



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 12:38 PM UTC

PDB ID : 9KN5 / pdb_00009kn5
EMDB ID : EMD-62453
Title : Structure of the human 40S ribosome complexed with HCV IRES, eIF1A and eIF3
Authors : Iwasaki, W.; Kashiwagi, K.; Sakamoto, A.; Nishimoto, M.; Takahashi, M.; Machida, K.; Imataka, H.; Matsumoto, A.; Shichino, Y.; Iwasaki, S.; Imami, K.; Ito, T.
Deposited on : 2024-11-18
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

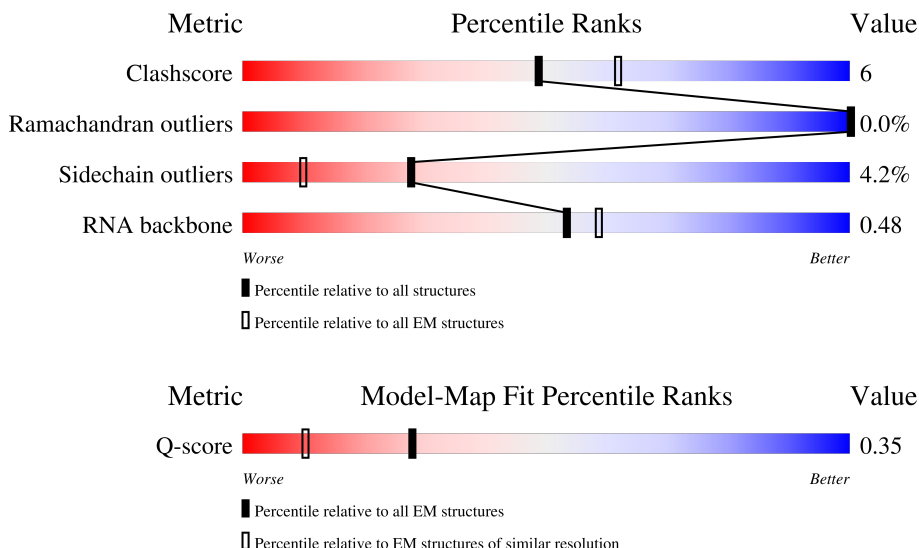
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



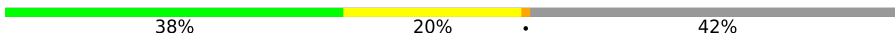
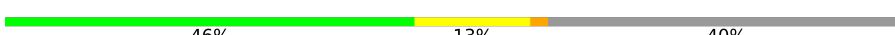
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1A	144	
2	SA	295	
3	SB	264	

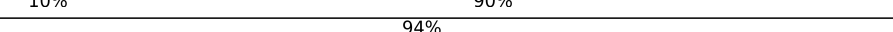
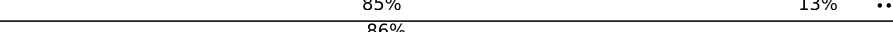
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	SC	293	
5	SD	243	
6	SE	263	
7	SF	204	
8	SG	249	
9	SH	194	
10	SI	208	
11	SJ	194	
12	SK	165	
13	SL	158	
14	Sf	132	
15	SN	151	
16	SO	151	
17	SP	145	
18	SQ	146	
19	SR	135	
20	SS	152	
21	ST	145	
22	SU	119	
23	SV	83	
24	SW	130	
25	SX	143	
26	SY	133	
27	SZ	125	
28	Sa	115	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Sb	84	 88% 11% .
30	Sc	69	 57% 32% . 10%
31	Sd	56	 79% 18% . .
32	Se	59	 76% 12% 12%
33	sh	156	 29% 11% . 59%
34	Sg	317	 79% 19% . .
35	Ln	25	 64% 32% .
36	S2	1869	 60% 31% . 6%
37	zz	332	 41% 41% 8% 9%
38	3m	374	 93% 76% 21% . .
39	3f	357	 51% 59% 16% 25%
40	3a	1382	 22% 35% 7% . 57%
41	3e	445	 83% 87% 9% .
42	3c	913	 38% 52% 7% 41%
43	3h	352	 36% 70% 20% 10%
44	3d	548	 7% 10% 90%
45	3k	218	 94% 85% 13% . .
46	3l	564	 86% 73% 18% . 8%

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 108797 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	98	Total	C	N	O	S	0	0
			780	492	137	147	4		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SA	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SB	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SC	219	Total	C	N	O	S	0	0
			1700	1100	292	298	10		

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SD	226	Total	C	N	O	S	0	0
			1756	1119	316	314	7		

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SE	260	Total	C	N	O	S	0	0
			2065	1319	384	354	8		

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SF	192	Total	C	N	O	S	0	0
			1518	948	287	276	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

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

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SH	187	Total	C	N	O	S	0	0
			1506	961	277	267	1		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SI	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 11 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SJ	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 12 is a protein called 40S ribosomal protein S10.

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

- Molecule 13 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SL	150	Total	C	N	O	S	0	0
			1220	776	228	210	6		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Sf	121	Total	C	N	O	S	0	0
			935	586	165	175	9		

- Molecule 15 is a protein called 40S ribosomal protein S13.

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

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SO	135	Total	C	N	O	S	0	0
			1007	617	198	186	6		

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SP	119	Total	C	N	O	S	0	0
			984	625	187	165	7		

- Molecule 18 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SQ	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 19 is a protein called 40S ribosomal protein S17.

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

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SS	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 21 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	ST	142	Total	C	N	O	S	0	0
			1103	691	212	197	3		

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 23 is a protein called 40S ribosomal protein S21.

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

- Molecule 24 is a protein called 40S ribosomal protein S15a.

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

- Molecule 25 is a protein called 40S ribosomal protein S23.

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

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SY	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 27 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SZ	75	Total	C	N	O	S	0	0
			601	385	111	104	1		

- Molecule 28 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sa	100	Total	C	N	O	S	0	0
			803	501	166	131	5		

- Molecule 29 is a protein called 40S ribosomal protein S27.

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

- Molecule 30 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Sc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 31 is a protein called 40S ribosomal protein S29.

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

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Se	52	Total	C	N	O	S	0	0
			417	259	92	65	1		

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	sh	64	Total	C	N	O	S	0	0
			518	327	99	85	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 35 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 36 is a RNA chain called Chains: S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	S2	1759	Total	C	N	O	P	6	0
			37669	16814	6767	12324	1764		

- Molecule 37 is a RNA chain called Chains: zz.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	zz	302	Total	C	N	O	P	0	0
			6443	2871	1148	2122	302		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	3m	363	Total	C	N	O	S	0	0
			2639	1666	450	511	12		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3f	269	Total	C	N	O	S	0	0
			2063	1303	354	394	12		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3a	592	Total	C	N	O	S	0	0
			4475	2834	803	817	21		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3e	430	Total	C	N	O	S	0	0
			3224	2053	561	594	16		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3c	543	Total	C	N	O	S	0	0
			3924	2463	721	716	24		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3h	318	Total	C	N	O	S	0	0
			2520	1599	431	475	15		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3d	55	Total	C	N	O	S	0	0
			347	222	65	59	1		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3k	215	Total	C	N	O	S	0	0
			1475	932	251	282	10		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit L.

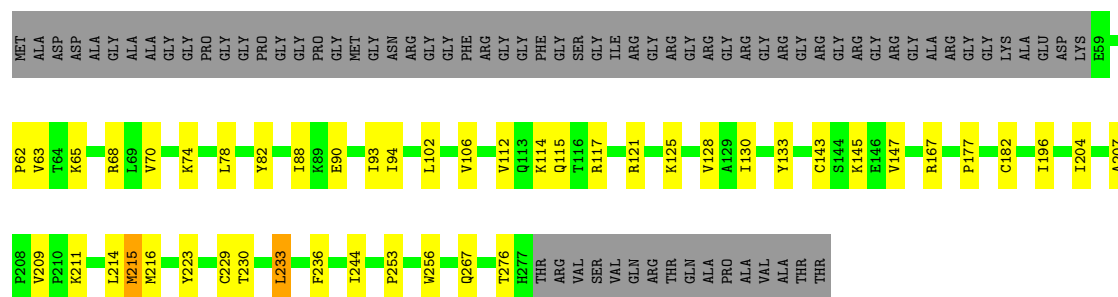
Mol	Chain	Residues	Atoms					AltConf	Trace
46	3l	520	Total	C	N	O	S	0	0
			4335	2808	715	793	19		

- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

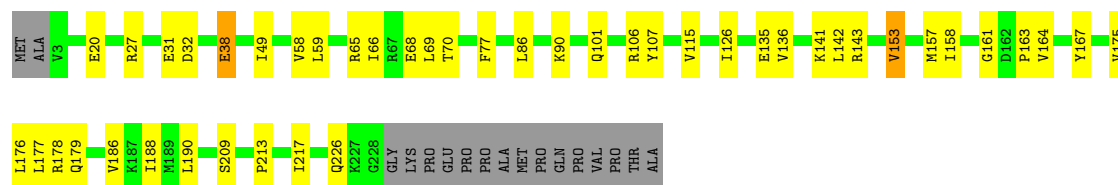
Mol	Chain	Residues	Atoms		AltConf
47	Sa	1	Total	Zn	0
			1	1	
47	sh	1	Total	Zn	0
			1	1	

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

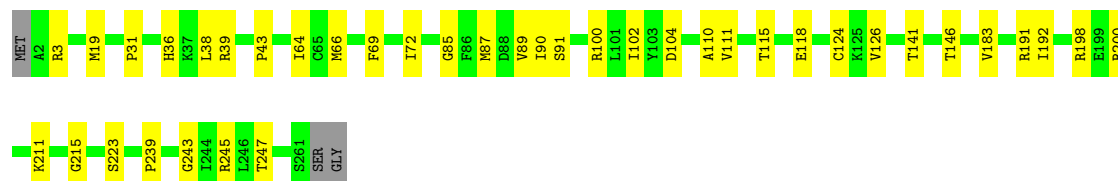
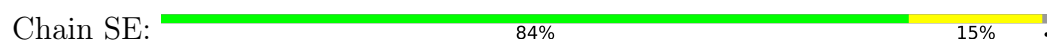
Mol	Chain	Residues	Atoms		AltConf
48	S2	8	Total	Mg	0
			8	8	



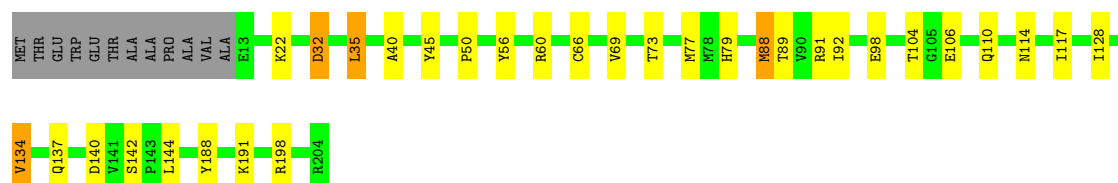
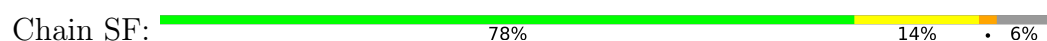
• Molecule 5: 40S ribosomal protein S3



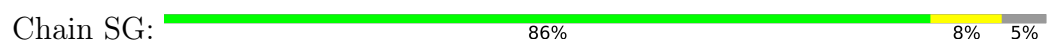
• Molecule 6: 40S ribosomal protein S4, X isoform



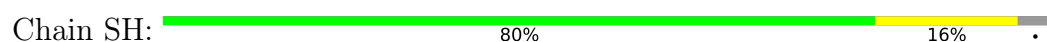
• Molecule 7: 40S ribosomal protein S5

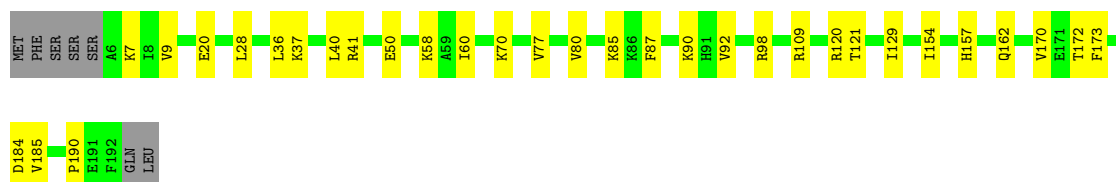


• Molecule 8: 40S ribosomal protein S6



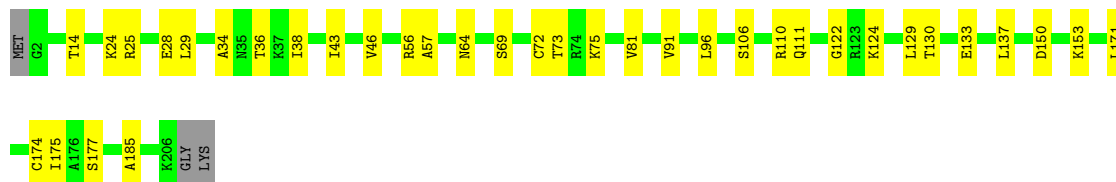
• Molecule 9: 40S ribosomal protein S7





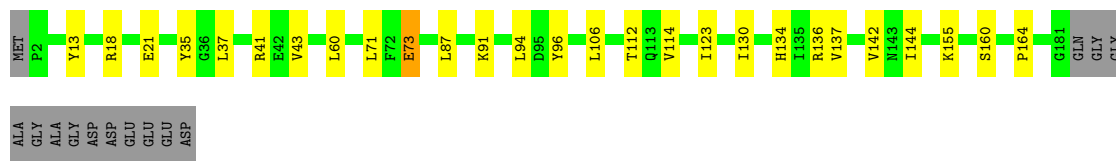
- Molecule 10: 40S ribosomal protein S8

Chain SI: 81% 17% .



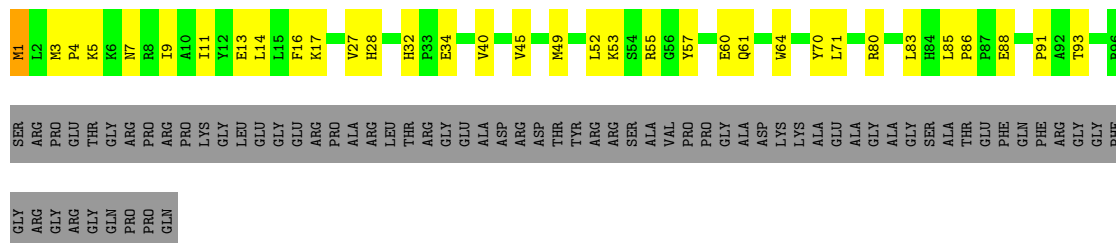
- Molecule 11: 40S ribosomal protein S9

Chain SJ: 79% 13% . 7%



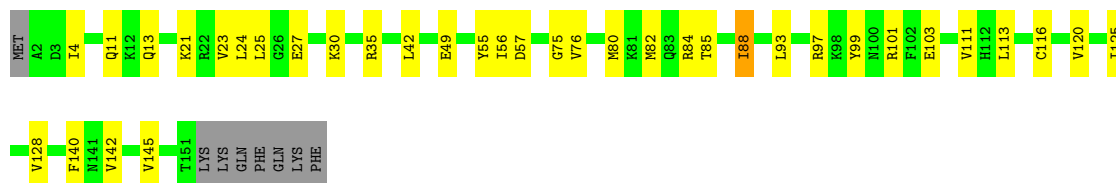
- Molecule 12: 40S ribosomal protein S10

Chain SK: 38% 20% . 42%

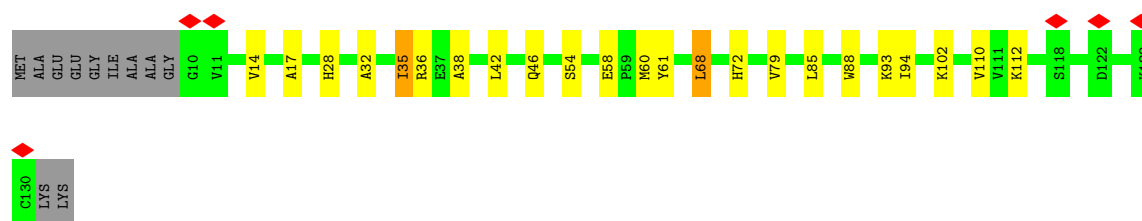
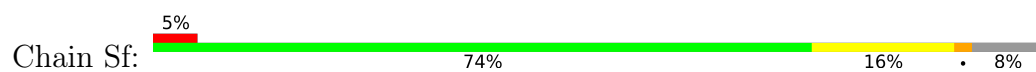


- Molecule 13: 40S ribosomal protein S11

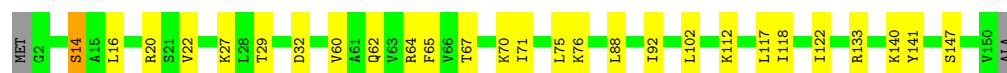
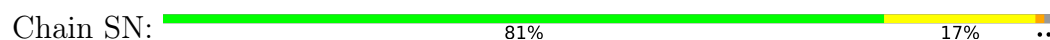
Chain SL: 72% 22% . 5%



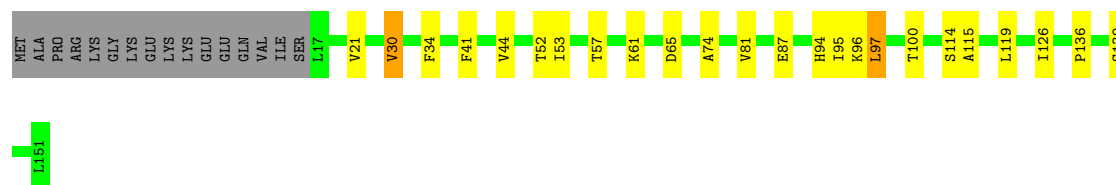
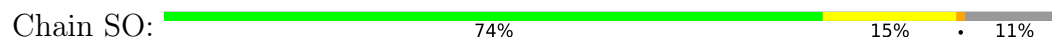
- Molecule 14: 40S ribosomal protein S12



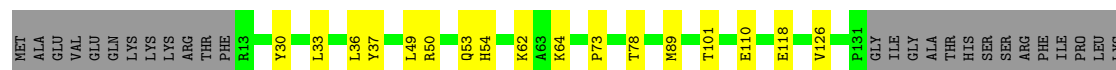
- Molecule 15: 40S ribosomal protein S13



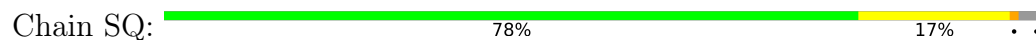
- Molecule 16: 40S ribosomal protein S14



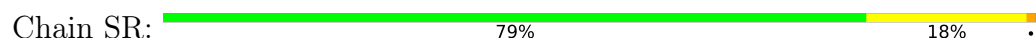
- Molecule 17: 40S ribosomal protein S15



- Molecule 18: 40S ribosomal protein S16

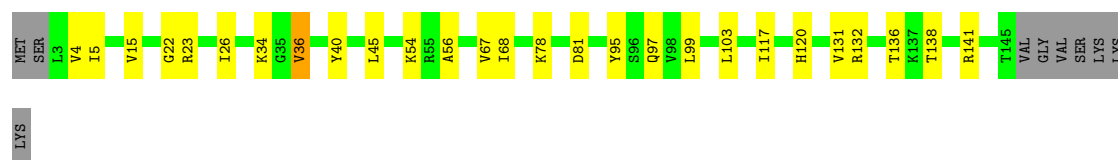


- Molecule 19: 40S ribosomal protein S17



- Molecule 20: 40S ribosomal protein S18

Chain SS:  76% 17% 6%



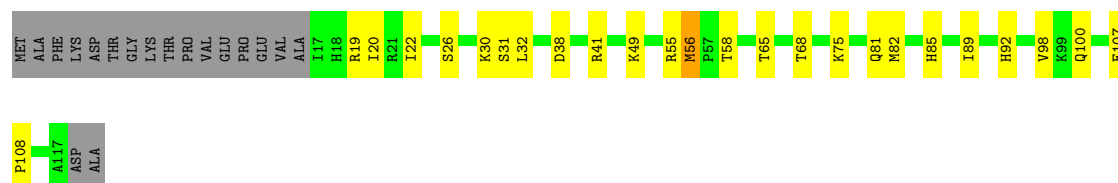
- Molecule 21: 40S ribosomal protein S19

Chain ST:  88% 10% 2%



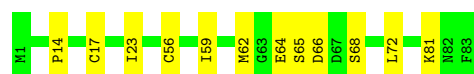
- Molecule 22: 40S ribosomal protein S20

Chain SU:  64% 20% 15%



- Molecule 23: 40S ribosomal protein S21

Chain SV:  86% 14%



- Molecule 24: 40S ribosomal protein S15a

Chain SW:  85% 12% 3%



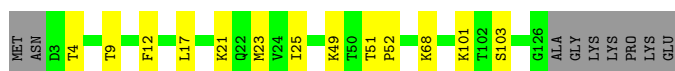
- Molecule 25: 40S ribosomal protein S23

Chain SX:  87% 11% 2%

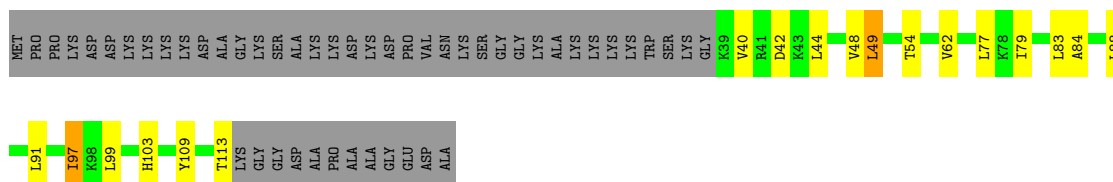


- Molecule 26: 40S ribosomal protein S24

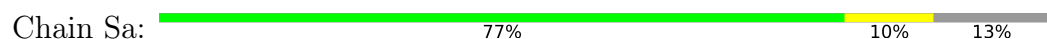
Chain SY:  83% 10% 7%



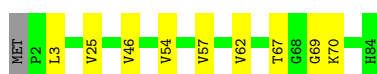
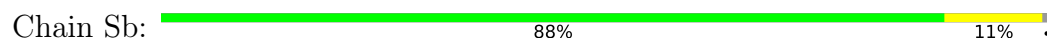
- Molecule 27: 40S ribosomal protein S25



- Molecule 28: 40S ribosomal protein S26



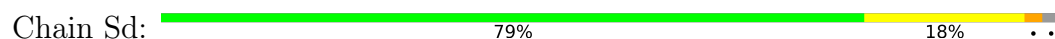
- Molecule 29: 40S ribosomal protein S27



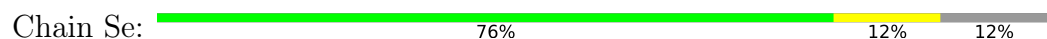
- Molecule 30: 40S ribosomal protein S28



- Molecule 31: 40S ribosomal protein S29

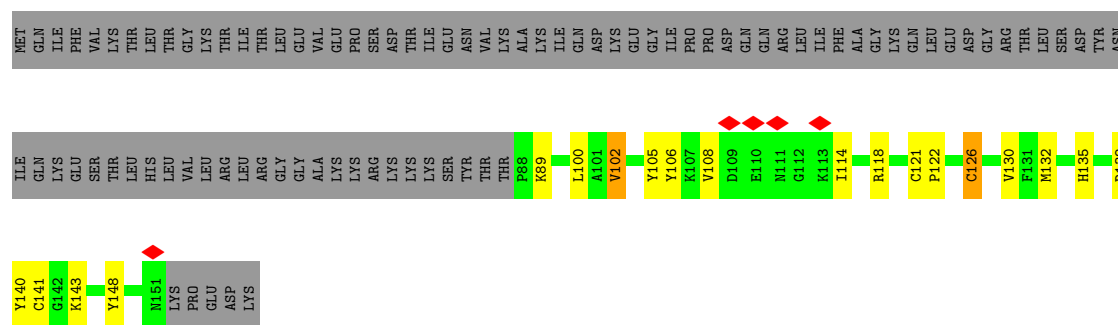


- Molecule 32: 40S ribosomal protein S30



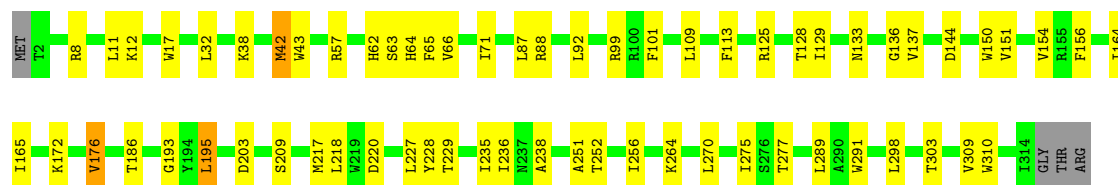
- Molecule 33: Ubiquitin-40S ribosomal protein S27a

Chain sh:  29% 11% 59%



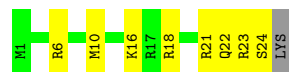
- Molecule 34: Receptor of activated protein C kinase 1

Chain Sg:  79% 19% 2%



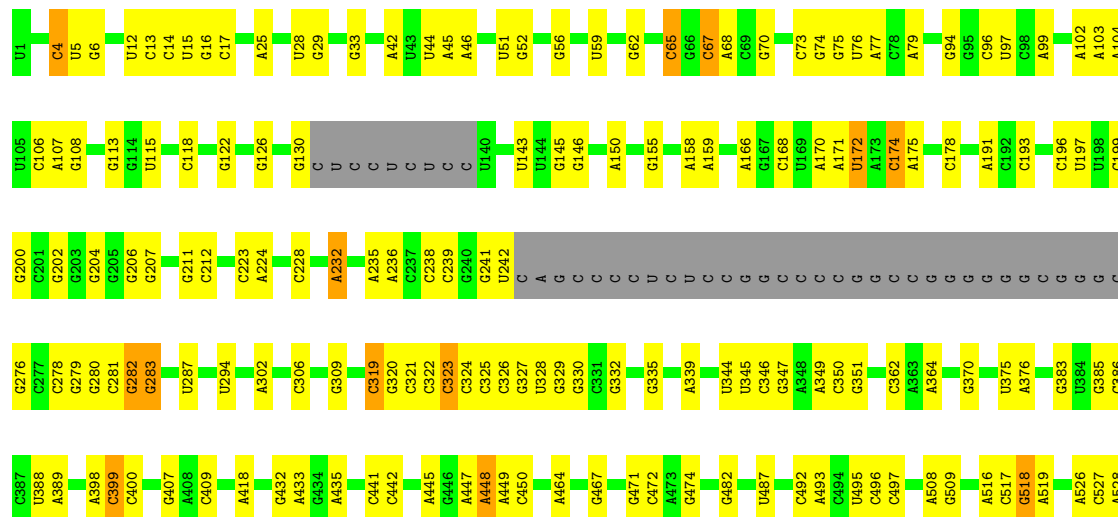
- Molecule 35: 60S ribosomal protein L41

