



Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 01:12 PM JST

PDB ID : 9KKF / pdb_00009kkf
EMDB ID : EMD-62386
Title : Structure of the human 40S ribosome complexed with HCV IRES 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 : 2024-11-13
Resolution : 3.30 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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.47

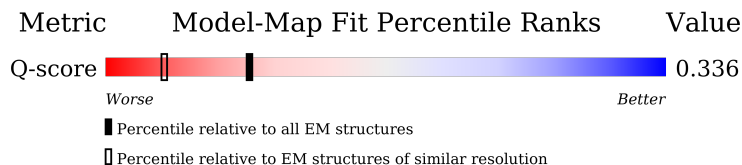
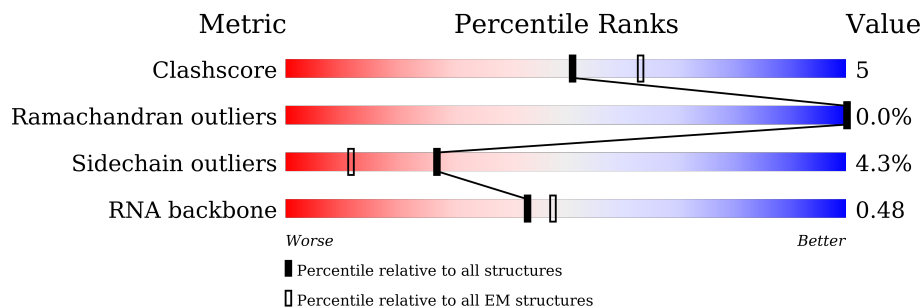
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.










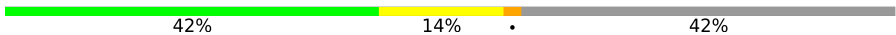














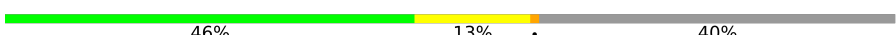


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	SA	295	
2	SB	264	
3	SC	293	











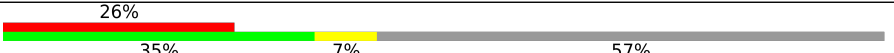

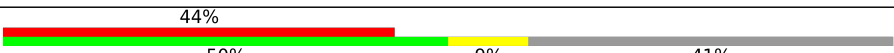
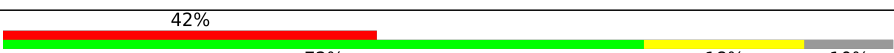

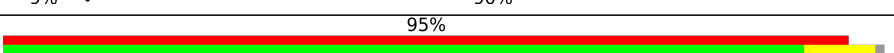

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	SD	243	
5	SE	263	
6	SF	204	
7	SG	249	
8	SH	194	
9	SI	208	
10	SJ	194	
11	SK	165	
12	SL	158	
13	Sf	132	
14	SN	151	
15	SO	151	
16	SP	145	
17	SQ	146	
18	SR	135	
19	SS	152	
20	ST	145	
21	SU	119	
22	SV	83	
23	SW	130	
24	SX	143	
25	SY	133	
26	SZ	125	
27	Sa	115	
28	Sb	84	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Sc	69	
30	Sd	56	
31	Se	59	
32	sh	156	
33	Sg	317	
34	Ln	25	
35	S2	1869	
36	zz	332	
37	3m	374	
38	3f	357	
39	3a	1382	
40	3e	445	
41	3c	913	
42	3h	352	
43	3d	548	
44	3k	218	
45	3l	564	

2 Entry composition [i](#)

There are 47 unique types of molecules in this entry. The entry contains 108043 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 Small ribosomal subunit protein uS2.

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

- Molecule 2 is a protein called 40S ribosomal protein S3a.

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

- Molecule 3 is a protein called 40S ribosomal protein S2.

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

- Molecule 4 is a protein called 40S ribosomal protein S3.

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

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 6 is a protein called 40S ribosomal protein S5.

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

- Molecule 7 is a protein called 40S ribosomal protein S6.

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

- Molecule 8 is a protein called 40S ribosomal protein S7.

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

- Molecule 9 is a protein called 40S ribosomal protein S8.

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

- Molecule 10 is a protein called 40S ribosomal protein S9.

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

- Molecule 11 is a protein called 40S ribosomal protein S10.

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

- Molecule 12 is a protein called 40S ribosomal protein S11.

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

- Molecule 13 is a protein called 40S ribosomal protein S12.

