



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 07:05 PM UTC

PDB ID : 7SYX / pdb_00007syx
EMDB ID : EMD-25544
Title : Structure of the delta dII IRES eIF5B-containing 48S initiation complex, closed conformation. Structure 15(delta dII)
Authors : Brown, Z.P.; Abaeva, I.S.; De, S.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on : 2021-11-25
Resolution : 3.70 Å(reported)
Based on initial models : 4UJD, 6D9J, 5K0Y, 5FLX

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:

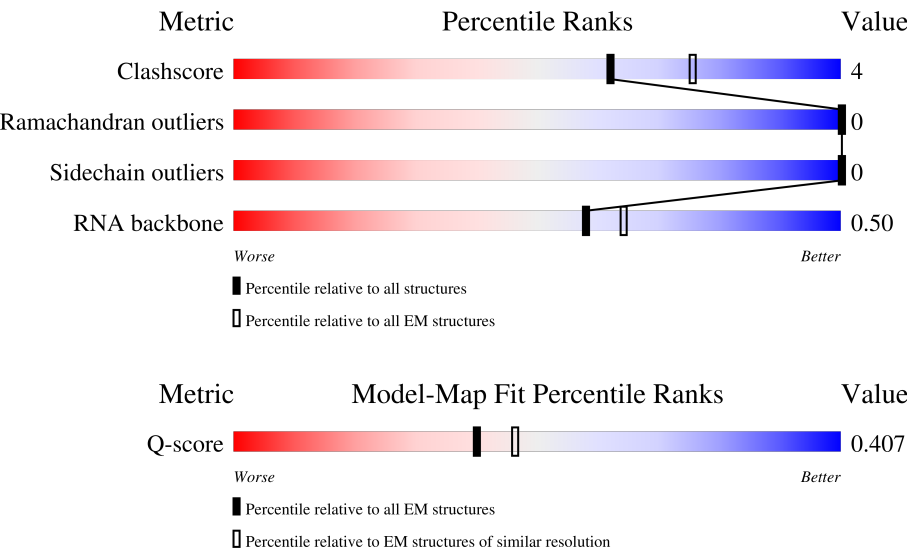
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	1870	10% 62% 26% 9%
2	A	144	68% 55% 14% 31%
3	B	295	11% 63% 11% 26%

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Mol	Chain	Length	Quality of chain
4	C	264	
5	D	221	
6	E	281	
7	F	262	
8	G	204	
9	H	249	
10	I	432	
11	J	208	
12	K	194	
13	L	149	
14	M	158	
15	N	132	
16	O	151	
17	P	168	
18	Q	145	
19	R	172	
20	S	135	
21	T	152	
22	U	145	
23	V	119	
24	W	83	
25	X	130	
26	Y	143	
27	Z	131	
28	a	124	

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Mol	Chain	Length	Quality of chain
29	b	101	
30	c	84	
31	d	69	
32	e	56	
33	f	133	
34	g	188	
35	h	317	
36	i	75	
37	n	25	
38	x	627	
39	z	400	

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 86744 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1697	Total	C	N	O	P	0	0
			36227	16170	6504	11857	1696		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	99	Total	C	N	O	S	0	0
			798	503	143	148	4		

- Molecule 3 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 4 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 5 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 6 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 7 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	262	Total	C	N	O	S	0	0
			2073	1323	384	357	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17

- Molecule 8 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 9 is a protein called eS6.

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

- Molecule 10 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 11 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	206	Total	C	N	O	S	1	0
			1691	1061	333	292	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 12 is a protein called uS4.

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

- Molecule 13 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 14 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	151	Total	C	N	O	S	0	0
			1233	785	231	211	6		

- Molecule 15 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 16 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 17 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 18 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 19 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 20 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 21 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 22 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 23 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 24 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	83	Total	C	N	O	S	0	0
			628	384	117	122	5		

- Molecule 25 is a protein called uS8.

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

- Molecule 26 is a protein called uS12.

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

- Molecule 27 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 28 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	77	Total	C	N	O	S	0	0
			614	393	114	106	1		

- Molecule 29 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	101	Total	C	N	O	S	0	0
			811	506	167	132	6		

- Molecule 30 is a protein called eS27.

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

- Molecule 31 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	67	Total	C	N	O	S	0	0
			530	321	108	99	2		

- Molecule 32 is a protein called eS29.

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

- Molecule 33 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 35 is a protein called RACK1.

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

- Molecule 36 is a RNA chain called Met-tRNA-i-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 37 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	x	627	Total	C	N	O	S	0	0
			4965	3157	856	929	23		

- Molecule 39 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	z	188	Total	C	N	O	P	0	0
			4017	1789	721	1319	188		

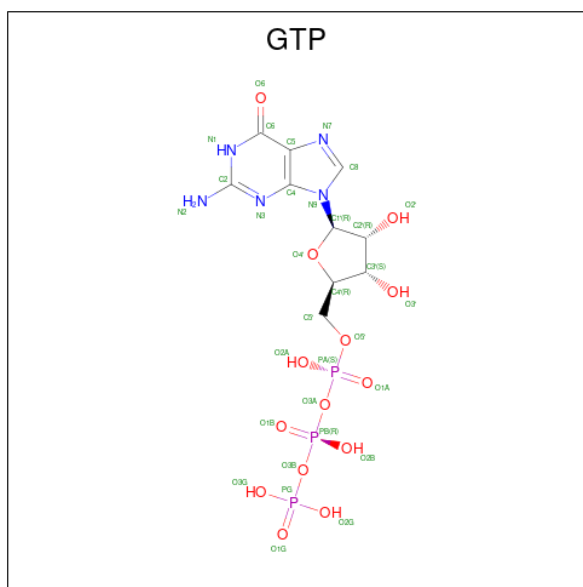
- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	b	1	Total	Zn	0
			1	1	

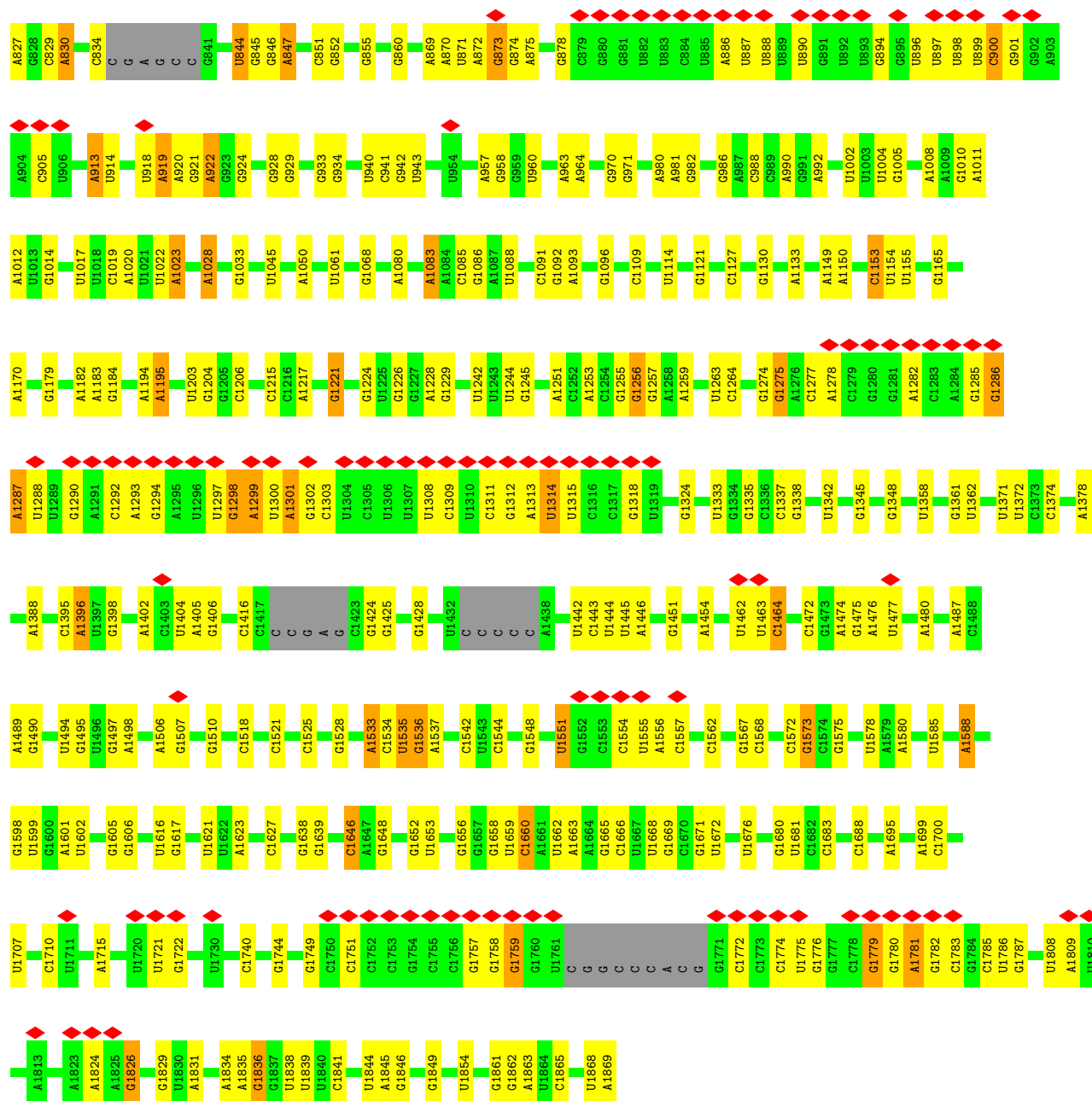
- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
41	x	1	Total	Mg	0
			1	1	

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

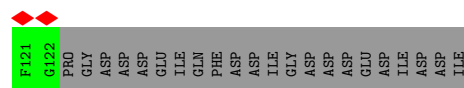


Mol	Chain	Residues	Atoms					AltConf
42	x	1	Total	C	N	O	P	0
			32	10	5	14	3	

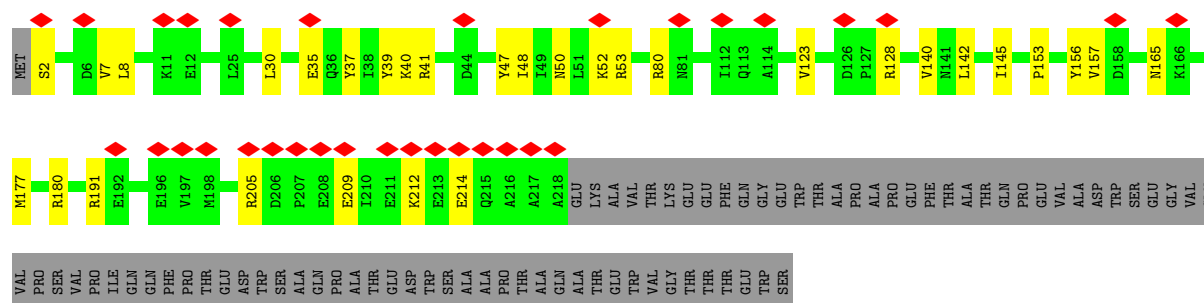


• Molecule 2: Eukaryotic translation initiation factor 1A, X-chromosomal

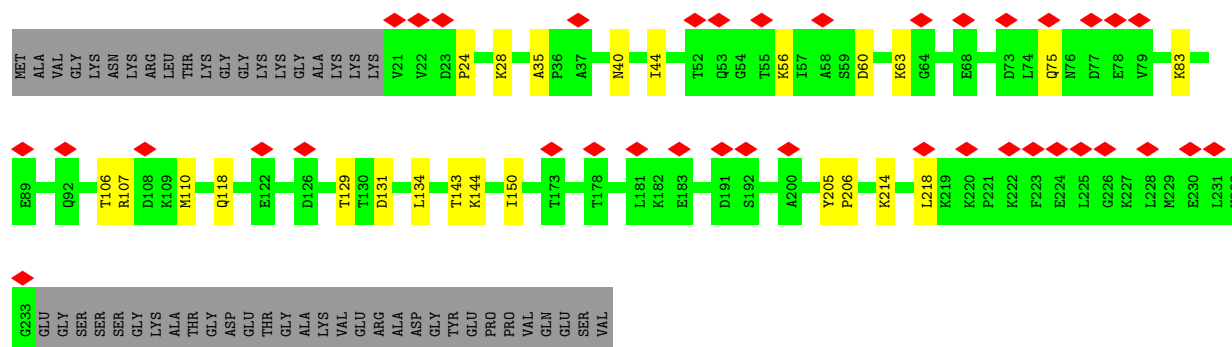




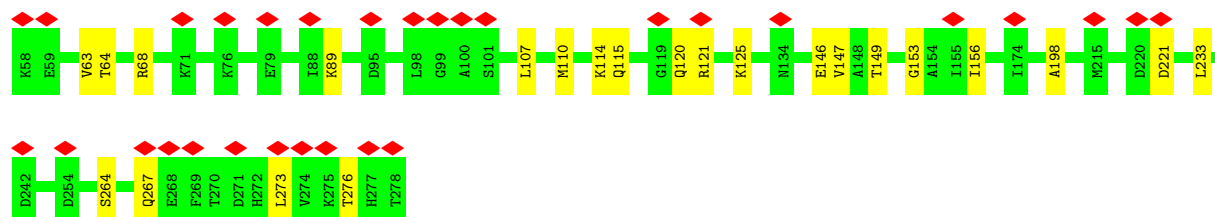
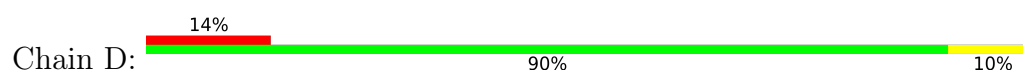
• Molecule 3: uS2



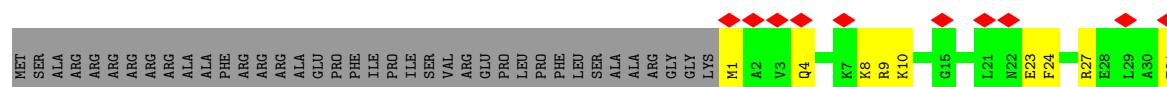
• Molecule 4: eS1

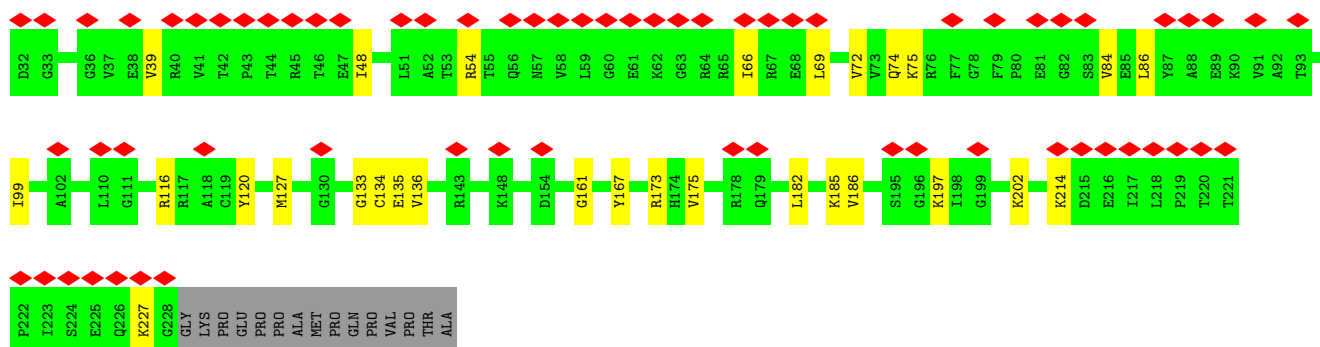


• Molecule 5: uS5

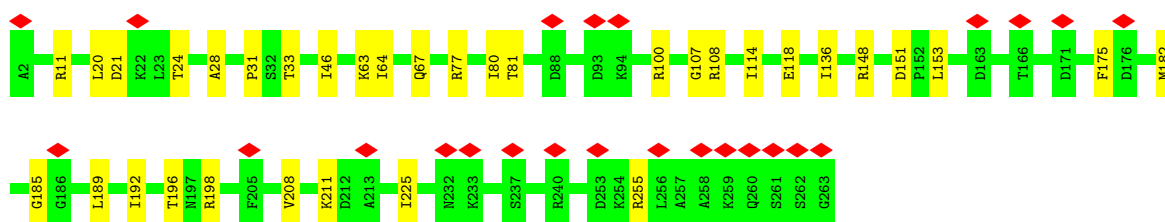
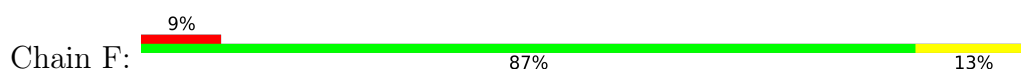


• Molecule 6: uS3

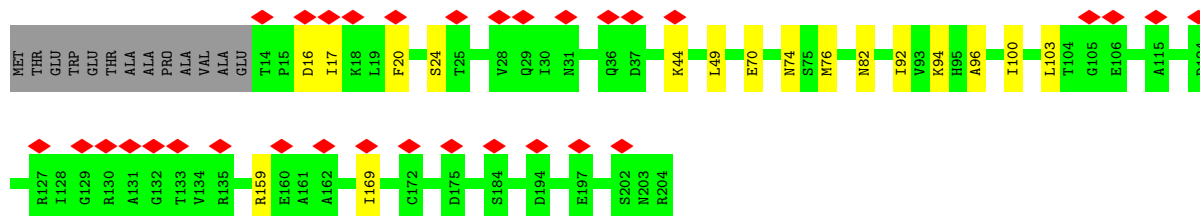
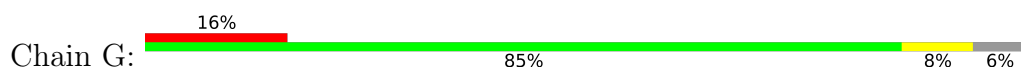




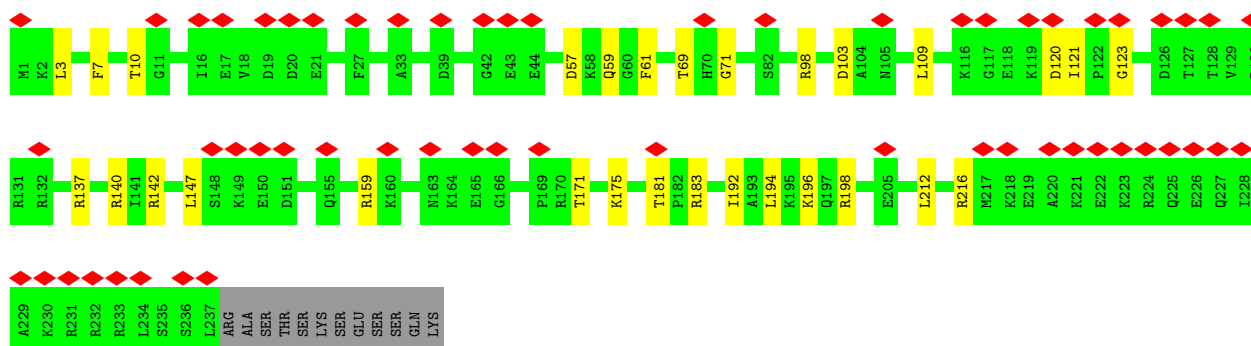
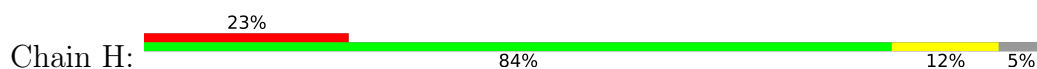
• Molecule 7: eS4



