



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:01 AM UTC

PDB ID : 7OHV / pdb_00007ohv
EMDB ID : EMD-12910
Title : Nog1-TAP associated immature ribosomal particles from *S. cerevisiae* after
rpL2 expression shut down, population C
Authors : Milkereit, P.; Poell, G.
Deposited on : 2021-05-11
Resolution : 3.90 Å(reported)
Based on initial model : 6ELZ

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:

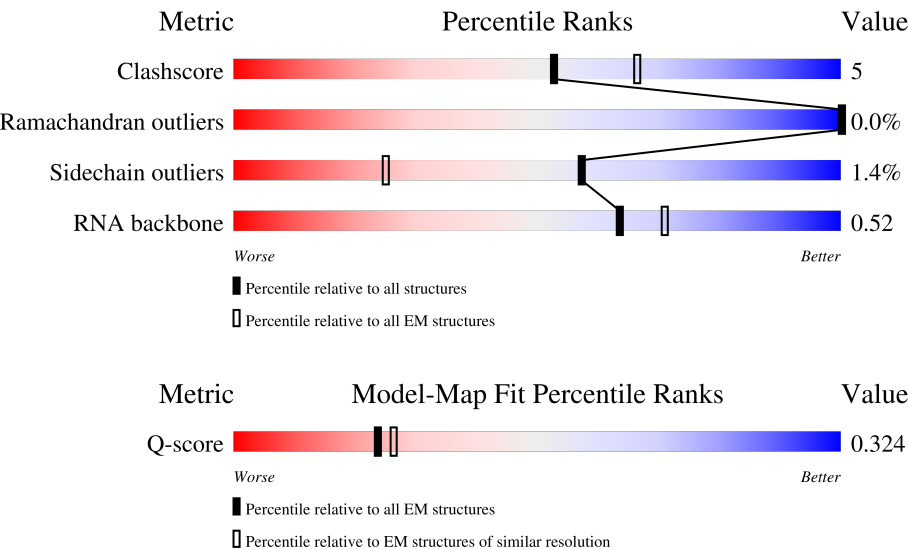
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

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



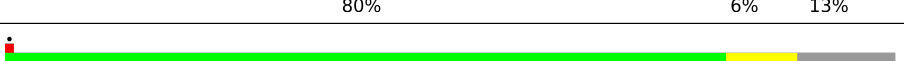
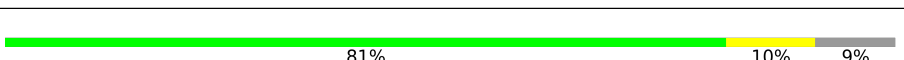
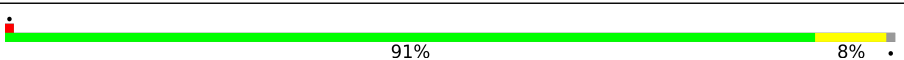
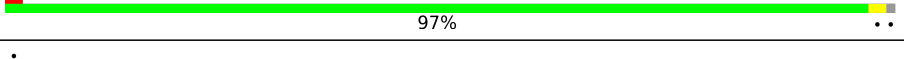
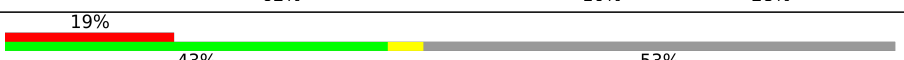
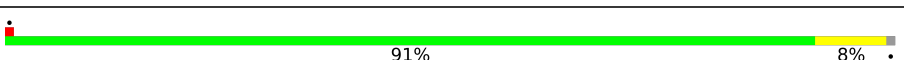
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	1	3396	40%18%5%37%
2	2	158	60%30%8%
3	6	232	12%10%6%72%

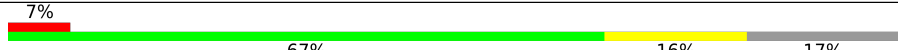
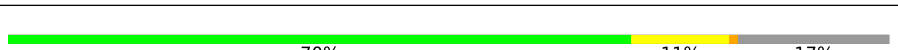
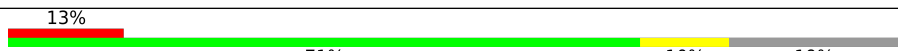
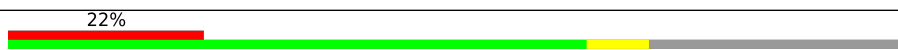
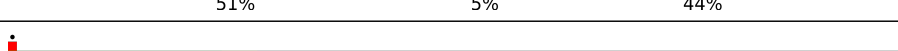
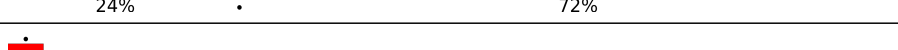
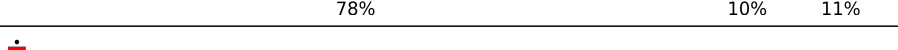
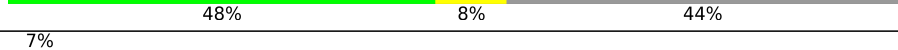
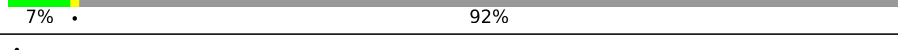
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	A	291	
5	B	387	
6	C	362	
7	D	505	
8	E	176	
9	F	244	
10	G	256	
11	H	191	
12	J	427	
13	K	376	
14	L	199	
15	M	138	
16	N	204	
17	O	199	
18	P	184	
19	Q	186	
20	R	189	
21	S	172	
22	U	121	
23	V	137	
24	W	236	
25	X	142	
26	Y	127	
27	Z	136	
28	a	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	b	647	
30	d	113	
31	e	130	
32	f	107	
33	h	120	
34	i	100	
35	j	88	
36	k	78	
37	m	807	
38	n	605	
39	o	220	
40	p	460	
41	r	261	
42	t	322	
43	u	199	
44	v	231	
45	w	841	
46	y	245	

2 Entry composition [i](#)

There are 47 unique types of molecules in this entry. The entry contains 205079 atoms, of which 91259 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 25S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	2141	Total	C	H	N	O	P	0	0
			68875	20469	23027	8298	14940	2141		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	155	Total	C	H	N	O	P	0	0
			4955	1472	1664	577	1087	155		

- Molecule 3 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	6	65	Total	C	H	N	O	P	0	0
			2061	614	691	228	463	65		

- Molecule 4 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	198	Total	C	H	N	O	S	0	0
			3250	1043	1627	284	290	6		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	341	Total	C	H	N	O	S	0	0
			5483	1715	2781	501	480	6		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	C	359	Total	C	H	N	O	S	0	0
			5584	1720	2853	518	490	3		

- Molecule 7 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D	437	Total	C	H	N	O	S	0	0
			7106	2247	3620	600	627	12		

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	E	156	Total	C	H	N	O	S	0	0
			2567	800	1328	222	216	1		

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	F	222	Total	C	H	N	O	S	0	0
			3647	1151	1863	324	308	1		

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	G	184	Total	C	H	N	O	S	0	0
			2960	930	1522	249	257	2		

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	H	190	Total	C	H	N	O	S	0	0
			3086	957	1576	273	276	4		

- Molecule 12 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	J	79	Total	C	H	N	O	S	0	0
			1318	420	656	116	124	2		

- Molecule 13 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	K	257	Total	C	H	N	O	S	0	0
			4230	1337	2157	341	392	3		

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	117	Total	C	H	N	O	0	0
			1962	601	1004	202	155		

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
15	M	136	Total	C	H	N	O	S	0	0
			2203	675	1150	199	177	2		

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
16	N	186	Total	C	H	N	O	S	0	0
			3224	994	1637	333	259	1		

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	O	197	Total	C	H	N	O	S	0	0
			3215	1003	1660	289	262	1		

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	163	Total	C	H	N	O	0	0
			2608	799	1321	255	233		

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
19	Q	134	Total	C	H	N	O	S	0	0
			2151	659	1116	196	179	1		

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	89	Total	C	H	N	O	0	0
			1521	460	796	147	118		

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	S	170	Total	C	H	N	O	S	0	0
			2903	922	1471	265	242	3		

- Molecule 22 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	U	94	Total	C	H	N	O		0	0
			1519	489	767	123	140			

- Molecule 23 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	V	124	Total	C	H	N	O	S	0	0
			1897	584	974	171	161	7		

- Molecule 24 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	W	232	Total	C	H	N	O	S	0	0
			3773	1184	1903	321	360	5		

- Molecule 25 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	X	127	Total	C	H	N	O	S	0	0
			2076	645	1075	175	179	2		

- Molecule 26 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Y	126	Total	C	H	N	O		0	0
			2075	625	1082	192	176			

- Molecule 27 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Z	130	Total	C	H	N	O		0	0
			2154	680	1105	195	174			

- Molecule 28 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	73	Total	C	H	N	O	0	0
			1188	375	618	98	97		

- Molecule 29 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
29	b	421	Total	C	H	N	O	S	0	0
			6876	2180	3466	585	627	18		

- Molecule 30 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	d	100	Total	C	H	N	O	S	0	0
			1687	521	871	157	137	1		

- Molecule 31 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
31	e	124	Total	C	H	N	O	S	0	0
			2071	635	1070	202	163	1		

- Molecule 32 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	f	106	Total	C	H	N	O	S	0	0
			1731	540	881	165	144	1		

- Molecule 33 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
33	h	118	Total	C	H	N	O	S	0	0
			2038	612	1074	185	166	1		

- Molecule 34 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
34	i	83	Total	C	H	N	O	S	0	0
			1371	408	713	135	113	2		

- Molecule 35 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	j	73	Total	C	H	N	O	S	0	0
			1169	353	589	126	96	5		

- Molecule 36 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	k	63	Total	C	H	N	O		0	0
			1123	340	600	99	84			

- Molecule 37 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	m	583	Total	C	H	N	O	S	0	0
			9518	3033	4766	834	870	15		

- Molecule 38 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	n	411	Total	C	H	N	O	S	0	0
			6868	2179	3499	585	592	13		

- Molecule 39 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	o	133	Total	C	H	N	O	S	0	0
			2267	716	1160	198	189	4		

- Molecule 40 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	p	257	Total	C	H	N	O	S	0	0
			3984	1247	1990	353	388	6		

- Molecule 41 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	r	73	Total	C	H	N	O	S	0	0
			1288	388	660	133	106	1		

- Molecule 42 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	t	286	Total	C	H	N	O	S	0	0
			4752	1455	2455	426	413	3		

- Molecule 43 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	u	116	Total	C	H	N	O	S	0	0
			1987	612	1011	200	155	9		

- Molecule 44 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	v	130	Total	C	H	N	O	S	0	0
			2223	678	1136	211	195	3		

- Molecule 45 is a protein called 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	w	69	Total	C	H	N	O	S	0	0
			1136	351	577	105	100	3		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	y	225	Total	C	H	N	O	S	0	0
			3398	1056	1697	295	343	7		

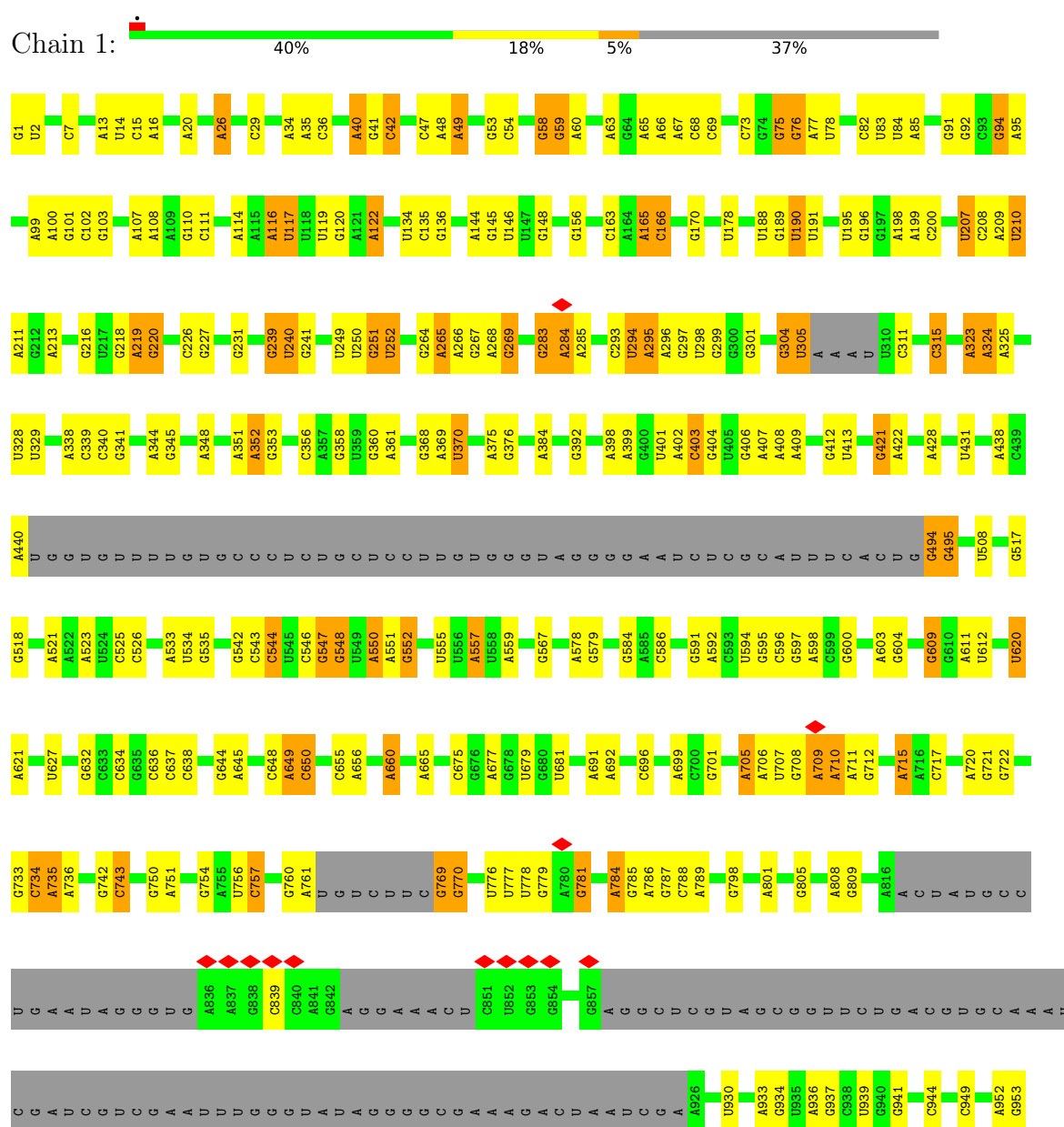
- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
47	j	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.

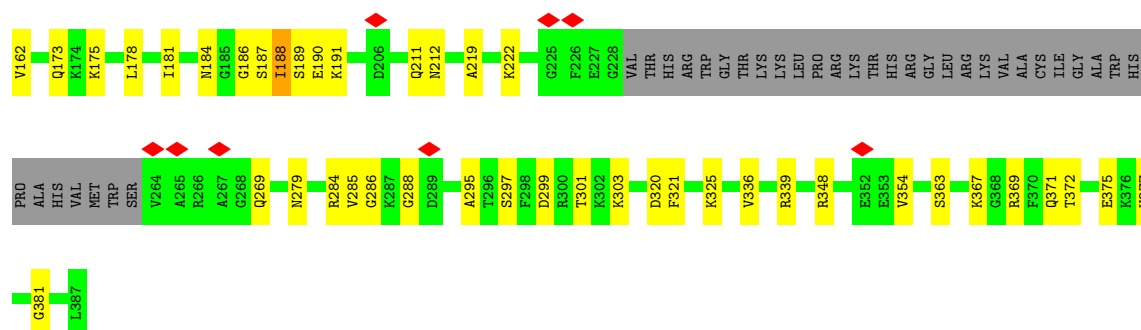
• Molecule 1: 25S rRNA





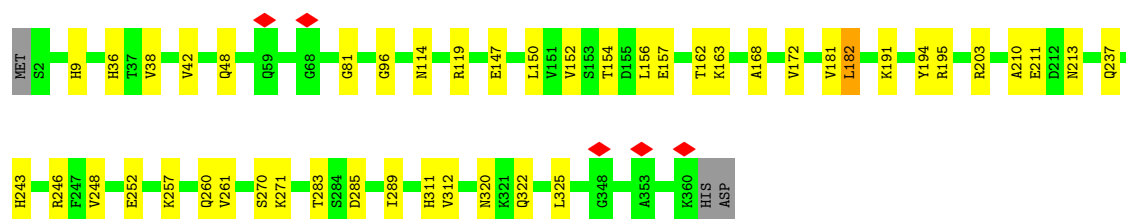


NET	SER	HIS	ARG	LYS	TYR	GLU	ALA	PRO	ARG	HIS	G12	G15	K20	A31	K34	D35	D36	V41	T55	I56	V57	K66	R70	V73	V76	V79	R85	R86	R87	G88	R89	V90	R100	T104	R117	A129	K132	D140	V160	L161
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------



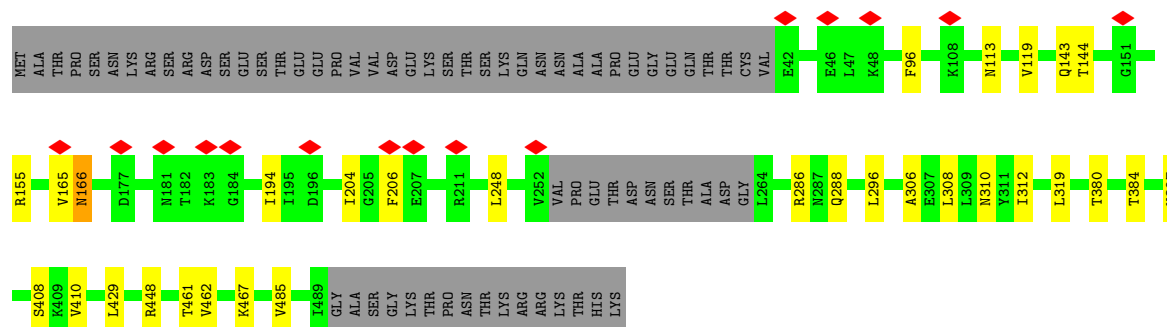
- Molecule 6: 60S ribosomal protein L4-A

Chain C: 86% 12%



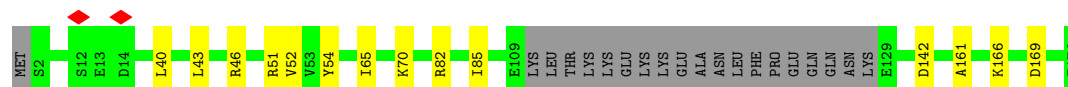
- Molecule 7: ATP-dependent RNA helicase HAS1

Chain D: 80% 6% 13%



- Molecule 8: 60S ribosomal protein L6-A

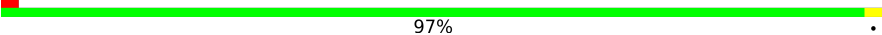
Chain E: 81% 8% 11%

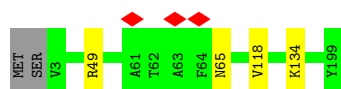


- Molecule 9: 60S ribosomal protein L7-A

Chain F: 81% 10% 9%

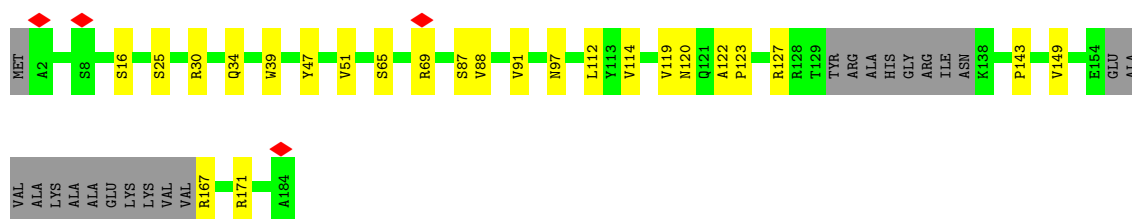


Chain O:  97% ..



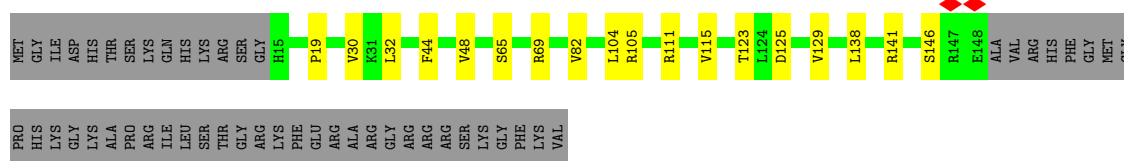
- Molecule 18: 60S ribosomal protein L17-A

Chain P:  76% 13% 11%



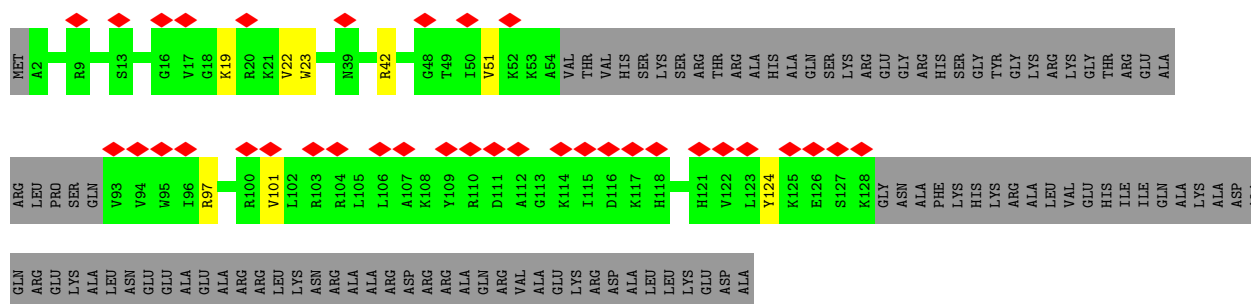
- Molecule 19: 60S ribosomal protein L18-A

Chain Q:  62% 10% 28%



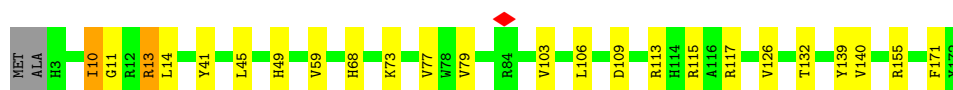
- Molecule 20: 60S ribosomal protein L19-A

Chain R:  19% 43% 53%

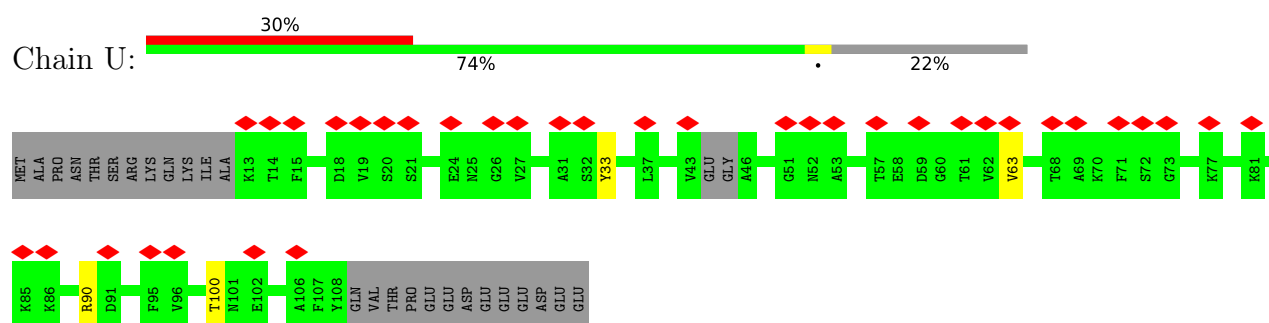


- Molecule 21: 60S ribosomal protein L20-A

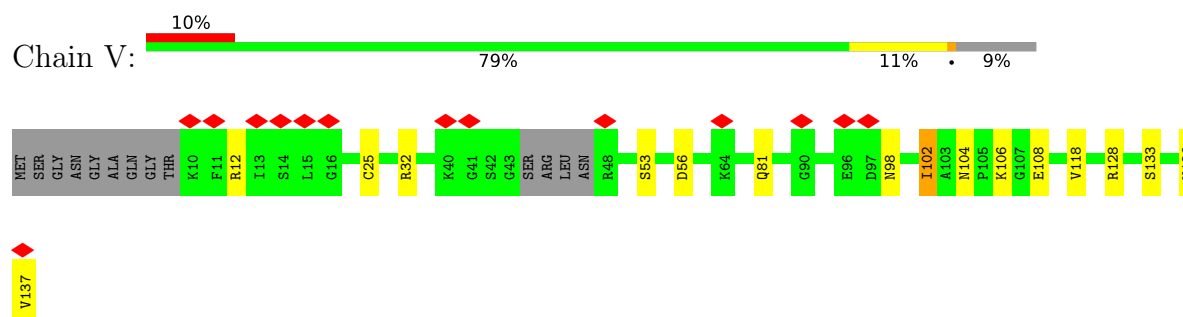
Chain S:  85% 13% ..