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

- Molecule 14 is a protein called 40S ribosomal protein S13.

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

- Molecule 15 is a protein called 40S ribosomal protein S14.

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

- Molecule 16 is a protein called 40S ribosomal protein S15.

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

- Molecule 17 is a protein called 40S ribosomal protein S16.

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

- Molecule 18 is a protein called 40S ribosomal protein S17.

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

- Molecule 19 is a protein called 40S ribosomal protein S18.

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

- Molecule 20 is a protein called 40S ribosomal protein S19.

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

- Molecule 21 is a protein called 40S ribosomal protein S20.

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

- Molecule 22 is a protein called 40S ribosomal protein S21.

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

- Molecule 23 is a protein called 40S ribosomal protein S15a.

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

- Molecule 24 is a protein called 40S ribosomal protein S23.

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

- Molecule 25 is a protein called 40S ribosomal protein S24.

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

- Molecule 26 is a protein called 40S ribosomal protein S25.

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

- Molecule 27 is a protein called 40S ribosomal protein S26.

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

- Molecule 28 is a protein called 40S ribosomal protein S27.

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

- Molecule 29 is a protein called 40S ribosomal protein S28.

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

- Molecule 30 is a protein called 40S ribosomal protein S29.

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

- Molecule 31 is a protein called 40S ribosomal protein S30.

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

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	sh	64	Total	C	N	O	S	0	0
			522	329	99	87	7		

- Molecule 33 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 34 is a protein called 60S ribosomal protein L41.

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

- Molecule 35 is a RNA chain called 18S ribosomal RNA.

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

- Molecule 36 is a RNA chain called HCV-IRES RNA.

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

- Molecule 37 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3m	363	Total	C	N	O	S	0	0
			2639	1666	450	511	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	3f	269	Total	C	N	O	S	0	0
			2063	1303	354	394	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3a	592	Total	C	N	O	S	0	0
			4497	2849	805	822	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3e	430	Total	C	N	O	S	0	0
			3224	2053	561	594	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3c	543	Total	C	N	O	S	0	0
			3924	2463	721	716	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3h	318	Total	C	N	O	S	0	0
			2520	1599	431	475	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3d	55	Total	C	N	O	S	0	0
			347	222	65	59	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3k	215	Total	C	N	O	S	0	0
			1475	932	251	282	10		

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


Mol	Chain	Residues	Atoms					AltConf	Trace
45	3l	520	Total	C	N	O	S	0	0
			4335	2808	715	793	19		

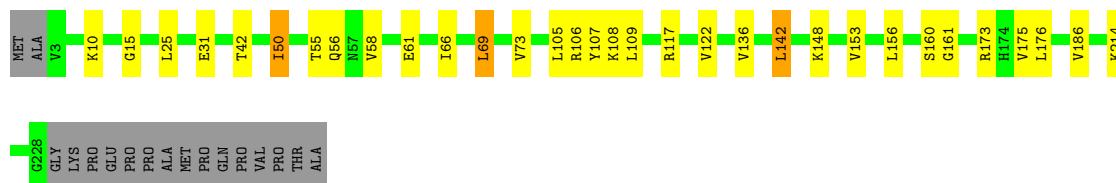
- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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


- Molecule 47 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

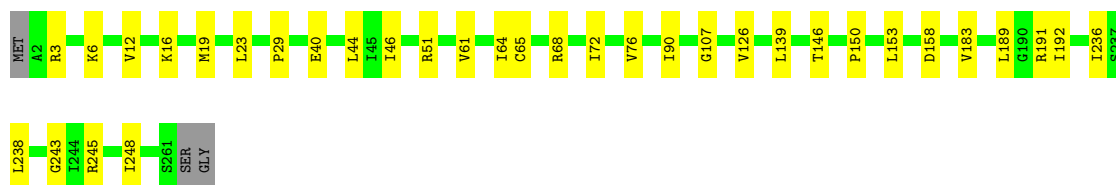
Mol	Chain	Residues	Atoms		AltConf
47	S2	8	Total	Mg	0
			8	8	