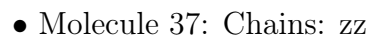
Chain Ln:  64% 32% 4%

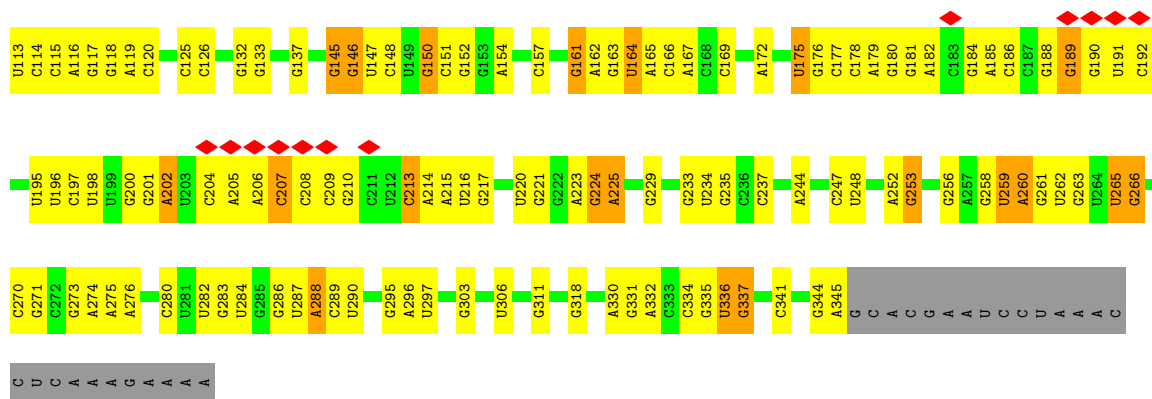


- Molecule 36: Chains: S2

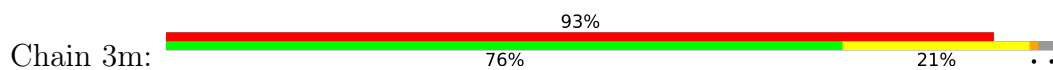
Chain S2:  60% 31% 6%





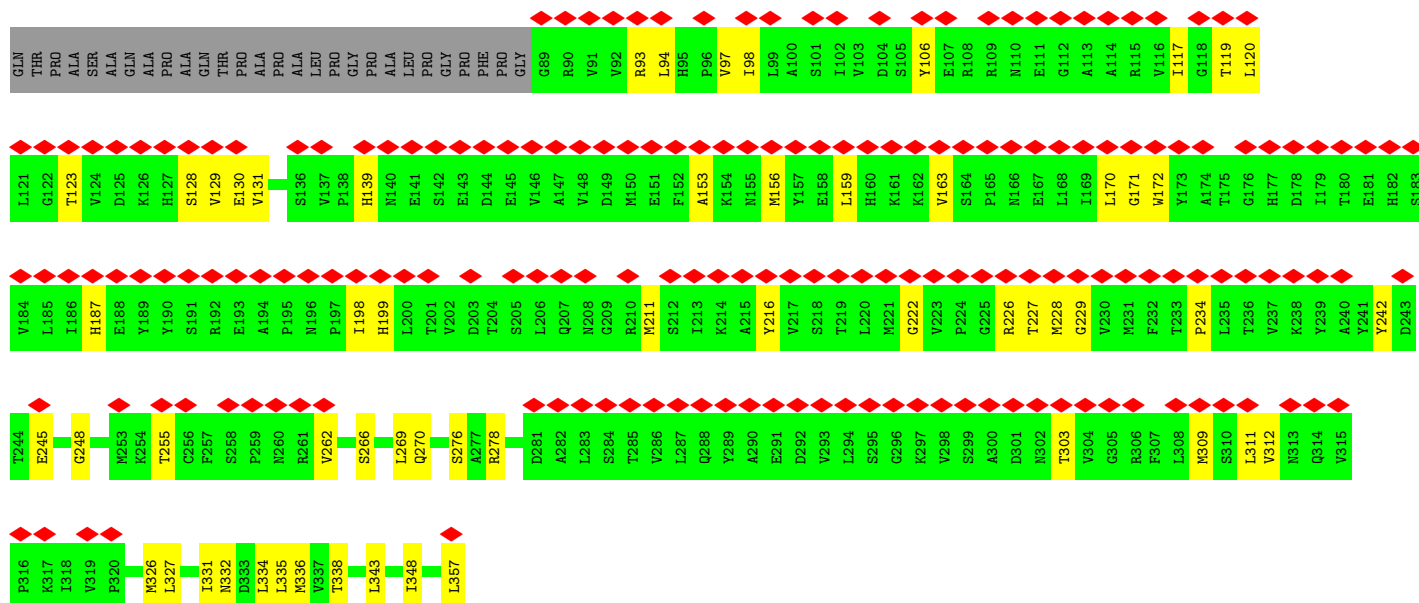


• Molecule 38: Eukaryotic translation initiation factor 3 subunit M

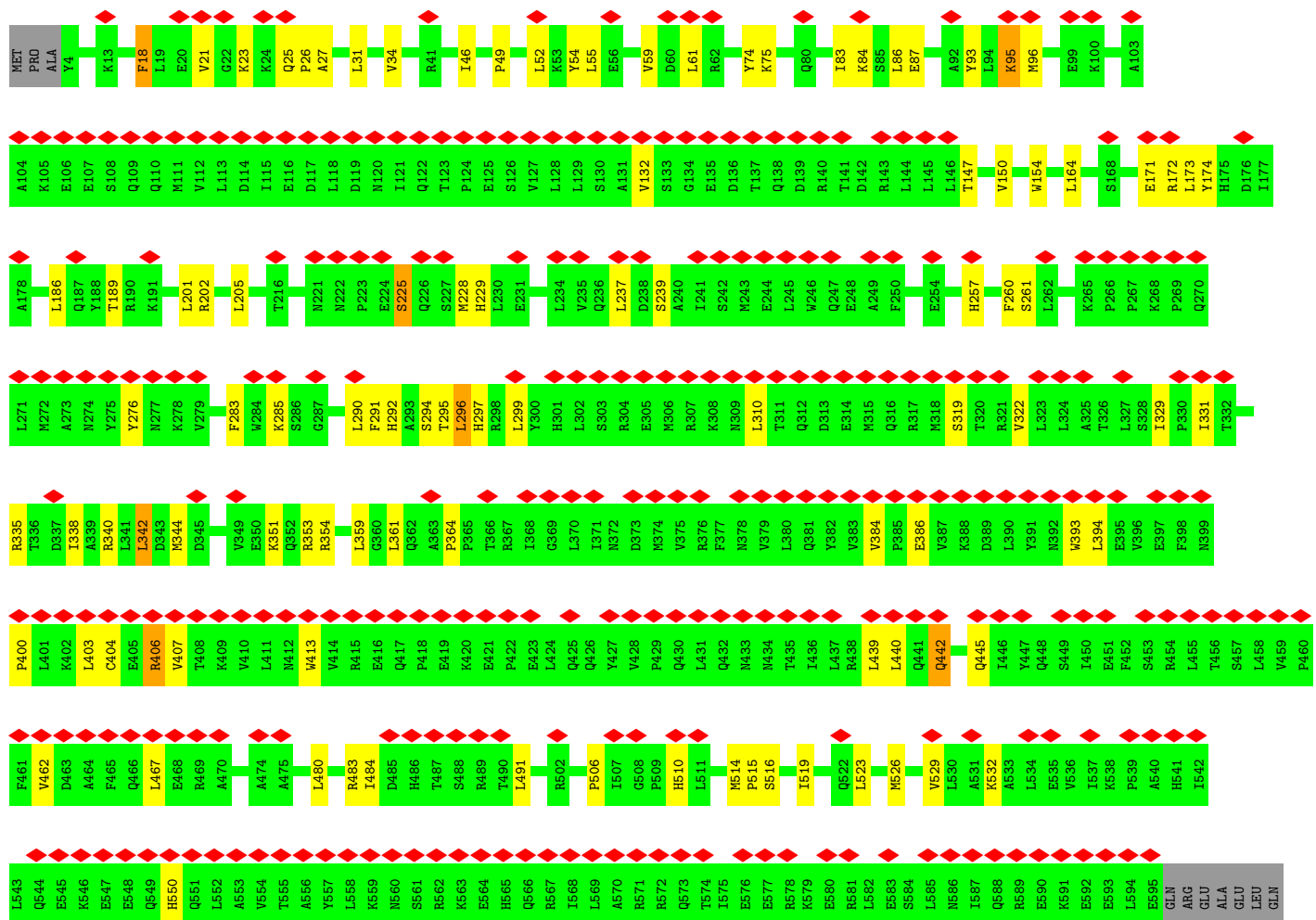
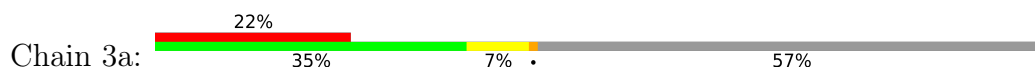


• Molecule 39: Eukaryotic translation initiation factor 3 subunit F

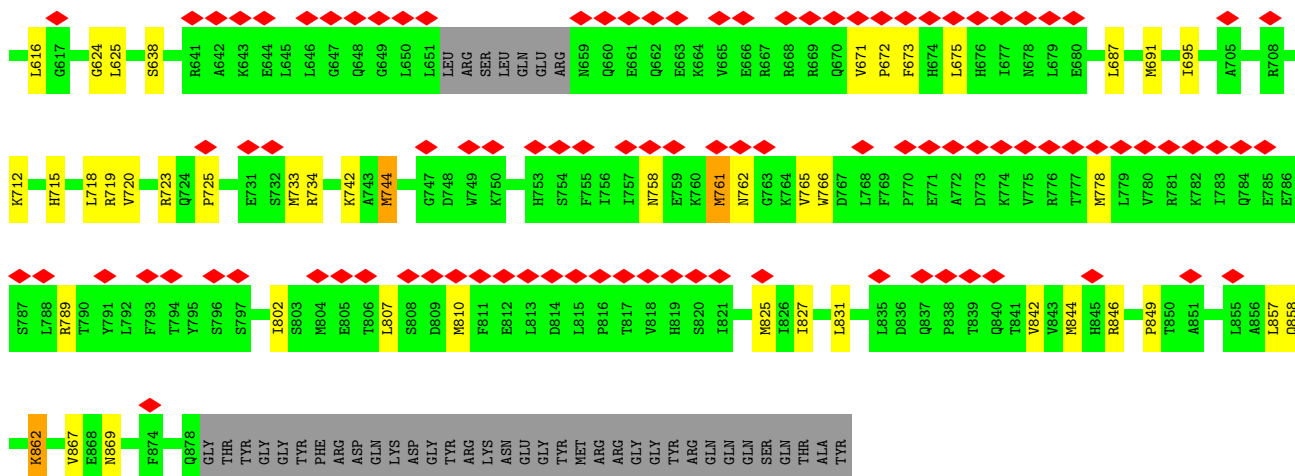




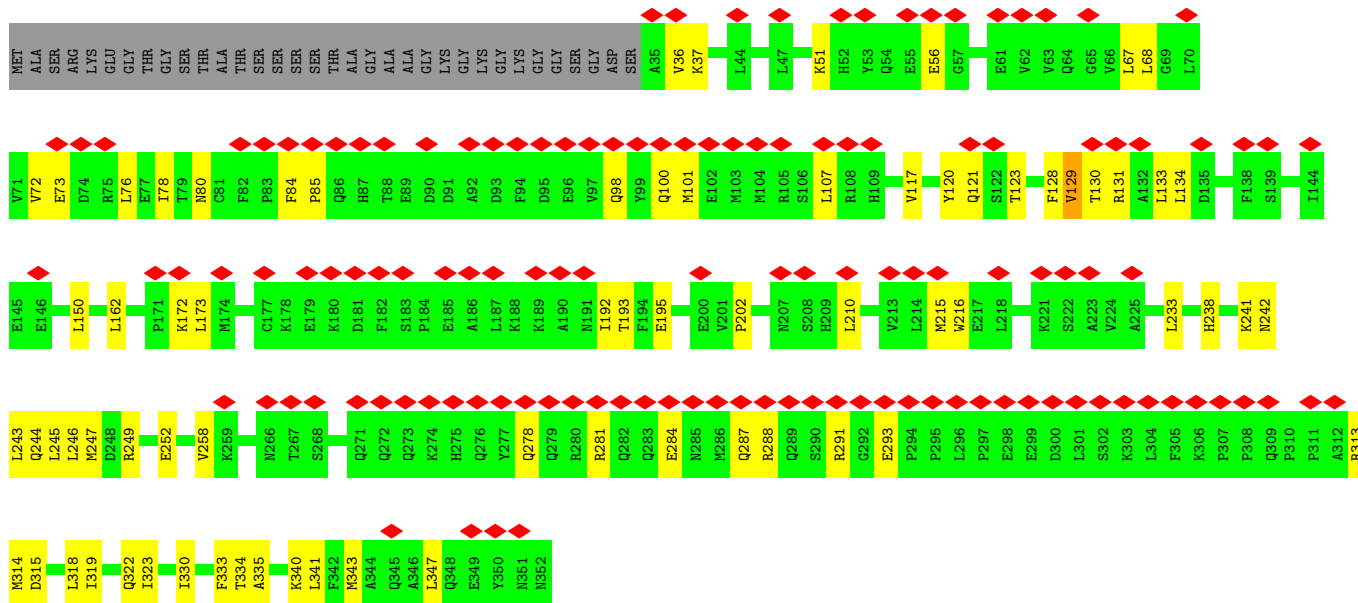
• Molecule 40: Eukaryotic translation initiation factor 3 subunit A



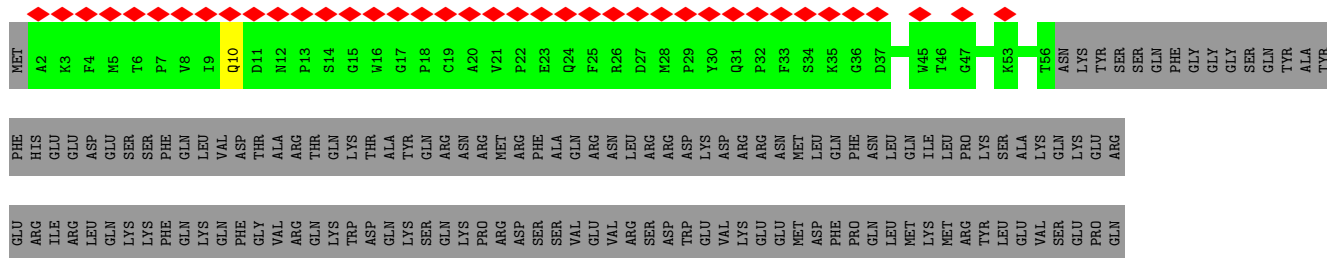




• Molecule 43: Eukaryotic translation initiation factor 3 subunit H



• Molecule 44: Eukaryotic translation initiation factor 3 subunit D





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46337	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	636.0, 636.0, 636.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.272, 1.272, 1.272	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, MG

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	1A	0.17	0/790	0.52	0/1058
2	SA	0.17	0/1742	0.42	0/2367
3	SB	0.16	0/1749	0.42	0/2340
4	SC	0.20	0/1737	0.52	0/2347
5	SD	0.15	0/1784	0.40	0/2402
6	SE	0.17	0/2107	0.45	0/2836
7	SF	0.18	0/1540	0.45	0/2071
8	SG	0.14	0/1946	0.41	0/2590
9	SH	0.19	0/1529	0.51	0/2048
10	SI	0.15	0/1711	0.39	0/2282
11	SJ	0.16	0/1524	0.41	0/2035
12	SK	0.27	0/834	0.74	0/1125
13	SL	0.20	0/1241	0.48	0/1662
14	Sf	0.16	0/945	0.49	0/1269
15	SN	0.18	0/1226	0.46	0/1649
16	SO	0.18	0/1020	0.43	0/1368
17	SP	0.23	0/1003	0.61	0/1340
18	SQ	0.20	0/1133	0.53	0/1517
19	SR	0.25	0/1082	0.64	0/1452
20	SS	0.19	0/1202	0.48	0/1610
21	ST	0.19	0/1122	0.51	0/1504
22	SU	0.20	0/813	0.54	0/1092
23	SV	0.21	0/643	0.53	0/860
24	SW	0.18	0/1051	0.45	0/1406
25	SX	0.17	0/1116	0.47	0/1490
26	SY	0.16	0/1031	0.38	0/1370
27	SZ	0.23	0/607	0.58	0/815
28	Sa	0.16	0/817	0.42	0/1095
29	Sb	0.20	0/665	0.43	0/891
30	Sc	0.19	0/490	0.50	0/656
31	Sd	0.22	0/470	0.56	0/623
32	Se	0.14	0/422	0.35	0/555

