-NBP	5.97	1.44	1.35
40	2	201	M7M	CBM-NBV	5.83	1.45	1.35
40	2	201	M7M	CBO-NBN	5.72	1.47	1.37
40	2	201	M7M	CBM-NBE	5.67	1.45	1.32
40	2	201	M7M	CBM-NBN	5.13	1.48	1.36
40	2	201	M7M	OBR-CBQ	-5.02	1.30	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	2	201	M7M	CBF-NBE	3.30	1.43	1.38
40	2	201	M7M	OCB-CBY	3.08	1.50	1.43
40	2	201	M7M	OCA-CBX	-2.98	1.35	1.43
40	2	201	M7M	CBG-CBO	2.95	1.44	1.36
40	2	201	M7M	OBB-CBF	-2.60	1.19	1.23
40	2	201	M7M	CBI-NBH	2.10	1.52	1.42
41	C	1101	GTP	C5-N7	-2.09	1.34	1.39
40	2	201	M7M	PBK-OBU	2.01	1.67	1.59
41	C	1101	GTP	O4'-C4'	-2.01	1.40	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	C	1101	GTP	C5-C4-N3	-4.95	120.51	128.39
41	C	1101	GTP	C2-N3-C4	4.44	119.95	112.30
40	2	201	M7M	CBO-CBG-NBH	4.07	109.86	106.86
41	C	1101	GTP	N9-C4-N3	3.36	132.68	125.95
41	C	1101	GTP	C2-N1-C6	-3.01	119.66	125.11
41	C	1101	GTP	N9-C8-N7	-2.71	108.37	113.40
41	C	1101	GTP	O6-C6-C5	-2.69	119.44	126.53
40	2	201	M7M	NBP-CBI-NBH	2.66	107.14	103.37
41	C	1101	GTP	C5-C6-N1	2.60	119.87	113.25
40	2	201	M7M	CBY-CBX-CBQ	2.40	106.00	101.46
41	C	1101	GTP	C8-N7-C5	2.39	108.52	104.26
41	C	1101	GTP	C3'-C2'-C1'	2.17	105.57	101.46
41	C	1101	GTP	O2G-PG-O3B	2.14	111.80	104.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

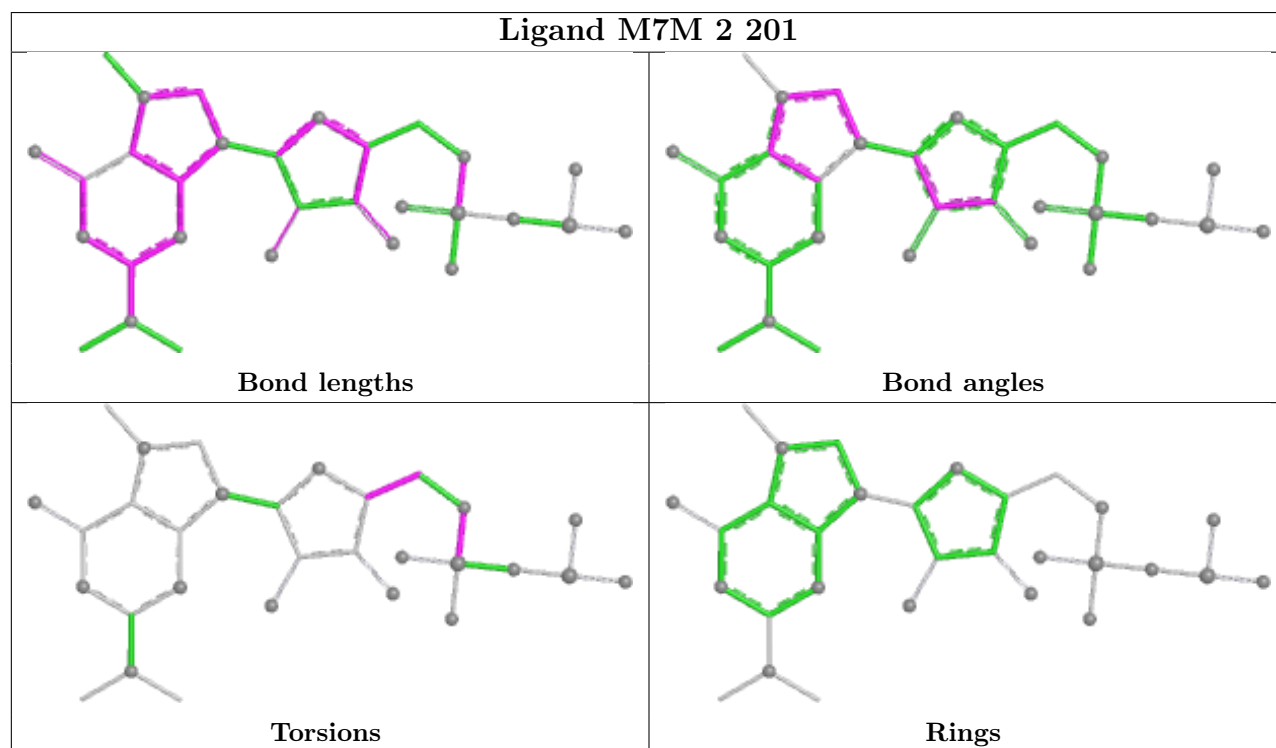
Mol	Chain	Res	Type	Atoms
40	2	201	M7M	CBT-OBU-PBK-OB
40	2	201	M7M	CBT-OBU-PBK-OB
41	C	1101	GTP	C3'-C4'-C5'-O5'
40	2	201	M7M	CBY-CBS-CBT-OB
41	C	1101	GTP	PA-O3A-PB-O1B
41	C	1101	GTP	O4'-C4'-C5'-O5'