Chain SD:  80% 12% 7%




- Molecule 5: 40S ribosomal protein S4, X isoform

Chain SE:  86% 13% 1%




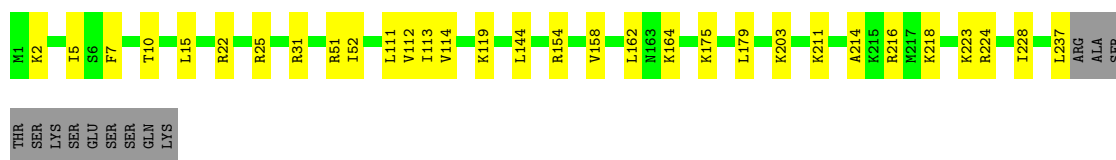
- Molecule 6: 40S ribosomal protein S5

Chain SF:  84% 9% 6%




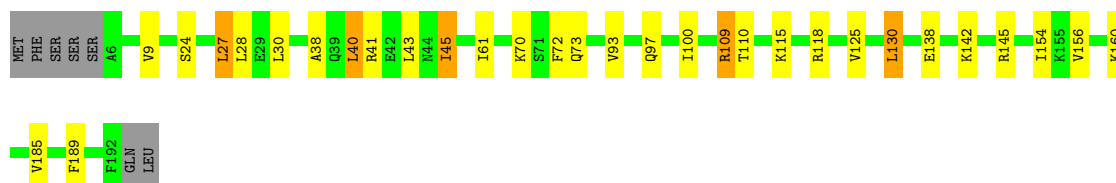
- Molecule 7: 40S ribosomal protein S6

Chain SG:  83% 12% 5%




- Molecule 8: 40S ribosomal protein S7

Chain SH:  80% 13% 7%



- Molecule 9: 40S ribosomal protein S8

Chain SI:  86% 12% 2%



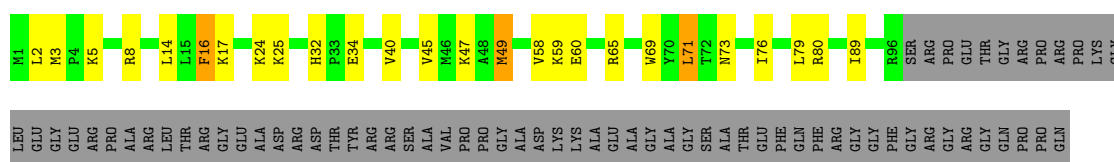
- Molecule 10: 40S ribosomal protein S9

Chain SJ: 82% 11% 7%



- Molecule 11: 40S ribosomal protein S10

Chain SK: 42% 14% 42%



- Molecule 12: 40S ribosomal protein S11

Chain SL: 83% 11% 5%



- Molecule 13: 40S ribosomal protein S12

Chain Sf: 68% 21% 8%



- Molecule 14: 40S ribosomal protein S13

Chain SN: 88% 11% 1%



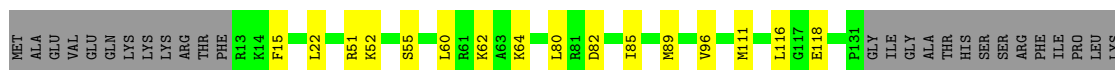
- Molecule 15: 40S ribosomal protein S14

Chain SO: 74% 15% 11%



- Molecule 16: 40S ribosomal protein S15

Chain SP: 71% 11% 18%



- Molecule 17: 40S ribosomal protein S16

Chain SQ: 76% 19% ..



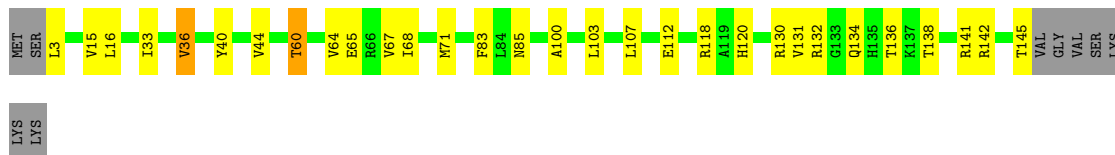
- Molecule 18: 40S ribosomal protein S17

Chain SR: 80% 16% ..



- Molecule 19: 40S ribosomal protein S18

Chain SS: 74% 18% 6%



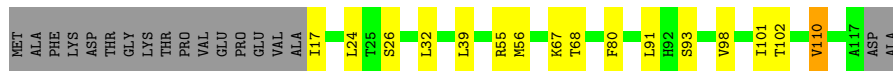
- Molecule 20: 40S ribosomal protein S19

Chain ST: 83% 14% ..




- Molecule 21: 40S ribosomal protein S20

Chain SU: 71% 13% 15%



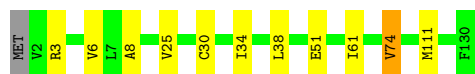
- Molecule 22: 40S ribosomal protein S21

Chain SV:  87% 13%




- Molecule 23: 40S ribosomal protein S15a

Chain SW:  91% 8% ..




