



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:31 PM UTC

PDB ID : 7SYO / pdb_00007syo
EMDB ID : EMD-25535
Title : Structure of the HCV IRES bound to the 40S ribosomal subunit, head open.
Structure 9(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 : 4.60 Å(reported)
Based on initial models : 6D9J, 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:

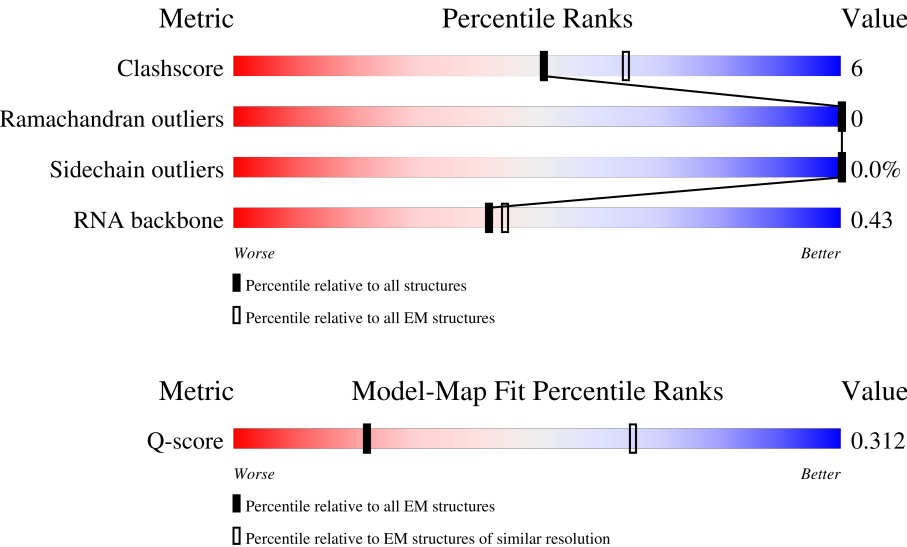
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 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	2407 (4.10 - 5.10)

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	6% 53% 32% 6% 9%
2	B	295	14% 61% 12% 26%
3	C	264	9% 67% 14% 19%

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Mol	Chain	Length	Quality of chain
4	D	221	
5	F	263	
6	G	204	
7	H	249	
8	I	432	
9	J	208	
10	K	194	
11	L	149	
12	M	158	
13	N	132	
14	O	151	
15	P	168	
16	Q	145	
17	R	172	
18	T	152	
19	U	145	
20	V	119	
21	W	83	
22	X	130	
23	Y	143	
24	Z	131	
25	a	124	
26	b	101	
27	c	84	
28	d	69	

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Mol	Chain	Length	Quality of chain
29	e	56	
30	f	133	
31	g	188	
32	h	317	
33	n	25	
34	E	281	
35	S	135	
36	z	400	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 78846 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 uS2 (SA).

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 3 is a protein called eS1.

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

- Molecule 4 is a protein called 40S ribosomal protein S2.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	73	MET	VAL	conflict	UNP G1TUT9
D	101	SER	ALA	conflict	UNP G1TUT9
D	119	GLY	ALA	conflict	UNP G1TUT9
D	194	ARG	HIS	conflict	UNP G1TUT9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	215	MET	LEU	conflict	UNP G1TUT9
D	227	ARG	TRP	conflict	UNP G1TUT9
D	228	GLY	SER	conflict	UNP G1TUT9

- Molecule 5 is a protein called eS4 (S4 X isoform).

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	51	ARG	LYS	conflict	UNP G1TK17
F	78	THR	ALA	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 6 is a protein called uS7.

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

- Molecule 7 is a protein called eS6.

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

- Molecule 8 is a protein called eS7.

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

- Molecule 9 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	206	Total	C	N	O	S	0	0
			1686	1058	332	291	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 10 is a protein called uS4.

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

- Molecule 11 is a protein called eS10.

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

- Molecule 12 is a protein called uS17.

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

- Molecule 13 is a protein called eS12.

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

- Molecule 14 is a protein called uS15.

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

- Molecule 15 is a protein called uS11.

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

- Molecule 16 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	115	Total	C	N	O	S	0	0
			956	610	176	163	7		

- Molecule 17 is a protein called uS9.

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

- Molecule 18 is a protein called uS13.

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

- Molecule 19 is a protein called eS19.

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

- Molecule 20 is a protein called uS10.

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

- Molecule 21 is a protein called eS21.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82

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Chain	Residue	Modelled	Actual	Comment	Reference
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 22 is a protein called uS8.

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

- Molecule 23 is a protein called uS12.

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

- Molecule 24 is a protein called eS24.

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

- Molecule 25 is a protein called eS25.

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

- Molecule 26 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	28	ARG	CYS	conflict	UNP G1TFE8
b	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 27 is a protein called eS27.

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

- Molecule 28 is a protein called eS28.

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

- Molecule 29 is a protein called uS14.

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

- Molecule 30 is a protein called eS30.

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

- Molecule 31 is a protein called eS31.

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

- Molecule 32 is a protein called Receptor for Activated C Kinase 1 (RACK1).

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

- Molecule 33 is a protein called eL41.

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

- Molecule 34 is a protein called uS3.

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

- Molecule 35 is a protein called eS17.

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

- Molecule 36 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	z	166	Total	C	N	O	P	0	0
			3550	1580	637	1167	166		

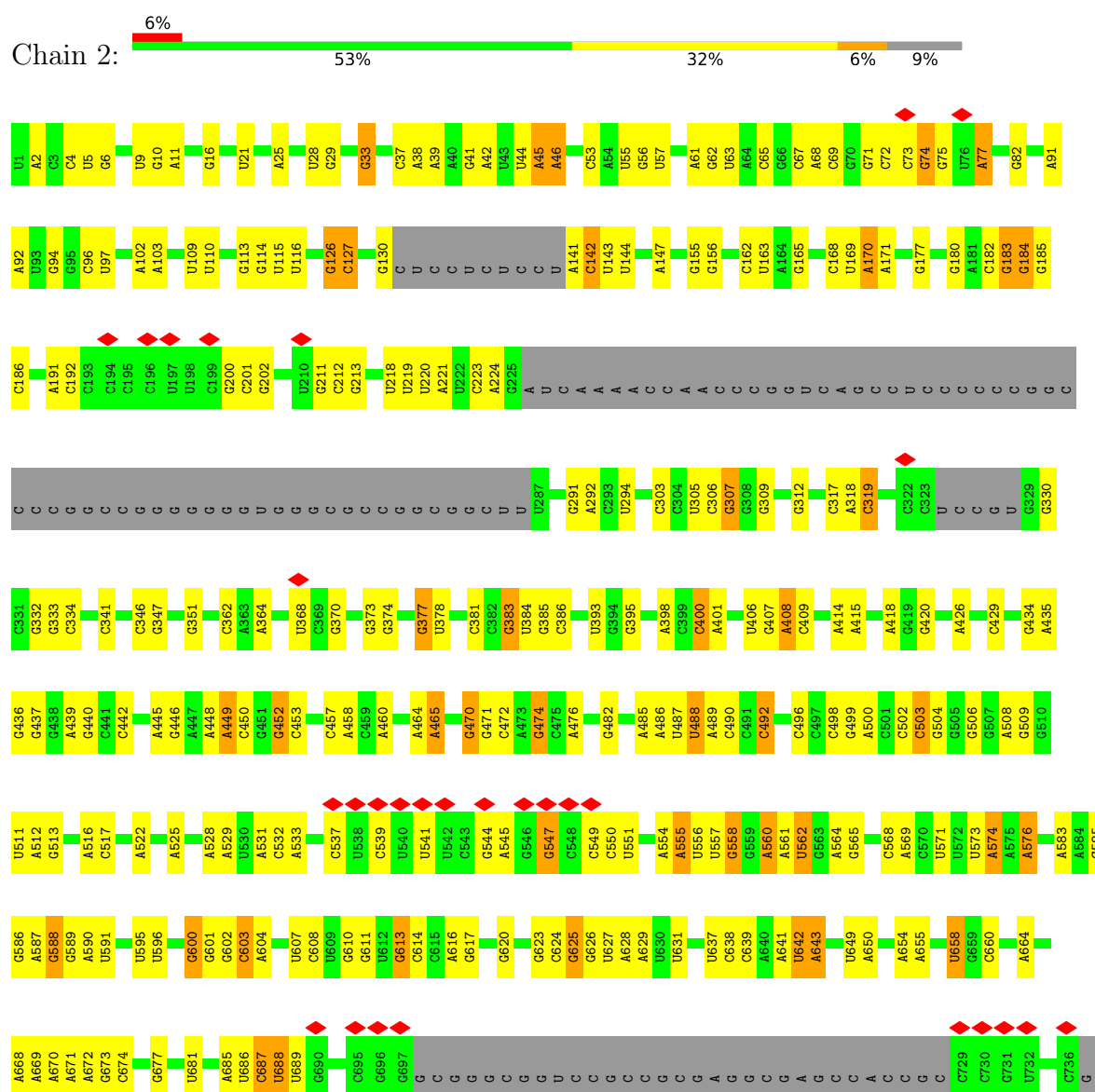
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

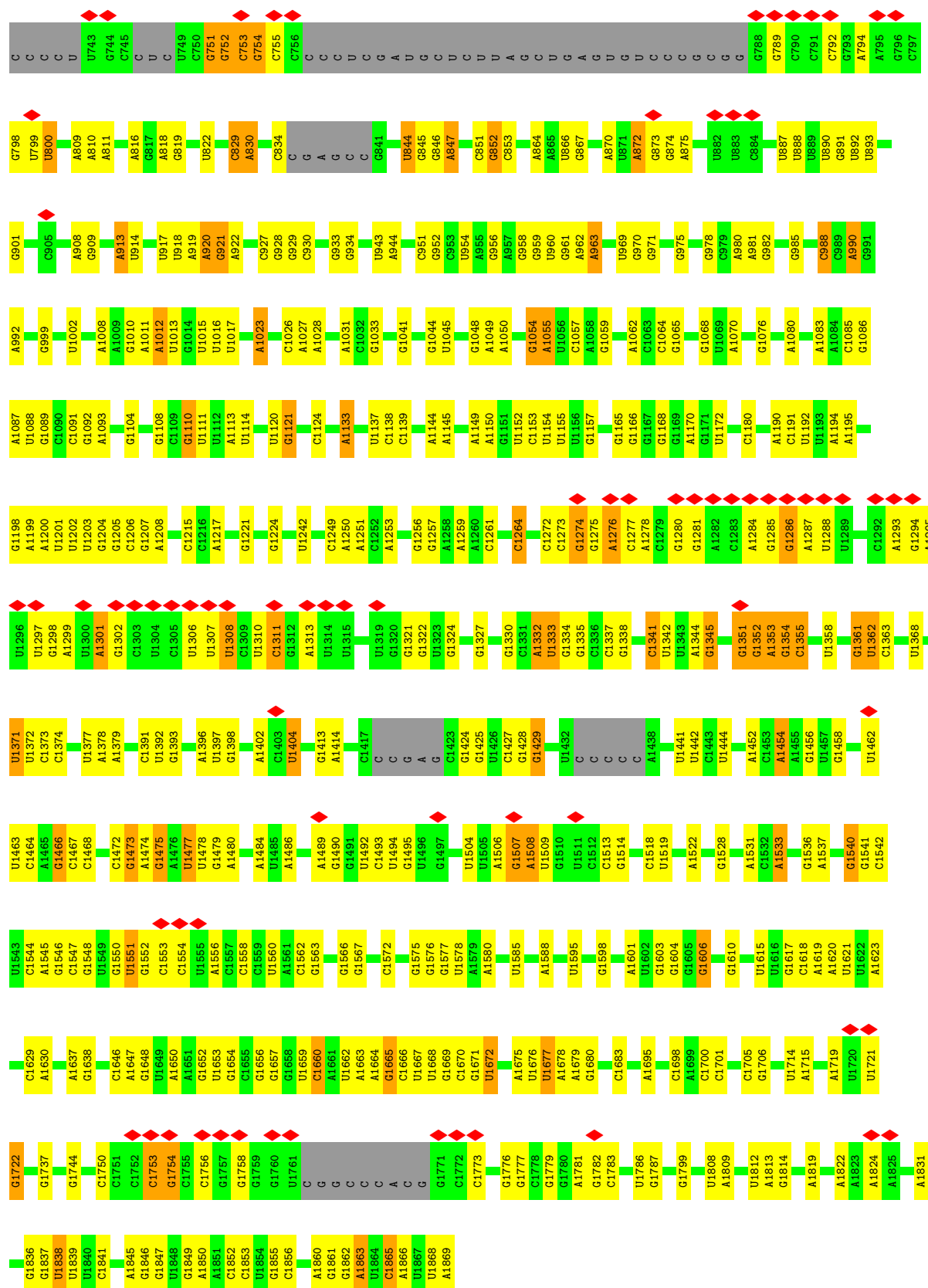
Mol	Chain	Residues	Atoms		AltConf
37	b	1	Total	Zn	0
			1	1	
37	g	1	Total	Zn	0
			1	1	

3 Residue-property plots

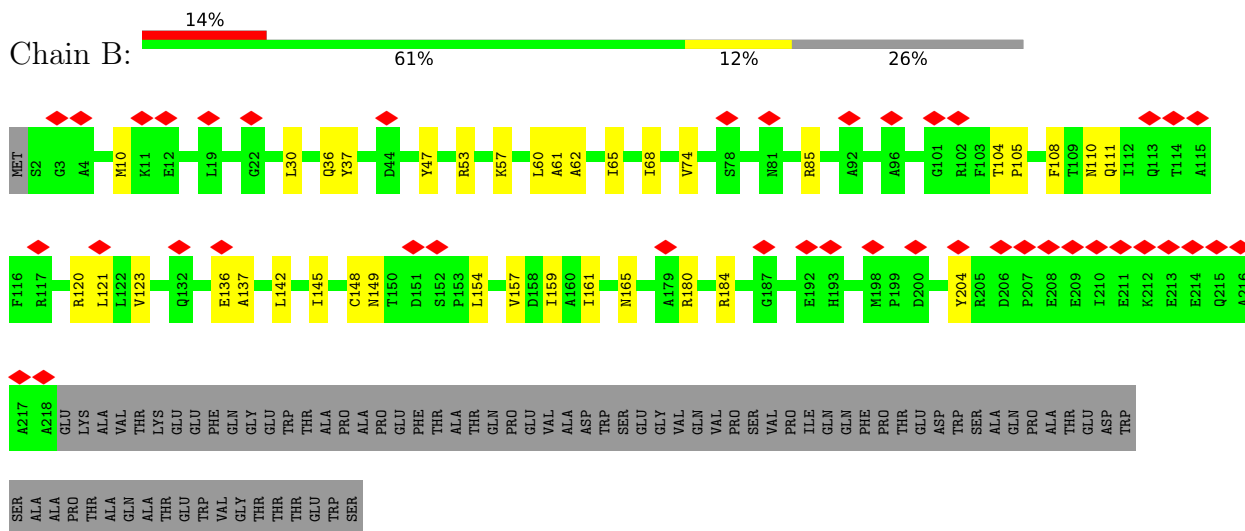
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 18S rRNA

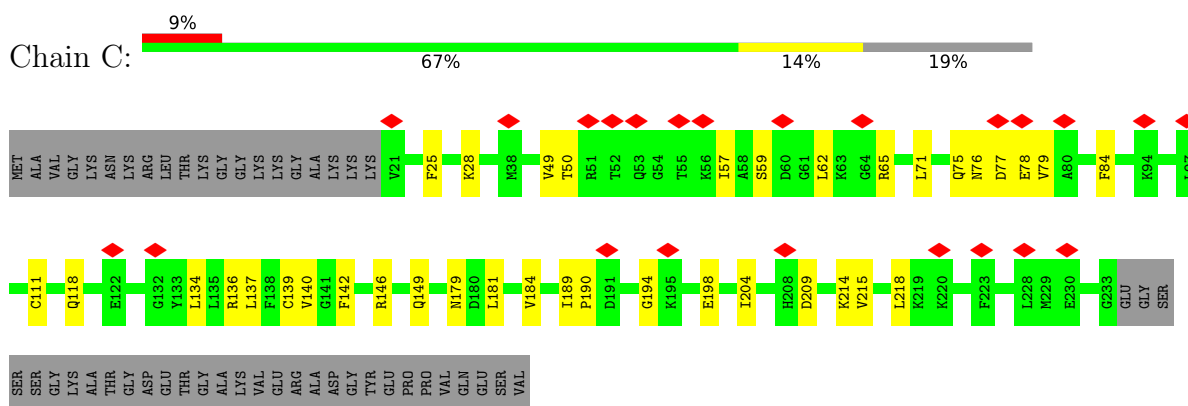




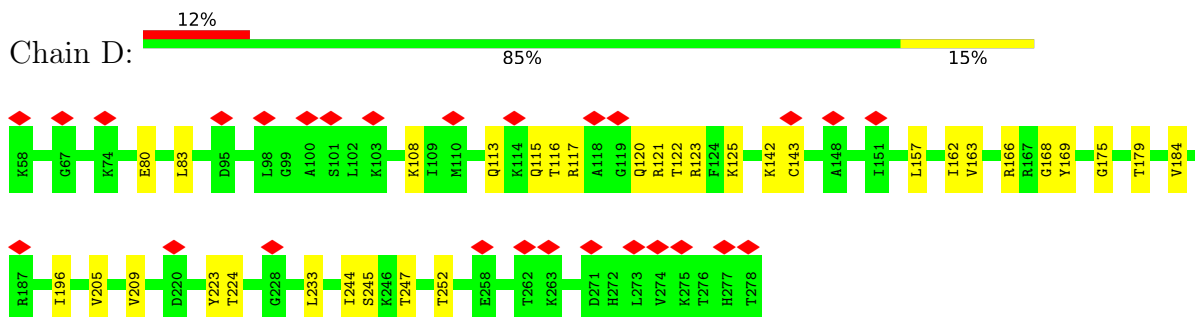
• Molecule 2: uS2 (SA)



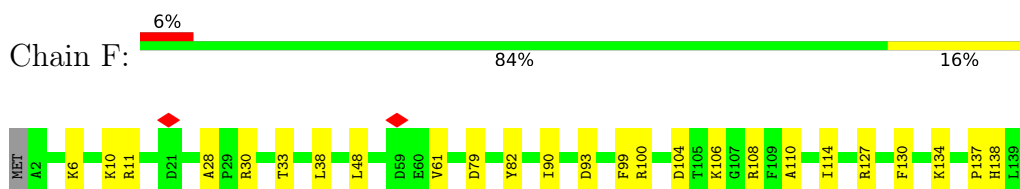
- Molecule 3: eS1



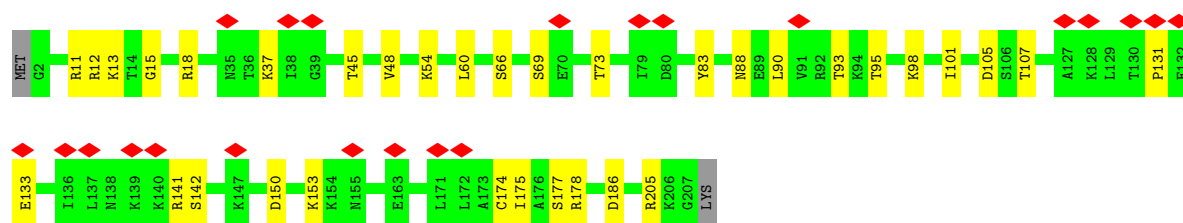
- Molecule 4: 40S ribosomal protein S2



- Molecule 5: eS4 (S4 X isoform)

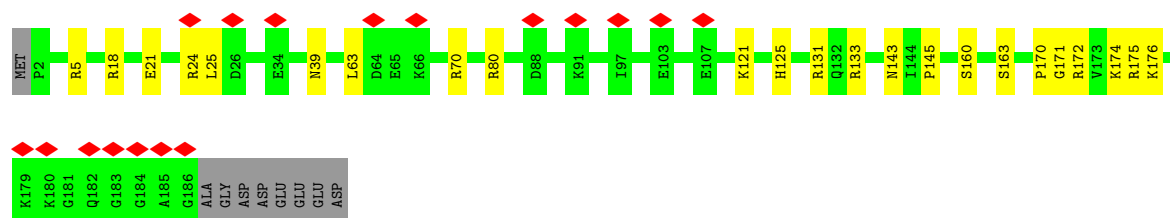


Chain J: 