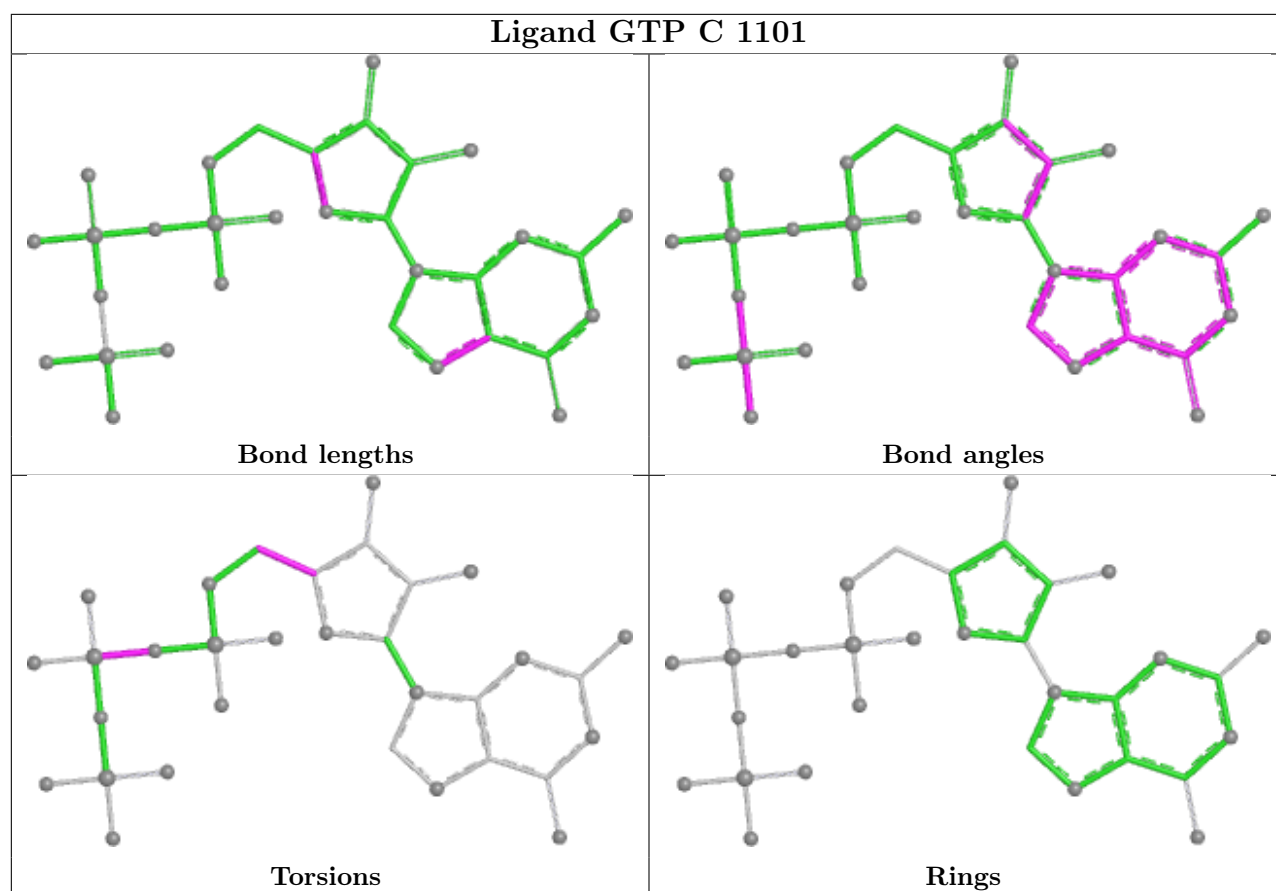
There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

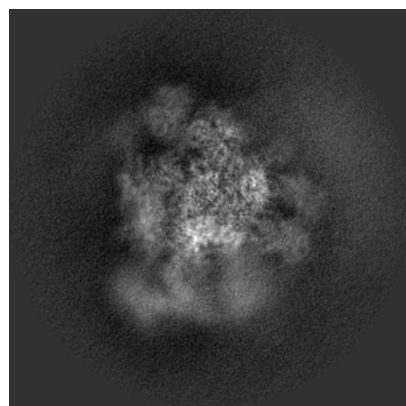
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62843. These allow visual inspection of the internal detail of the map and identification of artifacts.

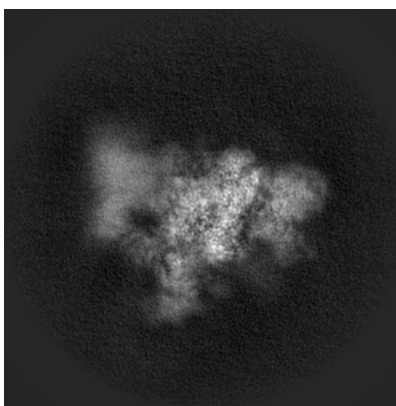
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

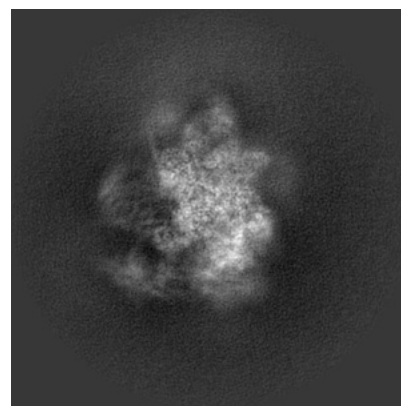
6.1.1 Primary map



X

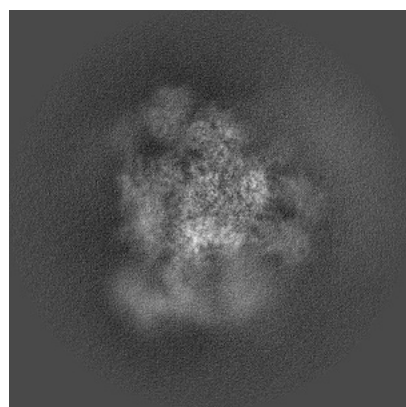


Y

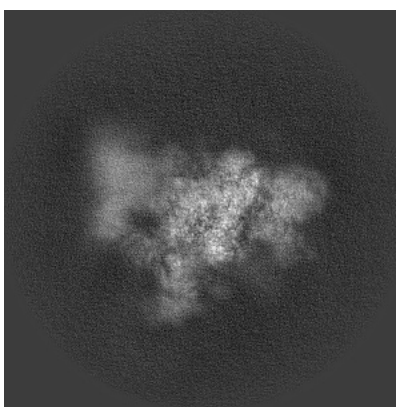


Z

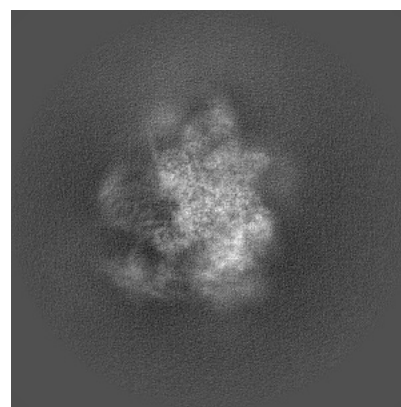
6.1.2 Raw map



X



Y

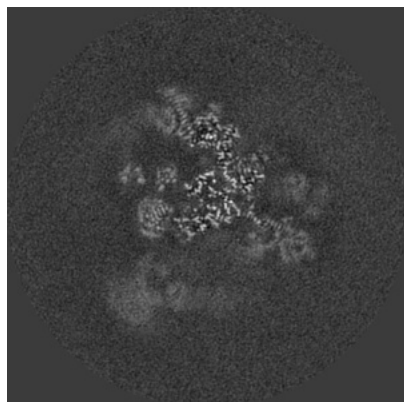


Z

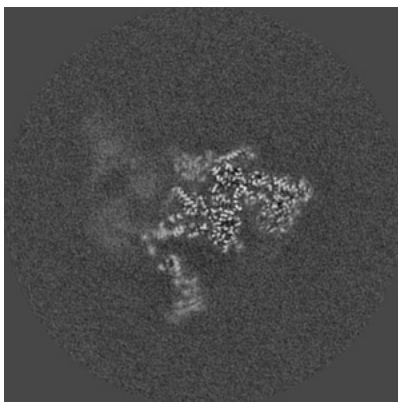
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