- Molecule 24: 40S ribosomal protein S23

Chain SX:  81% 17% ..



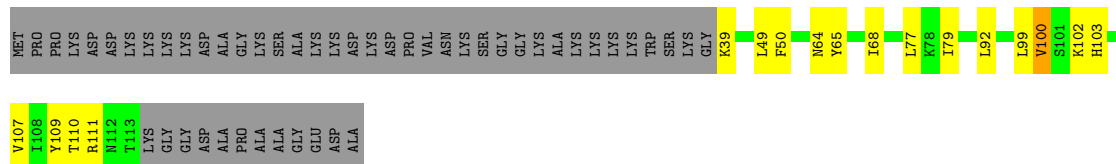
- Molecule 25: 40S ribosomal protein S24

Chain SY:  81% 11% • 7%




- Molecule 26: 40S ribosomal protein S25

Chain SZ:  46% 13% • 40%



- Molecule 27: 40S ribosomal protein S26

Chain Sa:  80% 7% 13%



- Molecule 28: 40S ribosomal protein S27

Chain Sb:  85% 14% •




- Molecule 29: 40S ribosomal protein S28

Chain Sc:  70% 20% 10%




- Molecule 30: 40S ribosomal protein S29

Chain Sd:  80% 18% .



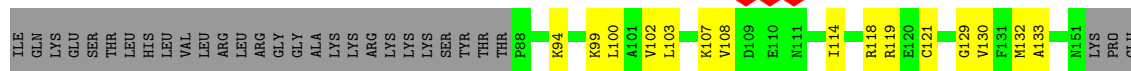
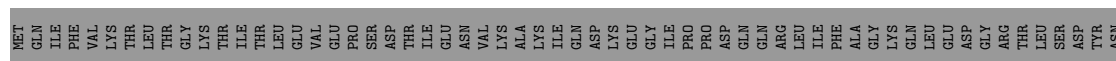
- Molecule 31: 40S ribosomal protein S30

Chain Se:  76% 12% 12%




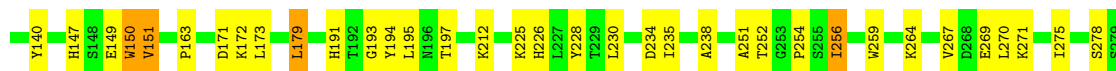
- Molecule 32: Ubiquitin-40S ribosomal protein S27a

Chain sh:  31% 10% 59%



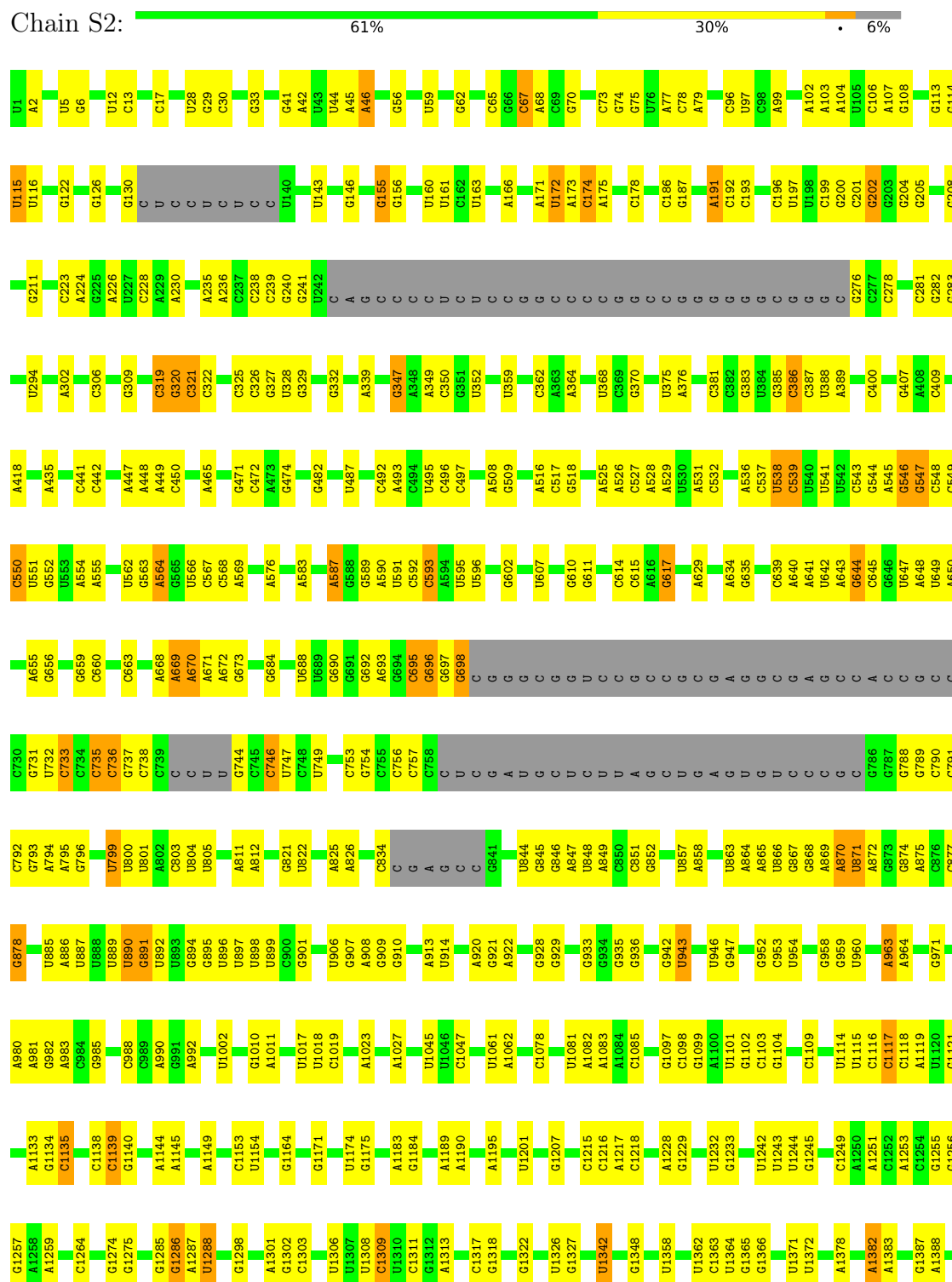
- Molecule 33: Receptor of activated protein C kinase 1