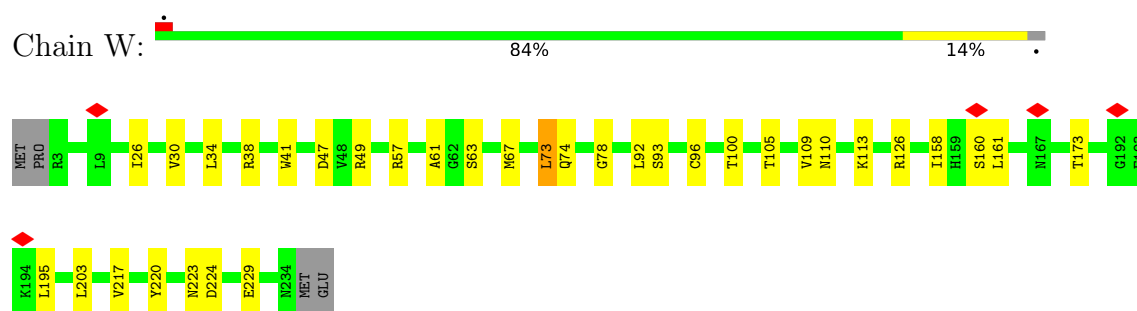
- Molecule 22: 60S ribosomal protein L22-A



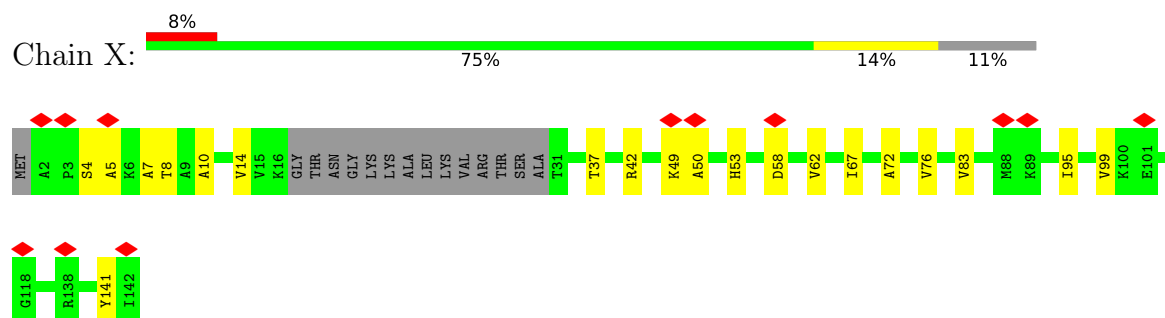
- Molecule 23: 60S ribosomal protein L23-A



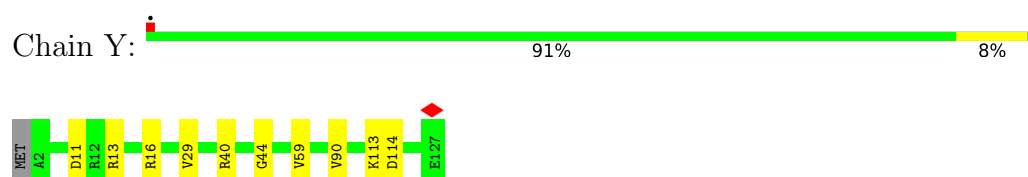
- Molecule 24: Ribosome assembly factor MRT4



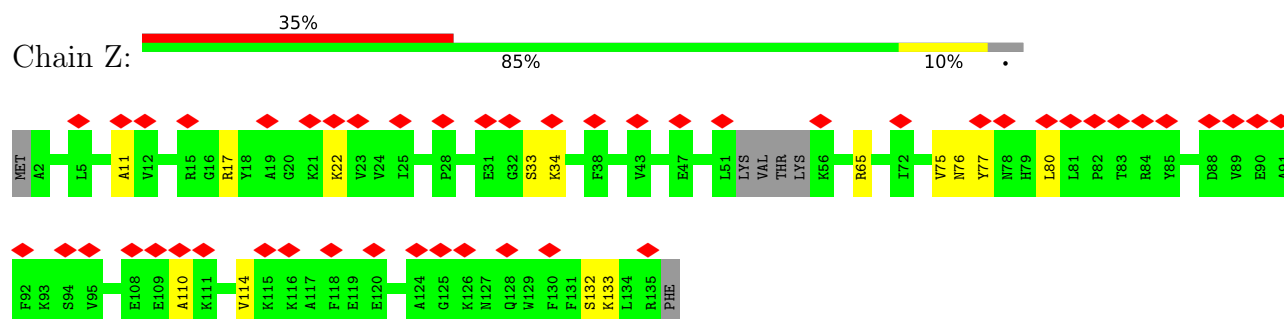
- Molecule 25: 60S ribosomal protein L25



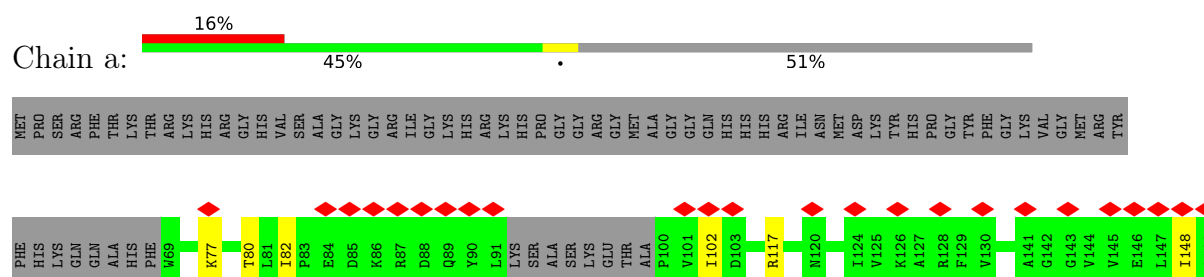
- Molecule 26: 60S ribosomal protein L26-A



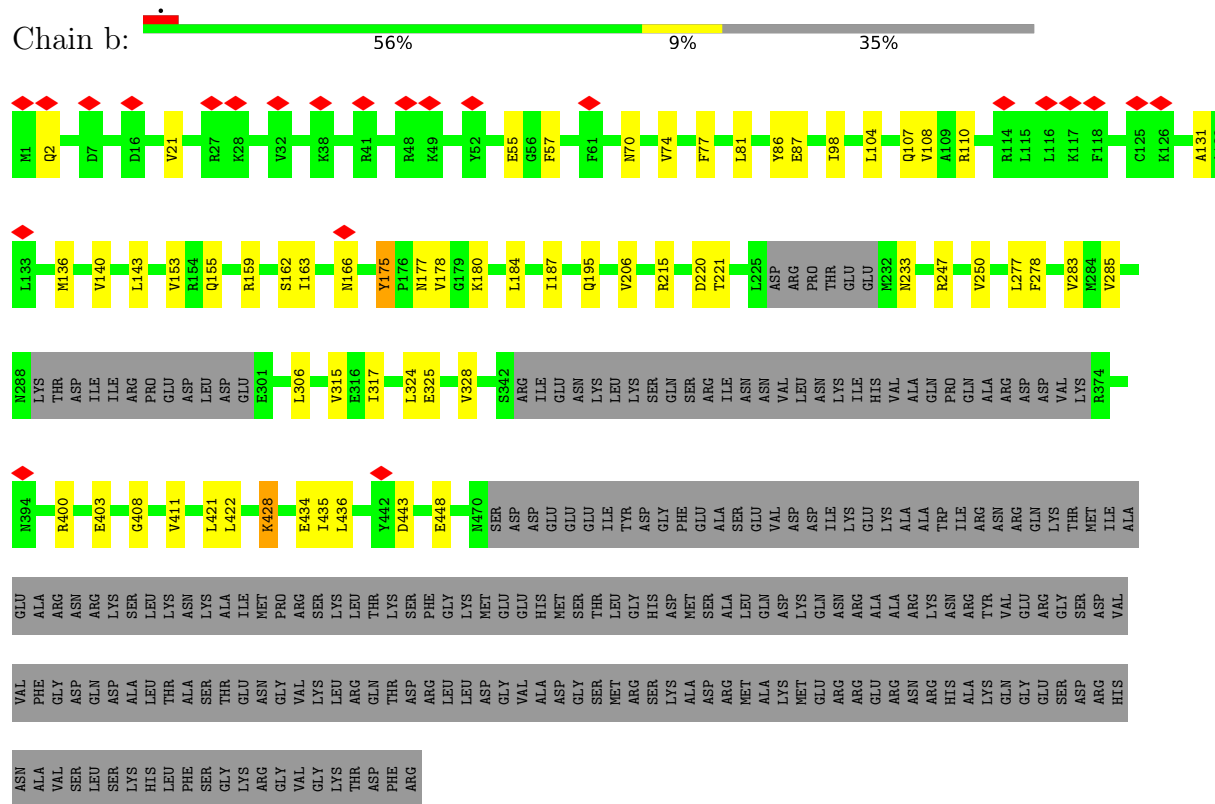
- Molecule 27: 60S ribosomal protein L27-A



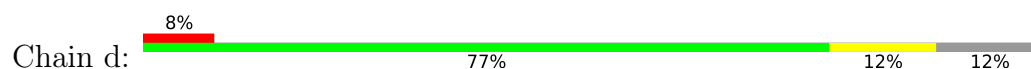
- Molecule 28: 60S ribosomal protein L28

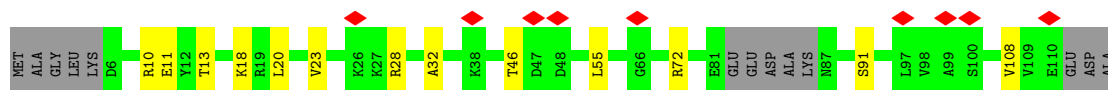


- Molecule 29: Nucleolar GTP-binding protein 1

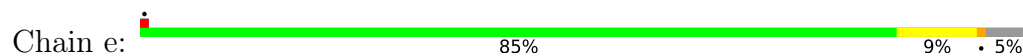


- Molecule 30: 60S ribosomal protein L31-A

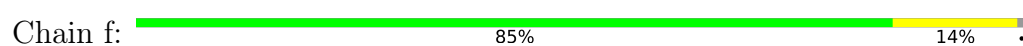




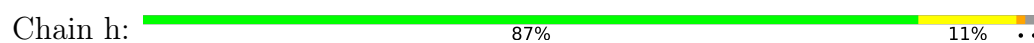
- Molecule 31: 60S ribosomal protein L32



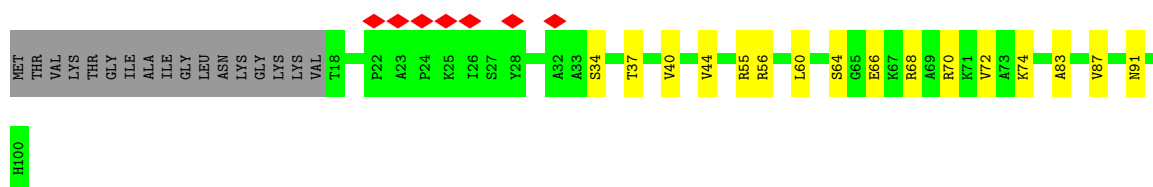
- Molecule 32: 60S ribosomal protein L33-A



- Molecule 33: 60S ribosomal protein L35-A



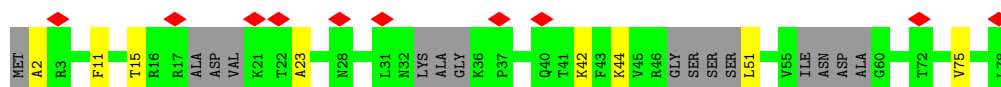
- Molecule 34: 60S ribosomal protein L36-A



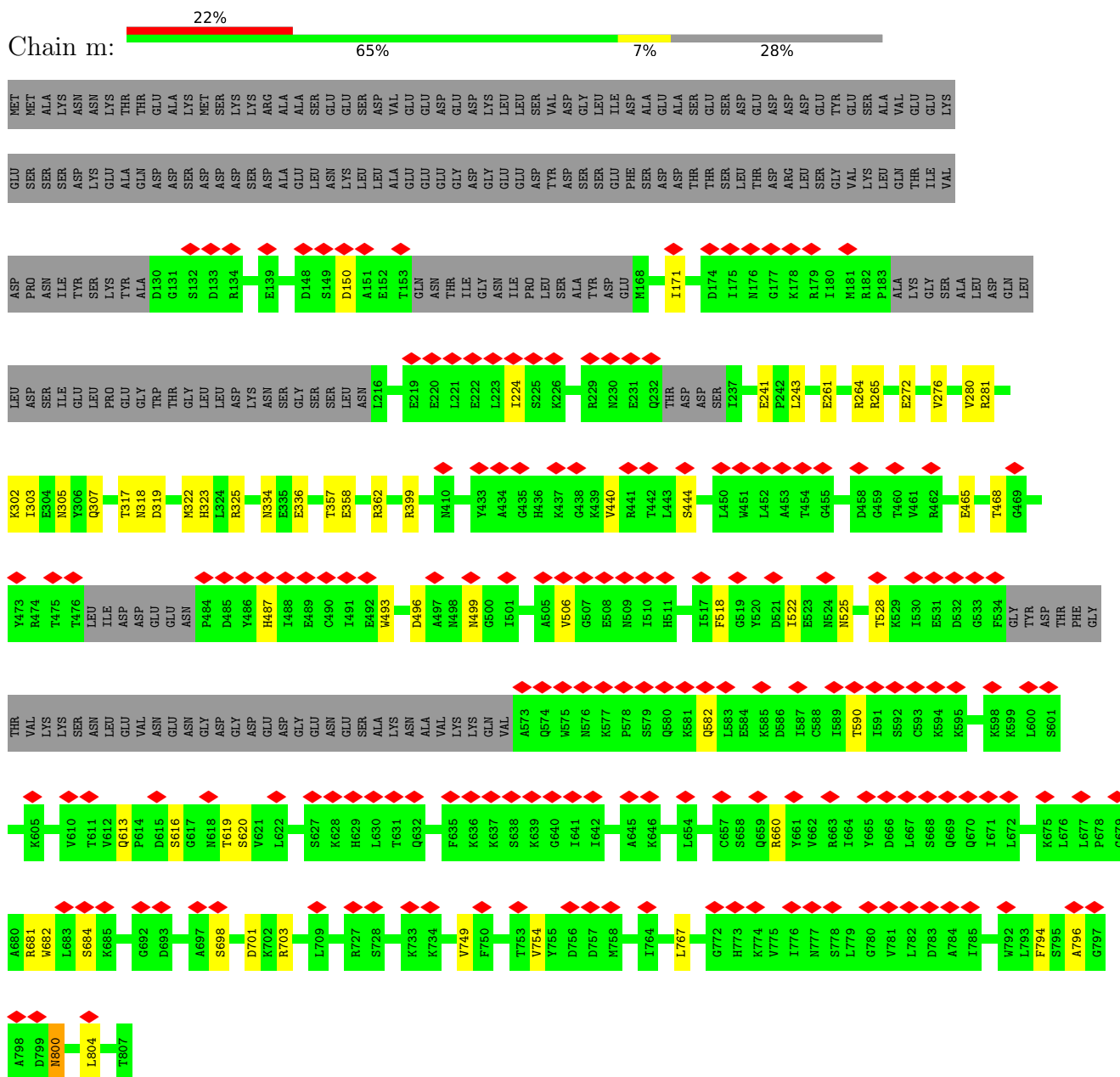
- Molecule 35: 60S ribosomal protein L37-A



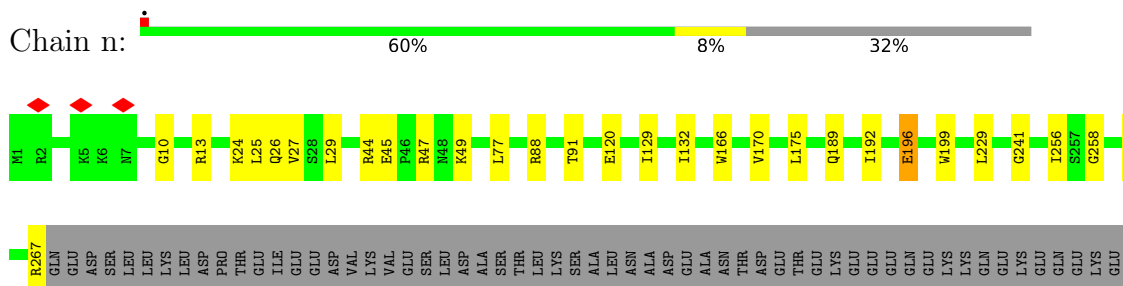
- Molecule 36: 60S ribosomal protein L38

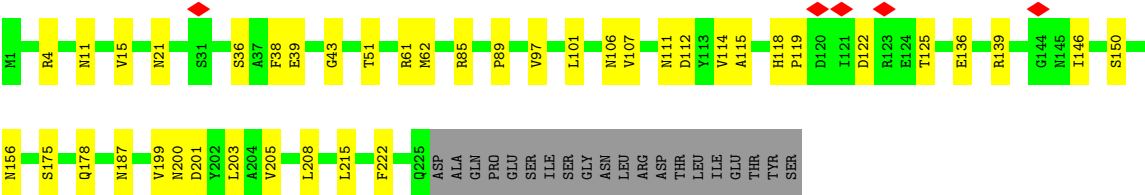


Chain m:



Chain n:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19178	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	86.45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.038	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	425.40002, 425.40002, 425.40002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	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	1	0.07	0/51295	0.22	0/79910
2	2	0.07	0/3676	0.21	0/5721
3	6	0.10	0/1527	0.30	1/2371 (0.0%)
4	A	0.09	0/1663	0.22	0/2248
5	B	0.11	0/2756	0.26	0/3702
6	C	0.10	0/2782	0.26	0/3766
7	D	0.09	0/3552	0.23	0/4789
8	E	0.10	0/1260	0.23	0/1694
9	F	0.11	0/1821	0.27	0/2451
10	G	0.10	0/1463	0.26	0/1978
11	H	0.08	0/1531	0.26	0/2062
12	J	0.11	0/675	0.23	0/908
13	K	0.09	0/2107	0.24	0/2845
14	L	0.12	0/976	0.27	0/1311
15	M	0.10	0/1068	0.21	0/1438
16	N	0.12	0/1619	0.23	0/2166
17	O	0.10	0/1585	0.23	0/2128
18	P	0.11	0/1306	0.23	0/1752
19	Q	0.10	0/1050	0.22	0/1419
20	R	0.11	0/733	0.23	0/980
21	S	0.11	0/1468	0.24	0/1973
22	U	0.09	0/767	0.19	0/1038
23	V	0.11	0/937	0.25	0/1259
24	W	0.09	0/1902	0.24	0/2564
25	X	0.10	0/1016	0.22	0/1369
26	Y	0.11	0/1004	0.23	0/1341
27	Z	0.12	0/1073	0.28	0/1436
28	a	0.11	0/580	0.21	0/784
29	b	0.09	0/3474	0.25	0/4683
30	d	0.11	0/829	0.22	0/1112
31	e	0.10	0/1022	0.24	0/1367
32	f	0.11	0/868	0.24	0/1168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.13	0/973	0.27	0/1294
34	i	0.12	0/665	0.27	0/884
35	j	0.11	0/592	0.24	0/785
36	k	0.11	0/525	0.21	0/694
37	m	0.10	0/4874	0.24	0/6600
38	n	0.08	0/3441	0.24	0/4625
39	o	0.10	0/1129	0.24	0/1502
40	p	0.09	0/2027	0.24	0/2744
41	r	0.09	0/638	0.27	0/837
42	t	0.11	0/2323	0.28	0/3113
43	u	0.10	0/996	0.29	0/1324
44	v	0.10	0/1100	0.20	0/1456
45	w	0.10	0/565	0.16	0/748
46	y	0.08	0/1722	0.23	0/2343
All	All	0.09	0/120955	0.23	1/174682 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	1	C	C2'-C3'-O3'	5.46	117.69	109.50