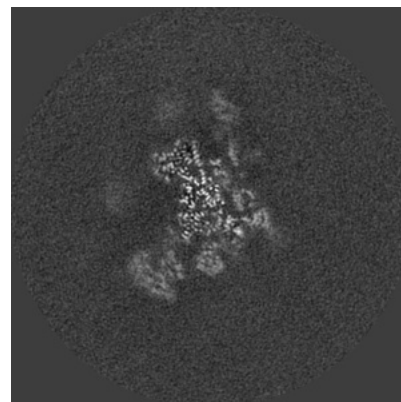
6.2.1 Primary map



X Index: 240

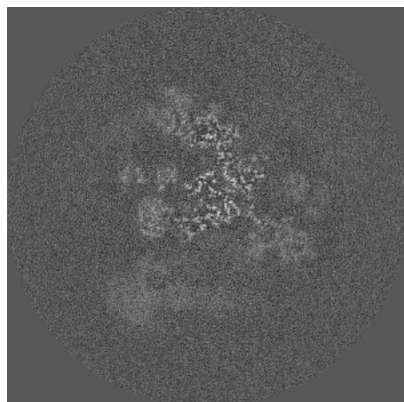


Y Index: 240

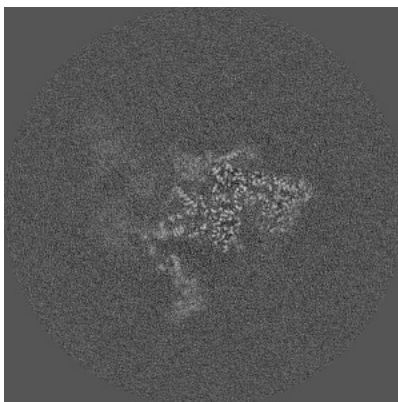


Z Index: 240

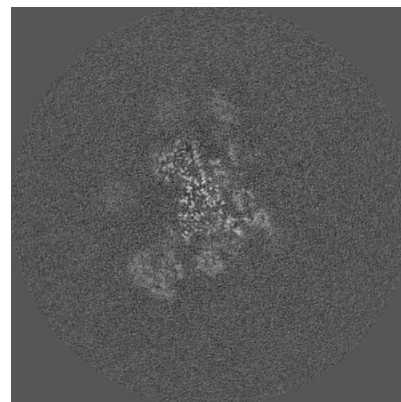
6.2.2 Raw map



X Index: 240



Y Index: 240

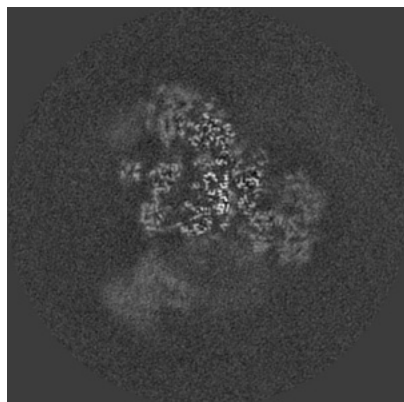


Z Index: 240

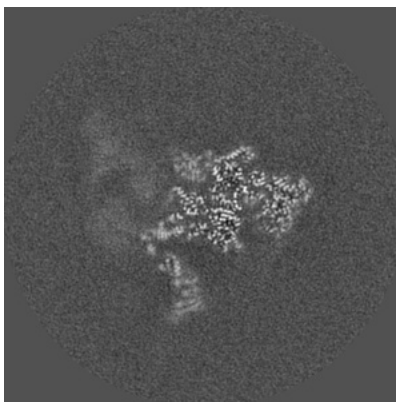
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