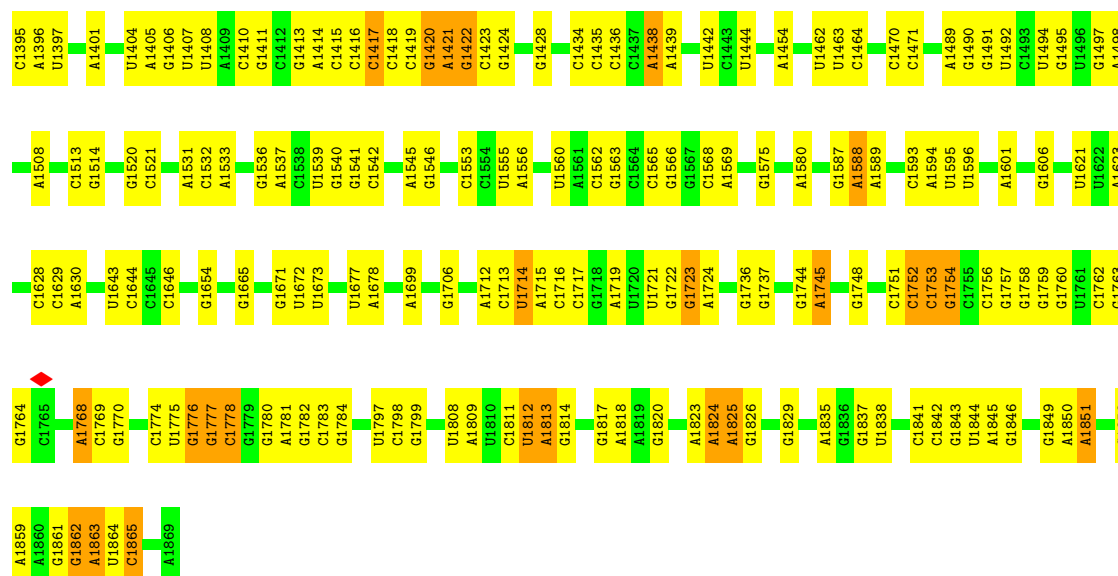
Chain Sg:  75% 22% ..