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	1	45848	23027	23061	484	0
2	2	3291	1664	1665	46	0
3	6	1370	691	692	33	0
4	A	1623	1627	1624	24	0
5	B	2702	2781	2779	44	0
6	C	2731	2853	2852	34	0
7	D	3486	3620	3618	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	1239	1328	1326	10	0
9	F	1784	1863	1862	18	0
10	G	1438	1522	1520	16	0
11	H	1510	1576	1576	22	0
12	J	662	656	654	8	0
13	K	2073	2157	2155	36	0
14	L	958	1004	1003	17	0
15	M	1053	1150	1149	12	0
16	N	1587	1637	1635	26	0
17	O	1555	1660	1659	3	0
18	P	1287	1321	1318	18	0
19	Q	1035	1116	1115	12	0
20	R	725	796	794	7	0
21	S	1432	1471	1470	16	0
22	U	752	767	765	3	0
23	V	923	974	972	11	0
24	W	1870	1903	1902	19	0
25	X	1001	1075	1073	12	0
26	Y	993	1082	1081	9	0
27	Z	1049	1105	1103	8	0
28	a	570	618	617	2	0
29	b	3410	3466	3463	36	0
30	d	816	871	869	9	0
31	e	1001	1070	1070	11	0
32	f	850	881	880	11	0
33	h	964	1074	1073	9	0
34	i	658	713	712	12	0
35	j	580	589	584	11	0
36	k	523	600	595	7	0
37	m	4752	4766	4761	41	0
38	n	3369	3499	3496	31	0
39	o	1107	1160	1159	16	0
40	p	1994	1990	1984	11	0
41	r	628	660	660	7	0
42	t	2297	2455	2452	18	0
43	u	976	1011	1011	9	0
44	v	1087	1136	1133	14	0
45	w	559	577	574	4	0
46	y	1701	1697	1697	23	0
47	j	1	0	0	0	0
All	All	113820	91259	91213	1039	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1039) 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)
1:1:1560:G:O2'	1:1:1561:G:O5'	1.75	1.04
1:1:1254:C:O2'	1:1:1255:C:O4'	1.83	0.95
3:6:16:U:O2'	3:6:17:G:OP2	1.86	0.94
1:1:3049:A:HO2'	5:B:55:THR:HG1	1.00	0.92
1:1:399:A:HO2'	1:1:403:C:HO2'	1.12	0.91
1:1:3149:G:O2'	5:B:129:ALA:O	1.88	0.90
1:1:953:G:O6	1:1:1143:A:N7	2.06	0.88
1:1:1456:A:O2'	1:1:1457:U:O5'	1.93	0.87
1:1:304:G:O2'	1:1:305:U:OP1	1.94	0.86
1:1:408:A:N3	1:1:655:C:O2'	2.09	0.85
1:1:1497:C:HO2'	1:1:1602:A:HO2'	1.15	0.84
1:1:596:C:OP1	9:F:37:ASN:ND2	2.09	0.84
3:6:33:U:O2'	3:6:34:A:OP2	1.95	0.83
46:y:106:ASN:OD1	46:y:150:SER:OG	1.94	0.82
1:1:94:G:O2'	1:1:95:A:O4'	1.96	0.82
3:6:25:G:O2'	3:6:26:U:OP1	1.97	0.82
1:1:1560:G:HO2'	1:1:1561:G:P	2.02	0.82
1:1:3184:A:N3	1:1:3187:A:O2'	2.13	0.82
1:1:421:G:O6	1:1:2383:C:O2'	1.96	0.82
1:1:3352:U:O2'	1:1:3353:G:O5'	1.98	0.82
1:1:769:G:O2'	1:1:770:G:OP1	1.98	0.81
1:1:534:U:OP1	21:S:132:THR:OG1	1.97	0.81
1:1:116:A:O2'	1:1:117:U:OP1	1.98	0.81
1:1:399:A:O2'	1:1:403:C:O2'	1.97	0.81
3:6:15:C:O2'	3:6:16:U:OP2	1.99	0.80
1:1:360:G:O2'	1:1:361:A:O4'	1.97	0.80
1:1:733:G:N2	1:1:736:A:OP2	2.14	0.80
1:1:952:A:N3	1:1:1114:U:O2'	2.13	0.80
1:1:3060:C:O2	1:1:3332:U:O2'	2.00	0.80
1:1:600:G:N2	1:1:603:A:OP2	2.15	0.80
1:1:708:G:N2	1:1:711:A:OP2	2.15	0.80
1:1:1329:U:O2'	1:1:1330:A:OP1	1.99	0.80
1:1:3288:G:O2'	1:1:3289:G:O5'	1.99	0.80
1:1:3164:C:O2'	1:1:3165:A:O5'	1.98	0.80
1:1:3042:U:OP2	1:1:3092:C:N4	2.14	0.79
42:t:90:THR:HG23	42:t:93:ILE:HD11	1.63	0.79
1:1:84:U:O2	1:1:102:C:N4	2.16	0.78
1:1:297:G:N2	1:1:297:G:OP2	2.17	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:68:C:OP2	1:1:301:G:N2	2.16	0.78
1:1:627:U:O2'	1:1:1399:A:N3	2.16	0.78
1:1:1394:A:N6	1:1:1416:C:O2	2.16	0.78
4:A:190:THR:OG1	4:A:215:ILE:O	2.01	0.78
1:1:2887:A:O2'	1:1:2888:U:OP1	2.00	0.78
1:1:1655:G:N2	1:1:1801:U:O4	2.17	0.78
1:1:1152:G:N2	1:1:1152:G:OP2	2.17	0.78
1:1:1188:U:OP1	1:1:1210:U:O2'	2.01	0.78
1:1:1493:G:N2	1:1:1493:G:OP2	2.17	0.78
1:1:3028:G:O2'	29:b:215:ARG:NH2	2.17	0.78
1:1:3110:C:OP1	41:r:26:LYS:NZ	2.16	0.78
1:1:2992:U:OP1	1:1:3310:A:O2'	2.00	0.78
1:1:239:G:O2'	1:1:240:U:O5'	2.03	0.77
1:1:1188:U:O2'	1:1:1190:A:N7	2.15	0.77
37:m:496:ASP:O	37:m:499:ASN:ND2	2.16	0.77
46:y:15:VAL:HG22	46:y:61:ARG:HG3	1.66	0.77
1:1:1600:U:OP1	20:R:42:ARG:NH2	2.18	0.77
24:W:34:LEU:O	24:W:223:ASN:ND2	2.17	0.77
1:1:294:U:OP2	16:N:15:GLN:NE2	2.19	0.76
1:1:717:C:OP1	1:1:751:A:O2'	2.02	0.76
13:K:183:ASP:O	13:K:187:VAL:HG23	1.86	0.76
29:b:177:ASN:ND2	29:b:195:GLN:O	2.19	0.76
3:6:1:C:O2'	3:6:2:C:OP2	2.02	0.76
37:m:616:SER:OG	37:m:619:THR:OG1	2.03	0.75
1:1:1237:G:O6	1:1:1251:A:N6	2.20	0.75
31:e:98:HIS:O	31:e:125:ARG:NH2	2.19	0.74
38:n:448:LEU:N	38:n:451:GLU:OE2	2.19	0.74
1:1:1765:U:O2'	1:1:1766:G:O5'	2.05	0.74
1:1:1112:A:N3	1:1:1370:G:O2'	2.20	0.74
1:1:69:C:HO2'	1:1:101:G:HO2'	1.29	0.74
1:1:1129:A:O2'	1:1:1130:A:OP1	2.02	0.74
2:2:147:U:O2	25:X:37:THR:OG1	2.06	0.74
21:S:155:ARG:NH1	21:S:171:PHE:O	2.20	0.74
1:1:981:U:O2'	1:1:1105:A:O2'	1.99	0.74
1:1:3079:U:O2'	1:1:3080:G:OP1	2.05	0.74
2:2:21:C:OP2	6:C:194:TYR:OH	2.06	0.74
1:1:675:C:O2'	1:1:679:U:OP1	2.06	0.74
1:1:1404:G:N2	1:1:1407:A:OP2	2.19	0.73
2:2:103:G:OP2	2:2:105:A:O2'	2.06	0.73
1:1:3228:C:O2'	1:1:3229:G:OP2	2.04	0.73
1:1:165:A:O2'	1:1:166:C:OP2	2.06	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:184:ASP:OD1	13:K:208:SER:OG	2.07	0.73
1:1:3114:A:OP2	1:1:3115:C:O2'	2.02	0.73
1:1:324:A:O2'	1:1:325:A:O4'	2.06	0.73
1:1:1593:A:O2'	1:1:1594:A:O4'	2.05	0.73
1:1:1861:G:O2'	1:1:1862:U:OP1	2.05	0.73
1:1:116:A:OP1	1:1:265:A:O2'	2.06	0.73
1:1:1157:G:O2'	1:1:1169:A:N3	2.22	0.73
3:6:51:U:O2'	3:6:54:A:N7	2.22	0.73
1:1:1227:C:O2'	1:1:1228:C:OP1	2.07	0.72
3:6:227:C:N4	42:t:151:LEU:O	2.22	0.72
2:2:150:G:O2'	10:G:59:GLN:NE2	2.22	0.72
1:1:267:G:O4'	16:N:50:ARG:NH1	2.23	0.71
1:1:1259:A:N3	1:1:1280:C:O2'	2.22	0.71
1:1:53:G:OP2	35:j:48:ASN:ND2	2.24	0.71
37:m:317:THR:OG1	37:m:319:ASP:OD1	2.08	0.71
37:m:465:GLU:OE2	37:m:468:THR:OG1	2.09	0.71
1:1:3115:C:O2	1:1:3117:C:N4	2.24	0.71
1:1:75:G:O2'	1:1:76:G:OP1	2.09	0.70
5:B:367:LYS:O	5:B:369:ARG:NH2	2.24	0.70
43:u:23:ARG:NH2	43:u:25:ASP:OD1	2.24	0.70
37:m:318:ASN:ND2	38:n:120:GLU:O	2.24	0.70
21:S:68:HIS:O	21:S:73:LYS:NZ	2.24	0.70
1:1:3306:U:O2'	1:1:3308:C:OP2	2.08	0.70
35:j:54:LYS:O	35:j:58:THR:HG23	1.92	0.70
1:1:406:G:O2'	1:1:407:A:OP2	2.10	0.70
1:1:798:G:O3'	14:L:15:ARG:NH2	2.24	0.70
1:1:1682:U:O4	22:U:90:ARG:NH1	2.25	0.69
1:1:3028:G:N2	29:b:162:SER:OG	2.25	0.69
16:N:99:ARG:NH2	16:N:118:SER:O	2.25	0.69
1:1:219:A:O2'	1:1:220:G:N2	2.25	0.69
1:1:494:G:O2'	1:1:495:G:O5'	2.08	0.69
1:1:1481:A:O2'	1:1:1858:A:O2'	2.10	0.69
1:1:1637:A:O2'	1:1:1709:C:O2'	2.10	0.69
1:1:3355:U:O2'	1:1:3356:G:OP2	2.08	0.69
9:F:88:ARG:NH1	9:F:90:LYS:O	2.26	0.69
1:1:1176:C:OP2	1:1:1177:G:O2'	2.07	0.69
1:1:2857:C:O2'	1:1:2858:U:O5'	2.07	0.69
21:S:109:ASP:OD1	21:S:113:ARG:NH1	2.25	0.69
1:1:1145:G:N2	1:1:1331:U:O2'	2.26	0.69
1:1:296:A:N3	1:1:299:G:O2'	2.23	0.69
1:1:3287:U:O2'	1:1:3288:G:O5'	2.10	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:54:A:OP1	10:G:213:LYS:NZ	2.26	0.69
4:A:153:LYS:O	4:A:157:VAL:HG23	1.93	0.69
46:y:200:ASN:OD1	46:y:203:LEU:N	2.25	0.69
1:1:58:G:O2'	1:1:59:G:O5'	2.04	0.69
1:1:264:G:O2'	7:D:155:ARG:NH1	2.26	0.69
1:1:518:G:OP2	1:1:518:G:N2	2.18	0.69
2:2:85:G:OP2	26:Y:113:LYS:NZ	2.26	0.69
2:2:141:C:O2	16:N:112:ASN:ND2	2.26	0.69
13:K:277:ARG:NE	39:o:200:MET:SD	2.66	0.69
13:K:236:VAL:HG21	13:K:246:VAL:HG22	1.74	0.68
1:1:2897:A:OP2	1:1:2899:C:N4	2.26	0.68
38:n:45:GLU:OE1	38:n:49:LYS:NZ	2.26	0.68
1:1:1283:C:O2'	1:1:1284:C:OP1	2.10	0.68
1:1:1277:C:O2'	1:1:1278:A:O5'	2.09	0.68
29:b:70:ASN:O	29:b:74:VAL:HG23	1.92	0.68
1:1:1816:A:O2'	1:1:1817:G:OP1	2.10	0.68
2:2:36:G:OP2	33:h:85:THR:OG1	2.11	0.68
2:2:50:C:OP2	2:2:51:G:N2	2.26	0.68
1:1:144:A:OP1	10:G:193:LYS:NZ	2.18	0.68
1:1:620:U:O2	32:f:60:ARG:NH1	2.27	0.68
1:1:1260:A:O2'	1:1:1279:C:O2	2.12	0.68
7:D:288:GLN:NE2	13:K:115:ALA:O	2.27	0.68
13:K:41:VAL:HG21	13:K:260:VAL:HG22	1.76	0.68
3:6:29:G:N1	3:6:50:U:O4	2.26	0.68
1:1:3112:G:OP1	11:H:77:ASN:ND2	2.26	0.68
44:v:175:ARG:O	44:v:225:ARG:NH2	2.27	0.68
1:1:705:A:N6	1:1:715:A:OP2	2.25	0.68
12:J:236:ILE:O	12:J:242:ARG:NH1	2.26	0.67
1:1:40:A:O2'	1:1:42:C:N4	2.27	0.67
1:1:103:G:HO2'	1:1:699:A:HO2'	1.43	0.67
38:n:358:SER:O	38:n:361:SER:OG	2.09	0.67
23:V:81:GLN:O	23:V:98:ASN:ND2	2.27	0.67
1:1:392:G:O2'	26:Y:90:VAL:HG11	1.95	0.67
9:F:48:ASN:ND2	9:F:182:ASP:OD2	2.28	0.67
5:B:57:VAL:HG12	5:B:73:VAL:HG22	1.76	0.66
10:G:81:THR:HG21	10:G:181:LYS:HG3	1.77	0.66
1:1:2887:A:HO2'	1:1:2888:U:P	2.18	0.66
13:K:81:ILE:HG23	13:K:248:LEU:HD11	1.76	0.66
24:W:41:TRP:HH2	24:W:109:VAL:HG23	1.60	0.66
1:1:3313:U:OP1	5:B:173:GLN:NE2	2.28	0.66
37:m:684:SER:OG	37:m:698:SER:OG	2.14	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:358:G:N2	1:1:361:A:OP2	2.28	0.65
1:1:2391:G:H22	1:1:2989:U:H3	1.44	0.65
1:1:91:G:N2	1:1:95:A:OP2	2.29	0.65
29:b:166:ASN:O	29:b:247:ARG:NH2	2.30	0.65
1:1:209:A:O2'	1:1:211:A:OP2	2.08	0.65
13:K:38:ILE:HG13	13:K:260:VAL:HG11	1.77	0.65
14:L:123:ILE:HG22	33:h:118:ILE:HG12	1.76	0.65
23:V:106:LYS:O	23:V:128:ARG:NH1	2.29	0.65
46:y:4:ARG:HB3	46:y:208:LEU:HD23	1.77	0.65
1:1:54:C:HO2'	1:1:1547:G:HO2'	1.41	0.65
1:1:656:A:O2'	2:2:17:A:O2'	2.15	0.65
1:1:1699:A:N6	1:1:1747:G:O6	2.29	0.65
1:1:3084:C:O2'	1:1:3332:U:OP1	2.13	0.65
21:S:79:VAL:HG21	21:S:106:LEU:HD21	1.78	0.65
1:1:1633:C:O2'	37:m:682:TRP:NE1	2.29	0.65
1:1:1702:U:O2	1:1:1743:G:O6	2.13	0.65
1:1:59:G:OP2	2:2:33:A:O2'	2.15	0.65
13:K:256:PRO:O	13:K:260:VAL:HG23	1.97	0.64
18:P:51:VAL:HG11	18:P:88:VAL:HG21	1.79	0.64
1:1:165:A:N3	44:v:216:LYS:NZ	2.46	0.64
2:2:14:C:O2'	2:2:15:G:OP1	2.16	0.64
1:1:1748:G:OP1	36:k:44:LYS:NZ	2.22	0.64
1:1:1187:C:O2'	1:1:1295:G:N2	2.27	0.64
1:1:1693:C:O2'	1:1:1772:U:O3'	2.16	0.64
1:1:1339:C:O2'	1:1:1405:U:O4	2.16	0.64
21:S:11:GLY:N	21:S:41:TYR:OH	2.30	0.64
1:1:3276:G:O6	18:P:171:ARG:NH1	2.30	0.64
42:t:234:ILE:O	42:t:238:GLN:NE2	2.29	0.64
1:1:1624:G:OP1	38:n:560:SER:OG	2.12	0.64
6:C:154:THR:OG1	6:C:252:GLU:OE1	2.16	0.64
6:C:325:LEU:O	9:F:41:ARG:NH2	2.31	0.64
1:1:188:U:O2'	1:1:207:U:O2	2.16	0.63
4:A:168:LYS:NZ	37:m:150:ASP:OD2	2.29	0.63
1:1:1405:U:H3	31:e:55:ILE:HD12	1.61	0.63
1:1:2990:G:OP1	5:B:20:LYS:N	2.31	0.63
29:b:155:GLN:O	29:b:159:ARG:NH2	2.30	0.63
1:1:1620:U:OP1	38:n:47:ARG:NE	2.32	0.63
1:1:1747:G:OP1	36:k:42:LYS:NZ	2.30	0.63
1:1:58:G:HO2'	1:1:59:G:P	2.20	0.63
1:1:1807:G:OP1	27:Z:133:LYS:NZ	2.26	0.63
1:1:63:A:N3	1:1:78:U:O2'	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:62:GLU:OE1	34:i:74:LYS:NZ	2.31	0.63
9:F:186:HIS:O	9:F:190:THR:OG1	2.09	0.63
24:W:57:ARG:O	24:W:61:ALA:N	2.31	0.63
37:m:302:LYS:O	37:m:305:ASN:ND2	2.31	0.63
1:1:345:G:O2'	2:2:25:G:N3	2.30	0.63
5:B:299:ASP:OD2	5:B:301:THR:OG1	2.09	0.63
1:1:1657:C:N4	1:1:1798:A:OP2	2.31	0.63
4:A:38:SER:O	4:A:41:VAL:HG23	1.99	0.63
1:1:1294:A:C2	1:1:1295:G:N7	2.67	0.63
27:Z:75:VAL:HG11	27:Z:80:LEU:HD21	1.79	0.63
46:y:199:VAL:HG11	46:y:222:PHE:CZ	2.34	0.63
3:6:38:U:O2	3:6:42:G:N2	2.32	0.62
25:X:58:ASP:O	25:X:62:VAL:HG23	1.99	0.62
1:1:1320:C:O2'	21:S:115:ARG:NH2	2.31	0.62
1:1:3113:A:OP1	11:H:69:ARG:NH1	2.32	0.62
38:n:369:ARG:NE	42:t:249:ASP:OD1	2.31	0.62
1:1:3349:C:O2	1:1:3356:G:N2	2.31	0.62
28:a:77:LYS:O	28:a:80:THR:OG1	2.13	0.62
24:W:41:TRP:HE3	24:W:217:VAL:HG21	1.64	0.62
1:1:2899:C:O2'	1:1:2901:G:OP2	2.15	0.62
1:1:294:U:O2'	1:1:295:A:O5'	2.16	0.62
5:B:187:SER:O	5:B:189:SER:N	2.33	0.62
7:D:397:ASN:ND2	7:D:467:LYS:O	2.32	0.62
1:1:598:A:OP1	9:F:41:ARG:NE	2.33	0.62
1:1:1456:A:O2'	1:1:1457:U:O4'	2.17	0.62
44:v:177:GLN:OE1	44:v:225:ARG:NH1	2.32	0.62
1:1:542:G:O6	1:1:550:A:N6	2.33	0.61
1:1:3092:C:O2'	1:1:3094:A:OP2	2.12	0.61
1:1:3158:G:O6	1:1:3292:A:N1	2.32	0.61
18:P:47:TYR:O	18:P:51:VAL:HG23	1.99	0.61
46:y:156:ASN:ND2	46:y:201:ASP:OD2	2.34	0.61
1:1:634:C:O3'	31:e:47:ARG:NH2	2.33	0.61
1:1:949:C:O2'	1:1:971:G:OP1	2.17	0.61
1:1:3085:G:OP1	43:u:34:SER:OG	2.18	0.61
2:2:57:C:O2	2:2:61:A:O2'	2.18	0.61
5:B:303:LYS:NZ	5:B:371:GLN:OE1	2.33	0.61
25:X:72:ALA:O	25:X:76:VAL:HG23	1.99	0.61
46:y:175:SER:O	46:y:178:GLN:NE2	2.33	0.61
1:1:1191:U:OP2	17:O:49:ARG:NE	2.33	0.61
1:1:428:A:N6	1:1:632:G:O6	2.34	0.61
1:1:1120:A:N6	1:1:1139:G:O6	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:90:GLU:N	4:A:98:TYR:O	2.33	0.61
13:K:224:ASN:OD1	13:K:225:ASN:N	2.33	0.61
3:6:35:C:O2'	13:K:84:ASN:ND2	2.33	0.61
6:C:152:VAL:O	6:C:252:GLU:N	2.34	0.61
1:1:1820:U:O2	1:1:1822:C:N4	2.33	0.61
1:1:3089:C:OP1	5:B:222:LYS:NZ	2.33	0.61
2:2:12:A:C2	2:2:13:A:C8	2.89	0.61
5:B:212:ASN:OD1	5:B:354:VAL:HG22	2.00	0.61
13:K:229:VAL:HG22	13:K:233:GLN:OE1	2.01	0.61
1:1:1481:A:N6	1:1:1872:C:O2	2.34	0.61
5:B:31:ALA:O	5:B:339:ARG:NH1	2.34	0.61
37:m:325:ARG:NH1	37:m:399:ARG:O	2.34	0.61
1:1:3275:U:O2'	32:f:99:ARG:NH1	2.34	0.60
46:y:11:ASN:OD1	46:y:187:ASN:ND2	2.33	0.60
1:1:1167:U:O2'	9:F:210:PRO:O	2.18	0.60
4:A:148:HIS:CE1	4:A:223:VAL:HG21	2.36	0.60
6:C:289:ILE:HG21	19:Q:32:LEU:HD11	1.83	0.60
36:k:11:PHE:O	36:k:15:THR:HG23	2.02	0.60
1:1:1222:G:HO2'	1:1:1285:G:H1	1.46	0.60
5:B:284:ARG:NH1	5:B:295:ALA:O	2.34	0.60
1:1:163:C:OP1	44:v:213:GLY:N	2.34	0.60
1:1:1307:G:O2'	1:1:1308:A:OP2	2.19	0.60
29:b:77:PHE:CZ	29:b:163:ILE:HD11	2.36	0.60
24:W:92:LEU:HD12	24:W:93:SER:N	2.17	0.60
1:1:508:U:C2	1:1:584:G:C2	2.89	0.60
44:v:184:TRP:CZ2	44:v:188:LEU:HD11	2.37	0.60
3:6:229:U:OP2	42:t:48:LYS:NZ	2.23	0.59
16:N:122:ASN:OD1	16:N:123:GLN:N	2.34	0.59
42:t:58:ALA:O	42:t:62:VAL:HG23	2.02	0.59
46:y:101:LEU:HD22	46:y:107:VAL:HG21	1.84	0.59
1:1:707:U:O2'	1:1:754:G:N3	2.35	0.59
1:1:508:U:C2	1:1:584:G:N1	2.70	0.59
1:1:2988:C:OP1	17:O:65:ASN:ND2	2.35	0.59
1:1:644:G:H1'	1:1:1117:G:H21	1.67	0.59
8:E:51:ARG:NH1	8:E:161:ALA:O	2.36	0.59
1:1:15:C:OP1	25:X:42:ARG:NE	2.36	0.59
1:1:3060:C:O3'	1:1:3371:G:N2	2.36	0.59
8:E:40:LEU:N	8:E:52:VAL:O	2.30	0.59
23:V:104:ASN:OD1	23:V:108:GLU:N	2.35	0.59
29:b:180:LYS:NZ	29:b:221:THR:O	2.30	0.59
37:m:261:GLU:OE1	37:m:265:ARG:NH1	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1383:G:HO2'	6:C:243:HIS:HD1	1.50	0.59
18:P:39:TRP:O	18:P:114:VAL:HG12	2.02	0.59
1:1:283:G:N2	1:1:284:A:N7	2.51	0.58
44:v:155:GLU:O	44:v:159:VAL:HG23	2.03	0.58
1:1:1149:G:OP2	32:f:21:ARG:NH2	2.36	0.58
1:1:1508:C:HO2'	1:1:2353:G:HO2'	1.46	0.58
9:F:189:ILE:HG23	9:F:190:THR:HG23	1.84	0.58
1:1:1776:G:O2'	1:1:1777:U:O4'	2.20	0.58
18:P:30:ARG:HA	18:P:119:VAL:HG11	1.84	0.58
39:o:92:ILE:HG23	39:o:167:LEU:HB2	1.85	0.58
1:1:120:G:O2'	37:m:264:ARG:O	2.18	0.58
1:1:392:G:HO2'	26:Y:90:VAL:HG11	1.66	0.58
1:1:438:A:OP1	31:e:118:LYS:NZ	2.36	0.58
1:1:660:A:N1	1:1:941:G:O2'	2.35	0.58
4:A:41:VAL:HG13	4:A:45:HIS:HB2	1.86	0.58
6:C:157:GLU:OE2	6:C:210:ALA:N	2.37	0.58
32:f:9:VAL:HG21	32:f:44:TYR:HE1	1.68	0.58
1:1:3016:A:O2'	1:1:3017:A:O5'	2.21	0.58
7:D:286:ARG:NH2	13:K:69:ASP:OD1	2.36	0.58
29:b:86:TYR:CZ	29:b:153:VAL:HG23	2.38	0.58
37:m:616:SER:O	37:m:620:SER:OG	2.05	0.58
8:E:70:LYS:N	8:E:142:ASP:OD2	2.36	0.58
37:m:701:ASP:OD2	37:m:703:ARG:NH1	2.37	0.58
5:B:288:GLY:N	5:B:320:ASP:OD1	2.36	0.57
29:b:163:ILE:HG22	29:b:206:VAL:HG11	1.84	0.57
30:d:11:GLU:OE1	30:d:72:ARG:NE	2.36	0.57
6:C:261:VAL:O	6:C:271:LYS:NZ	2.37	0.57
1:1:594:U:OP1	1:1:609:G:N1	2.32	0.57
10:G:89:GLU:HG3	39:o:156:LEU:HD12	1.85	0.57
2:2:70:G:O2'	2:2:87:G:N2	2.38	0.57
12:J:225:SER:OG	12:J:228:ASN:ND2	2.36	0.57
13:K:88:PHE:O	13:K:89:THR:HG22	2.05	0.57
1:1:1283:C:HO2'	1:1:1284:C:P	2.28	0.57
1:1:3348:G:O2'	1:1:3349:C:O5'	2.22	0.57
5:B:35:ASP:OD1	5:B:36:ASP:N	2.38	0.57
5:B:90:VAL:HG22	5:B:104:THR:HG22	1.87	0.57
46:y:119:PRO:O	46:y:139:ARG:NH1	2.38	0.57
1:1:1103:A:O2'	1:1:1104:G:OP1	2.22	0.57
23:V:102:ILE:O	23:V:102:ILE:HD12	2.04	0.57
1:1:3329:U:O2'	5:B:363:SER:OG	2.21	0.57
24:W:63:SER:HG	24:W:105:THR:CB	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:e:6:HIS:O	31:e:6:HIS:ND1	2.37	0.57
38:n:24:LYS:O	38:n:26:GLN:NE2	2.38	0.57
44:v:36:ILE:O	44:v:40:TRP:N	2.36	0.57
46:y:85:ARG:NH1	46:y:89:PRO:O	2.38	0.56
1:1:1151:U:OP1	32:f:21:ARG:NH2	2.38	0.56
1:1:1866:C:O2'	1:1:1867:A:O4'	2.23	0.56
31:e:42:VAL:O	31:e:52:GLN:NE2	2.38	0.56
5:B:86:VAL:HG22	5:B:162:VAL:HG12	1.86	0.56
25:X:4:SER:O	25:X:7:ALA:N	2.38	0.56
37:m:276:VAL:O	37:m:280:VAL:HG23	2.06	0.56
39:o:149:GLN:HG3	39:o:166:VAL:HG23	1.86	0.56
39:o:190:THR:O	39:o:190:THR:HG22	2.06	0.56
13:K:182:ALA:HB3	13:K:187:VAL:HG22	1.87	0.56
40:p:241:MET:O	40:p:277:ARG:NH1	2.38	0.56
1:1:99:A:OP1	16:N:194:GLN:NE2	2.38	0.56
1:1:1468:A:N1	1:1:1881:A:O2'	2.34	0.56
6:C:211:GLU:OE1	6:C:213:ASN:ND2	2.38	0.56
7:D:312:ILE:HG22	7:D:312:ILE:O	2.06	0.56
1:1:216:G:OP1	26:Y:16:ARG:NH1	2.39	0.56
37:m:224:ILE:HD11	45:w:669:LEU:HD12	1.88	0.56
37:m:272:GLU:O	37:m:276:VAL:HG23	2.05	0.56
1:1:1278:A:O2'	1:1:1279:C:O5'	2.19	0.56
46:y:39:GLU:O	46:y:43:GLY:N	2.38	0.56
29:b:175:TYR:O	29:b:178:VAL:HG23	2.06	0.56
1:1:69:C:O2'	1:1:101:G:O2'	2.06	0.56
1:1:102:C:O2'	14:L:62:THR:OG1	2.24	0.56
3:6:231:A:O2'	3:6:232:A:O4'	2.19	0.56
16:N:9:GLU:HB3	34:i:44:VAL:HG21	1.87	0.56
2:2:129:C:OP1	38:n:10:GLY:N	2.37	0.55
32:f:75:HIS:N	32:f:80:VAL:O	2.38	0.55
1:1:1:G:OP2	1:1:1:G:N2	2.35	0.55
1:1:1187:C:O3'	1:1:1295:G:N2	2.38	0.55
1:1:3041:U:OP1	23:V:12:ARG:NH1	2.38	0.55
2:2:56:G:OP1	35:j:68:LYS:NZ	2.35	0.55
1:1:323:A:N6	1:1:324:A:N1	2.54	0.55
10:G:140:VAL:HG21	16:N:3:ALA:HB2	1.89	0.55
1:1:1524:A:O2'	1:1:1526:U:OP1	2.17	0.55
2:2:157:U:N3	42:t:55:PHE:O	2.39	0.55
23:V:53:SER:OG	23:V:56:ASP:OD2	2.18	0.55
1:1:696:C:OP2	6:C:119:ARG:NH2	2.40	0.55
1:1:75:G:HO2'	1:1:76:G:P	2.30	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:114:A:N1	1:1:266:A:O2'	2.33	0.55
1:1:2830:G:N2	1:1:2831:G:C5	2.75	0.55
11:H:22:SER:O	11:H:24:ILE:N	2.40	0.55
1:1:1560:G:HO2'	1:1:1561:G:C5'	2.08	0.55
1:1:1601:U:OP1	20:R:42:ARG:NH1	2.37	0.55
1:1:3329:U:HO2'	5:B:363:SER:HG	1.54	0.55
14:L:61:PRO:O	14:L:62:THR:OG1	2.25	0.55
1:1:166:C:OP2	44:v:217:ARG:NE	2.40	0.54
1:1:358:G:O2'	1:1:360:G:O6	2.25	0.54
10:G:134:TYR:CG	10:G:190:VAL:HG21	2.42	0.54
15:M:99:TRP:CE2	15:M:103:ILE:HD11	2.42	0.54
35:j:67:LEU:HD13	35:j:67:LEU:O	2.06	0.54
38:n:166:TRP:O	38:n:170:VAL:HG23	2.07	0.54
1:1:1412:G:OP1	31:e:105:ARG:NH1	2.39	0.54
1:1:1657:C:O2'	1:1:1797:A:OP1	2.15	0.54
12:J:252:ASP:O	12:J:256:VAL:HG23	2.07	0.54
1:1:36:C:O2'	1:1:934:G:N3	2.41	0.54
29:b:57:PHE:CE1	29:b:140:VAL:HG21	2.43	0.54
37:m:303:ILE:O	37:m:307:GLN:NE2	2.41	0.54
5:B:76:VAL:HG12	5:B:325:LYS:HA	1.89	0.54
29:b:2:GLN:NE2	29:b:74:VAL:O	2.37	0.54
46:y:122:ASP:OD1	46:y:125:THR:N	2.41	0.54
1:1:1408:G:OP2	31:e:31:ASN:ND2	2.40	0.54
3:6:15:C:HO2'	3:6:16:U:P	2.25	0.54
1:1:508:U:N3	1:1:584:G:C6	2.76	0.54
3:6:33:U:O2'	3:6:34:A:P	2.66	0.54
29:b:400:ARG:N	46:y:36:SER:OG	2.41	0.54
36:k:23:ALA:HB3	36:k:75:VAL:HG22	1.90	0.54
1:1:805:G:N1	1:1:939:U:O4	2.41	0.54
1:1:1201:C:O2'	1:1:1202:A:O4'	2.24	0.54
1:1:3265:C:N4	1:1:3266:G:O6	2.41	0.54
1:1:3292:A:O2'	5:B:132:LYS:NZ	2.40	0.54
1:1:3395:G:O2'	1:1:3396:U:OP2	2.22	0.54
16:N:27:VAL:HG23	16:N:129:TYR:CE2	2.42	0.54
1:1:2371:G:OP2	1:1:2372:A:N6	2.31	0.54
3:6:8:A:OP2	42:t:132:LYS:NZ	2.40	0.54
27:Z:22:LYS:NZ	27:Z:132:SER:OG	2.40	0.54
18:P:16:SER:HB3	18:P:149:VAL:HG22	1.90	0.53
1:1:3009:G:N2	5:B:15:GLY:O	2.40	0.53
1:1:3017:A:O2'	1:1:3018:C:O5'	2.27	0.53
6:C:237:GLN:O	6:C:246:ARG:NH1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:71:VAL:HG21	10:G:76:ALA:HB2	1.91	0.53
30:d:46:THR:HG21	30:d:91:SER:HB2	1.91	0.53
34:i:68:ARG:O	34:i:72:VAL:HG23	2.07	0.53
1:1:3367:C:OP2	1:1:3368:U:O2'	2.14	0.53
21:S:139:TYR:CD2	21:S:140:VAL:HG23	2.44	0.53
3:6:38:U:O2	3:6:42:G:C2	2.62	0.53
42:t:223:GLU:N	42:t:224:PRO:CD	2.72	0.53
1:1:1481:A:HO2'	1:1:1858:A:HO2'	1.46	0.53
1:1:1650:G:C6	1:1:1806:A:N6	2.77	0.53
40:p:336:ALA:N	40:p:345:ALA:O	2.42	0.53
1:1:665:A:N6	1:1:798:G:O6	2.41	0.53
1:1:649:A:O2'	1:1:650:C:P	2.67	0.53
1:1:1666:G:O2'	1:1:1743:G:O5'	2.26	0.53
1:1:3244:A:OP2	5:B:100:ARG:NH1	2.42	0.53
1:1:353:G:OP2	44:v:7:ARG:NE	2.39	0.53
11:H:41:ILE:CG2	11:H:43:VAL:HG22	2.39	0.53
1:1:406:G:OP1	1:1:1415:U:O2'	2.25	0.53
2:2:123:G:O2'	2:2:124:G:P	2.67	0.53
1:1:3199:G:OP1	11:H:21:LYS:NZ	2.41	0.52
1:1:3267:A:OP1	1:1:3268:A:N6	2.41	0.52
1:1:586:C:HO2'	1:1:1164:G:HO2'	1.44	0.52
12:J:250:SER:O	12:J:254:VAL:HG23	2.09	0.52
1:1:1227:C:HO2'	1:1:1228:C:P	2.29	0.52
1:1:2432:A:N1	1:1:2598:G:C6	2.78	0.52
11:H:71:VAL:O	11:H:75:VAL:HG23	2.09	0.52
19:Q:123:THR:OG1	19:Q:125:ASP:OD1	2.25	0.52
34:i:60:LEU:O	34:i:64:SER:N	2.36	0.52
37:m:440:VAL:HG23	37:m:796:ALA:HB1	1.91	0.52
37:m:613:GLN:NE2	37:m:619:THR:O	2.42	0.52
8:E:166:LYS:N	8:E:169:ASP:OD2	2.43	0.52
16:N:9:GLU:CB	34:i:44:VAL:HG21	2.40	0.52
16:N:124:ASP:OD2	16:N:125:SER:N	2.41	0.52
21:S:45:LEU:HD13	21:S:49:HIS:ND1	2.24	0.52
22:U:33:TYR:HD2	22:U:63:VAL:HG21	1.74	0.52
1:1:2832:C:O2	1:1:2833:A:N7	2.42	0.52
1:1:210:U:OP2	6:C:162:THR:N	2.43	0.52
2:2:99:C:P	25:X:53:HIS:HE2	2.32	0.52
19:Q:104:LEU:HD22	19:Q:105:ARG:HE	1.75	0.52
37:m:582:GLN:NE2	37:m:590:THR:OG1	2.43	0.52
4:A:144:GLU:OE1	4:A:150:GLN:NE2	2.41	0.52
1:1:84:U:OP2	1:1:85:A:O2'	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:547:G:O2'	1:1:548:G:O5'	2.26	0.52
38:n:431:TRP:NE1	38:n:442:VAL:HG13	2.25	0.52
2:2:12:A:C2	2:2:13:A:N7	2.78	0.52
29:b:77:PHE:CE2	29:b:163:ILE:HD11	2.45	0.52
1:1:3005:A:N1	1:1:3140:G:O2'	2.33	0.51
12:J:226:GLU:O	12:J:227:THR:OG1	2.24	0.51
1:1:1203:A:O2'	1:1:1204:A:OP2	2.25	0.51
1:1:3026:G:OP1	11:H:174:LYS:NZ	2.43	0.51
2:2:88:A:O2'	2:2:89:A:O5'	2.28	0.51
6:C:311:HIS:O	6:C:311:HIS:ND1	2.43	0.51
7:D:143:GLN:OE1	7:D:166:ASN:ND2	2.38	0.51
29:b:435:ILE:HD12	43:u:1:MET:HE3	1.91	0.51
40:p:109:LEU:C	40:p:109:LEU:HD13	2.36	0.51
1:1:1277:C:HO2'	1:1:1278:A:P	2.33	0.51
14:L:46:ILE:HG22	14:L:46:ILE:O	2.10	0.51
23:V:104:ASN:ND2	23:V:108:GLU:OE1	2.43	0.51
27:Z:76:ASN:OD1	27:Z:77:TYR:N	2.43	0.51
34:i:34:SER:O	34:i:37:THR:N	2.40	0.51
1:1:1595:U:C2	1:1:1596:C:C5	2.98	0.51
4:A:36:ILE:CD1	4:A:74:LEU:HD21	2.40	0.51
1:1:649:A:O2'	1:1:650:C:O5'	2.27	0.51
41:r:6:TYR:O	41:r:10:HIS:N	2.32	0.51
1:1:508:U:N3	1:1:584:G:N1	2.59	0.51
1:1:3187:A:OP1	11:H:23:ARG:NH2	2.44	0.51
1:1:3303:G:O2'	1:1:3305:A:N7	2.43	0.51
37:m:487:HIS:O	37:m:506:VAL:HG23	2.11	0.51
1:1:1129:A:HO2'	1:1:1130:A:P	2.29	0.51
1:1:1494:U:O2'	1:1:1496:C:N4	2.43	0.51
1:1:1456:A:HO2'	1:1:1457:U:C5'	2.20	0.51
1:1:35:A:O2'	1:1:809:G:N3	2.40	0.50
39:o:124:ARG:NH1	39:o:129:GLY:O	2.44	0.50
1:1:839:C:O2'	1:1:1724:U:OP1	2.24	0.50
11:H:167:VAL:HG12	11:H:170:LYS:HB2	1.92	0.50
37:m:444:SER:HG	37:m:493:TRP:CD1	2.29	0.50
46:y:21:ASN:ND2	46:y:112:ASP:OD2	2.43	0.50
1:1:431:U:OP1	32:f:65:ARG:NH1	2.42	0.50
2:2:95:G:O2'	35:j:81:GLY:O	2.30	0.50
1:1:2364:G:O6	1:1:2984:C:O2'	2.28	0.50
5:B:34:LYS:O	5:B:184:ASN:ND2	2.44	0.50
5:B:57:VAL:CG1	5:B:73:VAL:HG22	2.41	0.50
6:C:181:VAL:O	6:C:182:LEU:HD23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:122:ALA:HB1	18:P:123:PRO:HD2	1.92	0.50
37:m:487:HIS:C	37:m:506:VAL:HG23	2.37	0.50
43:u:61:LYS:O	43:u:111:ARG:NE	2.45	0.50
1:1:409:A:H62	2:2:15:G:N2	2.10	0.50
4:A:31:GLN:OE1	4:A:158:HIS:ND1	2.45	0.50
1:1:1861:G:O2'	1:1:1862:U:P	2.69	0.50
11:H:67:ALA:O	11:H:71:VAL:HG23	2.11	0.50
30:d:13:THR:OG1	30:d:72:ARG:NH1	2.40	0.50
1:1:269:G:OP2	16:N:44:ARG:NH1	2.43	0.50
2:2:81:U:O2'	2:2:83:C:OP1	2.29	0.50
3:6:33:U:O5'	13:K:285:ARG:NH1	2.44	0.50
5:B:219:ALA:CB	5:B:336:VAL:HG12	2.42	0.50
6:C:38:VAL:O	6:C:42:VAL:HG23	2.12	0.50
14:L:43:ALA:O	14:L:47:ALA:N	2.45	0.50
42:t:74:ARG:O	42:t:78:VAL:HG23	2.12	0.50
42:t:318:LEU:O	42:t:322:ASN:N	2.45	0.50
1:1:3020:U:OP1	29:b:400:ARG:NH2	2.44	0.50
11:H:57:VAL:HG23	11:H:68:LEU:HD23	1.92	0.50
13:K:102:VAL:HG22	13:K:262:ASN:OD1	2.12	0.50
20:R:23:TRP:CE3	20:R:51:VAL:HG22	2.47	0.49
24:W:220:TYR:N	24:W:229:GLU:O	2.45	0.49
39:o:95:VAL:HG12	39:o:98:LEU:HD11	1.93	0.49
39:o:149:GLN:CG	39:o:166:VAL:HG23	2.42	0.49
46:y:118:HIS:CE1	46:y:146:ILE:HD11	2.46	0.49
1:1:213:A:N6	1:1:227:G:O2'	2.43	0.49
5:B:187:SER:O	5:B:190:GLU:N	2.42	0.49
7:D:380:THR:O	7:D:384:THR:OG1	2.30	0.49
11:H:61:GLY:O	11:H:65:VAL:HG23	2.11	0.49
37:m:322:MET:N	37:m:322:MET:SD	2.85	0.49
1:1:67:A:O2'	1:1:315:C:O2	2.26	0.49
1:1:3287:U:HO2'	1:1:3288:G:C5'	2.25	0.49
29:b:250:VAL:HG11	29:b:278:PHE:CD2	2.47	0.49
42:t:208:ILE:HG21	42:t:251:ILE:HG13	1.94	0.49
1:1:54:C:O2'	1:1:1547:G:O2'	2.12	0.49
1:1:1710:C:C2	1:1:1711:C:C5	3.01	0.49
3:6:15:C:O2'	3:6:16:U:P	2.70	0.49
18:P:87:SER:O	18:P:91:VAL:HG23	2.13	0.49
1:1:117:U:O2'	1:1:119:U:OP2	2.24	0.49
4:A:133:SER:O	4:A:175:HIS:NE2	2.23	0.49
24:W:26:ILE:O	24:W:30:VAL:HG23	2.12	0.49
27:Z:11:ALA:HB1	27:Z:80:LEU:HD22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:103:G:O2'	1:1:699:A:O2'	2.16	0.49
6:C:168:ALA:O	6:C:172:VAL:HG23	2.12	0.49
13:K:259:PHE:O	13:K:263:VAL:HG23	2.11	0.49
1:1:3123:A:OP1	17:O:134:LYS:NZ	2.44	0.49
2:2:71:A:H4'	2:2:72:A:O5'	2.13	0.49
1:1:406:G:HO2'	1:1:407:A:P	2.36	0.49
1:1:734:C:O2'	1:1:735:A:OP1	2.31	0.49
1:1:1158:A:OP2	9:F:90:LYS:NZ	2.46	0.49
1:1:1561:G:O2'	1:1:1562:C:OP2	2.28	0.49
2:2:95:G:OP2	35:j:72:ARG:NH1	2.44	0.49
4:A:148:HIS:HB2	12:J:201:MET:HE1	1.95	0.49
16:N:6:TYR:CZ	34:i:40:VAL:HG22	2.48	0.49
1:1:1626:U:OP1	37:m:681:ARG:NH1	2.41	0.49
5:B:372:THR:OG1	5:B:375:GLU:OE2	2.31	0.49
44:v:184:TRP:CH2	44:v:188:LEU:HD11	2.48	0.49
1:1:409:A:N6	2:2:14:C:H42	2.11	0.48
1:1:2995:A:O2'	1:1:2996:U:OP1	2.23	0.48
11:H:36:LYS:NZ	11:H:152:GLU:OE2	2.37	0.48
18:P:122:ALA:HB1	18:P:123:PRO:CD	2.43	0.48
24:W:73:LEU:HD12	24:W:100:THR:HB	1.94	0.48
1:1:1419:A:OP1	2:2:20:U:O2'	2.31	0.48
25:X:10:ALA:O	25:X:14:VAL:HG23	2.13	0.48
1:1:494:G:HO2'	1:1:495:G:C5'	2.26	0.48
1:1:1637:A:HO2'	1:1:1709:C:HO2'	1.45	0.48