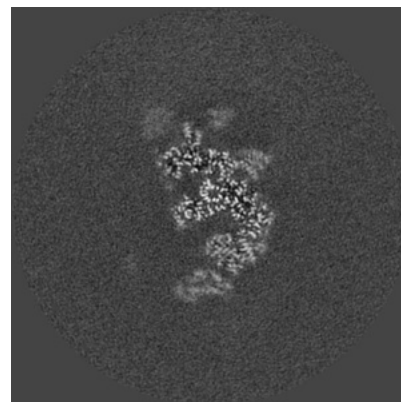
6.3.1 Primary map



X Index: 247

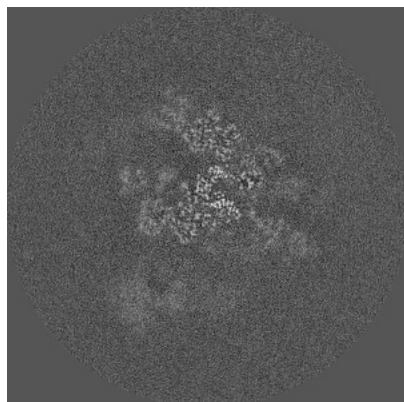


Y Index: 239

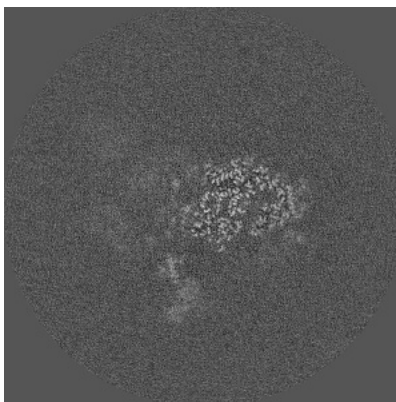


Z Index: 276

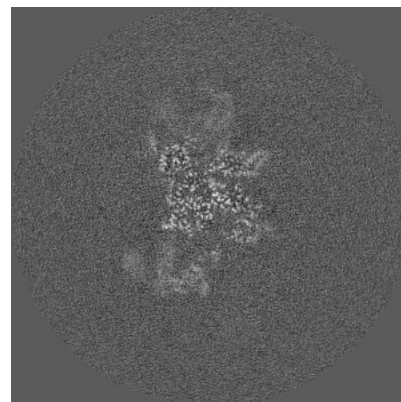
6.3.2 Raw map



X Index: 235



Y Index: 249

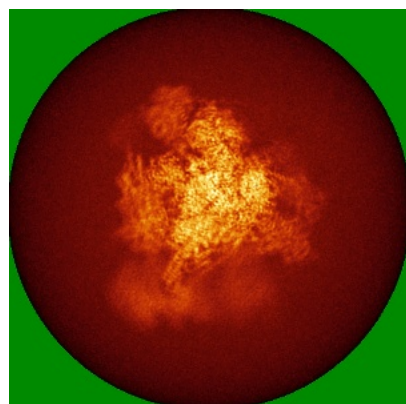


Z Index: 259

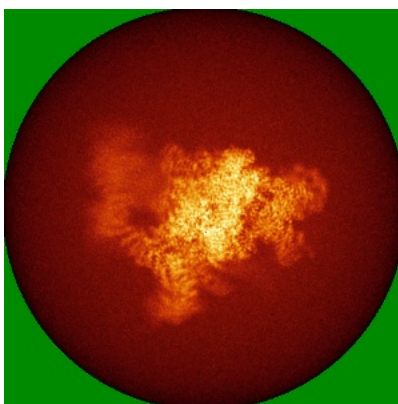
The images above show the largest variance slices of the map in three orthogonal directions.

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

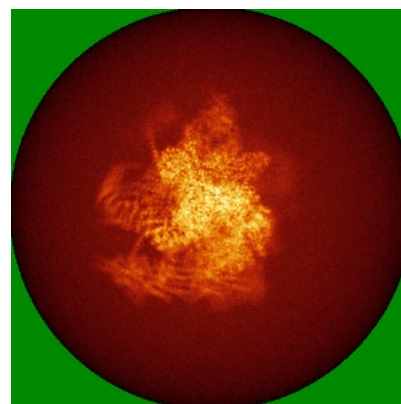
6.4.1 Primary map



X

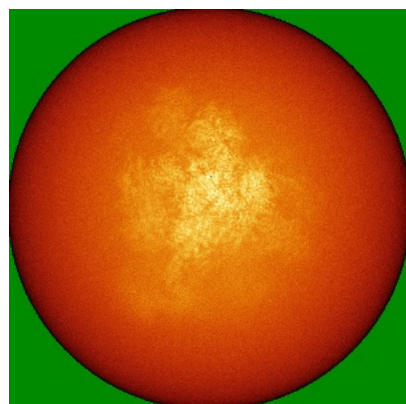


Y

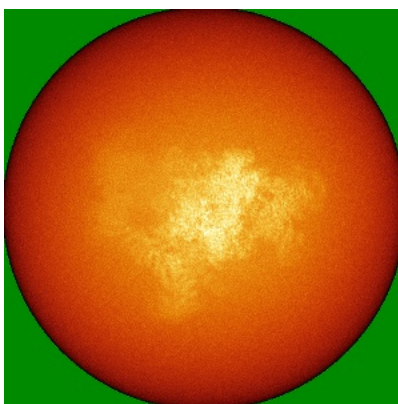


Z

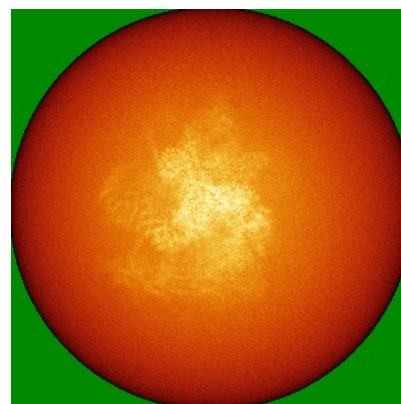
6.4.2 Raw map



X



Y

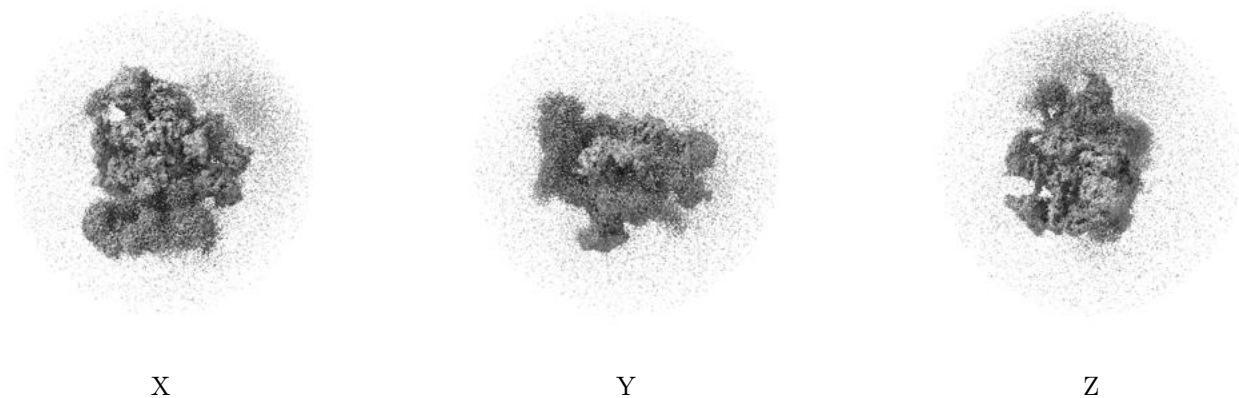


Z

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.

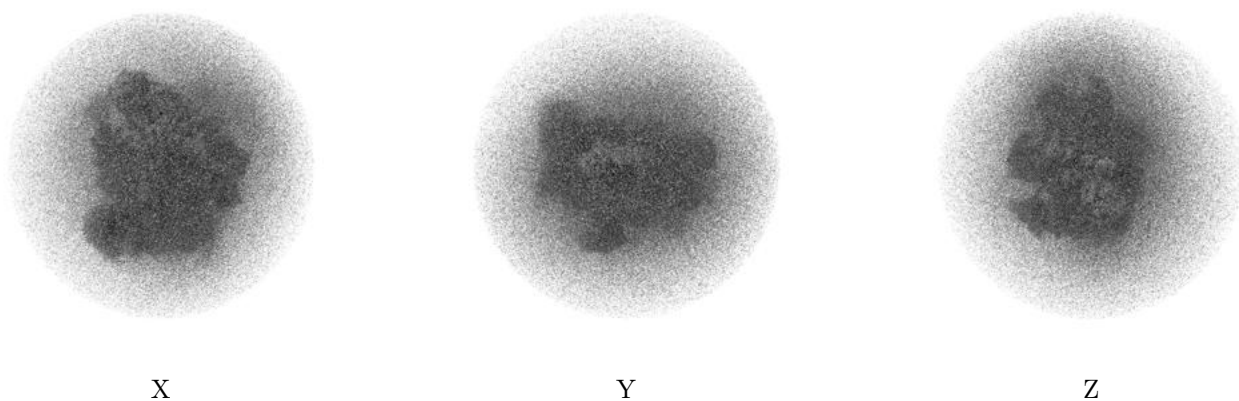
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