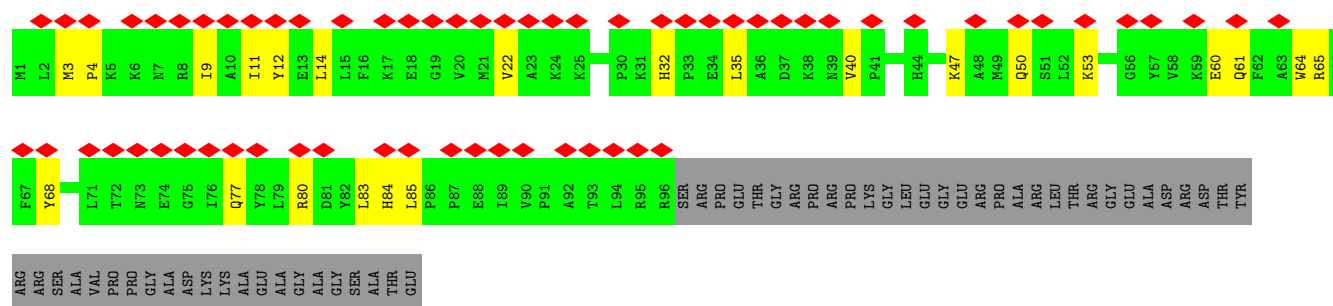
• Molecule 10: uS4

Chain K: 



• Molecule 11: eS10

Chain L: 

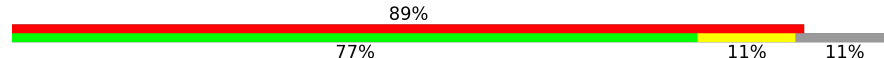


• Molecule 12: uS17

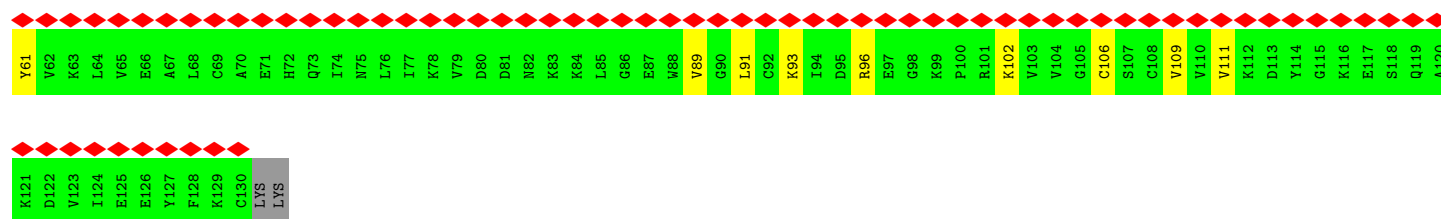
Chain M: 



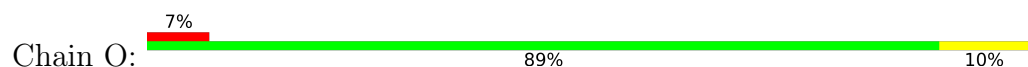
• Molecule 13: eS12

Chain N: 

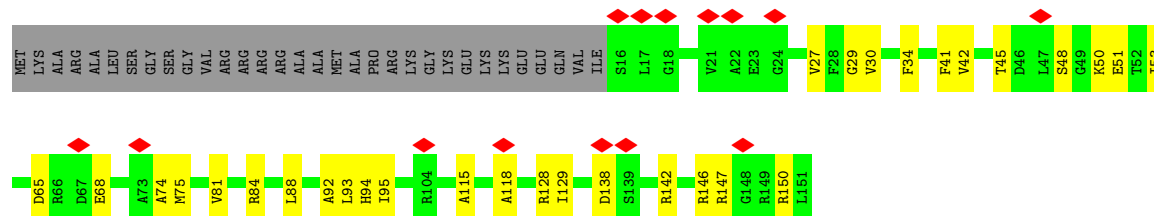




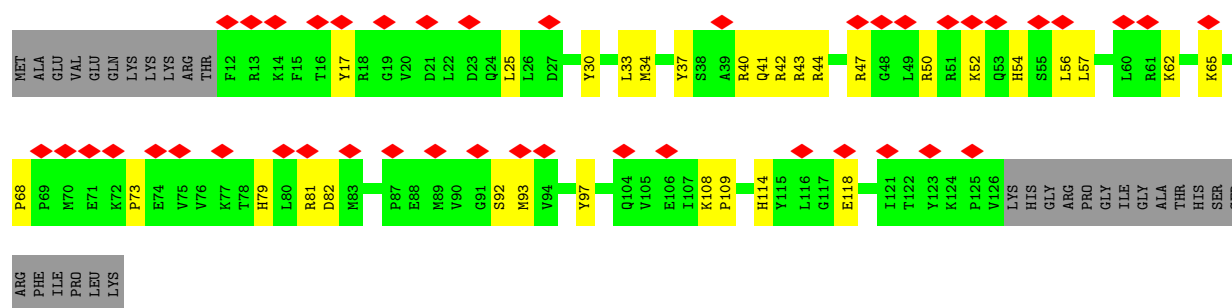
• Molecule 14: uS15



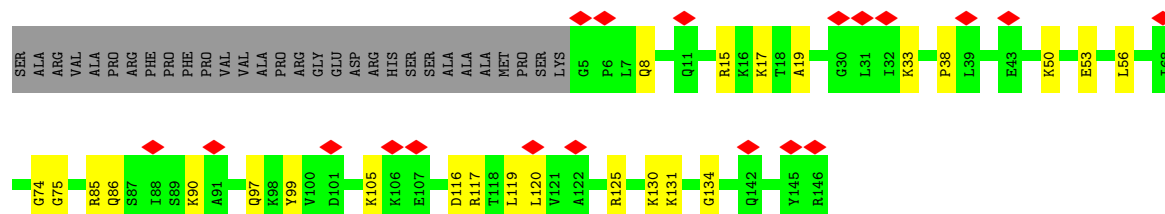
• Molecule 15: uS11



• Molecule 16: uS19

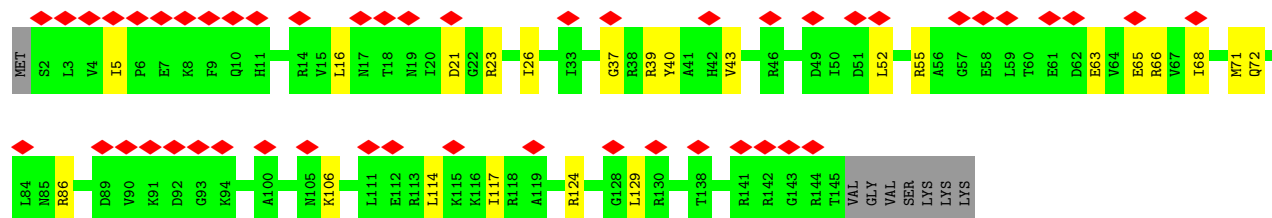


• Molecule 17: uS9



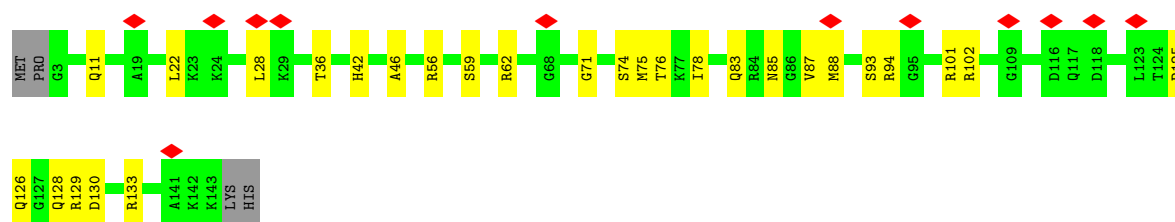
- Molecule 18: uS13

Chain T: 



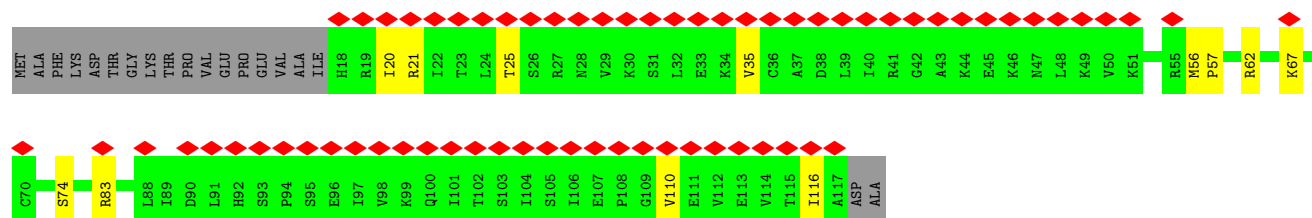
- Molecule 19: eS19

Chain U: 

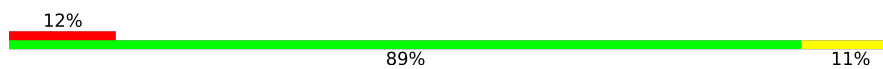


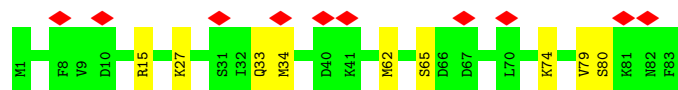
- Molecule 20: uS10

Chain V: 



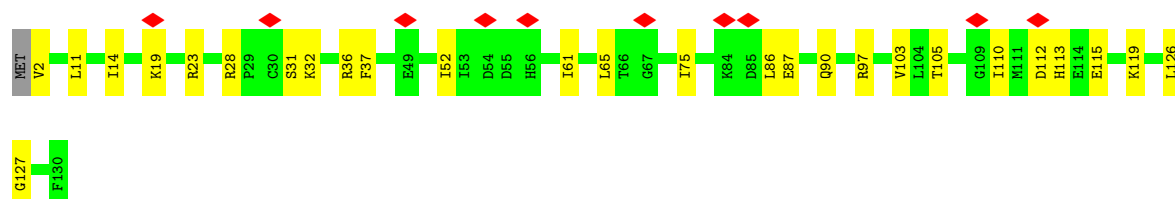
- Molecule 21: eS21

Chain W: 



- Molecule 22: uS8

Chain X: 



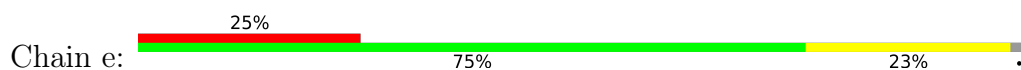
NET ASN ASP T4 M13 T14 N15 R20 K21 Q22 F60 G71 M74 K99 K100 K101 T102 S103 Q106 N112 K115 A127 GLY LYS LYS LYS

[illegible]

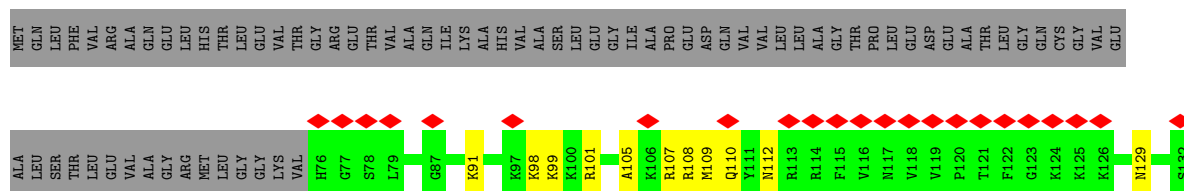
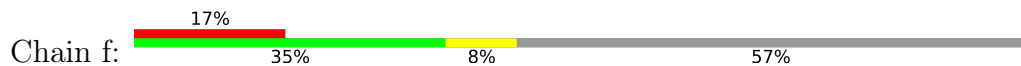
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T2	100	Yellow	
K3	100	Yellow	
K4	100	Yellow	
A11	100	Yellow	
K12	100	Green	
K13	100	Green	
T21	100	Red	Red Diamond
R22	100	Red	
C23	100	Red	
D33	100	Yellow	
K37	100	Yellow	
T44	100	Yellow	
V45	100	Red	Red Diamond
E46	100	Red	Red Diamond
A47	100	Red	Red Diamond
A48	100	Red	Red Diamond
A49	100	Red	Red Diamond
V50	100	Red	Red Diamond
E55	100	Yellow	
F59	100	Yellow	Red Diamond
D60	100	Yellow	
Y68	100	Yellow	
C74	100	Yellow	
C77	100	Yellow	
R87	100	Yellow	
A91	100	Yellow	
T96	100	Red	Red Diamond
R100	100	Red	Red Diamond
F101	100	Red	Red Diamond
R102	100	Red	Red Diamond

Category	Count
P2	100
D6	100
E14	100
E15	100
K16	100
R17	100
K18	100
H19	100
K20	100
K21	100
K22	100
K36	100
G39	100
C40	100
Y41	100
K42	100
I43	100
Q51	100
L55	100
C56	100
V57	100
C64	100
Q65	100
P66	100
T67	100
K70	100
A71	100
R72	100
G76	100
C77	100
S78	100
F79	100
R80	100
R81	100
H81	100

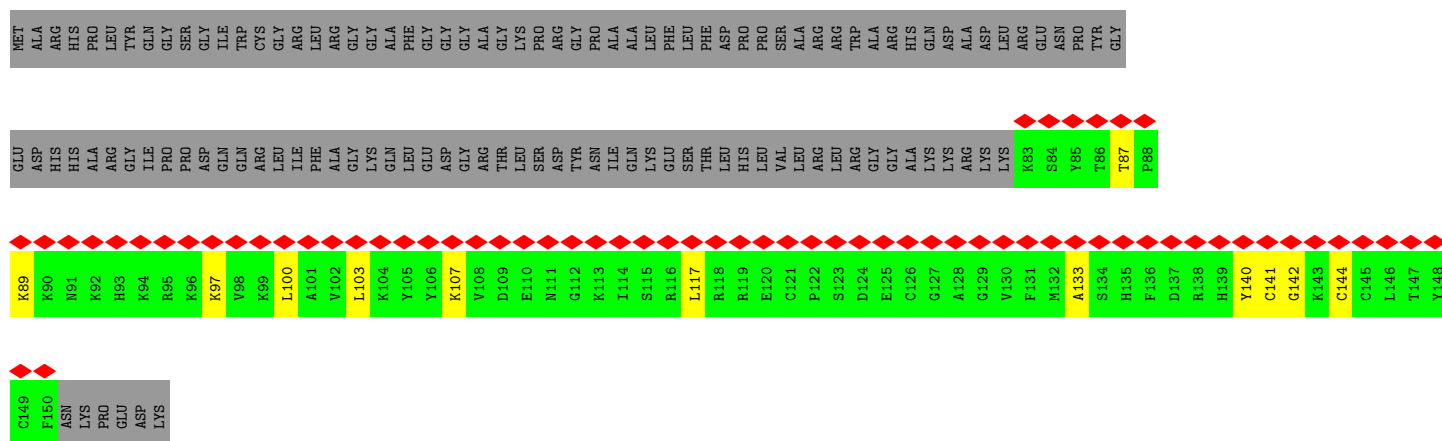
MET	ASP
T3	
S4	
R5	
V6	
Q7	
P8	
I9	
K10	
L11	
A12	
R13	
L18	
R31	
M35	
D36	
D37	
R40	
S41	
I42	
I43	
R44	
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S61	
E62	
R63	
E64	
A65	
R66	
R67	
L68	
P69	



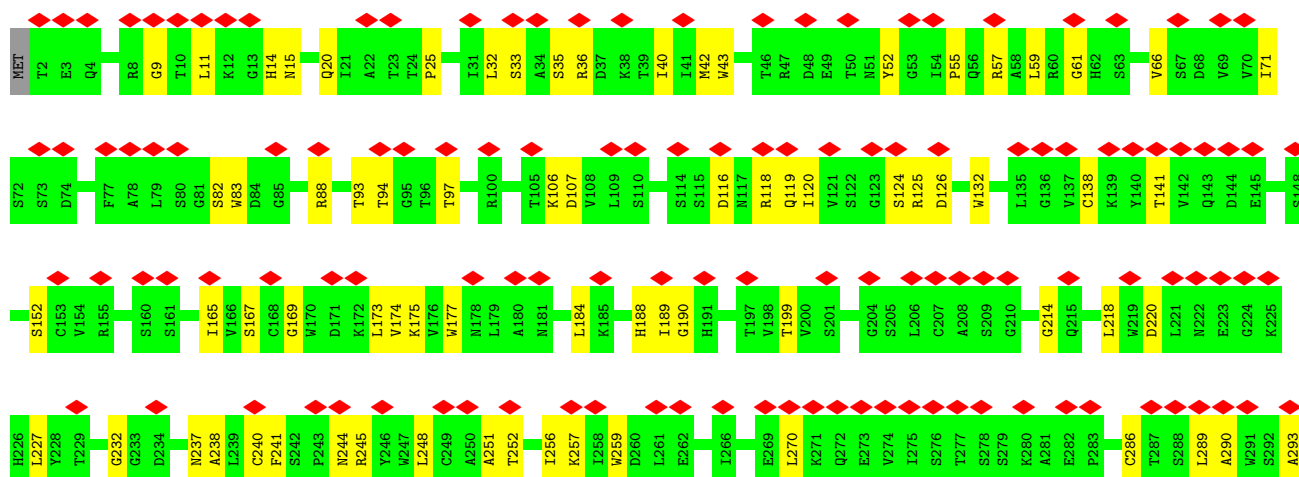
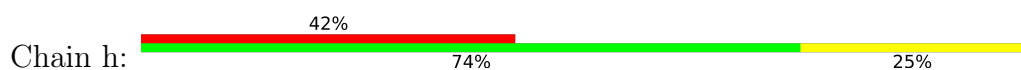
• Molecule 30: eS30

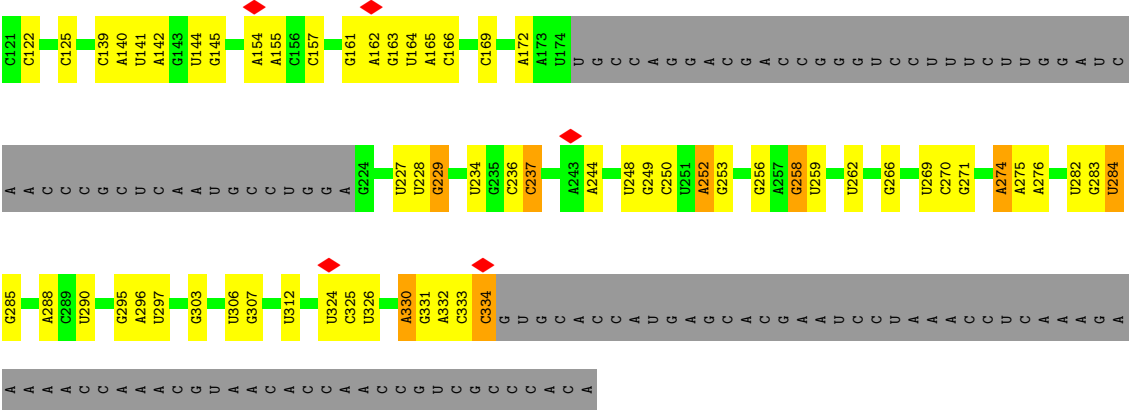


• Molecule 31: eS31



• Molecule 32: Receptor for Activated C Kinase 1 (RACK1)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46095	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	0.048	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	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:
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	0.15	0/40506	0.35	1/63123 (0.0%)
2	B	0.24	0/1747	0.59	0/2374
3	C	0.21	0/1756	0.58	0/2350
4	D	0.22	0/1753	0.56	0/2369
5	F	0.18	0/2118	0.48	0/2849
6	G	0.23	0/1531	0.58	1/2059 (0.0%)
7	H	0.18	0/1946	0.46	0/2590
8	I	0.21	0/1510	0.49	0/2022
9	J	0.19	0/1715	0.47	0/2287
10	K	0.24	0/1550	0.57	0/2069
11	L	0.26	0/834	0.67	0/1125
12	M	0.18	0/1254	0.51	0/1677
13	N	0.18	0/918	0.47	0/1233
14	O	0.20	0/1226	0.48	0/1649
15	P	0.18	0/1029	0.47	0/1380
16	Q	0.24	0/974	0.62	0/1301
17	R	0.21	0/1146	0.50	0/1534
18	T	0.24	0/1208	0.62	2/1618 (0.1%)
19	U	0.21	0/1115	0.56	0/1493
20	V	0.20	0/805	0.48	0/1081
21	W	0.18	0/643	0.47	0/860
22	X	0.24	0/1051	0.59	0/1406
23	Y	0.20	0/1116	0.51	0/1490
24	Z	0.18	0/1028	0.45	0/1366
25	a	0.19	0/620	0.51	0/831
26	b	0.20	0/828	0.44	0/1109
27	c	0.20	0/665	0.53	0/891
28	d	0.18	0/532	0.62	2/712 (0.3%)
29	e	0.21	0/470	0.45	0/623
30	f	0.19	0/462	0.50	0/607
31	g	0.12	0/567	0.36	0/753
32	h	0.18	0/2493	0.50	0/3394