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	sh	0.16	0/529	0.42	0/701
34	Sg	0.14	0/2493	0.41	0/3394
35	Ln	0.19	0/231	0.64	1/294 (0.3%)
36	S2	0.14	0/42121	0.31	0/65651
37	zz	0.14	0/7199	0.34	0/11223
38	3m	0.15	0/2676	0.45	0/3635
39	3f	0.14	0/2099	0.36	0/2856
40	3a	0.13	0/4560	0.40	0/6207
41	3e	0.12	0/3288	0.35	0/4475
42	3c	0.13	0/3990	0.35	0/5424
43	3h	0.19	0/2571	0.39	0/3484
44	3d	0.11	0/358	0.30	0/493
45	3k	0.17	0/1502	0.44	0/2052
46	3l	0.13	0/4446	0.38	0/6013
All	All	0.16	0/115155	0.39	1/165627 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	Ln	22	GLN	N-CA-C	-5.29	107.84	114.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	780	0	786	20	0
2	SA	1705	0	1706	26	0
3	SB	1722	0	1794	20	0
4	SC	1700	0	1784	28	0
5	SD	1756	0	1851	25	0
6	SE	2065	0	2169	22	0
7	SF	1518	0	1569	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	SG	1923	0	2089	14	0
9	SH	1506	0	1603	16	0
10	SI	1682	0	1769	17	0
11	SJ	1499	0	1618	17	0
12	SK	810	0	836	27	0
13	SL	1220	0	1289	22	0
14	Sf	935	0	964	14	0
15	SN	1202	0	1289	17	0
16	SO	1007	0	1032	13	0
17	SP	984	0	1033	11	0
18	SQ	1116	0	1185	13	0
19	SR	1068	0	1121	17	0
20	SS	1184	0	1244	18	0
21	ST	1103	0	1133	7	0
22	SU	803	0	873	14	0
23	SV	636	0	637	6	0
24	SW	1034	0	1080	8	0
25	SX	1098	0	1167	8	0
26	SY	1014	0	1082	7	0
27	SZ	601	0	662	12	0
28	Sa	803	0	850	6	0
29	Sb	651	0	672	6	0
30	Sc	488	0	514	14	0
31	Sd	459	0	452	9	0
32	Se	417	0	463	4	0
33	sh	518	0	527	9	0
34	Sg	2436	0	2393	34	0
35	Ln	230	0	276	2	0
36	S2	37669	0	19037	275	0
37	zz	6443	0	3259	60	0
38	3m	2639	0	2442	46	0
39	3f	2063	0	2054	39	0
40	3a	4475	0	4192	75	0
41	3e	3224	0	2925	24	0
42	3c	3924	0	3512	47	0
43	3h	2520	0	2445	52	0
44	3d	347	0	259	0	0
45	3k	1475	0	1239	21	0
46	3l	4335	0	4272	68	0
47	Sa	1	0	0	0	0
47	sh	1	0	0	0	0
48	S2	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	108797	0	87148	1128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1128) 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)
37:zz:61:U:H3	37:zz:107:G:H1	1.08	0.94
37:zz:52:G:N2	37:zz:111:C:O2	2.08	0.87
36:S2:197:U:H3	36:S2:202:G:H1	0.88	0.85
36:S2:1748:G:H1	36:S2:1786:U:H3	1.26	0.83
40:3a:276:TYR:HB3	40:3a:299:LEU:HD23	1.61	0.81
5:SD:177:LEU:HD13	5:SD:179:GLN:H	1.47	0.79
43:3h:244:GLN:HA	43:3h:247:MET:HG3	1.68	0.76
46:3l:330:GLN:HE22	46:3l:499:ASN:HB2	1.52	0.75
5:SD:27:ARG:HB3	12:SK:61:GLN:HE21	1.53	0.74
36:S2:171:A:H3'	36:S2:172:U:H6	1.54	0.73
20:SS:36:VAL:HG23	20:SS:40:TYR:HB3	1.71	0.72
34:Sg:87:LEU:HB2	34:Sg:101:PHE:HB2	1.71	0.72
4:SC:209:VAL:HG21	4:SC:233:LEU:HD21	1.71	0.70
24:SW:8:ALA:HA	24:SW:74:VAL:HG11	1.73	0.70
29:Sb:67:THR:HG23	29:Sb:69:GLY:H	1.57	0.70
40:3a:18:PHE:HB3	40:3a:27:ALA:HB2	1.73	0.69
43:3h:278:GLN:HA	43:3h:281:ARG:HB2	1.75	0.69
16:SO:74:ALA:HB1	16:SO:115:ALA:HB2	1.75	0.69
34:Sg:109:LEU:HD11	34:Sg:125:ARG:HG3	1.75	0.69
2:SA:10:MET:HE3	2:SA:15:VAL:HG22	1.74	0.68
36:S2:870:A:H4'	36:S2:871:U:H3'	1.76	0.68
2:SA:30:LEU:HD21	2:SA:35:GLU:HG2	1.75	0.68
4:SC:204:ILE:HD13	4:SC:215:MET:HG2	1.75	0.68
2:SA:184:ARG:HD2	2:SA:191:ARG:HG2	1.76	0.68
4:SC:102:LEU:HD12	4:SC:130:ILE:HG12	1.75	0.68
46:3l:454:GLN:HE22	46:3l:496:LYS:HG3	1.59	0.68
37:zz:52:G:N1	37:zz:111:C:N3	2.35	0.67
5:SD:213:PRO:HG3	19:SR:19:LYS:HB3	1.77	0.67
36:S2:546:G:H4'	36:S2:547:G:H5'	1.76	0.67
16:SO:34:PHE:HB3	16:SO:41:PHE:HB2	1.76	0.67
45:3k:108:LEU:HD21	45:3k:117:PHE:HA	1.75	0.67
42:3c:720:VAL:HA	42:3c:723:ARG:HB2	1.77	0.66
12:SK:14:LEU:HA	12:SK:17:LYS:HB2	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SF:188:TYR:HA	7:SF:191:LYS:HZ2	1.60	0.66
36:S2:851:C:H5''	36:S2:852:G:H5'	1.77	0.66
42:3c:802:ILE:HD12	42:3c:807:LEU:HD11	1.76	0.66
12:SK:16:PHE:HE2	12:SK:91:PRO:HD3	1.61	0.66
22:SU:49:LYS:HB2	22:SU:92:HIS:HB2	1.78	0.66
1:1A:62:ARG:HD3	1:1A:90:ASP:HB3	1.78	0.65
36:S2:172:U:H3	36:S2:174:C:H41	1.42	0.65
42:3c:825:MET:HB3	42:3c:831:LEU:HB2	1.77	0.65
28:Sa:26:CYS:HB3	28:Sa:77:CYS:SG	2.36	0.65
19:SR:71:ILE:HD12	19:SR:74:GLN:HB3	1.77	0.65
6:SE:100:ARG:HG2	6:SE:102:ILE:HG12	1.78	0.65
37:zz:162:A:N1	37:zz:164:U:C4	2.65	0.64
3:SB:136:ARG:HB2	3:SB:218:LEU:HD21	1.78	0.64
15:SN:29:THR:HG22	15:SN:32:ASP:HB2	1.79	0.64
15:SN:102:LEU:HD21	15:SN:112:LYS:HG2	1.78	0.64
42:3c:869:ASN:HD21	43:3h:258:VAL:HG13	1.62	0.64
4:SC:196:ILE:HB	4:SC:223:TYR:HB2	1.79	0.64
36:S2:1751:C:H42	36:S2:1782:G:H21	1.46	0.64
40:3a:296:LEU:HD21	40:3a:322:VAL:HA	1.80	0.64
9:SH:50:GLU:HG3	9:SH:58:LYS:HE3	1.79	0.64
42:3c:733:MET:HG3	42:3c:761:MET:HE2	1.80	0.64
45:3k:212:SER:HB3	46:3l:555:ARG:HH12	1.62	0.64
36:S2:239:C:H42	36:S2:278:C:H42	1.43	0.63
10:SI:25:ARG:HB2	10:SI:28:GLU:HG3	1.81	0.63
22:SU:31:SER:HB2	22:SU:107:GLU:HG3	1.80	0.63
36:S2:898:U:H2'	36:S2:899:U:H6	1.63	0.63
46:3l:349:MET:HA	46:3l:352:ARG:HD2	1.81	0.63
46:3l:48:ILE:HB	46:3l:53:LYS:HE3	1.80	0.63
40:3a:351:LYS:HA	40:3a:354:ARG:HE	1.64	0.63
3:SB:217:MET:HE1	3:SB:220:LYS:HG3	1.81	0.63
6:SE:3:ARG:HG2	36:S2:447:A:H4'	1.81	0.62
33:sh:126:CYS:HB3	33:sh:143:LYS:HD2	1.80	0.62
37:zz:262:U:O2	37:zz:271:G:O6	2.16	0.62
39:3f:334:LEU:HB3	43:3h:334:THR:HG23	1.82	0.62
46:3l:380:MET:HG2	46:3l:538:ARG:HH12	1.65	0.62
37:zz:98:G:H2'	37:zz:99:A:C8	2.35	0.62
37:zz:175:U:H3'	37:zz:176:G:H8	1.64	0.62
45:3k:124:ASN:HD22	45:3k:127:LEU:HD12	1.64	0.62
36:S2:1756:C:H2'	36:S2:1757:G:H8	1.65	0.61
41:3e:110:GLY:HA2	41:3e:113:LEU:HD12	1.82	0.61
5:SD:161:GLY:HA3	36:S2:1388:A:H61	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:3m:83:ILE:HG23	38:3m:86:LEU:HD23	1.83	0.61
41:3e:155:ARG:HH11	41:3e:169:LEU:HD11	1.63	0.61
7:SF:104:THR:HG23	7:SF:106:GLU:H	1.65	0.61
36:S2:649:U:H2'	36:S2:650:A:H8	1.65	0.61
5:SD:177:LEU:HD22	5:SD:178:ARG:H	1.66	0.61
17:SP:33:LEU:HD23	17:SP:36:LEU:HD12	1.82	0.61
18:SQ:86:GLN:HE22	18:SQ:122:ALA:HA	1.65	0.61
40:3a:18:PHE:HE1	40:3a:23:LYS:HD2	1.66	0.61
38:3m:16:ALA:HA	38:3m:19:ARG:HH21	1.66	0.61
36:S2:1536:G:H2'	36:S2:1537:A:H8	1.65	0.61
18:SQ:111:ILE:HA	18:SQ:114:GLN:HE21	1.66	0.60
42:3c:858:GLN:HB2	43:3h:247:MET:HE1	1.83	0.60
3:SB:35:ALA:HB2	3:SB:44:ILE:HD11	1.81	0.60
27:SZ:79:ILE:HD12	27:SZ:83:LEU:HD13	1.82	0.60
36:S2:375:U:H2'	36:S2:376:A:C8	2.36	0.60
46:3l:349:MET:HE3	46:3l:349:MET:H	1.65	0.60
46:3l:464:LEU:HD22	46:3l:530:ILE:HD11	1.82	0.60
5:SD:226:GLN:HG3	34:Sg:186:THR:HG23	1.84	0.60
36:S2:518:G:H2'	36:S2:519:A:H8	1.67	0.60
39:3f:94:LEU:HG	39:3f:98:ILE:HD11	1.84	0.60
46:3l:278:LEU:HD21	46:3l:294:LEU:HB2	1.83	0.59
13:SL:113:LEU:HD22	13:SL:142:VAL:HG11	1.83	0.59
38:3m:165:LEU:HD12	38:3m:188:LEU:HD13	1.85	0.59
36:S2:792:C:H2'	36:S2:793:G:C8	2.37	0.59
40:3a:55:LEU:HD13	40:3a:93:TYR:HB2	1.85	0.59
46:3l:382:ILE:HG13	46:3l:387:HIS:HB2	1.85	0.59
36:S2:171:A:H3'	36:S2:172:U:C6	2.37	0.59
36:S2:928:G:H2'	36:S2:929:G:C8	2.38	0.59
17:SP:110:GLU:HG3	20:SS:117:ILE:HD11	1.84	0.59
25:SX:101:LEU:HB3	25:SX:124:LYS:HB2	1.85	0.59
37:zz:61:U:O2	37:zz:107:G:N2	2.28	0.59
39:3f:163:VAL:HG22	43:3h:85:PRO:HG3	1.84	0.59
3:SB:82:ARG:HG3	3:SB:103:MET:HE2	1.85	0.59
6:SE:192:ILE:HB	6:SE:243:GLY:HA3	1.84	0.59
38:3m:15:ALA:HA	38:3m:18:LEU:HD12	1.83	0.59
40:3a:523:LEU:HD23	43:3h:233:LEU:HD11	1.85	0.59
30:Sc:60:GLU:HG2	30:Sc:63:ARG:HH11	1.67	0.59
36:S2:150:A:H62	36:S2:168:C:H42	1.50	0.59
31:Sd:55:LEU:HD23	36:S2:1391:C:H4'	1.85	0.58
46:3l:148:PRO:HB2	46:3l:153:ARG:HE	1.68	0.58
14:Sf:32:ALA:HB3	14:Sf:110:VAL:HB	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:S2:1562:C:H2'	36:S2:1563:G:H8	1.68	0.58
38:3m:69:SER:HA	38:3m:72:LEU:HD12	1.85	0.58
38:3m:156:LEU:HD11	38:3m:160:LYS:HD2	1.84	0.58
46:3l:213:ASP:HA	46:3l:216:ARG:HD2	1.86	0.58
1:1A:29:LYS:HB2	1:1A:35:TYR:HE1	1.68	0.58
27:SZ:40:VAL:HG12	27:SZ:42:ASP:H	1.68	0.58
36:S2:1757:G:H1	36:S2:1775:U:H3	1.51	0.58
36:S2:1764:G:O6	36:S2:1768:A:N7	2.35	0.58
1:1A:33:GLN:HB3	1:1A:78:LEU:HD11	1.85	0.58
36:S2:1536:G:H2'	36:S2:1537:A:C8	2.38	0.58
19:SR:83:ASN:C	19:SR:83:ASN:HD22	2.10	0.58
30:Sc:18:LEU:HD11	30:Sc:43:ILE:HD11	1.87	0.57
42:3c:424:ILE:HG21	42:3c:439:ARG:HD2	1.86	0.57
11:SJ:91:LYS:HB3	11:SJ:96:TYR:HD1	1.69	0.57
43:3h:284:GLU:HA	43:3h:287:GLN:HG2	1.86	0.57
45:3k:146:VAL:HG12	45:3k:189:ILE:HG12	1.87	0.57
39:3f:120:LEU:HD13	39:3f:131:VAL:HG22	1.86	0.57
39:3f:357:LEU:HD22	41:3e:425:LYS:HE3	1.85	0.57
45:3k:150:TYR:HB3	45:3k:189:ILE:HG21	1.87	0.57
39:3f:98:ILE:HG21	39:3f:131:VAL:HG12	1.87	0.57
39:3f:338:THR:HB	43:3h:334:THR:HG21	1.87	0.57
22:SU:22:ILE:HG13	22:SU:89:ILE:HB	1.87	0.57
36:S2:150:A:H62	36:S2:168:C:N4	2.02	0.57
38:3m:143:GLU:HG2	38:3m:146:GLN:H	1.70	0.57
41:3e:411:LEU:HD12	42:3c:867:VAL:HG11	1.86	0.57
12:SK:4:PRO:HD2	12:SK:7:ASN:HD21	1.69	0.57
34:Sg:32:LEU:HD11	34:Sg:92:LEU:HD21	1.87	0.57
39:3f:276:SER:HB2	43:3h:343:MET:HE1	1.87	0.57
2:SA:122:LEU:HB2	2:SA:142:LEU:HD12	1.85	0.56
36:S2:1758:G:H2'	36:S2:1759:G:H8	1.69	0.56
20:SS:23:ARG:HB3	27:SZ:48:VAL:HG21	1.88	0.56
22:SU:38:ASP:HA	22:SU:41:ARG:HH12	1.69	0.56
37:zz:252:A:H4'	37:zz:253:G:H5'	1.87	0.56
40:3a:462:VAL:HG21	40:3a:467:LEU:HD13	1.86	0.56
36:S2:1723:G:H2'	36:S2:1724:A:C8	2.40	0.56
1:1A:37:GLN:HG3	1:1A:114:LYS:HZ2	1.70	0.56
7:SF:88:MET:HE2	7:SF:92:ILE:HD11	1.88	0.56
12:SK:32:HIS:HE1	12:SK:34:GLU:HB3	1.69	0.56
14:Sf:35:ILE:HD12	14:Sf:36:ARG:HG2	1.85	0.56
34:Sg:238:ALA:H	34:Sg:251:ALA:HB3	1.70	0.56
2:SA:34:MET:HE1	2:SA:162:PRO:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SC:90:GLU:HB2	4:SC:93:ILE:HD13	1.88	0.56
6:SE:104:ASP:HB3	6:SE:110:ALA:HB2	1.88	0.56
45:3k:188:PHE:HZ	45:3k:191:SER:HB2	1.71	0.56
6:SE:64:ILE:HG23	26:SY:17:LEU:HD12	1.87	0.56
16:SO:95:ILE:HD11	16:SO:126:ILE:HD12	1.86	0.56
37:zz:87:G:H2'	37:zz:88:G:H8	1.69	0.56
38:3m:57:ASP:HB3	38:3m:98:ARG:HE	1.71	0.56
46:3l:330:GLN:HG3	46:3l:378:TYR:HE1	1.71	0.56
15:SN:20:ARG:HG3	15:SN:65:PHE:HE1	1.71	0.56
33:sh:121:CYS:HA	33:sh:132:MET:HE1	1.87	0.56
38:3m:29:ILE:HG12	38:3m:44:GLN:HG3	1.88	0.56
2:SA:108:PHE:HB3	2:SA:140:VAL:HG21	1.88	0.56
17:SP:49:LEU:HD22	17:SP:53:GLN:HE21	1.70	0.55
23:SV:14:PRO:HG2	23:SV:23:ILE:HD11	1.87	0.55
40:3a:483:ARG:HH12	42:3c:846:ARG:HD3	1.71	0.55
9:SH:50:GLU:HB2	9:SH:60:ILE:HG22	1.88	0.55
30:Sc:22:GLY:HA2	30:Sc:68:LEU:HB2	1.88	0.55
36:S2:874:G:H2'	36:S2:875:A:H8	1.70	0.55
42:3c:573:ILE:HD11	42:3c:616:LEU:HD22	1.87	0.55
4:SC:70:VAL:HG11	4:SC:93:ILE:HG13	1.88	0.55
34:Sg:42:MET:HE3	34:Sg:57:ARG:HB3	1.89	0.55
36:S2:70:G:H21	36:S2:79:A:H62	1.54	0.55
42:3c:624:GLY:H	42:3c:778:MET:HE1	1.71	0.55
42:3c:460:GLN:HG3	42:3c:672:PRO:HG3	1.89	0.55
42:3c:611:ARG:HH21	42:3c:671:VAL:HG11	1.71	0.55
5:SD:106:ARG:HG3	5:SD:175:VAL:HG22	1.88	0.55
36:S2:1545:A:H2'	36:S2:1546:G:C8	2.42	0.55
41:3e:341:PHE:HA	41:3e:344:PHE:HB2	1.87	0.55
43:3h:131:ARG:HH12	43:3h:315:ASP:HA	1.72	0.55
43:3h:242:ASN:HA	43:3h:245:LEU:HD12	1.89	0.55
45:3k:181:ALA:HB2	45:3k:187:ILE:HG12	1.89	0.55
3:SB:87:ILE:HG22	3:SB:101:HIS:HB2	1.88	0.55
4:SC:68:ARG:HE	4:SC:276:THR:HG21	1.71	0.55
6:SE:66:MET:HE2	6:SE:66:MET:HA	1.89	0.55
36:S2:197:U:O4	36:S2:202:G:O6	2.25	0.55
40:3a:529:VAL:HG23	40:3a:532:LYS:HE3	1.89	0.55
46:3l:339:ILE:HD12	46:3l:342:TYR:HB3	1.88	0.55
36:S2:1762:C:H2'	36:S2:1763:G:H8	1.72	0.55
37:zz:259:U:H2'	37:zz:260:A:H8	1.71	0.55
42:3c:691:MET:HE1	42:3c:695:ILE:HD13	1.89	0.55
9:SH:80:VAL:HG23	9:SH:92:VAL:HB	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SL:99:TYR:CE2	25:SX:13:LEU:HB3	2.41	0.55
19:SR:83:ASN:O	19:SR:83:ASN:ND2	2.36	0.55
33:sh:135:HIS:HB2	33:sh:138:ARG:HG2	1.89	0.55
5:SD:115:VAL:HG11	5:SD:142:LEU:HD12	1.88	0.55
36:S2:508:A:H3'	36:S2:509:G:H8	1.71	0.55
36:S2:1776:G:H2'	36:S2:1777:G:H4'	1.88	0.55
40:3a:342:LEU:HD11	42:3c:718:LEU:HD23	1.89	0.55
4:SC:62:PRO:HG2	4:SC:68:ARG:HD2	1.88	0.54
4:SC:106:VAL:HG22	4:SC:128:VAL:HG22	1.88	0.54
9:SH:154:ILE:HB	9:SH:185:VAL:HG22	1.89	0.54
13:SL:23:VAL:HG13	13:SL:25:LEU:H	1.72	0.54
36:S2:1101:U:H2'	36:S2:1102:G:C8	2.43	0.54
36:S2:647:U:H2'	36:S2:648:A:H8	1.72	0.54
39:3f:248:GLY:HA2	43:3h:162:LEU:HD11	1.88	0.54
43:3h:67:LEU:HD21	43:3h:78:ILE:HD13	1.88	0.54
36:S2:388:U:H2'	36:S2:389:A:C8	2.42	0.54
36:S2:753:C:H2'	36:S2:754:G:H8	1.72	0.54
40:3a:186:LEU:HD21	40:3a:239:SER:HA	1.89	0.54
20:SS:26:ILE:HG22	20:SS:45:LEU:HD21	1.89	0.54
36:S2:1550:G:H3'	36:S2:1579:A:H61	1.72	0.54
45:3k:174:MET:HE3	45:3k:187:ILE:HG21	1.89	0.54
36:S2:1748:G:O6	36:S2:1786:U:O4	2.26	0.54
46:3l:198:SER:HA	46:3l:201:ARG:HE	1.73	0.54
36:S2:877:C:H2'	36:S2:878:G:C8	2.42	0.54
12:SK:53:LYS:HZ2	12:SK:60:GLU:HG2	1.72	0.54
36:S2:1797:U:H2'	36:S2:1798:C:C6	2.43	0.54
46:3l:346:THR:HB	46:3l:349:MET:HE1	1.89	0.54
14:Sf:58:GLU:HG3	14:Sf:60:MET:H	1.73	0.54
16:SO:34:PHE:HE1	16:SO:100:THR:HA	1.73	0.54
23:SV:59:ILE:HA	23:SV:62:MET:HE3	1.89	0.54
4:SC:114:LYS:HD2	4:SC:121:ARG:HE	1.73	0.54
36:S2:981:A:H2'	36:S2:982:G:C8	2.43	0.54
36:S2:1189:A:H2'	36:S2:1190:A:H8	1.73	0.54
36:S2:1751:C:H3'	36:S2:1752:C:H4'	1.90	0.54
39:3f:311:LEU:HG	40:3a:529:VAL:HG13	1.89	0.54
11:SJ:91:LYS:HB3	11:SJ:96:TYR:CD1	2.43	0.53
34:Sg:172:LYS:HG2	34:Sg:193:GLY:H	1.73	0.53
37:zz:179:A:H2'	37:zz:180:G:H8	1.73	0.53
39:3f:156:MET:HA	39:3f:159:LEU:HD12	1.90	0.53
7:SF:50:PRO:HB3	7:SF:69:VAL:HG23	1.90	0.53
39:3f:343:LEU:HD21	41:3e:411:LEU:HD21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:3a:514:MET:HG2	40:3a:515:PRO:HD2	1.89	0.53
42:3c:602:ASP:HB2	42:3c:604:PRO:HD2	1.91	0.53
21:ST:22:LEU:HD12	21:ST:28:LEU:HD22	1.90	0.53
37:zz:181:G:H2'	37:zz:182:A:C8	2.42	0.53
43:3h:193:THR:HG22	43:3h:195:GLU:H	1.74	0.53
43:3h:120:TYR:HB2	43:3h:150:LEU:HB3	1.91	0.53
2:SA:34:MET:HG2	2:SA:154:LEU:HD21	1.91	0.53
6:SE:115:THR:HG23	6:SE:118:GLU:H	1.73	0.53
39:3f:222:GLY:HA3	39:3f:226:ARG:HD3	1.91	0.53
41:3e:299:LEU:HD21	41:3e:340:ILE:HG12	1.90	0.53
36:S2:375:U:H2'	36:S2:376:A:H8	1.73	0.53
37:zz:259:U:O2	37:zz:274:A:N7	2.42	0.53
6:SE:19:MET:HE2	36:S2:846:G:C5	2.44	0.53
8:SG:7:PHE:HD2	8:SG:10:THR:HG22	1.74	0.53
34:Sg:195:LEU:HD11	34:Sg:209:SER:HB2	1.91	0.53
45:3k:165:LEU:HD13	45:3k:169:GLN:HB3	1.91	0.53
40:3a:172:ARG:HD3	40:3a:228:MET:HE2	1.91	0.53
40:3a:296:LEU:HD12	40:3a:299:LEU:HD11	1.91	0.53
40:3a:296:LEU:HG	40:3a:322:VAL:HG23	1.90	0.53
10:SI:150:ASP:HA	10:SI:153:LYS:HE2	1.91	0.52
36:S2:756:C:H2'	36:S2:757:C:H6	1.74	0.52
17:SP:64:LYS:HA	17:SP:73:PRO:HB3	1.89	0.52
36:S2:587:A:H5'	36:S2:592:C:H41	1.74	0.52
43:3h:243:LEU:HD23	43:3h:246:LEU:HD23	1.90	0.52
12:SK:32:HIS:CE1	12:SK:34:GLU:HB3	2.44	0.52
1:1A:29:LYS:HB2	1:1A:35:TYR:CE1	2.44	0.52
36:S2:878:G:H22	36:S2:908:A:H2	1.58	0.52
8:SG:57:ASP:HA	8:SG:106:LEU:HA	1.90	0.52
30:Sc:13:ARG:HH21	30:Sc:35:MET:HE1	1.74	0.52
39:3f:187:HIS:CE1	39:3f:199:HIS:HB2	2.44	0.52
13:SL:11:GLN:HB3	13:SL:56:ILE:HG21	1.92	0.52
38:3m:22:LEU:HB3	38:3m:27:ALA:HB3	1.92	0.52
45:3k:105:LEU:HD23	45:3k:108:LEU:HD23	1.92	0.52
46:3l:521:PHE:HB3	46:3l:530:ILE:HG12	1.91	0.52
8:SG:4:ASN:HB3	8:SG:110:ASN:HD22	1.73	0.52
39:3f:106:TYR:HD2	43:3h:210:LEU:HD11	1.75	0.52
34:Sg:289:LEU:HD22	34:Sg:298:LEU:HD11	1.92	0.52
36:S2:12:U:H2'	36:S2:13:C:C6	2.45	0.52
36:S2:1228:A:H2'	36:S2:1229:G:C8	2.45	0.52
46:3l:369:ALA:HB1	46:3l:412:LEU:HD21	1.92	0.52
13:SL:111:VAL:HG11	13:SL:128:VAL:HG11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:S2:279:G:H2'	36:S2:280:G:C8	2.45	0.52
36:S2:398:A:H4'	36:S2:399:C:H5''	1.92	0.52
36:S2:1736:G:H2'	36:S2:1737:G:C8	2.45	0.52
41:3e:400:PRO:HB3	42:3c:849:PRO:HG3	1.92	0.52
43:3h:72:VAL:HG22	43:3h:73:GLU:HG2	1.92	0.52
2:SA:18:PHE:CZ	2:SA:177:MET:HE1	2.45	0.52
36:S2:197:U:O2	36:S2:202:G:N2	2.31	0.52
36:S2:595:U:H2'	36:S2:596:U:C6	2.45	0.52
41:3e:264:ASN:HD22	41:3e:270:ARG:HG3	1.74	0.52
8:SG:154:ARG:HG2	36:S2:77:A:C8	2.44	0.51
11:SJ:37:LEU:HD11	11:SJ:106:LEU:HD21	1.91	0.51
12:SK:32:HIS:CD2	12:SK:45:VAL:HG11	2.45	0.51
36:S2:866:U:H2'	36:S2:867:G:C8	2.45	0.51
7:SF:140:ASP:HB2	30:Sc:46:VAL:HG12	1.92	0.51
13:SL:4:ILE:HD11	13:SL:55:TYR:HA	1.91	0.51
36:S2:1232:U:H2'	36:S2:1233:G:H8	1.74	0.51
38:3m:260:LYS:HE2	38:3m:260:LYS:HA	1.92	0.51
40:3a:225:SER:HA	40:3a:228:MET:HB3	1.92	0.51
40:3a:403:LEU:HD22	40:3a:439:LEU:HB2	1.93	0.51
17:SP:50:ARG:HH12	36:S2:1618:C:H4'	1.75	0.51
31:Sd:50:ILE:HD12	31:Sd:50:ILE:H	1.75	0.51
36:S2:527:C:H2'	36:S2:528:A:H8	1.74	0.51
37:zz:51:G:H2'	37:zz:52:G:C8	2.45	0.51
7:SF:77:MET:HG2	7:SF:89:THR:HG21	1.93	0.51
18:SQ:58:LEU:HB3	18:SQ:62:ARG:HD3	1.91	0.51
34:Sg:256:ILE:HG23	34:Sg:270:LEU:HB2	1.92	0.51
36:S2:1762:C:H2'	36:S2:1763:G:C8	2.45	0.51
37:zz:51:G:H2'	37:zz:52:G:H8	1.76	0.51
37:zz:145:G:N2	37:zz:248:U:O2	2.43	0.51
9:SH:60:ILE:HD11	9:SH:92:VAL:HG22	1.93	0.51
36:S2:1759:G:H2'	36:S2:1760:G:H8	1.75	0.51
38:3m:221:ASP:HA	38:3m:224:LEU:HD12	1.93	0.51
39:3f:172:TRP:HE1	39:3f:187:HIS:CG	2.28	0.51
46:3l:150:LEU:HD21	46:3l:200:TYR:CE2	2.45	0.51
3:SB:83:LYS:HG3	3:SB:106:THR:HG22	1.93	0.51
34:Sg:38:LYS:HA	34:Sg:66:VAL:HG23	1.92	0.51
37:zz:118:G:H3'	37:zz:119:A:H8	1.76	0.51
37:zz:179:A:H2'	37:zz:180:G:C8	2.46	0.51
12:SK:16:PHE:CE2	12:SK:91:PRO:HD3	2.45	0.51
36:S2:1736:G:H2'	36:S2:1737:G:H8	1.76	0.51
40:3a:445:GLN:HE22	40:3a:510:HIS:HA	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SN:64:ARG:HD3	15:SN:70:LYS:HG2	1.92	0.51
21:ST:88:MET:HA	21:ST:88:MET:HE2	1.92	0.51
36:S2:649:U:H2'	36:S2:650:A:C8	2.46	0.51
10:SI:110:ARG:HH21	10:SI:122:GLY:HA3	1.76	0.51
14:Sf:85:LEU:HA	14:Sf:88:TRP:HB2	1.92	0.51
36:S2:1491:G:H2'	36:S2:1492:U:C6	2.46	0.51
37:zz:180:G:H2'	37:zz:181:G:C8	2.46	0.51
37:zz:180:G:H2'	37:zz:181:G:H8	1.76	0.51
2:SA:118:GLU:HG3	4:SC:65:LYS:HG3	1.92	0.51
29:Sb:70:LYS:HD2	36:S2:1106:C:H5''	1.92	0.51
36:S2:1098:C:H2'	36:S2:1099:G:C8	2.46	0.51
43:3h:241:LYS:HA	43:3h:244:GLN:HG3	1.93	0.51
2:SA:206:ASP:HB3	2:SA:209:GLU:HG2	1.91	0.50
20:SS:22:GLY:HA2	20:SS:56:ALA:HB3	1.92	0.50
30:Sc:17:VAL:HA	30:Sc:30:VAL:HG12	1.93	0.50
36:S2:1763:G:H2'	36:S2:1764:G:H8	1.76	0.50
37:zz:213:C:H2'	37:zz:214:A:C8	2.46	0.50
38:3m:278:ARG:CZ	38:3m:278:ARG:HA	2.41	0.50
8:SG:113:ILE:HD12	8:SG:113:ILE:H	1.75	0.50
37:zz:205:A:H2'	37:zz:206:A:C8	2.46	0.50
42:3c:844:MET:HE2	42:3c:844:MET:HA	1.92	0.50
36:S2:1513:C:H2'	36:S2:1514:G:H8	1.76	0.50
40:3a:319:SER:HA	40:3a:322:VAL:HG12	1.93	0.50
17:SP:78:THR:HA	36:S2:1298:G:H4'	1.93	0.50
36:S2:1174:U:H2'	36:S2:1175:G:H8	1.75	0.50
37:zz:259:U:H2'	37:zz:260:A:C8	2.47	0.50
43:3h:123:THR:HG21	43:3h:128:PHE:HB3	1.94	0.50
1:1A:65:LEU:HB3	1:1A:69:VAL:HG22	1.94	0.50
1:1A:101:ARG:CZ	1:1A:101:ARG:HA	2.41	0.50
36:S2:1228:A:H2'	36:S2:1229:G:H8	1.77	0.50
40:3a:171:GLU:HA	40:3a:174:TYR:HB3	1.92	0.50
2:SA:119:PRO:HG2	2:SA:142:LEU:HD11	1.94	0.50
36:S2:28:U:H2'	36:S2:29:G:H8	1.77	0.50
32:Se:31:ARG:HH22	36:S2:526:A:H5'	1.77	0.50
38:3m:83:ILE:HA	38:3m:86:LEU:HB3	1.93	0.50
41:3e:18:LEU:HA	41:3e:178:LEU:HD21	1.93	0.50
33:sh:122:PRO:HD3	33:sh:132:MET:HE1	1.93	0.50
34:Sg:154:VAL:HG12	34:Sg:165:ILE:HD11	1.94	0.50
36:S2:793:G:H2'	36:S2:794:A:O4'	2.12	0.50
36:S2:1652:G:H1	36:S2:1672:U:H3	1.59	0.50
43:3h:129:VAL:HG12	43:3h:318:LEU:HG	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SG:172:LYS:HE3	36:S2:65:C:H4'	1.94	0.49
38:3m:240:LEU:HA	38:3m:243:ILE:HD12	1.93	0.49
40:3a:484:ILE:HG12	40:3a:491:LEU:HD23	1.94	0.49
34:Sg:275:ILE:HG22	34:Sg:277:THR:H	1.77	0.49
36:S2:551:U:H2'	36:S2:552:G:C8	2.48	0.49
36:S2:791:C:H2'	36:S2:792:C:C6	2.47	0.49
37:zz:184:G:H21	37:zz:215:A:H62	1.58	0.49
42:3c:573:ILE:HG13	42:3c:585:ALA:HB1	1.93	0.49
2:SA:77:ILE:HG13	2:SA:99:ILE:HB	1.94	0.49
21:ST:99:VAL:O	21:ST:103:VAL:HG23	2.12	0.49
36:S2:496:C:H2'	36:S2:497:C:H6	1.77	0.49
39:3f:309:MET:HA	39:3f:312:VAL:HG22	1.95	0.49
5:SD:70:THR:HB	5:SD:86:LEU:HG	1.94	0.49
24:SW:86:LEU:HD21	24:SW:113:HIS:HB2	1.95	0.49
36:S2:982:G:H2'	36:S2:983:A:C8	2.48	0.49
38:3m:18:LEU:HD11	38:3m:70:LEU:HG	1.94	0.49
46:3l:341:LEU:HD11	46:3l:549:LYS:HE3	1.94	0.49
2:SA:6:ASP:HA	2:SA:9:GLN:HG2	1.94	0.49
16:SO:30:VAL:HG23	16:SO:94:HIS:HB2	1.93	0.49
36:S2:235:A:H2'	36:S2:236:A:C8	2.47	0.49
36:S2:388:U:H2'	36:S2:389:A:H8	1.77	0.49
41:3e:169:LEU:HB3	41:3e:192:LEU:HD12	1.92	0.49
46:3l:324:LEU:HD21	46:3l:374:ALA:HB2	1.94	0.49
34:Sg:63:SER:HB3	36:S2:1398:G:H1'	1.94	0.49
38:3m:93:PHE:HB2	38:3m:102:ARG:HH22	1.76	0.49
40:3a:295:THR:HG22	40:3a:359:LEU:HD12	1.94	0.49
43:3h:129:VAL:HB	43:3h:322:GLN:HG3	1.94	0.49
1:1A:26:LEU:HD11	1:1A:103:LEU:HD13	1.95	0.49
6:SE:19:MET:HE2	36:S2:846:G:C4	2.47	0.49
10:SI:69:SER:HB2	13:SL:21:LYS:HB2	1.93	0.49
11:SJ:134:HIS:HE1	11:SJ:164:PRO:HD2	1.77	0.49
19:SR:71:ILE:HG13	19:SR:75:GLU:HG2	1.94	0.49
36:S2:322:C:H2'	36:S2:323:C:C6	2.48	0.49
41:3e:353:ILE:HD13	41:3e:368:GLU:HB2	1.94	0.49
46:3l:103:THR:HG22	46:3l:112:TRP:HE1	1.76	0.49
1:1A:24:ARG:HH21	1:1A:95:TYR:HD1	1.60	0.49
36:S2:1221:G:H2'	36:S2:1222:G:C8	2.48	0.49
36:S2:1653:U:H3	36:S2:1671:G:H1	1.60	0.49
42:3c:512:TYR:HE2	42:3c:675:LEU:HA	1.76	0.49
43:3h:288:ARG:HG2	43:3h:293:GLU:HG3	1.95	0.49
18:SQ:70:VAL:HG11	18:SQ:84:ILE:HG23	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:3m:124:TYR:HA	38:3m:127:LEU:HD12	1.95	0.49
39:3f:216:TYR:HA	39:3f:234:PRO:HA	1.94	0.49
12:SK:53:LYS:NZ	12:SK:60:GLU:HG2	2.28	0.49
18:SQ:78:VAL:HG22	36:S2:1673:U:H5'	1.93	0.49
40:3a:164:LEU:HB3	40:3a:174:TYR:HB2	1.95	0.49
40:3a:404:CYS:HA	40:3a:407:VAL:HB	1.95	0.49
20:SS:97:GLN:HG3	20:SS:99:LEU:HD21	1.94	0.48
36:S2:982:G:H2'	36:S2:983:A:H8	1.77	0.48
38:3m:269:LEU:HD12	38:3m:271:GLU:HB2	1.93	0.48
40:3a:394:LEU:HD22	40:3a:406:ARG:HH22	1.78	0.48
20:SS:132:ARG:HH11	36:S2:1623[A]:A:H62	1.60	0.48
27:SZ:79:ILE:HG23	27:SZ:83:LEU:HB3	1.95	0.48
36:S2:736:C:H2'	36:S2:737:G:C8	2.48	0.48
36:S2:1413:G:H2'	36:S2:1414:A:H8	1.78	0.48
12:SK:64:TRP:CD2	31:Sd:23:VAL:HG22	2.49	0.48
19:SR:98:VAL:HG21	19:SR:117:LEU:HD23	1.94	0.48
36:S2:844:U:H2'	36:S2:845:G:H8	1.77	0.48
37:zz:265:U:HO2'	37:zz:266:G:H8	1.60	0.48
38:3m:245:VAL:HA	38:3m:339:HIS:CE1	2.48	0.48
45:3k:17:GLY:HA2	46:3l:232:HIS:CD2	2.48	0.48
33:sh:106:TYR:HB3	33:sh:114:ILE:HD11	1.95	0.48
36:S2:106:C:H2'	36:S2:107:A:C8	2.48	0.48
36:S2:1588:A:H2'	36:S2:1589:A:C8	2.49	0.48
38:3m:64:MET:HE2	38:3m:64:MET:HA	1.94	0.48
40:3a:59:VAL:HG11	40:3a:96:MET:HE1	1.95	0.48
41:3e:403:GLN:NE2	42:3c:857:LEU:HD22	2.28	0.48
1:1A:110:PRO:HG2	1:1A:112:HIS:HE1	1.78	0.48
36:S2:321:C:H2'	36:S2:322:C:C6	2.49	0.48
36:S2:746:C:H1'	36:S2:747:U:H5	1.76	0.48
36:S2:1809:A:H2'	36:S2:1810:U:C6	2.49	0.48
40:3a:283:PHE:HB3	40:3a:292:HIS:HB2	1.96	0.48
42:3c:570:LEU:HD22	42:3c:612:THR:HG21	1.95	0.48
2:SA:205:ARG:HH21	2:SA:210:ILE:HA	1.77	0.48
4:SC:214:LEU:HD21	4:SC:244:ILE:HD11	1.94	0.48
27:SZ:91:LEU:HD23	27:SZ:97:ILE:HD13	1.96	0.48
36:S2:5:U:H2'	36:S2:6:G:H8	1.78	0.48
36:S2:528:A:H2'	36:S2:529:A:C8	2.48	0.48
36:S2:996:A:H2'	36:S2:997:A:C8	2.49	0.48
37:zz:161:G:H2'	37:zz:162:A:H8	1.78	0.48
38:3m:60:VAL:HB	38:3m:101:LEU:HD11	1.95	0.48
42:3c:515:ASP:H	42:3c:579:HIS:CE1	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SH:37:LYS:HD3	9:SH:41:ARG:HH21	1.79	0.48
10:SI:34:ALA:HB2	10:SI:56:ARG:HE	1.79	0.48
20:SS:132:ARG:HH21	36:S2:1609:C:H3'	1.79	0.48
36:S2:106:C:H2'	36:S2:107:A:H8	1.79	0.48
1:1A:37:GLN:HG3	1:1A:114:LYS:NZ	2.29	0.48
18:SQ:110:ASP:O	18:SQ:114:GLN:HG3	2.13	0.48
19:SR:78:ARG:HA	19:SR:81:ARG:HG2	1.94	0.48
38:3m:172:LEU:HB2	38:3m:177:LYS:HZ1	1.77	0.48
43:3h:172:LYS:HD3	43:3h:192:ILE:HG22	1.94	0.48
17:SP:30:TYR:HA	17:SP:33:LEU:HB2	1.95	0.48
36:S2:536:A:H3'	36:S2:537:C:H5''	1.95	0.48
36:S2:929:G:H2'	36:S2:930:C:O4'	2.14	0.48
38:3m:144:LEU:HD11	38:3m:184:VAL:HG22	1.96	0.48
4:SC:133:TYR:CD2	4:SC:216:MET:HA	2.49	0.48
6:SE:72:ILE:HG12	6:SE:90:ILE:HD13	1.96	0.48
7:SF:91:ARG:HD2	27:SZ:103:HIS:CE1	2.49	0.48
46:3l:274:LEU:O	46:3l:278:LEU:HD12	2.13	0.48
7:SF:110:GLN:HE21	7:SF:114:ASN:ND2	2.12	0.47
10:SI:38:ILE:HD12	10:SI:96:LEU:HD21	1.96	0.47
10:SI:175:ILE:HD13	10:SI:185:ALA:HB1	1.95	0.47
11:SJ:60:LEU:HD11	11:SJ:73:GLU:HB3	1.96	0.47
31:Sd:53:ILE:HG13	31:Sd:55:LEU:HD13	1.96	0.47
3:SB:229:MET:HE3	3:SB:229:MET:HA	1.96	0.47
7:SF:32:ASP:HB3	7:SF:35:LEU:HD23	1.96	0.47
9:SH:36:LEU:HD13	9:SH:40:LEU:HD22	1.96	0.47
13:SL:97:ARG:NH1	13:SL:97:ARG:HB2	2.29	0.47
32:Se:56:ASN:HB3	36:S2:606:G:H5''	1.96	0.47
37:zz:78:U:H2'	37:zz:79:C:C6	2.49	0.47
40:3a:393:TRP:CD2	40:3a:406:ARG:HD2	2.48	0.47
42:3c:672:PRO:HD2	42:3c:675:LEU:HD12	1.96	0.47
46:3l:469:THR:HG23	46:3l:529:HIS:HA	1.96	0.47
1:1A:42:LEU:HD13	1:1A:48:GLU:HB2	1.96	0.47
25:SX:68:LYS:HB3	25:SX:91:LEU:HD22	1.97	0.47
36:S2:1628:C:H2'	36:S2:1629:C:C6	2.48	0.47
37:zz:220:U:H2'	37:zz:221:G:C8	2.48	0.47
38:3m:172:LEU:HB2	38:3m:177:LYS:NZ	2.29	0.47
34:Sg:125:ARG:HG2	34:Sg:150:TRP:CG	2.49	0.47
36:S2:232:A:H5''	36:S2:890:U:H3	1.79	0.47
36:S2:1382:A:H2'	36:S2:1383:A:H8	1.80	0.47
37:zz:73:A:H2'	37:zz:74:A:H8	1.79	0.47
38:3m:280:LEU:HD22	38:3m:339:HIS:CE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:3a:83:ILE:HD12	40:3a:83:ILE:H	1.78	0.47
46:3l:201:ARG:HB3	46:3l:215:LEU:HD12	1.96	0.47
1:1A:76:ILE:HG22	1:1A:95:TYR:HD2	1.79	0.47
2:SA:15:VAL:HG11	19:SR:106:LEU:HD11	1.96	0.47
36:S2:51:U:H2'	36:S2:52:G:H8	1.79	0.47
36:S2:319:C:H2'	36:S2:320:G:O4'	2.14	0.47
36:S2:863:U:H2'	36:S2:864:A:H8	1.79	0.47
36:S2:1337:C:H2'	36:S2:1338:G:H8	1.79	0.47
13:SL:80:MET:HE1	13:SL:120:VAL:HG13	1.97	0.47
15:SN:122:ILE:HG21	15:SN:141:TYR:HD2	1.78	0.47
20:SS:138:THR:HA	20:SS:141:ARG:HH21	1.80	0.47
27:SZ:77:LEU:HB3	27:SZ:79:ILE:HG12	1.96	0.47
36:S2:639:C:H2'	36:S2:640:A:C8	2.49	0.47
36:S2:974:C:H2'	36:S2:975:G:H8	1.80	0.47
6:SE:124:CYS:HB3	6:SE:141:THR:HB	1.96	0.47
12:SK:1:MET:HE2	12:SK:1:MET:HA	1.97	0.47
12:SK:53:LYS:HE3	12:SK:53:LYS:HA	1.96	0.47
36:S2:1595:U:H2'	36:S2:1596:U:C6	2.50	0.47
39:3f:93:ARG:HD2	39:3f:130:GLU:HB3	1.96	0.47
40:3a:23:LYS:HB3	40:3a:26:PRO:HG2	1.96	0.47
40:3a:59:VAL:HG21	40:3a:96:MET:HE1	1.96	0.47
46:3l:336:PHE:HB2	46:3l:371:LEU:HD13	1.96	0.47
4:SC:74:LYS:HA	4:SC:74:LYS:HD3	1.76	0.47
4:SC:78:LEU:HG	4:SC:82:TYR:HE1	1.80	0.47
6:SE:198:ARG:HH22	6:SE:200:ARG:HH12	1.63	0.47
9:SH:85:LYS:HE3	9:SH:85:LYS:HB3	1.64	0.47
12:SK:11:ILE:HD13	12:SK:45:VAL:HA	1.97	0.47
15:SN:16:LEU:HD11	15:SN:62:GLN:HE21	1.79	0.47
15:SN:112:LYS:HE2	15:SN:112:LYS:HB3	1.76	0.47
22:SU:56:MET:HE3	36:S2:1580:A:H8	1.80	0.47
36:S2:963:A:H2'	36:S2:964:A:C8	2.50	0.47
37:zz:151:C:H2'	37:zz:152:G:C8	2.49	0.47
43:3h:249:ARG:HH21	43:3h:319:ILE:HG23	1.79	0.47
2:SA:121:LEU:HD12	2:SA:122:LEU:H	1.80	0.47
8:SG:10:THR:HA	8:SG:129:VAL:HG12	1.96	0.47
24:SW:3:ARG:HD3	24:SW:6:VAL:HG22	1.96	0.47
30:Sc:12:ALA:HB1	30:Sc:32:VAL:HB	1.96	0.47
36:S2:1221:G:H2'	36:S2:1222:G:H8	1.79	0.47
36:S2:1756:C:H2'	36:S2:1757:G:C8	2.48	0.47
41:3e:405:ILE:HA	41:3e:408:THR:HG22	1.96	0.47
42:3c:742:LYS:HE3	42:3c:742:LYS:HB3	1.73	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3l:183:LEU:HD22	46:3l:272:PHE:HD2	1.80	0.47
4:SC:114:LYS:HE3	36:S2:1358:U:H5'	1.97	0.47
7:SF:40:ALA:HB1	7:SF:45:TYR:CG	2.50	0.47
39:3f:171:GLY:HA3	39:3f:198:ILE:H	1.80	0.47
42:3c:807:LEU:HD22	42:3c:810:MET:HE2	1.96	0.47
8:SG:217:MET:HE2	8:SG:217:MET:HB3	1.86	0.46
13:SL:111:VAL:HG12	13:SL:140:PHE:HB2	1.97	0.46
20:SS:132:ARG:HD3	36:S2:1623[B]:A:C6	2.50	0.46
22:SU:20:ILE:HD13	22:SU:98:VAL:HG21	1.97	0.46
24:SW:6:VAL:HG12	24:SW:34:ILE:HD11	1.96	0.46
30:Sc:21:THR:HG23	30:Sc:27:CYS:HB2	1.98	0.46
36:S2:656:G:H21	36:S2:663:C:H5''	1.80	0.46
36:S2:1410:C:H2'	36:S2:1411:G:H8	1.80	0.46
38:3m:255:PHE:HE2	38:3m:263:ILE:HD11	1.80	0.46
39:3f:332:ASN:O	39:3f:336:MET:HE3	2.15	0.46
5:SD:101:GLN:HG2	5:SD:126:ILE:HD11	1.96	0.46
36:S2:1365:G:H2'	36:S2:1366:G:H8	1.80	0.46
37:zz:259:U:C2	37:zz:274:A:N7	2.83	0.46
40:3a:21:VAL:HG23	40:3a:23:LYS:HG3	1.98	0.46
41:3e:319:LEU:HD23	41:3e:325:LEU:HD13	1.96	0.46
11:SJ:136:ARG:HG2	11:SJ:160:SER:HA	1.96	0.46
14:Sf:46:GLN:HG2	14:Sf:112:LYS:HD3	1.98	0.46
15:SN:140:LYS:HB3	15:SN:140:LYS:HE3	1.75	0.46
22:SU:30:LYS:HE2	22:SU:30:LYS:HB2	1.83	0.46
36:S2:794:A:H2'	36:S2:795:A:C8	2.50	0.46
36:S2:1858:G:H2'	36:S2:1859:A:H8	1.79	0.46
37:zz:206:A:H1'	37:zz:207:C:H5'	1.97	0.46
40:3a:132:VAL:HA	42:3c:673:PHE:HE2	1.80	0.46
46:3l:380:MET:HG2	46:3l:538:ARG:NH1	2.29	0.46
12:SK:9:ILE:HD12	12:SK:83:LEU:HD11	1.97	0.46
25:SX:129:SER:HB3	36:S2:29:G:H4'	1.96	0.46
31:Sd:13:LYS:N	31:Sd:13:LYS:HE2	2.30	0.46
36:S2:1232:U:H2'	36:S2:1233:G:C8	2.50	0.46
39:3f:242:TYR:H	39:3f:245:GLU:HB2	1.81	0.46
36:S2:885:U:H3	36:S2:901:G:H22	1.62	0.46
36:S2:942:G:H2'	36:S2:943:U:C6	2.50	0.46
36:S2:1101:U:H2'	36:S2:1102:G:H8	1.78	0.46
36:S2:1808:U:H2'	36:S2:1809:A:C8	2.50	0.46
39:3f:97:VAL:HG11	43:3h:51:LYS:HD3	1.96	0.46
39:3f:326:MET:HE1	40:3a:519:ILE:HD13	1.98	0.46
46:3l:496:LYS:HD2	46:3l:496:LYS:HA	1.71	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SH:9:VAL:HG21	9:SH:20:GLU:HB3	1.96	0.46
9:SH:87:PHE:HB3	9:SH:90:LYS:HD2	1.97	0.46
18:SQ:19:ALA:HB2	18:SQ:75:GLY:HA3	1.98	0.46
23:SV:59:ILE:HD11	29:Sb:3:LEU:HD11	1.98	0.46
33:sh:102:VAL:HA	33:sh:105:TYR:HD2	1.81	0.46
36:S2:538:U:H2'	36:S2:539:C:O4'	2.16	0.46
39:3f:97:VAL:HG21	43:3h:51:LYS:HD3	1.97	0.46
40:3a:331:ILE:HG22	40:3a:506:PRO:HB3	1.98	0.46
36:S2:102:A:H4'	36:S2:104:A:C8	2.50	0.46
36:S2:282:G:H2'	36:S2:283:G:H8	1.80	0.46
36:S2:496:C:H2'	36:S2:497:C:C6	2.51	0.46
36:S2:527:C:H2'	36:S2:528:A:C8	2.50	0.46
36:S2:1304:U:H2'	36:S2:1305:C:C6	2.50	0.46
36:S2:1692:U:H2'	36:S2:1693:G:H8	1.81	0.46
36:S2:1723:G:H2'	36:S2:1724:A:H8	1.78	0.46
43:3h:340:LYS:HB3	43:3h:340:LYS:HE3	1.71	0.46
46:3l:127:VAL:HG11	46:3l:176:LEU:HD11	1.97	0.46
46:3l:545:ARG:HG2	46:3l:549:LYS:HD3	1.98	0.46
17:SP:118:GLU:HB3	20:SS:120:HIS:H	1.81	0.46
34:Sg:164:ILE:HD11	34:Sg:176:VAL:HG22	1.97	0.46
36:S2:639:C:H2'	36:S2:640:A:H8	1.81	0.46
36:S2:1413:G:H2'	36:S2:1414:A:C8	2.51	0.46
36:S2:1629:C:H2'	36:S2:1630:A:H8	1.80	0.46
36:S2:1761:U:H2'	36:S2:1762:C:C6	2.50	0.46
42:3c:579:HIS:HB2	42:3c:581:ARG:NH1	2.30	0.46
3:SB:25:PHE:HZ	16:SO:53:ILE:HA	1.81	0.46
10:SI:129:LEU:HB3	10:SI:133:GLU:HB2	1.97	0.46
10:SI:153:LYS:HE2	10:SI:153:LYS:HB2	1.82	0.46
14:Sf:14:VAL:HA	14:Sf:17:ALA:HB3	1.98	0.46
36:S2:107:A:H2'	36:S2:108:G:C8	2.51	0.46
36:S2:1758:G:H2'	36:S2:1759:G:C8	2.48	0.46
39:3f:242:TYR:HB2	39:3f:245:GLU:HB2	1.98	0.46
43:3h:130:THR:HA	43:3h:318:LEU:HD21	1.98	0.46
46:3l:470:MET:HE2	46:3l:470:MET:HB2	1.79	0.46
24:SW:38:LEU:HB3	24:SW:47:ILE:HD11	1.97	0.46
36:S2:1759:G:H2'	36:S2:1760:G:C8	2.51	0.46
36:S2:1798:C:H2'	36:S2:1799:G:O4'	2.15	0.46
36:S2:1842:C:H2'	36:S2:1843:G:H8	1.81	0.46
40:3a:400:PRO:HB3	40:3a:442:GLN:HB3	1.98	0.46
41:3e:372:VAL:HG23	41:3e:384:ILE:HD13	1.98	0.46
4:SC:167:ARG:HB3	4:SC:177:PRO:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SG:149:LYS:HA	8:SG:149:LYS:HD3	1.76	0.45
9:SH:157:HIS:HB3	9:SH:190:PRO:HG3	1.97	0.45
36:S2:540:U:H3	36:S2:543:C:H41	1.64	0.45
40:3a:25:GLN:HB2	40:3a:61:LEU:HD21	1.97	0.45
34:Sg:62:HIS:CE1	34:Sg:88:ARG:HG3	2.51	0.45
37:zz:147:U:H2'	37:zz:148:C:C6	2.51	0.45
39:3f:269:LEU:HD11	43:3h:335:ALA:HB1	1.98	0.45
41:3e:229:ARG:HH22	41:3e:328:CYS:HB3	1.82	0.45
11:SJ:37:LEU:HD12	11:SJ:43:VAL:HG23	1.98	0.45
34:Sg:12:LYS:HD2	34:Sg:12:LYS:HA	1.83	0.45
36:S2:958:G:H2'	36:S2:959:G:C8	2.51	0.45
37:zz:188:G:HO2'	37:zz:189:G:H8	1.60	0.45
40:3a:84:LYS:H	40:3a:84:LYS:HG3	1.50	0.45
41:3e:346:ARG:HE	41:3e:380:LEU:HD21	1.81	0.45
42:3c:733:MET:HE1	42:3c:765:VAL:HG22	1.98	0.45
2:SA:24:HIS:HB3	2:SA:51:LEU:HD21	1.97	0.45
4:SC:230:THR:HB	4:SC:236:PHE:CE2	2.52	0.45
5:SD:59:LEU:HA	5:SD:66:ILE:HG13	1.98	0.45
10:SI:25:ARG:HA	36:S2:448:A:H5''	1.98	0.45
18:SQ:31:LEU:HD11	18:SQ:33:LYS:HD2	1.98	0.45
19:SR:76:GLU:HB2	19:SR:80:ARG:HH21	1.81	0.45
34:Sg:17:TRP:CE2	34:Sg:303:THR:HB	2.52	0.45
37:zz:79:C:H2'	37:zz:80:U:C6	2.52	0.45
40:3a:296:LEU:HA	40:3a:299:LEU:HG	1.97	0.45
46:3l:320:GLY:HA2	46:3l:323:TYR:HB2	1.97	0.45
33:sh:89:LYS:HA	33:sh:89:LYS:HD3	1.77	0.45
36:S2:96:C:H2'	36:S2:97:U:C6	2.51	0.45
36:S2:1144:A:H5'	36:S2:1355:C:H41	1.81	0.45
46:3l:367:MET:HA	46:3l:370:LEU:HB2	1.99	0.45
7:SF:128:ILE:HD13	7:SF:137:GLN:HB2	1.97	0.45
8:SG:155:GLN:HB2	8:SG:156:TYR:HD1	1.81	0.45
36:S2:321:C:H2'	36:S2:322:C:H6	1.81	0.45
36:S2:698:G:H2'	36:S2:733:C:N4	2.31	0.45
30:Sc:15:THR:HB	30:Sc:31:ARG:HG2	1.98	0.45
36:S2:158:A:H2'	36:S2:159:A:O4'	2.16	0.45
36:S2:241:G:H22	36:S2:276:G:H22	1.63	0.45
36:S2:1692:U:H2'	36:S2:1693:G:C8	2.52	0.45
36:S2:1103:C:H2'	36:S2:1104:G:C8	2.52	0.45
36:S2:1103:C:H2'	36:S2:1104:G:H8	1.82	0.45
36:S2:1531:A:H2'	36:S2:1532:C:C6	2.52	0.45
37:zz:52:G:N2	37:zz:53:A:H1'	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3f:227:THR:HG23	39:3f:229:GLY:H	1.82	0.45
40:3a:440:LEU:HB3	40:3a:480:LEU:HD21	1.99	0.45
41:3e:352:SER:HB3	41:3e:390:HIS:CD2	2.52	0.45
5:SD:157:MET:HA	5:SD:157:MET:HE2	1.98	0.45
17:SP:50:ARG:H	17:SP:53:GLN:NE2	2.14	0.45
36:S2:952:G:H2'	36:S2:953:C:C6	2.51	0.45
36:S2:1417:C:H2'	36:S2:1418:C:C2	2.51	0.45
38:3m:58:LYS:HD3	38:3m:58:LYS:HA	1.85	0.45
38:3m:241:LEU:O	38:3m:245:VAL:HG12	2.16	0.45
42:3c:715:HIS:CE1	42:3c:719:ARG:HD2	2.52	0.45
3:SB:25:PHE:HD1	3:SB:28:LYS:HD2	1.81	0.45
3:SB:146:ARG:HE	3:SB:206:PRO:HG2	1.82	0.45
19:SR:126:MET:HE1	36:S2:1108:G:H21	1.82	0.45
20:SS:54:LYS:H	20:SS:54:LYS:HG2	1.57	0.45
36:S2:674:C:H2'	36:S2:675:U:C6	2.51	0.45
36:S2:1667:U:H2'	36:S2:1668:U:C6	2.51	0.45
39:3f:153:ALA:HA	39:3f:156:MET:HG2	1.98	0.45
40:3a:342:LEU:HD21	42:3c:718:LEU:HB3	1.99	0.45
42:3c:512:TYR:CE2	42:3c:675:LEU:HA	2.52	0.45
45:3k:79:HIS:H	46:3l:513:PHE:HZ	1.64	0.45
13:SL:99:TYR:HE2	25:SX:13:LEU:HB3	1.81	0.44
14:Sf:42:LEU:HB2	14:Sf:72:HIS:CD2	2.52	0.44
14:Sf:79:VAL:HG11	14:Sf:85:LEU:HD13	1.99	0.44
29:Sb:46:VAL:HG11	29:Sb:54:VAL:HG21	1.98	0.44
34:Sg:64:HIS:CG	34:Sg:65:PHE:H	2.35	0.44
36:S2:1562:C:H2'	36:S2:1563:G:C8	2.49	0.44
37:zz:81:A:H2'	37:zz:84:C:H42	1.81	0.44
37:zz:177:C:H2'	37:zz:178:C:C6	2.52	0.44
43:3h:242:ASN:HB3	43:3h:330:ILE:HD12	1.99	0.44
46:3l:150:LEU:HD21	46:3l:200:TYR:CZ	2.52	0.44
36:S2:107:A:H2'	36:S2:108:G:H8	1.82	0.44
36:S2:804:U:H2'	36:S2:805:U:C6	2.52	0.44
36:S2:964:A:H2'	36:S2:965:U:C6	2.53	0.44
40:3a:351:LYS:HG3	40:3a:354:ARG:HH21	1.82	0.44
4:SC:93:ILE:HG22	4:SC:94:ILE:HD13	2.00	0.44
9:SH:170:VAL:HA	9:SH:173:PHE:HB2	1.99	0.44
12:SK:80:ARG:HA	12:SK:85:LEU:HD23	1.99	0.44
19:SR:106:LEU:HD12	19:SR:111:PHE:HB2	1.99	0.44
36:S2:145:G:H2'	36:S2:146:G:C8	2.53	0.44
36:S2:656:G:N2	36:S2:663:C:H5''	2.32	0.44
37:zz:224:G:H2'	37:zz:225:A:C8	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3f:117:ILE:HB	39:3f:139:HIS:CD2	2.52	0.44
40:3a:353:ARG:HH22	40:3a:364:PRO:HD3	1.82	0.44
43:3h:172:LYS:HD2	43:3h:173:LEU:HG	2.00	0.44
46:3l:207:LYS:HE3	46:3l:215:LEU:HG	1.99	0.44
2:SA:89:LYS:NZ	2:SA:201:LEU:HG	2.33	0.44
9:SH:70:LYS:HE2	9:SH:70:LYS:HB2	1.83	0.44
12:SK:91:PRO:HB2	12:SK:93:THR:HG22	2.00	0.44
18:SQ:102:GLU:HB2	18:SQ:105:LYS:HD3	1.98	0.44
19:SR:71:ILE:HD11	19:SR:78:ARG:HH22	1.83	0.44
36:S2:550:C:H2'	36:S2:551:U:C6	2.52	0.44
36:S2:1203:G:H2'	36:S2:1204:A:C8	2.52	0.44
43:3h:243:LEU:HA	43:3h:246:LEU:HD23	1.97	0.44
2:SA:155:ARG:HG2	2:SA:156:TYR:CD2	2.52	0.44
16:SO:30:VAL:HG21	16:SO:96:LYS:HE2	1.99	0.44
25:SX:73:GLN:HB2	25:SX:80:LYS:HG3	1.99	0.44
34:Sg:217:MET:HB3	34:Sg:229:THR:HG23	1.99	0.44
36:S2:1434:C:H4'	36:S2:1435:C:OP2	2.17	0.44
38:3m:189:LEU:HA	38:3m:192:TYR:HB2	1.99	0.44
46:3l:341:LEU:HD22	46:3l:545:ARG:HH22	1.82	0.44
3:SB:83:LYS:HE2	3:SB:106:THR:HA	2.00	0.44
6:SE:102:ILE:HG21	6:SE:239:PRO:HD3	1.98	0.44
34:Sg:220:ASP:HB2	34:Sg:227:LEU:HD11	2.00	0.44
36:S2:907:G:H2'	36:S2:908:A:C8	2.53	0.44
38:3m:156:LEU:HG	38:3m:160:LYS:HB3	1.99	0.44
46:3l:461:ARG:HD2	46:3l:519:VAL:HG21	2.00	0.44
1:1A:35:TYR:HB2	1:1A:52:PHE:HD2	1.82	0.44
3:SB:153:THR:HG22	3:SB:155:TYR:HE2	1.82	0.44
5:SD:32:ASP:OD1	5:SD:58:VAL:HG13	2.18	0.44
6:SE:39:ARG:H	6:SE:39:ARG:HG2	1.61	0.44
11:SJ:134:HIS:CE1	11:SJ:164:PRO:HD2	2.52	0.44
13:SL:57:ASP:HB2	13:SL:84:ARG:HH12	1.82	0.44
26:SY:12:PHE:HZ	26:SY:21:LYS:HD3	1.82	0.44
36:S2:1279:C:H2'	36:S2:1280:G:C8	2.53	0.44
36:S2:1410:C:H2'	36:S2:1411:G:C8	2.53	0.44
36:S2:1415:C:H2'	36:S2:1416:C:C6	2.53	0.44
38:3m:22:LEU:HD21	38:3m:45:ILE:HD12	1.99	0.44
41:3e:391:VAL:HG12	41:3e:393:MET:HE3	2.00	0.44
42:3c:762:ASN:HA	42:3c:766:TRP:HB2	1.99	0.44
45:3k:108:LEU:HD12	45:3k:113:HIS:HB2	2.00	0.44
30:Sc:46:VAL:HG21	30:Sc:50:VAL:HG11	2.00	0.44
34:Sg:8:ARG:HB3	34:Sg:309:VAL:HG23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:S2:1740:C:H2'	36:S2:1741:U:C6	2.53	0.44
36:S2:1769:C:H2'	36:S2:1770:G:C8	2.52	0.44
37:zz:59:U:H3	37:zz:109:A:N6	2.16	0.44
38:3m:13:ASP:O	38:3m:17:GLU:HG3	2.18	0.44
40:3a:147:THR:HA	40:3a:150:VAL:HG22	2.00	0.44
40:3a:526:MET:HA	40:3a:529:VAL:HG12	2.00	0.44
41:3e:384:ILE:HG23	41:3e:391:VAL:HG22	2.00	0.44
46:3l:470:MET:HB3	46:3l:474:LYS:HD2	2.00	0.44
7:SF:22:LYS:HB3	7:SF:22:LYS:HE2	1.73	0.44
8:SG:164:LYS:HB2	36:S2:67:C:H41	1.83	0.44
12:SK:7:ASN:O	12:SK:11:ILE:HG13	2.17	0.44
26:SY:101:LYS:HB2	26:SY:101:LYS:HE2	1.67	0.44
36:S2:825:A:H2'	36:S2:826:A:C8	2.53	0.44
37:zz:146:G:H2'	37:zz:147:U:C6	2.53	0.44
40:3a:172:ARG:HH11	40:3a:228:MET:HG2	1.82	0.44
42:3c:862:LYS:HB2	42:3c:862:LYS:HE3	1.72	0.44
5:SD:136:VAL:HG22	5:SD:186:VAL:HG22	1.99	0.43
6:SE:191:ARG:HD3	6:SE:245:ARG:HB2	1.99	0.43
9:SH:109:ARG:HD2	36:S2:799:U:H5'	1.99	0.43
14:Sf:102:LYS:HD3	14:Sf:102:LYS:HA	1.74	0.43
37:zz:336:U:HO2'	37:zz:337:G:H8	1.64	0.43
42:3c:638:SER:HB2	42:3c:712:LYS:HB3	2.00	0.43
6:SE:31:PRO:HG3	6:SE:43:PRO:HG3	2.00	0.43
36:S2:441:C:H2'	36:S2:442:C:C6	2.53	0.43
36:S2:1453:C:H2'	36:S2:1454:A:H4'	2.00	0.43
36:S2:1844:U:H2'	36:S2:1845:A:C8	2.53	0.43
46:3l:182:TRP:HA	46:3l:185:ASP:HB3	1.99	0.43
2:SA:76:VAL:HG12	2:SA:123:VAL:HB	2.00	0.43
3:SB:174:ARG:HG2	3:SB:174:ARG:HH11	1.83	0.43
4:SC:211:LYS:O	4:SC:215:MET:HG3	2.18	0.43
6:SE:38:LEU:HB2	36:S2:346:C:H5''	2.00	0.43
13:SL:30:LYS:HE2	13:SL:30:LYS:HA	2.00	0.43
16:SO:136:PRO:HB2	16:SO:139:SER:HB3	2.01	0.43
26:SY:68:LYS:HB3	26:SY:68:LYS:HE2	1.71	0.43
33:sh:114:ILE:HD12	33:sh:114:ILE:HA	1.78	0.43
36:S2:885:U:H3	36:S2:901:G:H1	1.66	0.43
36:S2:1189:A:H2'	36:S2:1190:A:C8	2.53	0.43
37:zz:287:U:H2'	37:zz:288:A:H8	1.83	0.43
38:3m:46:ILE:HG23	38:3m:89:LYS:HG2	2.00	0.43
4:SC:78:LEU:HG	4:SC:82:TYR:CE1	2.53	0.43
14:Sf:58:GLU:HB3	14:Sf:61:TYR:HE1	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:SR:58:MET:HA	19:SR:61:ILE:HB	2.00	0.43
36:S2:150:A:N6	36:S2:168:C:H42	2.14	0.43
36:S2:841:G:H2'	36:S2:842:C:H6	1.83	0.43
37:zz:104:C:H2'	37:zz:105:G:C8	2.53	0.43
40:3a:95:LYS:HA	40:3a:95:LYS:HD3	1.82	0.43
40:3a:335:ARG:HH12	40:3a:340:ARG:NH2	2.16	0.43
41:3e:303:PHE:CZ	42:3c:827:ILE:HG21	2.54	0.43
42:3c:589:MET:C	42:3c:589:MET:HE2	2.43	0.43
43:3h:252:GLU:HG2	43:3h:319:ILE:HG21	2.00	0.43
43:3h:287:GLN:O	43:3h:291:ARG:HG2	2.18	0.43
46:3l:367:MET:HB3	46:3l:367:MET:HE3	1.79	0.43
46:3l:549:LYS:HB2	46:3l:549:LYS:HE2	1.73	0.43
3:SB:165:ARG:HA	3:SB:168:MET:HB2	1.99	0.43
13:SL:49:GLU:HG3	13:SL:116:CYS:HA	2.00	0.43
21:ST:104:LEU:HD13	21:ST:121:ARG:HD2	2.01	0.43
22:SU:19:ARG:HA	22:SU:19:ARG:HH11	1.83	0.43
36:S2:959:G:H2'	36:S2:960:U:C6	2.53	0.43
37:zz:53:A:H3'	37:zz:54:A:H8	1.83	0.43
38:3m:274:MET:HA	38:3m:274:MET:HE2	2.01	0.43
39:3f:327:LEU:HD12	43:3h:341:LEU:HD22	2.01	0.43
7:SF:134:VAL:HG21	37:zz:87:G:O4'	2.19	0.43
7:SF:142:SER:HB2	30:Sc:50:VAL:HG12	2.01	0.43
27:SZ:84:ALA:O	27:SZ:88:LEU:HB2	2.19	0.43
36:S2:349:A:H2'	36:S2:350:C:C6	2.54	0.43
36:S2:1842:C:H2'	36:S2:1843:G:C8	2.54	0.43
42:3c:425:LEU:HA	42:3c:441:ARG:HD3	2.00	0.43
3:SB:167:LYS:HA	3:SB:167:LYS:HD2	1.87	0.43
6:SE:36:HIS:CG	6:SE:85:GLY:HA3	2.52	0.43
10:SI:106:SER:HB3	10:SI:171:LEU:HG	2.00	0.43
13:SL:42:LEU:HD23	13:SL:42:LEU:HA	1.89	0.43
13:SL:56:ILE:HD13	13:SL:56:ILE:HA	1.86	0.43
34:Sg:235:ILE:O	34:Sg:252:THR:HA	2.19	0.43
36:S2:432:G:H2'	36:S2:433:A:C8	2.54	0.43
36:S2:893:U:H2'	36:S2:894:G:C8	2.53	0.43
36:S2:1769:C:H2'	36:S2:1770:G:H8	1.84	0.43
36:S2:1813:A:H3'	36:S2:1814:G:H8	1.84	0.43
46:3l:324:LEU:HB3	46:3l:325:MET:HE2	2.01	0.43
1:1A:21:SER:O	1:1A:22:GLU:HG3	2.19	0.43
5:SD:135:GLU:HG2	5:SD:153:VAL:HB	2.00	0.43
8:SG:159:ARG:HH21	8:SG:171:THR:HG23	1.84	0.43
12:SK:5:LYS:O	12:SK:9:ILE:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:SO:44:VAL:HG12	16:SO:53:ILE:HB	2.01	0.43
18:SQ:76:GLY:O	18:SQ:80:GLN:HG3	2.18	0.43
19:SR:67:ARG:HH12	36:S2:1376:A:P	2.41	0.43
20:SS:81:ASP:HB2	20:SS:95:TYR:CD2	2.54	0.43
25:SX:130:LEU:HD23	25:SX:130:LEU:HA	1.88	0.43
26:SY:49:LYS:HE2	26:SY:49:LYS:HB2	1.80	0.43
37:zz:103:U:H2'	37:zz:104:C:O4'	2.19	0.43
37:zz:178:C:H2'	37:zz:179:A:C8	2.54	0.43
37:zz:275:A:H2'	37:zz:276:A:H8	1.83	0.43
40:3a:237:LEU:HD23	40:3a:237:LEU:HA	1.90	0.43
42:3c:802:ILE:HG13	42:3c:842:VAL:HB	2.01	0.43
46:3l:471:PRO:HA	46:3l:527:MET:HA	2.01	0.43
2:SA:10:MET:HG3	2:SA:55:TRP:CD2	2.53	0.43
3:SB:71:LEU:HD22	3:SB:71:LEU:HA	1.86	0.43
11:SJ:112:THR:HG22	11:SJ:123:ILE:HD11	2.00	0.43
12:SK:61:GLN:HA	12:SK:61:GLN:OE1	2.19	0.43
18:SQ:50:LYS:HA	18:SQ:50:LYS:HD2	1.84	0.43
20:SS:132:ARG:HH11	36:S2:1623[B]:A:N6	2.17	0.43
31:Sd:31:ILE:HG21	31:Sd:36:LEU:HD22	2.01	0.43
37:zz:262:U:O2	37:zz:271:G:C6	2.72	0.43
40:3a:201:LEU:HD23	40:3a:202:ARG:HH21	1.83	0.43
40:3a:483:ARG:HH22	42:3c:846:ARG:HD3	1.83	0.43
41:3e:420:MET:C	41:3e:420:MET:HE3	2.44	0.43
45:3k:105:LEU:HD11	45:3k:124:ASN:HD21	1.83	0.43
46:3l:112:TRP:HB2	46:3l:136:TYR:HD2	1.83	0.43
46:3l:400:ARG:HB2	46:3l:408:VAL:HG21	2.00	0.43
13:SL:24:LEU:HA	13:SL:27:GLU:HB3	2.00	0.43
16:SO:61:LYS:HA	16:SO:61:LYS:HD2	1.76	0.43
28:Sa:37:LYS:HB2	28:Sa:37:LYS:HE2	1.71	0.43
36:S2:1643:U:H2'	36:S2:1644:C:C6	2.54	0.43
39:3f:129:VAL:HG13	39:3f:170:LEU:HD22	2.01	0.43
45:3k:95:GLU:CD	45:3k:95:GLU:H	2.27	0.43
3:SB:97:LEU:HD13	3:SB:232:HIS:HD2	1.84	0.42
5:SD:20:GLU:HG2	5:SD:77:PHE:HZ	1.84	0.42
10:SI:129:LEU:HD12	10:SI:129:LEU:H	1.84	0.42
11:SJ:94:LEU:HD12	11:SJ:94:LEU:HA	1.92	0.42
13:SL:13:GLN:NE2	13:SL:35:ARG:HG3	2.33	0.42
17:SP:62:LYS:HA	17:SP:62:LYS:HD3	1.78	0.42
21:ST:61:ALA:HB2	21:ST:107:LEU:HD21	2.01	0.42
21:ST:130:ASP:O	21:ST:134:ILE:HG22	2.19	0.42
34:Sg:164:ILE:HD11	34:Sg:176:VAL:HG13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Sg:291:TRP:CD2	34:Sg:298:LEU:HD23	2.54	0.42
36:S2:754:G:C6	36:S2:791:C:H1'	2.54	0.42
38:3m:278:ARG:HH22	38:3m:281:THR:HB	1.83	0.42
40:3a:354:ARG:NH1	42:3c:725:PRO:HB3	2.34	0.42
42:3c:789:ARG:HE	42:3c:825:MET:HE3	1.84	0.42
43:3h:243:LEU:HD23	43:3h:243:LEU:HA	1.75	0.42
46:3l:474:LYS:HE2	46:3l:478:PHE:HE2	1.83	0.42
5:SD:188:ILE:HG22	5:SD:190:LEU:HD12	2.01	0.42
7:SF:60:ARG:HD2	36:S2:1679:A:H2'	1.99	0.42
7:SF:144:LEU:HD23	30:Sc:49:PRO:HG2	2.01	0.42
11:SJ:13:TYR:HE2	11:SJ:41:ARG:HE	1.67	0.42
27:SZ:79:ILE:HD13	27:SZ:79:ILE:HA	1.86	0.42
36:S2:1139:C:H2'	36:S2:1140:G:O4'	2.19	0.42
36:S2:1198:G:H2'	36:S2:1199:A:C8	2.54	0.42
36:S2:1768:A:H2'	36:S2:1769:C:C6	2.54	0.42
40:3a:514:MET:SD	40:3a:516:SER:HB3	2.59	0.42
43:3h:68:LEU:HD11	43:3h:80:ASN:HB3	2.01	0.42
46:3l:469:THR:HG22	46:3l:527:MET:SD	2.59	0.42
14:Sf:38:ALA:O	14:Sf:42:LEU:HG	2.19	0.42
16:SO:95:ILE:HD13	16:SO:126:ILE:HG23	2.00	0.42
19:SR:11:LYS:HE2	19:SR:11:LYS:HB2	1.90	0.42
34:Sg:228:TYR:CG	34:Sg:264:LYS:HE2	2.54	0.42
36:S2:118:C:H1'	36:S2:445:A:C5	2.55	0.42
40:3a:340:ARG:HA	40:3a:340:ARG:HH11	1.85	0.42
46:3l:52:ILE:HG12	46:3l:102:LEU:HD11	2.01	0.42
46:3l:555:ARG:O	46:3l:559:LYS:HG2	2.20	0.42
2:SA:205:ARG:HE	2:SA:210:ILE:HD13	1.83	0.42
4:SC:233:LEU:HD22	4:SC:233:LEU:HA	1.82	0.42
6:SE:211:LYS:HE2	6:SE:215:GLY:HA2	2.01	0.42
12:SK:27:VAL:HG23	12:SK:28:HIS:CD2	2.54	0.42
15:SN:27:LYS:HA	15:SN:27:LYS:HD2	1.80	0.42
17:SP:89:MET:HE3	17:SP:89:MET:HB3	1.93	0.42
22:SU:58:THR:HG22	22:SU:85:HIS:HA	2.00	0.42
36:S2:1405:A:H2'	36:S2:1406:G:O4'	2.18	0.42
36:S2:1417:C:H5''	36:S2:1418:C:C6	2.55	0.42
36:S2:1670:C:H2'	36:S2:1671:G:C8	2.54	0.42
37:zz:108:C:H2'	37:zz:109:A:H8	1.84	0.42
38:3m:39:HIS:HA	38:3m:82:LEU:HD21	2.01	0.42
46:3l:327:ARG:HD3	46:3l:450:GLU:CD	2.44	0.42
28:Sa:42:ARG:HH12	28:Sa:67:LEU:HD23	1.85	0.42
36:S2:15:U:H2'	36:S2:16:G:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:S2:495:U:H2'	36:S2:496:C:O4'	2.20	0.42
36:S2:518:G:H2'	36:S2:519:A:C8	2.50	0.42
36:S2:540:U:H2'	36:S2:541:U:H5	1.85	0.42
37:zz:201:G:H5''	37:zz:202:A:H5''	2.01	0.42
40:3a:338:ILE:HG22	40:3a:342:LEU:HD13	2.02	0.42
42:3c:744:MET:HE2	42:3c:744:MET:HB2	1.97	0.42
43:3h:134:LEU:HD23	43:3h:314:MET:HE1	2.01	0.42
45:3k:88:MET:HE3	45:3k:88:MET:HA	2.01	0.42
46:3l:277:LEU:HG	46:3l:293:VAL:HG21	2.02	0.42
22:SU:19:ARG:HA	22:SU:19:ARG:NH1	2.34	0.42
35:Ln:23:ARG:HD3	35:Ln:24:SER:N	2.35	0.42
36:S2:980:A:H2'	36:S2:981:A:C8	2.55	0.42
36:S2:1217:A:H2'	36:S2:1218:C:C6	2.55	0.42
36:S2:1671:G:H2'	36:S2:1672:U:H6	1.84	0.42
37:zz:145:G:H2'	37:zz:146:G:C8	2.55	0.42
40:3a:74:TYR:HD2	40:3a:86:LEU:HD13	1.84	0.42
40:3a:205:LEU:HD21	40:3a:229:HIS:HE2	1.83	0.42
46:3l:498:LYS:HE3	46:3l:514:GLN:HA	2.02	0.42
3:SB:38:MET:HE1	3:SB:231:LEU:HD21	2.01	0.42
5:SD:158:ILE:HG23	5:SD:164:VAL:HG12	2.00	0.42
9:SH:98:ARG:HB3	36:S2:913:A:N6	2.34	0.42
20:SS:78:LYS:HB2	20:SS:78:LYS:HE2	1.70	0.42
28:Sa:26:CYS:SG	28:Sa:28:ARG:HB3	2.59	0.42
36:S2:1755:C:H2'	36:S2:1756:C:H6	1.84	0.42
38:3m:137:ILE:HD12	38:3m:137:ILE:HA	1.91	0.42
46:3l:316:TYR:HB3	46:3l:335:VAL:HG13	2.00	0.42
2:SA:17:LYS:HA	19:SR:91:LEU:HD12	2.00	0.42
6:SE:69:PHE:HD2	26:SY:17:LEU:HD13	1.85	0.42
13:SL:13:GLN:HE22	13:SL:35:ARG:HG3	1.85	0.42
22:SU:26:SER:HB3	22:SU:32:LEU:HG	2.02	0.42
22:SU:75:LYS:H	22:SU:75:LYS:HG2	1.55	0.42
32:Se:53:LYS:HA	32:Se:53:LYS:HD2	1.88	0.42
36:S2:223:C:H2'	36:S2:224:A:C8	2.55	0.42
36:S2:889:U:H2'	36:S2:890:U:C5	2.54	0.42
37:zz:73:A:H2'	37:zz:74:A:C8	2.55	0.42
39:3f:278:ARG:HD2	39:3f:278:ARG:HA	1.81	0.42
40:3a:384:VAL:HG12	40:3a:386:GLU:H	1.85	0.42
46:3l:328:ARG:HG2	46:3l:331:ASP:HB2	2.02	0.42
46:3l:551:GLU:HA	46:3l:554:ASN:ND2	2.34	0.42
1:1A:62:ARG:HG2	1:1A:91:VAL:O	2.20	0.42
5:SD:38:GLU:HG3	5:SD:49:ILE:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SN:71:ILE:HG13	36:S2:1018:U:H5''	2.02	0.42
20:SS:34:LYS:HB3	20:SS:103:LEU:HD23	2.01	0.42
38:3m:42:LEU:HD23	38:3m:45:ILE:HG21	2.02	0.42
39:3f:331:ILE:HG13	43:3h:341:LEU:HD13	2.02	0.42
42:3c:573:ILE:HB	42:3c:588:LEU:HD23	2.02	0.42
43:3h:76:LEU:HD21	43:3h:117:VAL:HG21	2.01	0.42
43:3h:131:ARG:NH1	43:3h:315:ASP:HA	2.33	0.42
4:SC:133:TYR:HD2	4:SC:216:MET:HA	1.85	0.42
4:SC:207:ALA:HB2	36:S2:4:C:H4'	2.00	0.42
12:SK:55:ARG:HD3	12:SK:57:TYR:CE2	2.54	0.42
12:SK:64:TRP:CE2	31:Sd:23:VAL:HG22	2.55	0.42
34:Sg:235:ILE:HD12	34:Sg:236:ILE:H	1.85	0.42
36:S2:531:A:H2'	36:S2:532:C:C6	2.54	0.42
36:S2:1597:C:H4'	36:S2:1603:G:O6	2.20	0.42
36:S2:1845:A:H2'	36:S2:1846:G:C8	2.55	0.42
37:zz:260:A:H2'	37:zz:261:G:O4'	2.20	0.42
38:3m:114:ASP:HB3	38:3m:117:THR:HG23	2.02	0.42
40:3a:75:LYS:HE3	40:3a:75:LYS:HB3	1.59	0.42
40:3a:257:HIS:HA	40:3a:260:PHE:HB2	2.01	0.42
40:3a:354:ARG:H	40:3a:354:ARG:HG3	1.68	0.42
1:1A:76:ILE:HD11	1:1A:114:LYS:HD2	2.02	0.41
4:SC:117:ARG:H	4:SC:117:ARG:HD3	1.83	0.41
5:SD:68:GLU:HB2	12:SK:70:TYR:HE1	1.85	0.41
15:SN:88:LEU:O	15:SN:92:ILE:HD12	2.20	0.41
29:Sb:3:LEU:HD23	29:Sb:3:LEU:HA	1.89	0.41
36:S2:1653:U:H2'	36:S2:1654:G:C8	2.55	0.41
40:3a:49:PRO:HA	40:3a:52:LEU:HD12	2.02	0.41
40:3a:329:ILE:HD12	40:3a:329:ILE:H	1.84	0.41
45:3k:158:LEU:HD22	45:3k:158:LEU:HA	1.82	0.41
3:SB:35:ALA:HB3	3:SB:42:ARG:HA	2.03	0.41
4:SC:125:LYS:HG2	4:SC:143:CYS:HB2	2.01	0.41
7:SF:32:ASP:HB2	7:SF:117:ILE:HD13	2.02	0.41
12:SK:86:PRO:HB2	12:SK:88:GLU:OE1	2.21	0.41
34:Sg:133:ASN:HD21	34:Sg:137:VAL:HG13	1.84	0.41
36:S2:1259:A:H1'	36:S2:1264:C:N4	2.35	0.41
40:3a:46:ILE:HD12	40:3a:46:ILE:HA	1.92	0.41
40:3a:550:HIS:CD2	43:3h:216:TRP:HB3	2.55	0.41
45:3k:74:LEU:HD12	45:3k:109:LEU:HD12	2.02	0.41
1:1A:114:LYS:HD3	1:1A:114:LYS:HA	1.83	0.41
4:SC:253:PRO:HA	4:SC:256:TRP:CE2	2.55	0.41
5:SD:31:GLU:HA	5:SD:107:TYR:HE1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SI:124:LYS:HD2	10:SI:124:LYS:HA	1.94	0.41
11:SJ:142:VAL:HG12	11:SJ:144:ILE:H	1.84	0.41
30:Sc:9:ILE:HD11	30:Sc:59:LEU:HD13	2.01	0.41
31:Sd:45:GLN:HG2	31:Sd:46:TYR:HD1	1.86	0.41
36:S2:1144:A:H2'	36:S2:1145:A:C8	2.55	0.41
36:S2:1714:U:H2'	36:S2:1715:A:C8	2.54	0.41
36:S2:1764:G:C6	36:S2:1768:A:N7	2.88	0.41
37:zz:265:U:O2'	37:zz:266:G:H8	2.03	0.41
39:3f:335:LEU:HD23	39:3f:335:LEU:HA	1.80	0.41
40:3a:285:LYS:HE2	40:3a:285:LYS:HB2	1.89	0.41
40:3a:294:SER:HA	40:3a:297:HIS:ND1	2.35	0.41
45:3k:198:PRO:HB3	46:3l:533:THR:HG23	2.02	0.41
46:3l:556:THR:O	46:3l:560:MET:HG3	2.21	0.41
13:SL:75:GLY:HA3	13:SL:88:ILE:HD12	2.03	0.41
15:SN:71:ILE:O	15:SN:75:LEU:HD12	2.19	0.41
18:SQ:34:VAL:HG11	18:SQ:84:ILE:HG21	2.02	0.41
33:sh:108:VAL:HG13	33:sh:114:ILE:HD13	2.02	0.41
36:S2:917:U:H2'	36:S2:918:U:C6	2.55	0.41
36:S2:1025:U:H2'	36:S2:1026:C:O4'	2.21	0.41
36:S2:1395:C:H2'	36:S2:1396:A:N3	2.36	0.41
37:zz:150:G:H2'	37:zz:151:C:C6	2.55	0.41
46:3l:268:MET:HE1	46:3l:307:ARG:HB2	2.03	0.41
2:SA:49:ILE:HG21	2:SA:162:PRO:O	2.21	0.41
5:SD:31:GLU:HA	5:SD:107:TYR:CE1	2.56	0.41
5:SD:141:LYS:HD3	36:S2:1332:A:O2'	2.20	0.41
11:SJ:87:LEU:HD12	11:SJ:87:LEU:HA	1.89	0.41
15:SN:16:LEU:HD11	15:SN:62:GLN:NE2	2.35	0.41
16:SO:97:LEU:HD13	28:Sa:44:ILE:HD11	2.02	0.41
36:S2:1162:C:H2'	36:S2:1163:C:O4'	2.21	0.41
43:3h:36:VAL:HG11	43:3h:76:LEU:HB2	2.01	0.41
8:SG:137:ARG:HD3	8:SG:178:ARG:HD2	2.03	0.41
10:SI:64:ASN:HA	10:SI:75:LYS:HA	2.03	0.41
20:SS:132:ARG:HH11	36:S2:1623[A]:A:N6	2.19	0.41
34:Sg:99:ARG:HH21	34:Sg:136:GLY:HA3	1.86	0.41
36:S2:344:U:H2'	36:S2:345:U:C6	2.55	0.41
36:S2:1010:G:H2'	36:S2:1011:A:C8	2.56	0.41
36:S2:1174:U:H2'	36:S2:1175:G:C8	2.56	0.41
36:S2:1539:U:H2'	36:S2:1540:G:C8	2.55	0.41
38:3m:196:ASN:HB2	38:3m:199:GLN:NE2	2.35	0.41
40:3a:87:GLU:HG3	40:3a:173:LEU:HD22	2.02	0.41
45:3k:109:LEU:HD23	45:3k:109:LEU:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3l:177:GLU:HA	46:3l:265:LEU:HG	2.03	0.41
5:SD:163:PRO:O	5:SD:167:TYR:HB2	2.21	0.41
23:SV:81:LYS:HE3	23:SV:81:LYS:HB3	1.90	0.41
34:Sg:129:ILE:HD13	34:Sg:129:ILE:HA	1.93	0.41
39:3f:348:ILE:HG21	43:3h:323:ILE:HG21	2.02	0.41
40:3a:96:MET:HE2	40:3a:96:MET:C	2.46	0.41
43:3h:98:GLN:HA	43:3h:101:MET:HB2	2.03	0.41
43:3h:313:ARG:HA	43:3h:313:ARG:HD3	1.74	0.41
46:3l:490:LEU:HD12	46:3l:490:LEU:HA	1.91	0.41
6:SE:87:MET:HE3	6:SE:87:MET:HA	2.02	0.41
9:SH:7:LYS:HB3	9:SH:28:LEU:HD11	2.02	0.41
13:SL:101:ARG:HB2	25:SX:10:ALA:HB2	2.01	0.41
24:SW:55:ASP:HB2	29:Sb:25:VAL:HG13	2.03	0.41
30:Sc:60:GLU:HG2	30:Sc:63:ARG:HD3	2.03	0.41
36:S2:320:G:H2'	36:S2:321:C:C6	2.56	0.41
36:S2:669:A:H8	36:S2:1164:G:O2'	2.03	0.41
36:S2:1220:A:H2'	36:S2:1221:G:O4'	2.21	0.41
36:S2:1365:G:H2'	36:S2:1366:G:C8	2.55	0.41
36:S2:1407:U:H2'	36:S2:1408:U:C6	2.56	0.41
38:3m:120:ARG:HA	38:3m:123:VAL:HB	2.01	0.41
40:3a:31:LEU:HD12	40:3a:54:TYR:CD1	2.56	0.41
1:1A:35:TYR:CE2	1:1A:103:LEU:HD21	2.55	0.41
3:SB:86:LEU:HB3	3:SB:98:THR:OG1	2.21	0.41
5:SD:65:ARG:HA	5:SD:68:GLU:HG2	2.02	0.41
12:SK:71:LEU:HD12	12:SK:71:LEU:HA	1.88	0.41
14:Sf:42:LEU:HD22	14:Sf:68:LEU:HB3	2.02	0.41
15:SN:20:ARG:HG3	15:SN:65:PHE:CE1	2.53	0.41
15:SN:76:LYS:HE2	15:SN:76:LYS:HB2	1.79	0.41
15:SN:118:ILE:HD13	15:SN:118:ILE:HA	1.89	0.41
20:SS:15:VAL:HG13	20:SS:68:ILE:HD12	2.02	0.41
36:S2:554:A:H4'	36:S2:555:A:H8	1.84	0.41
36:S2:799:U:O2'	36:S2:800:U:H5''	2.21	0.41
36:S2:931:C:H2'	36:S2:932:G:C8	2.56	0.41
37:zz:260:A:H62	37:zz:273:G:H21	1.68	0.41
38:3m:49:CYS:HA	38:3m:52:CYS:HB3	2.02	0.41
39:3f:211:MET:H	39:3f:211:MET:HG3	1.67	0.41
40:3a:172:ARG:HD3	40:3a:172:ARG:HA	1.84	0.41
42:3c:687:LEU:HD13	42:3c:734:ARG:HH11	1.85	0.41
42:3c:758:ASN:HB3	42:3c:761:MET:HG2	2.02	0.41
43:3h:238:HIS:HB3	43:3h:333:PHE:CE2	2.55	0.41
46:3l:487:ARG:HH12	46:3l:528:ILE:HD11	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SA:211:GLU:HA	2:SA:214:GLU:HB2	2.02	0.41
13:SL:76:VAL:HG12	13:SL:125:ILE:HG12	2.03	0.41
21:ST:104:LEU:HD23	21:ST:104:LEU:HA	1.94	0.41
22:SU:100:GLN:H	22:SU:100:GLN:HG3	1.65	0.41
27:SZ:99:LEU:HD23	27:SZ:109:TYR:CE1	2.56	0.41
31:Sd:45:GLN:HG2	31:Sd:46:TYR:CD1	2.56	0.41
35:Ln:21:ARG:HH12	36:S2:1174:U:H5''	1.85	0.41
36:S2:634:A:H2'	36:S2:635:G:H8	1.85	0.41
36:S2:1703:C:H2'	36:S2:1704:C:O4'	2.21	0.41
36:S2:1755:C:H2'	36:S2:1756:C:C6	2.56	0.41
39:3f:266:SER:HB2	39:3f:270:GLN:HB2	2.02	0.41
46:3l:390:LEU:HD12	46:3l:394:TYR:HD2	1.85	0.41
4:SC:145:LYS:HB3	4:SC:145:LYS:NZ	2.36	0.40
6:SE:146:THR:HG21	36:S2:122:G:H21	1.86	0.40
10:SI:46:VAL:HG21	10:SI:56:ARG:HH11	1.85	0.40
12:SK:49:MET:HA	12:SK:52:LEU:HG	2.02	0.40
14:Sf:93:LYS:HE3	14:Sf:102:LYS:HG2	2.02	0.40
15:SN:14:SER:HB2	36:S2:1016:U:H5''	2.03	0.40
18:SQ:107:GLU:O	18:SQ:111:ILE:HG13	2.20	0.40
19:SR:83:ASN:C	19:SR:83:ASN:ND2	2.75	0.40
36:S2:1277:C:H2'	36:S2:1278:A:H8	1.86	0.40
36:S2:1326:U:H4'	36:S2:1327:G:OP1	2.21	0.40
38:3m:230:LYS:HA	38:3m:233:GLU:HG3	2.02	0.40
43:3h:84:PHE:CE1	43:3h:100:GLN:HB3	2.56	0.40
45:3k:197:LYS:HE3	45:3k:197:LYS:HB2	1.90	0.40
10:SI:137:LEU:HD23	10:SI:137:LEU:HA	1.93	0.40
23:SV:17:CYS:HB2	23:SV:56:CYS:HB3	2.02	0.40
24:SW:38:LEU:O	24:SW:42:MET:HG3	2.21	0.40
27:SZ:44:LEU:HD12	27:SZ:44:LEU:HA	1.96	0.40
27:SZ:49:LEU:HD13	27:SZ:49:LEU:HA	1.95	0.40
28:Sa:51:ARG:O	28:Sa:55:GLU:HG2	2.20	0.40
36:S2:1380:C:H2'	36:S2:1381:G:C8	2.56	0.40
38:3m:149:LYS:HD2	38:3m:149:LYS:HA	1.87	0.40
38:3m:241:LEU:HD23	38:3m:241:LEU:HA	1.94	0.40
39:3f:119:THR:HA	39:3f:172:TRP:HA	2.03	0.40
40:3a:526:MET:HG2	43:3h:347:LEU:HD11	2.02	0.40
1:1A:33:GLN:HG3	1:1A:80:GLY:HA2	2.03	0.40
8:SG:237:LEU:HD22	8:SG:237:LEU:HA	1.96	0.40
10:SI:43:ILE:HG13	10:SI:57:ALA:HA	2.02	0.40
11:SJ:18:ARG:HH22	36:S2:4:C:H1'	1.87	0.40
16:SO:119:LEU:HD12	16:SO:119:LEU:HA	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:SV:68:SER:O	23:SV:72:LEU:HG	2.21	0.40
34:Sg:11:LEU:HB3	34:Sg:43:TRP:CH2	2.56	0.40
34:Sg:236:ILE:HD13	34:Sg:236:ILE:HA	1.90	0.40
36:S2:14:C:H2'	36:S2:15:U:C6	2.57	0.40
36:S2:1010:G:H2'	36:S2:1011:A:H8	1.86	0.40
36:S2:1689:C:H2'	36:S2:1690:U:C6	2.56	0.40
37:zz:200:G:H2'	37:zz:201:G:C8	2.56	0.40
40:3a:386:GLU:HG2	40:3a:413:TRP:CG	2.56	0.40
7:SF:56:TYR:HE2	7:SF:66:CYS:HA	1.87	0.40
11:SJ:35:TYR:HD2	11:SJ:35:TYR:HA	1.78	0.40
11:SJ:114:VAL:HG21	11:SJ:130:ILE:HD11	2.02	0.40
11:SJ:155:LYS:HE2	11:SJ:155:LYS:HB3	1.81	0.40
14:Sf:58:GLU:HB3	14:Sf:61:TYR:CE1	2.57	0.40
22:SU:107:GLU:HA	22:SU:108:PRO:HD3	1.97	0.40
26:SY:51:THR:HA	26:SY:52:PRO:HD3	1.97	0.40
34:Sg:298:LEU:HB3	34:Sg:310:TRP:HB2	2.04	0.40
36:S2:528:A:H2'	36:S2:529:A:H8	1.85	0.40
42:3c:582:TRP:HZ2	42:3c:625:LEU:HD13	1.86	0.40
46:3l:194:PHE:CG	46:3l:227:VAL:HG21	2.56	0.40
2:SA:107:THR:HG23	2:SA:115:ALA:O	2.22	0.40
24:SW:28:ARG:HB3	24:SW:60:LYS:HG2	2.03	0.40
32:Se:39:ASN:ND2	36:S2:552:G:H5''	2.37	0.40
36:S2:5:U:H2'	36:S2:6:G:C8	2.56	0.40
36:S2:647:U:H2'	36:S2:648:A:C8	2.54	0.40
36:S2:1317:C:H2'	36:S2:1318:G:C8	2.57	0.40
41:3e:383:LYS:HD2	41:3e:383:LYS:HA	1.93	0.40
43:3h:37:LYS:HD2	43:3h:202:PRO:HD2	2.04	0.40
46:3l:330:GLN:HG3	46:3l:378:TYR:CE1	2.55	0.40
46:3l:376:THR:HG21	46:3l:401:MET:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	96/144 (67%)	88 (92%)	7 (7%)	1 (1%)	12	45
2	SA	214/295 (72%)	207 (97%)	7 (3%)	0	100	100
3	SB	210/264 (80%)	207 (99%)	3 (1%)	0	100	100
4	SC	217/293 (74%)	209 (96%)	8 (4%)	0	100	100
5	SD	224/243 (92%)	221 (99%)	3 (1%)	0	100	100
6	SE	258/263 (98%)	249 (96%)	9 (4%)	0	100	100
7	SF	190/204 (93%)	178 (94%)	12 (6%)	0	100	100
8	SG	235/249 (94%)	229 (97%)	6 (3%)	0	100	100
9	SH	185/194 (95%)	177 (96%)	8 (4%)	0	100	100
10	SI	203/208 (98%)	195 (96%)	8 (4%)	0	100	100
11	SJ	178/194 (92%)	177 (99%)	1 (1%)	0	100	100
12	SK	94/165 (57%)	86 (92%)	8 (8%)	0	100	100
13	SL	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
14	Sf	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
15	SN	147/151 (97%)	142 (97%)	5 (3%)	0	100	100
16	SO	133/151 (88%)	125 (94%)	8 (6%)	0	100	100
17	SP	117/145 (81%)	112 (96%)	5 (4%)	0	100	100
18	SQ	138/146 (94%)	135 (98%)	3 (2%)	0	100	100
19	SR	130/135 (96%)	123 (95%)	7 (5%)	0	100	100
20	SS	141/152 (93%)	134 (95%)	7 (5%)	0	100	100
21	ST	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
22	SU	99/119 (83%)	99 (100%)	0	0	100	100
23	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
24	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
25	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
26	SY	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
27	SZ	73/125 (58%)	69 (94%)	4 (6%)	0	100	100
28	Sa	98/115 (85%)	95 (97%)	3 (3%)	0	100	100
29	Sb	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
30	Sc	60/69 (87%)	56 (93%)	4 (7%)	0	100	100
31	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
32	Se	50/59 (85%)	49 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	sh	62/156 (40%)	55 (89%)	7 (11%)	0	100	100
34	Sg	311/317 (98%)	297 (96%)	14 (4%)	0	100	100
35	Ln	22/25 (88%)	20 (91%)	2 (9%)	0	100	100
38	3m	361/374 (96%)	345 (96%)	16 (4%)	0	100	100
39	3f	267/357 (75%)	260 (97%)	7 (3%)	0	100	100
40	3a	590/1382 (43%)	568 (96%)	22 (4%)	0	100	100
41	3e	428/445 (96%)	418 (98%)	10 (2%)	0	100	100
42	3c	537/913 (59%)	521 (97%)	16 (3%)	0	100	100
43	3h	316/352 (90%)	306 (97%)	10 (3%)	0	100	100
44	3d	53/548 (10%)	50 (94%)	3 (6%)	0	100	100
45	3k	213/218 (98%)	204 (96%)	9 (4%)	0	100	100
46	3l	518/564 (92%)	501 (97%)	17 (3%)	0	100	100
All	All	8178/10798 (76%)	7886 (96%)	291 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	112	HIS