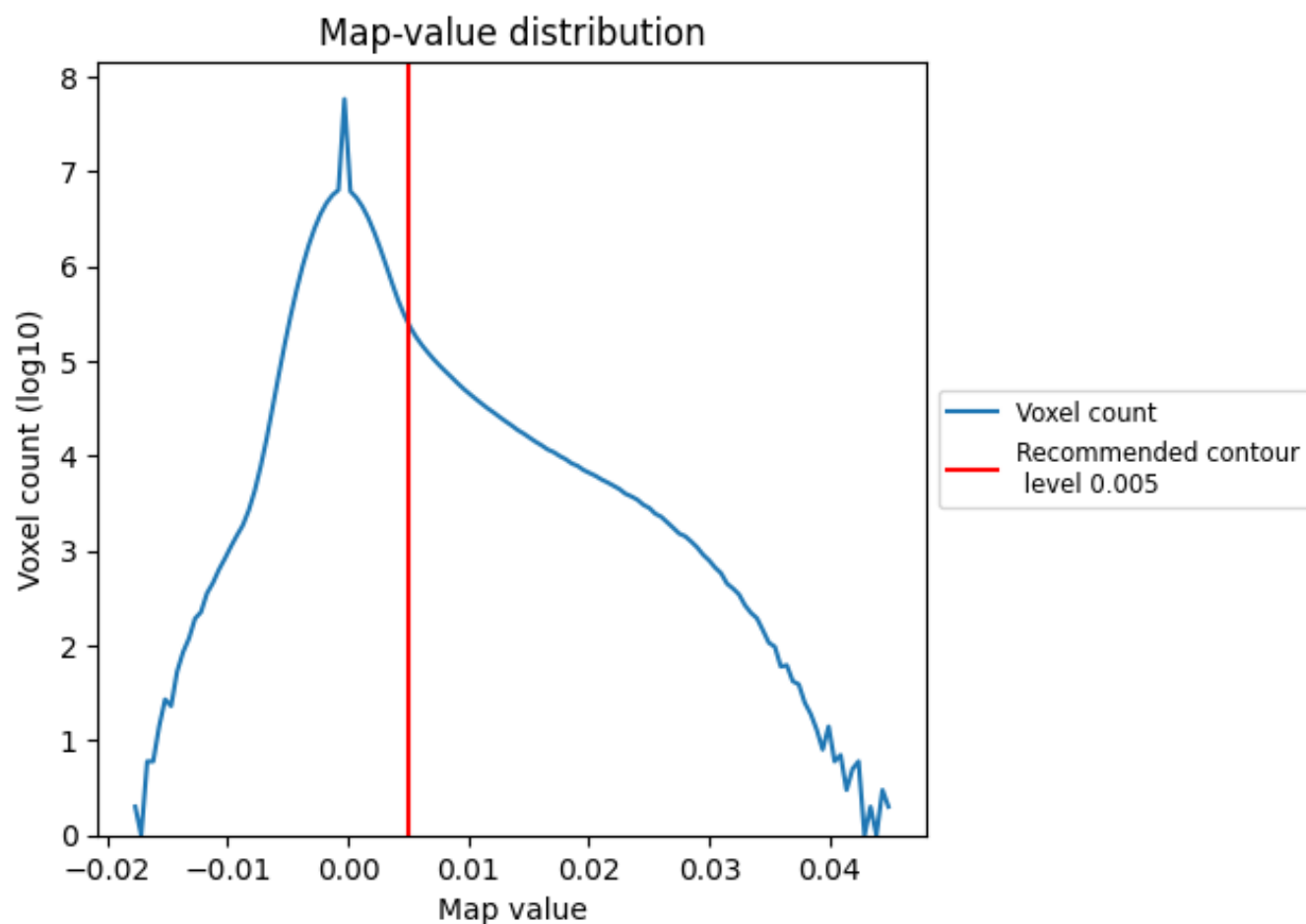
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

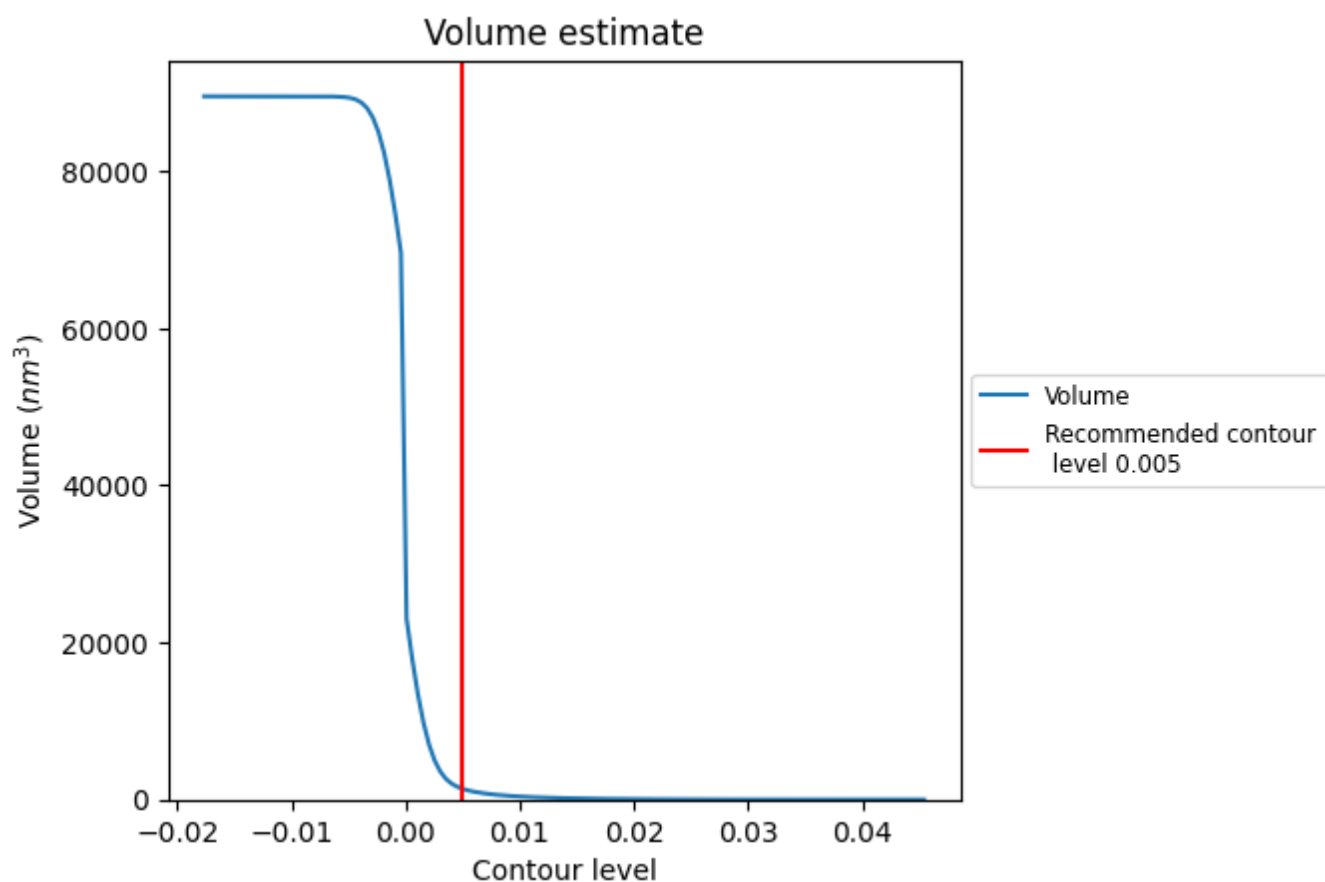
This section contains the results of statistical analysis of the map.