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	n	0.21	0/240	0.59	0/305
34	E	0.21	0/1796	0.55	0/2417
35	S	0.25	0/1082	0.64	0/1452
36	z	0.15	0/3966	0.35	0/6182
All	All	0.18	0/84200	0.44	6/122581 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	6	VAL	CA-C-N	6.68	130.56	121.20
28	d	6	VAL	C-N-CA	6.68	130.56	121.20
1	2	688	U	P-O3'-C3'	5.38	128.27	120.20
18	T	16	LEU	CA-C-N	5.28	131.62	121.54
18	T	16	LEU	C-N-CA	5.28	131.62	121.54
6	G	195	GLU	CA-CB-CG	5.21	124.52	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	36227	0	18299	319	0
2	B	1710	0	1708	23	0
3	C	1729	0	1803	24	0
4	D	1716	0	1806	19	0
5	F	2076	0	2177	28	0
6	G	1509	0	1563	12	0
7	H	1923	0	2089	22	0
8	I	1488	0	1582	17	0
9	J	1686	0	1772	22	0
10	K	1525	0	1640	18	0
11	L	810	0	836	15	0
12	M	1233	0	1310	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	908	0	939	10	0
14	O	1202	0	1289	10	0
15	P	1016	0	1039	23	0
16	Q	956	0	1002	19	0
17	R	1128	0	1195	17	0
18	T	1190	0	1249	15	0
19	U	1097	0	1130	22	0
20	V	795	0	862	10	0
21	W	636	0	637	7	0
22	X	1034	0	1080	21	0
23	Y	1098	0	1167	13	0
24	Z	1011	0	1083	7	0
25	a	614	0	678	7	0
26	b	814	0	863	15	0
27	c	651	0	672	13	0
28	d	530	0	561	10	0
29	e	459	0	452	12	0
30	f	457	0	502	8	0
31	g	555	0	563	9	0
32	h	2436	0	2393	49	0
33	n	239	0	289	2	0
34	E	1768	0	1866	26	0
35	S	1068	0	1121	17	0
36	z	3550	0	1795	16	0
37	b	1	0	0	0	0
37	g	1	0	0	0	0
All	All	78846	0	61012	727	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 6.