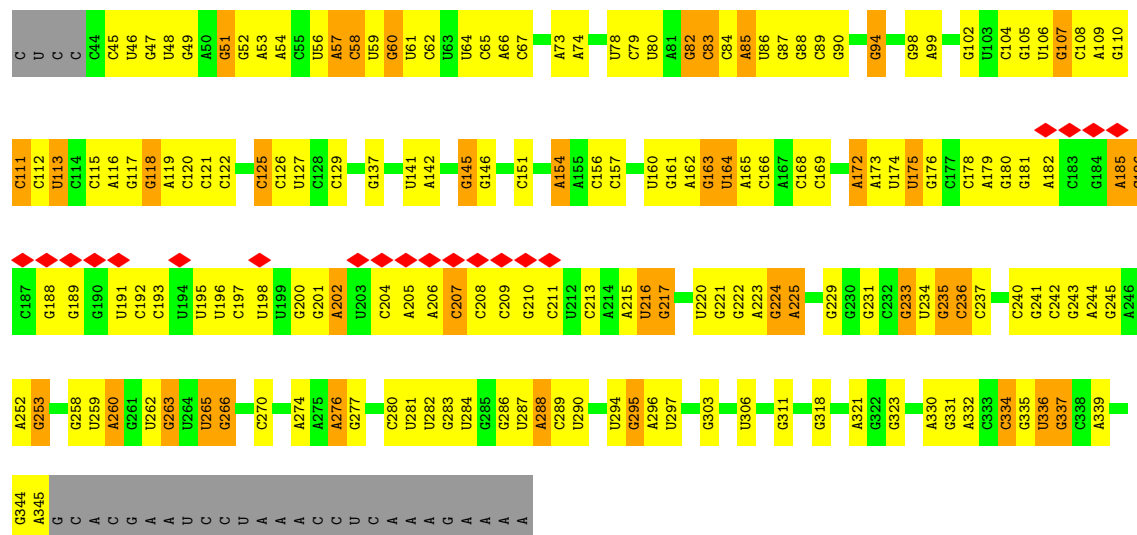
- Molecule 34: 60S ribosomal protein L41

Chain Ln:  88% 8% .