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.

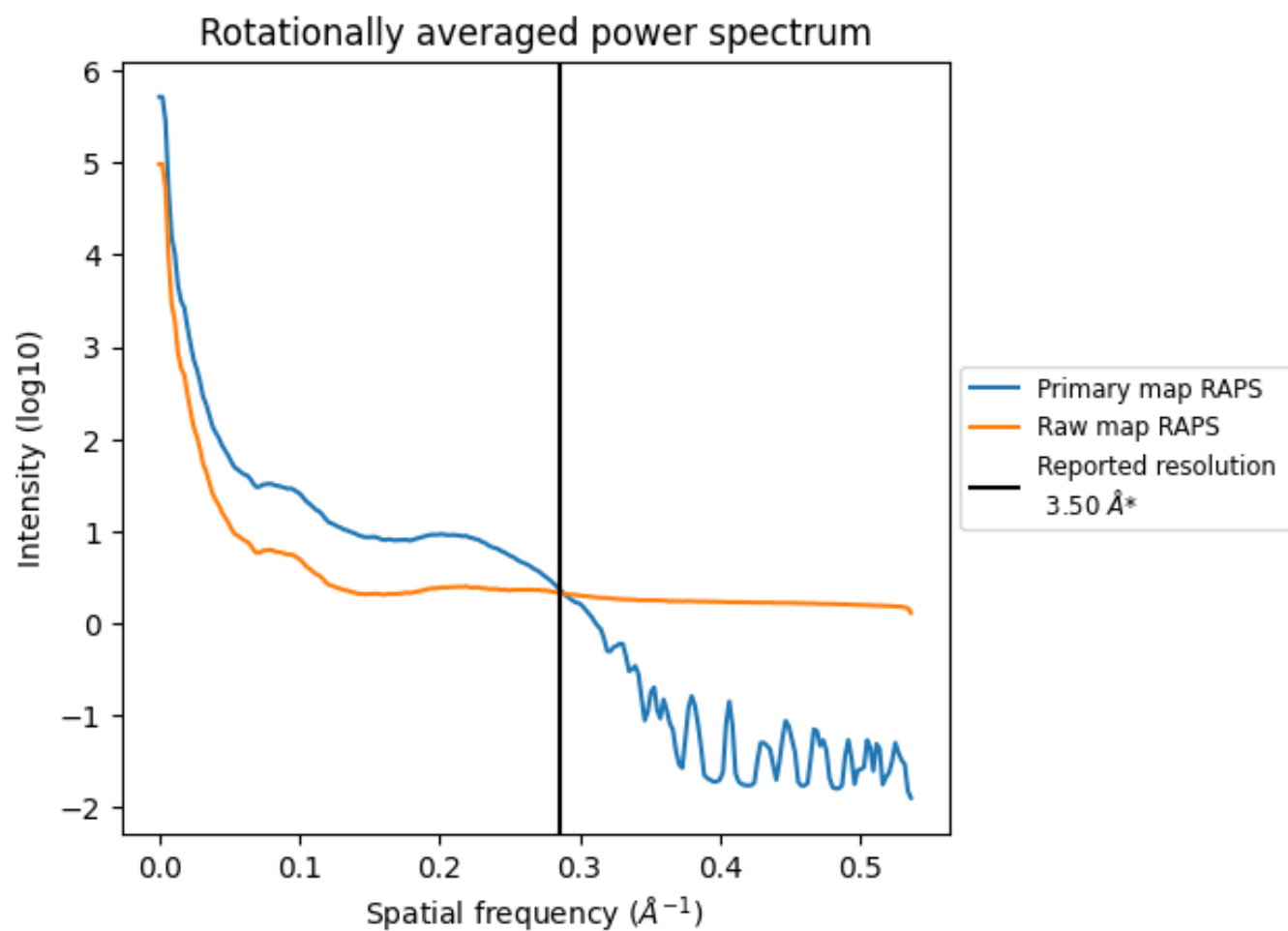
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1361 nm³; this corresponds to an approximate mass of 1229 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 ⓘ