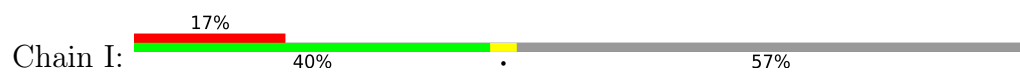
• Molecule 8: uS7



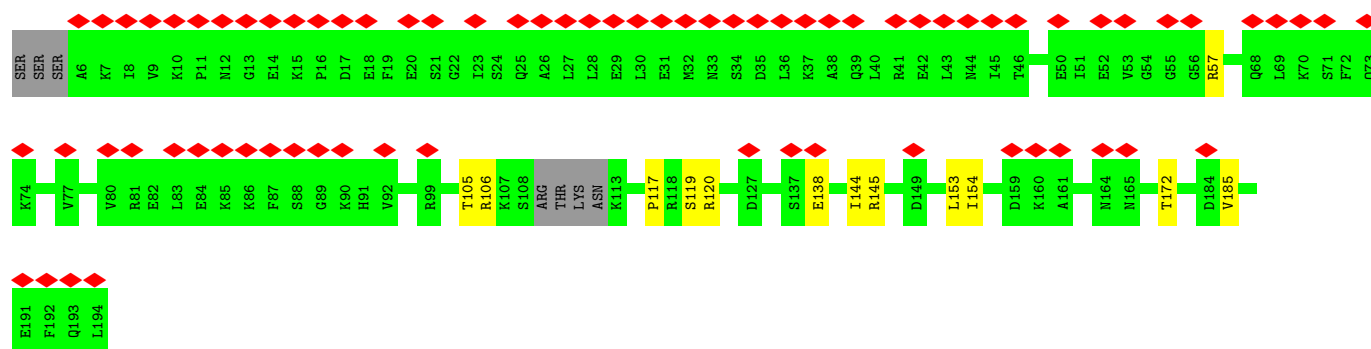
• Molecule 9: eS6



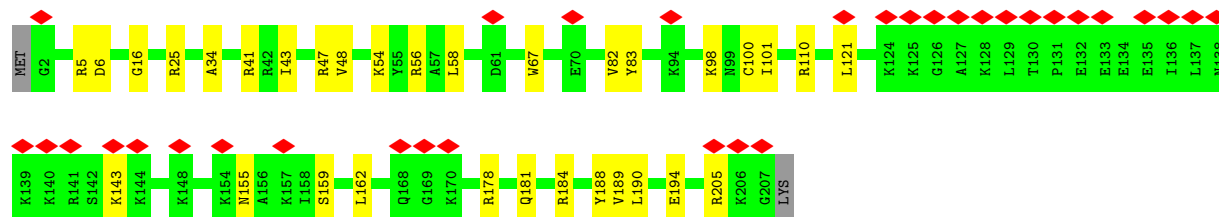
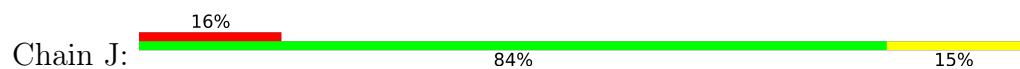
• Molecule 10: 40S ribosomal protein S7



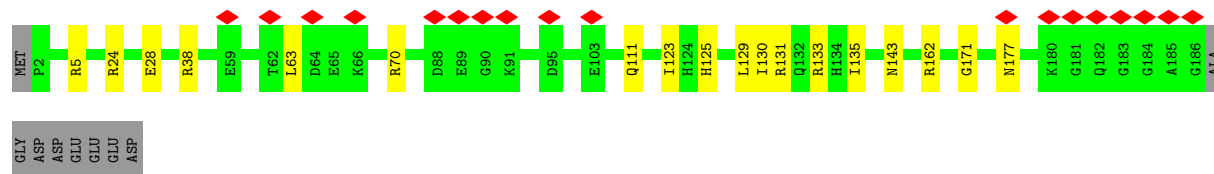
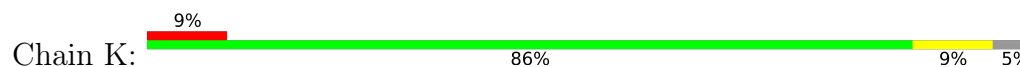
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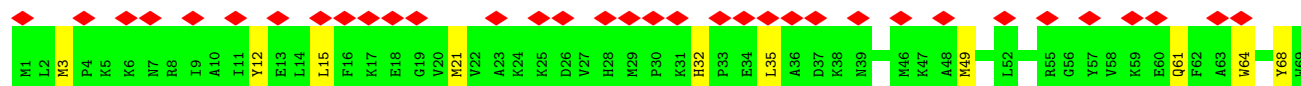
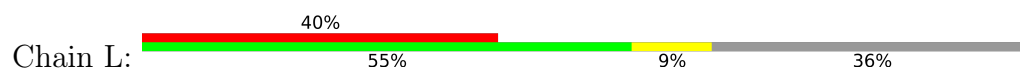
• Molecule 11: eS8

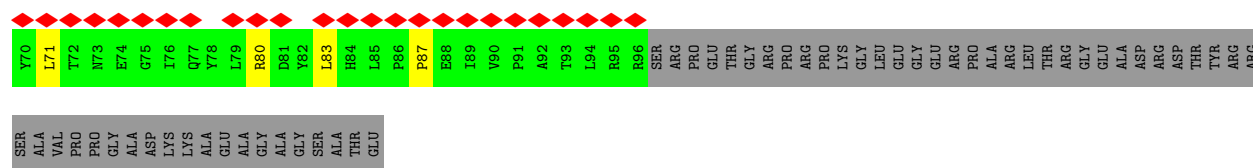


• Molecule 12: uS4

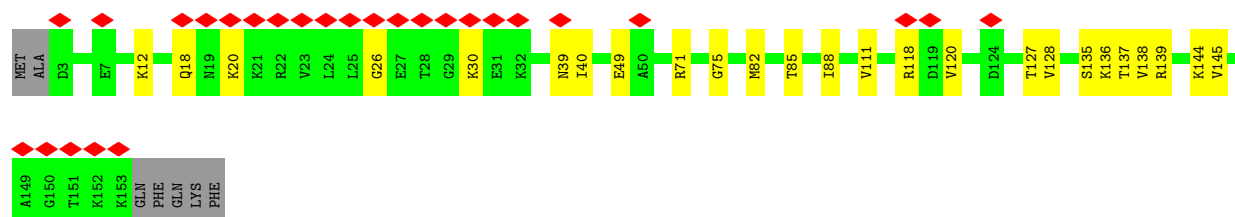
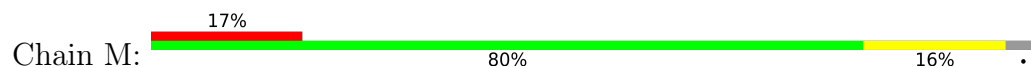


• Molecule 13: eS10

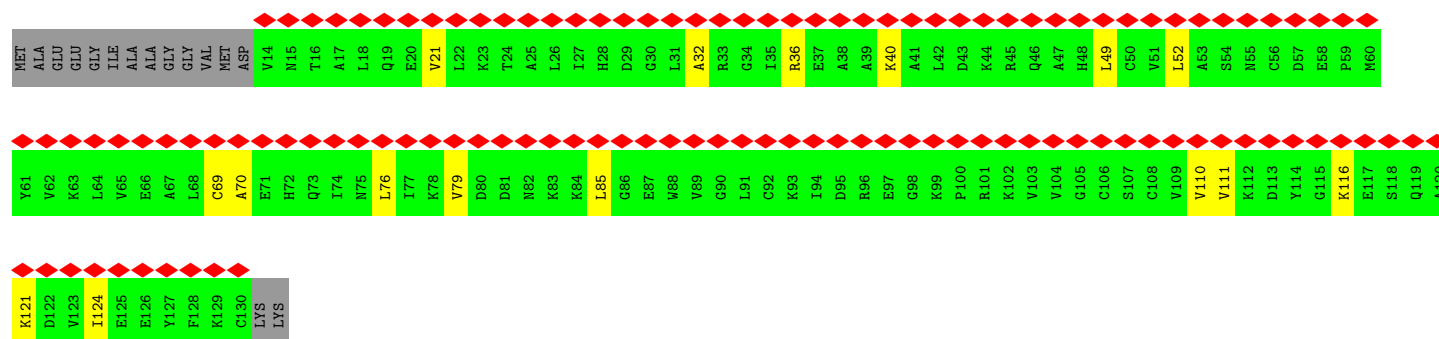
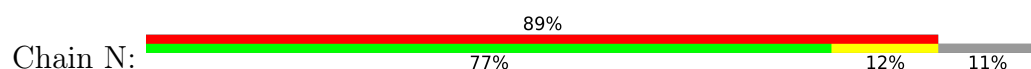




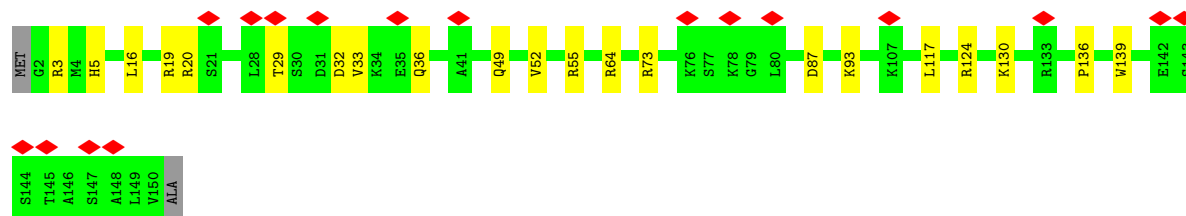
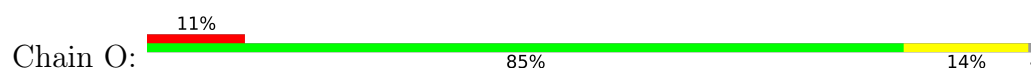
• Molecule 14: uS17



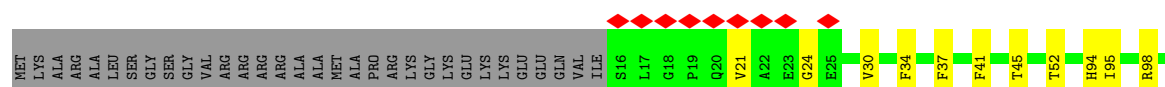
• Molecule 15: eS12

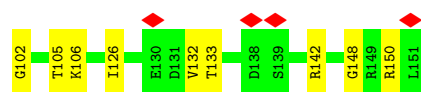


• Molecule 16: uS15

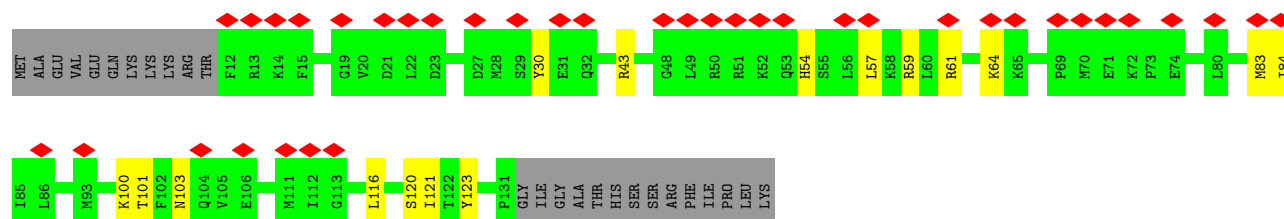
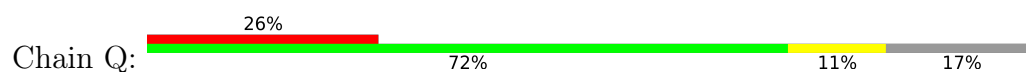


• Molecule 17: uS11

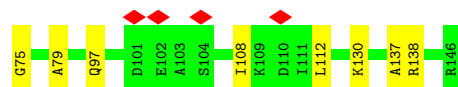
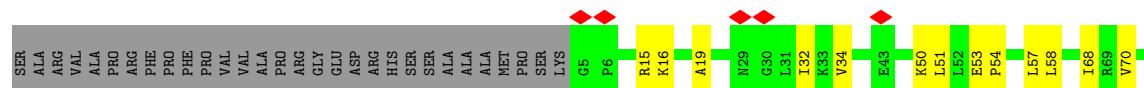




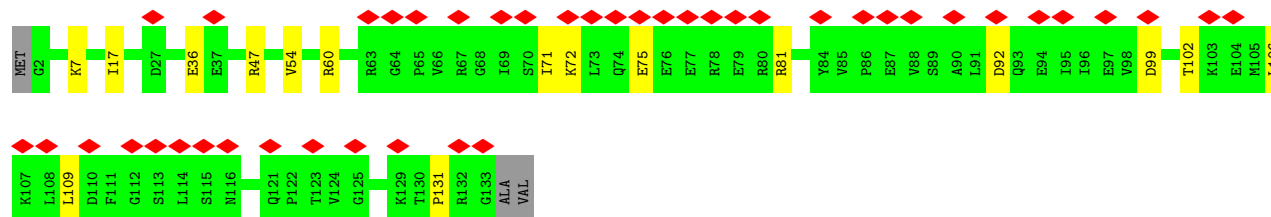
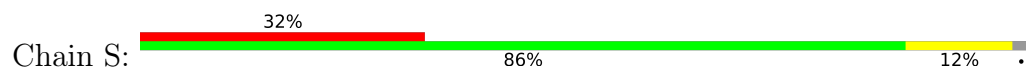
• Molecule 18: uS19



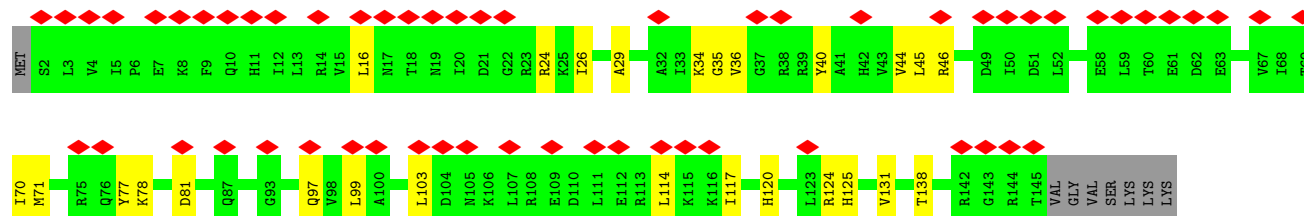
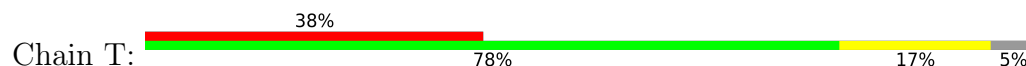
• Molecule 19: uS9



• Molecule 20: eS17

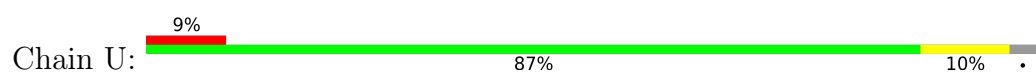


• Molecule 21: uS13

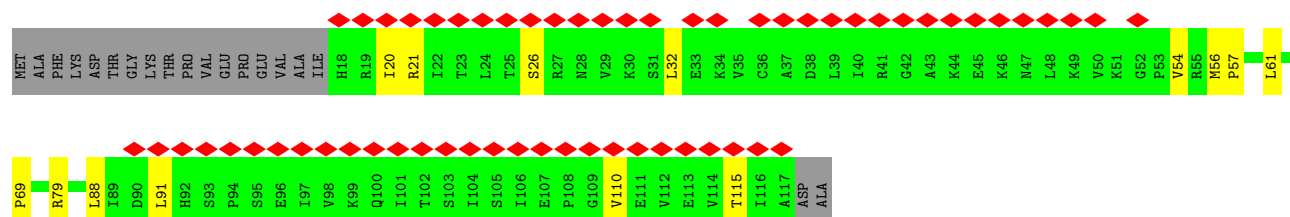
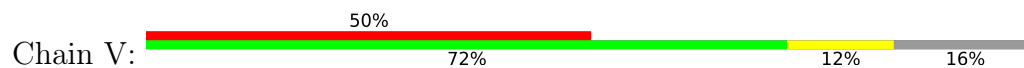


• Molecule 22: eS19

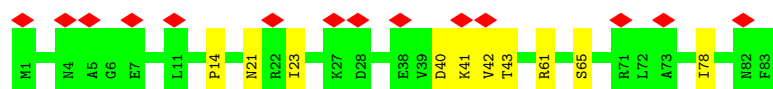
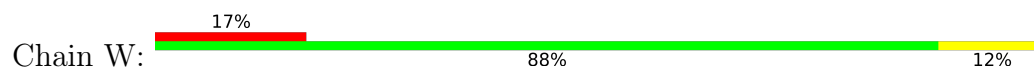




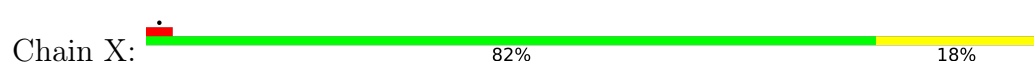
• Molecule 23: uS10



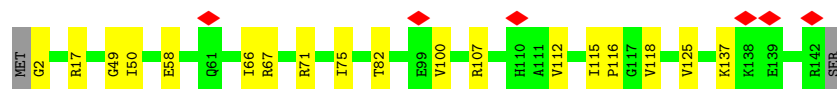
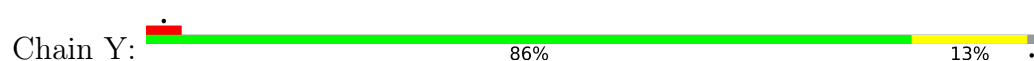
• Molecule 24: eS21



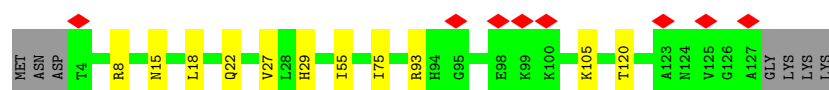
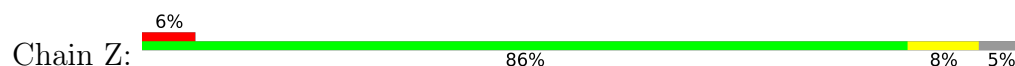
• Molecule 25: uS8



• Molecule 26: uS12

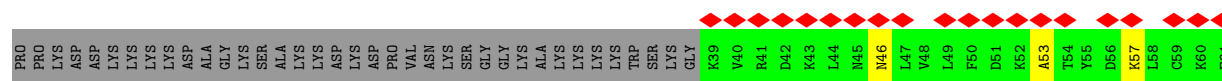


• Molecule 27: 40S ribosomal protein S24

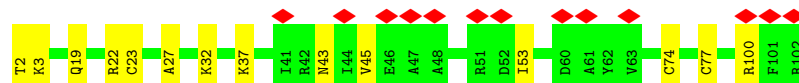
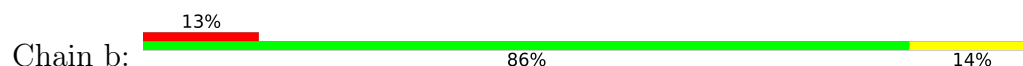


• Molecule 28: 40S ribosomal protein S25

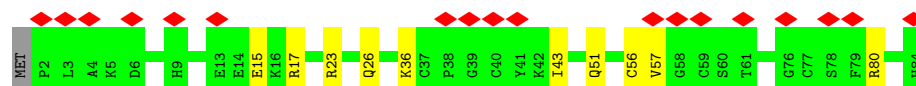
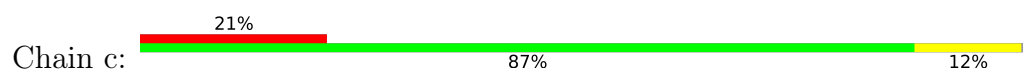




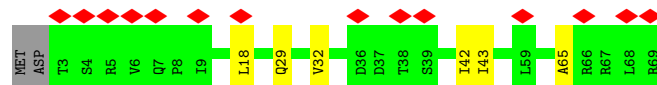
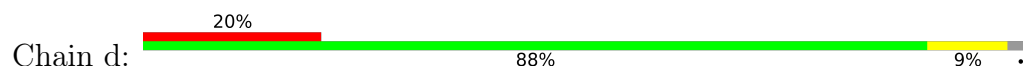
• Molecule 29: eS26



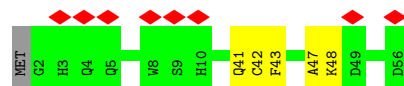
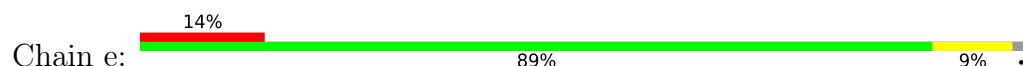
• Molecule 30: eS27



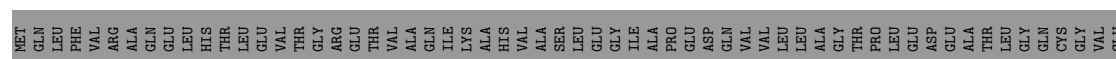
• Molecule 31: eS28



• Molecule 32: eS29



• Molecule 33: eS30



• Molecule 34: 40S ribosomal protein S27a



MET ALA ARG HIS HIS PRO LEU LEU TVR GLN GLY SER ASP GLY ASP GLN ILE TRP CYS GLY LEU ARG LEU ARG GLY GLY ALA PHE GLY PHE GLY GLY GLY ALA THR LYS PRO ARG ARG GLY PRO ALA ALA PHE LEU PHE LEU PHE ASP PRO LEU PRO VAL SER ALA ARG ARG TRP ALA GLY GLY HIS ASP GLN ASP ALA ASP LYS LEU ARG GLU ASN PRO TYR GLY