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	
1	1A	82/123 (67%)	79 (96%)	3 (4%)	30	63
2	SA	180/243 (74%)	172 (96%)	8 (4%)	25	59
3	SB	193/231 (84%)	186 (96%)	7 (4%)	31	63
4	SC	185/225 (82%)	175 (95%)	10 (5%)	20	53
5	SD	189/202 (94%)	181 (96%)	8 (4%)	26	60
6	SE	223/225 (99%)	216 (97%)	7 (3%)	35	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	SF	162/170 (95%)	154 (95%)	8 (5%)	22	55
8	SG	207/218 (95%)	204 (99%)	3 (1%)	59	77
9	SH	167/174 (96%)	160 (96%)	7 (4%)	26	60
10	SI	178/180 (99%)	166 (93%)	12 (7%)	15	47
11	SJ	160/168 (95%)	156 (98%)	4 (2%)	42	69
12	SK	87/136 (64%)	83 (95%)	4 (5%)	24	58
13	SL	134/142 (94%)	128 (96%)	6 (4%)	24	58
14	Sf	102/108 (94%)	97 (95%)	5 (5%)	22	55
15	SN	130/131 (99%)	123 (95%)	7 (5%)	20	53
16	SO	104/119 (87%)	95 (91%)	9 (9%)	9	36
17	SP	107/130 (82%)	103 (96%)	4 (4%)	30	63
18	SQ	116/121 (96%)	110 (95%)	6 (5%)	21	54
19	SR	119/122 (98%)	110 (92%)	9 (8%)	12	42
20	SS	124/132 (94%)	118 (95%)	6 (5%)	23	56
21	ST	112/115 (97%)	108 (96%)	4 (4%)	31	63
22	SU	93/107 (87%)	87 (94%)	6 (6%)	15	47
23	SV	67/67 (100%)	64 (96%)	3 (4%)	24	58
24	SW	112/113 (99%)	105 (94%)	7 (6%)	16	48
25	SX	113/115 (98%)	105 (93%)	8 (7%)	13	44
26	SY	108/115 (94%)	103 (95%)	5 (5%)	24	58
27	SZ	67/103 (65%)	62 (92%)	5 (8%)	12	42
28	Sa	87/98 (89%)	84 (97%)	3 (3%)	32	64
29	Sb	75/76 (99%)	73 (97%)	2 (3%)	39	68
30	Sc	55/62 (89%)	52 (94%)	3 (6%)	19	52
31	Sd	48/49 (98%)	45 (94%)	3 (6%)	16	48
32	Se	42/48 (88%)	39 (93%)	3 (7%)	13	44
33	sh	56/140 (40%)	48 (86%)	8 (14%)	3	16
34	Sg	272/275 (99%)	261 (96%)	11 (4%)	28	61
35	Ln	23/24 (96%)	19 (83%)	4 (17%)	2	10
38	3m	252/335 (75%)	240 (95%)	12 (5%)	23	56
39	3f	229/289 (79%)	223 (97%)	6 (3%)	40	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	3a	434/1259 (34%)	418 (96%)	16 (4%)	30	63
41	3e	302/406 (74%)	295 (98%)	7 (2%)	44	70
42	3c	347/811 (43%)	341 (98%)	6 (2%)	53	75
43	3h	272/310 (88%)	266 (98%)	6 (2%)	45	71
44	3d	20/494 (4%)	19 (95%)	1 (5%)	22	55
45	3k	121/193 (63%)	115 (95%)	6 (5%)	22	55
46	3l	475/515 (92%)	461 (97%)	14 (3%)	37	67
All	All	6731/9419 (72%)	6449 (96%)	282 (4%)	28	60