All (727) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1332:A:H62	1:2:1493:C:N4	1.57	1.01
1:2:16:G:N2	1:2:1195:A:H62	1.60	0.98
1:2:1332:A:N6	1:2:1493:C:H42	1.61	0.96
1:2:16:G:H21	1:2:1195:A:N6	1.62	0.96
1:2:1048:G:N2	1:2:1070:A:H62	1.63	0.95
1:2:1048:G:H21	1:2:1070:A:N6	1.64	0.94
31:g:141:CYS:SG	31:g:144:CYS:HB2	2.11	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:677:G:H21	1:2:1028:A:H62	1.04	0.91
1:2:1288:U:H3	1:2:1311:C:H42	1.03	0.91
1:2:1335:G:H1	1:2:1492:U:H3	1.17	0.88
1:2:1048:G:H21	1:2:1070:A:H62	0.91	0.87
1:2:1288:U:H3	1:2:1311:C:N4	1.72	0.86
15:P:27:VAL:O	15:P:92:ALA:HB3	1.82	0.80
1:2:677:G:N2	1:2:1028:A:H62	1.79	0.80
1:2:1657:G:H1	1:2:1667:U:H3	1.31	0.78
1:2:1324:G:H1	1:2:1504:U:H3	1.30	0.76
1:2:1656:G:H1	1:2:1668:U:H3	1.33	0.76
1:2:1368:U:HO2'	35:S:2:GLY:N	1.86	0.73
1:2:1332:A:H62	1:2:1493:C:H42	0.81	0.73
1:2:934:G:H1	1:2:1008:A:H2	1.38	0.71
36:z:256:G:N2	36:z:276:A:H62	1.89	0.69
1:2:16:G:H21	1:2:1195:A:H62	0.81	0.69
32:h:118:ARG:HG3	32:h:119:GLN:HG2	1.76	0.68
22:X:105:THR:HG23	22:X:126:LEU:HD11	1.75	0.68
36:z:256:G:H21	36:z:276:A:N6	1.93	0.66
15:P:34:PHE:HB3	15:P:41:PHE:HB2	1.76	0.66
5:F:79:ASP:HB3	5:F:82:TYR:HB2	1.78	0.65
36:z:256:G:N2	36:z:276:A:N6	2.45	0.65
18:T:39:ARG:HH22	19:U:46:ALA:HB2	1.61	0.65
1:2:317:C:H42	1:2:334:C:H42	1.44	0.65
1:2:1091:C:HO2'	22:X:2:VAL:N	1.95	0.65
1:2:1274:G:H1	29:e:7:TYR:HH	0.71	0.64
1:2:1351:G:H21	1:2:1352:G:H3'	1.62	0.64
32:h:120:ILE:HB	32:h:132:TRP:HB2	1.78	0.64
32:h:116:ASP:OD1	32:h:118:ARG:NH1	2.31	0.63
7:H:14:LYS:HD2	7:H:123:GLY:HA3	1.81	0.63
35:S:27:ASP:O	35:S:31:ASN:ND2	2.32	0.63
1:2:677:G:H21	1:2:1028:A:N6	1.86	0.62
32:h:106:LYS:HD2	32:h:126:ASP:HB3	1.81	0.62
32:h:199:THR:HG21	32:h:240:CYS:HA	1.82	0.62
34:E:125:PHE:O	34:E:129:SER:HB2	2.00	0.62
18:T:86:ARG:HG3	18:T:106:LYS:HZ2	1.64	0.62
22:X:52:ILE:HG12	22:X:61:ILE:HG12	1.81	0.62
29:e:19:ARG:HH12	29:e:32:ARG:HH11	1.47	0.61
34:E:32:ASP:HB2	34:E:54:ARG:HB2	1.82	0.61
32:h:238:ALA:H	32:h:251:ALA:HB3	1.64	0.61
1:2:1495:G:N2	29:e:42:CYS:SG	2.72	0.61
22:X:87:GLU:OE1	22:X:90:GLN:NE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1277:C:H2'	1:2:1278:A:H8	1.66	0.61
20:V:35:VAL:HG21	20:V:110:VAL:HG21	1.83	0.61
13:N:93:LYS:HB3	13:N:96:ARG:HD2	1.84	0.60
1:2:658:U:H1'	23:Y:17:ARG:HH12	1.66	0.60
2:B:123:VAL:HG12	2:B:145:ILE:HB	1.82	0.60
1:2:1273:C:O2	1:2:1508:A:N6	2.35	0.59
1:2:442:C:H42	1:2:449:A:H62	1.50	0.59
19:U:129:ARG:HG2	19:U:133:ARG:HE	1.67	0.59
1:2:38:A:OP1	10:K:5:ARG:NH2	2.35	0.59
32:h:40:ILE:HB	32:h:59:LEU:HB2	1.82	0.59
1:2:1477:U:OP1	35:S:3:ARG:NH2	2.36	0.59
1:2:1540:G:H5''	19:U:56:ARG:HH21	1.66	0.58
7:H:106:LEU:HD13	7:H:109:LEU:HD21	1.84	0.58
18:T:68:ILE:O	18:T:72:GLN:NE2	2.36	0.58
13:N:91:LEU:HD11	13:N:106:CYS:HB2	1.84	0.58
19:U:83:GLN:OE1	19:U:85:ASN:ND2	2.37	0.58
1:2:141:A:H61	1:2:177:G:H21	1.51	0.58
1:2:1311:C:OP2	13:N:36:ARG:NH2	2.37	0.58
1:2:921:G:H3'	22:X:28:ARG:HH22	1.69	0.58
25:a:66:LYS:HG2	25:a:111:ARG:HH21	1.69	0.58
1:2:927:C:O2	27:c:51:GLN:NE2	2.37	0.57
8:I:76:GLN:HA	8:I:79:LEU:HB2	1.86	0.57
3:C:111:CYS:HB3	26:b:68:TYR:HB2	1.86	0.57
21:W:74:LYS:NZ	21:W:80:SER:O	2.37	0.57
32:h:308:ARG:NH2	32:h:309:VAL:O	2.37	0.57
1:2:511:U:O2'	1:2:576:A:N6	2.37	0.57
34:E:103:GLU:OE1	34:E:173:ARG:NH1	2.37	0.57
1:2:457:C:H2'	1:2:458:A:H8	1.69	0.57
3:C:28:LYS:HE3	3:C:50:THR:HG22	1.85	0.57
7:H:7:PHE:HB2	7:H:124:LEU:HD23	1.86	0.57
11:L:9:ILE:HA	11:L:12:TYR:HD2	1.70	0.57
26:b:102:ARG:NH2	36:z:330:A:O2'	2.37	0.57
27:c:36:LYS:HB3	27:c:43:ILE:HG22	1.86	0.57
13:N:89:VAL:HG21	13:N:109:VAL:HG11	1.85	0.57
1:2:346:C:H5''	5:F:38:LEU:HB2	1.87	0.57
1:2:1786:U:H2'	1:2:1787:G:H8	1.70	0.57
1:2:919:A:N7	14:O:64:ARG:NH1	2.52	0.56
1:2:1706:G:N3	1:2:1850:A:O2'	2.37	0.56
17:R:53:GLU:HG3	17:R:85:ARG:HH21	1.68	0.56
27:c:56:CYS:SG	27:c:57:VAL:N	2.79	0.56
26:b:87:ARG:NH1	26:b:91:ALA:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:g:141:CYS:SG	31:g:142:GLY:N	2.78	0.56
32:h:107:ASP:OD2	35:S:33:ARG:NH1	2.38	0.56
34:E:46:THR:HB	34:E:84:VAL:HG12	1.86	0.56
1:2:400:C:OP1	23:Y:11:ARG:NH1	2.39	0.56
1:2:829:C:O2'	1:2:845:G:N2	2.39	0.56
1:2:1191:C:H5''	23:Y:119:ARG:HH21	1.71	0.56
1:2:1276:A:H62	1:2:1321:G:H21	1.53	0.56
1:2:1615:U:OP2	16:Q:43:ARG:NH2	2.38	0.56
1:2:1542:C:OP1	19:U:62:ARG:NH1	2.38	0.56
4:D:108:LYS:HD2	4:D:233:LEU:HD23	1.88	0.56
1:2:1124:C:O2'	35:S:127:ASN:ND2	2.38	0.56
32:h:252:THR:HG21	32:h:257:LYS:HE3	1.88	0.56
1:2:1618:C:OP1	16:Q:52:LYS:NZ	2.39	0.56
20:V:20:ILE:HG12	20:V:116:ILE:HG22	1.88	0.56
5:F:137:PRO:HB2	5:F:150:PRO:HD2	1.87	0.56
32:h:138:CYS:SG	32:h:141:THR:OG1	2.64	0.55
2:B:37:TYR:OH	2:B:57:LYS:NZ	2.39	0.55
1:2:603:C:N4	1:2:620:G:O6	2.40	0.55
1:2:1507:G:N2	31:g:87:THR:O	2.38	0.55
1:2:1838:U:H1'	15:P:150:ARG:HH22	1.71	0.55
4:D:196:ILE:HB	4:D:223:TYR:HB2	1.88	0.55
11:L:35:LEU:HD23	11:L:40:VAL:HG11	1.89	0.55
27:c:65:GLN:HB3	27:c:72:ARG:HB3	1.87	0.55
1:2:378:U:OP2	9:J:178:ARG:NH1	2.38	0.55
1:2:1669:G:H4'	20:V:62:ARG:HH22	1.70	0.55
1:2:1545:A:H4'	17:R:74:GLY:HA2	1.89	0.55
5:F:197:ASN:HB2	5:F:209:HIS:HB2	1.88	0.55
18:T:114:LEU:HD13	18:T:117:ILE:HD11	1.89	0.55
1:2:851:C:O2'	1:2:852:G:N2	2.40	0.55
5:F:130:PHE:HB3	5:F:138:HIS:HB2	1.89	0.55
1:2:637:U:O2	30:f:129:ASN:ND2	2.40	0.54
28:d:31:ARG:HB2	28:d:43:ILE:HG22	1.88	0.54
36:z:141:U:H2'	36:z:142:A:H8	1.72	0.54
36:z:144:U:O2	36:z:249:G:O6	2.25	0.54
1:2:1338:G:H4'	20:V:74:SER:H	1.72	0.54
15:P:45:THR:OG1	15:P:51:GLU:O	2.23	0.54
6:G:71:ARG:NH2	6:G:148:ASN:OD1	2.41	0.54
21:W:15:ARG:NH1	21:W:33:GLN:OE1	2.41	0.54
1:2:395:G:H5'	12:M:82:MET:HE1	1.89	0.54
1:2:674:C:H42	1:2:1031:A:H61	1.55	0.54
8:I:50:GLU:HG3	8:I:60:ILE:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:63:ARG:NH1	28:d:64:GLU:O	2.41	0.54
1:2:1563:G:H1	1:2:1572:C:H42	1.56	0.54
14:O:75:LEU:HB3	14:O:81:ALA:HB2	1.88	0.54
1:2:844:U:OP2	5:F:240:ARG:NH1	2.41	0.54
1:2:1653:U:H3	1:2:1671:G:H1	1.55	0.54
9:J:174:CYS:SG	9:J:175:ILE:N	2.81	0.54
15:P:142:ARG:NH1	26:b:23:CYS:O	2.41	0.54
26:b:55:GLU:OE1	28:d:5:ARG:NH1	2.40	0.54
34:E:1:MET:HG2	34:E:3:VAL:HG12	1.88	0.54
1:2:460:A:H1'	1:2:470:G:H22	1.73	0.54
1:2:560:A:H5'	10:K:174:LYS:HB2	1.90	0.54
4:D:121:ARG:HH12	4:D:123:ARG:HD3	1.72	0.54
11:L:61:GLN:HB2	11:L:68:TYR:HB2	1.88	0.54
1:2:1398:G:O2'	32:h:88:ARG:NH2	2.40	0.53
1:2:1049:A:OP2	1:2:1068:G:N2	2.41	0.53
8:I:73:GLN:OE1	8:I:76:GLN:NE2	2.40	0.53
18:T:26:ILE:HD11	18:T:52:LEU:HA	1.91	0.53
1:2:97:U:O2	1:2:434:G:N2	2.41	0.53
3:C:75:GLN:NE2	3:C:76:ASN:OD1	2.41	0.53
28:d:18:LEU:HB3	36:z:330:A:H61	1.72	0.53
32:h:107:ASP:O	32:h:124:SER:OG	2.27	0.53
34:E:29:LEU:HD11	34:E:58:VAL:HG23	1.89	0.53
28:d:69:ARG:HE	36:z:334:C:H5'	1.73	0.53
1:2:383:G:H21	12:M:133:PRO:HG3	1.73	0.53
1:2:685:A:H5''	22:X:31:SER:HB3	1.90	0.53
1:2:1288:U:O2	1:2:1311:C:N3	2.41	0.53
1:2:1617:G:N1	1:2:1620:A:OP2	2.42	0.53
1:2:943:U:OP1	3:C:214:LYS:NZ	2.41	0.53
1:2:1110:G:O2'	35:S:126:MET:SD	2.66	0.53
4:D:123:ARG:NE	4:D:143:CYS:SG	2.74	0.53
1:2:1033:G:H1	1:2:1080:A:HO2'	1.55	0.53
2:B:148:CYS:SG	2:B:149:ASN:N	2.80	0.53
1:2:1566:G:N7	19:U:101:ARG:NH2	2.57	0.53
32:h:173:LEU:HD22	32:h:189:ILE:HG12	1.91	0.53
1:2:1144:A:OP1	1:2:1355:C:N4	2.42	0.52
1:2:1547:C:H1'	1:2:1670:C:H4'	1.91	0.52
3:C:142:PHE:HB2	3:C:209:ASP:HB2	1.91	0.52
9:J:83:TYR:HD2	9:J:101:ILE:HD13	1.74	0.52
32:h:42:MET:HE2	32:h:57:ARG:HB3	1.92	0.52
1:2:846:G:OP2	5:F:108:ARG:NH1	2.42	0.52
2:B:30:LEU:HB2	2:B:47:TYR:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:41:ARG:NH1	8:I:42:GLU:OE1	2.42	0.52
18:T:23:ARG:O	18:T:55:ARG:NH2	2.42	0.52
1:2:522:A:O2'	10:K:131:ARG:NH1	2.42	0.52
1:2:960:U:O2'	1:2:963:A:N6	2.39	0.52
1:2:1133:A:O3'	26:b:13:LYS:NZ	2.42	0.52
1:2:1332:A:O2'	34:E:145:GLN:O	2.28	0.52
1:2:1424:G:H2'	1:2:1425:G:H8	1.73	0.52
2:B:108:PHE:HB2	2:B:136:GLU:HG2	1.91	0.52
4:D:142:LYS:HB2	4:D:157:LEU:HD12	1.92	0.52
4:D:205:VAL:O	4:D:224:THR:OG1	2.28	0.52
1:2:1533:A:OP1	6:G:164:ARG:NH2	2.43	0.52
15:P:65:ASP:HA	15:P:68:GLU:HG3	1.92	0.52
22:X:11:LEU:HD11	22:X:37:PHE:HE2	1.74	0.52
32:h:82:SER:OG	32:h:83:TRP:N	2.43	0.52
1:2:377:G:H5'	9:J:98:LYS:HB3	1.92	0.52
15:P:42:VAL:HG11	15:P:81:VAL:HG11	1.92	0.52
1:2:65:C:OP1	7:H:136:LYS:NZ	2.42	0.52
1:2:74:G:N2	1:2:77:A:OP2	2.43	0.52
1:2:573:U:N3	1:2:576:A:OP2	2.40	0.52
11:L:77:GLN:HA	11:L:80:ARG:HG2	1.92	0.52
1:2:1172:U:O3'	33:n:14:LYS:NZ	2.36	0.51
1:2:1863:A:OP2	26:b:4:LYS:NZ	2.38	0.51
10:K:170:PRO:O	10:K:175:ARG:NH2	2.43	0.51
11:L:83:LEU:HG	11:L:85:LEU:HD23	1.91	0.51
32:h:93:THR:HG23	32:h:94:THR:HG23	1.91	0.51
1:2:638:C:H5''	30:f:109:MET:HE1	1.92	0.51
13:N:33:ARG:HE	13:N:89:VAL:HG22	1.75	0.51
4:D:80:GLU:HA	4:D:83:LEU:HB3	1.93	0.51
18:T:65:GLU:HA	18:T:68:ILE:HG12	1.93	0.51
35:S:130:THR:O	35:S:132:ARG:NH1	2.43	0.51
1:2:53:C:OP1	24:Z:112:ASN:ND2	2.40	0.51
1:2:142:C:H1'	7:H:180:VAL:HG11	1.92	0.51
1:2:922:A:OP1	22:X:28:ARG:NH2	2.44	0.51
1:2:1719:A:H62	1:2:1814:G:HO2'	1.56	0.51
32:h:237:ASN:ND2	32:h:286:CYS:O	2.44	0.51
1:2:1057:C:O2'	1:2:1059:G:N7	2.39	0.51
1:2:1660:C:OP1	29:e:16:GLN:NE2	2.44	0.51
9:J:37:LYS:NZ	9:J:93:THR:OG1	2.44	0.51
1:2:71:G:N7	7:H:170:ARG:NH2	2.59	0.51
1:2:830:A:OP2	1:2:846:G:N2	2.44	0.51
1:2:1652:G:H1	1:2:1672:U:H3	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:108:LYS:HD3	16:Q:109:PRO:HD2	1.93	0.51
1:2:33:G:O2'	1:2:564:A:O2'	2.28	0.51
1:2:346:C:O2'	5:F:30:ARG:NH2	2.39	0.51
1:2:516:A:N1	1:2:643:A:O2'	2.43	0.51
15:P:84:ARG:HH21	15:P:88:LEU:HB2	1.75	0.51
19:U:42:HIS:HB3	19:U:83:GLN:HG2	1.91	0.51
24:Z:99:LYS:O	24:Z:101:LYS:NZ	2.44	0.51
20:V:67:LYS:O	29:e:44:ARG:NH1	2.44	0.51
23:Y:100:VAL:HG12	23:Y:125:VAL:HG22	1.92	0.51
26:b:74:CYS:SG	26:b:77:CYS:HB2	2.51	0.51
1:2:600:G:H2'	1:2:601:G:H8	1.76	0.51
1:2:658:U:O3'	23:Y:17:ARG:NH2	2.44	0.51
27:c:14:GLU:O	27:c:18:LYS:NZ	2.44	0.51
34:E:105:LEU:HD12	34:E:122:VAL:HG21	1.92	0.51
1:2:319:C:N4	7:H:186:GLN:OE1	2.45	0.50
4:D:113:GLN:HG3	4:D:122:THR:HG22	1.93	0.50
6:G:169:ILE:HA	6:G:172:CYS:HB2	1.93	0.50
35:S:58:MET:HA	35:S:61:ILE:HG22	1.93	0.50
36:z:165:A:N6	36:z:237:C:O2'	2.44	0.50
1:2:141:A:H61	1:2:177:G:N2	2.08	0.50
16:Q:81:ARG:NH2	16:Q:97:TYR:O	2.45	0.50
22:X:86:LEU:HD21	22:X:113:HIS:HB2	1.93	0.50
2:B:149:ASN:ND2	2:B:165:ASN:OD1	2.44	0.50
1:2:918:U:O2'	1:2:919:A:O4'	2.30	0.50
1:2:1838:U:O3'	15:P:150:ARG:NH1	2.44	0.50
8:I:10:LYS:HD2	8:I:14:GLU:HB3	1.93	0.50
27:c:19:HIS:HB3	27:c:22:LYS:HG3	1.93	0.50
1:2:65:C:N4	1:2:169:U:O2'	2.44	0.50
6:G:49:LEU:HD12	17:R:50:LYS:HB2	1.94	0.50
1:2:587:A:O2'	1:2:588:G:N2	2.44	0.50
1:2:1297:U:H2'	1:2:1298:G:H2'	1.94	0.50
1:2:1551:U:OP1	34:E:9:ARG:NH2	2.45	0.50
3:C:78:GLU:HG2	3:C:79:VAL:H	1.76	0.50
9:J:66:SER:HA	9:J:73:THR:HG22	1.93	0.50
17:R:116:ASP:HB3	17:R:119:LEU:HD23	1.94	0.50
19:U:11:GLN:HG2	19:U:62:ARG:HH21	1.76	0.50
35:S:41:ILE:HG22	35:S:43:SER:H	1.77	0.50
22:X:75:ILE:HG12	22:X:127:GLY:HA2	1.94	0.50
35:S:98:VAL:O	35:S:120:THR:OG1	2.30	0.50
1:2:818:A:N7	1:2:847:A:N6	2.60	0.49
1:2:872:A:O2'	1:2:874:G:OP2	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1473:G:O2'	1:2:1475:G:N2	2.44	0.49
3:C:181:LEU:HA	3:C:184:VAL:HG22	1.93	0.49
4:D:115:GLN:HA	4:D:120:GLN:HA	1.93	0.49
7:H:37:ALA:HA	7:H:49:VAL:HA	1.94	0.49
22:X:87:GLU:OE2	22:X:97:ARG:NH1	2.45	0.49
27:c:40:CYS:SG	27:c:41:TYR:N	2.85	0.49
32:h:257:LYS:HD3	32:h:259:TRP:HE1	1.76	0.49
5:F:255:ARG:HH11	5:F:259:LYS:HD3	1.77	0.49
30:f:98:LYS:NZ	30:f:99:LYS:O	2.45	0.49
34:E:132:LYS:HE2	34:E:191:PRO:HA	1.93	0.49
1:2:1121:G:O2'	3:C:204:ILE:O	2.30	0.49
1:2:1299:A:H5'	16:Q:56:LEU:HD13	1.95	0.49
1:2:1598:G:O6	25:a:85:ARG:NH2	2.46	0.49
1:2:1841:C:OP2	33:n:2:ARG:NH1	2.44	0.49
7:H:70:HIS:HB3	7:H:101:ILE:HB	1.94	0.49
1:2:681:U:OP1	12:M:104:LYS:NZ	2.42	0.49
1:2:1544:C:O2'	17:R:75:GLY:O	2.29	0.49
1:2:1620:A:H2'	16:Q:40:ARG:HH21	1.77	0.49
7:H:63:MET:HA	7:H:98:ARG:HB2	1.94	0.49
11:L:53:LYS:HE3	11:L:60:GLU:HB2	1.93	0.49
24:Z:15:ASN:OD1	24:Z:22:GLN:NE2	2.46	0.49
32:h:167:SER:OG	32:h:175:LYS:O	2.28	0.49
1:2:127:C:O2	5:F:134:LYS:NZ	2.40	0.49
1:2:539:C:N4	1:2:545:A:N1	2.60	0.49
1:2:1606:G:H5''	19:U:87:VAL:HB	1.94	0.49
3:C:139:CYS:SG	3:C:140:VAL:N	2.85	0.49
6:G:175:ASP:O	6:G:179:ASN:ND2	2.46	0.49
1:2:109:U:O2'	12:M:71:ARG:NH2	2.45	0.49
1:2:482:G:N2	1:2:485:A:OP2	2.43	0.49
1:2:1374:C:O2'	1:2:1464:C:O2	2.31	0.49
24:Z:13:MET:SD	24:Z:15:ASN:ND2	2.86	0.49
27:c:80:ARG:NH2	36:z:236:C:O3'	2.46	0.49
3:C:136:ARG:HB2	3:C:218:LEU:HD11	1.95	0.49
5:F:246:LEU:HD12	5:F:250:GLU:HG2	1.94	0.49
23:Y:109:GLY:HA2	23:Y:119:ARG:HD3	1.94	0.49
1:2:21:U:H3	1:2:654:A:H2	1.61	0.49
1:2:1475:G:OP2	17:R:117:ARG:NH2	2.45	0.49
4:D:169:TYR:OH	4:D:175:GLY:O	2.28	0.49
5:F:100:ARG:HB2	5:F:114:ILE:HD13	1.94	0.49
6:G:55:ARG:HH22	17:R:125:ARG:HD3	1.78	0.49
9:J:105:ASP:OD2	9:J:107:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:72:C:O2'	1:2:74:G:OP2	2.31	0.48
1:2:307:G:N2	9:J:45:THR:O	2.44	0.48
1:2:547:G:O2'	1:2:549:C:N4	2.46	0.48
1:2:555:A:H61	1:2:589:G:H21	1.60	0.48
1:2:1629:C:H4'	18:T:40:TYR:HE1	1.76	0.48
22:X:23:ARG:O	22:X:65:LEU:N	2.45	0.48
1:2:944:A:N1	1:2:982:G:O6	2.46	0.48
3:C:189:ILE:HG23	3:C:190:PRO:HD3	1.95	0.48
10:K:63:LEU:O	10:K:70:ARG:NH1	2.46	0.48
1:2:990:A:OP2	26:b:37:LYS:NZ	2.44	0.48
1:2:1286:G:H21	1:2:1313:A:H62	1.60	0.48
10:K:171:GLY:O	10:K:175:ARG:NE	2.47	0.48
12:M:33:LEU:HD12	12:M:34:PRO:HD2	1.95	0.48
34:E:193:ASP:N	34:E:193:ASP:OD1	2.46	0.48
1:2:687:C:O4'	8:I:118:ARG:NH1	2.47	0.48
13:N:26:LEU:HG	13:N:31:LEU:HD21	1.95	0.48
1:2:586:G:OP1	10:K:176:LYS:NZ	2.41	0.48
1:2:610:G:H2'	1:2:611:G:H8	1.78	0.48
1:2:1108:G:N2	1:2:1124:C:O2	2.41	0.48
1:2:1276:A:H4'	11:L:50:GLN:HE22	1.78	0.48
4:D:116:THR:HG22	4:D:117:ARG:H	1.78	0.48
1:2:751:G:H1	1:2:792:C:H2'	1.78	0.48
4:D:168:GLY:N	4:D:179:THR:O	2.46	0.48
1:2:486:A:O2'	1:2:513:G:N2	2.47	0.48
2:B:157:VAL:O	21:W:65:SER:OG	2.31	0.48
14:O:22:VAL:HG22	14:O:66:VAL:HG12	1.96	0.48
32:h:61:GLY:O	32:h:88:ARG:NH2	2.46	0.48
32:h:174:VAL:HB	32:h:188:HIS:HB2	1.95	0.48
1:2:184:G:H2'	1:2:185:G:H8	1.78	0.48
29:e:50:ILE:HG23	34:E:15:GLY:HA3	1.95	0.48
1:2:29:G:OP1	23:Y:124:LYS:NZ	2.40	0.48
2:B:10:MET:SD	2:B:10:MET:N	2.87	0.48
3:C:134:LEU:HG	3:C:218:LEU:HD12	1.96	0.48
32:h:9:GLY:O	32:h:308:ARG:NH1	2.44	0.48
32:h:32:LEU:HB2	32:h:71:ILE:HD11	1.95	0.48
32:h:244:ASN:OD1	32:h:245:ARG:NH1	2.46	0.48
1:2:1337:C:H2'	1:2:1338:G:H8	1.79	0.47
5:F:141:THR:HB	5:F:145:ARG:H	1.79	0.47
17:R:19:ALA:HB2	17:R:75:GLY:HA3	1.95	0.47
17:R:97:GLN:HG3	17:R:105:LYS:HE3	1.95	0.47
1:2:980:A:H2'	1:2:981:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:90:ILE:HB	5:F:99:PHE:HB2	1.95	0.47
5:F:127:ARG:HB3	5:F:140:VAL:HG23	1.95	0.47
6:G:90:VAL:HA	6:G:93:VAL:HG12	1.96	0.47
9:J:150:ASP:HA	9:J:153:LYS:HB2	1.96	0.47
14:O:14:SER:OG	14:O:15:ALA:N	2.47	0.47
16:Q:44:ARG:NH2	16:Q:82:ASP:O	2.47	0.47
32:h:256:ILE:HB	32:h:270:LEU:HB2	1.96	0.47
34:E:105:LEU:HD22	34:E:184:ILE:HG21	1.95	0.47
1:2:69:C:OP2	7:H:164:LYS:NZ	2.47	0.47
1:2:1113:A:N6	1:2:1121:G:O6	2.48	0.47
1:2:1536:G:H2'	1:2:1537:A:H8	1.79	0.47
2:B:57:LYS:HD2	2:B:159:ILE:HG23	1.96	0.47
2:B:121:LEU:HD11	2:B:145:ILE:HG12	1.96	0.47
4:D:125:LYS:HZ3	4:D:143:CYS:HB2	1.80	0.47
6:G:176:GLU:HA	6:G:179:ASN:HB2	1.95	0.47
11:L:65:ARG:NH2	29:e:21:CYS:O	2.47	0.47
1:2:490:C:O2'	1:2:574:A:N1	2.43	0.47
1:2:1092:G:H2'	1:2:1093:A:H8	1.79	0.47
3:C:57:ILE:HG22	3:C:59:SER:H	1.80	0.47
1:2:1562:C:OP1	19:U:74:SER:N	2.48	0.47
1:2:292:A:O2'	12:M:39:ASN:O	2.33	0.47
1:2:602:G:H3'	1:2:603:C:H2'	1.96	0.47
1:2:1373:C:O2'	35:S:10:LYS:NZ	2.38	0.47
12:M:59:LYS:O	12:M:112:HIS:NE2	2.48	0.47
15:P:30:VAL:HG12	15:P:94:HIS:HB2	1.97	0.47
17:R:90:LYS:NZ	17:R:120:LEU:O	2.43	0.47
26:b:60:ASP:OD1	26:b:60:ASP:N	2.46	0.47
36:z:262:U:O2	36:z:271:G:O6	2.33	0.47
1:2:1528:G:O2'	1:2:1666:C:OP1	2.32	0.47
5:F:154:ILE:HG23	5:F:158:ASP:HB2	1.95	0.47
11:L:84:HIS:HB3	13:N:27:ILE:HG23	1.95	0.47
1:2:934:G:O6	1:2:1008:A:N1	2.47	0.47
2:B:57:LYS:HG3	2:B:161:ILE:HD13	1.97	0.47
26:b:74:CYS:SG	26:b:77:CYS:CB	2.94	0.47
34:E:58:VAL:HA	34:E:65:ARG:HH21	1.78	0.47
1:2:677:G:N1	1:2:1027:A:OP2	2.38	0.47
15:P:138:ASP:N	15:P:138:ASP:OD1	2.48	0.47
28:d:44:ARG:HA	28:d:65:ALA:HB2	1.97	0.47
1:2:1855:G:OP2	15:P:147:ARG:NH2	2.47	0.46
2:B:68:ILE:HD11	2:B:74:VAL:HG23	1.97	0.46
10:K:131:ARG:NH2	10:K:143:ASN:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:25:THR:HG21	34:E:7:LYS:HE2	1.98	0.46
32:h:152:SER:H	32:h:169:GLY:HA2	1.80	0.46
1:2:930:C:H42	1:2:1012:A:H61	1.61	0.46
9:J:88:ASN:OD1	9:J:205:ARG:NH2	2.43	0.46
18:T:21:ASP:OD1	18:T:21:ASP:N	2.46	0.46
1:2:928:G:H2'	1:2:929:G:C8	2.50	0.46
1:2:1120:U:OP1	27:c:72:ARG:NH1	2.49	0.46
1:2:1152:U:O2'	22:X:19:LYS:NZ	2.48	0.46
1:2:1281:G:OP2	13:N:102:LYS:NZ	2.46	0.46
25:a:73:VAL:HG12	25:a:79:ILE:HD11	1.96	0.46
32:h:124:SER:OG	32:h:125:ARG:N	2.48	0.46
1:2:641:A:OP2	30:f:107:ARG:NE	2.48	0.46
4:D:162:ILE:O	21:W:27:LYS:NZ	2.48	0.46
5:F:104:ASP:HB2	5:F:110:ALA:HB2	1.96	0.46
9:J:98:LYS:HD2	9:J:178:ARG:HD2	1.97	0.46
1:2:5:U:H2'	1:2:6:G:H8	1.81	0.46
5:F:11:ARG:HA	5:F:28:ALA:HB2	1.96	0.46
12:M:86:ILE:HG13	12:M:113:LEU:HD13	1.97	0.46
15:P:75:MET:HG2	15:P:118:ALA:HB2	1.98	0.46
15:P:129:ILE:HD12	26:b:44:ILE:HD11	1.97	0.46
18:T:124:ARG:HD2	18:T:129:LEU:HD11	1.98	0.46
1:2:220:U:H2'	1:2:221:A:H8	1.81	0.46
1:2:1301:A:HO2'	29:e:2:GLY:N	2.14	0.46
1:2:1856:C:OP2	15:P:146:ARG:N	2.49	0.46
4:D:244:ILE:HA	4:D:247:THR:HG23	1.98	0.46
1:2:5:U:H2'	1:2:6:G:C8	2.51	0.46
1:2:1444:U:OP1	17:R:15:ARG:NH2	2.48	0.46
32:h:14:HIS:CE1	32:h:35:SER:HG	2.33	0.46