GLU ASP HIS HIS LYS PRO ARG GLY ILE ASP PRO ASP ASP LYS K83 K84 Y85 Y86 Y87 Y88

K89 K90 N91 K92 ARG K93 K94 R95 K96 K97 V98 K99 L100 A101 V102 L103 K104 L105 Y106 K107 V108 D109 E110 N111 G112 K113 I114 S115 R116 L117 R118 R119 E120 C121 P122 S123 D124 E125 C126 G127 A128 G129 V130 F131 M132 A133 S134 H135 F136 D137 R138 H139 Y140 C141 G142 K143 C144 C145 L146 T147 Y148

C149 F150 ASN PRO GLU ASP LYS

• Molecule 35: RACK1

Chain h: 33% 82% 17%

MET T2 E3 Q4 M5 T6 L7 R8 L11 N15 G16 W17 V18 T24 P25 Q26 I31 S35 R36 T40 T41 M42 E49 T50 N51 Y52 G53 I54 P55 Q56 R57 R60 V66 S67 D68 I71 S72 D74 Q76 F77 S80 L87 D91 L92 F101 H104 D107 V108 L109 S110 V111 S115 D116 M117 R118 Q119 I120 V121 S122 G123 S124 D126 L131 T134 L135 G136 V137 C138 K139 Y140 Q143 D144 E145 S146 H147 S148 S152 S157 P158 N159 S160 S161 M162 P163 I164 K172 N178 L179 A180 N181 C182 K185 H191 S201 P202 D203 G204 S205 L206 C207 A208 S209 G210 G211 D212 D213 G214 Q215 L218 W219 D220 L221 N222 E223 L227 L230 D231 G232 G233 D234 I235 Y246 W247 A251 T252 T256 K257 W259 D260 L261 E262 G263 K264 T265 T266 V267 D268 E269 K271 Q272 E273 V274 I275 S276 T277 S278 K280 A281 E282 S288 L289 A290 W291 S292 A293 D294 G295 A300 D304 N305 L306 V307 R308 V312 T313 I314 GLY THR ARG

• Molecule 36: Met-tRNA-i-Met

Chain i: 43% 69% 28%

A1 G2 C3 A4 G5 U8 G12 C13 A14 G15 C16 G17 G18 A19 A20 U27 G28 G45 U46 C47 G48 A49 U50 G51 G52 A53 U54 C55 G56 A57 A58 A59 C60 A62 U63 C64 C65 U66 C67 U68 U71 A72 C73 C74 A75

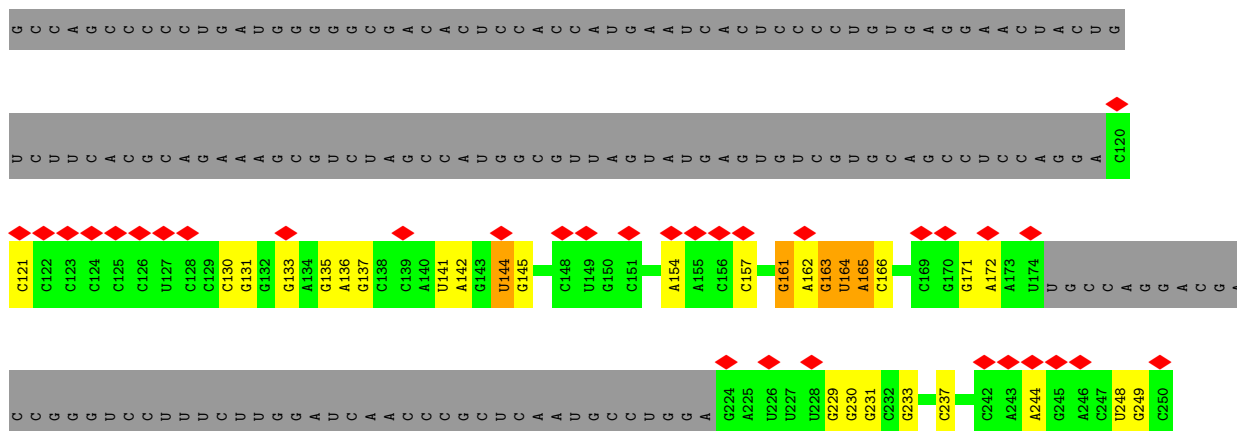
• Molecule 37: 60s ribosomal protein 141

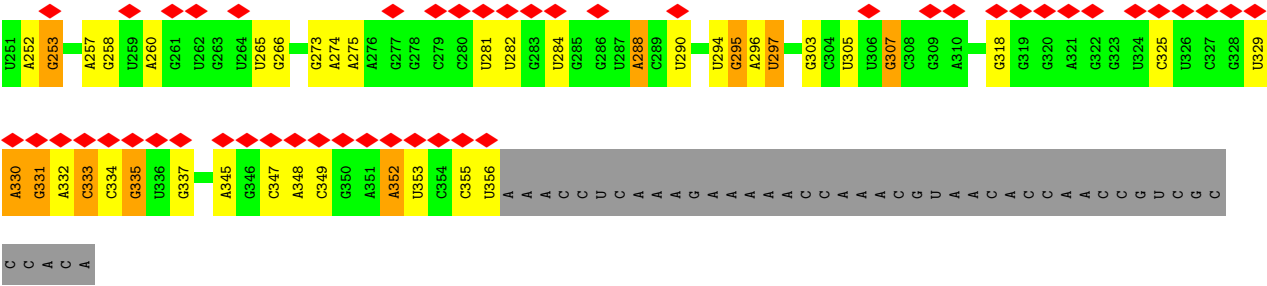
Chain n: 24% 80% 20%

H1 R2 R9 M10 R11 K16 M20 R21 Q22 R23 S24 K25

• Molecule 38: Eukaryotic translation initiation factor 5B

Chain x: 52% 85% 15%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	52000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.051	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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, MG, ZN

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	0.14	0/40506	0.31	0/63123
2	A	0.17	0/809	0.48	0/1083
3	B	0.20	0/1747	0.50	0/2374
4	C	0.18	0/1756	0.45	0/2350
5	D	0.19	0/1753	0.49	0/2369
6	E	0.21	0/1796	0.52	0/2417
7	F	0.18	0/2115	0.44	0/2843
8	G	0.20	0/1531	0.50	1/2059 (0.0%)
9	H	0.17	0/1946	0.40	0/2590
10	I	0.20	0/1510	0.50	0/2022
11	J	0.23	0/1723	0.58	0/2298
12	K	0.18	0/1550	0.43	0/2069
13	L	0.19	0/834	0.47	0/1125
14	M	0.19	0/1254	0.48	0/1677
15	N	0.21	0/918	0.51	0/1233
16	O	0.20	0/1226	0.46	0/1649
17	P	0.16	0/1029	0.41	0/1380
18	Q	0.18	0/1017	0.46	0/1358
19	R	0.22	0/1146	0.48	0/1534
20	S	0.19	0/1082	0.53	0/1452
21	T	0.20	0/1208	0.53	0/1618
22	U	0.20	0/1115	0.46	0/1493
23	V	0.18	0/805	0.45	0/1081
24	W	0.16	0/634	0.44	0/848
25	X	0.21	0/1051	0.50	0/1406
26	Y	0.36	1/1116 (0.1%)	0.65	5/1490 (0.3%)
27	Z	0.21	0/1028	0.51	0/1366
28	a	0.28	0/620	0.70	0/831
29	b	0.18	0/825	0.44	0/1106
30	c	0.18	0/665	0.43	0/891
31	d	0.23	0/532	0.53	0/712
32	e	0.15	0/470	0.40	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.14	0/462	0.43	0/607
34	g	0.11	0/567	0.32	0/753
35	h	0.17	0/2493	0.45	0/3394
36	i	0.12	0/1795	0.23	0/2798
37	n	0.19	0/240	0.42	0/305
38	x	0.20	0/5047	0.51	1/6803 (0.0%)
39	z	0.14	0/4488	0.30	0/6995
All	All	0.17	1/92409 (0.0%)	0.40	7/134125 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	116	PRO	CG-CD	-8.70	1.21	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	116	PRO	N-CD-CG	-11.34	86.20	103.20
26	Y	116	PRO	CA-N-CD	-10.64	97.11	112.00
38	x	956	VAL	N-CA-C	-8.71	104.99	113.53
26	Y	116	PRO	CA-CB-CG	-6.04	93.02	104.50
26	Y	116	PRO	N-CA-C	5.19	123.17	112.47
26	Y	116	PRO	N-CA-CB	-5.10	97.90	103.25
8	G	44	LYS	N-CA-C	-5.01	107.83	114.04

There are no chirality outliers.

There are no planarity outliers.

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	36227	0	18299	209	0
2	A	798	0	807	15	0
3	B	1710	0	1711	21	0
4	C	1729	0	1803	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1716	0	1806	13	0
6	E	1768	0	1866	25	0
7	F	2073	0	2175	23	0
8	G	1509	0	1563	10	0
9	H	1923	0	2089	20	0
10	I	1488	0	1582	8	0
11	J	1691	0	1778	24	0
12	K	1525	0	1640	13	0
13	L	810	0	836	10	0
14	M	1233	0	1310	18	0
15	N	908	0	939	9	0
16	O	1202	0	1289	16	0
17	P	1016	0	1039	13	0
18	Q	997	0	1045	12	0
19	R	1128	0	1195	17	0
20	S	1068	0	1121	13	0
21	T	1190	0	1249	17	0
22	U	1097	0	1130	10	0
23	V	795	0	862	9	0
24	W	628	0	630	8	0
25	X	1034	0	1080	16	0
26	Y	1098	0	1167	15	0
27	Z	1011	0	1083	8	0
28	a	614	0	678	9	0
29	b	811	0	859	11	0
30	c	651	0	672	7	0
31	d	530	0	561	3	0
32	e	459	0	452	4	0
33	f	457	0	502	4	0
34	g	555	0	565	7	0
35	h	2436	0	2393	29	0
36	i	1604	0	816	8	0
37	n	239	0	289	5	0
38	x	4965	0	5126	57	0
39	z	4017	0	2033	30	0
40	b	1	0	0	0	0
41	x	1	0	0	0	0
42	x	32	0	12	1	0
All	All	86744	0	68052	635	0