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	27	VAL
1	1A	41	MET
1	1A	73	THR
2	SA	15	VAL
2	SA	23	THR
2	SA	38	ILE
2	SA	104	THR
2	SA	131	HIS
2	SA	141	ASN
2	SA	142	LEU
2	SA	197	VAL
3	SB	29	ASP
3	SB	69	VAL
3	SB	71	LEU
3	SB	88	THR
3	SB	127	VAL
3	SB	212	VAL
3	SB	218	LEU
4	SC	63	VAL
4	SC	88	ILE
4	SC	112	VAL
4	SC	115	GLN
4	SC	147	VAL
4	SC	182	CYS
4	SC	215	MET
4	SC	229	CYS
4	SC	233	LEU
4	SC	267	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	SD	38	GLU
5	SD	69	LEU
5	SD	90	LYS
5	SD	143	ARG
5	SD	153	VAL
5	SD	176	LEU
5	SD	209	SER
5	SD	217	ILE
6	SE	89	VAL
6	SE	91	SER
6	SE	111	VAL
6	SE	126	VAL
6	SE	183	VAL
6	SE	223	SER
6	SE	247	THR
7	SF	32	ASP
7	SF	35	LEU
7	SF	73	THR
7	SF	79	HIS
7	SF	88	MET
7	SF	98	GLU
7	SF	134	VAL
7	SF	198	ARG
8	SG	131	ARG
8	SG	158	VAL
8	SG	237	LEU
9	SH	77	VAL
9	SH	120	ARG
9	SH	121	THR
9	SH	129	ILE
9	SH	162	GLN
9	SH	172	THR
9	SH	184	ASP
10	SI	14	THR
10	SI	24	LYS
10	SI	29	LEU
10	SI	36	THR
10	SI	72	CYS
10	SI	73	THR
10	SI	81	VAL
10	SI	91	VAL
10	SI	111	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	SI	130	THR
10	SI	174	CYS
10	SI	177	SER
11	SJ	21	GLU
11	SJ	71	LEU
11	SJ	73	GLU
11	SJ	137	VAL
12	SK	1	MET
12	SK	3	MET
12	SK	13	GLU
12	SK	40	VAL
13	SL	82	MET
13	SL	85	THR
13	SL	88	ILE
13	SL	93	LEU
13	SL	103	GLU
13	SL	145	VAL
14	Sf	28	HIS
14	Sf	35	ILE
14	Sf	54	SER
14	Sf	68	LEU
14	Sf	94	ILE
15	SN	14	SER
15	SN	22	VAL
15	SN	60	VAL
15	SN	67	THR
15	SN	117	LEU
15	SN	133	ARG
15	SN	147	SER
16	SO	21	VAL
16	SO	30	VAL
16	SO	52	THR
16	SO	57	THR
16	SO	65	ASP
16	SO	81	VAL
16	SO	87	GLU
16	SO	97	LEU
16	SO	114	SER
17	SP	37	TYR
17	SP	54	HIS
17	SP	101	THR
17	SP	126	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	SQ	8	GLN
18	SQ	46	THR
18	SQ	66	VAL
18	SQ	78	VAL
18	SQ	108	ILE
18	SQ	113	ILE
19	SR	7	LYS
19	SR	9	VAL
19	SR	30	THR
19	SR	60	ARG
19	SR	66	VAL
19	SR	83	ASN
19	SR	85	VAL
19	SR	91	LEU
19	SR	101	ASP
20	SS	4	VAL
20	SS	5	ILE
20	SS	36	VAL
20	SS	67	VAL
20	SS	131	VAL
20	SS	136	THR
21	ST	15	VAL
21	ST	24	LYS
21	ST	66	LEU
21	ST	83	GLN
22	SU	55	ARG
22	SU	56	MET
22	SU	65	THR
22	SU	68	THR
22	SU	81	GLN
22	SU	82	MET
23	SV	64	GLU
23	SV	65	SER
23	SV	66	ASP
24	SW	19	LYS
24	SW	28	ARG
24	SW	30	CYS
24	SW	74	VAL
24	SW	105	THR
24	SW	111	MET
24	SW	115	GLU
25	SX	13	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	SX	57	VAL
25	SX	66	ILE
25	SX	72	VAL
25	SX	112	VAL
25	SX	118	VAL
25	SX	128	VAL
25	SX	131	LEU
26	SY	4	THR
26	SY	9	THR
26	SY	23	MET
26	SY	25	ILE
26	SY	103	SER
27	SZ	49	LEU
27	SZ	54	THR
27	SZ	62	VAL
27	SZ	97	ILE
27	SZ	113	THR
28	Sa	30	VAL
28	Sa	40	VAL
28	Sa	96	THR
29	Sb	57	VAL
29	Sb	62	VAL
30	Sc	17	VAL
30	Sc	38	THR
30	Sc	56	LEU
31	Sd	7	TYR
31	Sd	40	ARG
31	Sd	53	ILE
32	Se	25	LYS
32	Se	36	MET
32	Se	45	VAL
33	sh	100	LEU
33	sh	102	VAL
33	sh	118	ARG
33	sh	126	CYS
33	sh	130	VAL
33	sh	140	TYR
33	sh	141	CYS
33	sh	148	TYR
34	Sg	42	MET
34	Sg	71	ILE
34	Sg	113	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	Sg	128	THR
34	Sg	144	ASP
34	Sg	151	VAL
34	Sg	156	PHE
34	Sg	176	VAL
34	Sg	195	LEU
34	Sg	203	ASP
34	Sg	218	LEU
35	Ln	6	ARG
35	Ln	10	MET
35	Ln	16	LYS
35	Ln	18	ARG
38	3m	44	GLN
38	3m	45	ILE
38	3m	90	LEU
38	3m	103	LEU
38	3m	129	LYS
38	3m	130	VAL
38	3m	138	GLN
38	3m	144	LEU
38	3m	161	LYS
38	3m	225	THR
38	3m	238	HIS
38	3m	257	GLN
39	3f	123	THR
39	3f	128	SER
39	3f	228	MET
39	3f	255	THR
39	3f	262	VAL
39	3f	303	THR
40	3a	18	PHE
40	3a	34	VAL
40	3a	95	LYS
40	3a	154	TRP
40	3a	189	THR
40	3a	225	SER
40	3a	261	SER
40	3a	290	LEU
40	3a	291	PHE
40	3a	296	LEU
40	3a	310	LEU
40	3a	342	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	3a	344	MET
40	3a	361	LEU
40	3a	406	ARG
40	3a	442	GLN
41	3e	17	HIS
41	3e	19	VAL
41	3e	117	LEU
41	3e	155	ARG
41	3e	209	GLN
41	3e	299	LEU
41	3e	338	LEU
42	3c	422	GLU
42	3c	517	LYS
42	3c	572	HIS
42	3c	744	MET
42	3c	761	MET
42	3c	862	LYS
43	3h	56	GLU
43	3h	107	LEU
43	3h	121	GLN
43	3h	129	VAL
43	3h	133	LEU
43	3h	215	MET
44	3d	10	GLN
45	3k	95	GLU
45	3k	103	LEU
45	3k	128	LEU
45	3k	157	LEU
45	3k	158	LEU
45	3k	214	MET
46	3l	101	LYS
46	3l	131	LEU
46	3l	182	TRP
46	3l	265	LEU
46	3l	295	GLU
46	3l	334	ARG
46	3l	361	ASN
46	3l	375	LEU
46	3l	382	ILE
46	3l	390	LEU
46	3l	495	HIS
46	3l	509	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	3l	514	GLN
46	3l	554	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	112	HIS
2	SA	29	ASN
2	SA	33	GLN
3	SB	186	ASN
7	SF	110	GLN
9	SH	33	ASN
9	SH	44	ASN
9	SH	126	HIS
10	SI	52	ASN
11	SJ	75	ASN
12	SK	28	HIS
12	SK	32	HIS
12	SK	61	GLN
13	SL	13	GLN
14	Sf	48	HIS
16	SO	32	HIS
16	SO	83	GLN
18	SQ	86	GLN
24	SW	98	GLN
25	SX	16	HIS
25	SX	61	GLN
32	Se	39	ASN
32	Se	58	ASN
34	Sg	26	GLN
34	Sg	62	HIS
34	Sg	147	HIS
34	Sg	305	ASN
34	Sg	311	GLN
38	3m	33	ASN
38	3m	222	HIS
38	3m	259	ASN
38	3m	339	HIS
39	3f	182	HIS
39	3f	314	GLN
39	3f	356	ASN
40	3a	76	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	3a	180	GLN
40	3a	292	HIS
40	3a	448	GLN
40	3a	518	GLN
41	3e	225	HIS
41	3e	348	HIS
41	3e	403	GLN
42	3c	417	ASN
42	3c	461	ASN
42	3c	579	HIS
42	3c	600	HIS
42	3c	615	GLN
42	3c	648	GLN
42	3c	819	HIS
42	3c	837	GLN
43	3h	255	GLN
43	3h	270	GLN
45	3k	124	ASN
46	3l	97	ASN
46	3l	109	ASN
46	3l	169	ASN
46	3l	195	GLN
46	3l	225	HIS
46	3l	232	HIS
46	3l	330	GLN
46	3l	338	ASN
46	3l	361	ASN
46	3l	402	GLN
46	3l	495	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	S2	1746/1869 (93%)	342 (19%)	6 (0%)
37	zz	301/332 (90%)	115 (38%)	0
All	All	2047/2201 (93%)	457 (22%)	6 (0%)