10:G:135:GLY:O	10:G:139:VAL:HG23	2.14	0.48
11:H:20:ILE:HB	15:M:7:VAL:HG22	1.95	0.48
26:Y:40:ARG:O	26:Y:44:GLY:N	2.41	0.48
43:u:82:ASN:O	43:u:86:VAL:HG23	2.12	0.48
13:K:225:ASN:O	13:K:229:VAL:HG23	2.13	0.48
38:n:25:LEU:O	38:n:27:VAL:HG23	2.14	0.48
1:1:709:A:H4'	1:1:710:A:OP1	2.13	0.48
1:1:2933:A:N7	1:1:3014:U:O2'	2.46	0.48
1:1:338:A:OP1	6:C:48:GLN:N	2.37	0.48
1:1:1613:A:OP1	36:k:51:LEU:N	2.47	0.48
1:1:3165:A:N6	1:1:3286:G:O6	2.47	0.48
1:1:3355:U:HO2'	1:1:3356:G:P	2.31	0.48
2:2:142:C:OP1	16:N:38:ARG:NH1	2.43	0.48
5:B:188:ILE:HG22	5:B:191:LYS:HE3	1.96	0.48
30:d:28:ARG:O	30:d:32:ALA:N	2.42	0.48
46:y:38:PHE:HE1	46:y:205:VAL:HG21	1.78	0.48
1:1:1380:G:OP1	6:C:191:LYS:N	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1508:C:N4	1:1:1880:U:O2'	2.47	0.48
1:1:3098:G:OP1	5:B:279:ASN:ND2	2.45	0.48
1:1:3288:G:O2'	1:1:3289:G:P	2.71	0.48
9:F:163:LEU:HD13	9:F:169:ILE:HD11	1.95	0.48
1:1:644:G:O2'	1:1:1117:G:N2	2.47	0.48
1:1:3266:G:O2'	1:1:3267:A:O4'	2.24	0.48
1:1:1188:U:P	1:1:1210:U:HO2'	2.31	0.48
1:1:1709:C:C2	1:1:1710:C:C5	3.01	0.48
1:1:77:A:OP2	14:L:73:ARG:NH2	2.47	0.47
1:1:208:C:OP2	6:C:163:LYS:NZ	2.41	0.47
1:1:595:G:OP2	9:F:30:ARG:NH2	2.46	0.47
1:1:784:A:N7	19:Q:65:SER:OG	2.36	0.47
1:1:960:U:O2	1:1:960:U:H2'	2.14	0.47
2:2:149:A:N3	10:G:55:TYR:OH	2.35	0.47
4:A:192:GLU:N	4:A:213:VAL:O	2.44	0.47
5:B:377:HIS:O	5:B:381:GLY:N	2.45	0.47
34:i:66:GLU:OE2	34:i:91:ASN:ND2	2.46	0.47
1:1:1383:G:OP1	6:C:203:ARG:NE	2.44	0.47
1:1:1561:G:O2'	1:1:1562:C:P	2.71	0.47
1:1:1855:U:O2	1:1:1856:C:C5	2.67	0.47
2:2:14:C:HO2'	2:2:15:G:P	2.35	0.47
35:j:54:LYS:O	35:j:58:THR:N	2.46	0.47
37:m:525:ASN:O	37:m:528:THR:OG1	2.31	0.47
1:1:3084:C:HO2'	1:1:3085:G:H5'	1.79	0.47
35:j:66:TYR:OH	35:j:73:ARG:NH2	2.47	0.47
45:w:834:ALA:O	45:w:838:HIS:N	2.48	0.47
1:1:1568:U:N3	1:1:1574:C:O4'	2.47	0.47
1:1:3017:A:HO2'	1:1:3018:C:H6	1.62	0.47
5:B:348:ARG:CZ	29:b:411:VAL:HG23	2.45	0.47
6:C:181:VAL:HG12	6:C:182:LEU:N	2.29	0.47
23:V:118:VAL:HG21	23:V:133:SER:HB3	1.97	0.47
24:W:41:TRP:CE3	24:W:217:VAL:HG21	2.47	0.47
1:1:100:A:H3'	1:1:101:G:H21	1.79	0.47
1:1:1405:U:H4'	1:1:1406:A:OP1	2.14	0.47
1:1:2986:U:C2'	1:1:2987:A:O5'	2.61	0.47
1:1:591:G:N2	1:1:612:U:OP1	2.39	0.47
4:A:224:ILE:O	4:A:225:LEU:HD22	2.15	0.47
1:1:20:A:OP2	33:h:86:ARG:NH2	2.43	0.47
1:1:47:C:OP2	1:1:48:A:O2'	2.12	0.47
1:1:1300:G:O2'	41:r:48:LYS:NZ	2.48	0.47
1:1:1712:G:N1	1:1:1733:G:O6	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:110:ALA:O	27:Z:114:VAL:HG23	2.14	0.47
29:b:107:GLN:OE1	29:b:110:ARG:NH1	2.48	0.47
35:j:54:LYS:C	35:j:58:THR:HG23	2.40	0.47
46:y:38:PHE:CE1	46:y:205:VAL:HG21	2.50	0.47
1:1:226:C:H4'	26:Y:29:VAL:HG12	1.96	0.47
1:1:1293:U:C2	1:1:1294:A:C8	3.02	0.47
1:1:2432:A:C6	1:1:2598:G:C6	3.03	0.47
3:6:1:C:O2'	3:6:2:C:P	2.73	0.47
3:6:16:U:C2'	3:6:17:G:OP2	2.62	0.47
1:1:251:G:OP1	37:m:281:ARG:NE	2.47	0.47
19:Q:44:PHE:O	19:Q:48:VAL:HG23	2.15	0.47
23:V:136:VAL:HG21	46:y:62:MET:SD	2.55	0.47
33:h:29:ALA:O	33:h:33:VAL:HG23	2.15	0.47
1:1:107:A:O2'	1:1:324:A:N3	2.42	0.47
4:A:140:ASP:OD2	4:A:141:GLN:N	2.48	0.47
9:F:157:ASN:C	9:F:157:ASN:OD1	2.57	0.47
25:X:95:ILE:O	25:X:99:VAL:HG23	2.15	0.47
29:b:86:TYR:CE2	29:b:153:VAL:HG23	2.50	0.47
40:p:152:TYR:O	40:p:216:VAL:HG21	2.14	0.47
1:1:175:G:O2'	1:1:176:G:P	2.72	0.46
1:1:189:G:O2'	1:1:190:U:O4'	2.32	0.46
1:1:1299:U:N3	1:1:1300:G:N7	2.63	0.46
1:1:1757:A:C6	1:1:1769:G:C6	3.03	0.46
7:D:119:VAL:HG13	7:D:194:ILE:HD11	1.97	0.46
10:G:54:GLU:O	10:G:58:VAL:HG23	2.14	0.46
10:G:184:ALA:O	10:G:188:THR:HG23	2.15	0.46
29:b:403:GLU:O	29:b:408:GLY:N	2.38	0.46
38:n:175:LEU:HD13	38:n:192:ILE:HD13	1.96	0.46
1:1:1565:G:C6	38:n:29:LEU:HD22	2.51	0.46
1:1:1812:G:O2'	1:1:1817:G:N3	2.47	0.46
1:1:2388:U:O2	18:P:69:ARG:NH2	2.48	0.46
11:H:12:VAL:HG22	11:H:79:ILE:HD13	1.97	0.46
30:d:46:THR:HG21	30:d:91:SER:CB	2.44	0.46
33:h:93:THR:HG22	33:h:94:LYS:H	1.81	0.46
37:m:323:HIS:O	38:n:44:ARG:NH2	2.49	0.46
1:1:701:G:N2	1:1:788:C:O3'	2.49	0.46
14:L:42:ARG:O	14:L:46:ILE:N	2.48	0.46
21:S:10:ILE:HD12	21:S:59:VAL:HG23	1.97	0.46
26:Y:11:ASP:OD1	26:Y:13:ARG:N	2.49	0.46
1:1:122:A:N6	1:1:146:U:O4'	2.48	0.46
1:1:3111:U:N3	1:1:3121:U:O4	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:98:ILE:HD13	29:b:143:LEU:HD23	1.98	0.46
37:m:794:PHE:CD1	37:m:804:LEU:HD23	2.50	0.46
1:1:1278:A:O2'	1:1:1279:C:P	2.73	0.46
1:1:1287:A:O2'	1:1:1288:U:O4'	2.31	0.46
3:6:33:U:O2	3:6:33:U:C2'	2.63	0.46
7:D:408:SER:OG	7:D:410:VAL:HG22	2.16	0.46
9:F:156:ILE:HD12	9:F:161:VAL:HG21	1.97	0.46
10:G:134:TYR:CD1	10:G:190:VAL:HG21	2.50	0.46
1:1:122:A:O2'	1:1:145:G:N2	2.49	0.46
2:2:11:C:C2	2:2:12:A:C8	3.04	0.46
8:E:82:ARG:O	32:f:105:SER:N	2.44	0.46
15:M:127:LYS:O	15:M:131:VAL:HG23	2.15	0.46
37:m:660:ARG:NE	37:m:681:ARG:O	2.47	0.46
1:1:786:A:OP2	19:Q:146:SER:OG	2.28	0.46
1:1:2986:U:H2'	1:1:2987:A:O5'	2.15	0.46
2:2:128:U:OP1	2:2:129:C:N4	2.46	0.46
21:S:139:TYR:CE2	21:S:140:VAL:HG23	2.51	0.46
1:1:2830:G:H2'	1:1:2830:G:N3	2.30	0.46
3:6:18:U:OP2	13:K:210:ARG:NH2	2.45	0.46
18:P:120:ASN:OD1	18:P:120:ASN:N	2.49	0.46
29:b:325:GLU:O	29:b:328:VAL:HG13	2.16	0.46
46:y:115:ALA:N	46:y:136:GLU:O	2.46	0.46
1:1:1242:G:OP2	29:b:233:ASN:ND2	2.46	0.46
1:1:3300:U:N3	1:1:3301:U:C5	2.84	0.46
1:1:3376:A:OP1	30:d:18:LYS:NZ	2.21	0.46
23:V:25:CYS:O	23:V:32:ARG:NH1	2.49	0.46
29:b:443:ASP:O	43:u:75:ARG:NH2	2.49	0.46
40:p:340:THR:HG23	40:p:341:LEU:N	2.30	0.46
1:1:3355:U:O2'	1:1:3356:G:P	2.73	0.46
24:W:158:ILE:HG22	24:W:160:SER:H	1.80	0.46
27:Z:33:SER:OG	27:Z:34:LYS:N	2.49	0.46
29:b:283:VAL:HB	29:b:315:VAL:HG12	1.98	0.46
34:i:83:ALA:O	34:i:87:VAL:HG23	2.16	0.46
1:1:348:A:N3	1:1:352:A:O2'	2.49	0.45
1:1:1187:C:HO2'	1:1:1295:G:N2	2.14	0.45
1:1:1747:G:H21	36:k:2:ALA:CB	2.29	0.45
3:6:32:A:C4	13:K:285:ARG:HD3	2.51	0.45
6:C:246:ARG:O	6:C:248:VAL:HG23	2.16	0.45
25:X:5:ALA:O	25:X:8:THR:OG1	2.26	0.45
29:b:104:LEU:O	29:b:108:VAL:HG23	2.16	0.45
41:r:11:ILE:O	41:r:15:GLY:N	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:u:56:ARG:NE	43:u:62:GLU:OE1	2.43	0.45
1:1:1224:C:C2	1:1:1225:A:C8	3.05	0.45
1:1:1743:G:N3	1:1:1743:G:H2'	2.31	0.45
5:B:295:ALA:HB2	5:B:301:THR:O	2.15	0.45
26:Y:59:VAL:HG12	26:Y:59:VAL:O	2.17	0.45
1:1:239:G:H4'	1:1:240:U:OP1	2.16	0.45
2:2:11:C:O2	2:2:12:A:C8	2.69	0.45
4:A:86:VAL:C	4:A:87:LEU:HD22	2.41	0.45
21:S:77:VAL:HG22	21:S:126:VAL:HG13	1.98	0.45
1:1:353:G:O6	35:j:55:ARG:NH2	2.50	0.45
1:1:413:U:OP1	18:P:34:GLN:NE2	2.48	0.45
5:B:161:LEU:HD22	5:B:178:LEU:HD11	1.98	0.45
14:L:47:ALA:O	44:v:50:TYR:OH	2.24	0.45
38:n:129:ILE:O	38:n:132:ILE:HG22	2.17	0.45
1:1:3036:G:H2'	1:1:3037:U:O4'	2.16	0.45
5:B:66:LYS:O	5:B:70:ARG:NH2	2.50	0.45
6:C:260:GLN:O	6:C:270:SER:OG	2.23	0.45
11:H:41:ILE:HG23	11:H:43:VAL:HG22	1.99	0.45
13:K:254:LEU:O	13:K:259:PHE:HB2	2.17	0.45
31:e:95:GLU:OE1	31:e:120:THR:OG1	2.16	0.45
37:m:749:VAL:HG13	37:m:767:LEU:HB2	1.98	0.45
38:n:368:SER:O	38:n:371:VAL:HG22	2.17	0.45
1:1:1698:C:N4	1:1:1699:A:H62	2.14	0.45
1:1:3287:U:H2'	1:1:3288:G:C8	2.51	0.45
3:6:27:G:OP1	39:o:130:ASN:ND2	2.46	0.45
7:D:306:ALA:O	7:D:310:ASN:ND2	2.50	0.45
14:L:119:TYR:O	14:L:123:ILE:HG23	2.16	0.45
16:N:14:LYS:HA	16:N:19:LEU:HD12	1.98	0.45
28:a:82:ILE:HD11	28:a:102:ILE:HD11	1.98	0.45
1:1:178:U:O2'	44:v:31:GLN:OE1	2.33	0.45
1:1:1423:C:C2	1:1:1424:C:C5	3.05	0.45
1:1:3258:U:O2'	1:1:3260:G:OP1	2.34	0.45
2:2:85:G:O6	26:Y:114:ASP:N	2.42	0.45
6:C:257:LYS:O	6:C:261:VAL:HG23	2.16	0.45
10:G:55:TYR:CZ	10:G:56:VAL:HG23	2.52	0.45
32:f:49:ILE:O	32:f:69:GLY:N	2.50	0.45
38:n:431:TRP:NE1	38:n:442:VAL:O	2.49	0.45
45:w:667:HIS:O	45:w:671:LEU:HD23	2.16	0.45
2:2:154:C:OP1	10:G:181:LYS:NZ	2.48	0.45
3:6:45:U:O2	13:K:243:THR:OG1	2.30	0.45
4:A:90:GLU:O	4:A:98:TYR:N	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1712:G:H4'	1:1:1713:G:OP1	2.16	0.45
1:1:3306:U:OP1	5:B:269:GLN:NE2	2.50	0.45
14:L:62:THR:O	14:L:64:LYS:N	2.50	0.45
1:1:1635:G:C4	1:1:1637:A:OP2	2.71	0.44
13:K:162:THR:HG23	13:K:163:VAL:N	2.32	0.44
19:Q:125:ASP:O	19:Q:129:VAL:HG23	2.17	0.44
1:1:1596:C:C2	1:1:1597:C:C5	3.05	0.44
20:R:23:TRP:HE3	20:R:51:VAL:HG22	1.82	0.44
23:V:118:VAL:O	23:V:137:VAL:N	2.50	0.44
29:b:184:LEU:HA	29:b:187:ILE:HG22	1.98	0.44
1:1:494:G:H4'	1:1:495:G:OP1	2.17	0.44
1:1:1816:A:HO2'	1:1:1817:G:P	2.39	0.44
18:P:122:ALA:HB3	18:P:143:PRO:O	2.17	0.44
33:h:50:SER:O	33:h:54:VAL:HG23	2.17	0.44
42:t:90:THR:HG22	42:t:90:THR:O	2.17	0.44
1:1:195:U:H2'	1:1:196:G:O4'	2.18	0.44
1:1:196:G:N1	1:1:199:A:OP2	2.48	0.44
1:1:340:C:OP2	6:C:195:ARG:NH2	2.51	0.44
1:1:976:U:O2	1:1:976:U:O4'	2.35	0.44
1:1:1757:A:N6	1:1:1769:G:O6	2.50	0.44
8:E:52:VAL:HG11	8:E:65:ILE:HD13	1.99	0.44
15:M:99:TRP:NE1	15:M:103:ILE:HD11	2.33	0.44
16:N:66:VAL:HG11	16:N:102:ALA:HB2	1.99	0.44
25:X:67:ILE:O	25:X:141:TYR:OH	2.23	0.44
1:1:1160:C:N3	1:1:1366:A:O2'	2.49	0.44
2:2:88:A:C2'	2:2:89:A:O5'	2.65	0.44
1:1:525:C:OP2	15:M:77:ARG:NH2	2.51	0.44
1:1:1231:A:OP2	24:W:49:ARG:NE	2.51	0.44
1:1:1514:G:H2'	1:1:1514:G:N3	2.32	0.44
19:Q:19:PRO:HG3	19:Q:30:VAL:HG21	1.99	0.44
20:R:19:LYS:HA	20:R:22:VAL:HG22	1.99	0.44
21:S:77:VAL:HG12	21:S:79:VAL:HG23	2.00	0.44
29:b:250:VAL:HG13	29:b:283:VAL:HG13	1.99	0.44
37:m:171:ILE:O	37:m:171:ILE:HG22	2.17	0.44
1:1:369:A:O2'	1:1:370:U:H5''	2.17	0.44
1:1:1225:A:C4	1:1:1226:G:C8	3.06	0.44
1:1:1325:U:O4	1:1:1326:A:N6	2.50	0.44
1:1:1642:A:N3	1:1:1822:C:O2'	2.47	0.44
1:1:3214:U:OP2	15:M:128:ARG:NH2	2.42	0.44
11:H:160:ASP:O	11:H:164:ILE:HG23	2.18	0.44
39:o:156:LEU:HD13	39:o:157:LEU:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1117:G:O6	1:1:1142:G:N2	2.50	0.44
1:1:3019:U:O2	1:1:3019:U:O4'	2.36	0.44
3:6:33:U:C5'	13:K:285:ARG:HE	2.30	0.44
4:A:74:LEU:HD22	4:A:86:VAL:HG21	1.99	0.44
22:U:100:THR:HG23	22:U:100:THR:O	2.17	0.44
45:w:669:LEU:HD11	45:w:679:LEU:HD11	1.99	0.44
1:1:252:U:O2'	44:v:218:ARG:NH2	2.51	0.44
1:1:3151:U:OP1	5:B:132:LYS:NZ	2.51	0.44
1:1:3181:C:O2	1:1:3181:C:O4'	2.36	0.44
5:B:41:VAL:HG22	5:B:186:GLY:HA3	1.99	0.44
13:K:77:ASP:O	13:K:251:LEU:N	2.49	0.44
37:m:303:ILE:O	37:m:303:ILE:HG22	2.18	0.44
1:1:551:A:O2'	1:1:552:G:O5'	2.31	0.43
1:1:304:G:O2'	1:1:305:U:P	2.76	0.43
1:1:1121:U:O4	1:1:1137:C:N3	2.51	0.43
1:1:1300:G:O3'	41:r:48:LYS:NZ	2.47	0.43
1:1:3302:U:H2'	1:1:3303:G:O4'	2.18	0.43
4:A:31:GLN:OE1	4:A:85:ASN:ND2	2.51	0.43
14:L:79:GLU:OE2	14:L:112:ASN:ND2	2.49	0.43
16:N:180:PHE:O	16:N:184:LYS:N	2.51	0.43
1:1:1628:C:N4	38:n:561:ASN:OD1	2.51	0.43
5:B:117:ARG:HA	5:B:175:LYS:HD2	2.00	0.43
12:J:228:ASN:ND2	12:J:252:ASP:OD2	2.46	0.43
24:W:74:GLN:O	24:W:78:GLY:N	2.51	0.43
37:m:241:GLU:N	37:m:241:GLU:OE1	2.51	0.43
1:1:3017:A:O2'	1:1:3018:C:C5'	2.66	0.43
13:K:129:ASP:O	13:K:132:ILE:HG22	2.18	0.43
24:W:47:ASP:OD2	24:W:126:ARG:NH2	2.48	0.43
37:m:754:VAL:HG12	37:m:754:VAL:O	2.18	0.43
39:o:120:VAL:HG23	39:o:137:LEU:HB3	2.00	0.43
1:1:293:C:H2'	1:1:294:U:O4'	2.18	0.43
1:1:526:C:N4	1:1:567:G:O6	2.52	0.43
1:1:784:A:O5'	19:Q:69:ARG:NH1	2.52	0.43
1:1:1546:A:H4'	16:N:101:THR:HG23	1.99	0.43
1:1:3217:C:H6	1:1:3266:G:H21	1.65	0.43
14:L:29:ALA:O	14:L:33:VAL:HG23	2.17	0.43
19:Q:111:ARG:O	19:Q:115:VAL:HG23	2.18	0.43
1:1:36:C:O3'	1:1:934:G:N2	2.51	0.43
4:A:139:PHE:CE2	4:A:157:VAL:HG22	2.53	0.43
5:B:286:GLY:N	5:B:321:PHE:O	2.44	0.43
11:H:20:ILE:HB	15:M:7:VAL:HG13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:159:ASP:O	13:K:163:VAL:HG12	2.18	0.43
14:L:27:ASP:O	14:L:28:GLN:C	2.61	0.43
29:b:184:LEU:HD22	29:b:220:ASP:HB2	1.99	0.43
38:n:412:VAL:HG22	38:n:414:ARG:H	1.83	0.43
1:1:743:C:O2	19:Q:141:ARG:NE	2.47	0.43
1:1:1259:A:OP1	24:W:67:MET:N	2.50	0.43
1:1:3356:G:H2'	1:1:3356:G:N3	2.32	0.43
5:B:160:VAL:N	5:B:181:ILE:O	2.45	0.43
5:B:188:ILE:HG22	5:B:191:LYS:HD2	2.01	0.43
18:P:114:VAL:HG13	18:P:114:VAL:O	2.19	0.43
33:h:63:ARG:NH2	33:h:79:ASP:OD2	2.49	0.43
1:1:692:A:OP1	16:N:201:ARG:NH2	2.44	0.43
1:1:1293:U:O2	1:1:1294:A:C8	2.72	0.43
39:o:190:THR:O	39:o:190:THR:CG2	2.67	0.43
41:r:55:TYR:O	41:r:59:VAL:HG23	2.19	0.43
42:t:67:ALA:HB1	42:t:153:VAL:HG23	2.01	0.43
1:1:210:U:OP2	6:C:162:THR:OG1	2.37	0.43
1:1:1234:G:H2'	1:1:1235:U:C5	2.54	0.43
1:1:1660:C:H2'	1:1:1661:G:H8	1.84	0.43
1:1:1807:G:H4'	1:1:1808:G:OP1	2.18	0.43
1:1:2829:U:O2	1:1:2829:U:H2'	2.18	0.43
6:C:156:LEU:HD13	6:C:156:LEU:O	2.19	0.43
13:K:81:ILE:HG22	13:K:281:ILE:HA	2.01	0.43
39:o:121:ARG:NH1	39:o:176:LEU:O	2.52	0.43
1:1:384:A:C6	1:1:1465:A:C6	3.07	0.43
1:1:750:G:C2	1:1:751:A:C8	3.06	0.43
1:1:1505:C:OP1	18:P:127:ARG:NH1	2.47	0.43
1:1:1546:A:O2'	16:N:104:GLU:OE1	2.35	0.43
1:1:1724:U:O2'	1:1:1725:C:OP2	2.34	0.43
1:1:1856:C:O2	1:1:1857:C:C5	2.72	0.43
1:1:3268:A:OP1	8:E:46:ARG:NH2	2.52	0.43
43:u:34:SER:O	43:u:35:LYS:C	2.62	0.43
1:1:777:U:H2'	1:1:778:U:O4'	2.19	0.42
1:1:789:A:O2'	6:C:114:ASN:ND2	2.48	0.42
1:1:1340:G:H2'	1:1:1341:U:C6	2.54	0.42
1:1:1481:A:O2'	1:1:1859:A:OP2	2.37	0.42
1:1:1579:C:O3'	1:1:1580:A:O4'	2.37	0.42
1:1:1671:C:H2'	1:1:1672:U:O4'	2.20	0.42
1:1:2907:G:C2	1:1:2908:G:C8	3.07	0.42
1:1:3287:U:H2'	1:1:3288:G:H8	1.84	0.42
37:m:518:PHE:HB3	37:m:522:ILE:HG21	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:t:103:ILE:HG22	42:t:311:GLU:O	2.19	0.42
1:1:1252:A:H62	1:1:1263:A:H2'	1.83	0.42
1:1:3008:A:H61	1:1:3139:A:N6	2.17	0.42
1:1:3193:C:H2'	1:1:3194:C:O4'	2.19	0.42
6:C:320:ASN:O	6:C:322:GLN:N	2.52	0.42
32:f:19:SER:N	32:f:22:VAL:O	2.44	0.42
42:t:295:GLU:OE2	42:t:299:ARG:NH2	2.48	0.42
1:1:198:A:N7	1:1:219:A:N6	2.67	0.42
1:1:1447:G:OP1	18:P:65:SER:OG	2.33	0.42
8:E:40:LEU:HD11	8:E:54:TYR:HB2	2.00	0.42
8:E:65:ILE:HD12	8:E:65:ILE:C	2.44	0.42
29:b:422:LEU:HD12	29:b:428:LYS:HD3	2.02	0.42
38:n:189:GLN:NE2	38:n:196:GLU:OE1	2.51	0.42
1:1:341:G:N1	2:2:24:G:O6	2.53	0.42
1:1:712:G:N2	1:1:754:G:O2'	2.49	0.42
1:1:1650:G:O6	1:1:1806:A:N6	2.52	0.42
14:L:109:PHE:O	14:L:113:VAL:HG23	2.20	0.42
33:h:83:LYS:O	35:j:73:ARG:NH1	2.50	0.42
38:n:417:LEU:HD12	38:n:417:LEU:O	2.19	0.42
1:1:1404:G:O6	31:e:16:LYS:NZ	2.51	0.42
1:1:1447:G:N7	18:P:25:SER:OG	2.47	0.42
1:1:3086:A:N3	1:1:3086:A:H2'	2.34	0.42
1:1:3332:U:H2'	1:1:3333:G:O4'	2.18	0.42
5:B:88:GLY:O	5:B:161:LEU:N	2.49	0.42
13:K:38:ILE:CG1	13:K:260:VAL:HG11	2.48	0.42
13:K:108:LYS:HB3	13:K:109:PRO:HD3	2.02	0.42
1:1:34:A:H3'	1:1:48:A:H61	1.84	0.42
1:1:1565:G:C5	38:n:29:LEU:HD22	2.54	0.42
1:1:1721:U:OP2	20:R:124:TYR:OH	2.21	0.42
39:o:189:ILE:HG22	39:o:191:LYS:O	2.20	0.42
1:1:26:A:N3	1:1:328:U:O2'	2.45	0.42
1:1:1776:G:H2'	1:1:1777:U:N1	2.35	0.42
1:1:3165:A:HO2'	1:1:3166:C:C5'	2.32	0.42
3:6:56:U:O2	3:6:56:U:H2'	2.20	0.42
15:M:28:SER:OG	15:M:53:VAL:HG23	2.20	0.42
37:m:334:ASN:N	37:m:336:GLU:OE1	2.40	0.42
38:n:241:GLY:O	38:n:267:ARG:N	2.52	0.42
40:p:113:ASP:OD1	40:p:113:ASP:N	2.52	0.42
46:y:111:ASN:OD1	46:y:114:VAL:N	2.43	0.42
1:1:1581:C:C4'	1:1:1582:C:OP1	2.67	0.42
5:B:211:GLN:HG2	5:B:285:VAL:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:144:LEU:HD21	13:K:223:THR:HG23	2.01	0.42
29:b:21:VAL:HG11	29:b:57:PHE:CE2	2.55	0.42
29:b:285:VAL:HB	29:b:317:ILE:HG22	2.01	0.42
38:n:408:THR:C	38:n:409:HIS:HD1	2.27	0.42
1:1:1295:G:C5	1:1:1296:C:C5	3.08	0.42
1:1:2830:G:O4'	29:b:131:ALA:HA	2.19	0.42
1:1:3013:U:O2	1:1:3042:U:N3	2.53	0.42
2:2:19:C:C2	2:2:20:U:C5	3.07	0.42
37:m:357:THR:O	37:m:362:ARG:NH1	2.52	0.42
1:1:543:C:H2'	1:1:544:C:O4'	2.20	0.42
1:1:1765:U:H4'	1:1:1766:G:OP1	2.19	0.42
1:1:1857:C:H2'	1:1:1858:A:C8	2.54	0.42
13:K:254:LEU:O	13:K:255:ARG:C	2.63	0.42
19:Q:82:VAL:N	19:Q:138:LEU:O	2.44	0.42
46:y:101:LEU:CD2	46:y:107:VAL:HG21	2.49	0.42
1:1:82:C:C4	1:1:83:U:C4	3.08	0.41
1:1:148:G:OP1	16:N:49:ARG:NH1	2.53	0.41
1:1:412:G:C6	2:2:12:A:C6	3.08	0.41
11:H:20:ILE:HG13	15:M:7:VAL:HG22	2.02	0.41
13:K:83:VAL:HG13	13:K:279:ILE:HG12	2.01	0.41
16:N:94:TYR:O	16:N:94:TYR:CG	2.72	0.41
34:i:56:ARG:HD2	34:i:60:LEU:HD23	2.01	0.41
1:1:1126:G:H2'	1:1:1127:G:H4'	2.01	0.41
1:1:2901:G:N2	1:1:3030:G:O2'	2.52	0.41
1:1:3008:A:N6	1:1:3139:A:N6	2.68	0.41
1:1:3220:G:O6	1:1:3266:G:N1	2.53	0.41
2:2:158:U:O4	3:6:228:U:N3	2.48	0.41
16:N:94:TYR:O	16:N:94:TYR:CD2	2.73	0.41
25:X:49:LYS:O	25:X:50:ALA:C	2.62	0.41
1:1:3170:A:C2	1:1:3281:U:C4	3.07	0.41
3:6:36:U:OP2	39:o:203:LYS:NZ	2.38	0.41
7:D:448:ARG:HG3	7:D:485:VAL:HG13	2.03	0.41
13:K:124:LEU:O	13:K:181:LEU:N	2.52	0.41
30:d:20:LEU:HD11	30:d:32:ALA:HB2	2.01	0.41
40:p:111:VAL:O	40:p:433:LYS:NZ	2.51	0.41
1:1:356:C:O2'	6:C:81:GLY:O	2.33	0.41
6:C:9:HIS:NE2	6:C:147:GLU:OE1	2.51	0.41
11:H:20:ILE:CG1	15:M:7:VAL:HG22	2.50	0.41
34:i:70:ARG:HG2	34:i:87:VAL:HG21	2.02	0.41
39:o:93:ILE:CD1	39:o:166:VAL:HG22	2.51	0.41
40:p:312:ILE:HD12	40:p:346:CYS:SG	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:y:15:VAL:HG22	46:y:61:ARG:CG	2.44	0.41
1:1:595:G:OP1	9:F:33:ARG:NH2	2.54	0.41
1:1:1508:C:N4	1:1:1880:U:HO2'	2.17	0.41
1:1:1570:U:H2'	1:1:1570:U:O2	2.19	0.41
1:1:3153:U:O2	1:1:3153:U:O4'	2.38	0.41
3:6:38:U:C2	3:6:42:G:N1	2.89	0.41
30:d:10:ARG:HG2	30:d:108:VAL:HG22	2.02	0.41
38:n:264:LEU:H	38:n:264:LEU:HD23	1.86	0.41
1:1:1425:U:O2'	6:C:36:HIS:NE2	2.44	0.41
1:1:3116:G:H21	1:1:3116:G:P	2.42	0.41
1:1:3165:A:O2'	1:1:3166:C:O5'	2.39	0.41
32:f:9:VAL:N	32:f:100:ILE:O	2.52	0.41
43:u:4:TYR:OH	43:u:74:ARG:NH1	2.54	0.41
1:1:165:A:O2'	1:1:166:C:P	2.77	0.41
1:1:1157:G:P	9:F:90:LYS:HZ3	2.43	0.41
1:1:1186:G:N1	1:1:1321:G:C6	2.89	0.41
1:1:3104:U:H2'	1:1:3104:U:O2	2.20	0.41
2:2:129:C:OP2	38:n:13:ARG:NH2	2.52	0.41
6:C:283:THR:HG22	6:C:285:ASP:H	1.86	0.41
37:m:800:ASN:OD1	37:m:800:ASN:N	2.53	0.41
1:1:49:A:OP1	16:N:191:TRP:NE1	2.51	0.41
1:1:696:C:O2'	44:v:65:GLY:N	2.50	0.41
1:1:715:A:N1	1:1:781:G:O2'	2.47	0.41
1:1:756:U:H2'	1:1:757:C:C5	2.55	0.41
1:1:2836:C:H3'	1:1:2837:A:H5'	2.02	0.41
1:1:3139:A:H2'	1:1:3140:G:O4'	2.20	0.41
3:6:33:U:O2'	3:6:33:U:O2	2.38	0.41
9:F:228:SER:O	9:F:232:ARG:NH2	2.54	0.41
21:S:10:ILE:HD12	21:S:59:VAL:CG2	2.49	0.41
30:d:23:VAL:O	30:d:28:ARG:NH1	2.54	0.41
1:1:1:G:H21	1:1:1:G:P	2.40	0.41
1:1:29:C:O2'	16:N:162:ARG:O	2.38	0.41
1:1:220:G:N7	1:1:1389:G:N1	2.64	0.41
1:1:1190:A:N3	1:1:1190:A:H2'	2.35	0.41
1:1:1213:G:N1	1:1:1293:U:C4	2.89	0.41
1:1:1255:C:H3'	1:1:1255:C:O2	2.20	0.41
1:1:1412:G:OP1	31:e:105:ARG:NH2	2.54	0.41
1:1:3114:A:P	1:1:3115:C:HO2'	2.33	0.41
1:1:3299:A:C5	1:1:3300:U:C5	3.09	0.41
2:2:15:G:O3'	2:2:16:G:O4'	2.38	0.41
4:A:131:LYS:HA	12:J:279:VAL:HG23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:308:LEU:HD21	7:D:429:LEU:HD22	2.03	0.41
7:D:312:ILE:O	7:D:312:ILE:CG2	2.68	0.41
8:E:43:LEU:HD21	8:E:85:ILE:HD12	2.02	0.41
15:M:77:ARG:O	15:M:81:VAL:HG23	2.21	0.41
21:S:13:ARG:O	21:S:14:LEU:C	2.63	0.41
21:S:77:VAL:HG13	21:S:126:VAL:HG22	2.03	0.41
24:W:47:ASP:OD2	24:W:126:ARG:NH1	2.50	0.41
25:X:67:ILE:HD12	25:X:83:VAL:HG12	2.02	0.41
33:h:53:CYS:O	33:h:57:VAL:HG23	2.21	0.41
42:t:264:CYS:O	42:t:268:LEU:N	2.54	0.41
1:1:1278:A:HO2'	1:1:1279:C:P	2.43	0.41
7:D:165:VAL:O	7:D:165:VAL:HG13	2.20	0.41
9:F:236:ILE:O	9:F:240:VAL:HG23	2.21	0.41
14:L:93:ILE:HG22	14:L:93:ILE:O	2.21	0.41
24:W:195:LEU:HD21	24:W:203:LEU:CD1	2.50	0.41
38:n:417:LEU:HD13	38:n:420:LYS:HB2	2.03	0.41
40:p:209:ALA:O	40:p:210:PRO:C	2.64	0.41
1:1:555:U:H5'	1:1:557:A:H61	1.85	0.40
1:1:1712:G:C2	1:1:1733:G:C6	3.09	0.40
1:1:3348:G:N2	1:1:3357:U:O2	2.52	0.40
9:F:223:PHE:N	9:F:229:PHE:O	2.54	0.40
37:m:358:GLU:OE1	37:m:358:GLU:N	2.54	0.40
40:p:387:ASN:HB3	40:p:390:ILE:HG22	2.03	0.40
1:1:344:A:OP1	6:C:96:GLY:N	2.47	0.40
1:1:620:U:O5'	18:P:167:ARG:NH2	2.54	0.40
1:1:808:A:H2'	1:1:809:G:C8	2.57	0.40
1:1:1120:A:C6	1:1:1139:G:C6	3.09	0.40
1:1:3121:U:H4'	1:1:3122:A:OP1	2.20	0.40
24:W:38:ARG:NH2	24:W:224:ASP:OD2	2.54	0.40
40:p:290:VAL:O	40:p:290:VAL:HG13	2.21	0.40
1:1:1747:G:H21	36:k:2:ALA:HB1	1.86	0.40
1:1:2894:C:OP2	11:H:168:ARG:NH2	2.51	0.40
1:1:3186:A:N3	11:H:44:THR:OG1	2.49	0.40
2:2:123:G:O2'	2:2:124:G:O5'	2.35	0.40
3:6:7:C:O2'	3:6:8:A:P	2.79	0.40
7:D:461:THR:HG23	7:D:462:VAL:HG23	2.02	0.40
10:G:160:ILE:O	10:G:164:VAL:HG13	2.21	0.40
13:K:158:LYS:O	13:K:162:THR:HG22	2.21	0.40
16:N:17:ASP:OD2	34:i:55:ARG:NH2	2.54	0.40
20:R:97:ARG:O	20:R:101:VAL:HG23	2.21	0.40
29:b:136:MET:O	29:b:140:VAL:HG23	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:t:276:GLU:O	42:t:278:SER:N	2.55	0.40
1:1:1299:U:H4'	41:r:43:THR:HG22	2.03	0.40
1:1:1321:G:H2'	1:1:1322:U:O4'	2.22	0.40
1:1:1560:G:C2'	1:1:1561:G:C8	3.03	0.40
1:1:1809:A:OP1	27:Z:65:ARG:NH2	2.55	0.40
1:1:3200:G:OP2	15:M:8:LYS:NZ	2.46	0.40
4:A:44:ARG:NE	4:A:117:LEU:O	2.54	0.40
4:A:137:LEU:HD22	4:A:177:MET:HB2	2.03	0.40
7:D:204:ILE:HG21	7:D:206:PHE:CE2	2.56	0.40
24:W:110:ASN:O	24:W:113:LYS:HG3	2.21	0.40
38:n:189:GLN:OE1	38:n:460:TRP:NE1	2.49	0.40
1:1:59:G:H2'	2:2:33:A:C8	2.57	0.40
1:1:953:G:N2	1:1:1142:G:O2'	2.55	0.40
1:1:3192:U:H2'	1:1:3193:C:C6	2.56	0.40
14:L:58:VAL:HG12	14:L:59:ARG:N	2.37	0.40
38:n:88:ARG:O	38:n:91:THR:OG1	2.36	0.40
38:n:256:ILE:HG23	38:n:258:GLY:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	192/291 (66%)	185 (96%)	7 (4%)	0	100	100
5	B	337/387 (87%)	326 (97%)	10 (3%)	1 (0%)	36	69
6	C	357/362 (99%)	344 (96%)	13 (4%)	0	100	100
7	D	433/505 (86%)	419 (97%)	14 (3%)	0	100	100
8	E	152/176 (86%)	145 (95%)	7 (5%)	0	100	100
9	F	220/244 (90%)	212 (96%)	8 (4%)	0	100	100
10	G	180/256 (70%)	172 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	H	188/191 (98%)	182 (97%)	6 (3%)	0	100	100
12	J	75/427 (18%)	75 (100%)	0	0	100	100
13	K	253/376 (67%)	245 (97%)	8 (3%)	0	100	100
14	L	115/199 (58%)	106 (92%)	9 (8%)	0	100	100
15	M	134/138 (97%)	133 (99%)	1 (1%)	0	100	100
16	N	182/204 (89%)	176 (97%)	6 (3%)	0	100	100
17	O	195/199 (98%)	191 (98%)	4 (2%)	0	100	100
18	P	157/184 (85%)	152 (97%)	5 (3%)	0	100	100
19	Q	132/186 (71%)	129 (98%)	3 (2%)	0	100	100
20	R	85/189 (45%)	85 (100%)	0	0	100	100
21	S	168/172 (98%)	159 (95%)	9 (5%)	0	100	100
22	U	90/121 (74%)	87 (97%)	3 (3%)	0	100	100
23	V	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
24	W	230/236 (98%)	226 (98%)	4 (2%)	0	100	100
25	X	123/142 (87%)	119 (97%)	4 (3%)	0	100	100
26	Y	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
27	Z	126/136 (93%)	122 (97%)	4 (3%)	0	100	100
28	a	69/149 (46%)	68 (99%)	1 (1%)	0	100	100
29	b	413/647 (64%)	401 (97%)	12 (3%)	0	100	100
30	d	96/113 (85%)	96 (100%)	0	0	100	100
31	e	122/130 (94%)	120 (98%)	2 (2%)	0	100	100
32	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
33	h	116/120 (97%)	109 (94%)	7 (6%)	0	100	100
34	i	81/100 (81%)	74 (91%)	7 (9%)	0	100	100
35	j	71/88 (81%)	70 (99%)	1 (1%)	0	100	100
36	k	53/78 (68%)	53 (100%)	0	0	100	100
37	m	571/807 (71%)	558 (98%)	13 (2%)	0	100	100
38	n	403/605 (67%)	394 (98%)	9 (2%)	0	100	100
39	o	131/220 (60%)	126 (96%)	5 (4%)	0	100	100
40	p	243/460 (53%)	234 (96%)	9 (4%)	0	100	100
41	r	71/261 (27%)	66 (93%)	5 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	t	280/322 (87%)	265 (95%)	15 (5%)	0	100	100
43	u	114/199 (57%)	110 (96%)	4 (4%)	0	100	100
44	v	124/231 (54%)	120 (97%)	4 (3%)	0	100	100
45	w	61/841 (7%)	61 (100%)	0	0	100	100
46	y	223/245 (91%)	217 (97%)	6 (3%)	0	100	100
All	All	7714/11308 (68%)	7471 (97%)	242 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	188	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	185/263 (70%)	183 (99%)	2 (1%)	65	74
5	B	284/323 (88%)	281 (99%)	3 (1%)	65	74
6	C	286/289 (99%)	283 (99%)	3 (1%)	68	75
7	D	381/440 (87%)	374 (98%)	7 (2%)	51	67
8	E	134/153 (88%)	134 (100%)	0	100	100
9	F	186/205 (91%)	184 (99%)	2 (1%)	65	74
10	G	150/208 (72%)	143 (95%)	7 (5%)	23	48
11	H	170/171 (99%)	163 (96%)	7 (4%)	27	51
12	J	73/383 (19%)	72 (99%)	1 (1%)	59	71
13	K	238/346 (69%)	236 (99%)	2 (1%)	73	77
14	L	96/159 (60%)	96 (100%)	0	100	100
15	M	107/109 (98%)	107 (100%)	0	100	100
16	N	161/176 (92%)	161 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	O	160/162 (99%)	159 (99%)	1 (1%)	78	80
18	P	131/146 (90%)	129 (98%)	2 (2%)	57	70
19	Q	110/151 (73%)	110 (100%)	0	100	100
20	R	76/154 (49%)	76 (100%)	0	100	100
21	S	155/156 (99%)	151 (97%)	4 (3%)	40	60
22	U	83/107 (78%)	83 (100%)	0	100	100
23	V	96/105 (91%)	95 (99%)	1 (1%)	68	75
24	W	209/213 (98%)	205 (98%)	4 (2%)	50	66
25	X	107/118 (91%)	107 (100%)	0	100	100
26	Y	109/110 (99%)	109 (100%)	0	100	100
27	Z	110/116 (95%)	109 (99%)	1 (1%)	70	75
28	a	60/119 (50%)	58 (97%)	2 (3%)	33	56
29	b	377/573 (66%)	365 (97%)	12 (3%)	34	56
30	d	88/97 (91%)	87 (99%)	1 (1%)	65	74
31	e	107/111 (96%)	106 (99%)	1 (1%)	70	75
32	f	90/91 (99%)	89 (99%)	1 (1%)	65	74
33	h	104/105 (99%)	103 (99%)	1 (1%)	68	75
34	i	69/82 (84%)	69 (100%)	0	100	100
35	j	60/71 (84%)	58 (97%)	2 (3%)	33	56
36	k	59/69 (86%)	59 (100%)	0	100	100
37	m	529/723 (73%)	527 (100%)	2 (0%)	84	83
38	n	371/548 (68%)	364 (98%)	7 (2%)	50	66
39	o	118/199 (59%)	116 (98%)	2 (2%)	53	68
40	p	229/413 (55%)	224 (98%)	5 (2%)	45	64
41	r	65/229 (28%)	64 (98%)	1 (2%)	57	70
42	t	256/287 (89%)	250 (98%)	6 (2%)	44	63
43	u	101/180 (56%)	100 (99%)	1 (1%)	68	75
44	v	116/205 (57%)	115 (99%)	1 (1%)	70	75
45	w	58/745 (8%)	58 (100%)	0	100	100
46	y	193/211 (92%)	190 (98%)	3 (2%)	55	69
All	All	6847/9821 (70%)	6752 (99%)	95 (1%)	57	71