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

All (635) 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)
39:z:260:A:H62	39:z:273:G:H21	1.07	0.99
1:2:1288:U:H3	1:2:1311:C:N4	1.65	0.93
1:2:1288:U:H3	1:2:1311:C:H42	0.85	0.82
1:2:934:G:H1	1:2:1008:A:H2	1.26	0.81
39:z:145:G:H1	39:z:248:U:H3	1.30	0.77
17:P:34:PHE:HB3	17:P:41:PHE:HB2	1.70	0.74
39:z:144:U:H3	39:z:249:G:H1	1.36	0.74
39:z:307:G:N1	39:z:329:U:C2	2.58	0.72
1:2:1533:A:H62	1:2:1602:U:H3	1.35	0.70
2:A:66:ARG:HG3	2:A:67:LYS:HG2	1.73	0.70
35:h:107:ASP:HB2	35:h:125:ARG:HG3	1.74	0.70
1:2:1091:C:HO2'	25:X:2:VAL:N	1.91	0.69
19:R:53:GLU:O	19:R:57:LEU:HB2	1.93	0.68
35:h:87:LEU:HB2	35:h:101:PHE:HB2	1.78	0.66
39:z:260:A:H62	39:z:273:G:N2	1.88	0.65
38:x:641:GLY:HA2	42:x:1302:GTP:H5''	1.78	0.65
3:B:123:VAL:HG12	3:B:145:ILE:HB	1.80	0.64
7:F:63:LYS:O	7:F:67:GLN:HB2	1.97	0.63
39:z:260:A:N6	39:z:273:G:H21	1.89	0.63
1:2:1646:C:H5'	19:R:138:ARG:HD3	1.80	0.62
38:x:665:GLN:HG3	38:x:987:GLY:HA3	1.80	0.62
38:x:722:ILE:HD11	38:x:836:LEU:HD11	1.82	0.62
39:z:161:G:H2'	39:z:163:G:H1	1.65	0.61
1:2:1050:A:H62	1:2:1068:G:H21	1.46	0.61
21:T:24:ARG:HB2	21:T:29:ALA:HB2	1.82	0.61
38:x:727:ILE:HG22	38:x:788:ARG:HH11	1.64	0.61
1:2:1542:C:OP1	22:U:62:ARG:NH1	2.33	0.61
27:Z:15:ASN:HB2	27:Z:22:GLN:HE22	1.66	0.61
1:2:1033:G:H1	1:2:1080:A:HO2'	1.49	0.60
9:H:69:THR:HG22	9:H:71:GLY:H	1.64	0.60
23:V:56:MET:HE3	23:V:57:PRO:HD2	1.81	0.60
15:N:32:ALA:HB3	15:N:110:VAL:HB	1.84	0.60
35:h:11:LEU:HB2	35:h:307:VAL:HB	1.83	0.60
1:2:940:U:H3	1:2:1002:U:H3	1.49	0.59
6:E:75:LYS:NZ	13:L:21:MET:SD	2.73	0.59
35:h:40:ILE:HD11	35:h:66:VAL:HG21	1.83	0.59
2:A:51:CYS:SG	2:A:52:PHE:N	2.75	0.59
13:L:32:HIS:HB3	13:L:35:LEU:HB2	1.84	0.59
6:E:74:GLN:HE21	6:E:84:VAL:HG22	1.68	0.59
3:B:191:ARG:NH1	24:W:42:VAL:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:318:A:C2	1:2:333:G:C2	2.90	0.59
1:2:318:A:N1	1:2:333:G:C6	2.71	0.58
8:G:103:LEU:HD21	28:a:67:LEU:HB2	1.85	0.58
1:2:1335:G:OP1	6:E:185:LYS:NZ	2.35	0.58
1:2:1183:A:H2'	1:2:1184:G:H8	1.68	0.58
1:2:377:G:H5'	11:J:98:LYS:HB3	1.86	0.58
13:L:61:GLN:HB2	13:L:68:TYR:HB2	1.86	0.58
19:R:54:PRO:O	19:R:58:LEU:HB2	2.03	0.58
34:g:139:HIS:HB2	34:g:148:TYR:HB2	1.84	0.58
7:F:196:THR:HG21	7:F:211:LYS:HD2	1.87	0.57
15:N:40:LYS:HG2	34:g:129:GLY:HA3	1.86	0.57
1:2:1658:G:OP2	1:2:1660:C:N4	2.37	0.57
6:E:66:ILE:HG23	6:E:86:LEU:HB2	1.86	0.57
2:A:39:ILE:HD11	2:A:50:MET:HE2	1.85	0.57
39:z:252:A:H4'	39:z:253:G:H5'	1.87	0.57
1:2:1179:G:N2	1:2:1182:A:OP2	2.38	0.57
1:2:1616:U:OP2	18:Q:43:ARG:NH2	2.38	0.57
18:Q:83:MET:HB3	18:Q:116:LEU:HD13	1.86	0.57
38:x:1101:ASN:ND2	38:x:1105:PRO:O	2.37	0.56
1:2:457:C:H2'	1:2:458:A:H8	1.70	0.56
13:L:12:TYR:HB3	13:L:83:LEU:HD21	1.87	0.56
1:2:919:A:OP2	16:O:64:ARG:NH2	2.38	0.56
7:F:136:ILE:HG21	7:F:148:ARG:HD2	1.86	0.56
17:P:45:THR:HA	17:P:52:THR:HA	1.85	0.56
23:V:54:VAL:HB	23:V:88:LEU:HB2	1.87	0.56
38:x:858:VAL:HG22	38:x:873:VAL:HG12	1.86	0.56
1:2:918:U:H4'	16:O:20:ARG:HH22	1.70	0.56
14:M:26:GLY:H	14:M:30:LYS:HZ3	1.53	0.56
6:E:116:ARG:NH2	6:E:120:TYR:OH	2.38	0.56
1:2:677:G:H21	1:2:1028:A:H62	1.51	0.56
9:H:137:ARG:HB3	9:H:140:ARG:HG3	1.87	0.56
10:I:145:ARG:HB3	10:I:153:LEU:HB3	1.87	0.56
1:2:1656:G:H1	1:2:1668:U:H3	1.54	0.56
1:2:1605:G:OP1	22:U:84:ARG:NH2	2.39	0.55
16:O:5:HIS:HB3	16:O:117:LEU:HD13	1.88	0.55
1:2:642:U:O4	33:f:106:LYS:NZ	2.39	0.55
29:b:43:ASN:ND2	29:b:45:VAL:O	2.39	0.55
1:2:1669:G:OP2	19:R:130:LYS:NZ	2.39	0.55
5:D:107:LEU:HB3	5:D:233:LEU:HD21	1.89	0.55
1:2:1396:A:O2'	1:2:1398:G:N7	2.37	0.55
1:2:1534:C:O2'	1:2:1598:G:N2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1551:U:OP1	6:E:9:ARG:NH2	2.40	0.55
25:X:111:MET:HE2	25:X:115:GLU:HB3	1.88	0.55
30:c:80:ARG:HH21	39:z:233:G:H2'	1.71	0.55
36:i:72:A:N6	38:x:1103:ARG:O	2.39	0.55
4:C:107:ARG:NH1	17:P:133:THR:O	2.39	0.55
3:B:30:LEU:HB2	3:B:47:TYR:HE1	1.70	0.55
13:L:21:MET:HG2	13:L:49:MET:HE3	1.87	0.55
19:R:34:VAL:HG23	19:R:70:VAL:HB	1.88	0.55
35:h:191:HIS:NE2	35:h:213:ASP:OD1	2.40	0.55
3:B:205:ARG:NH2	20:S:81:ARG:O	2.39	0.54
4:C:40:ASN:OD1	4:C:75:GLN:NE2	2.40	0.54
1:2:851:C:H5''	1:2:852:G:H5'	1.88	0.54
1:2:1562:C:H5''	22:U:71:GLY:HA3	1.89	0.54
9:H:98:ARG:NH2	9:H:103:ASP:OD1	2.41	0.54
38:x:1119:GLN:NE2	38:x:1137:THR:O	2.41	0.54
1:2:934:G:O6	1:2:1008:A:N1	2.41	0.54
6:E:175:VAL:HB	6:E:182:LEU:HB3	1.89	0.54
14:M:136:LYS:O	14:M:139:ARG:NH1	2.39	0.54
26:Y:58:GLU:HA	26:Y:66:ILE:HA	1.90	0.54
3:B:2:SER:N	24:W:78:ILE:O	2.41	0.54
38:x:978:GLY:H	38:x:1004:ALA:HB2	1.72	0.54
1:2:1495:G:N2	32:e:42:CYS:SG	2.77	0.54
10:I:117:PRO:HG2	10:I:120:ARG:HD3	1.90	0.54
16:O:16:LEU:O	30:c:26:GLN:NE2	2.38	0.54
35:h:277:THR:HA	35:h:281:ALA:HB3	1.89	0.54
3:B:214:GLU:OE2	20:S:81:ARG:NH2	2.41	0.54
14:M:135:SER:OG	14:M:136:LYS:N	2.41	0.54
3:B:177:MET:HE1	3:B:180:ARG:HH21	1.72	0.53
12:K:131:ARG:NH1	12:K:143:ASN:O	2.42	0.53
1:2:490:C:OP2	27:Z:105:LYS:NZ	2.40	0.53
1:2:898:U:OP2	1:2:900:C:N4	2.42	0.53
1:2:1841:C:OP2	37:n:2:ARG:NH1	2.41	0.53
1:2:1826:G:H4'	2:A:41:MET:HE1	1.89	0.53
9:H:159:ARG:NH2	9:H:171:THR:O	2.41	0.53
21:T:34:LYS:HG2	21:T:103:LEU:HD12	1.90	0.53
38:x:689:GLU:HG2	38:x:692:ARG:HD3	1.89	0.53
1:2:520:A:O2'	1:2:825:A:N3	2.40	0.53
10:I:144:ILE:HB	25:X:52:ILE:HB	1.89	0.53
1:2:1286:G:OP2	15:N:36:ARG:NH1	2.42	0.53
16:O:136:PRO:HG2	16:O:139:TRP:HB2	1.89	0.53
1:2:379:C:O2	11:J:5:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:x:1175:GLU:HG2	38:x:1177:THR:H	1.73	0.53
38:x:886:ILE:HG22	38:x:947:VAL:HG22	1.91	0.53
6:E:134:CYS:SG	6:E:135:GLU:N	2.82	0.52
2:A:82:ARG:NH1	2:A:84:TYR:OH	2.42	0.52
17:P:45:THR:HG22	17:P:52:THR:HG22	1.90	0.52
1:2:16:G:H21	1:2:1195:A:H62	1.56	0.52
1:2:1153:C:OP2	25:X:71:LYS:NZ	2.37	0.52
22:U:76:THR:HG21	22:U:97:LYS:HG2	1.92	0.52
1:2:218:U:O2	11:J:184:ARG:NH2	2.43	0.52
1:2:919:A:O2'	1:2:1020:A:N6	2.43	0.52
1:2:1020:A:OP1	16:O:73:ARG:NH2	2.42	0.52
11:J:190:LEU:HD22	11:J:194:GLU:HB3	1.92	0.52
1:2:1004:U:H2'	1:2:1005:G:H8	1.75	0.52
4:C:118:GLN:HB2	4:C:143:THR:HB	1.92	0.52
24:W:14:PRO:HG2	24:W:23:ILE:HD11	1.90	0.52
1:2:190:G:O2'	1:2:209:A:N6	2.43	0.52
1:2:202:G:OP1	11:J:143:LYS:NZ	2.41	0.52
1:2:560:A:OP2	12:K:177:ASN:ND2	2.42	0.52
1:2:581:U:OP1	12:K:133:ARG:NH1	2.43	0.52
15:N:116:LYS:HB3	15:N:121:LYS:HE2	1.92	0.52
1:2:1130:G:N2	1:2:1130:G:OP2	2.41	0.51
1:2:1669:G:OP1	23:V:79:ARG:NH2	2.41	0.51
3:B:30:LEU:HD21	3:B:35:GLU:HG3	1.92	0.51
39:z:307:G:C6	39:z:329:U:N3	2.78	0.51
1:2:98:C:OP2	1:2:426:A:O2'	2.25	0.51
1:2:663:C:OP2	26:Y:2:GLY:N	2.43	0.51
1:2:1535:U:O2'	8:G:82:ASN:OD1	2.28	0.51
1:2:1710:C:H1'	2:A:42:LEU:HD21	1.92	0.51
6:E:31:GLU:O	6:E:54:ARG:NH2	2.44	0.51
28:a:72:VAL:HG22	28:a:76:ARG:HE	1.74	0.51
39:z:288:A:H61	39:z:297:U:H3	1.58	0.51
20:S:71:ILE:O	20:S:75:GLU:N	2.43	0.51
1:2:575:A:OP2	27:Z:93:ARG:NH2	2.43	0.51
1:2:626:G:H21	2:A:64:LYS:HG2	1.76	0.51
1:2:637:U:O2	33:f:129:ASN:ND2	2.42	0.51
18:Q:83:MET:HE3	18:Q:84:ILE:H	1.74	0.51
26:Y:71:ARG:HG2	26:Y:82:THR:HG22	1.92	0.51
19:R:97:GLN:OE1	35:h:60:ARG:NH2	2.44	0.51
35:h:26:GLN:HE22	35:h:75:GLY:HA3	1.76	0.51
38:x:1192:LEU:HA	38:x:1196:PHE:HB2	1.93	0.51
1:2:1277:C:H2'	1:2:1278:A:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1416:C:OP1	22:U:133:ARG:NH2	2.43	0.51
1:2:561:A:H5'	12:K:171:GLY:HA3	1.93	0.51
3:B:128:ARG:HH21	3:B:153:PRO:HD3	1.76	0.51
7:F:153:LEU:HD23	9:H:216:ARG:HH11	1.75	0.51
21:T:36:VAL:HG23	21:T:40:TYR:HB3	1.92	0.51
38:x:705:GLU:OE2	38:x:734:GLN:NE2	2.43	0.51
39:z:260:A:N6	39:z:274:A:N1	2.59	0.51
1:2:1314:U:O2'	13:L:3:MET:SD	2.69	0.50
1:2:1533:A:N6	1:2:1602:U:H3	2.07	0.50
7:F:107:GLY:HA2	7:F:189:LEU:HD23	1.93	0.50
21:T:35:GLY:O	21:T:97:GLN:NE2	2.41	0.50
3:B:37:TYR:HA	3:B:53:ARG:HD3	1.92	0.50
38:x:1094:ILE:HA	38:x:1110:VAL:HG12	1.92	0.50
1:2:731:G:O2'	25:X:118:ARG:NH2	2.45	0.50
1:2:960:U:H1'	1:2:963:A:H62	1.75	0.50
5:D:115:GLN:HG3	5:D:120:GLN:HB3	1.92	0.50
3:B:40:LYS:NZ	3:B:41:ARG:O	2.45	0.50
39:z:248:U:H2'	39:z:249:G:H8	1.75	0.50
1:2:918:U:O2'	1:2:919:A:O4'	2.29	0.50
1:2:1472:C:H42	1:2:1476:A:H62	1.60	0.50
20:S:17:ILE:HD11	20:S:54:VAL:HG13	1.92	0.50
6:E:8:LYS:HB3	23:V:61:LEU:HD21	1.94	0.50
31:d:18:LEU:HD12	31:d:29:GLN:HG2	1.93	0.50
38:x:678:GLU:O	38:x:681:LYS:NZ	2.40	0.50
6:E:39:VAL:HG12	6:E:48:ILE:HG22	1.93	0.50
38:x:626:LYS:H	38:x:692:ARG:HH21	1.59	0.50
12:K:63:LEU:HD22	12:K:70:ARG:HB2	1.94	0.50
37:n:20:MET:HA	37:n:23:ARG:HG2	1.92	0.50
1:2:1444:U:OP1	19:R:15:ARG:NH1	2.45	0.50
9:H:7:PHE:HD2	9:H:10:THR:HG22	1.77	0.49
10:I:57:ARG:NH2	10:I:172:THR:OG1	2.45	0.49
14:M:120:VAL:HG22	14:M:145:VAL:HG21	1.94	0.49
26:Y:107:ARG:HG3	26:Y:112:VAL:HG22	1.94	0.49
38:x:626:LYS:O	38:x:850:HIS:NE2	2.42	0.49
1:2:943:U:OP1	4:C:214:LYS:NZ	2.44	0.49
1:2:1544:C:N4	1:2:1588:A:OP2	2.45	0.49
39:z:294:U:H2'	39:z:295:G:H2'	1.95	0.49
1:2:1290:G:N7	34:g:95:ARG:NH1	2.59	0.49
7:F:11:ARG:HA	7:F:28:ALA:HB2	1.94	0.49
8:G:16:ASP:N	8:G:16:ASP:OD1	2.44	0.49
1:2:639:C:H2'	1:2:640:A:H8	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:52:LEU:HB2	15:N:76:LEU:HD22	1.94	0.49
22:U:42:HIS:ND1	22:U:93:SER:OG	2.44	0.49
5:D:147:VAL:HG21	39:z:352:A:H2'	1.93	0.49
5:D:198:ALA:HB3	5:D:221:ASP:HB3	1.94	0.49
17:P:98:ARG:HB2	17:P:132:VAL:HG23	1.95	0.49
7:F:31:PRO:HA	7:F:81:THR:HB	1.94	0.49
1:2:1014:G:N2	30:c:51:GLN:OE1	2.46	0.49
1:2:847:A:OP1	7:F:108:ARG:NH2	2.39	0.49
9:H:57:ASP:HB3	9:H:61:PHE:H	1.78	0.49
9:H:142:ARG:HG2	9:H:147:LEU:HB2	1.95	0.49
14:M:135:SER:HB3	14:M:138:VAL:HB	1.94	0.49
36:i:8:U:H3	36:i:14:A:H62	1.61	0.49
39:z:130:C:H2'	39:z:131:G:H8	1.78	0.49
39:z:307:G:C6	39:z:329:U:C4	3.01	0.49
1:2:1345:G:OP1	1:2:1688:C:O2'	2.31	0.48
15:N:49:LEU:HD11	15:N:124:ILE:HG12	1.94	0.48
21:T:70:ILE:HD13	21:T:77:TYR:HD2	1.78	0.48
38:x:954:ILE:HG12	38:x:956:VAL:HG23	1.94	0.48
1:2:177:G:H22	1:2:313:A:H5'	1.78	0.48
19:R:19:ALA:HB2	19:R:75:GLY:HA3	1.93	0.48
1:2:1544:C:O2'	19:R:75:GLY:O	2.30	0.48
9:H:194:LEU:HB3	9:H:198:ARG:HH21	1.78	0.48
13:L:80:ARG:HD3	13:L:87:PRO:HB3	1.95	0.48
23:V:69:PRO:HB3	32:e:41:GLN:HG2	1.94	0.48
35:h:41:ILE:HD12	35:h:55:PRO:HB3	1.95	0.48
38:x:1032:ILE:HB	38:x:1054:ILE:HG13	1.95	0.48
1:2:928:G:H2'	1:2:929:G:C8	2.47	0.48
14:M:111:VAL:HG11	14:M:128:VAL:HG11	1.94	0.48
23:V:20:ILE:HD11	23:V:91:LEU:HB3	1.94	0.48
1:2:1405:A:H2	1:2:1443:C:H42	1.62	0.48
1:2:1844:U:OP1	37:n:11:ARG:NH2	2.45	0.48
35:h:206:LEU:HB3	35:h:218:LEU:HD11	1.95	0.48
35:h:247:TRP:HB3	35:h:258:ILE:HD11	1.94	0.48
36:i:20:A:N6	36:i:45:G:O2'	2.47	0.48
1:2:151:C:OP1	27:Z:120:THR:OG1	2.27	0.48
1:2:1845:A:H2'	1:2:1846:G:H8	1.79	0.48
1:2:1012:A:OP1	16:O:3:ARG:NH1	2.47	0.48
1:2:1525:C:N4	21:T:138:THR:OG1	2.47	0.48
16:O:130:LYS:NZ	16:O:139:TRP:O	2.45	0.48
36:i:57:A:O2'	36:i:59:A:OP2	2.31	0.48
2:A:57:ARG:NH2	2:A:86:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:32:ILE:HG12	19:R:68:ILE:HD12	1.95	0.48
22:U:18:LEU:HD13	22:U:134:ILE:HG21	1.95	0.48
25:X:105:THR:N	25:X:124:LYS:O	2.45	0.48
26:Y:75:ILE:HA	38:x:1017:MET:HE1	1.96	0.48
29:b:32:LYS:O	29:b:37:LYS:NZ	2.39	0.48
1:2:1255:G:OP1	1:2:1256:G:O2'	2.31	0.48
5:D:110:MET:HE2	5:D:125:LYS:HD3	1.96	0.48
9:H:192:ILE:HG22	9:H:196:LYS:HE3	1.95	0.48
38:x:1198:ASP:OD1	38:x:1198:ASP:N	2.43	0.48
1:2:119:U:O2	7:F:33:THR:OG1	2.32	0.47
1:2:291:G:N2	14:M:40:ILE:O	2.43	0.47
3:B:140:VAL:HG23	3:B:142:LEU:HB2	1.96	0.47
1:2:1127:C:H4'	30:c:17:ARG:HD2	1.96	0.47
1:2:1374:C:OP2	20:S:7:LYS:NZ	2.47	0.47
9:H:121:ILE:HG22	9:H:123:GLY:H	1.80	0.47
20:S:106:LEU:HD23	20:S:109:LEU:HD12	1.96	0.47
35:h:212:LYS:HA	35:h:235:ILE:HG13	1.96	0.47
1:2:1286:G:N2	1:2:1312:G:O2'	2.46	0.47
6:E:99:ILE:HG23	6:E:173:ARG:HH21	1.79	0.47
10:I:138:GLU:OE1	16:O:19:ARG:NH2	2.47	0.47
17:P:102:GLY:O	17:P:106:LYS:NZ	2.39	0.47
38:x:871:ILE:HB	38:x:931:ILE:HB	1.95	0.47
1:2:855:G:O2'	14:M:71:ARG:NH1	2.47	0.47
7:F:64:ILE:HD11	27:Z:18:LEU:HD22	1.97	0.47
9:H:120:ASP:OD1	9:H:120:ASP:N	2.46	0.47
17:P:95:ILE:HD11	17:P:126:ILE:HD12	1.97	0.47
19:R:16:LYS:HD3	19:R:79:ALA:HA	1.97	0.47
25:X:106:THR:HG22	25:X:108:ALA:H	1.79	0.47
1:2:645:C:H2'	1:2:646:G:H8	1.80	0.47
8:G:20:PHE:O	8:G:94:LYS:NZ	2.47	0.47
26:Y:50:ILE:HD11	38:x:1021:VAL:HG21	1.95	0.47
38:x:627:LEU:HD22	38:x:844:LEU:HG	1.95	0.47
38:x:905:PRO:HG3	38:x:911:LEU:HD22	1.96	0.47
1:2:445:A:H5''	11:J:47:ARG:HH21	1.80	0.47
1:2:614:C:OP1	2:A:62:ARG:NH2	2.46	0.47
1:2:860:G:H21	25:X:107:SER:HB3	1.79	0.47
1:2:981:A:H2'	1:2:982:G:C8	2.50	0.47
1:2:1023:A:OP2	16:O:124:ARG:NH2	2.47	0.47
1:2:1662:U:O4	1:2:1663:A:N6	2.47	0.47
9:H:181:THR:HG22	9:H:183:ARG:H	1.79	0.47
21:T:99:LEU:O	21:T:103:LEU:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:85:ASN:HB2	22:U:88:MET:HB2	1.96	0.47
38:x:889:PRO:HB3	38:x:965:LEU:HD21	1.95	0.47
39:z:307:G:C2	39:z:329:U:C2	3.03	0.47
1:2:643:A:OP1	12:K:38:ARG:NH1	2.47	0.47
1:2:659:G:H21	26:Y:17:ARG:HH22	1.63	0.47
38:x:633:CYS:HB2	38:x:718:CYS:HB2	1.43	0.47
1:2:596:U:OP1	26:Y:137:LYS:NZ	2.48	0.47
1:2:986:G:OP2	1:2:988:C:N4	2.47	0.47
11:J:188:TYR:OH	14:M:12:LYS:NZ	2.47	0.47
18:Q:123:TYR:OH	21:T:124:ARG:NH1	2.48	0.47
20:S:92:ASP:OD1	20:S:92:ASP:N	2.48	0.47
1:2:1464:C:H4'	20:S:60:ARG:HH22	1.79	0.47
18:Q:54:HIS:HD2	18:Q:57:LEU:HB2	1.79	0.47
1:2:587:A:O2'	1:2:588:G:N2	2.47	0.46
1:2:963:A:H2'	1:2:964:A:C8	2.50	0.46
26:Y:67:ARG:HG3	26:Y:115:ILE:HG22	1.96	0.46
39:z:333:C:O2'	39:z:335:G:OP1	2.28	0.46
1:2:1361:G:H5''	1:2:1362:U:H2'	1.97	0.46
5:D:273:LEU:HA	5:D:276:THR:HG22	1.97	0.46
6:E:136:VAL:HG22	6:E:186:VAL:HG12	1.97	0.46
10:I:154:ILE:HB	10:I:185:VAL:HG22	1.96	0.46
1:2:1096:G:OP1	25:X:20:ARG:NH2	2.47	0.46
1:2:1740:C:H5''	11:J:58:LEU:HD21	1.97	0.46
1:2:924:G:O6	1:2:1019:C:N4	2.48	0.46
1:2:1451:G:H21	1:2:1474:A:H61	1.62	0.46
1:2:1854:U:OP1	17:P:150:ARG:NH2	2.41	0.46
6:E:167:TYR:OH	6:E:202:LYS:O	2.30	0.46
12:K:111:GLN:HE21	12:K:123:ILE:HG13	1.79	0.46
25:X:82:GLN:H	25:X:85:ASP:HB3	1.79	0.46
38:x:688:ARG:NH2	38:x:690:ASN:OD1	2.48	0.46
38:x:889:PRO:HA	38:x:894:PRO:HA	1.97	0.46
39:z:307:G:O6	39:z:329:U:C4	2.68	0.46
1:2:373:G:H4'	14:M:85:THR:HG21	1.97	0.46
1:2:1228:A:H2'	1:2:1229:G:C8	2.51	0.46
4:C:56:LYS:HE2	4:C:56:LYS:HB2	1.81	0.46
11:J:6:ASP:OD1	11:J:6:ASP:N	2.45	0.46
34:g:137:ASP:N	34:g:137:ASP:OD1	2.49	0.46
29:b:22:ARG:HH21	29:b:27:ALA:HB1	1.80	0.46
3:B:80:ARG:NH2	3:B:165:ASN:O	2.49	0.46
6:E:24:PHE:HA	6:E:27:ARG:HE	1.80	0.46
6:E:197:LYS:HE3	6:E:197:LYS:HB3	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:100:ARG:HB2	7:F:114:ILE:HD13	1.97	0.46
3:B:157:VAL:O	24:W:65:SER:OG	2.34	0.46
7:F:185:GLY:H	7:F:189:LEU:HD13	1.81	0.46
26:Y:115:ILE:HD12	26:Y:118:VAL:HG23	1.97	0.46
1:2:64:A:H2	1:2:83:A:H62	1.63	0.46
8:G:17:ILE:HD11	8:G:24:SER:HB2	1.98	0.46
23:V:26:SER:HB3	23:V:32:LEU:HD13	1.98	0.46
35:h:49:GLU:HG2	35:h:50:THR:HG23	1.97	0.46
1:2:384:U:O4	11:J:5:ARG:NH2	2.41	0.45
1:2:830:A:OP2	1:2:846:G:N2	2.49	0.45
7:F:100:ARG:NH2	7:F:118:GLU:O	2.49	0.45
12:K:130:ILE:HG13	12:K:135:ILE:HD13	1.98	0.45
1:2:28:U:H2'	1:2:29:G:H8	1.81	0.45
7:F:21:ASP:OD1	7:F:21:ASP:N	2.49	0.45
38:x:625:GLU:HG2	38:x:692:ARG:HH21	1.82	0.45
1:2:433:A:OP1	11:J:25:ARG:NH2	2.49	0.45
1:2:617:G:N7	26:Y:67:ARG:NH1	2.63	0.45
1:2:829:C:O2'	1:2:845:G:N2	2.49	0.45
11:J:34:ALA:HB2	11:J:56:ARG:HD2	1.98	0.45
11:J:159:SER:HB3	11:J:162:LEU:HD12	1.99	0.45
38:x:759:LEU:HB2	38:x:762:TRP:HB2	1.98	0.45
39:z:171:G:H3'	39:z:172:A:H8	1.82	0.45
2:A:46:ARG:NH1	26:Y:58:GLU:OE2	2.49	0.45
4:C:24:PRO:O	4:C:28:LYS:NZ	2.49	0.45
11:J:110:ARG:HA	11:J:121:LEU:HD23	1.97	0.45
31:d:43:ILE:HG22	31:d:65:ALA:HB2	1.98	0.45
34:g:141:CYS:SG	34:g:144:CYS:N	2.88	0.45
35:h:178:ASN:HB2	35:h:185:LYS:HE3	1.98	0.45
1:2:1165:G:OP2	1:2:1165:G:N2	2.44	0.45
35:h:72:SER:OG	35:h:74:ASP:OD1	2.34	0.45
1:2:373:G:OP1	14:M:137:THR:OG1	2.35	0.45
1:2:476:A:N3	1:2:488:U:O2'	2.45	0.45