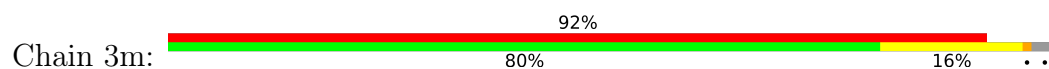


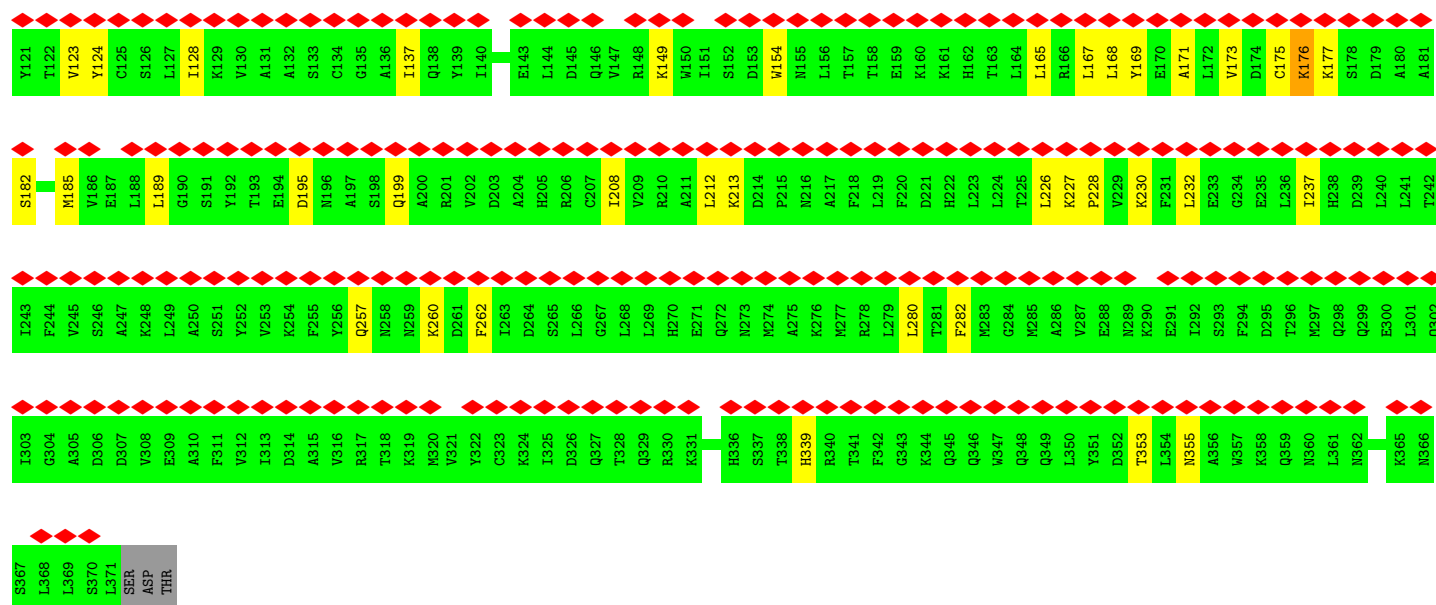


• Molecule 36: HCV-IRES RNA

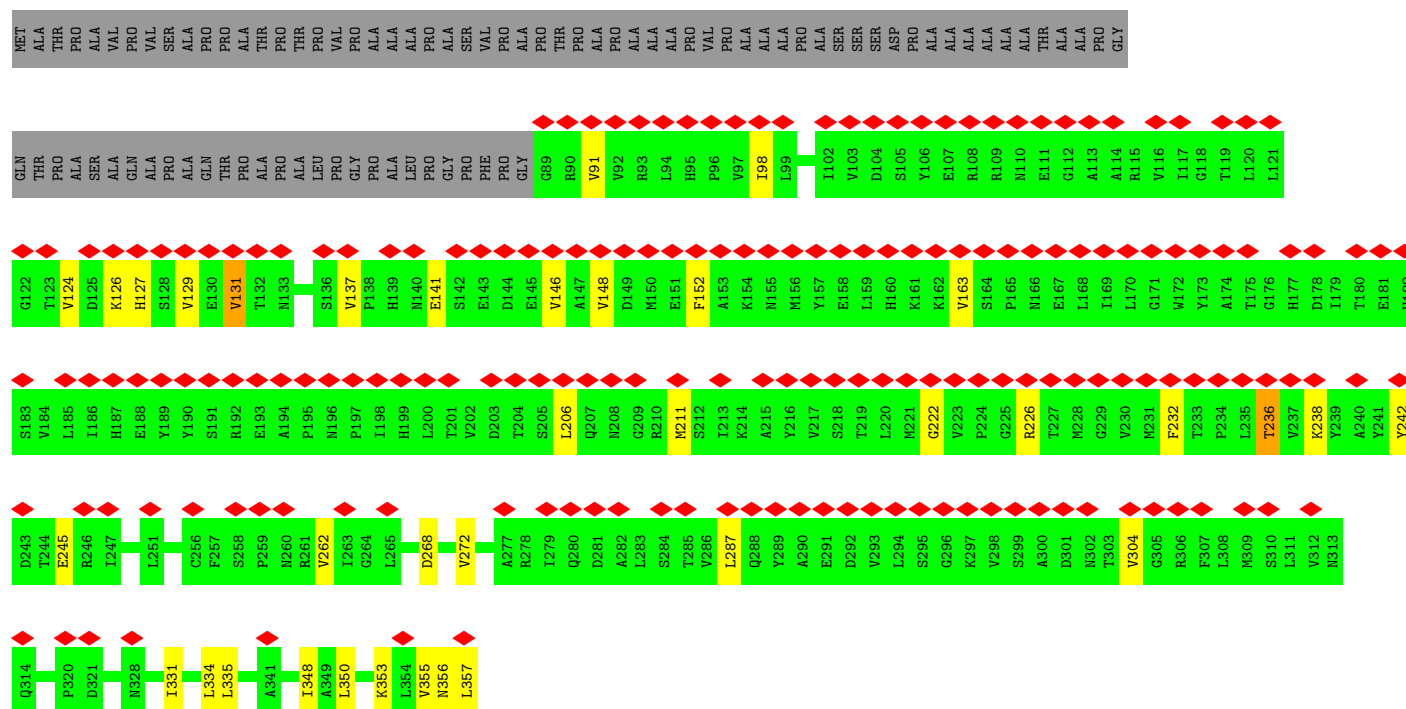


• Molecule 37: Eukaryotic translation initiation factor 3 subunit M

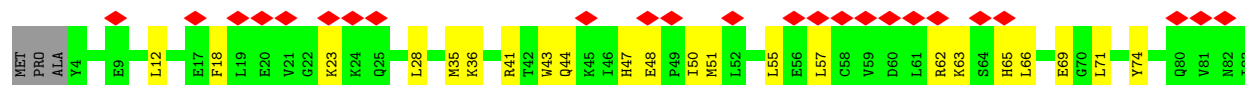
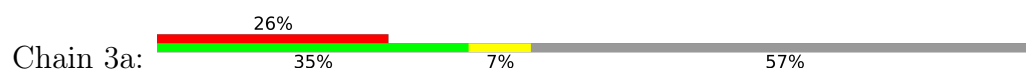