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	137	LEU
4	A	225	LEU
5	B	79	VAL
5	B	85	VAL
5	B	297	SER
6	C	150	LEU
6	C	182	LEU
6	C	312	VAL
7	D	96	PHE
7	D	113	ASN
7	D	144	THR
7	D	166	ASN
7	D	248	LEU
7	D	296	LEU
7	D	319	LEU
9	F	46	GLU
9	F	82	LYS
10	G	79	GLN
10	G	84	ARG
10	G	144	GLU
10	G	150	LEU
10	G	162	LEU
10	G	189	LEU
10	G	228	GLU
11	H	1	MET
11	H	16	VAL
11	H	70	THR
11	H	144	ILE
11	H	157	ASN
11	H	161	LEU
11	H	162	GLN
12	J	236	ILE
13	K	48	THR
13	K	261	ASP
17	O	118	VAL
18	P	97	ASN
18	P	112	LEU
21	S	10	ILE
21	S	13	ARG
21	S	103	VAL
21	S	117	ARG
23	V	102	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	W	73	LEU
24	W	96	CYS
24	W	161	LEU
24	W	173	THR
27	Z	17	ARG
28	a	117	ARG
28	a	148	ILE
29	b	55	GLU
29	b	81	LEU
29	b	87	GLU
29	b	175	TYR
29	b	277	LEU
29	b	306	LEU
29	b	324	LEU
29	b	421	LEU
29	b	428	LYS
29	b	434	GLU
29	b	436	LEU
29	b	448	GLU
30	d	55	LEU
31	e	120	THR
32	f	106	ASN
33	h	93	THR
35	j	67	LEU
35	j	75	LYS
37	m	243	LEU
37	m	800	ASN
38	n	77	LEU
38	n	196	GLU
38	n	199	TRP
38	n	229	LEU
38	n	359	LEU
38	n	417	LEU
38	n	551	GLU
39	o	137	LEU
39	o	176	LEU
40	p	229	ASN
40	p	331	SER
40	p	342	ASN
40	p	409	SER
40	p	438	VAL
41	r	4	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	t	160	PHE
42	t	187	LEU
42	t	229	LEU
42	t	271	PHE
42	t	303	ASN
42	t	311	GLU
43	u	27	LYS
44	v	157	GLU
46	y	51	THR
46	y	97	VAL
46	y	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	84	ASN
4	A	85	ASN
4	A	95	GLN
4	A	165	ASN
6	C	114	ASN
6	C	140	HIS
6	C	196	ASN
7	D	337	ASN
7	D	413	ASN
8	E	4	GLN
8	E	28	GLN
8	E	61	ASN
9	F	93	ASN
9	F	186	HIS
10	G	59	GLN
10	G	95	ASN
11	H	139	ASN
12	J	228	ASN
13	K	79	GLN
13	K	84	ASN
13	K	85	ASN
13	K	101	ASN
13	K	212	HIS
17	O	72	HIS
18	P	92	GLN
18	P	96	GLN
18	P	121	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Q	58	ASN
21	S	122	HIS
22	U	87	ASN
23	V	132	ASN
26	Y	110	HIS
27	Z	40	HIS
29	b	70	ASN
29	b	72	ASN
29	b	177	ASN
29	b	259	GLN
30	d	57	GLN
31	e	35	GLN
31	e	52	GLN
31	e	98	HIS
33	h	59	ASN
37	m	228	GLN
37	m	230	ASN
37	m	307	GLN
37	m	403	ASN
37	m	436	HIS
37	m	613	GLN
37	m	694	ASN
38	n	11	ASN
39	o	199	ASN
40	p	300	ASN
40	p	368	GLN
41	r	49	GLN
42	t	172	ASN
42	t	269	GLN
42	t	303	ASN
46	y	33	ASN
46	y	170	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2116/3396 (62%)	373 (17%)	42 (1%)
2	2	153/158 (96%)	27 (17%)	2 (1%)
3	6	64/232 (27%)	20 (31%)	4 (6%)
All	All	2333/3786 (61%)	420 (18%)	48 (2%)