All (457) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
36	S2	4	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	S2	17	C
36	S2	25	A
36	S2	33	G
36	S2	42	A
36	S2	44	U
36	S2	45	A
36	S2	46	A
36	S2	56	G
36	S2	59	U
36	S2	62	G
36	S2	65	C
36	S2	67	C
36	S2	68	A
36	S2	73	C
36	S2	74	G
36	S2	75	G
36	S2	76	U
36	S2	94	G
36	S2	99	A
36	S2	103	A
36	S2	113	G
36	S2	115	U
36	S2	126	G
36	S2	130	G
36	S2	143	U
36	S2	155	G
36	S2	166	A
36	S2	170	A
36	S2	172	U
36	S2	175	A
36	S2	178	C
36	S2	191	A
36	S2	193	C
36	S2	196	C
36	S2	199	C
36	S2	200	G
36	S2	204	G
36	S2	206	G
36	S2	207	G
36	S2	211	G
36	S2	212	C
36	S2	228	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	S2	232	A
36	S2	238	C
36	S2	242	U
36	S2	281	C
36	S2	282	G
36	S2	283	G
36	S2	287	U
36	S2	294	U
36	S2	302	A
36	S2	306	C
36	S2	309	G
36	S2	319	C
36	S2	323	C
36	S2	324	C
36	S2	325	C
36	S2	326	C
36	S2	327	G
36	S2	328	U
36	S2	329	G
36	S2	330	G
36	S2	332	G
36	S2	335	G
36	S2	339	A
36	S2	347	G
36	S2	351	G
36	S2	362	C
36	S2	364	A
36	S2	370	G
36	S2	383	G
36	S2	385	G
36	S2	386	C
36	S2	399	C
36	S2	400	C
36	S2	407	G
36	S2	409	C
36	S2	418	A
36	S2	435	A
36	S2	448	A
36	S2	449	A
36	S2	450	C
36	S2	464	A
36	S2	467	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	S2	471	G
36	S2	472	C
36	S2	474	G
36	S2	482	G
36	S2	487	U
36	S2	492	C
36	S2	493	A
36	S2	516	A
36	S2	517	C
36	S2	518	G
36	S2	532	C
36	S2	533	A
36	S2	534	G
36	S2	536	A
36	S2	537	C
36	S2	538	U
36	S2	540	U
36	S2	541	U
36	S2	543	C
36	S2	545	A
36	S2	546	G
36	S2	547	G
36	S2	548	C
36	S2	549	C
36	S2	550	C
36	S2	554	A
36	S2	555	A
36	S2	559	G
36	S2	564	A
36	S2	568	C
36	S2	576	A
36	S2	583	A
36	S2	587	A
36	S2	589	G
36	S2	590	A
36	S2	591	U
36	S2	604	A
36	S2	606	G
36	S2	607	U
36	S2	614	C
36	S2	617	G
36	S2	629	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	S2	643	A
36	S2	644	G
36	S2	655	A
36	S2	660	C
36	S2	669	A
36	S2	670	A
36	S2	671	A
36	S2	672	A
36	S2	673	G
36	S2	684	G
36	S2	688	U
36	S2	690	G
36	S2	692	G
36	S2	693	A
36	S2	695	C
36	S2	696	G
36	S2	697	G
36	S2	698	G
36	S2	731	G
36	S2	732	U
36	S2	733	C
36	S2	735	C
36	S2	736	C
36	S2	738	C
36	S2	739	C
36	S2	746	C
36	S2	749	U
36	S2	790	C
36	S2	793	G
36	S2	795	A
36	S2	796	G
36	S2	798	G
36	S2	799	U
36	S2	800	U
36	S2	801	U
36	S2	821	G
36	S2	822	U
36	S2	827	A
36	S2	834	C
36	S2	847	A
36	S2	869	A
36	S2	870	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	S2	871	U
36	S2	872	A
36	S2	878	G
36	S2	883	U
36	S2	885	U
36	S2	886	A
36	S2	890	U
36	S2	891	G
36	S2	893	U
36	S2	894	G
36	S2	895	G
36	S2	896	U
36	S2	897	U
36	S2	906	U
36	S2	913	A
36	S2	914	U
36	S2	920	A
36	S2	922	A
36	S2	933	G
36	S2	943	U
36	S2	954	U
36	S2	985	G
36	S2	990	A
36	S2	992	A
36	S2	1002	U
36	S2	1017	U
36	S2	1023	A
36	S2	1045	U
36	S2	1061	U
36	S2	1062	A
36	S2	1081	U
36	S2	1082	A
36	S2	1083	A
36	S2	1085	C
36	S2	1109	C
36	S2	1114	U
36	S2	1115	U
36	S2	1117	C
36	S2	1118	C
36	S2	1119	A
36	S2	1121	G
36	S2	1133	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	S2	1138	C
36	S2	1139	C
36	S2	1149	A
36	S2	1153	C
36	S2	1154	U
36	S2	1171	G
36	S2	1195	A
36	S2	1207	G
36	S2	1215	C
36	S2	1216	C
36	S2	1242	U
36	S2	1243	U
36	S2	1244	U
36	S2	1248	U
36	S2	1249	C
36	S2	1251	A
36	S2	1253	A
36	S2	1256	G
36	S2	1257	G
36	S2	1259	A
36	S2	1264	C
36	S2	1274	G
36	S2	1275	G
36	S2	1283	C
36	S2	1286	G
36	S2	1288	U
36	S2	1291	A
36	S2	1295	A
36	S2	1301	A
36	S2	1302	G
36	S2	1303	C
36	S2	1306	U
36	S2	1308	U
36	S2	1309	C
36	S2	1312	G
36	S2	1320	G
36	S2	1322	G
36	S2	1326	U
36	S2	1327	G
36	S2	1333	U
36	S2	1342	U
36	S2	1348	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	S2	1371	U
36	S2	1372	U
36	S2	1378	A
36	S2	1382	A
36	S2	1397	U
36	S2	1406	G
36	S2	1417	C
36	S2	1418	C
36	S2	1419	C
36	S2	1420	G
36	S2	1421	A
36	S2	1422	G
36	S2	1423	C
36	S2	1424	G
36	S2	1435	C
36	S2	1436	C
36	S2	1438	A
36	S2	1452	A
36	S2	1454	A
36	S2	1462	U
36	S2	1463	U
36	S2	1489	A
36	S2	1490	G
36	S2	1494	U
36	S2	1495	G
36	S2	1497	G
36	S2	1498	A
36	S2	1508	A
36	S2	1521	C
36	S2	1522	A
36	S2	1523	C
36	S2	1533	A
36	S2	1535	U
36	S2	1544	C
36	S2	1553	C
36	S2	1555	U
36	S2	1575	G
36	S2	1580	A
36	S2	1585	U
36	S2	1588	A
36	S2	1601	A
36	S2	1606	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	S2	1621	U
36	S2	1654	G
36	S2	1661	A
36	S2	1664	A
36	S2	1665	G
36	S2	1680	G
36	S2	1683	C
36	S2	1699	A
36	S2	1710	C
36	S2	1712	A
36	S2	1713	C
36	S2	1715	A
36	S2	1719	A
36	S2	1722	G
36	S2	1723	G
36	S2	1744	G
36	S2	1745	A
36	S2	1748	G
36	S2	1752	C
36	S2	1753	C
36	S2	1754	G
36	S2	1768	A
36	S2	1776	G
36	S2	1777	G
36	S2	1778	C
36	S2	1780	G
36	S2	1781	A
36	S2	1782	G
36	S2	1783	C
36	S2	1784	G
36	S2	1812	U
36	S2	1813	A
36	S2	1820	G
36	S2	1821	U
36	S2	1823	A
36	S2	1824	A
36	S2	1825	A
36	S2	1826	G
36	S2	1829	G
36	S2	1838	U
36	S2	1849	G
36	S2	1851	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	S2	1861	G
36	S2	1862	G
36	S2	1863	A
36	S2	1864	U
36	S2	1865	C
37	zz	45	C
37	zz	46	U
37	zz	47	G
37	zz	48	U
37	zz	50	A
37	zz	51	G
37	zz	53	A
37	zz	56	U
37	zz	58	C
37	zz	59	U
37	zz	63	U
37	zz	64	U
37	zz	70	A
37	zz	82	G
37	zz	83	C
37	zz	84	C
37	zz	85	A
37	zz	94	G
37	zz	97	U
37	zz	102	G
37	zz	104	C
37	zz	105	G
37	zz	106	U
37	zz	107	G
37	zz	110	G
37	zz	111	C
37	zz	112	C
37	zz	113	U
37	zz	114	C
37	zz	115	C
37	zz	116	A
37	zz	117	G
37	zz	120	C
37	zz	125	C
37	zz	126	C
37	zz	132	G
37	zz	133	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	zz	137	G
37	zz	145	G
37	zz	146	G
37	zz	150	G
37	zz	154	A
37	zz	157	C
37	zz	161	G
37	zz	163	G
37	zz	164	U
37	zz	165	A
37	zz	166	C
37	zz	167	A
37	zz	169	C
37	zz	172	A
37	zz	175	U
37	zz	185	A
37	zz	186	C
37	zz	189	G
37	zz	190	G
37	zz	191	U
37	zz	192	C
37	zz	195	U
37	zz	196	U
37	zz	197	C
37	zz	198	U
37	zz	202	A
37	zz	204	C
37	zz	207	C
37	zz	208	C
37	zz	209	C
37	zz	210	G
37	zz	213	C
37	zz	216	U
37	zz	217	G
37	zz	223	A
37	zz	224	G
37	zz	225	A
37	zz	229	G
37	zz	233	G
37	zz	234	U
37	zz	235	G
37	zz	237	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	zz	244	A
37	zz	247	C
37	zz	253	G
37	zz	256	G
37	zz	258	G
37	zz	259	U
37	zz	260	A
37	zz	263	G
37	zz	265	U
37	zz	266	G
37	zz	270	C
37	zz	280	C
37	zz	282	U
37	zz	283	G
37	zz	284	U
37	zz	286	G
37	zz	288	A
37	zz	289	C
37	zz	290	U
37	zz	295	G
37	zz	296	A
37	zz	297	U
37	zz	303	G
37	zz	306	U
37	zz	311	G
37	zz	318	G
37	zz	330	A
37	zz	331	G
37	zz	332	A
37	zz	334	C
37	zz	335	G
37	zz	336	U
37	zz	337	G
37	zz	341	C
37	zz	344	G
37	zz	345	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	S2	174	C
36	S2	517	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	S2	531	A
36	S2	871	U
36	S2	1326	U
36	S2	1434	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