1:2:922:A:OP1	25:X:28:ARG:NH2	2.49	0.45
1:2:1324:G:O2'	1:2:1510:G:O2'	2.32	0.45
1:2:1652:G:H1	1:2:1672:U:H3	1.65	0.45
25:X:86:LEU:HD21	25:X:113:HIS:HB2	1.98	0.45
1:2:45:A:H4'	1:2:46:A:H5'	1.98	0.45
1:2:442:C:H42	1:2:449:A:H62	1.63	0.45
6:E:1:MET:O	6:E:4:GLN:NE2	2.43	0.45
1:2:165:G:OP2	1:2:165:G:N2	2.49	0.45
1:2:1700:C:H5	1:2:1836:G:H1	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:87:ASP:OD1	16:O:87:ASP:N	2.49	0.45
1:2:1536:G:H2'	1:2:1537:A:H8	1.82	0.45
9:H:3:LEU:HD23	9:H:109:LEU:HB3	1.99	0.45
19:R:58:LEU:HD13	19:R:108:ILE:HD11	1.98	0.45
1:2:155:G:H2'	1:2:156:G:H8	1.82	0.45
1:2:871:U:O2'	1:2:873:G:OP1	2.34	0.45
1:2:1083:A:N7	1:2:1841:C:O2'	2.42	0.45
1:2:1264:C:H42	1:2:1518:C:H41	1.63	0.45
1:2:1808:U:H2'	1:2:1809:A:H8	1.82	0.45
36:i:52:G:H2'	36:i:53:A:H8	1.82	0.45
38:x:727:ILE:HG12	38:x:753:LEU:HD23	1.99	0.45
2:A:40:LYS:NZ	2:A:48:GLU:OE1	2.45	0.44
3:B:50:ASN:HB2	3:B:53:ARG:HD2	1.99	0.44
9:H:212:LEU:HD11	9:H:216:ARG:HH21	1.82	0.44
1:2:1244:U:H2'	1:2:1245:G:H8	1.82	0.44
8:G:92:ILE:HD13	8:G:169:ILE:HD13	1.99	0.44
14:M:82:MET:HG3	14:M:85:THR:HG23	1.99	0.44
20:S:36:GLU:HB2	20:S:47:ARG:HD2	1.98	0.44
30:c:36:LYS:HD3	30:c:43:ILE:HG12	1.98	0.44
11:J:100:CYS:SG	11:J:101:ILE:N	2.90	0.44
21:T:81:ASP:OD1	21:T:81:ASP:N	2.46	0.44
25:X:55:ASP:OD2	25:X:56:HIS:N	2.50	0.44
29:b:74:CYS:SG	29:b:77:CYS:CB	2.98	0.44
38:x:1033:LEU:HD12	38:x:1063:LEU:HD21	2.00	0.44
1:2:613:G:N2	1:2:626:G:OP1	2.47	0.44
1:2:466:G:H1'	9:H:59:GLN:HE21	1.82	0.44
1:2:1228:A:H2'	1:2:1229:G:H8	1.82	0.44
3:B:156:TYR:OH	24:W:61:ARG:NH1	2.50	0.44
8:G:96:ALA:O	8:G:100:ILE:HG12	2.18	0.44
29:b:74:CYS:SG	29:b:77:CYS:HB2	2.58	0.44
30:c:15:GLU:O	30:c:23:ARG:NE	2.46	0.44
1:2:38:A:H5''	12:K:5:ARG:HB3	1.98	0.44
2:A:77:ILE:HG22	2:A:94:LYS:HG3	2.00	0.44
2:A:98:ASP:OD1	2:A:98:ASP:N	2.49	0.44
1:2:171:A:OP2	9:H:137:ARG:NH2	2.51	0.44
1:2:1424:G:H2'	1:2:1425:G:H8	1.83	0.44
22:U:9:VAL:O	22:U:11:GLN:NE2	2.51	0.44
1:2:77:A:O2'	9:H:175:LYS:NZ	2.43	0.44
1:2:1599:U:OP2	28:a:46:ASN:ND2	2.47	0.44
21:T:44:VAL:HG21	21:T:71:MET:HB3	1.99	0.44
36:i:27:U:H2'	36:i:28:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:550:C:O2'	1:2:551:U:O4'	2.35	0.44
1:2:1528:G:O2'	1:2:1666:C:OP1	2.34	0.44
5:D:153:GLY:HA2	5:D:156:ILE:HG22	2.00	0.44
8:G:49:LEU:HD13	19:R:50:LYS:HE2	1.99	0.44
14:M:127:THR:HG22	14:M:144:LYS:HG2	2.00	0.44
15:N:79:VAL:HG11	15:N:85:LEU:HD23	2.00	0.44
18:Q:30:TYR:OH	18:Q:61:ARG:NH2	2.51	0.44
1:2:1572:C:H2'	1:2:1573:G:C8	2.53	0.43
4:C:144:LYS:HB3	4:C:206:PRO:HB2	2.00	0.43
17:P:142:ARG:NH1	29:b:23:CYS:O	2.51	0.43
18:Q:64:LYS:HD2	18:Q:64:LYS:HA	1.85	0.43
23:V:26:SER:HB2	23:V:110:VAL:HA	1.99	0.43
29:b:2:THR:OG1	29:b:3:LYS:N	2.51	0.43
35:h:289:LEU:HA	35:h:300:ALA:HA	2.00	0.43
1:2:104:A:H62	1:2:356:C:H5	1.64	0.43
1:2:223:C:OP1	14:M:20:LYS:NZ	2.41	0.43
1:2:823:U:N3	12:K:143:ASN:OD1	2.41	0.43
1:2:1388:A:H61	6:E:161:GLY:HA3	1.83	0.43
5:D:89:LYS:HE2	5:D:89:LYS:HB2	1.84	0.43
16:O:49:GLN:HA	16:O:52:VAL:HG12	2.00	0.43
17:P:21:VAL:HG13	17:P:24:GLY:H	1.83	0.43
34:g:99:LYS:HD2	34:g:99:LYS:HA	1.78	0.43
38:x:743:LYS:HD3	38:x:801:LEU:HD11	2.00	0.43
11:J:178:ARG:HB3	11:J:181:GLN:HE21	1.82	0.43
35:h:124:SER:OG	35:h:126:ASP:OD1	2.31	0.43
38:x:790:LYS:HA	38:x:793:ILE:HG12	2.00	0.43
38:x:1091:LYS:HG2	38:x:1181:VAL:HG12	2.01	0.43
39:z:307:G:C2	39:z:329:U:O2	2.71	0.43
1:2:33:G:O2'	1:2:564:A:O2'	2.37	0.43
6:E:10:LYS:HD3	6:E:10:LYS:HA	1.75	0.43
19:R:130:LYS:HA	19:R:137:ALA:HA	2.00	0.43
3:B:37:TYR:HD1	3:B:53:ARG:HB3	1.83	0.43
21:T:46:ARG:NH1	22:U:50:GLU:OE1	2.51	0.43
32:e:43:PHE:O	32:e:47:ALA:HB2	2.18	0.43
38:x:785:PHE:HZ	38:x:820:PRO:HB3	1.83	0.43
1:2:1779:G:H2'	1:2:1780:G:C8	2.53	0.43
5:D:114:LYS:HD3	5:D:121:ARG:HH21	1.84	0.43
14:M:75:GLY:HA3	14:M:88:ILE:HD12	2.00	0.43
1:2:150:A:H62	1:2:168:C:H42	1.67	0.43
1:2:223:C:H2'	1:2:224:A:C8	2.54	0.43
13:L:15:LEU:HD13	13:L:71:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:32:VAL:N	31:d:42:ILE:O	2.44	0.43
35:h:35:SER:OG	35:h:36:ARG:N	2.52	0.43
1:2:373:G:H2'	1:2:374:G:H8	1.83	0.43
35:h:17:TRP:O	35:h:36:ARG:N	2.52	0.43
11:J:82:VAL:O	11:J:205:ARG:NH2	2.52	0.43
35:h:109:LEU:HG	35:h:152:SER:HA	2.01	0.43
39:z:305:U:O2	39:z:325:C:N4	2.51	0.43
1:2:1183:A:H5'	37:n:11:ARG:HE	1.84	0.43
9:H:216:ARG:HD3	9:H:216:ARG:HA	1.89	0.43
15:N:69:CYS:SG	15:N:70:ALA:N	2.91	0.43
16:O:29:THR:HG23	16:O:32:ASP:H	1.83	0.43
20:S:72:LYS:HE3	20:S:72:LYS:HB3	1.78	0.43
1:2:1337:C:H2'	1:2:1338:G:H8	1.83	0.42
1:2:1568:C:O2	1:2:1627:C:O2'	2.37	0.42
1:2:1598:G:H2'	28:a:81:GLY:H	1.84	0.42
3:B:209:GLU:HA	3:B:212:LYS:HB3	2.01	0.42
4:C:134:LEU:HD22	4:C:218:LEU:HB2	2.01	0.42
5:D:264:SER:HB3	5:D:267:GLN:HG2	2.01	0.42
36:i:3:C:H2'	36:i:4:A:H8	1.84	0.42
39:z:135:G:O2'	39:z:297:U:OP1	2.30	0.42
1:2:844:U:O2'	7:F:255:ARG:NH1	2.41	0.42
1:2:980:A:H2'	1:2:981:A:C8	2.54	0.42
1:2:1445:U:O4	1:2:1446:A:N6	2.52	0.42
1:2:1653:U:H3	1:2:1671:G:H1	1.67	0.42
7:F:80:ILE:HG13	7:F:81:THR:HG23	2.01	0.42
29:b:45:VAL:HG11	29:b:53:ILE:HG13	2.01	0.42
38:x:992:LEU:HD23	38:x:992:LEU:HA	1.87	0.42
1:2:64:A:N6	1:2:83:A:OP2	2.43	0.42
1:2:183:G:O2'	1:2:184:G:O4'	2.34	0.42
1:2:1681:U:O2	1:2:1683:C:N4	2.45	0.42
32:e:48:LYS:HA	32:e:48:LYS:HD2	1.77	0.42
33:f:97:LYS:HB3	33:f:97:LYS:HE3	1.83	0.42
35:h:272:GLN:OE1	35:h:308:ARG:NH1	2.51	0.42
5:D:146:GLU:HG2	5:D:149:THR:HG22	2.01	0.42
17:P:37:PHE:HE2	17:P:105:THR:HG21	1.84	0.42
19:R:112:LEU:HD23	19:R:112:LEU:HA	1.90	0.42
1:2:60:A:O2'	1:2:316:G:O2'	2.37	0.42
1:2:1092:G:H2'	1:2:1093:A:H8	1.84	0.42
1:2:1277:C:H2'	1:2:1278:A:C8	2.54	0.42
17:P:30:VAL:HG22	17:P:94:HIS:HB2	2.00	0.42
35:h:68:ASP:HB3	35:h:111:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:104:HIS:NE2	35:h:122:SER:OG	2.43	0.42
1:2:482:G:N1	1:2:485:A:OP2	2.49	0.42
38:x:642:LYS:HE2	38:x:642:LYS:HB2	1.94	0.42
38:x:670:ASN:HD21	38:x:697:LEU:HD12	1.85	0.42
38:x:825:THR:OG1	38:x:827:ASP:OD1	2.34	0.42
1:2:318:A:C2	1:2:333:G:N1	2.87	0.42
1:2:658:U:O2	26:Y:17:ARG:NH1	2.52	0.42
6:E:23:GLU:O	6:E:27:ARG:HG2	2.20	0.42
21:T:26:ILE:HG13	21:T:45:LEU:HD21	2.01	0.42
21:T:114:LEU:HA	21:T:117:ILE:HG22	2.02	0.42
39:z:144:U:O4	39:z:249:G:O6	2.37	0.42
1:2:678:U:H2'	1:2:679:A:H8	1.85	0.42
1:2:1290:G:OP2	34:g:95:ARG:NH2	2.53	0.42
3:B:52:LYS:NZ	20:S:109:LEU:HB3	2.35	0.42
5:D:68:ARG:HA	5:D:68:ARG:HD3	1.77	0.42
7:F:151:ASP:OD1	9:H:216:ARG:NH2	2.51	0.42
38:x:693:ILE:HA	38:x:694:PRO:HD3	1.86	0.42
1:2:292:A:O2'	14:M:39:ASN:O	2.32	0.42
4:C:129:THR:OG1	4:C:131:ASP:OD1	2.35	0.42
18:Q:121:ILE:HG22	21:T:120:HIS:HD2	1.85	0.42
1:2:677:G:N2	1:2:1028:A:H62	2.15	0.42
1:2:941:C:H2'	1:2:942:G:C8	2.55	0.42
5:D:63:VAL:HG23	5:D:64:THR:HG23	2.02	0.42
11:J:41:ARG:HD3	11:J:43:ILE:HD12	2.01	0.42
11:J:98:LYS:HD2	11:J:178:ARG:HG3	2.02	0.42
21:T:125:HIS:CD2	21:T:131:VAL:HG11	2.55	0.42
1:2:1617:G:O6	18:Q:43:ARG:NH1	2.53	0.41
8:G:70:GLU:OE1	8:G:74:ASN:ND2	2.52	0.41
1:2:1781:A:H61	1:2:1785:C:H41	1.67	0.41
18:Q:103:ASN:HD22	18:Q:120:SER:HB2	1.85	0.41
20:S:99:ASP:HB3	20:S:102:THR:HG22	2.01	0.41
28:a:53:ALA:O	28:a:57:LYS:HB2	2.20	0.41
28:a:102:LYS:HD2	28:a:102:LYS:HA	1.81	0.41
38:x:775:LYS:HA	38:x:775:LYS:HD2	1.81	0.41
1:2:17:C:O2'	1:2:1194:A:N1	2.48	0.41
1:2:1707:U:H5'	37:n:9:ARG:HH22	1.85	0.41
6:E:69:LEU:HA	6:E:72:VAL:HG12	2.02	0.41
7:F:20:LEU:HD21	7:F:46:ILE:HD12	2.02	0.41
7:F:182:MET:HB3	7:F:192:ILE:HD13	2.01	0.41
16:O:93:LYS:HA	16:O:93:LYS:HD2	1.83	0.41
17:P:148:GLY:HA2	29:b:27:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:18:VAL:HA	35:h:35:SER:HA	2.02	0.41
35:h:42:MET:SD	35:h:57:ARG:NH1	2.93	0.41
38:x:1031:VAL:HG12	38:x:1053:ARG:HB2	2.01	0.41
1:2:957:A:H2'	1:2:958:G:H8	1.86	0.41
3:B:39:TYR:HB3	3:B:48:ILE:HG13	2.01	0.41
16:O:33:VAL:HA	16:O:36:GLN:HB2	2.01	0.41
1:2:1808:U:H2'	1:2:1809:A:C8	2.56	0.41
4:C:150:ILE:HG23	20:S:131:PRO:HA	2.01	0.41
12:K:24:ARG:O	12:K:28:GLU:HG2	2.21	0.41
1:2:1221:G:O2'	1:2:1676:U:O2	2.35	0.41
1:2:1868:U:O2	29:b:100:ARG:NH1	2.53	0.41
6:E:214:LYS:HD3	6:E:214:LYS:HA	1.75	0.41
12:K:162:ARG:HE	12:K:162:ARG:HB3	1.63	0.41
23:V:21:ARG:O	23:V:115:THR:OG1	2.38	0.41
27:Z:55:ILE:HG23	27:Z:75:ILE:HG13	2.03	0.41
35:h:3:GLU:HA	35:h:314:ILE:HD11	2.02	0.41
1:2:1299:A:O5'	18:Q:59:ARG:NH1	2.53	0.41
7:F:198:ARG:HG3	7:F:208:VAL:HG12	2.02	0.41
35:h:292:SER:OG	35:h:293:ALA:N	2.53	0.41
35:h:294:ASP:OD1	35:h:294:ASP:N	2.54	0.41
38:x:632:ILE:HD13	38:x:720:ILE:HG23	2.02	0.41
38:x:1093:LYS:HD3	38:x:1179:ILE:HG12	2.03	0.41
38:x:1103:ARG:HD2	38:x:1169:MET:HE3	2.01	0.41
39:z:165:A:OP1	39:z:230:G:N2	2.42	0.41
1:2:1226:G:N1	1:2:1639:G:OP2	2.42	0.41
1:2:1759:G:H1	1:2:1774:C:H42	1.68	0.41
4:C:83:LYS:HE2	4:C:106:THR:HA	2.01	0.41
7:F:21:ASP:OD2	7:F:24:THR:OG1	2.38	0.41
21:T:16:LEU:HD12	21:T:99:LEU:HD21	2.02	0.41
30:c:56:CYS:SG	30:c:57:VAL:N	2.93	0.41
38:x:1076:LYS:HB2	38:x:1076:LYS:HE2	1.82	0.41
1:2:50:A:H62	1:2:477:G:H21	1.69	0.41
1:2:210:U:H2'	1:2:211:G:H8	1.86	0.41
1:2:223:C:H2'	1:2:224:A:H8	1.85	0.41
1:2:1275:G:N2	1:2:1506:A:OP2	2.43	0.41
1:2:1297:U:H2'	1:2:1298:G:H2'	2.02	0.41
3:B:7:VAL:HG13	3:B:8:LEU:HG	2.03	0.41
4:C:60:ASP:O	4:C:63:LYS:HB2	2.21	0.41
14:M:49:GLU:OE2	14:M:118:ARG:NH2	2.54	0.41
15:N:21:VAL:HG22	15:N:111:VAL:HG11	2.03	0.41
24:W:21:ASN:HB3	25:X:67:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:110:ILE:HD12	25:X:126:LEU:HD11	2.03	0.41
26:Y:100:VAL:HG12	26:Y:125:VAL:HG23	2.02	0.41
27:Z:8:ARG:HD2	27:Z:8:ARG:HA	1.94	0.41
28:a:99:LEU:HD11	28:a:102:LYS:HD3	2.01	0.41
38:x:632:ILE:HD12	38:x:836:LEU:HD13	2.02	0.41
39:z:141:U:H2'	39:z:142:A:C8	2.56	0.41
39:z:330:A:H4'	39:z:331:G:H5'	2.02	0.41
1:2:121:U:OP1	7:F:77:ARG:NH1	2.54	0.41
4:C:35:ALA:HB2	4:C:44:ILE:HD11	2.02	0.41
4:C:110:MET:HE3	4:C:110:MET:HB3	1.98	0.41
8:G:76:MET:O	8:G:159:ARG:NH2	2.47	0.41
10:I:105:THR:OG1	10:I:106:ARG:N	2.53	0.41
12:K:125:HIS:O	12:K:129:LEU:HB2	2.21	0.41
18:Q:100:LYS:HG2	18:Q:101:THR:HG23	2.02	0.41
19:R:58:LEU:HD23	19:R:58:LEU:HA	1.92	0.41
24:W:40:ASP:HB3	24:W:43:THR:HG22	2.03	0.41
27:Z:27:VAL:HG12	27:Z:29:HIS:HD2	1.85	0.41
28:a:71:ALA:O	28:a:74:SER:OG	2.34	0.41
38:x:980:TYR:HB3	38:x:1032:ILE:HD13	2.03	0.41
1:2:402:C:H5''	11:J:16:GLY:HA3	2.04	0.40
1:2:525:A:H2'	1:2:526:A:C8	2.56	0.40
1:2:934:G:N1	1:2:1008:A:H2	2.07	0.40
19:R:51:LEU:HD23	19:R:51:LEU:HA	1.97	0.40
24:W:40:ASP:OD1	24:W:41:LYS:N	2.53	0.40
25:X:80:ASP:HA	25:X:124:LYS:HA	2.02	0.40
26:Y:49:GLY:HA2	26:Y:75:ILE:HG13	2.02	0.40
39:z:164:U:OP2	39:z:231:G:O2'	2.31	0.40
1:2:552:G:H5'	33:f:116:VAL:HG11	2.03	0.40
1:2:913:A:N6	10:I:119:SER:O	2.52	0.40
2:A:39:ILE:HD13	2:A:39:ILE:HA	1.91	0.40
6:E:227:LYS:HB2	6:E:227:LYS:HE2	1.89	0.40
28:a:106:GLN:HE21	28:a:107:VAL:H	1.69	0.40
38:x:1092:MET:HE1	38:x:1112:VAL:HG22	2.04	0.40
38:x:1101:ASN:HB3	38:x:1107:VAL:H	1.85	0.40
1:2:1287:A:N3	1:2:1315:U:N3	2.69	0.40
1:2:1337:C:H2'	1:2:1338:G:C8	2.56	0.40
1:2:1786:U:H2'	1:2:1787:G:H8	1.87	0.40
14:M:12:LYS:HB2	14:M:18:GLN:HE22	1.86	0.40
21:T:78:LYS:HA	21:T:78:LYS:HD2	1.89	0.40
29:b:19:GLN:H	29:b:19:GLN:HG2	1.72	0.40
36:i:51:G:H2'	36:i:52:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:x:641:GLY:O	38:x:645:ILE:HG12	2.21	0.40
1:2:1010:G:H2'	1:2:1011:A:H8	1.86	0.40
2:A:40:LYS:HD2	2:A:42:LEU:HD13	2.03	0.40
6:E:127:MET:HE1	6:E:133:GLY:HA2	2.02	0.40
7:F:175:PHE:HE1	7:F:225:ILE:HG21	1.86	0.40
13:L:71:LEU:HD23	13:L:71:LEU:HA	1.89	0.40
38:x:755:LYS:HD2	38:x:758:ARG:HG3	2.02	0.40
38:x:1092:MET:HB2	38:x:1180:LEU:HB2	2.03	0.40
39:z:130:C:H2'	39:z:131:G:C8	2.55	0.40
1:2:598:G:O2'	1:2:605:A:N1	2.53	0.40
1:2:844:U:H2'	1:2:845:G:H8	1.86	0.40
1:2:1299:A:O2'	1:2:1301:A:OP1	2.39	0.40
4:C:143:THR:HG23	4:C:205:TYR:HE2	1.87	0.40
6:E:23:GLU:OE1	13:L:64:TRP:NE1	2.55	0.40
11:J:48:VAL:HG11	11:J:54:LYS:HD3	2.03	0.40
11:J:67:TRP:HD1	11:J:189:VAL:HG11	1.87	0.40
11:J:83:TYR:HB3	11:J:101:ILE:HB	2.02	0.40
16:O:52:VAL:HG23	16:O:55:ARG:NH2	2.35	0.40
35:h:25:PRO:HA	35:h:293:ALA:HB2	2.03	0.40
38:x:711:ARG:HD3	38:x:711:ARG:HA	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	97/144 (67%)	93 (96%)	4 (4%)	0	100	100
3	B	215/295 (73%)	197 (92%)	18 (8%)	0	100	100
4	C	211/264 (80%)	198 (94%)	13 (6%)	0	100	100
5	D	219/221 (99%)	207 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	226/281 (80%)	219 (97%)	7 (3%)	0	100	100
7	F	260/262 (99%)	250 (96%)	10 (4%)	0	100	100
8	G	189/204 (93%)	180 (95%)	9 (5%)	0	100	100
9	H	235/249 (94%)	232 (99%)	3 (1%)	0	100	100
10	I	181/432 (42%)	173 (96%)	8 (4%)	0	100	100
11	J	205/208 (99%)	195 (95%)	10 (5%)	0	100	100
12	K	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
13	L	94/149 (63%)	87 (93%)	7 (7%)	0	100	100
14	M	149/158 (94%)	138 (93%)	11 (7%)	0	100	100
15	N	115/132 (87%)	106 (92%)	9 (8%)	0	100	100
16	O	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
17	P	134/168 (80%)	127 (95%)	7 (5%)	0	100	100
18	Q	118/145 (81%)	114 (97%)	4 (3%)	0	100	100
19	R	140/172 (81%)	135 (96%)	5 (4%)	0	100	100
20	S	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
21	T	142/152 (93%)	133 (94%)	9 (6%)	0	100	100
22	U	139/145 (96%)	137 (99%)	2 (1%)	0	100	100
23	V	98/119 (82%)	97 (99%)	1 (1%)	0	100	100
24	W	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
25	X	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
26	Y	139/143 (97%)	129 (93%)	10 (7%)	0	100	100
27	Z	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
28	a	75/124 (60%)	71 (95%)	4 (5%)	0	100	100
29	b	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
30	c	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
31	d	65/69 (94%)	63 (97%)	2 (3%)	0	100	100
32	e	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
33	f	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
34	g	66/188 (35%)	65 (98%)	1 (2%)	0	100	100
35	h	311/317 (98%)	292 (94%)	19 (6%)	0	100	100
37	n	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	x	625/627 (100%)	584 (93%)	41 (7%)	0	100	100
All	All	5549/6591 (84%)	5293 (95%)	256 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	84/123 (68%)	84 (100%)	0	100	100
3	B	180/244 (74%)	180 (100%)	0	100	100
4	C	194/231 (84%)	194 (100%)	0	100	100
5	D	187/187 (100%)	187 (100%)	0	100	100
6	E	190/232 (82%)	190 (100%)	0	100	100
7	F	223/223 (100%)	223 (100%)	0	100	100
8	G	161/170 (95%)	161 (100%)	0	100	100
9	H	207/218 (95%)	207 (100%)	0	100	100
10	I	165/360 (46%)	165 (100%)	0	100	100
11	J	179/180 (99%)	179 (100%)	0	100	100
12	K	161/168 (96%)	161 (100%)	0	100	100
13	L	87/125 (70%)	87 (100%)	0	100	100
14	M	136/142 (96%)	136 (100%)	0	100	100
15	N	99/108 (92%)	99 (100%)	0	100	100
16	O	130/131 (99%)	130 (100%)	0	100	100
17	P	106/130 (82%)	106 (100%)	0	100	100
18	Q	109/130 (84%)	109 (100%)	0	100	100
19	R	117/140 (84%)	117 (100%)	0	100	100
20	S	119/121 (98%)	119 (100%)	0	100	100
21	T	125/132 (95%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	U	111/116 (96%)	111 (100%)	0	100	100
23	V	92/107 (86%)	92 (100%)	0	100	100
24	W	68/68 (100%)	68 (100%)	0	100	100
25	X	112/113 (99%)	112 (100%)	0	100	100
26	Y	113/115 (98%)	113 (100%)	0	100	100
27	Z	107/113 (95%)	107 (100%)	0	100	100
28	a	68/102 (67%)	68 (100%)	0	100	100
29	b	89/89 (100%)	89 (100%)	0	100	100
30	c	75/76 (99%)	75 (100%)	0	100	100
31	d	60/62 (97%)	60 (100%)	0	100	100
32	e	48/49 (98%)	48 (100%)	0	100	100
33	f	47/106 (44%)	47 (100%)	0	100	100
34	g	61/154 (40%)	61 (100%)	0	100	100
35	h	272/275 (99%)	272 (100%)	0	100	100
37	n	24/24 (100%)	24 (100%)	0	100	100
38	x	552/552 (100%)	552 (100%)	0	100	100
All	All	4858/5616 (86%)	4858 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	110	ASN
3	B	113	GLN
4	C	75	GLN
5	D	134	ASN
7	F	98	ASN
7	F	224	ASN
8	G	186	ASN
9	H	4	ASN
9	H	202	ASN
10	I	162	GLN
11	J	167	GLN
11	J	181	GLN
12	K	27	GLN