All (420) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	7	C
1	1	14	U
1	1	16	A
1	1	26	A
1	1	40	A
1	1	41	G
1	1	42	C
1	1	49	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	73	C
1	1	76	G
1	1	92	G
1	1	94	G
1	1	108	A
1	1	110	G
1	1	111	C
1	1	116	A
1	1	117	U
1	1	122	A
1	1	134	U
1	1	135	C
1	1	136	G
1	1	156	G
1	1	165	A
1	1	166	C
1	1	170	G
1	1	190	U
1	1	191	U
1	1	200	C
1	1	207	U
1	1	210	U
1	1	218	G
1	1	219	A
1	1	220	G
1	1	231	G
1	1	240	U
1	1	241	G
1	1	249	U
1	1	250	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	251	G
1	1	252	U
1	1	265	A
1	1	268	A
1	1	269	G
1	1	283	G
1	1	284	A
1	1	285	A
1	1	295	A
1	1	298	U
1	1	305	U
1	1	311	C
1	1	315	C
1	1	323	A
1	1	324	A
1	1	329	U
1	1	339	C
1	1	351	A
1	1	352	A
1	1	368	G
1	1	370	U
1	1	375	A
1	1	376	G
1	1	398	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	404	G
1	1	421	G
1	1	422	A
1	1	440	A
1	1	495	G
1	1	517	G
1	1	521	A
1	1	523	A
1	1	533	A
1	1	535	G
1	1	544	C
1	1	546	C
1	1	547	G
1	1	548	G
1	1	550	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	552	G
1	1	557	A
1	1	559	A
1	1	578	A
1	1	579	G
1	1	592	A
1	1	597	G
1	1	604	G
1	1	609	G
1	1	611	A
1	1	620	U
1	1	621	A
1	1	636	C
1	1	637	C
1	1	638	C
1	1	645	A
1	1	648	C
1	1	650	C
1	1	660	A
1	1	677	A
1	1	681	U
1	1	691	A
1	1	705	A
1	1	706	A
1	1	710	A
1	1	715	A
1	1	721	G
1	1	722	G
1	1	735	A
1	1	742	G
1	1	743	C
1	1	757	C
1	1	760	G
1	1	761	A
1	1	770	G
1	1	776	U
1	1	779	G
1	1	781	G
1	1	784	A
1	1	785	G
1	1	787	G
1	1	801	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	930	U
1	1	933	A
1	1	936	A
1	1	937	G
1	1	944	C
1	1	958	C
1	1	959	C
1	1	963	G
1	1	965	A
1	1	971	G
1	1	976	U
1	1	978	G
1	1	979	U
1	1	980	A
1	1	981	U
1	1	982	C
1	1	1103	A
1	1	1104	G
1	1	1105	A
1	1	1111	U
1	1	1112	A
1	1	1116	G
1	1	1123	U
1	1	1127	G
1	1	1129	A
1	1	1130	A
1	1	1135	A
1	1	1138	U
1	1	1144	U
1	1	1153	A
1	1	1155	C
1	1	1159	A
1	1	1174	G
1	1	1180	A
1	1	1181	U
1	1	1189	C
1	1	1192	C
1	1	1204	A
1	1	1218	U
1	1	1220	U
1	1	1221	A
1	1	1222	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1228	C
1	1	1242	G
1	1	1245	A
1	1	1246	G
1	1	1251	A
1	1	1252	A
1	1	1253	U
1	1	1254	C
1	1	1258	U
1	1	1263	A
1	1	1265	U
1	1	1278	A
1	1	1279	C
1	1	1284	C
1	1	1286	A
1	1	1287	A
1	1	1308	A
1	1	1330	A
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1351	U
1	1	1352	A
1	1	1353	U
1	1	1354	G
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1386	A
1	1	1392	G
1	1	1397	C
1	1	1399	A
1	1	1400	G
1	1	1406	A
1	1	1408	G
1	1	1417	G
1	1	1419	A
1	1	1434	G
1	1	1436	U
1	1	1437	C
1	1	1457	U
1	1	1470	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1496	C
1	1	1507	G
1	1	1508	C
1	1	1536	G
1	1	1549	U
1	1	1561	G
1	1	1562	C
1	1	1566	A
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1571	A
1	1	1572	U
1	1	1573	G
1	1	1574	C
1	1	1575	A
1	1	1580	A
1	1	1581	C
1	1	1582	C
1	1	1589	A
1	1	1593	A
1	1	1602	A
1	1	1603	A
1	1	1605	A
1	1	1608	C
1	1	1619	A
1	1	1620	U
1	1	1628	C
1	1	1631	C
1	1	1633	C
1	1	1639	C
1	1	1642	A
1	1	1643	A
1	1	1647	A
1	1	1656	A
1	1	1685	C
1	1	1705	U
1	1	1713	G
1	1	1724	U
1	1	1725	C
1	1	1728	G
1	1	1741	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1742	U
1	1	1750	A
1	1	1751	G
1	1	1766	G
1	1	1770	G
1	1	1775	G
1	1	1791	C
1	1	1792	C
1	1	1796	G
1	1	1797	A
1	1	1808	G
1	1	1813	A
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1821	U
1	1	1857	C
1	1	1862	U
1	1	1867	A
1	1	1869	C
1	1	1879	A
1	1	1880	U
1	1	1884	A
1	1	1886	A
1	1	2363	A
1	1	2366	C
1	1	2371	G
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2376	G
1	1	2391	G
1	1	2394	G
1	1	2434	U
1	1	2825	C
1	1	2836	C
1	1	2837	A
1	1	2857	C
1	1	2858	U
1	1	2888	U
1	1	2889	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2898	G
1	1	2935	U
1	1	2936	A
1	1	2987	A
1	1	2996	U
1	1	2997	G
1	1	3006	A
1	1	3012	A
1	1	3017	A
1	1	3019	U
1	1	3021	A
1	1	3022	G
1	1	3032	A
1	1	3056	U
1	1	3057	U
1	1	3059	G
1	1	3080	G
1	1	3086	A
1	1	3092	C
1	1	3099	C
1	1	3101	G
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3153	U
1	1	3155	U
1	1	3156	U
1	1	3157	U
1	1	3158	G
1	1	3162	C
1	1	3165	A
1	1	3170	A
1	1	3171	U
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3181	C
1	1	3187	A
1	1	3195	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	3207	U
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3229	G
1	1	3238	G
1	1	3245	A
1	1	3247	G
1	1	3252	G
1	1	3259	U
1	1	3260	G
1	1	3270	U
1	1	3273	A
1	1	3276	G
1	1	3281	U
1	1	3288	G
1	1	3289	G
1	1	3304	U
1	1	3316	A
1	1	3317	U
1	1	3319	U
1	1	3320	A
1	1	3334	U
1	1	3335	A
1	1	3341	U
1	1	3344	A
1	1	3349	C
1	1	3353	G
1	1	3356	G
1	1	3357	U
1	1	3369	G
1	1	3375	A
1	1	3378	C
1	1	3382	U
1	1	3390	G
1	1	3396	U
2	2	13	A
2	2	15	G
2	2	16	G
2	2	34	U
2	2	35	C
2	2	39	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	40	A
2	2	51	G
2	2	52	A
2	2	59	A
2	2	63	G
2	2	72	A
2	2	80	A
2	2	81	U
2	2	82	U
2	2	84	C
2	2	86	U
2	2	87	G
2	2	89	A
2	2	90	U
2	2	95	G
2	2	104	A
2	2	106	C
2	2	107	G
2	2	124	G
2	2	125	U
2	2	128	U
3	6	2	C
3	6	4	U
3	6	5	C
3	6	6	U
3	6	7	C
3	6	8	A
3	6	14	U
3	6	15	C
3	6	16	U
3	6	17	G
3	6	26	U
3	6	34	A
3	6	40	U
3	6	42	G
3	6	43	A
3	6	54	A
3	6	56	U
3	6	59	C
3	6	229	U
3	6	230	A