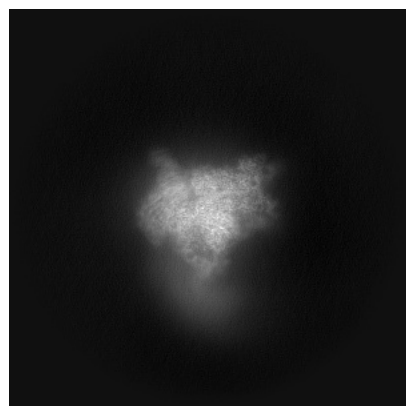
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62453. These allow visual inspection of the internal detail of the map and identification of artifacts.

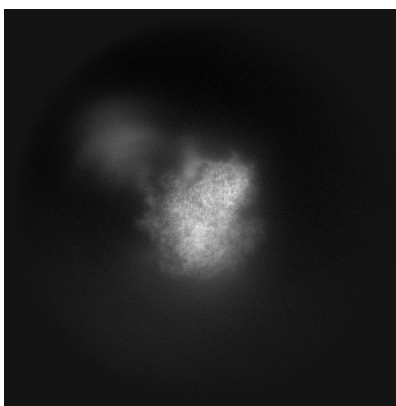
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

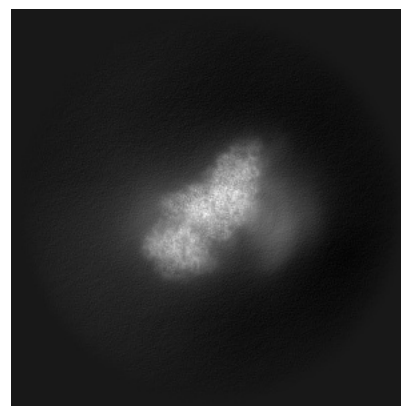
6.1.1 Primary map



X

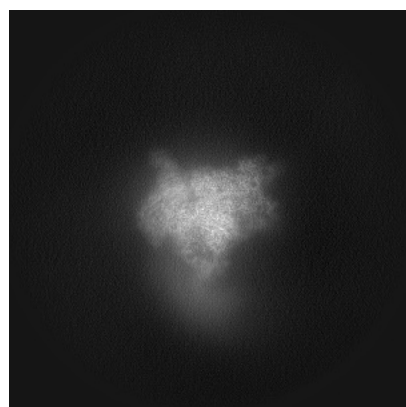


Y

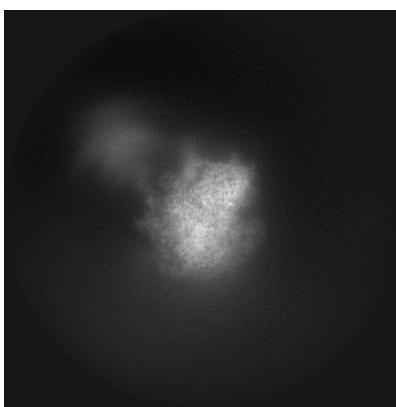


Z

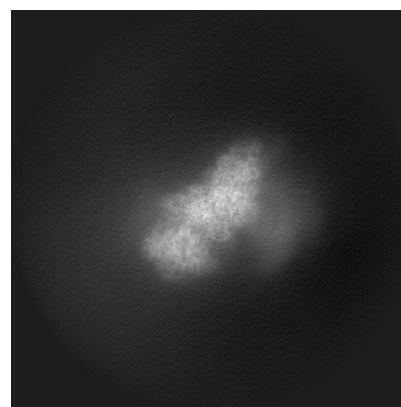
6.1.2 Raw map



X



Y

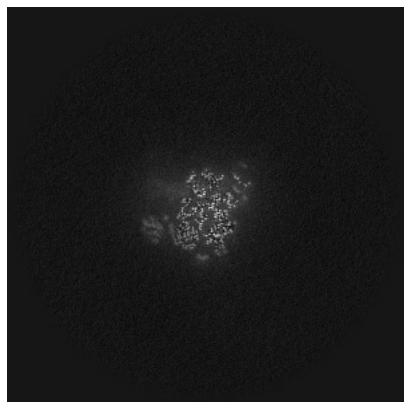


Z

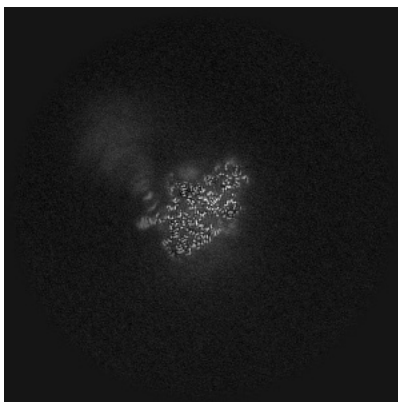
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

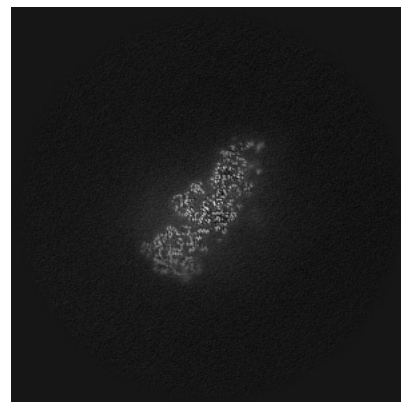
6.2.1 Primary map



X Index: 250

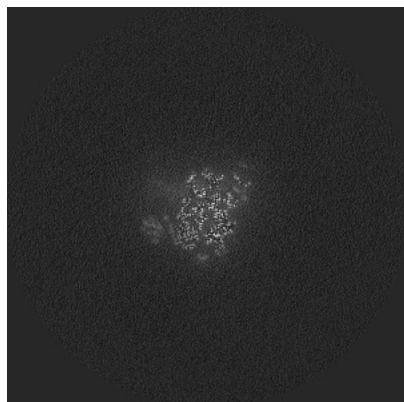


Y Index: 250

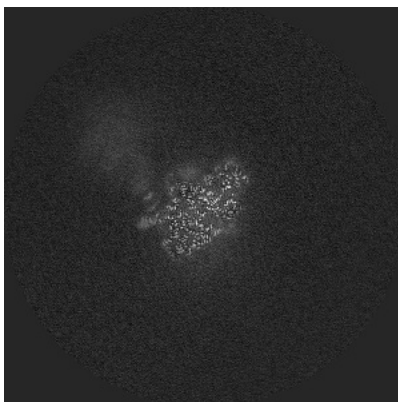


Z Index: 250

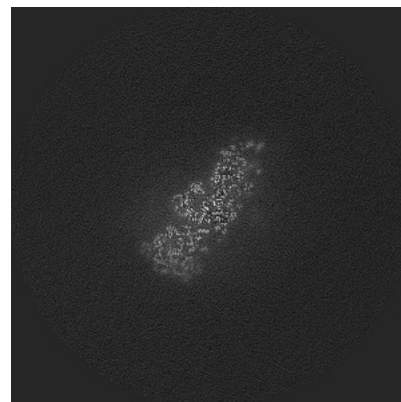
6.2.2 Raw map



X Index: 250



Y Index: 250

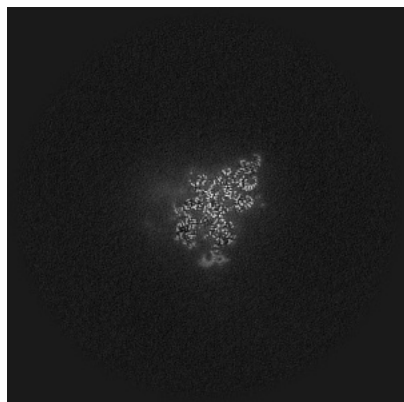


Z Index: 250

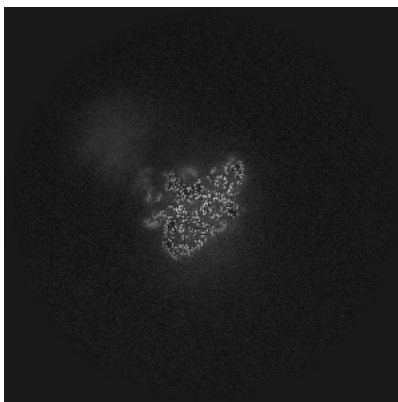
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

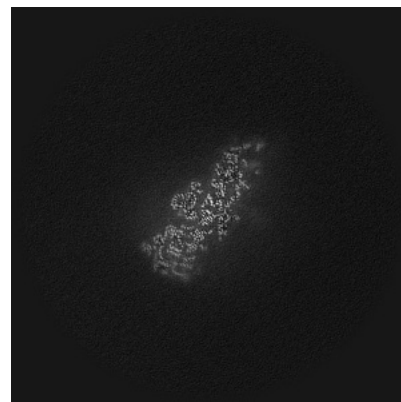
6.3.1 Primary map



X Index: 260

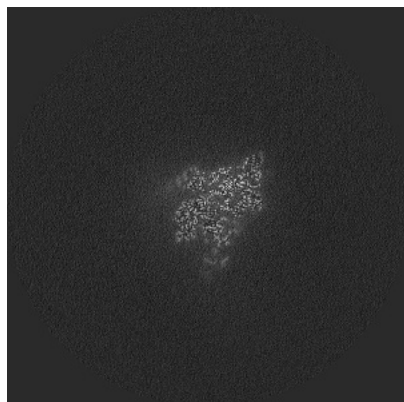


Y Index: 255

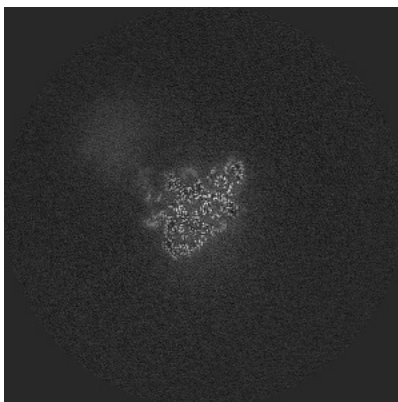


Z Index: 248

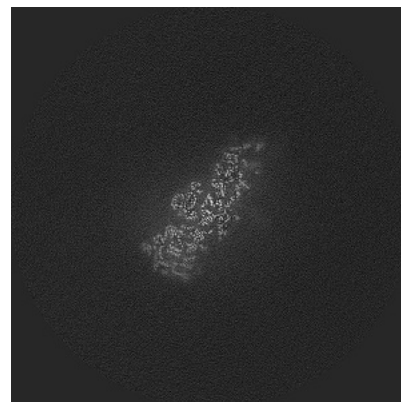
6.3.2 Raw map



X Index: 267



Y Index: 255

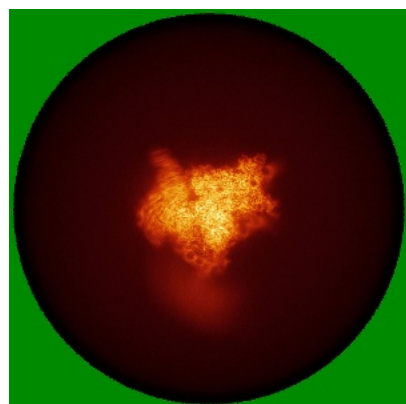


Z Index: 248

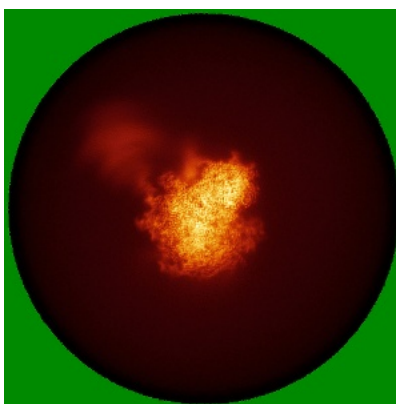
The images above show the largest variance slices of the map in three orthogonal directions.

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

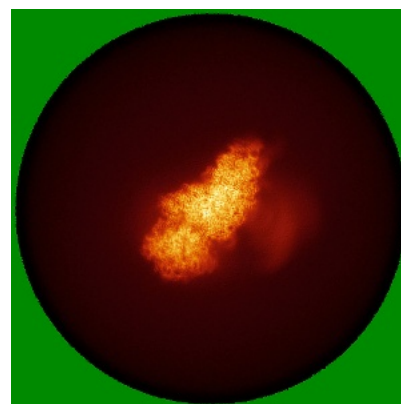
6.4.1 Primary map



X

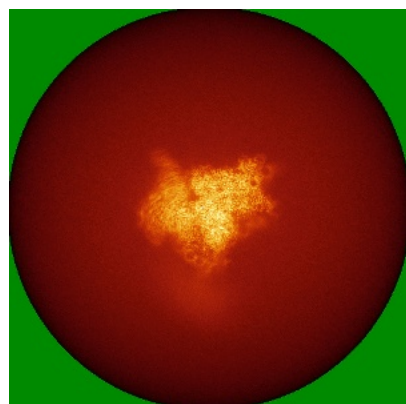


Y

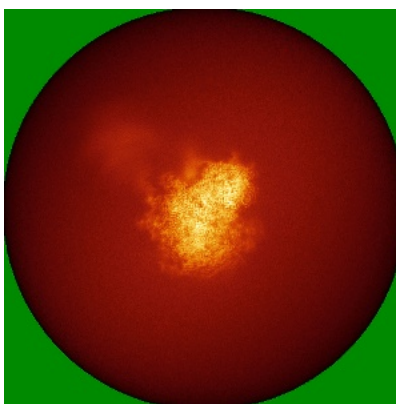


Z

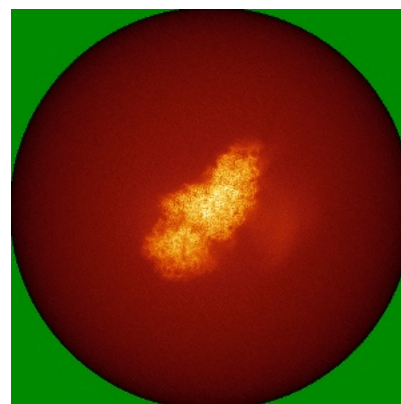
6.4.2 Raw map



X



Y

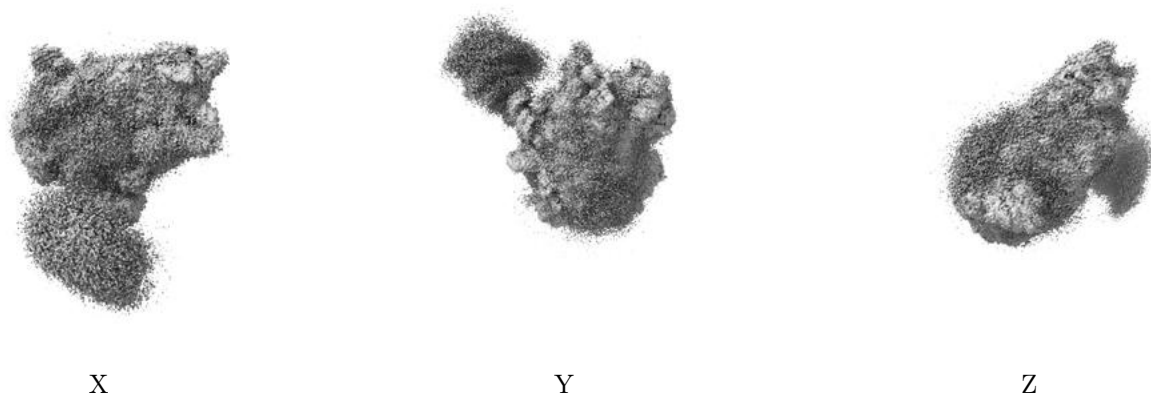


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

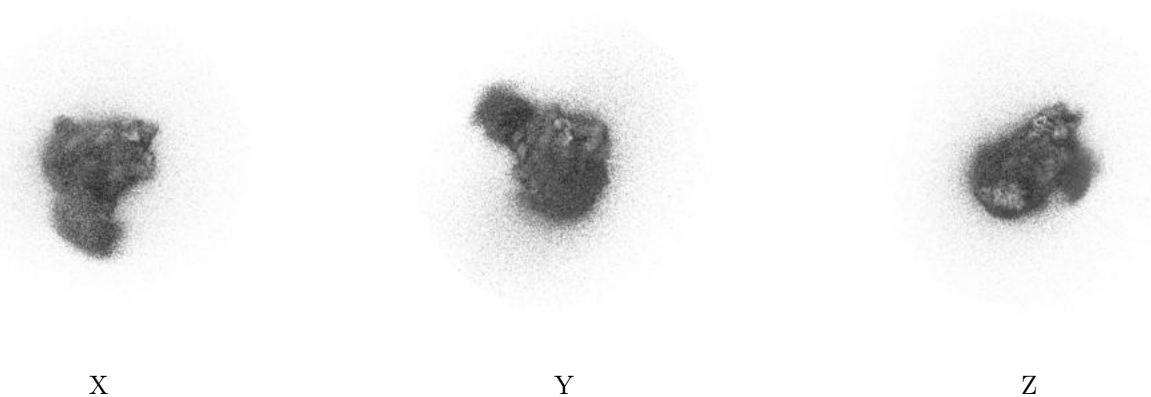
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