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Mol	Chain	Res	Type
12	K	111	GLN
15	N	82	ASN
16	O	69	ASN
16	O	105	ASN
20	S	48	ASN
20	S	118	GLN
21	T	11	HIS
22	U	10	ASN
22	U	137	GLN
23	V	47	ASN
23	V	85	HIS
25	X	24	GLN
25	X	90	GLN
26	Y	31	HIS
26	Y	92	ASN
27	Z	22	GLN
27	Z	85	ASN
28	a	112	ASN
31	d	45	ASN
33	f	88	GLN
35	h	4	GLN
35	h	76	GLN
35	h	188	HIS
35	h	215	GLN
35	h	285	GLN
35	h	305	ASN
38	x	665	GLN
38	x	704	HIS
38	x	754	ASN
38	x	799	GLN
38	x	927	GLN
38	x	970	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1870 (90%)	322 (19%)	10 (0%)
36	i	74/75 (98%)	11 (14%)	0
39	z	186/400 (46%)	48 (25%)	0
All	All	1945/2345 (82%)	381 (19%)	10 (0%)

All (381) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	C
1	2	4	C
1	2	26	U
1	2	33	G
1	2	41	G
1	2	42	A
1	2	44	U
1	2	46	A
1	2	56	G
1	2	61	A
1	2	67	C
1	2	68	A
1	2	69	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	103	A
1	2	113	G
1	2	115	U
1	2	116	U
1	2	126	G
1	2	128	U
1	2	130	G
1	2	142	C
1	2	143	U
1	2	147	A
1	2	149	A
1	2	162	C
1	2	164	A
1	2	170	A
1	2	180	G
1	2	182	C
1	2	183	G
1	2	184	G
1	2	192	C
1	2	199	C
1	2	207	G
1	2	208	G
1	2	214	U
1	2	292	A

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Mol	Chain	Res	Type
1	2	294	U
1	2	305	U
1	2	306	C
1	2	307	G
1	2	309	G
1	2	312	G
1	2	313	A
1	2	320	G
1	2	323	C
1	2	347	G
1	2	357	C
1	2	362	C
1	2	364	A
1	2	368	U
1	2	370	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	398	A
1	2	399	C
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	418	A
1	2	429	C
1	2	437	G
1	2	446	G
1	2	448	A
1	2	450	C
1	2	455	A
1	2	465	A
1	2	472	C
1	2	474	G
1	2	482	G
1	2	487	U
1	2	488	U
1	2	489	A
1	2	490	C
1	2	492	C
1	2	493	A
1	2	500	A

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Mol	Chain	Res	Type
1	2	502	C
1	2	508	A
1	2	525	A
1	2	530	U
1	2	532	C
1	2	537	C
1	2	538	U
1	2	541	U
1	2	542	U
1	2	544	G
1	2	547	G
1	2	549	C
1	2	550	C
1	2	551	U
1	2	552	G
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	561	A
1	2	562	U
1	2	576	A
1	2	583	A
1	2	588	G
1	2	590	A
1	2	591	U
1	2	606	G
1	2	608	C
1	2	614	C
1	2	617	G
1	2	622	C
1	2	623	G
1	2	627	U
1	2	628	A
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A

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Mol	Chain	Res	Type
1	2	684	G
1	2	688	U
1	2	689	U
1	2	691	G
1	2	694	G
1	2	696	G
1	2	730	C
1	2	731	G
1	2	745	C
1	2	750	C
1	2	752	G
1	2	753	C
1	2	754	G
1	2	795	A
1	2	799	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	827	A
1	2	830	A
1	2	834	C
1	2	844	U
1	2	847	A
1	2	869	A
1	2	870	A
1	2	872	A
1	2	873	G
1	2	874	G
1	2	875	A
1	2	878	G
1	2	886	A
1	2	887	U
1	2	888	U
1	2	890	U
1	2	894	G
1	2	896	U
1	2	897	U
1	2	899	U
1	2	900	C
1	2	901	G
1	2	905	C
1	2	913	A

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Mol	Chain	Res	Type
1	2	914	U
1	2	919	A
1	2	920	A
1	2	921	G
1	2	922	A
1	2	933	G
1	2	970	G
1	2	971	G
1	2	990	A
1	2	992	A
1	2	1017	U
1	2	1022	U
1	2	1023	A
1	2	1028	A
1	2	1045	U
1	2	1061	U
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1088	U
1	2	1109	C
1	2	1114	U
1	2	1121	G
1	2	1133	A
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1170	A
1	2	1195	A
1	2	1203	U
1	2	1204	G
1	2	1206	C
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1242	U
1	2	1251	A
1	2	1253	A
1	2	1256	G

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Mol	Chain	Res	Type
1	2	1257	G
1	2	1259	A
1	2	1263	U
1	2	1274	G
1	2	1275	G
1	2	1282	A
1	2	1285	G
1	2	1286	G
1	2	1287	A
1	2	1292	C
1	2	1293	A
1	2	1294	G
1	2	1298	G
1	2	1299	A
1	2	1300	U
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1308	U
1	2	1309	C
1	2	1313	A
1	2	1314	U
1	2	1318	G
1	2	1333	U
1	2	1342	U
1	2	1348	G
1	2	1358	U
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1396	A
1	2	1402	A
1	2	1404	U
1	2	1406	G
1	2	1428	G
1	2	1442	U
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1464	C
1	2	1475	G
1	2	1477	U

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Mol	Chain	Res	Type
1	2	1480	A
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1494	U
1	2	1497	G
1	2	1498	A
1	2	1507	G
1	2	1521	C
1	2	1533	A
1	2	1535	U
1	2	1536	G
1	2	1548	G
1	2	1551	U
1	2	1554	C
1	2	1555	U
1	2	1556	A
1	2	1557	C
1	2	1567	G
1	2	1573	G
1	2	1575	G
1	2	1578	U
1	2	1580	A
1	2	1585	U
1	2	1588	A
1	2	1601	A
1	2	1606	G
1	2	1621	U
1	2	1623	A
1	2	1638	G
1	2	1646	C
1	2	1648	G
1	2	1659	U
1	2	1660	C
1	2	1665	G
1	2	1680	G
1	2	1695	A
1	2	1699	A
1	2	1715	A
1	2	1721	U
1	2	1722	G
1	2	1744	G

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Mol	Chain	Res	Type
1	2	1749	G
1	2	1751	C
1	2	1757	G
1	2	1758	G
1	2	1759	G
1	2	1772	C
1	2	1775	U
1	2	1776	G
1	2	1779	G
1	2	1781	A
1	2	1782	G
1	2	1783	C
1	2	1824	A
1	2	1826	G
1	2	1829	G
1	2	1831	A
1	2	1834	A
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1849	G
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
1	2	1869	A
36	i	16	C
36	i	17	G
36	i	18	G
36	i	20	A
36	i	47	C
36	i	54	U
36	i	57	A
36	i	58	A
36	i	73	C
36	i	74	C
36	i	75	A
39	z	121	C
39	z	133	G
39	z	136	A
39	z	137	G

Continued on next page...

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Mol	Chain	Res	Type
39	z	144	U
39	z	154	A
39	z	157	C
39	z	161	G
39	z	162	A
39	z	163	G
39	z	164	U
39	z	165	A
39	z	166	C
39	z	229	G
39	z	237	C
39	z	244	A
39	z	253	G
39	z	257	A
39	z	258	G
39	z	265	U
39	z	266	G
39	z	275	A
39	z	281	U
39	z	282	U
39	z	284	U
39	z	288	A
39	z	290	U
39	z	295	G
39	z	296	A
39	z	297	U
39	z	303	G
39	z	307	G
39	z	318	G
39	z	330	A
39	z	331	G
39	z	332	A
39	z	333	C
39	z	334	C
39	z	335	G
39	z	337	G
39	z	345	A
39	z	347	C
39	z	348	A
39	z	349	C
39	z	352	A
39	z	353	U

Continued on next page...

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Mol	Chain	Res	Type
39	z	355	C
39	z	356	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	383	G
1	2	445	A
1	2	537	C
1	2	553	U
1	2	561	A
1	2	627	U
1	2	688	U
1	2	752	G
1	2	886	A
1	2	1395	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
42	GTP	x	1302	41	33,34,34	1.00	3 (9%)	50,54,54	1.68	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	x	1302	41	-	6/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	x	1302	GTP	PB-O3A	2.26	1.61	1.59
42	x	1302	GTP	C2-N3	2.20	1.38	1.33
42	x	1302	GTP	PA-O3A	2.07	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	x	1302	GTP	C5-C4-N3	-5.79	119.18	128.39
42	x	1302	GTP	C2-N3-C4	5.02	120.94	112.30
42	x	1302	GTP	N9-C4-N3	3.89	133.73	125.95
42	x	1302	GTP	C2-N1-C6	-3.11	119.48	125.11
42	x	1302	GTP	C5-C6-N1	2.58	119.82	113.25
42	x	1302	GTP	C3'-C2'-C1'	2.45	106.10	101.46
42	x	1302	GTP	C8-N7-C5	2.43	108.59	104.26
42	x	1302	GTP	O6-C6-C5	-2.41	120.17	126.53
42	x	1302	GTP	N9-C8-N7	-2.24	109.25	113.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

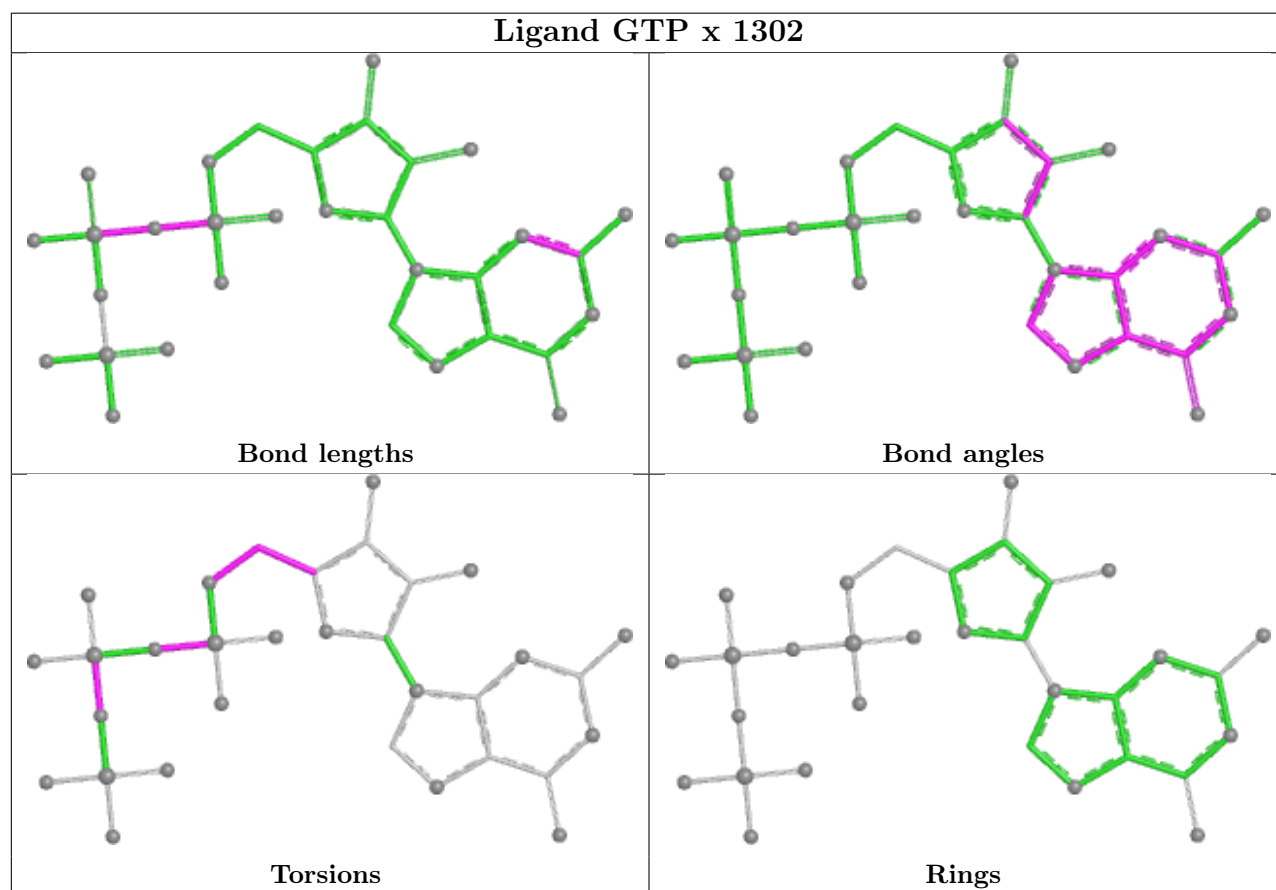
Mol	Chain	Res	Type	Atoms
42	x	1302	GTP	O4'-C4'-C5'-O5'
42	x	1302	GTP	C3'-C4'-C5'-O5'
42	x	1302	GTP	C4'-C5'-O5'-PA
42	x	1302	GTP	PB-O3A-PA-O1A
42	x	1302	GTP	PG-O3B-PB-O1B
42	x	1302	GTP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	x	1302	GTP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

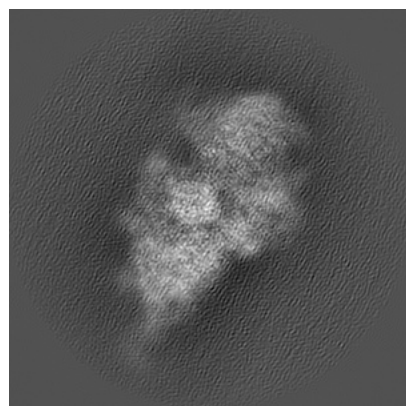
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25544. These allow visual inspection of the internal detail of the map and identification of artifacts.