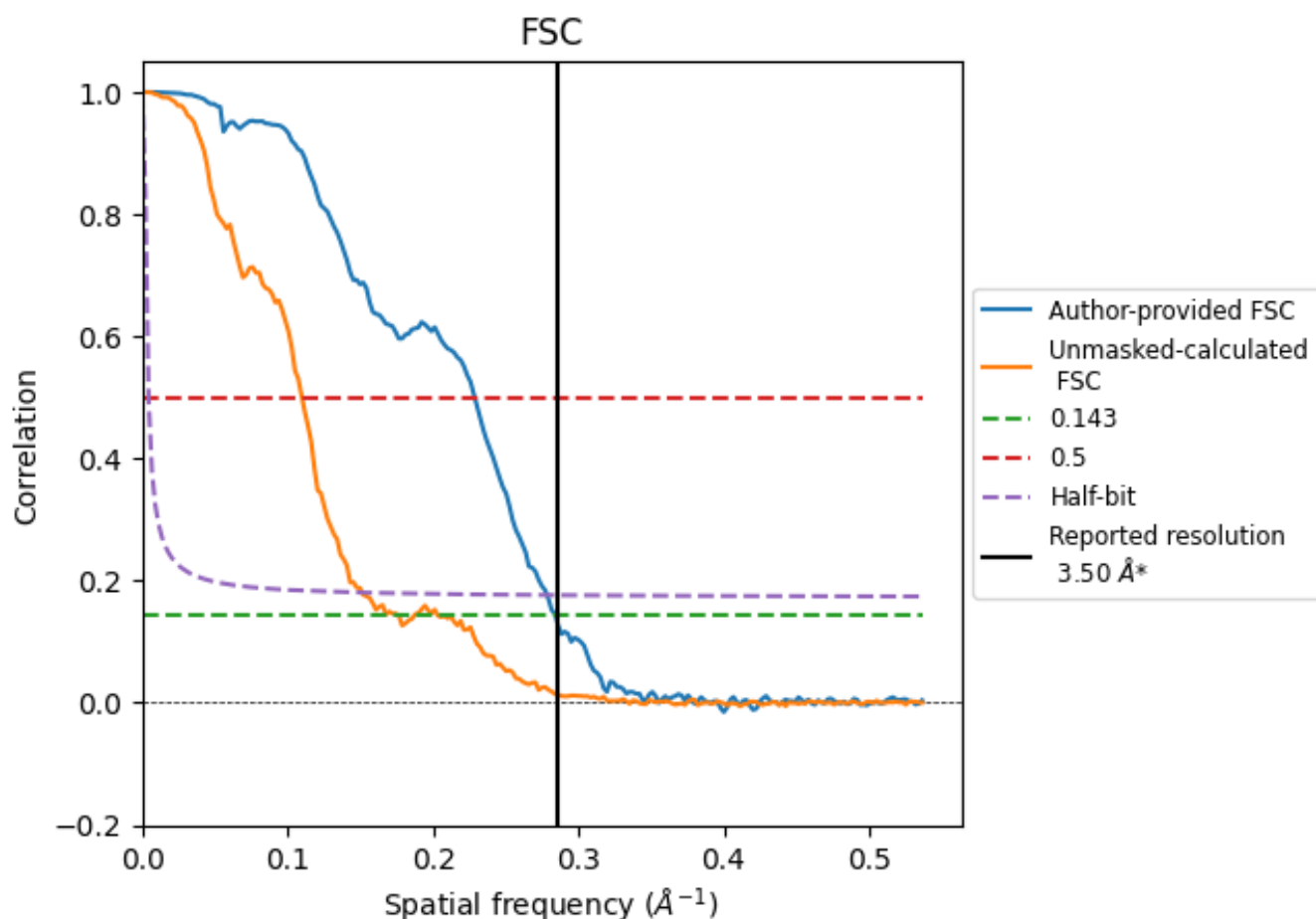


*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

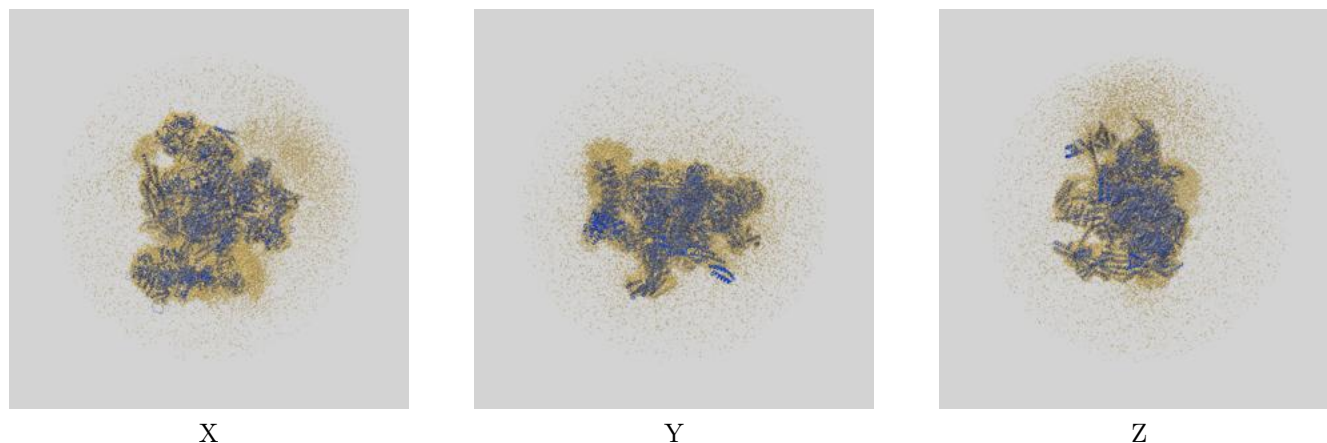
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	4.37	3.59
Unmasked-calculated*	5.68	9.10	6.61

*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 5.68 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

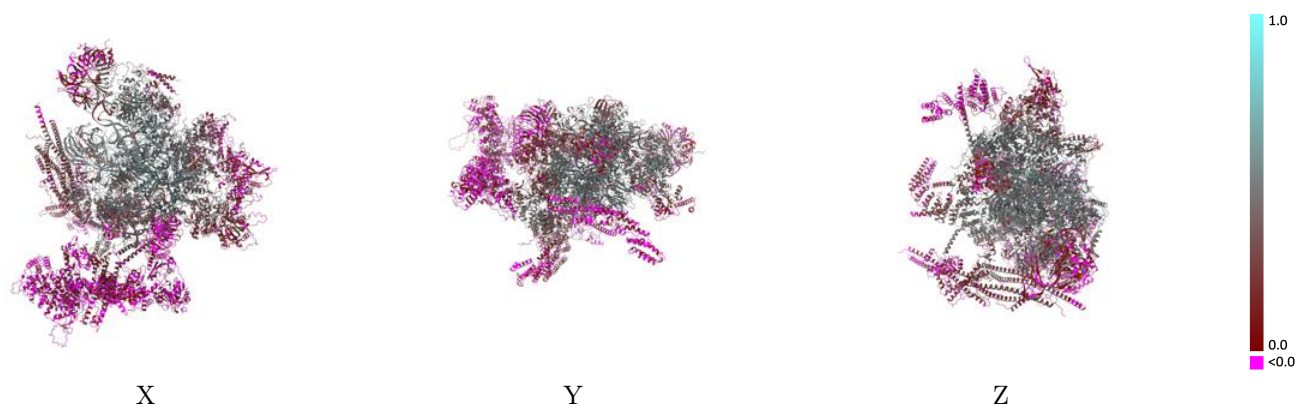
This section contains information regarding the fit between EMDB map EMD-62843 and PDB model 9L5T. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