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	13	A
1	1	58	G
1	1	75	G
1	1	116	A
1	1	165	A
1	1	239	G
1	1	294	U
1	1	304	G
1	1	494	G
1	1	649	A
1	1	709	A
1	1	720	A
1	1	734	C
1	1	769	G
1	1	1128	U
1	1	1129	A
1	1	1227	C
1	1	1241	U
1	1	1283	C
1	1	1307	G
1	1	1329	U
1	1	1355	A
1	1	1405	U
1	1	1456	A
1	1	1560	G
1	1	1574	C
1	1	1581	C
1	1	1712	G
1	1	1765	U
1	1	1807	G
1	1	1861	G
1	1	2857	C
1	1	2887	A
1	1	2986	U
1	1	2995	A
1	1	3079	U
1	1	3157	U
1	1	3228	C
1	1	3269	U
1	1	3352	U
1	1	3355	U
1	1	3389	U
2	2	14	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	123	G
3	6	1	C
3	6	15	C
3	6	16	U
3	6	33	U

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

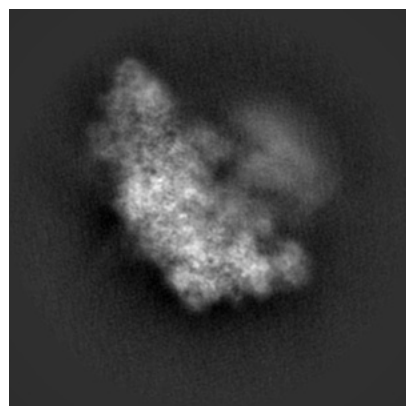
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12910. These allow visual inspection of the internal detail of the map and identification of artifacts.

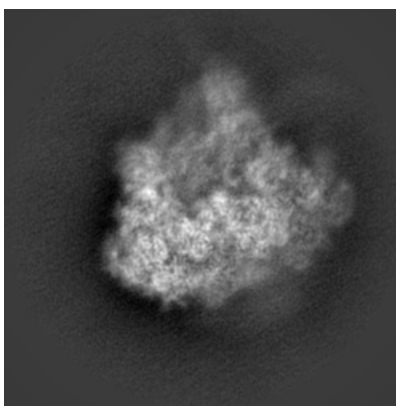
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

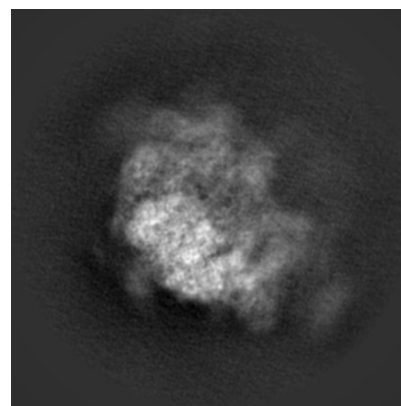
6.1.1 Primary map



X

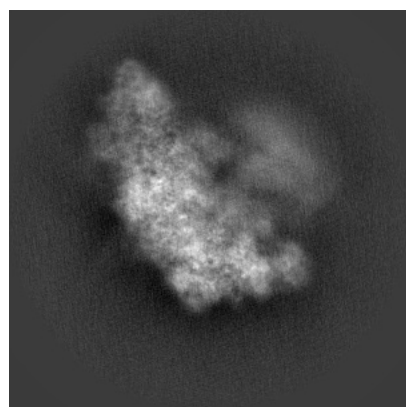


Y

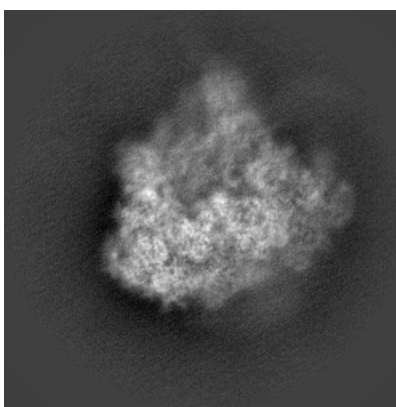


Z

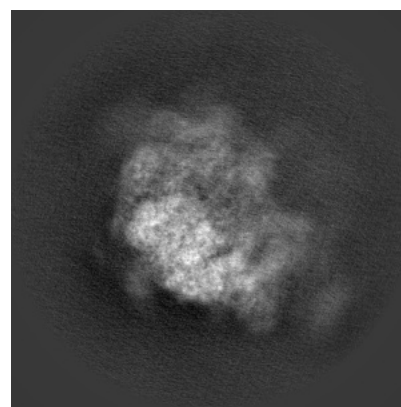
6.1.2 Raw map



X



Y

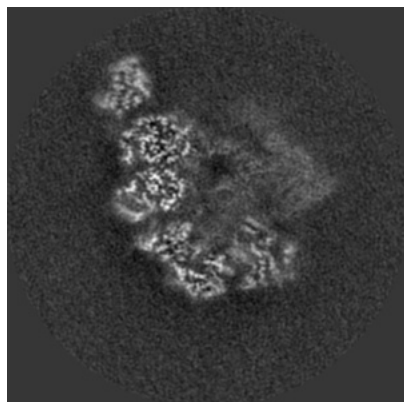


Z

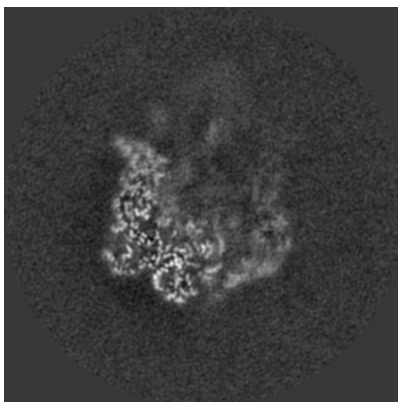
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

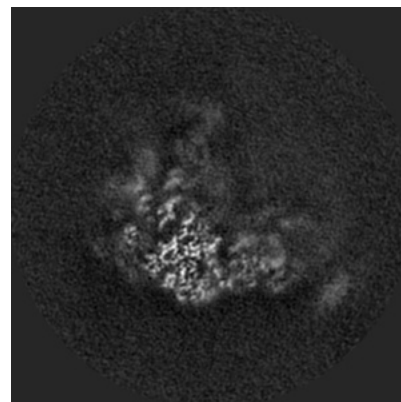
6.2.1 Primary map



X Index: 200

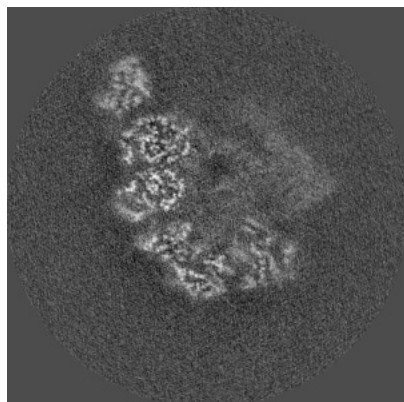


Y Index: 200

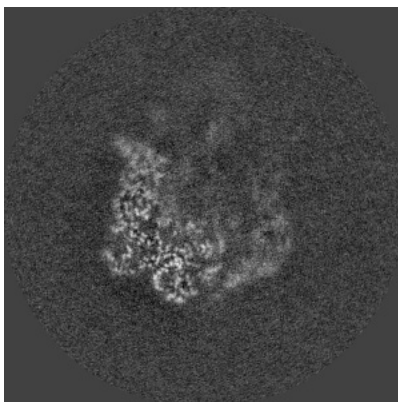


Z Index: 200

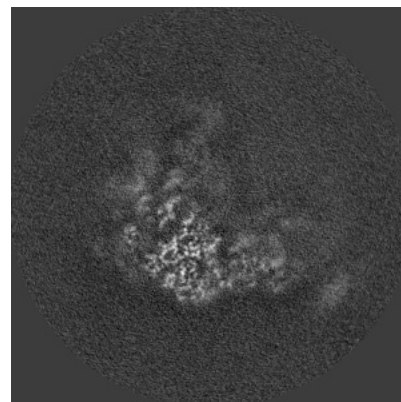
6.2.2 Raw map



X Index: 200



Y Index: 200

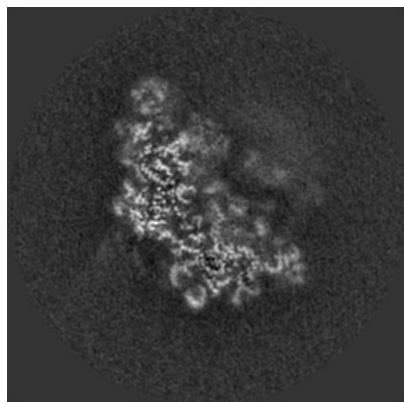


Z Index: 200

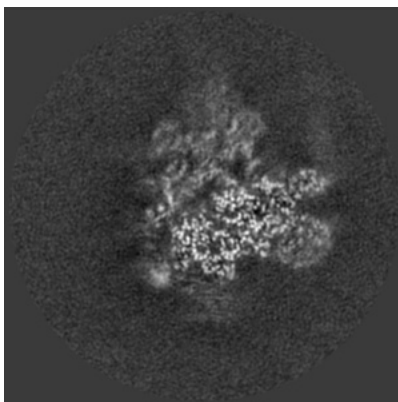
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

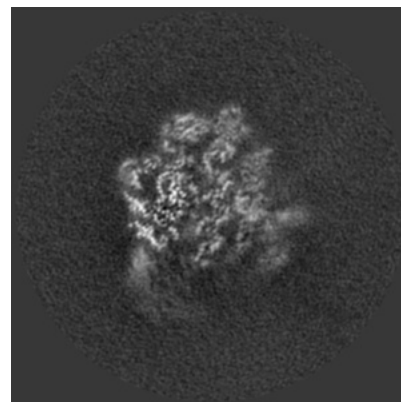
6.3.1 Primary map



X Index: 167

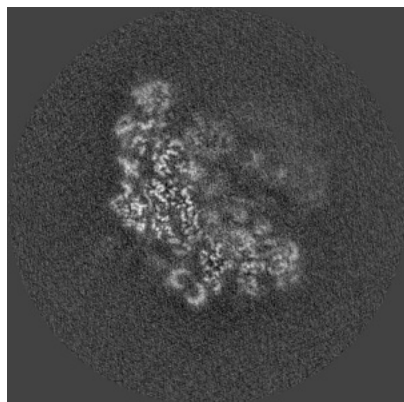


Y Index: 150

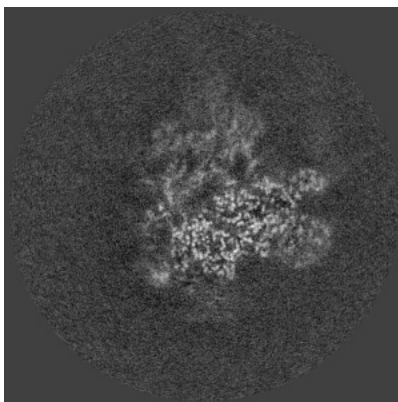


Z Index: 151

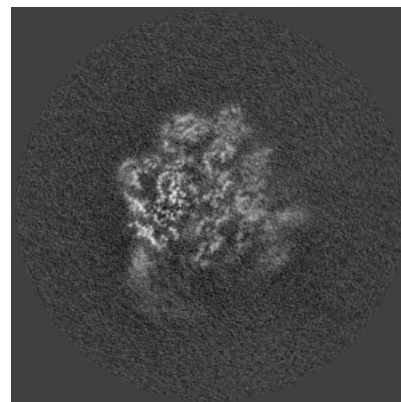
6.3.2 Raw map



X Index: 172



Y Index: 151

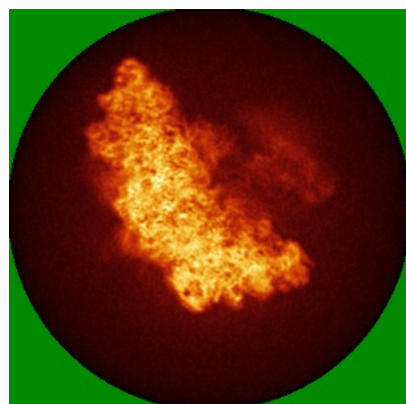


Z Index: 151

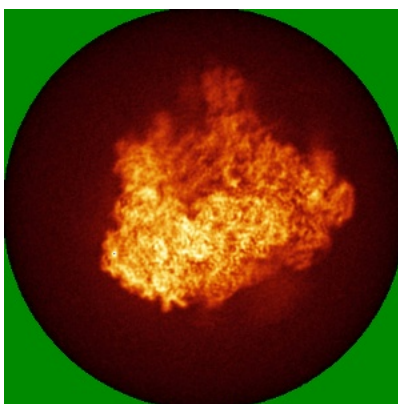
The images above show the largest variance slices of the map in three orthogonal directions.

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

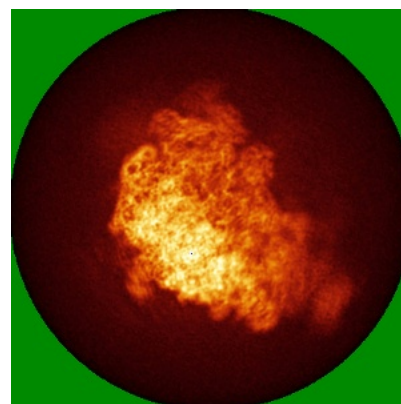
6.4.1 Primary map



X

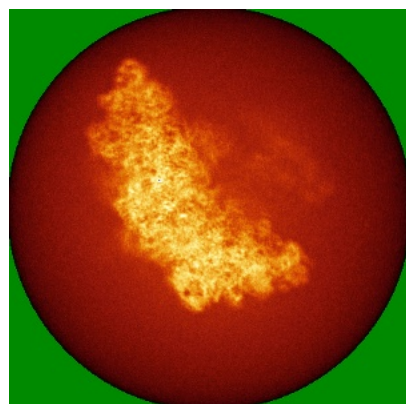


Y

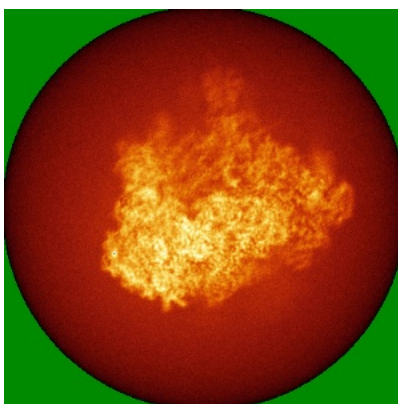


Z

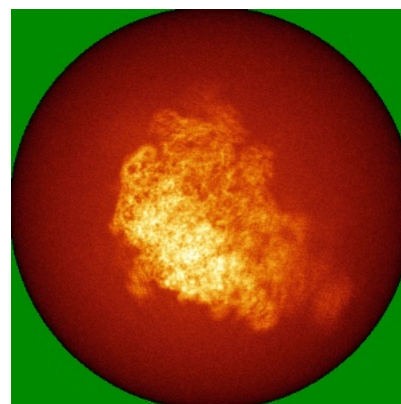
6.4.2 Raw map



X



Y

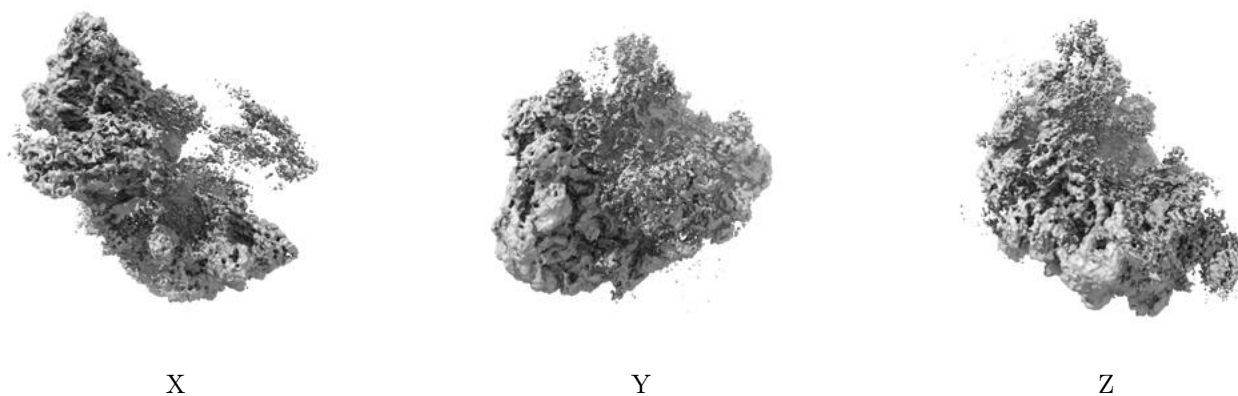


Z

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.