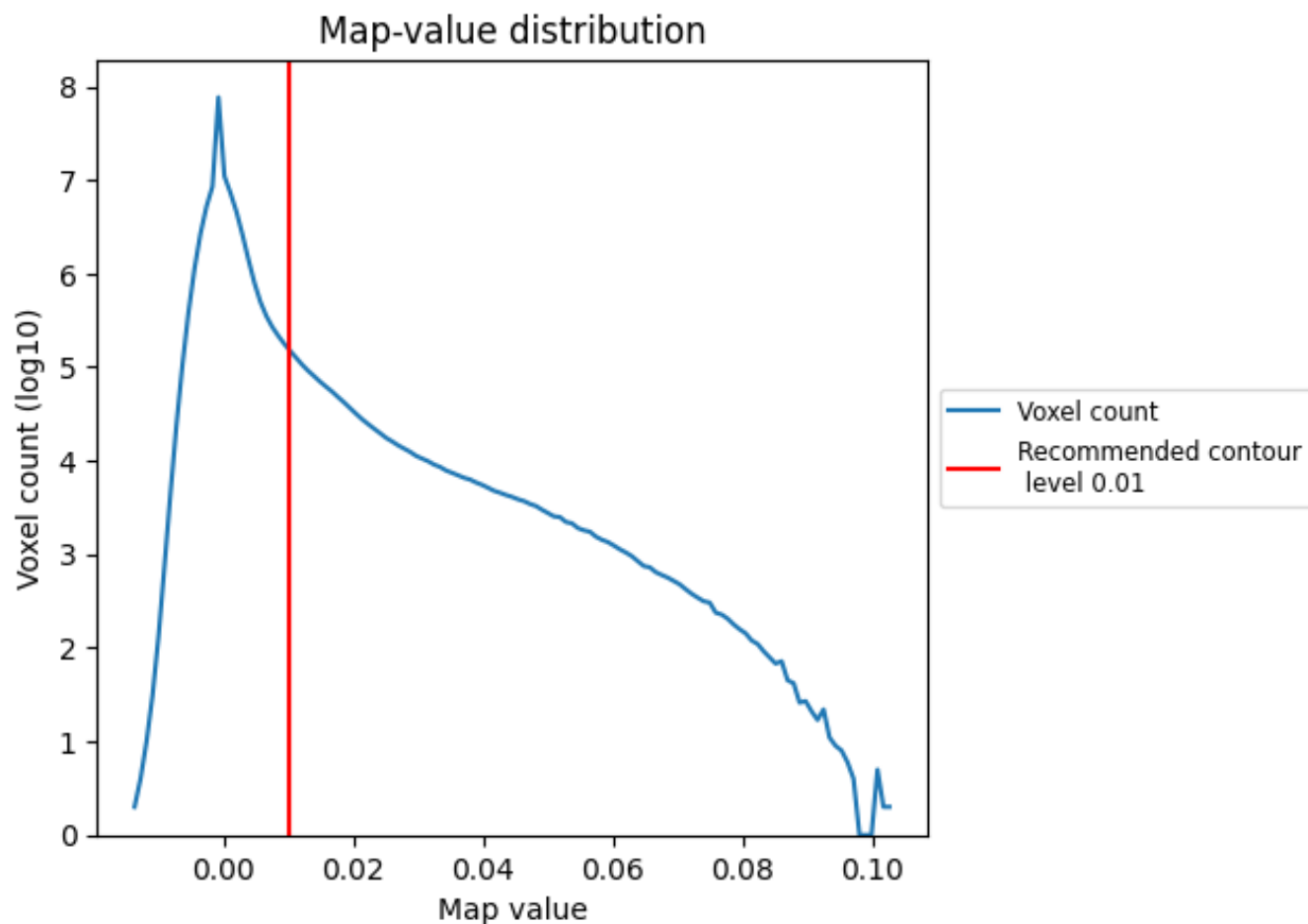
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

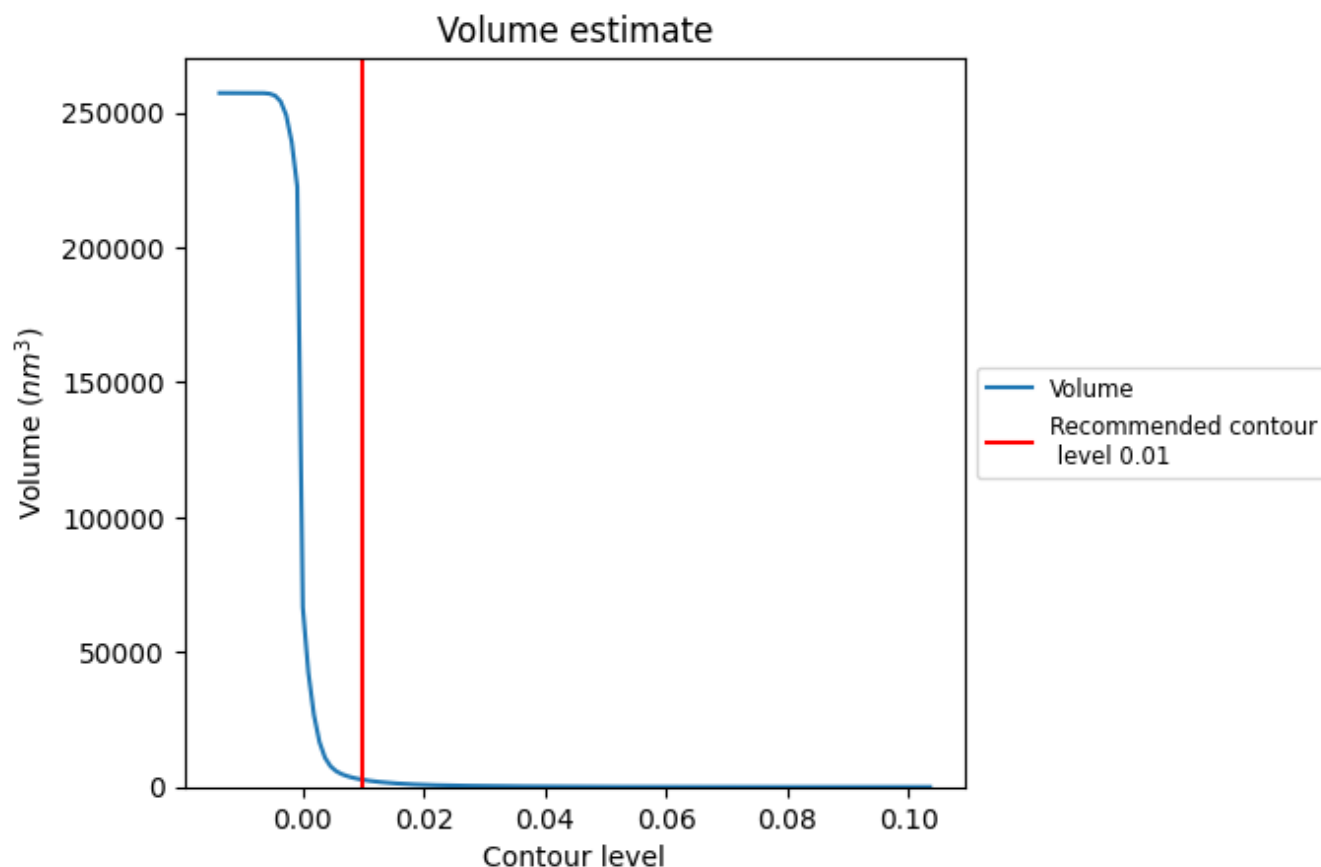
This section contains the results of statistical analysis of the map.

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.

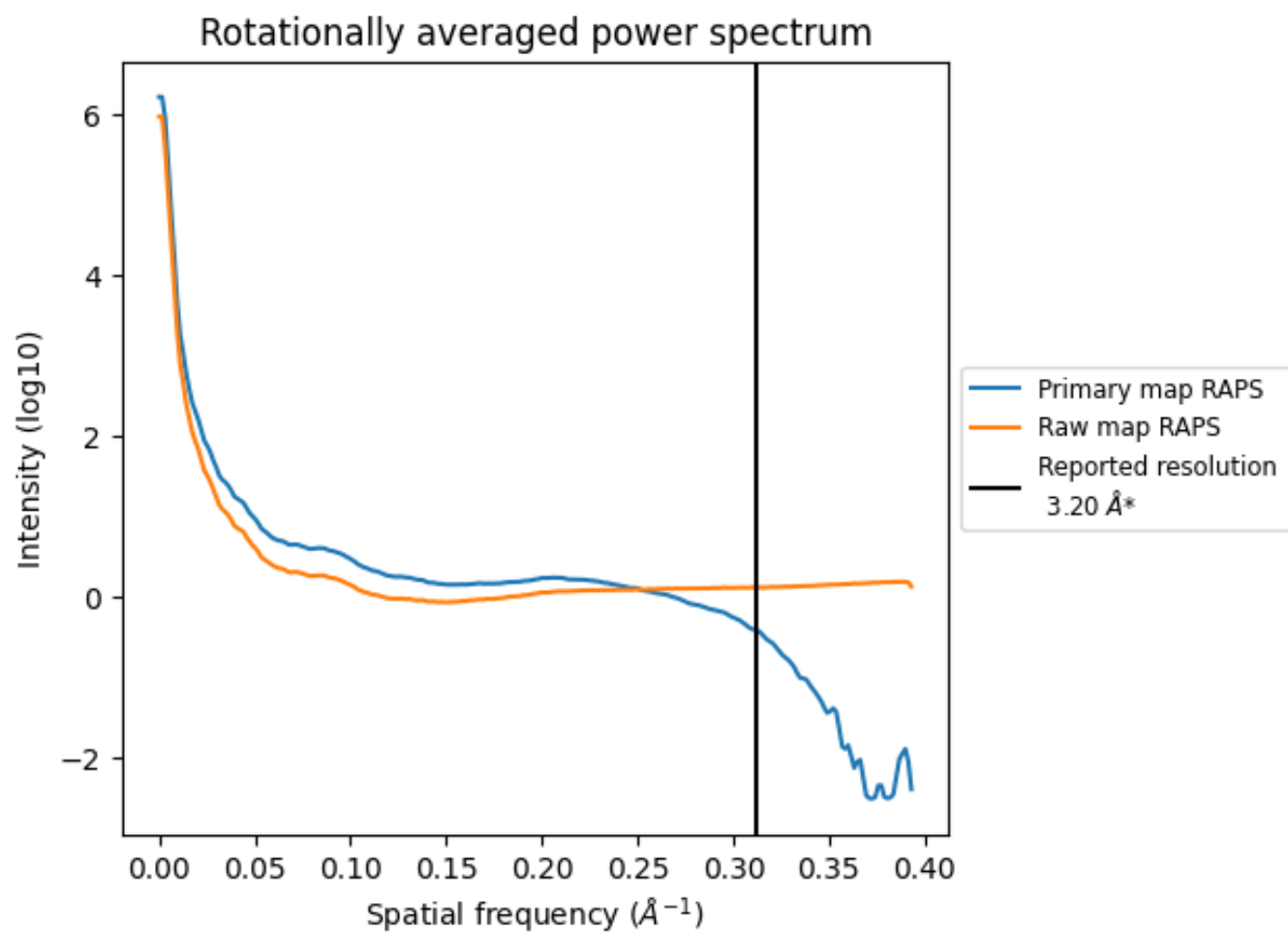
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2673 nm^3 ; this corresponds to an approximate mass of 2415 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 ⓘ

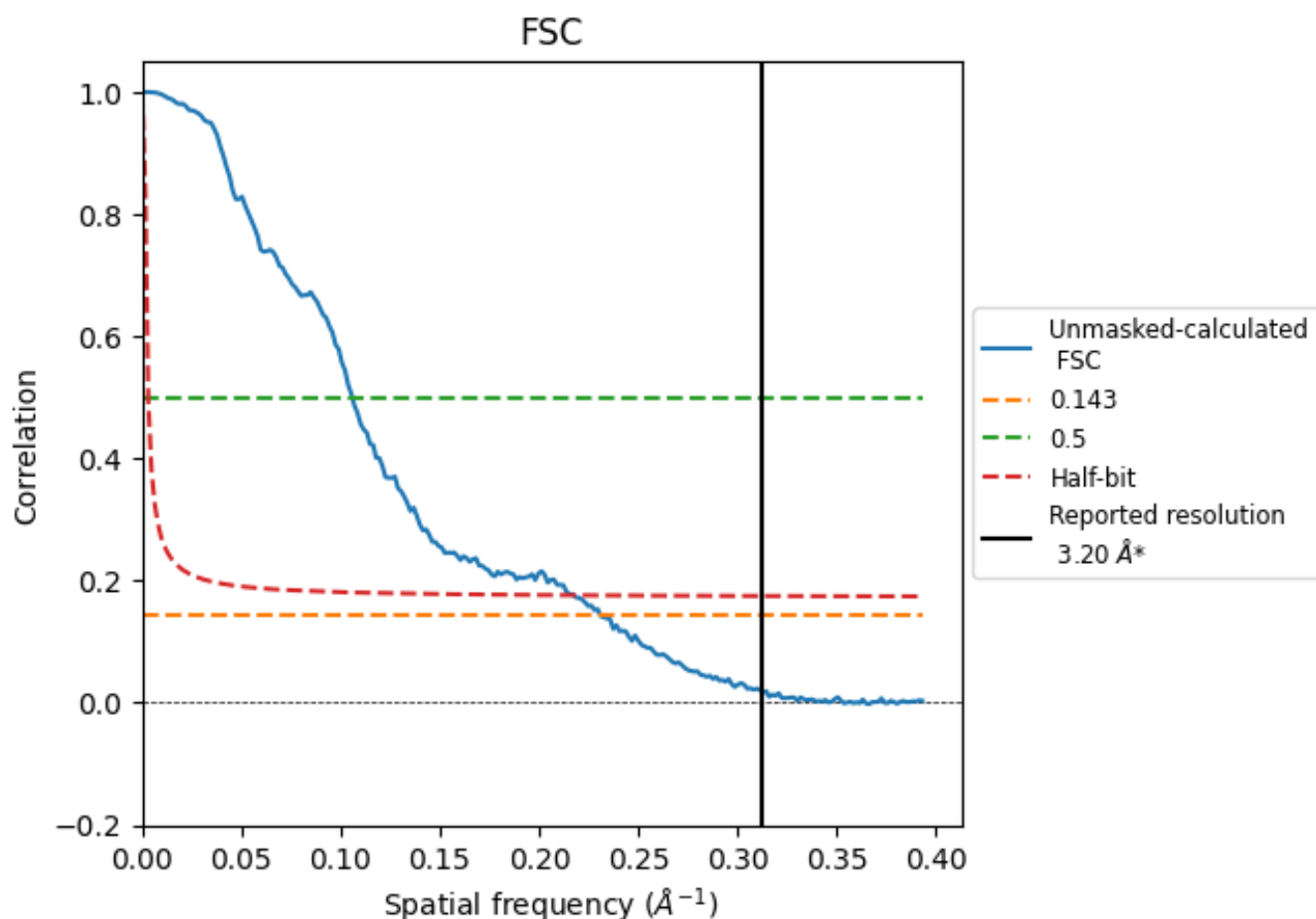


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

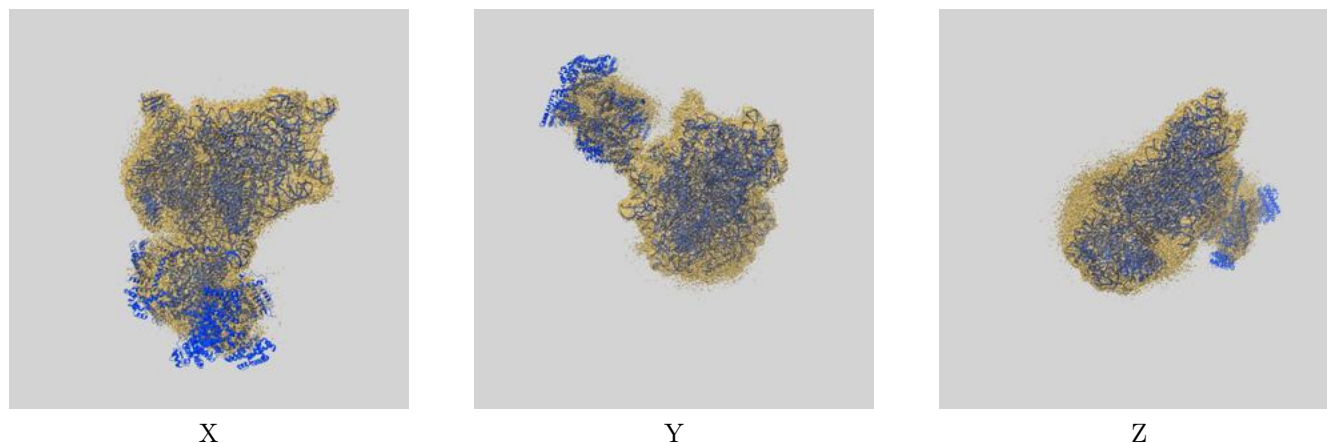
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.33	9.44	4.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.33 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

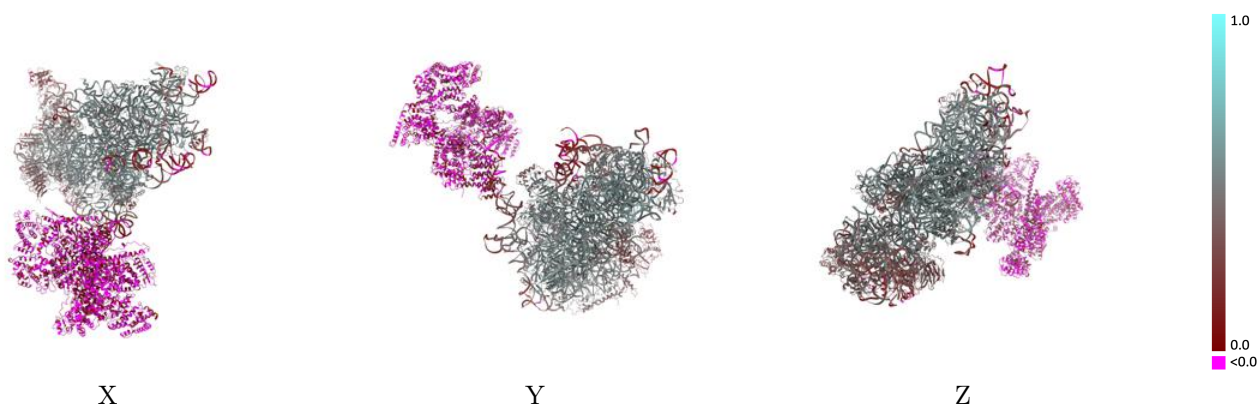
This section contains information regarding the fit between EMDB map EMD-62453 and PDB model 9KN5. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



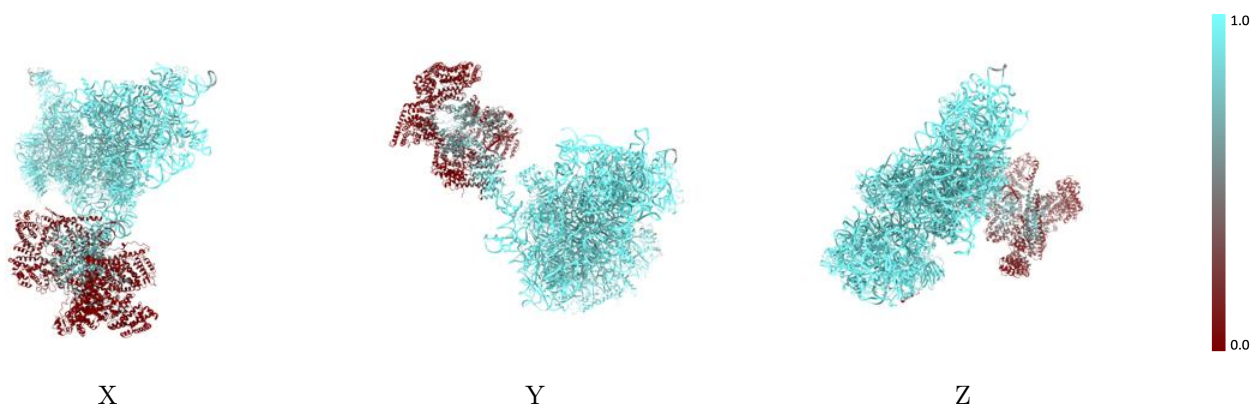
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



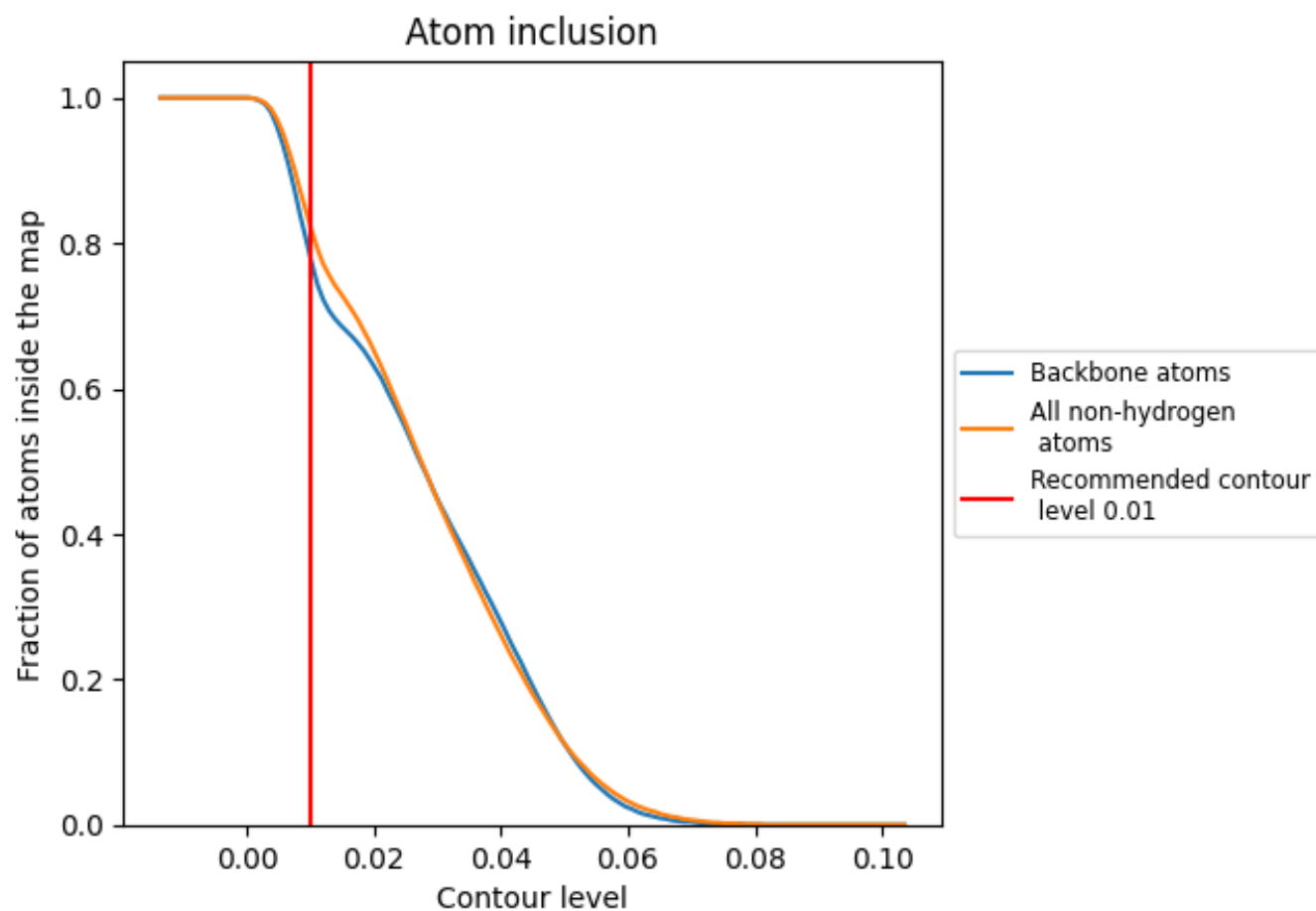
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8220	 0.3500
1A	 0.9920	 0.2970
3a	 0.4480	 0.0310
3c	 0.3590	 0.0140
3d	 0.2760	 -0.0030
3e	 0.1610	 0.0060
3f	 0.3230	 0.0050
3h	 0.4970	 0.0100
3k	 0.0420	 -0.0100
3l	 0.0780	 0.0030
3m	 0.0540	 -0.0050
Ln	 1.0000	 0.4880
S2	 0.9970	 0.4720
SA	 0.9990	 0.5180
SB	 0.9920	 0.5170
SC	 0.9990	 0.5220
SD	 0.9970	 0.4180
SE	 0.9990	 0.5160
SF	 0.9990	 0.4910
SG	 0.9780	 0.4410
SH	 0.9910	 0.4550
SI	 0.9910	 0.5000
SJ	 0.9980	 0.5290
SK	 1.0000	 0.3610
SL	 0.9920	 0.5030
SN	 1.0000	 0.5200
SO	 0.9980	 0.5180
SP	 0.9880	 0.3580
SQ	 1.0000	 0.4440
SR	 0.9990	 0.4520
SS	 0.9890	 0.3960
ST	 0.9960	 0.4060
SU	 0.9960	 0.3880
SV	 0.9970	 0.5160
SW	 1.0000	 0.5210



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SX	 1.0000	 0.5130
SY	 0.9980	 0.5080
SZ	 0.9970	 0.4360
Sa	 1.0000	 0.5370
Sb	 1.0000	 0.5140
Sc	 1.0000	 0.5220
Sd	 1.0000	 0.4420
Se	 1.0000	 0.4810
Sf	 0.8640	 0.1920
Sg	 0.9910	 0.3390
sh	 0.9050	 0.1990
zz	 0.9350	 0.3050