34:E:135:GLU:HB3	34:E:187:LYS:HB3	1.98	0.46
1:2:1264:C:H42	1:2:1518:C:H41	1.63	0.46
1:2:1630:A:OP1	18:T:37:GLY:N	2.46	0.46
19:U:76:THR:HG22	19:U:94:ARG:HB3	1.98	0.46
1:2:45:A:H4'	1:2:46:A:H5'	1.97	0.45
1:2:191:A:OP1	9:J:141:ARG:NH2	2.50	0.45
1:2:1705:C:H2'	1:2:1706:G:H8	1.81	0.45
1:2:1837:G:H5''	1:2:1838:U:H3'	1.97	0.45
32:h:220:ASP:HB2	32:h:227:LEU:HD21	1.97	0.45
34:E:140:GLY:HA3	34:E:182:LEU:HG	1.99	0.45
1:2:1427:C:O2'	1:2:1429:G:OP1	2.32	0.45
1:2:1650:A:N3	1:2:1675:A:N6	2.63	0.45
35:S:31:ASN:HA	35:S:34:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:440:G:O2'	1:2:1737:G:N3	2.48	0.45
23:Y:60:LYS:HD3	23:Y:60:LYS:HA	1.89	0.45
7:H:20:ASP:OD1	7:H:20:ASP:N	2.50	0.45
1:2:981:A:H2'	1:2:982:G:C8	2.51	0.45
15:P:53:ILE:HG23	15:P:88:LEU:HD13	1.99	0.45
19:U:125:PRO:HA	19:U:128:GLN:HG2	1.98	0.45
28:d:40:ARG:NH2	28:d:61:SER:O	2.48	0.45
32:h:218:LEU:HB3	32:h:227:LEU:HD12	1.98	0.45
32:h:289:LEU:HA	32:h:300:ALA:HA	1.99	0.45
1:2:800:U:H3	1:2:866:U:H3	1.63	0.45
2:B:154:LEU:HD22	2:B:157:VAL:HG11	1.98	0.45
10:K:160:SER:HB3	10:K:163:SER:HB2	1.99	0.45
11:L:11:ILE:HA	11:L:14:LEU:HG	1.99	0.45
18:T:68:ILE:HA	18:T:71:MET:HG2	1.99	0.45
1:2:94:G:OP1	5:F:6:LYS:NZ	2.49	0.45
1:2:96:C:H1'	1:2:474:G:H5'	1.98	0.45
1:2:436:G:H2'	1:2:437:G:C8	2.52	0.45
1:2:919:A:H4'	1:2:920:A:H5''	1.99	0.45
7:H:136:LYS:NZ	7:H:175:LYS:O	2.43	0.45
16:Q:54:HIS:HD2	16:Q:57:LEU:HD22	1.82	0.45
1:2:528:A:H2	1:2:558:G:H22	1.65	0.45
1:2:809:A:OP1	5:F:187:ALA:N	2.41	0.45
1:2:1454:A:N7	35:S:3:ARG:NH1	2.65	0.45
19:U:130:ASP:HA	19:U:133:ARG:HD2	1.99	0.45
1:2:453:C:O2'	7:H:92:ARG:O	2.33	0.45
1:2:639:C:H5''	30:f:110:GLN:HG3	1.99	0.45
1:2:1023:A:OP2	14:O:124:ARG:NH2	2.48	0.45
3:C:71:LEU:HD12	3:C:84:PHE:HE2	1.81	0.45
19:U:126:GLN:NE2	19:U:130:ASP:OD2	2.49	0.45
32:h:214:GLY:O	32:h:232:GLY:N	2.50	0.45
34:E:154:ASP:OD1	34:E:154:ASP:N	2.48	0.45
1:2:1392:U:H2'	1:2:1393:G:H8	1.82	0.45
5:F:48:LEU:HD23	5:F:61:VAL:HG23	1.98	0.45
15:P:29:GLY:O	15:P:93:LEU:HA	2.17	0.45
32:h:124:SER:OG	32:h:126:ASP:OD1	2.30	0.45
34:E:31:GLU:OE1	34:E:57:ASN:ND2	2.50	0.45
1:2:1392:U:H2'	1:2:1393:G:C8	2.52	0.44
1:2:1545:A:H2'	1:2:1546:G:C8	2.52	0.44
9:J:141:ARG:HE	9:J:142:SER:H	1.64	0.44
1:2:1308:U:H1'	31:g:133:ALA:HB1	1.99	0.44
1:2:1368:U:O2'	35:S:2:GLY:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:90:LEU:HD22	9:J:95:THR:HG21	1.99	0.44
15:P:128:ARG:HE	26:b:59:PHE:HE2	1.66	0.44
1:2:752:G:O2'	1:2:754:G:OP2	2.33	0.44
1:2:952:G:H1'	15:P:51:GLU:HA	1.99	0.44
1:2:1379:A:H2	2:B:110:ASN:HD21	1.65	0.44
1:2:464:A:H3'	1:2:465:A:H8	1.82	0.44
6:G:153:LEU:HD22	6:G:192:LYS:HZ2	1.83	0.44
8:I:7:LYS:NZ	8:I:40:LEU:O	2.51	0.44
9:J:12:ARG:HE	9:J:18:ARG:HG2	1.83	0.44
13:N:31:LEU:HA	13:N:111:VAL:HA	1.99	0.44
13:N:58:GLU:HB3	13:N:61:TYR:HB3	2.00	0.44
28:d:31:ARG:HA	28:d:43:ILE:HA	1.99	0.44
1:2:1013:U:O2'	1:2:1104:G:O2'	2.32	0.44
1:2:1541:G:H5''	19:U:59:SER:HB3	1.99	0.44
1:2:1753:C:O2'	1:2:1754:G:O5'	2.33	0.44
9:J:131:PRO:HB2	9:J:133:GLU:HG2	1.99	0.44
32:h:9:GLY:HA3	32:h:52:TYR:HB2	2.00	0.44
1:2:557:U:H2'	1:2:558:G:C2	2.52	0.44
1:2:624:C:N4	23:Y:63:ASN:OD1	2.50	0.44
1:2:1341:C:H42	1:2:1486:A:H61	1.65	0.44
16:Q:54:HIS:HA	16:Q:57:LEU:HD13	2.00	0.44
1:2:223:C:H2'	1:2:224:A:C8	2.53	0.44
1:2:571:U:O2'	24:Z:60:PHE:O	2.34	0.44
1:2:1813:A:H3'	1:2:1814:G:H8	1.83	0.44
2:B:68:ILE:HG21	2:B:120:ARG:HG2	1.99	0.44
8:I:86:LYS:HE3	8:I:86:LYS:HB2	1.81	0.44
16:Q:114:HIS:HB3	16:Q:118:GLU:HG3	1.99	0.44
18:T:5:ILE:HG13	25:a:49:LEU:HB2	1.99	0.44
27:c:67:THR:OG1	27:c:70:LYS:O	2.35	0.44
1:2:522:A:H5''	10:K:145:PRO:HD2	2.00	0.44
1:2:1865:C:OP1	26:b:87:ARG:NH2	2.50	0.44
7:H:231:ARG:HD3	7:H:234:LEU:HD21	1.99	0.44
8:I:100:ILE:HG22	8:I:125:VAL:HG21	1.98	0.44
9:J:11:ARG:NH1	9:J:15:GLY:O	2.51	0.44
15:P:74:ALA:HB1	15:P:115:ALA:HB2	2.00	0.44
30:f:108:ARG:O	30:f:112:ASN:ND2	2.50	0.44
1:2:642:U:OP2	10:K:39:ASN:ND2	2.36	0.44
1:2:1466:G:OP2	35:S:5:ARG:NH2	2.51	0.44
6:G:91:ARG:HD3	25:a:103:HIS:CE1	2.52	0.44
8:I:60:ILE:HG23	8:I:90:LYS:HD2	1.99	0.44
1:2:1273:C:N3	1:2:1508:A:N7	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1719:A:N6	1:2:1814:G:O2'	2.40	0.43
10:K:121:LYS:H	10:K:125:HIS:HD2	1.64	0.43
11:L:22:VAL:HG21	34:E:76:ARG:HA	2.00	0.43
19:U:22:LEU:HB3	19:U:28:LEU:HD21	2.00	0.43
19:U:42:HIS:ND1	19:U:93:SER:OG	2.50	0.43
32:h:40:ILE:HG13	32:h:66:VAL:HG11	1.99	0.43
32:h:190:GLY:HA2	34:E:219:PRO:HB2	1.99	0.43
1:2:908:A:H2'	1:2:909:G:C8	2.52	0.43
1:2:1335:G:O6	1:2:1492:U:O4	2.36	0.43
1:2:1647:A:N6	1:2:1676:U:OP2	2.39	0.43
1:2:1846:G:H2'	1:2:1847:G:C8	2.54	0.43
4:D:209:VAL:HG11	4:D:233:LEU:HD11	2.00	0.43
22:X:103:VAL:HG23	22:X:126:LEU:HB2	1.99	0.43
34:E:45:ARG:HD3	34:E:45:ARG:HA	1.80	0.43
3:C:137:LEU:HG	3:C:215:VAL:HG22	2.00	0.43
10:K:170:PRO:HB3	10:K:174:LYS:HD2	1.99	0.43
25:a:50:PHE:HZ	25:a:87:ALA:HB2	1.82	0.43
1:2:28:U:H2'	1:2:29:G:H8	1.84	0.43
1:2:908:A:H2'	1:2:909:G:H8	1.83	0.43
1:2:1545:A:H2	1:2:1671:G:H1'	1.82	0.43
1:2:1562:C:H5''	19:U:71:GLY:HA3	2.01	0.43
2:B:62:ALA:HA	2:B:65:ILE:HG22	2.01	0.43
2:B:137:ALA:HB1	2:B:142:LEU:HD23	2.00	0.43
7:H:64:LYS:HE3	7:H:82:SER:HB3	1.99	0.43
31:g:107:LYS:HB2	31:g:117:LEU:HD11	2.00	0.43
36:z:155:A:OP2	36:z:228:U:O2'	2.34	0.43
1:2:503:C:H3'	1:2:504:G:H8	1.83	0.43
1:2:1015:U:O2'	14:O:55:ARG:NH2	2.49	0.43
1:2:1662:U:O4	1:2:1663:A:N6	2.51	0.43
3:C:76:ASN:OD1	3:C:77:ASP:N	2.51	0.43
22:X:19:LYS:HB2	22:X:19:LYS:HE3	1.77	0.43
32:h:165:ILE:HD11	32:h:177:TRP:HD1	1.83	0.43
32:h:177:TRP:HA	32:h:184:LEU:HA	2.00	0.43
1:2:492:C:H41	1:2:506:G:H3'	1.82	0.43
1:2:613:G:N2	1:2:626:G:OP1	2.47	0.43
1:2:1201:U:O2'	1:2:1358:U:O2'	2.28	0.43
3:C:49:VAL:HG21	3:C:62:LEU:HD13	2.00	0.43
8:I:9:VAL:HB	8:I:44:ASN:HD21	1.83	0.43
16:Q:47:ARG:HG2	16:Q:50:ARG:HH22	1.83	0.43
27:c:21:LYS:HE3	27:c:21:LYS:HB3	1.86	0.43
34:E:9:ARG:HA	34:E:12:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:LEU:HD12	21:W:79:VAL:HG11	2.00	0.43
18:T:63:GLU:OE1	18:T:66:ARG:NE	2.42	0.43
28:d:13:ARG:HB3	28:d:35:MET:HE3	2.01	0.43
29:e:43:PHE:O	29:e:47:ALA:HB2	2.19	0.43
36:z:139:C:H2'	36:z:140:A:H8	1.83	0.43
5:F:93:ASP:OD1	5:F:93:ASP:N	2.52	0.43
12:M:82:MET:HB3	12:M:82:MET:HE2	1.74	0.43
22:X:115:GLU:O	22:X:119:LYS:HB2	2.19	0.43
1:2:1333:U:H2'	1:2:1334:G:H8	1.83	0.43
1:2:1337:C:H2'	1:2:1338:G:C8	2.54	0.43
2:B:61:ALA:HB2	2:B:159:ILE:HG21	2.00	0.43
9:J:13:LYS:HG3	12:M:137:THR:HG21	2.00	0.43
16:Q:34:MET:HB2	16:Q:42:ARG:HG2	2.00	0.43
22:X:11:LEU:HA	22:X:14:ILE:HG22	2.00	0.43
31:g:133:ALA:N	31:g:140:TYR:O	2.46	0.43
1:2:317:C:H2'	1:2:318:A:C8	2.53	0.43
1:2:1287:A:OP1	31:g:97:LYS:NZ	2.49	0.43
10:K:21:GLU:OE2	10:K:25:LEU:N	2.44	0.43
21:W:34:MET:HB3	21:W:34:MET:HE2	1.77	0.43
22:X:36:ARG:HA	22:X:36:ARG:HD3	1.89	0.43
1:2:212:C:H2'	1:2:213:G:H8	1.84	0.42
1:2:988:C:O2'	3:C:118:GLN:O	2.33	0.42
8:I:78:ARG:HB2	8:I:81:ARG:HH21	1.84	0.42
11:L:3:MET:HE3	11:L:4:PRO:HD2	2.01	0.42
31:g:89:LYS:HE2	31:g:89:LYS:HB3	1.78	0.42
1:2:71:G:O6	7:H:170:ARG:NH1	2.50	0.42
1:2:562:U:O4	10:K:172:ARG:NH2	2.52	0.42
1:2:1330:G:N2	1:2:1335:G:O6	2.52	0.42
1:2:1566:G:OP2	19:U:102:ARG:NH2	2.53	0.42
9:J:69:SER:HB2	12:M:21:LYS:HG2	2.01	0.42
11:L:64:TRP:CE2	29:e:23:VAL:HG23	2.54	0.42
14:O:26:LEU:HD23	14:O:28:LEU:H	1.83	0.42
22:X:36:ARG:HG3	22:X:110:ILE:HD13	2.01	0.42
24:Z:20:ARG:NH2	24:Z:22:GLN:OE1	2.52	0.42
32:h:11:LEU:HB2	32:h:307:VAL:HB	2.00	0.42
1:2:91:A:N6	7:H:89:THR:OG1	2.52	0.42
1:2:168:C:O2'	7:H:133:LEU:O	2.37	0.42
1:2:600:G:H2'	1:2:601:G:C8	2.53	0.42
8:I:58:LYS:HD2	8:I:90:LYS:HE2	2.01	0.42
1:2:183:G:O2'	1:2:184:G:O4'	2.34	0.42
1:2:1010:G:H2'	1:2:1011:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1456:G:OP1	35:S:59:LYS:NZ	2.39	0.42
15:P:95:ILE:HG12	15:P:129:ILE:HG22	2.02	0.42
32:h:290:ALA:O	32:h:299:PHE:N	2.53	0.42
34:E:179:GLN:HE21	34:E:182:LEU:HD11	1.84	0.42
1:2:452:G:O2'	7:H:91:GLU:OE1	2.37	0.42
1:2:664:A:O2'	1:2:670:A:N1	2.50	0.42
1:2:1472:C:O3'	32:h:15:ASN:ND2	2.49	0.42
1:2:220:U:H2'	1:2:221:A:C8	2.54	0.42
1:2:1404:U:OP1	20:V:21:ARG:NH2	2.45	0.42
5:F:33:THR:O	5:F:33:THR:OG1	2.37	0.42
5:F:182:MET:HB2	5:F:192:ILE:HD13	2.01	0.42
19:U:75:MET:HA	19:U:78:ILE:HG12	2.02	0.42
31:g:100:LEU:HD13	31:g:103:LEU:HD22	2.01	0.42
32:h:43:TRP:HA	32:h:55:PRO:HA	2.02	0.42
35:S:59:LYS:HB2	35:S:59:LYS:HE2	1.87	0.42
1:2:414:A:H2'	1:2:415:A:H8	1.84	0.42
1:2:913:A:N6	8:I:119:SER:O	2.51	0.42
14:O:76:LYS:HB3	14:O:76:LYS:HE2	1.87	0.42
16:Q:62:LYS:HD3	16:Q:65:LYS:HD3	2.00	0.42
32:h:25:PRO:HA	32:h:293:ALA:HB1	2.01	0.42
32:h:88:ARG:HD2	32:h:97:THR:HG21	2.00	0.42
34:E:136:VAL:HG12	34:E:186:VAL:HG12	2.01	0.42
1:2:28:U:H2'	1:2:29:G:C8	2.54	0.42
1:2:223:C:H2'	1:2:224:A:H8	1.84	0.42
1:2:616:A:H62	1:2:625:G:H21	1.67	0.42
1:2:686:U:OP1	22:X:32:LYS:N	2.52	0.42
1:2:1353:A:H5''	1:2:1354:G:C8	2.54	0.42
1:2:1647:A:N6	1:2:1677:U:O4	2.50	0.42
2:B:36:GLN:O	2:B:53:ARG:NH1	2.52	0.42
3:C:75:GLN:HG3	3:C:189:ILE:HD11	2.02	0.42
4:D:163:VAL:HG21	4:D:245:SER:HB2	2.02	0.42
21:W:62:MET:HB2	21:W:62:MET:HE2	1.77	0.42
30:f:101:ARG:HG3	30:f:105:ALA:H	1.84	0.42
3:C:146:ARG:HB2	3:C:149:GLN:HG3	2.01	0.42
3:C:179:ASN:OD1	3:C:179:ASN:N	2.52	0.42
7:H:27:PHE:HA	7:H:30:LYS:HE2	2.02	0.42
8:I:117:PRO:HG2	8:I:120:ARG:HD3	2.02	0.42
16:Q:17:TYR:HB2	16:Q:25:LEU:HD11	2.02	0.42
17:R:33:LYS:HA	17:R:38:PRO:HA	2.02	0.42
1:2:126:G:OP2	7:H:195:LYS:NZ	2.39	0.42
1:2:406:U:H2'	1:2:408:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:616:A:OP1	23:Y:68:LYS:NZ	2.53	0.42
1:2:1301:A:O2'	29:e:2:GLY:N	2.53	0.42
1:2:1550:G:O2'	1:2:1558:C:O2	2.30	0.42
32:h:36:ARG:HD2	32:h:36:ARG:HA	1.89	0.42
1:2:1144:A:H2'	1:2:1145:A:C8	2.55	0.41
3:C:25:PHE:HA	3:C:28:LYS:HD3	2.01	0.41
27:c:77:CYS:SG	27:c:78:SER:N	2.93	0.41
1:2:819:G:OP2	10:K:80:ARG:NH2	2.53	0.41
1:2:975:G:N2	15:P:50:LYS:O	2.51	0.41
1:2:1722:G:O6	1:2:1812:U:O2	2.38	0.41
2:B:85:ARG:HD2	2:B:204:TYR:HA	2.01	0.41
2:B:180:ARG:O	2:B:184:ARG:HG2	2.20	0.41
5:F:100:ARG:HH21	5:F:236:ILE:HG22	1.85	0.41
10:K:133:ARG:HB3	10:K:143:ASN:HD22	1.85	0.41
16:Q:30:TYR:HA	16:Q:33:LEU:HB3	2.01	0.41
36:z:258:G:N2	36:z:274:A:OP2	2.53	0.41
1:2:564:A:H3'	1:2:565:G:H8	1.85	0.41
1:2:1168:G:N2	1:2:1192:U:O2	2.53	0.41
1:2:1190:A:O2'	1:2:1714:U:O2'	2.29	0.41
1:2:1321:G:H2'	1:2:1322:G:C8	2.55	0.41
1:2:1345:G:N7	1:2:1371:U:O2'	2.40	0.41
1:2:1391:C:O2'	20:V:83:ARG:NH2	2.38	0.41
17:R:131:LYS:HD3	17:R:131:LYS:HA	1.76	0.41
34:E:44:THR:O	34:E:45:ARG:NH1	2.52	0.41
1:2:318:A:C2	1:2:333:G:C2	3.09	0.41
3:C:194:GLY:O	3:C:198:GLU:HB2	2.20	0.41
5:F:106:LYS:HE2	5:F:106:LYS:HB2	1.95	0.41
11:L:32:HIS:HB3	11:L:40:VAL:HG13	2.01	0.41
1:2:1361:G:H2'	1:2:1362:U:C4	2.55	0.41
1:2:1705:C:H2'	1:2:1706:G:C8	2.56	0.41
1:2:1054:G:H2'	1:2:1055:A:C8	2.55	0.41
32:h:20:GLN:O	32:h:33:SER:HA	2.21	0.41
1:2:1341:C:N4	1:2:1486:A:H61	2.19	0.41
1:2:1669:G:O2'	20:V:62:ARG:NH1	2.52	0.41
14:O:139:TRP:HE1	14:O:149:LEU:HD22	1.86	0.41
16:Q:79:HIS:HA	16:Q:97:TYR:HB2	2.02	0.41
24:Z:103:SER:OG	24:Z:106:GLN:OE1	2.33	0.41
27:c:16:LYS:HE2	27:c:16:LYS:HB2	1.94	0.41
1:2:57:U:O2'	1:2:499:G:N2	2.43	0.41
1:2:141:A:N6	1:2:177:G:H21	2.18	0.41
1:2:201:C:H3'	1:2:202:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:528:A:H2'	1:2:529:A:C8	2.56	0.41
1:2:1064:C:H2'	1:2:1065:G:H8	1.85	0.41
1:2:1478:U:H2'	1:2:1479:G:H8	1.85	0.41
1:2:1786:U:H2'	1:2:1787:G:C8	2.53	0.41
4:D:184:VAL:HG11	4:D:247:THR:HA	2.03	0.41
16:Q:68:PRO:HG3	16:Q:73:PRO:HB3	2.03	0.41
17:R:130:LYS:NZ	17:R:134:GLY:O	2.42	0.41
20:V:56:MET:SD	20:V:57:PRO:HD2	2.61	0.41
23:Y:88:ASP:OD1	23:Y:88:ASP:N	2.48	0.41
36:z:252:A:O2'	36:z:284:U:OP2	2.38	0.41
1:2:10:G:H1	1:2:1202:U:H3	1.69	0.41
1:2:165:G:OP2	1:2:165:G:N2	2.54	0.41
1:2:429:C:OP1	5:F:10:LYS:NZ	2.41	0.41
1:2:476:A:N3	1:2:488:U:O2'	2.42	0.41
1:2:498:C:H42	1:2:504:G:H1	1.69	0.41
1:2:602:G:OP2	1:2:603:C:O2'	2.34	0.41
1:2:951:C:H2'	1:2:952:G:C8	2.56	0.41
1:2:1050:A:OP1	1:2:1846:G:N2	2.54	0.41
1:2:1506:A:N1	1:2:1508:A:N6	2.68	0.41
2:B:104:THR:HA	2:B:105:PRO:HD3	1.88	0.41
6:G:14:THR:N	17:R:56:LEU:O	2.53	0.41
8:I:40:LEU:HD23	8:I:43:LEU:HD22	2.02	0.41
8:I:143:ARG:O	8:I:155:LYS:N	2.44	0.41
12:M:113:LEU:HD12	12:M:142:VAL:HG11	2.02	0.41
16:Q:37:TYR:CE2	16:Q:41:GLN:HG2	2.56	0.41
18:T:43:VAL:HG13	19:U:36:THR:HG22	2.02	0.41
1:2:63:U:O2'	1:2:170:A:N3	2.46	0.41
1:2:346:C:HO2'	5:F:30:ARG:HH21	1.65	0.41
1:2:1595:U:H5	25:a:104:ARG:HH12	1.68	0.41
1:2:1665:G:C8	19:U:88:MET:HE1	2.56	0.41
6:G:128:ILE:HD13	28:d:68:LEU:HA	2.03	0.41
10:K:18:ARG:O	10:K:24:ARG:NH2	2.54	0.41
14:O:34:LYS:HE3	14:O:34:LYS:HB2	1.86	0.41
23:Y:124:LYS:HE2	23:Y:124:LYS:HB3	1.91	0.41
32:h:126:ASP:OD1	32:h:126:ASP:N	2.49	0.41
36:z:166:C:P	36:z:229:G:H21	2.44	0.41
1:2:1494:U:H4'	1:2:1495:G:H5''	2.02	0.40
4:D:166:ARG:HH12	4:D:252:THR:HG21	1.86	0.40
9:J:60:LEU:HD23	9:J:60:LEU:HA	1.91	0.40
32:h:241:PHE:HE1	32:h:248:LEU:HD13	1.87	0.40
1:2:373:G:H2'	1:2:374:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:ARG:HB3	15:P:48:SER:HB2	2.03	0.40
22:X:103:VAL:HA	22:X:112:ASP:HA	2.04	0.40
26:b:11:ALA:HB3	26:b:33:ASP:HB2	2.02	0.40
1:2:212:C:H2'	1:2:213:G:C8	2.56	0.40
1:2:753:C:O2'	1:2:754:G:O4'	2.40	0.40
1:2:958:G:H3'	1:2:959:G:H8	1.85	0.40
1:2:1198:G:H2'	1:2:1199:A:C8	2.56	0.40
1:2:1413:G:H2'	1:2:1414:A:H8	1.87	0.40
1:2:1513:C:H2'	1:2:1514:G:C8	2.56	0.40
17:R:17:LYS:HE2	17:R:17:LYS:HB3	1.79	0.40
1:2:498:C:H2'	1:2:499:G:C8	2.55	0.40
1:2:1284:A:O4'	1:2:1313:A:N6	2.55	0.40
1:2:1618:C:C4	29:e:11:PRO:HD2	2.56	0.40
9:J:48:VAL:HG11	9:J:54:LYS:HD3	2.02	0.40
11:L:47:LYS:HA	11:L:47:LYS:HD3	1.79	0.40
16:Q:92:SER:OG	16:Q:93:MET:N	2.52	0.40
23:Y:17:ARG:HG3	23:Y:21:LYS:NZ	2.37	0.40
30:f:91:LYS:HE2	30:f:91:LYS:HB3	1.93	0.40
1:2:1576:G:H2'	1:2:1577:G:C8	2.56	0.40
1:2:1808:U:H2'	1:2:1809:A:C8	2.57	0.40
9:J:177:SER:OG	9:J:186:ASP:N	2.55	0.40
12:M:113:LEU:HG	12:M:142:VAL:HG21	2.04	0.40
17:R:8:GLN:HG3	17:R:99:TYR:CZ	2.56	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	B	215/295 (73%)	200 (93%)	15 (7%)	0	100	100
3	C	211/264 (80%)	201 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
5	F	260/263 (99%)	243 (94%)	17 (6%)	0	100	100
6	G	189/204 (93%)	176 (93%)	13 (7%)	0	100	100
7	H	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
8	I	181/432 (42%)	173 (96%)	8 (4%)	0	100	100
9	J	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
10	K	183/194 (94%)	178 (97%)	5 (3%)	0	100	100
11	L	94/149 (63%)	86 (92%)	8 (8%)	0	100	100
12	M	149/158 (94%)	136 (91%)	13 (9%)	0	100	100
13	N	115/132 (87%)	108 (94%)	7 (6%)	0	100	100
14	O	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
15	P	134/168 (80%)	129 (96%)	5 (4%)	0	100	100
16	Q	113/145 (78%)	104 (92%)	9 (8%)	0	100	100
17	R	140/172 (81%)	134 (96%)	6 (4%)	0	100	100
18	T	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
19	U	139/145 (96%)	131 (94%)	8 (6%)	0	100	100
20	V	98/119 (82%)	95 (97%)	3 (3%)	0	100	100
21	W	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
22	X	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
23	Y	139/143 (97%)	131 (94%)	8 (6%)	0	100	100
24	Z	122/131 (93%)	120 (98%)	2 (2%)	0	100	100
25	a	75/124 (60%)	71 (95%)	4 (5%)	0	100	100
26	b	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
27	c	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
28	d	65/69 (94%)	60 (92%)	5 (8%)	0	100	100
29	e	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
30	f	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
31	g	66/188 (35%)	58 (88%)	8 (12%)	0	100	100
32	h	311/317 (98%)	296 (95%)	15 (5%)	0	100	100
33	n	23/25 (92%)	23 (100%)	0	0	100	100
34	E	226/281 (80%)	218 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	S	130/135 (96%)	121 (93%)	9 (7%)	0	100	100
All	All	4821/5821 (83%)	4575 (95%)	246 (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	B	180/245 (74%)	179 (99%)	1 (1%)	78	80
3	C	194/231 (84%)	194 (100%)	0	100	100
4	D	187/187 (100%)	187 (100%)	0	100	100
5	F	224/225 (100%)	224 (100%)	0	100	100
6	G	161/170 (95%)	161 (100%)	0	100	100
7	H	207/218 (95%)	207 (100%)	0	100	100
8	I	165/360 (46%)	165 (100%)	0	100	100
9	J	178/180 (99%)	178 (100%)	0	100	100
10	K	161/168 (96%)	161 (100%)	0	100	100
11	L	87/125 (70%)	87 (100%)	0	100	100
12	M	136/142 (96%)	136 (100%)	0	100	100
13	N	99/108 (92%)	99 (100%)	0	100	100
14	O	130/131 (99%)	130 (100%)	0	100	100
15	P	106/130 (82%)	106 (100%)	0	100	100
16	Q	105/130 (81%)	105 (100%)	0	100	100
17	R	117/140 (84%)	116 (99%)	1 (1%)	70	76
18	T	125/132 (95%)	125 (100%)	0	100	100
19	U	111/116 (96%)	111 (100%)	0	100	100
20	V	92/107 (86%)	92 (100%)	0	100	100
21	W	67/67 (100%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	X	112/113 (99%)	112 (100%)	0	100	100
23	Y	113/115 (98%)	113 (100%)	0	100	100
24	Z	107/113 (95%)	107 (100%)	0	100	100
25	a	68/102 (67%)	68 (100%)	0	100	100
26	b	88/88 (100%)	88 (100%)	0	100	100
27	c	75/76 (99%)	75 (100%)	0	100	100
28	d	60/62 (97%)	60 (100%)	0	100	100
29	e	48/49 (98%)	48 (100%)	0	100	100
30	f	47/106 (44%)	47 (100%)	0	100	100
31	g	61/154 (40%)	61 (100%)	0	100	100
32	h	272/275 (99%)	272 (100%)	0	100	100
33	n	24/24 (100%)	24 (100%)	0	100	100
34	E	190/232 (82%)	190 (100%)	0	100	100
35	S	119/121 (98%)	119 (100%)	0	100	100
All	All	4216/4942 (85%)	4214 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	111	GLN
17	R	86	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	111	GLN
2	B	113	GLN
3	C	202	GLN
5	F	157	ASN
6	G	79	HIS
9	J	116	HIS
9	J	181	GLN
10	K	75	ASN
12	M	19	ASN
12	M	100	ASN
13	N	55	ASN