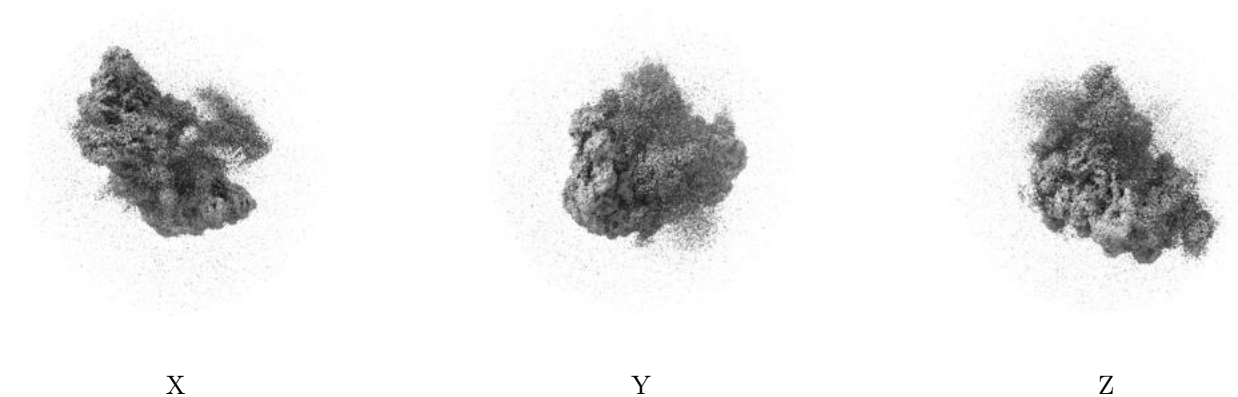
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

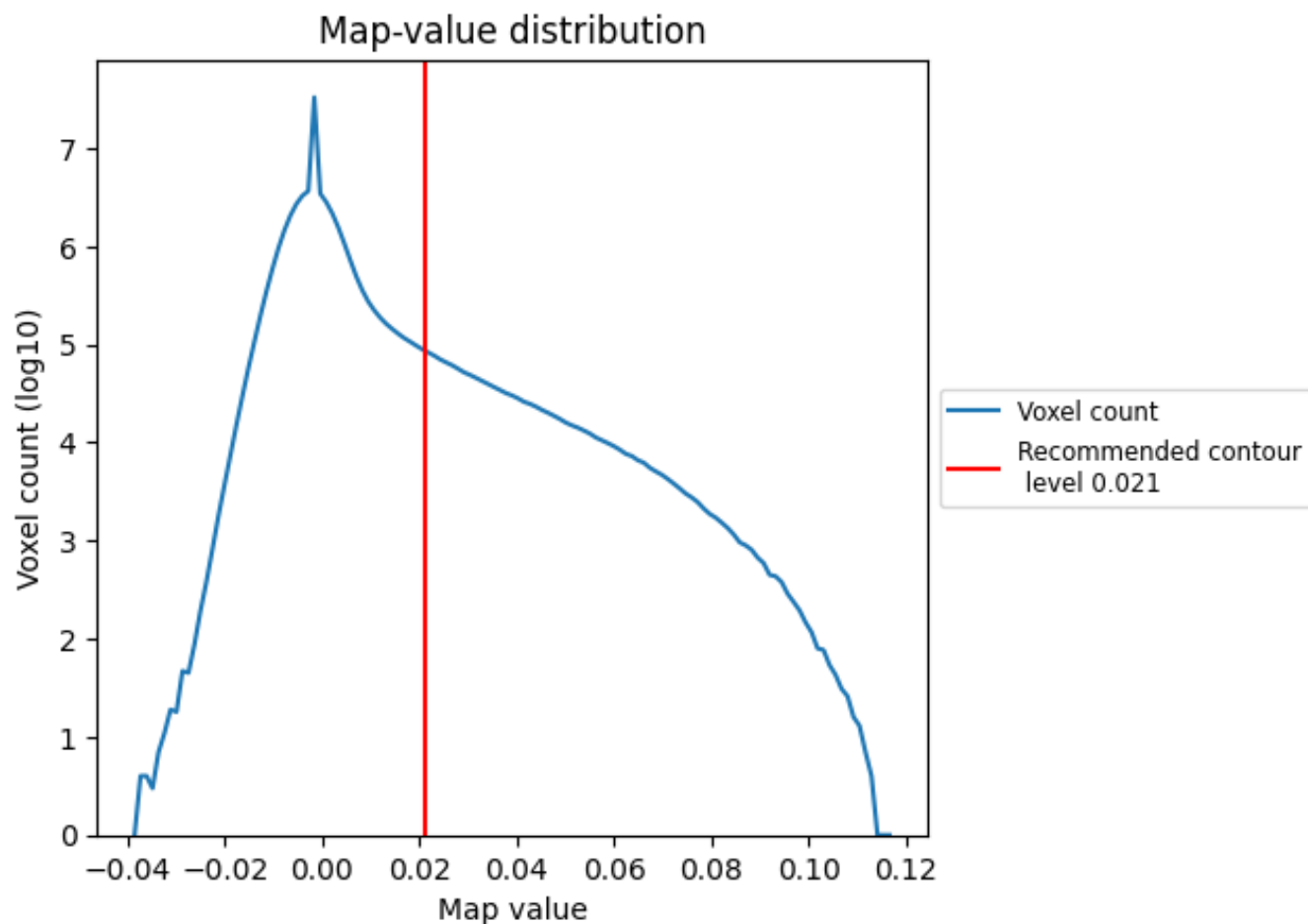
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

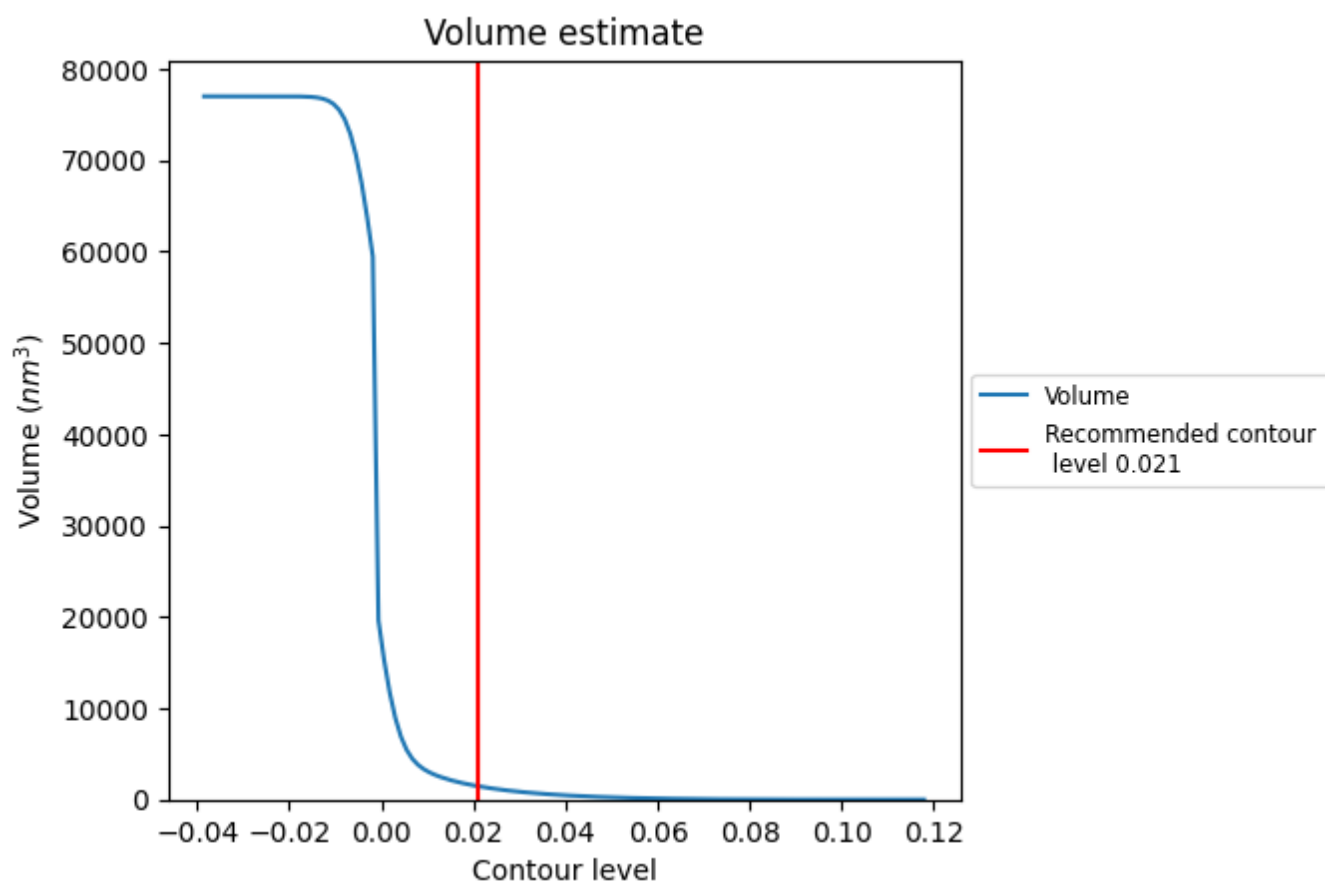
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

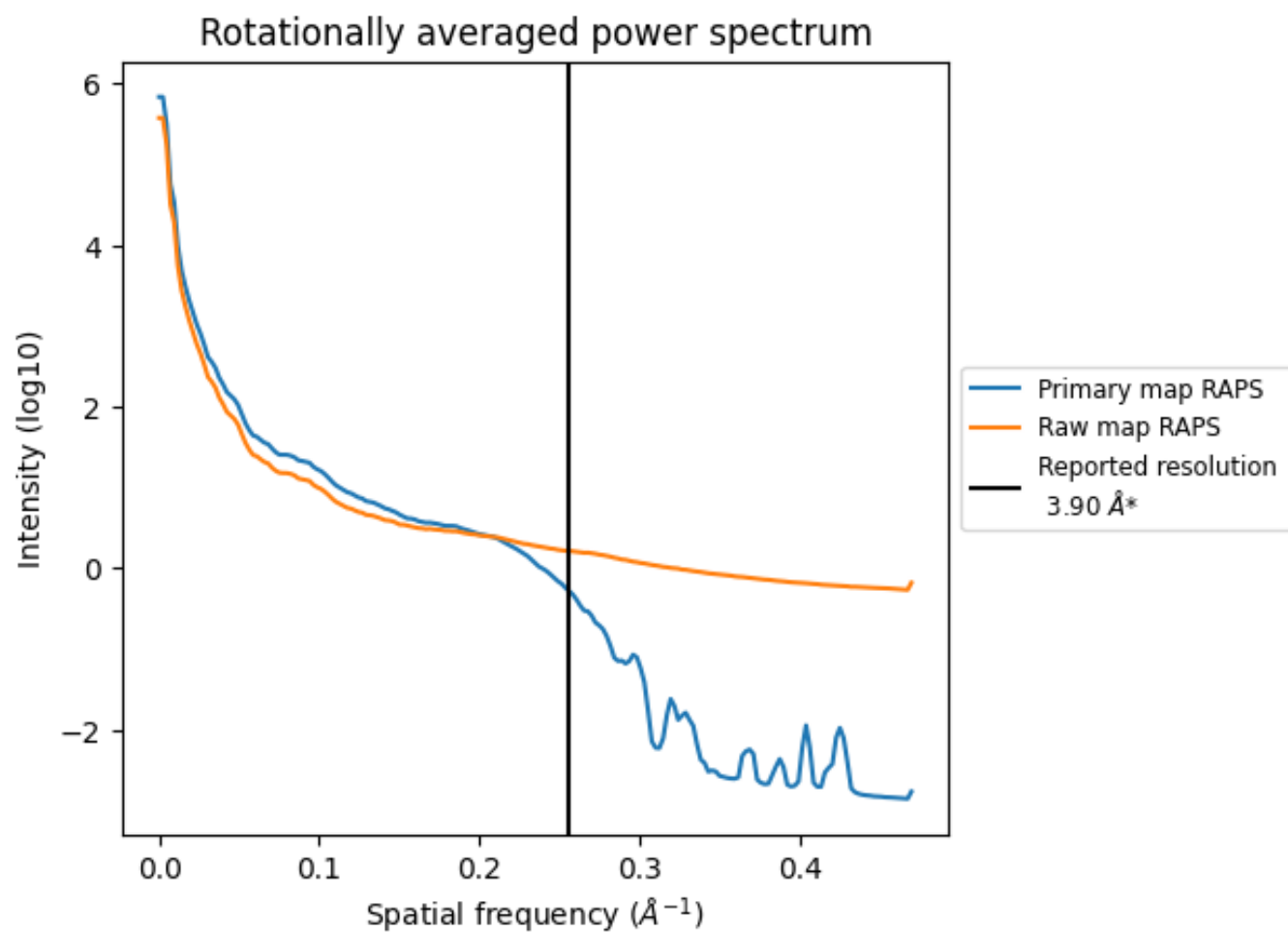
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1465 nm³; this corresponds to an approximate mass of 1324 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 ⓘ

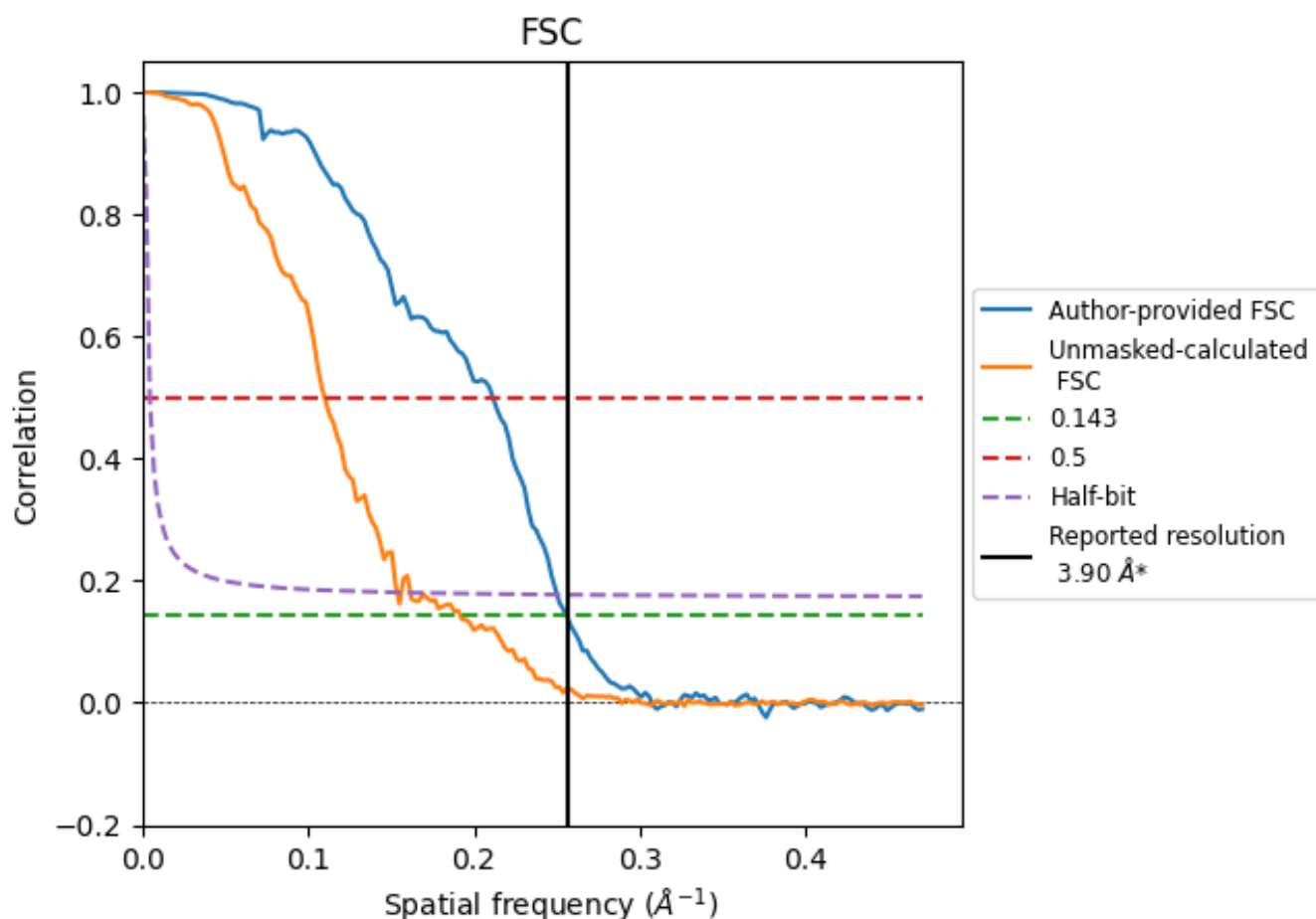


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

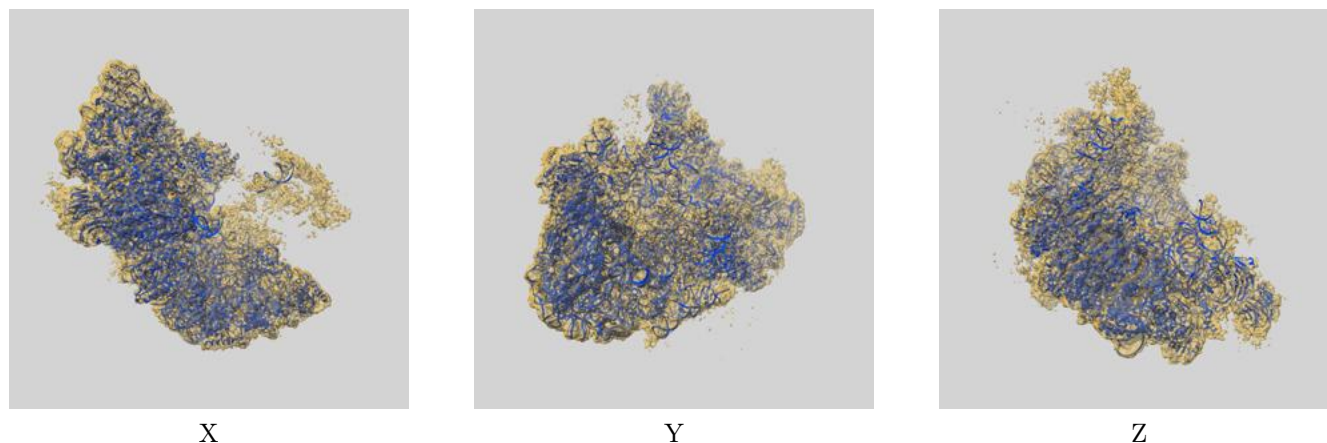
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.73	4.00
Unmasked-calculated*	5.22	9.10	6.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.22 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

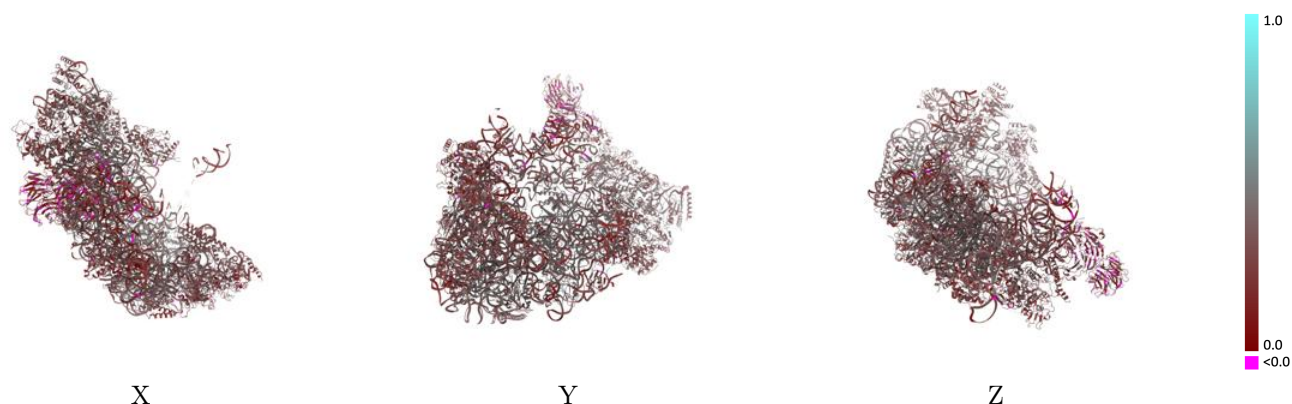
This section contains information regarding the fit between EMDB map EMD-12910 and PDB model 7OHV. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



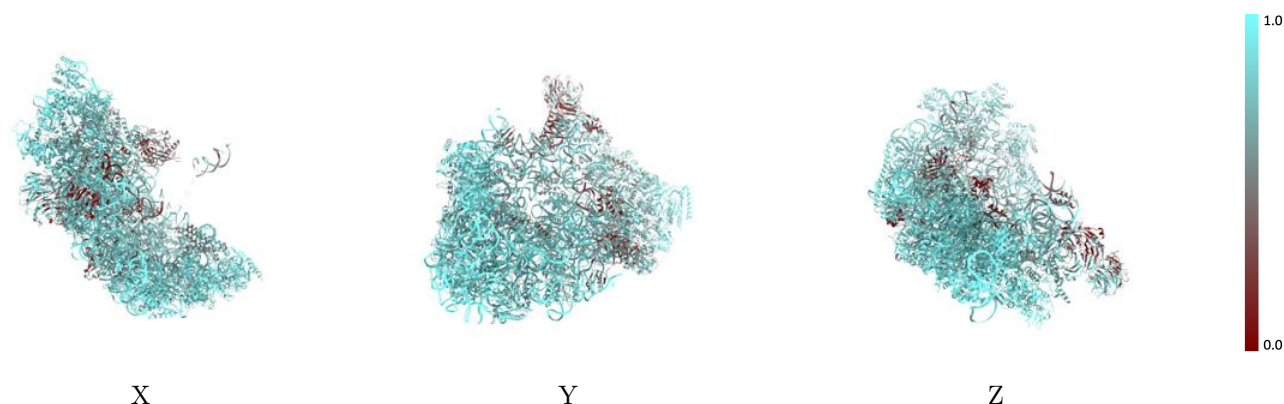
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



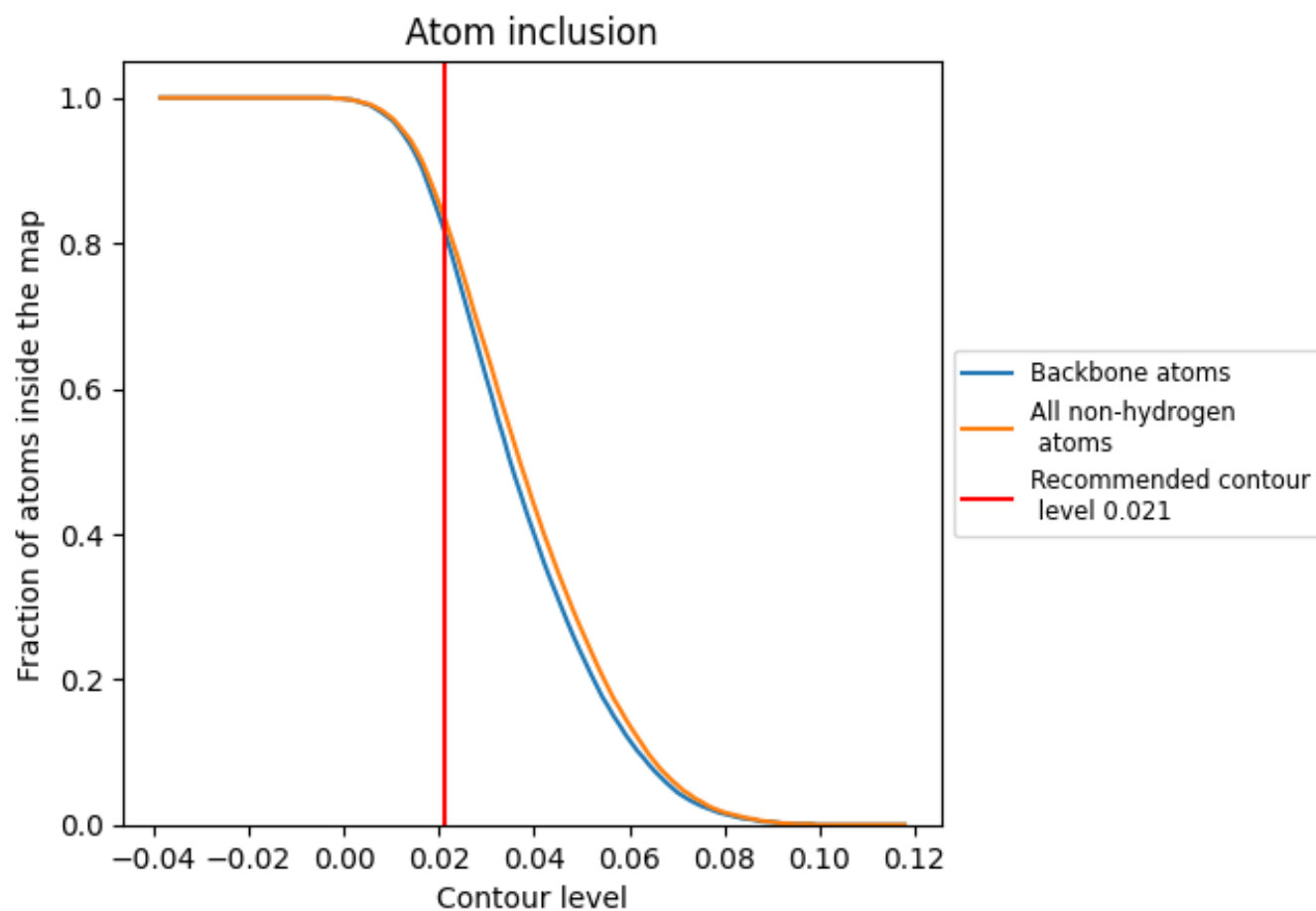
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 84% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8390	 0.3240
1	 0.9140	 0.3240
2	 0.9690	 0.3590
6	 0.9640	 0.3170
A	 0.5410	 0.2870
B	 0.8620	 0.3640
C	 0.8690	 0.4040
D	 0.7710	 0.3230
E	 0.8750	 0.3840
F	 0.8670	 0.3810
G	 0.7860	 0.3580
H	 0.7790	 0.3640
J	 0.3860	 0.2630
K	 0.8700	 0.3090
L	 0.8510	 0.3890
M	 0.8710	 0.3780
N	 0.8060	 0.3960
O	 0.8570	 0.3870
P	 0.8070	 0.3610
Q	 0.8290	 0.3770
R	 0.4740	 0.2690
S	 0.8830	 0.3790
U	 0.4760	 0.2490
V	 0.7380	 0.2610
W	 0.8160	 0.2730
X	 0.6770	 0.3480
Y	 0.8860	 0.4010
Z	 0.5090	 0.2200
a	 0.5210	 0.3310
b	 0.7440	 0.2670
d	 0.7050	 0.3250
e	 0.8300	 0.4200
f	 0.8760	 0.4380
h	 0.8710	 0.3650
i	 0.7470	 0.2750



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.8780	 0.4110
k	 0.5670	 0.2930
m	 0.5810	 0.2540
n	 0.8560	 0.3110
o	 0.8880	 0.3240
p	 0.5980	 0.1760
r	 0.7400	 0.3210
t	 0.8120	 0.3100
u	 0.8860	 0.2790
v	 0.8220	 0.3590
w	 0.2190	 0.2830
y	 0.8540	 0.2740