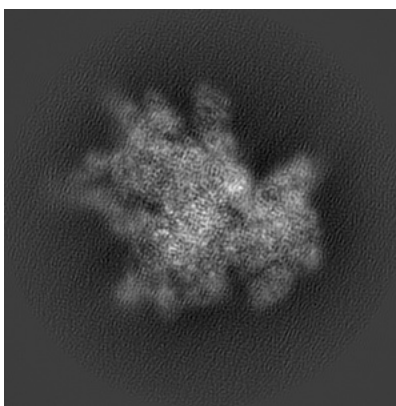
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

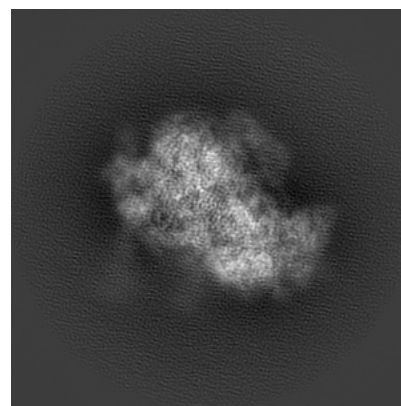
6.1.1 Primary map



X

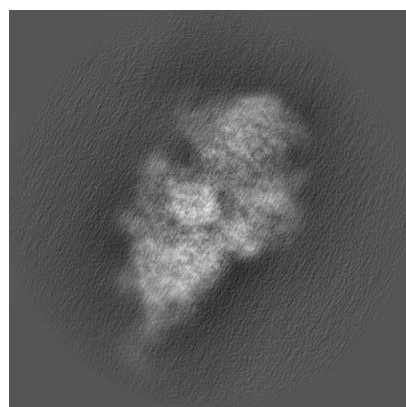


Y

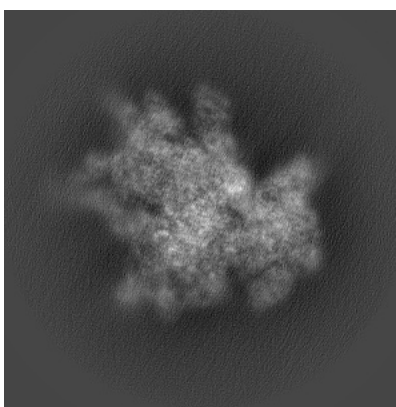


Z

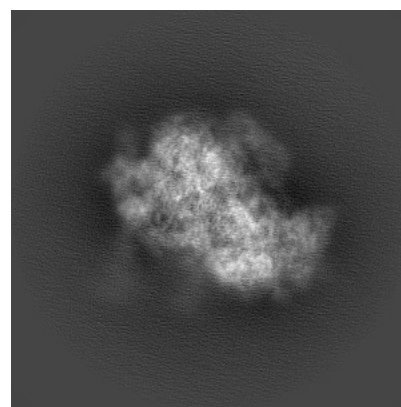
6.1.2 Raw map



X



Y

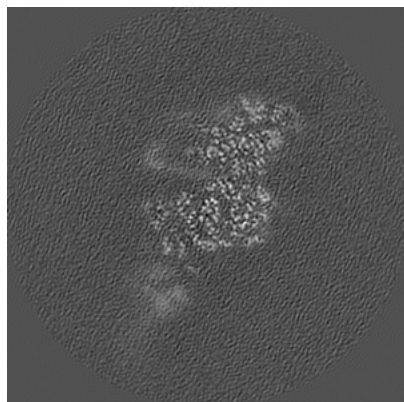


Z

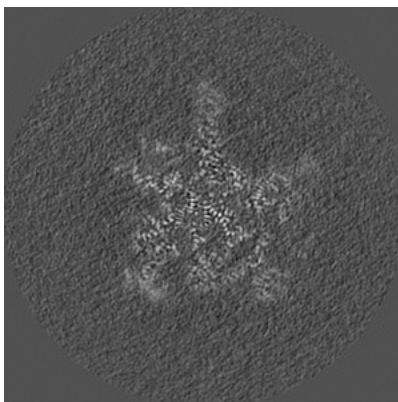
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

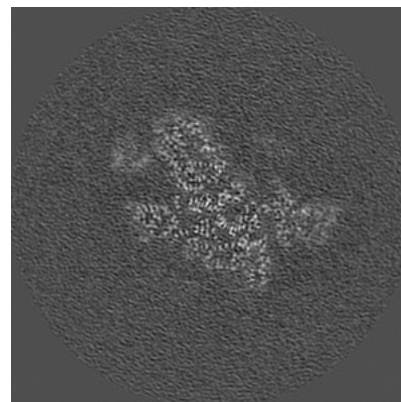
6.2.1 Primary map



X Index: 200

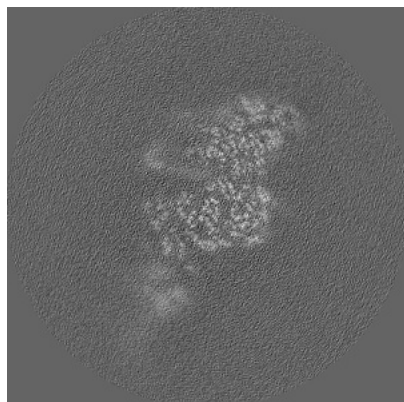


Y Index: 200

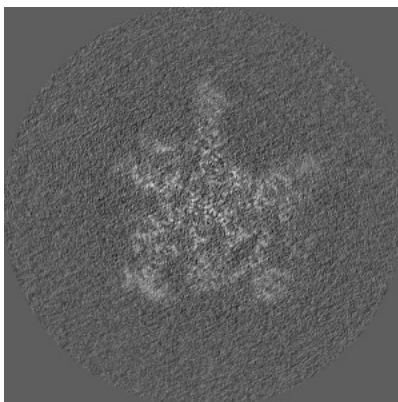


Z Index: 200

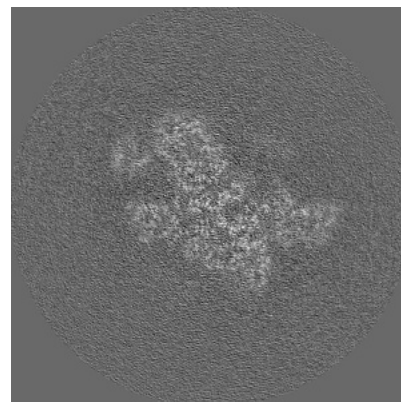
6.2.2 Raw map



X Index: 200



Y Index: 200

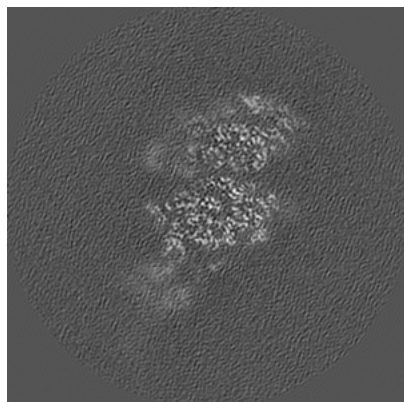


Z Index: 200

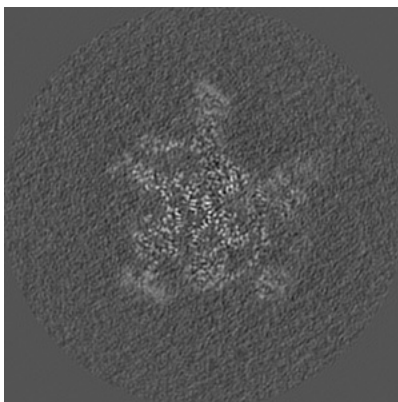
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

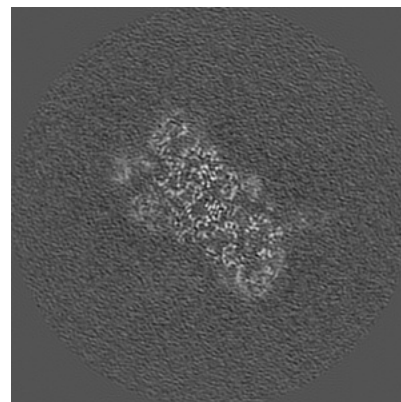
6.3.1 Primary map



X Index: 196

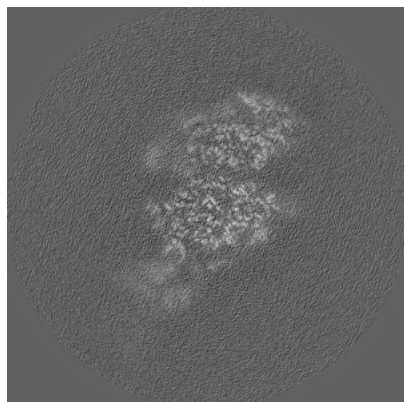


Y Index: 198

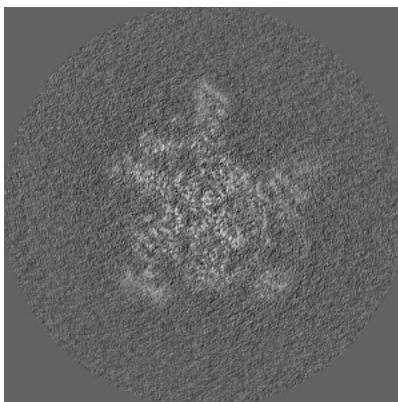


Z Index: 187

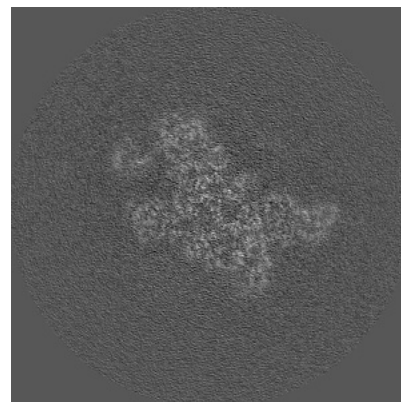
6.3.2 Raw map



X Index: 195



Y Index: 197

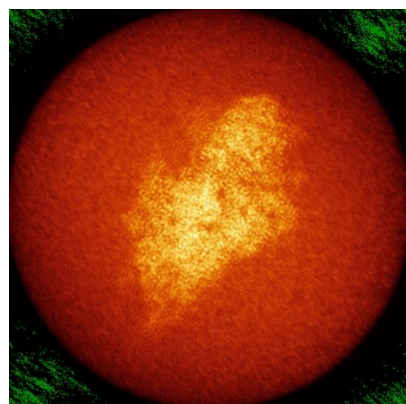


Z Index: 198

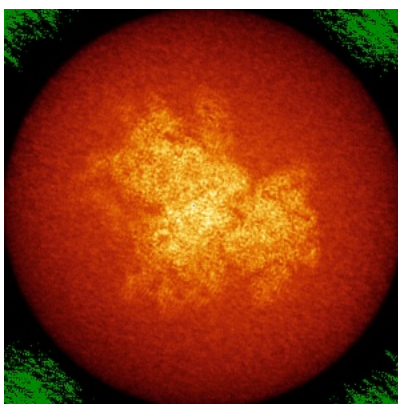
The images above show the largest variance slices of the map in three orthogonal directions.

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

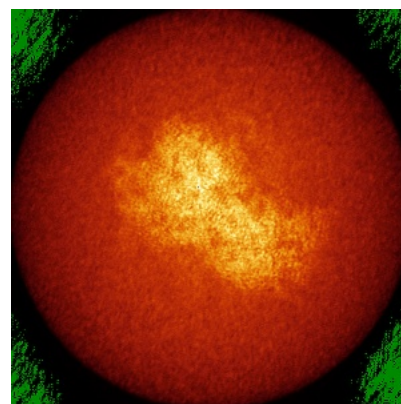
6.4.1 Primary map



X

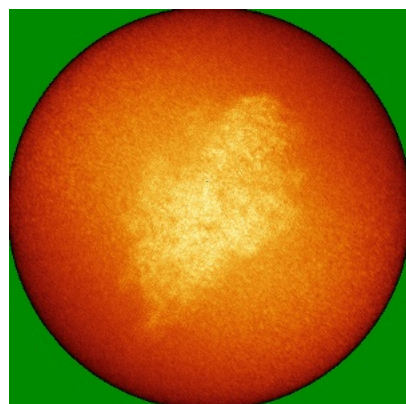


Y

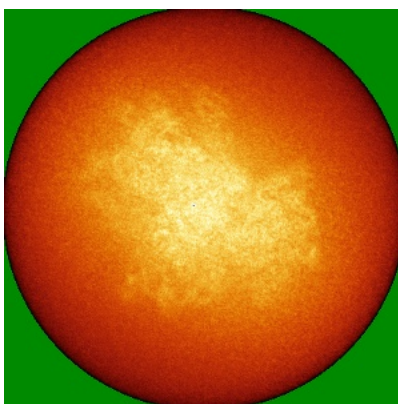


Z

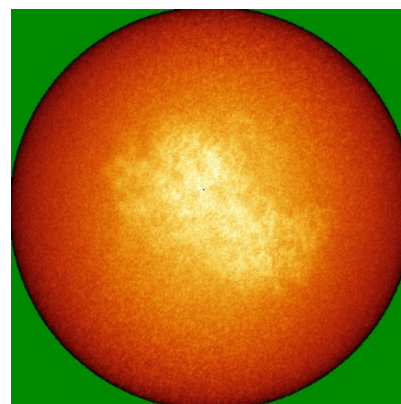
6.4.2 Raw map



X



Y

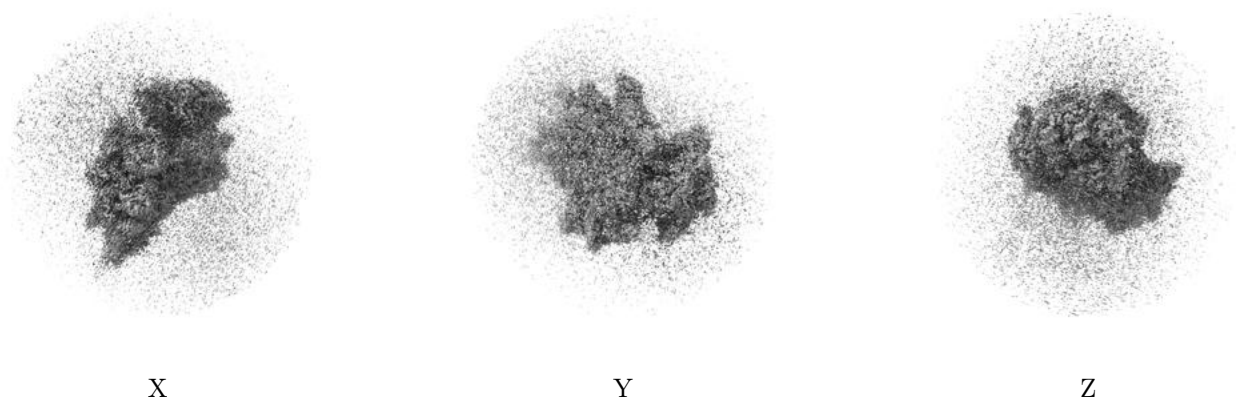


Z

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.

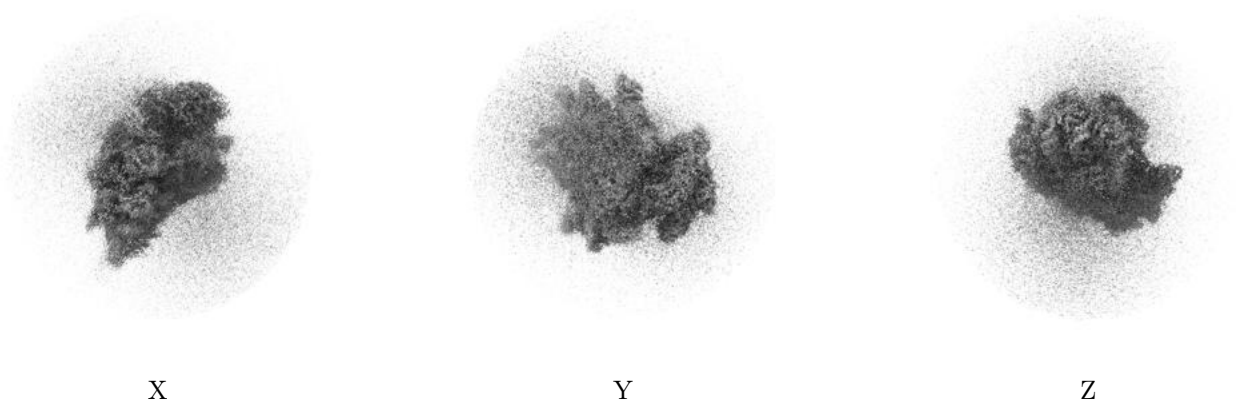
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

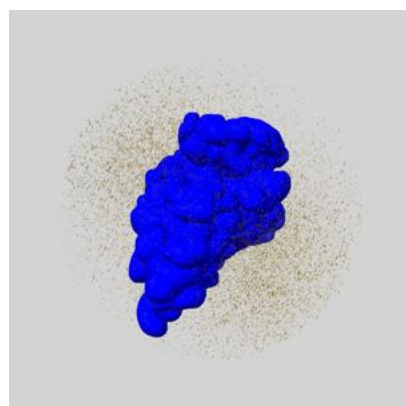
6.6 Mask visualisation [i](#)

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

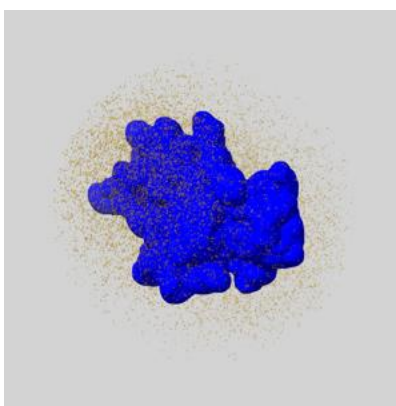
A mask typically either:

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

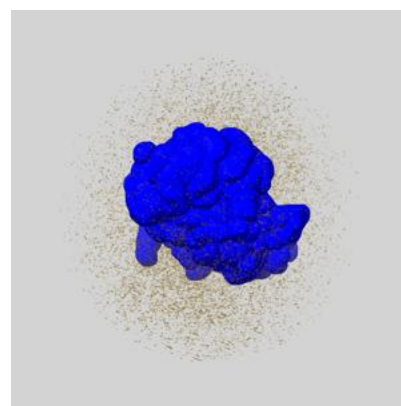
6.6.1 emd_25544_msk_1.map [i](#)



X



Y

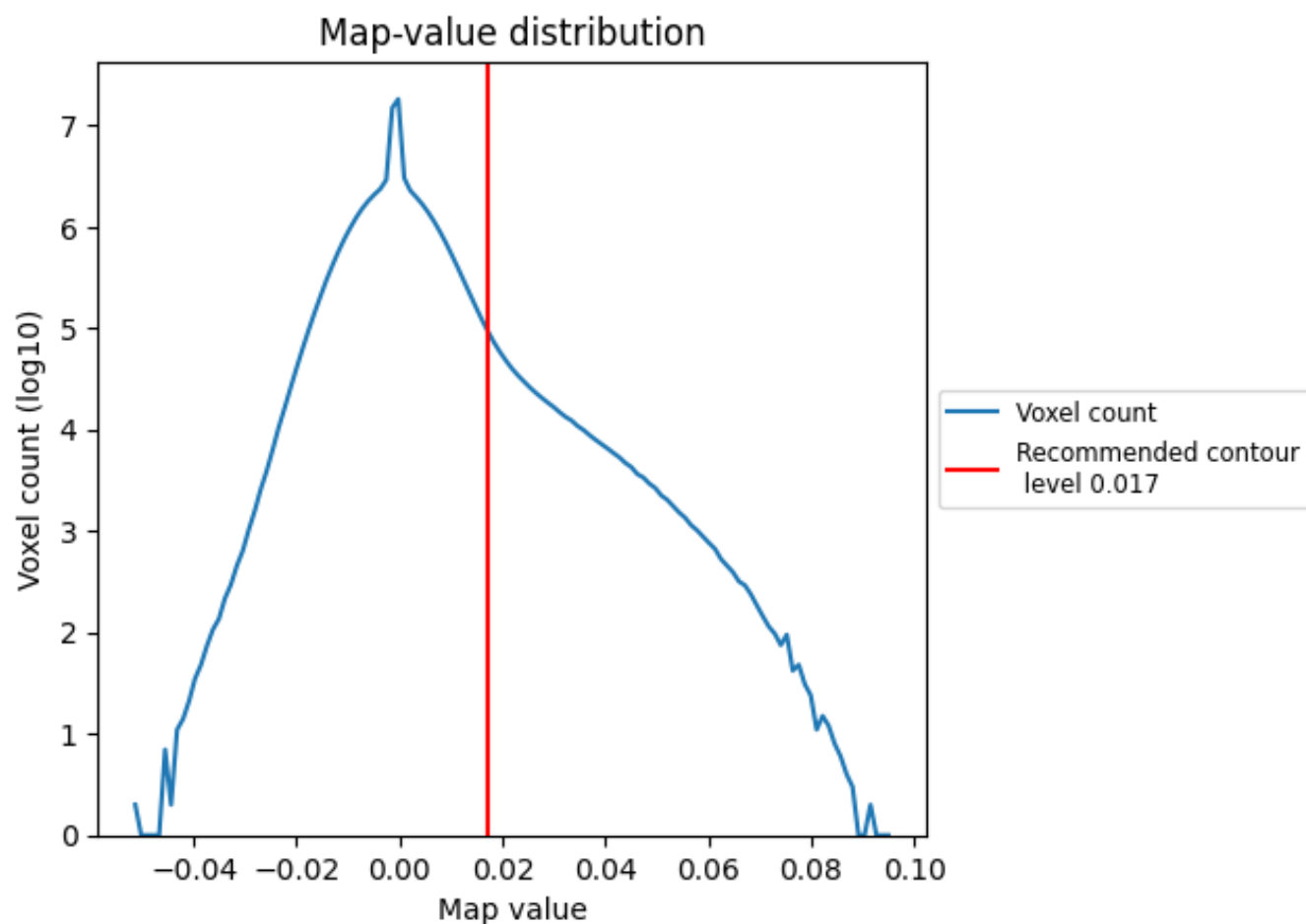


Z

7 Map analysis [i](#)

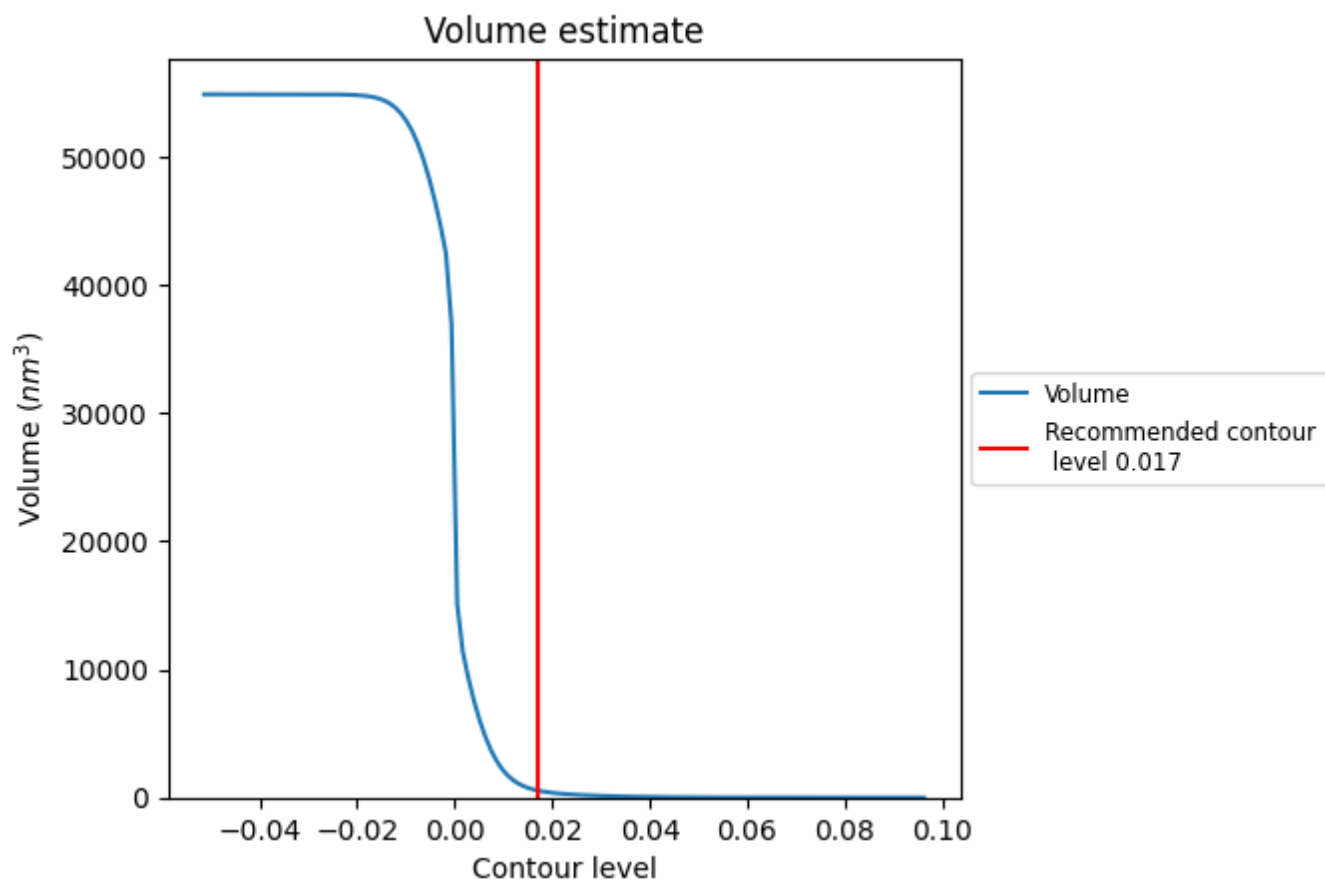
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