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Mol	Chain	Res	Type
16	Q	24	GLN
16	Q	54	HIS
18	T	17	ASN
18	T	72	GLN
18	T	101	ASN
19	U	63	HIS
19	U	83	GLN
19	U	85	ASN
19	U	128	GLN
20	V	81	GLN
22	X	70	ASN
23	Y	26	GLN
23	Y	46	HIS
24	Z	94	HIS
26	b	25	ASN
29	e	41	GLN
30	f	88	GLN
30	f	112	ASN
31	g	91	ASN
32	h	143	GLN
32	h	178	ASN
32	h	188	HIS
32	h	215	GLN
32	h	237	ASN
34	E	74	GLN
34	E	101	GLN
35	S	31	ASN
35	S	127	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1870 (90%)	423 (25%)	11 (0%)
36	z	164/400 (41%)	48 (29%)	0
All	All	1849/2270 (81%)	471 (25%)	11 (0%)

All (471) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C

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Mol	Chain	Res	Type
1	2	9	U
1	2	11	A
1	2	25	A
1	2	33	G
1	2	37	C
1	2	39	A
1	2	41	G
1	2	42	A
1	2	44	U
1	2	45	A
1	2	46	A
1	2	55	U
1	2	56	G
1	2	61	A
1	2	62	G
1	2	67	C
1	2	68	A
1	2	73	C
1	2	74	G
1	2	75	G
1	2	77	A
1	2	82	G
1	2	92	A
1	2	102	A
1	2	103	A
1	2	110	U
1	2	113	G
1	2	114	G
1	2	115	U
1	2	116	U
1	2	126	G
1	2	127	C
1	2	130	G
1	2	142	C
1	2	143	U
1	2	144	U
1	2	147	A
1	2	155	G
1	2	156	G
1	2	162	C
1	2	163	U
1	2	170	A

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Mol	Chain	Res	Type
1	2	171	A
1	2	180	G
1	2	182	C
1	2	183	G
1	2	184	G
1	2	186	C
1	2	192	C
1	2	200	G
1	2	211	G
1	2	218	U
1	2	219	U
1	2	291	G
1	2	294	U
1	2	303	C
1	2	305	U
1	2	306	C
1	2	307	G
1	2	309	G
1	2	312	G
1	2	319	C
1	2	330	G
1	2	332	G
1	2	341	C
1	2	347	G
1	2	351	G
1	2	362	C
1	2	364	A
1	2	368	U
1	2	370	G
1	2	377	G
1	2	381	C
1	2	383	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	393	U
1	2	398	A
1	2	400	C
1	2	401	A
1	2	407	G
1	2	408	A
1	2	409	C

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Mol	Chain	Res	Type
1	2	418	A
1	2	420	G
1	2	426	A
1	2	435	A
1	2	439	A
1	2	445	A
1	2	446	G
1	2	448	A
1	2	449	A
1	2	450	C
1	2	452	G
1	2	465	A
1	2	470	G
1	2	471	G
1	2	472	C
1	2	474	G
1	2	487	U
1	2	488	U
1	2	489	A
1	2	492	C
1	2	496	C
1	2	500	A
1	2	502	C
1	2	503	C
1	2	508	A
1	2	509	G
1	2	512	A
1	2	517	C
1	2	525	A
1	2	531	A
1	2	532	C
1	2	533	A
1	2	537	C
1	2	541	U
1	2	544	G
1	2	547	G
1	2	550	C
1	2	551	U
1	2	554	A
1	2	555	A
1	2	556	U
1	2	558	G

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Mol	Chain	Res	Type
1	2	560	A
1	2	561	A
1	2	562	U
1	2	568	C
1	2	569	A
1	2	574	A
1	2	576	A
1	2	583	A
1	2	585	C
1	2	588	G
1	2	590	A
1	2	591	U
1	2	595	U
1	2	596	U
1	2	600	G
1	2	603	C
1	2	604	A
1	2	607	U
1	2	608	C
1	2	613	G
1	2	614	C
1	2	617	G
1	2	623	G
1	2	625	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	631	U
1	2	642	U
1	2	643	A
1	2	649	U
1	2	650	A
1	2	655	A
1	2	658	U
1	2	660	C
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	687	C
1	2	688	U

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Mol	Chain	Res	Type
1	2	689	U
1	2	751	G
1	2	752	G
1	2	753	C
1	2	754	G
1	2	755	C
1	2	789	G
1	2	794	A
1	2	799	U
1	2	800	U
1	2	810	A
1	2	811	A
1	2	816	A
1	2	822	U
1	2	829	C
1	2	830	A
1	2	834	C
1	2	844	U
1	2	847	A
1	2	852	G
1	2	853	C
1	2	864	A
1	2	867	G
1	2	870	A
1	2	872	A
1	2	873	G
1	2	875	A
1	2	887	U
1	2	888	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	901	G
1	2	913	A
1	2	914	U
1	2	917	U
1	2	920	A
1	2	921	G
1	2	933	G
1	2	954	U
1	2	956	G

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Mol	Chain	Res	Type
1	2	961	G
1	2	962	A
1	2	963	A
1	2	969	U
1	2	970	G
1	2	971	G
1	2	978	G
1	2	985	G
1	2	988	C
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1002	U
1	2	1012	A
1	2	1016	U
1	2	1017	U
1	2	1023	A
1	2	1026	C
1	2	1041	G
1	2	1044	G
1	2	1045	U
1	2	1054	G
1	2	1055	A
1	2	1062	A
1	2	1076	G
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1087	A
1	2	1088	U
1	2	1089	G
1	2	1111	U
1	2	1114	U
1	2	1121	G
1	2	1133	A
1	2	1138	C
1	2	1139	C
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1155	U

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Mol	Chain	Res	Type
1	2	1157	G
1	2	1165	G
1	2	1166	G
1	2	1170	A
1	2	1180	C
1	2	1194	A
1	2	1200	A
1	2	1203	U
1	2	1204	G
1	2	1205	G
1	2	1206	C
1	2	1207	G
1	2	1208	A
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1242	U
1	2	1249	C
1	2	1250	A
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1261	C
1	2	1264	C
1	2	1272	C
1	2	1274	G
1	2	1275	G
1	2	1276	A
1	2	1280	G
1	2	1285	G
1	2	1286	G
1	2	1293	A
1	2	1294	G
1	2	1295	A
1	2	1301	A
1	2	1302	G
1	2	1306	U
1	2	1307	U
1	2	1308	U

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Mol	Chain	Res	Type
1	2	1310	U
1	2	1311	C
1	2	1327	G
1	2	1332	A
1	2	1333	U
1	2	1341	C
1	2	1342	U
1	2	1344	A
1	2	1345	G
1	2	1351	G
1	2	1352	G
1	2	1353	A
1	2	1354	G
1	2	1355	C
1	2	1361	G
1	2	1362	U
1	2	1363	C
1	2	1371	U
1	2	1372	U
1	2	1377	U
1	2	1378	A
1	2	1396	A
1	2	1397	U
1	2	1402	A
1	2	1404	U
1	2	1428	G
1	2	1429	G
1	2	1441	U
1	2	1442	U
1	2	1452	A
1	2	1454	A
1	2	1458	G
1	2	1462	U
1	2	1463	U
1	2	1466	G
1	2	1467	C
1	2	1468	C
1	2	1473	G
1	2	1474	A
1	2	1475	G
1	2	1477	U
1	2	1480	A

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Mol	Chain	Res	Type
1	2	1484	A
1	2	1489	A
1	2	1490	G
1	2	1507	G
1	2	1508	A
1	2	1509	U
1	2	1519	U
1	2	1522	A
1	2	1531	A
1	2	1533	A
1	2	1540	G
1	2	1548	G
1	2	1551	U
1	2	1552	G
1	2	1553	C
1	2	1554	C
1	2	1556	A
1	2	1560	U
1	2	1567	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	1603	G
1	2	1604	G
1	2	1606	G
1	2	1610	G
1	2	1619	A
1	2	1621	U
1	2	1623	A
1	2	1637	A
1	2	1638	G
1	2	1646	C
1	2	1648	G
1	2	1654	G
1	2	1659	U
1	2	1660	C
1	2	1665	G
1	2	1672	U
1	2	1677	U

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Mol	Chain	Res	Type
1	2	1678	A
1	2	1679	A
1	2	1680	G
1	2	1683	C
1	2	1695	A
1	2	1698	C
1	2	1700	C
1	2	1701	C
1	2	1715	A
1	2	1721	U
1	2	1722	G
1	2	1744	G
1	2	1750	C
1	2	1754	G
1	2	1756	C
1	2	1758	G
1	2	1773	C
1	2	1776	G
1	2	1777	G
1	2	1779	G
1	2	1781	A
1	2	1782	G
1	2	1783	C
1	2	1799	G
1	2	1819	A
1	2	1822	A
1	2	1824	A
1	2	1831	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1845	A
1	2	1849	G
1	2	1852	C
1	2	1853	C
1	2	1860	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
1	2	1866	A
1	2	1868	U

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Mol	Chain	Res	Type
1	2	1869	A
36	z	122	C
36	z	125	C
36	z	145	G
36	z	154	A
36	z	157	C
36	z	161	G
36	z	162	A
36	z	163	G
36	z	164	U
36	z	169	C
36	z	172	A
36	z	227	U
36	z	229	G
36	z	234	U
36	z	237	C
36	z	244	A
36	z	248	U
36	z	250	C
36	z	252	A
36	z	253	G
36	z	258	G
36	z	259	U
36	z	266	G
36	z	269	U
36	z	270	C
36	z	274	A
36	z	275	A
36	z	282	U
36	z	283	G
36	z	284	U
36	z	285	G
36	z	288	A
36	z	290	U
36	z	295	G
36	z	296	A
36	z	297	U
36	z	303	G
36	z	306	U
36	z	307	G
36	z	312	U
36	z	324	U

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Mol	Chain	Res	Type
36	z	325	C
36	z	326	U
36	z	330	A
36	z	331	G
36	z	332	A
36	z	333	C
36	z	334	C

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	383	G
1	2	445	A
1	2	561	A
1	2	688	U
1	2	752	G
1	2	798	G
1	2	1110	G
1	2	1137	U
1	2	1361	G
1	2	1664	A
1	2	1753	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

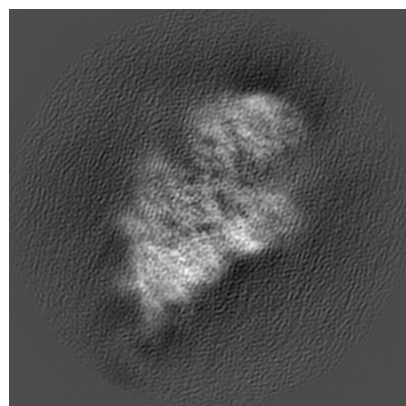
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25535. These allow visual inspection of the internal detail of the map and identification of artifacts.