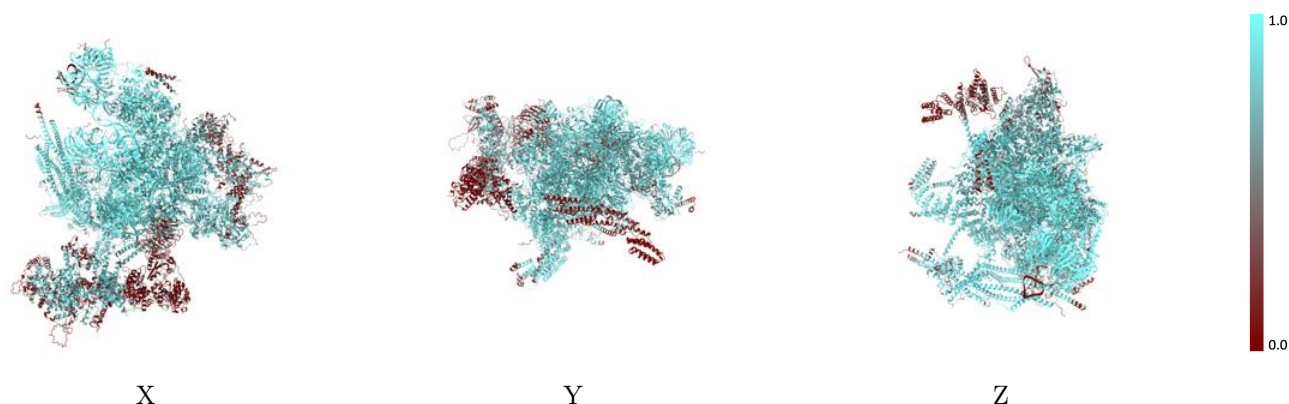
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



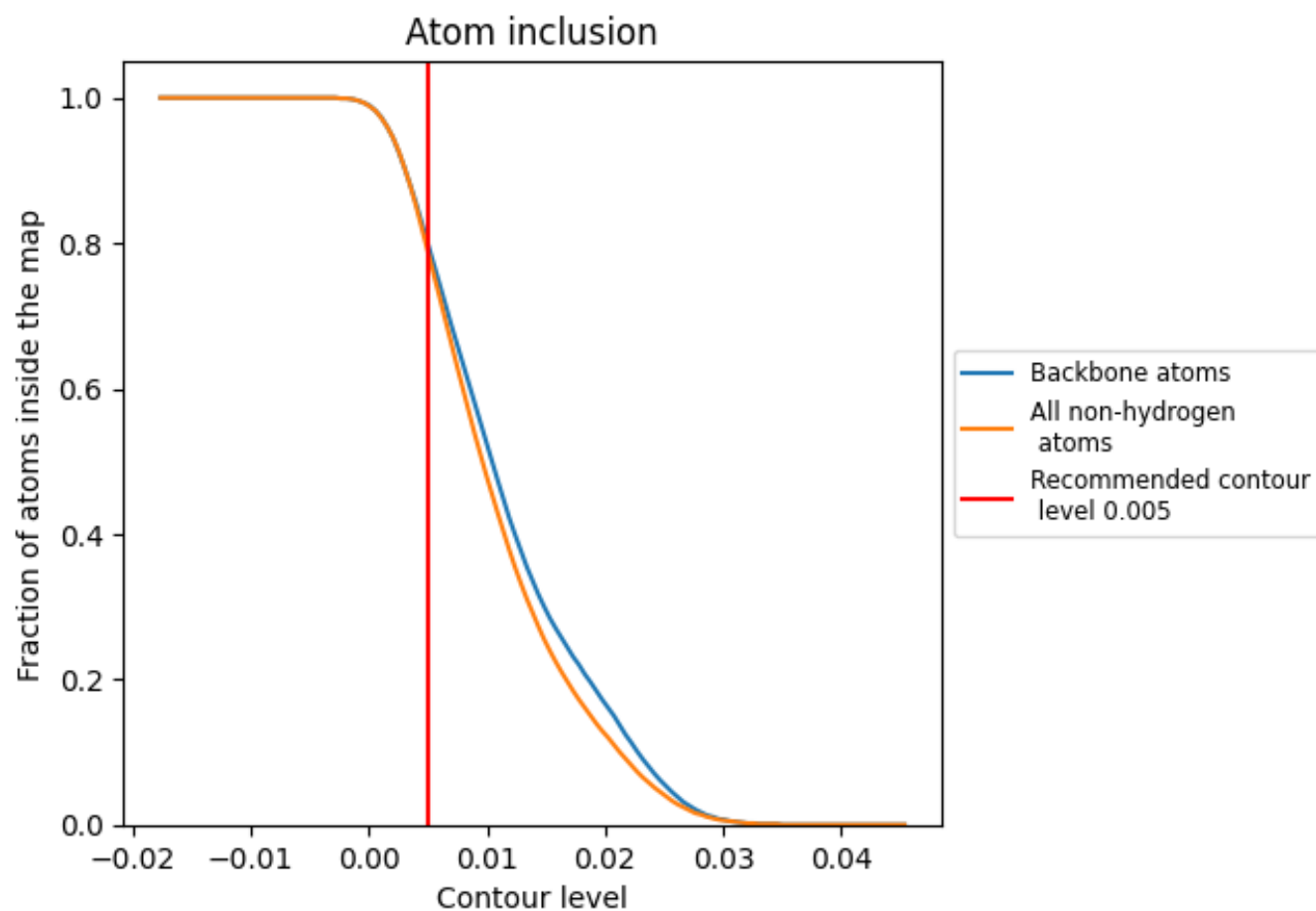
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 79% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7890	 0.3310
0	 0.9460	 0.4040
1	 0.7250	 0.3040
2	 0.9630	 0.4890
5	 0.8310	 0.3670
6	 0.9760	 0.4810
8	 0.9680	 0.3820
A	 0.8900	 0.4550
B	 0.8870	 0.4080
C	 0.9150	 0.4340
CY	 0.8030	 0.4330
Cb	 0.1660	 0.0260
Cc	 0.1070	 0.0260
Ck	 0.0490	 -0.0010
D	 0.8300	 0.3290
E	 0.9490	 0.4790
F	 0.8840	 0.2910
I	 0.8490	 0.2850
J	 0.9020	 0.3690
K	 0.8750	 0.2250
L	 0.8320	 0.3460
M	 0.8700	 0.3370
N	 0.9520	 0.5050
P	 0.9050	 0.4950
R	 0.8720	 0.4400
S	 0.9180	 0.4240
T	 0.9830	 0.5630
V	 0.5070	 0.2470
W	 0.4870	 0.1610
Y	 0.5210	 0.0280
Z	 0.5790	 0.3490
j	 0.9130	 0.1620
k	 0.9640	 0.3070
l	 0.8400	 0.0810
m	 0.8830	 0.1080



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Chain	Atom inclusion	Q-score
o	 0.8960	 0.1870
p	 0.8410	 0.3350
q	 0.8830	 0.2090
r	 0.9280	 0.2540
s	 0.7800	 0.1490
t	 0.7520	 0.0940
u	 0.9390	 0.4020
z	 0.7820	 0.2900