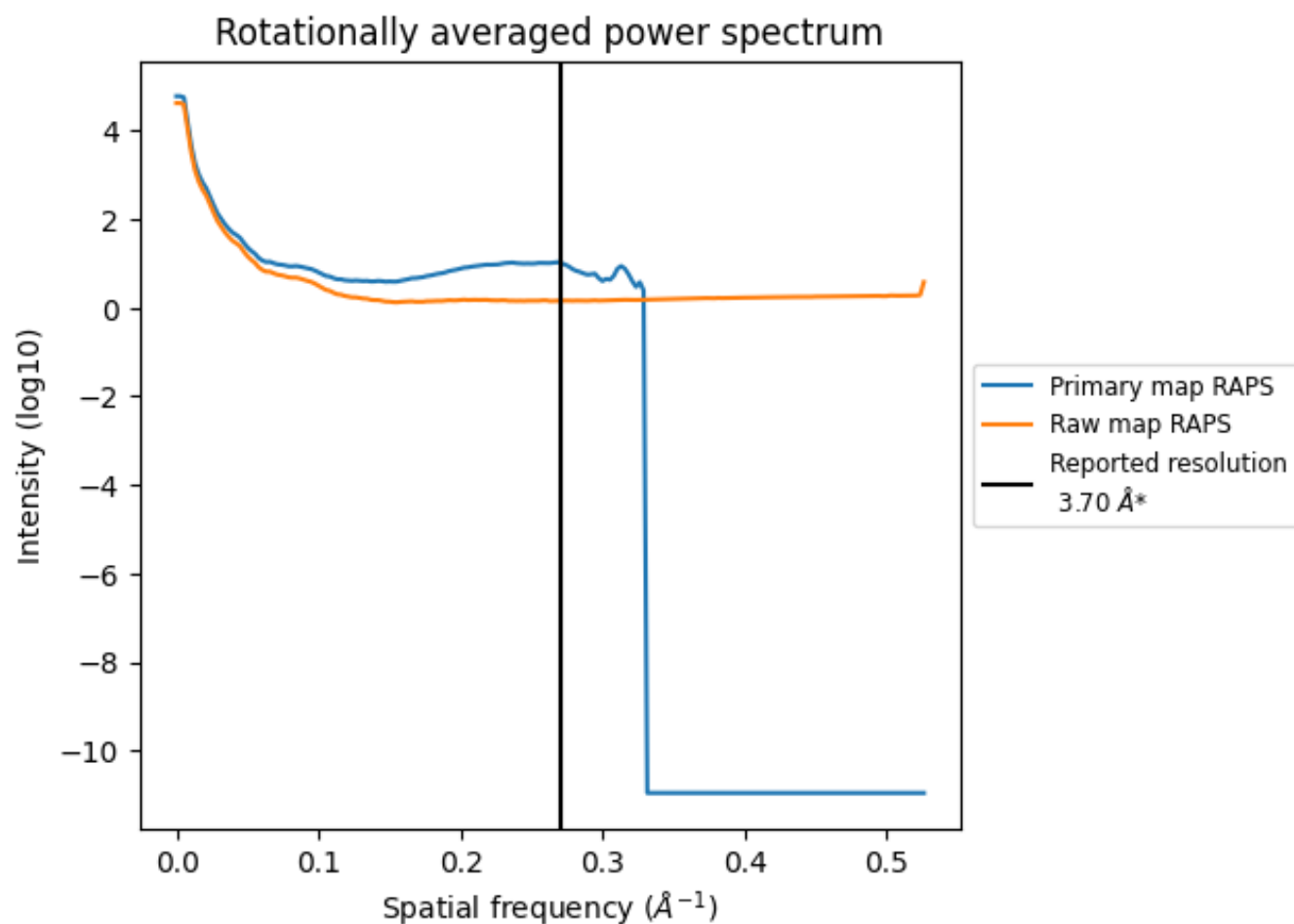
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 552 nm³; this corresponds to an approximate mass of 498 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 ⓘ

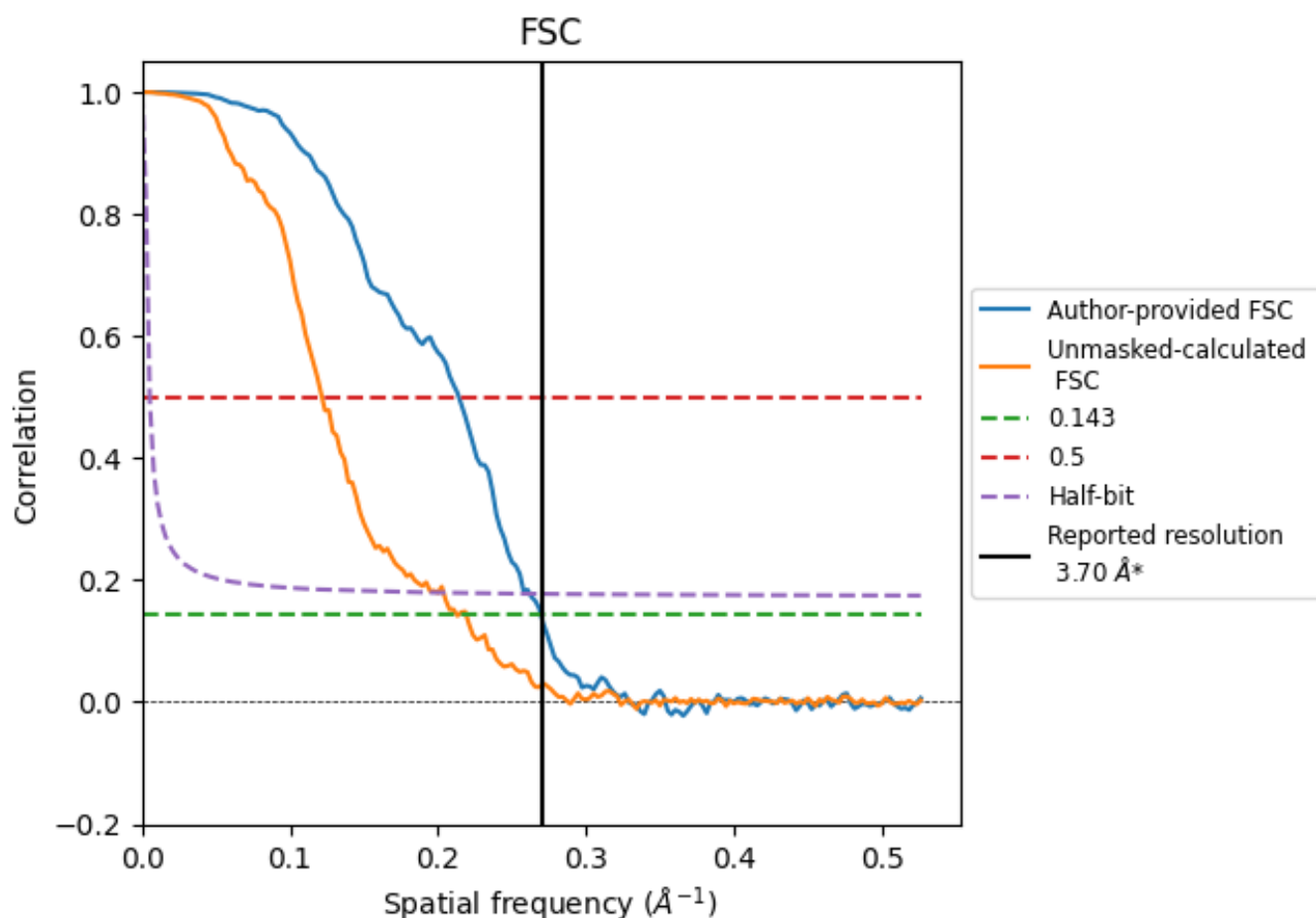


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.270 \text{ \AA}^{-1}$

8.2 Resolution estimates

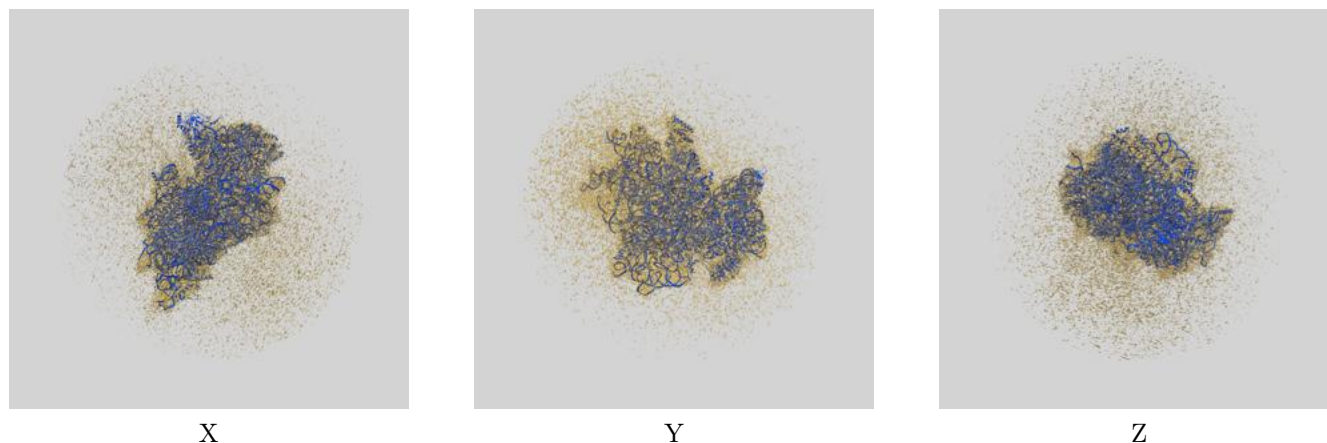
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.67	3.82
Unmasked-calculated*	4.70	8.23	5.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.70 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

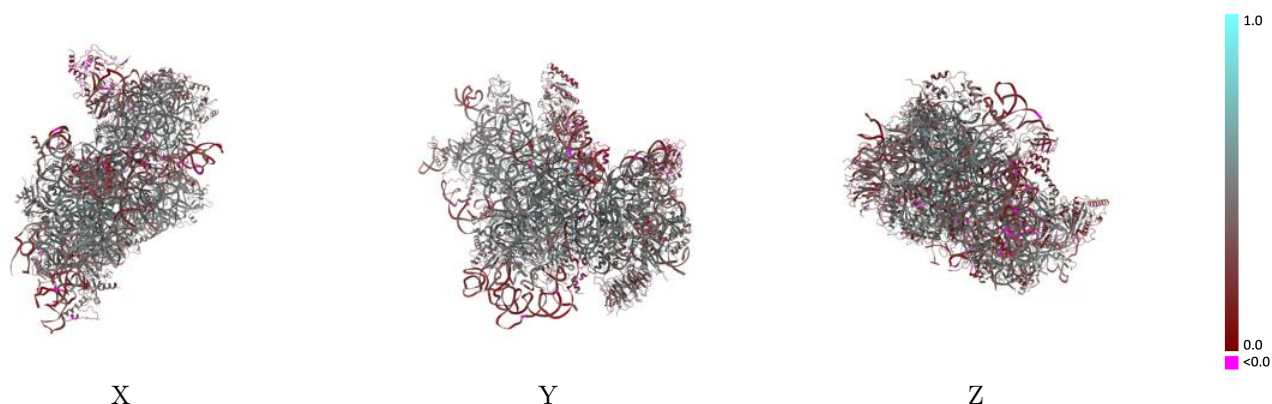
This section contains information regarding the fit between EMDB map EMD-25544 and PDB model 7SYX. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



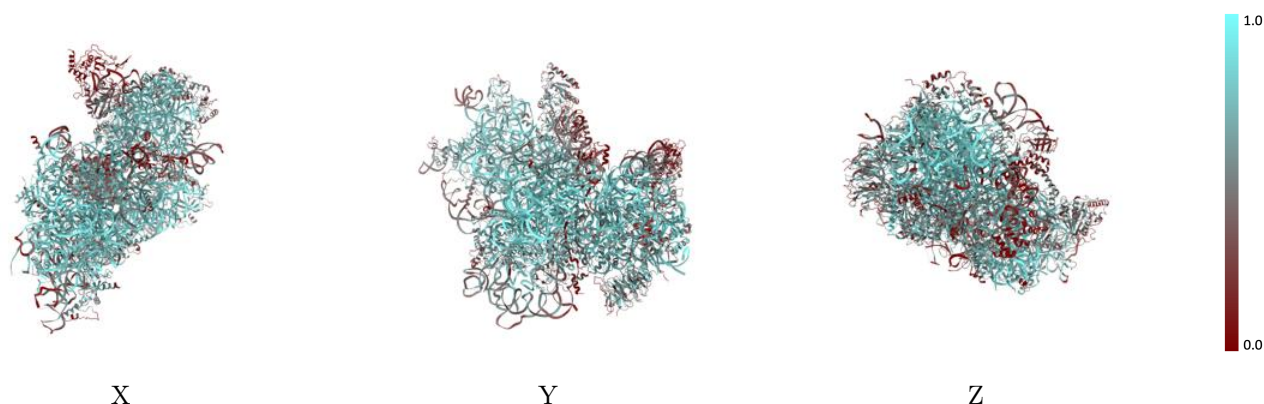
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



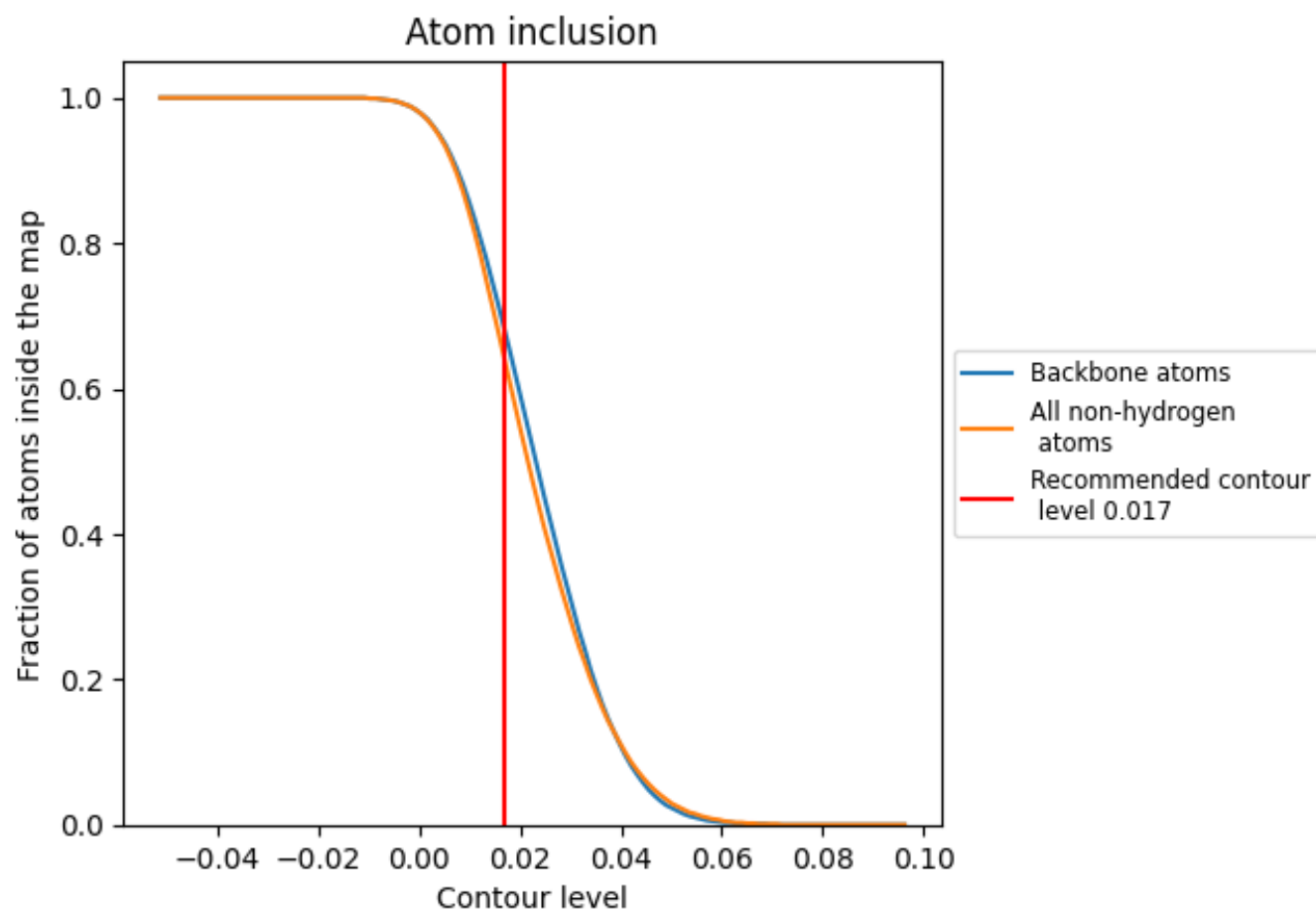
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 64% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6360	 0.4070
2	 0.7650	 0.4390
A	 0.0450	 0.1700
B	 0.6400	 0.4570
C	 0.6370	 0.4460
D	 0.6520	 0.4630
E	 0.4850	 0.3880
F	 0.6870	 0.4710
G	 0.6370	 0.4380
H	 0.5850	 0.4010
I	 0.4660	 0.3830
J	 0.6350	 0.4310
K	 0.6980	 0.4700
L	 0.3520	 0.3290
M	 0.6470	 0.4620
N	 0.0270	 0.1630
O	 0.6770	 0.4700
P	 0.6690	 0.4680
Q	 0.5290	 0.3840
R	 0.6910	 0.4710
S	 0.5280	 0.4040
T	 0.5020	 0.3930
U	 0.6970	 0.4630
V	 0.3590	 0.3250
W	 0.6450	 0.4680
X	 0.7070	 0.4960
Y	 0.7090	 0.4920
Z	 0.7030	 0.4540
a	 0.3990	 0.3510
b	 0.6950	 0.4760
c	 0.6070	 0.4300
d	 0.5490	 0.4180
e	 0.6420	 0.4650
f	 0.5500	 0.4040
g	 0.0320	 0.1920



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
h	 0.5090	 0.3790
i	 0.5170	 0.2700
n	 0.6100	 0.4360
x	 0.3980	 0.3060
z	 0.4550	 0.2140