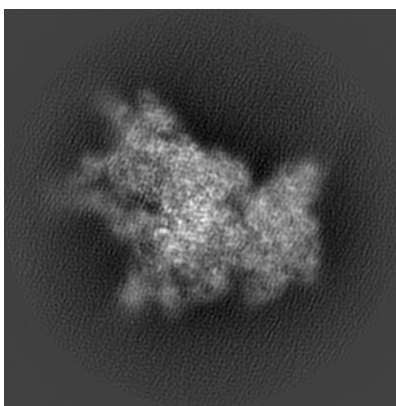
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

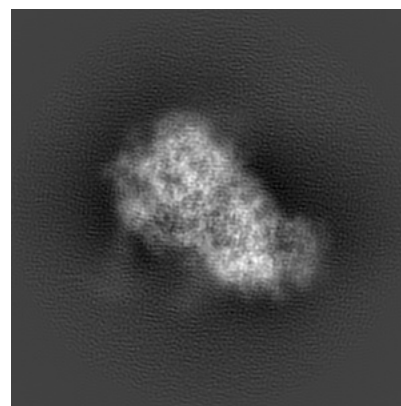
6.1.1 Primary map



X

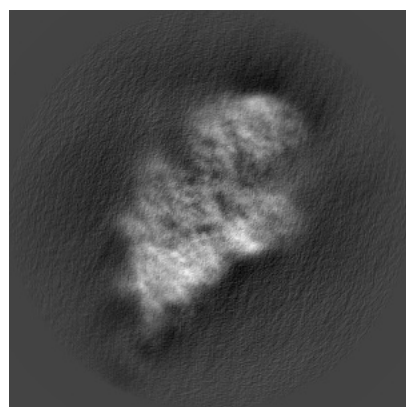


Y

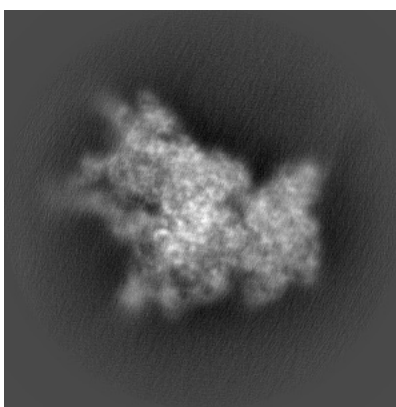


Z

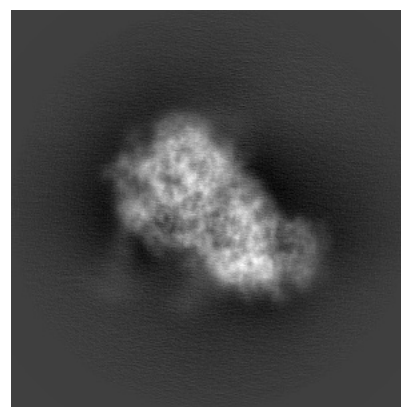
6.1.2 Raw map



X



Y

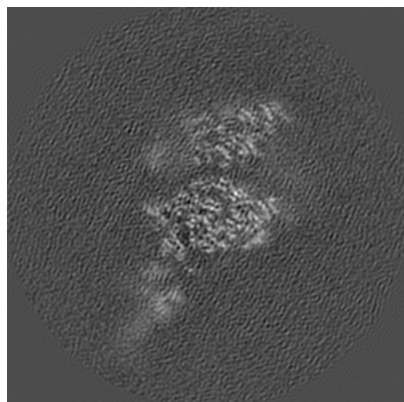


Z

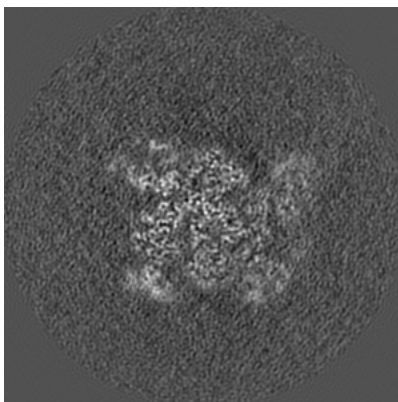
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

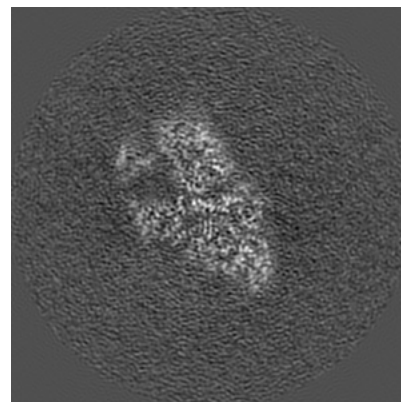
6.2.1 Primary map



X Index: 200

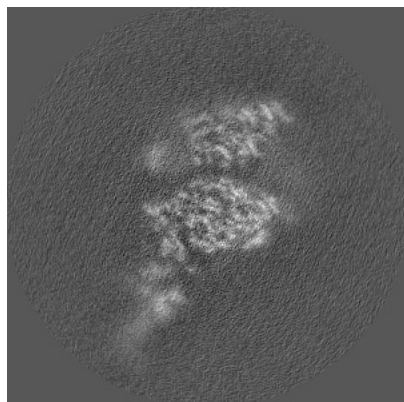


Y Index: 200

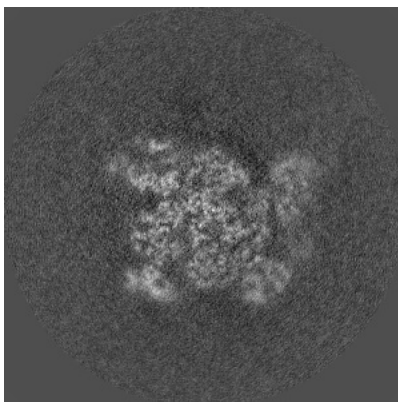


Z Index: 200

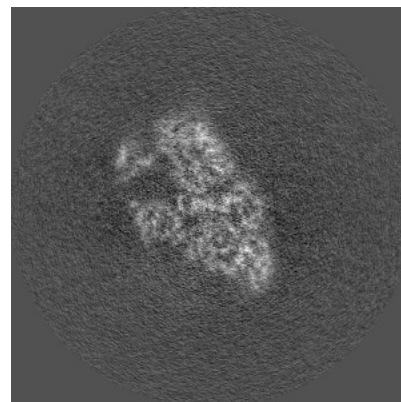
6.2.2 Raw map



X Index: 200



Y Index: 200

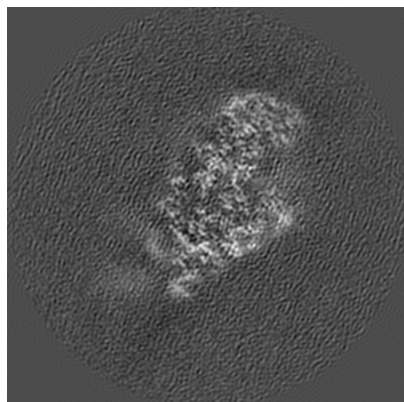


Z Index: 200

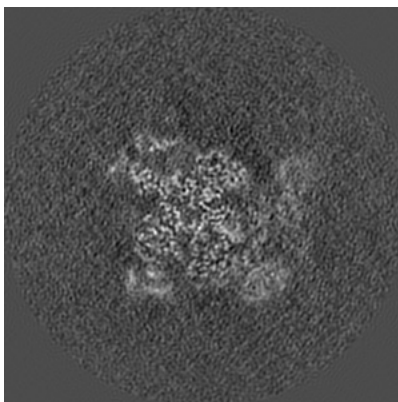
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

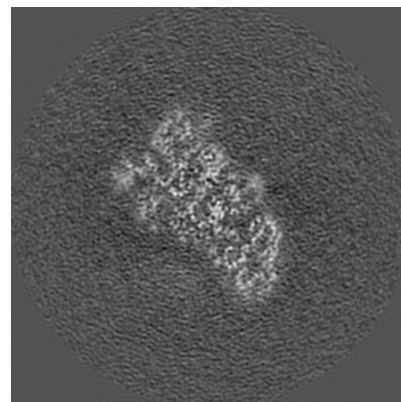
6.3.1 Primary map



X Index: 177

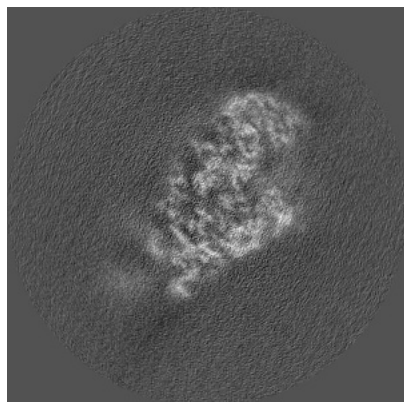


Y Index: 196

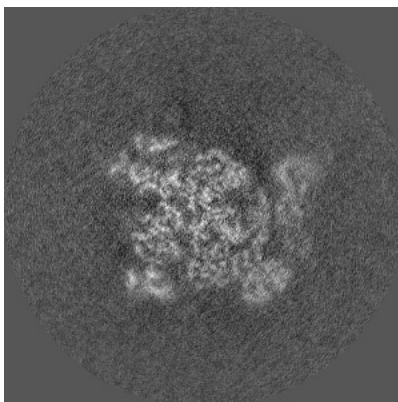


Z Index: 187

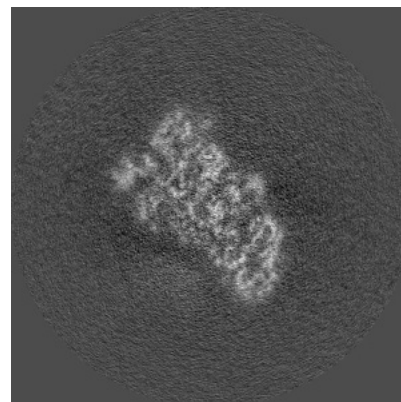
6.3.2 Raw map



X Index: 176



Y Index: 197

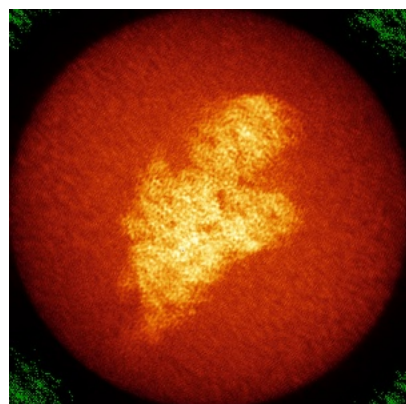


Z Index: 187

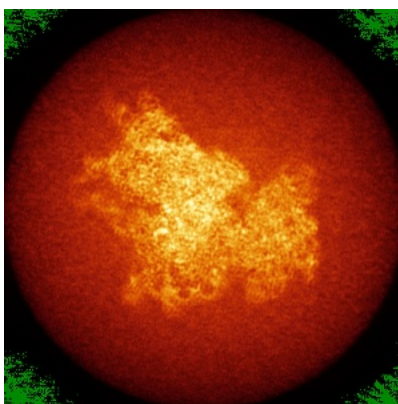
The images above show the largest variance slices of the map in three orthogonal directions.

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

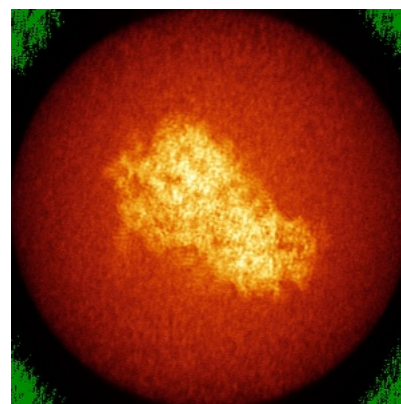
6.4.1 Primary map



X

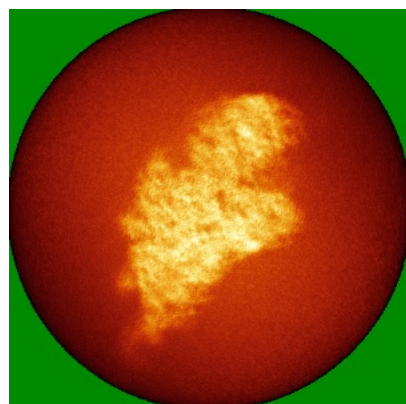


Y

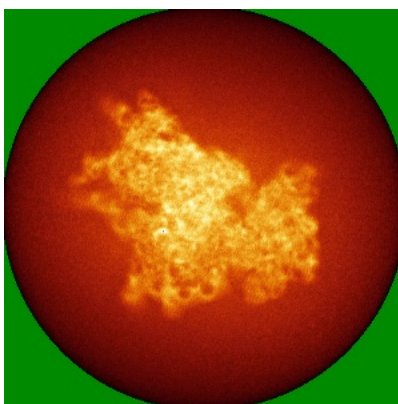


Z

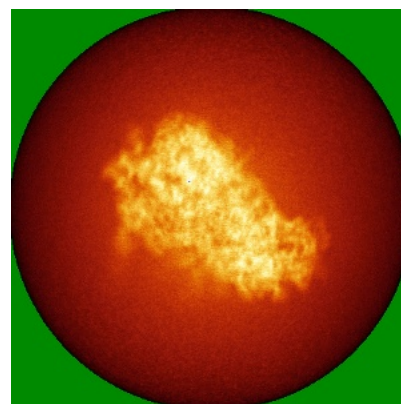
6.4.2 Raw map



X



Y

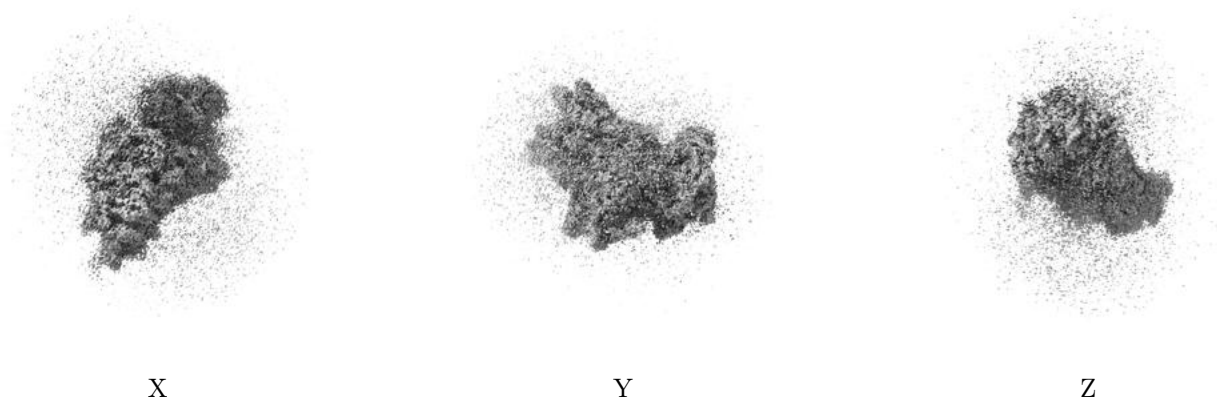


Z

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.

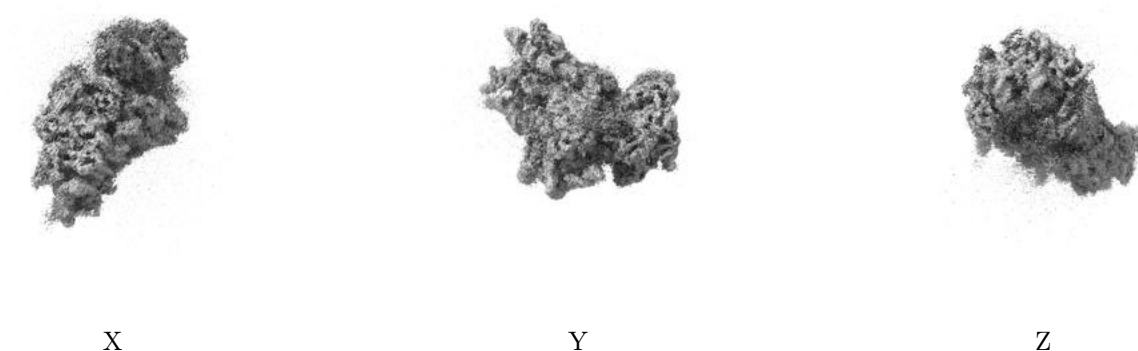
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

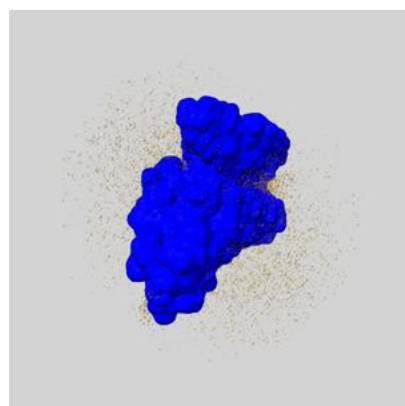
6.6 Mask visualisation [i](#)

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

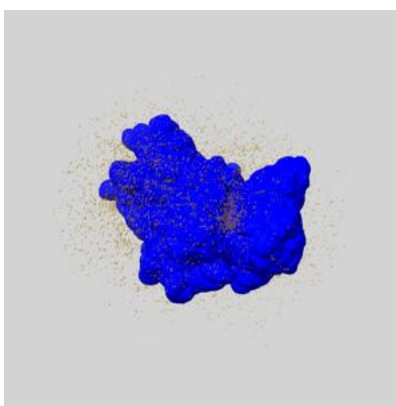
A mask typically either:

- 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_25535_msk_1.map [i](#)



X



Y

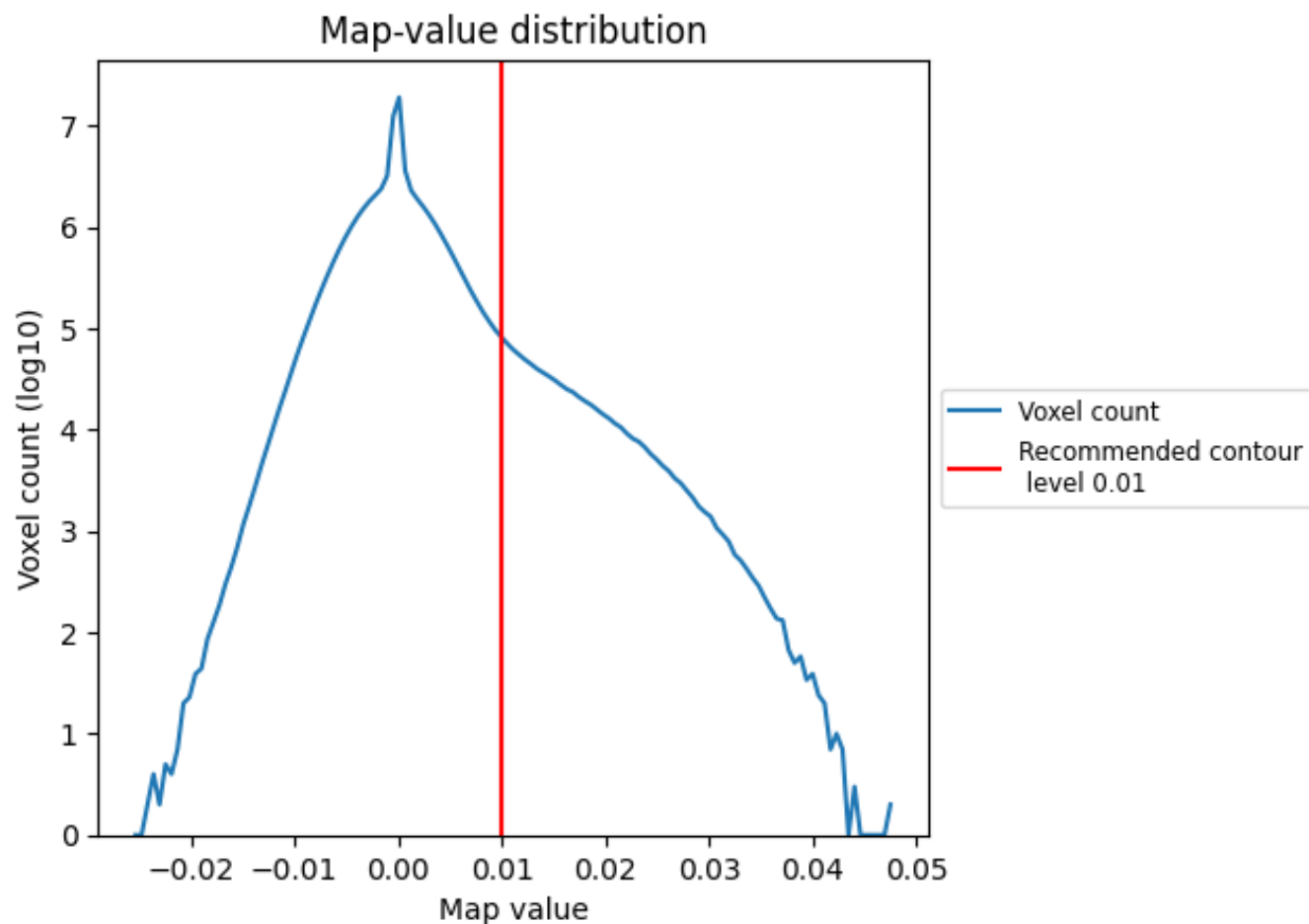


Z

7 Map analysis [i](#)

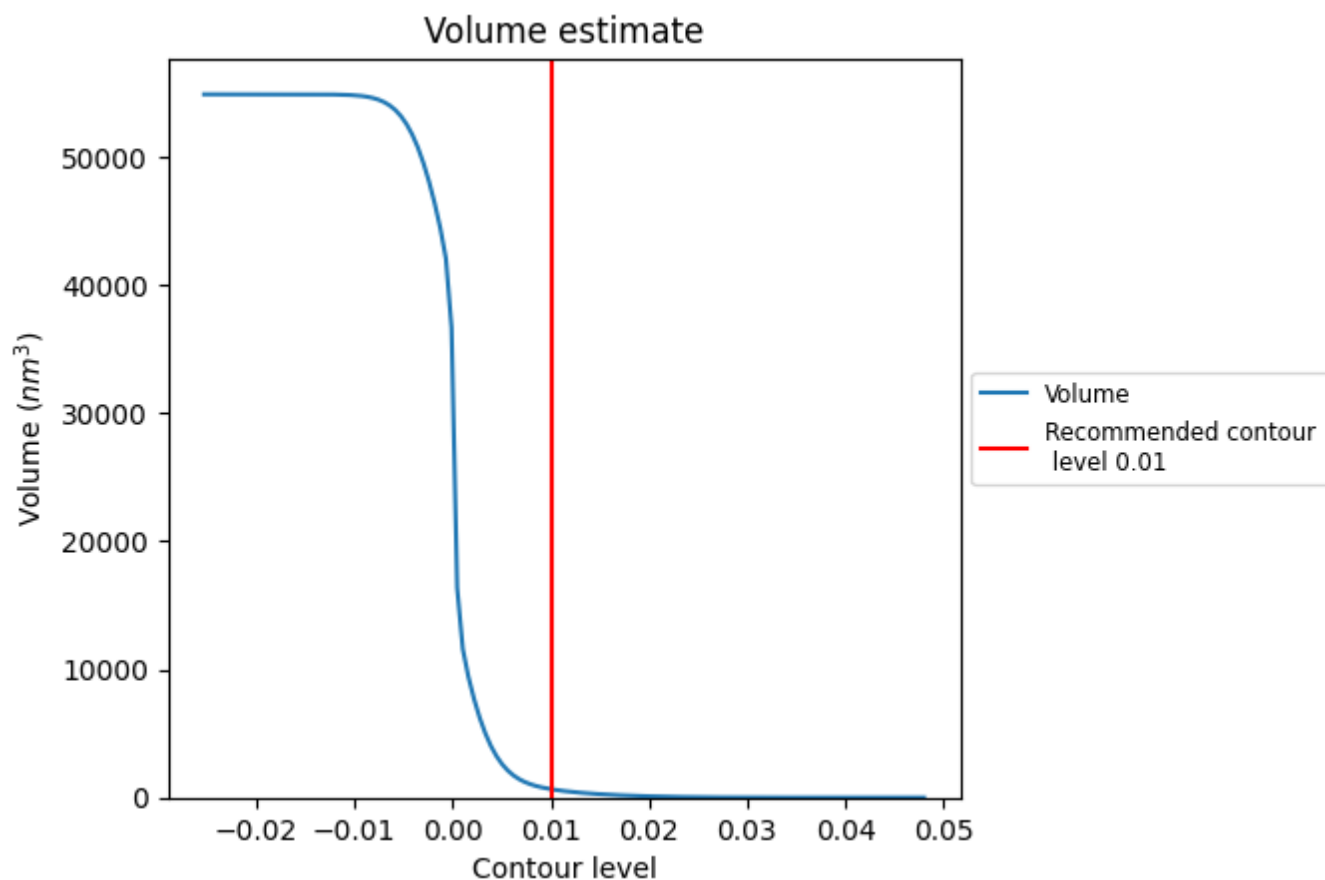
This section contains the results of statistical analysis of the map.

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.

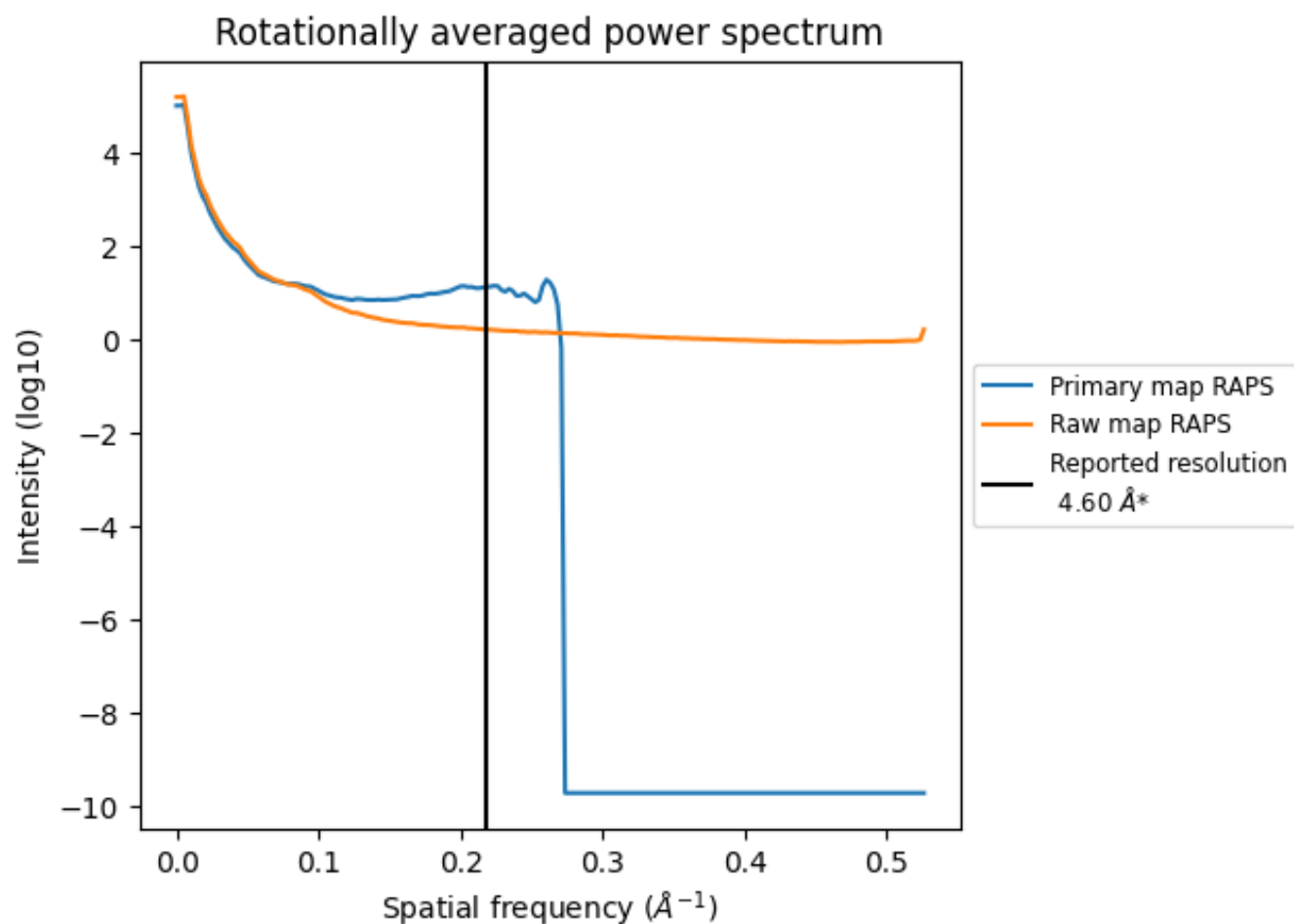
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 658 nm³; this corresponds to an approximate mass of 594 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 ⓘ

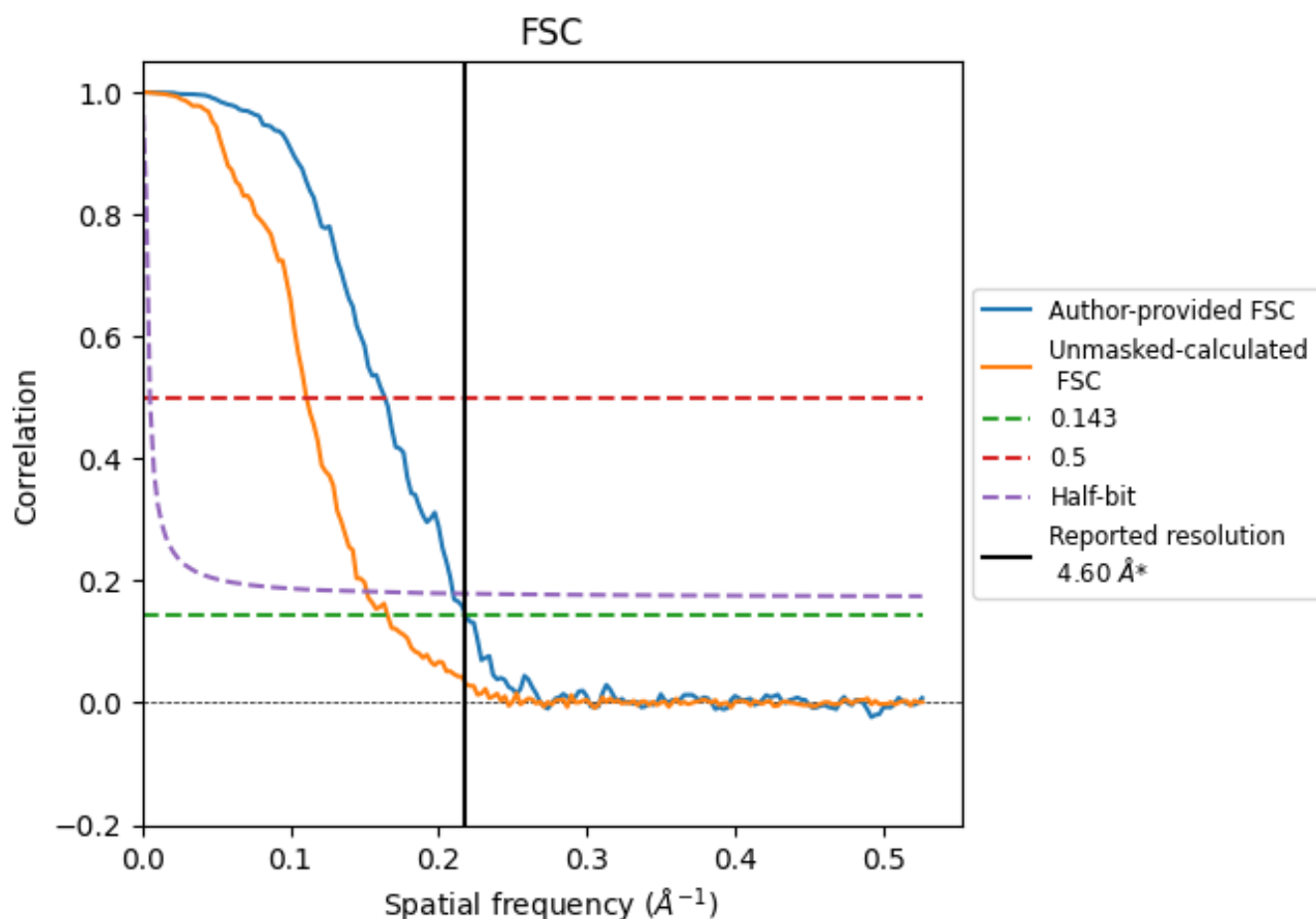


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

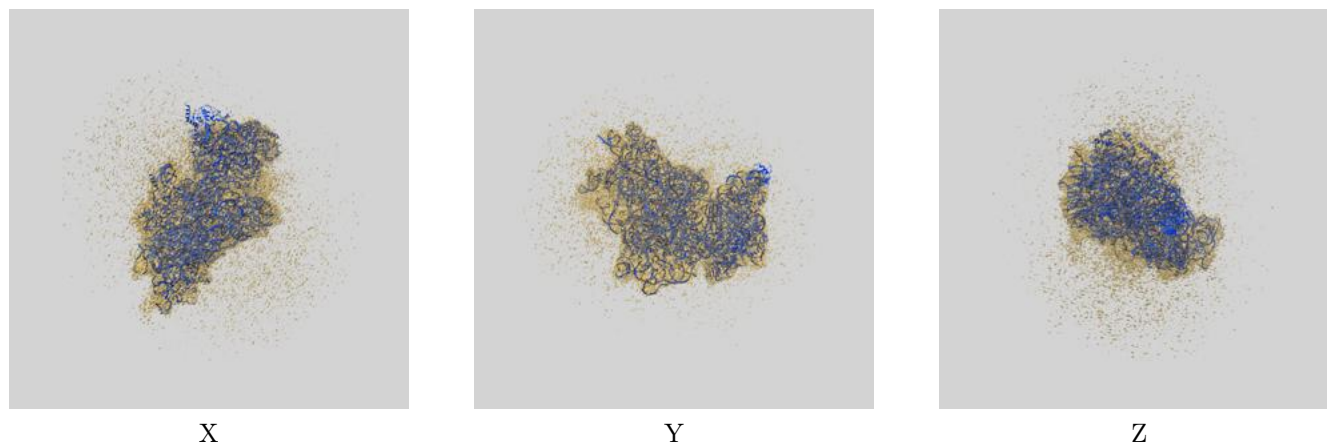
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.58	6.11	4.77
Unmasked-calculated*	6.04	9.02	6.60

*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 6.04 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

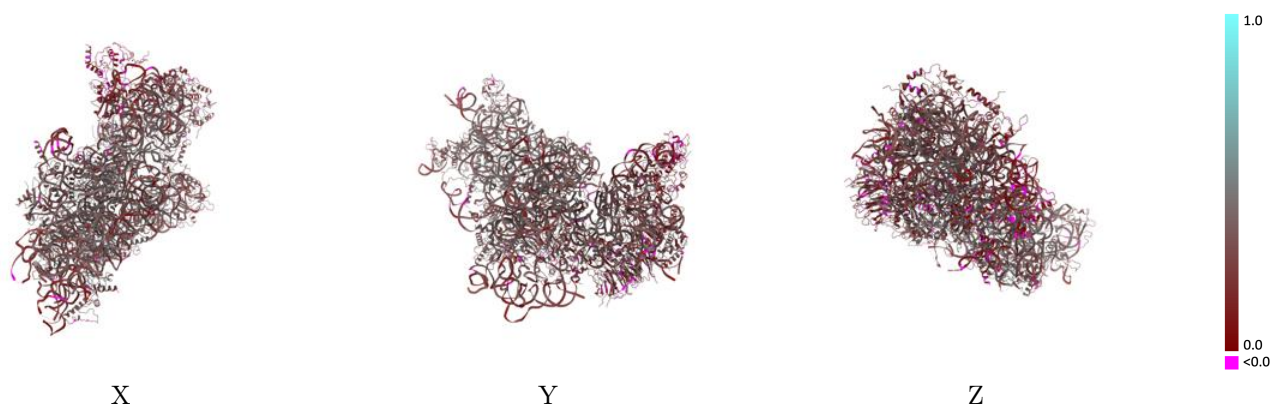
This section contains information regarding the fit between EMDB map EMD-25535 and PDB model 7SYO. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



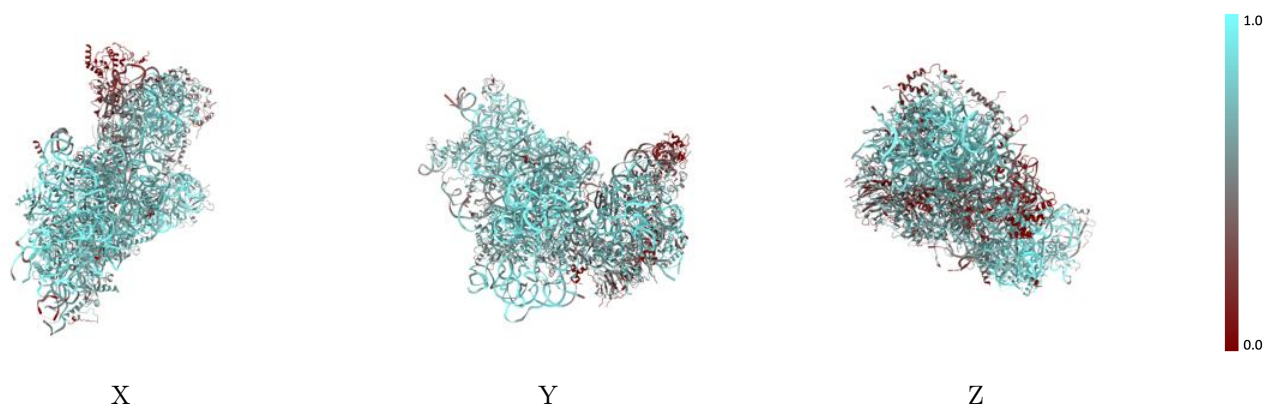
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



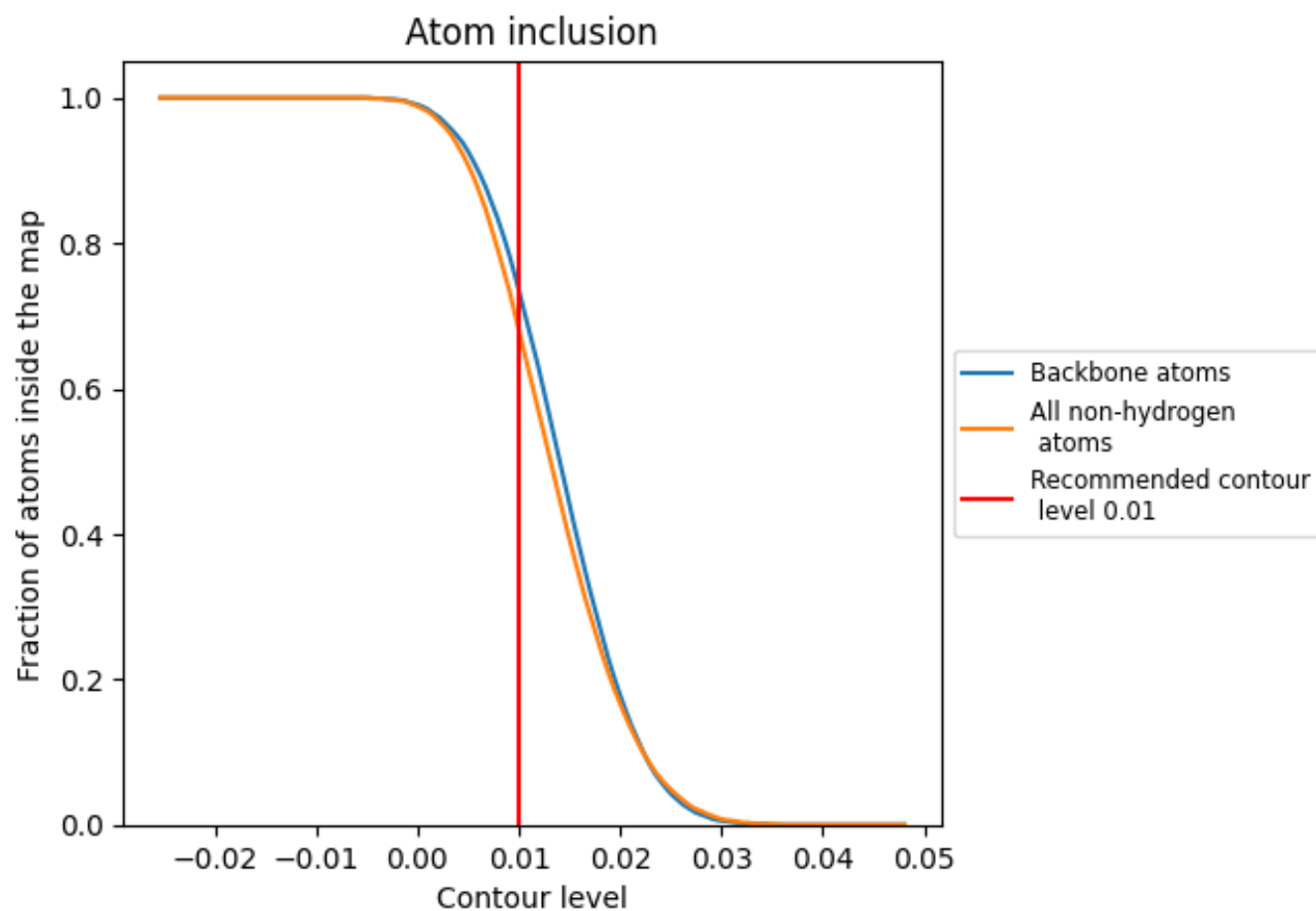
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 68% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6810	 0.3120
2	 0.7900	 0.3170
B	 0.5980	 0.3430
C	 0.6940	 0.3280
D	 0.6380	 0.3430
E	 0.3970	 0.2890
F	 0.7290	 0.3860
G	 0.5890	 0.3200
H	 0.6370	 0.3070
I	 0.5510	 0.3250
J	 0.6750	 0.3660
K	 0.7240	 0.3640
L	 0.3380	 0.2090
M	 0.6150	 0.3770
N	 0.0220	 0.1240
O	 0.7130	 0.3730
P	 0.7170	 0.3250
Q	 0.4720	 0.2120
R	 0.6460	 0.3260
S	 0.4320	 0.2740
T	 0.5060	 0.2720
U	 0.6800	 0.3250
V	 0.2800	 0.2290
W	 0.6330	 0.3500
X	 0.6560	 0.4080
Y	 0.6780	 0.3840
Z	 0.7780	 0.3700
a	 0.3310	 0.2290
b	 0.6650	 0.3740
c	 0.6370	 0.3830
d	 0.5060	 0.3120
e	 0.5310	 0.2930
f	 0.4820	 0.2440
g	 0.0390	 0.1610
h	 0.4530	 0.2300



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Chain	Atom inclusion	Q-score
n	 0.5780	 0.3330
z	 0.7360	 0.2340