• Molecule 38: Eukaryotic translation initiation factor 3 subunit F



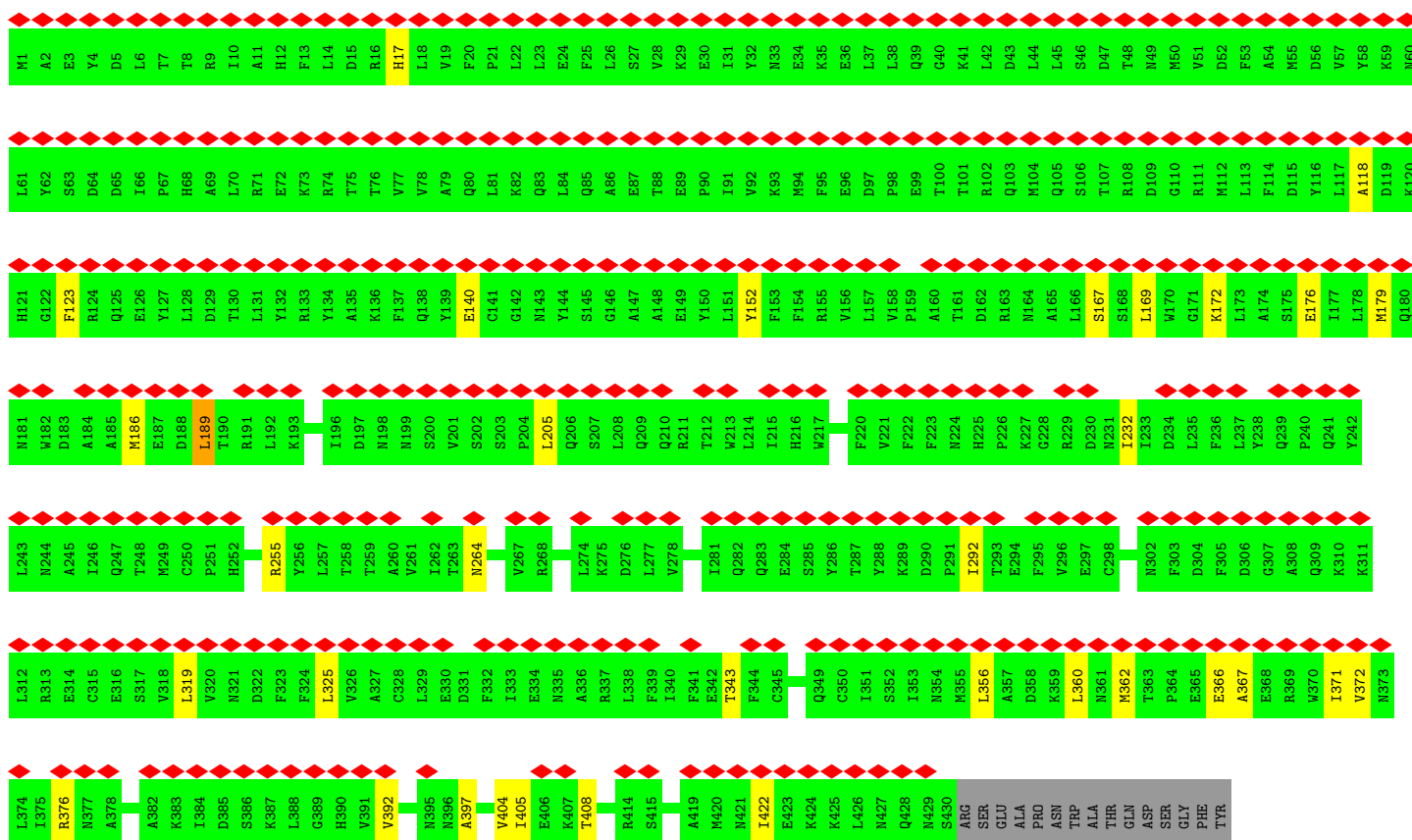
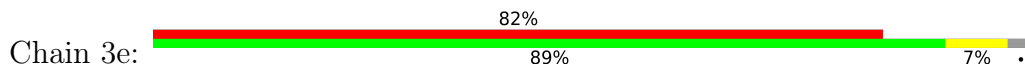
• Molecule 39: Eukaryotic translation initiation factor 3 subunit A





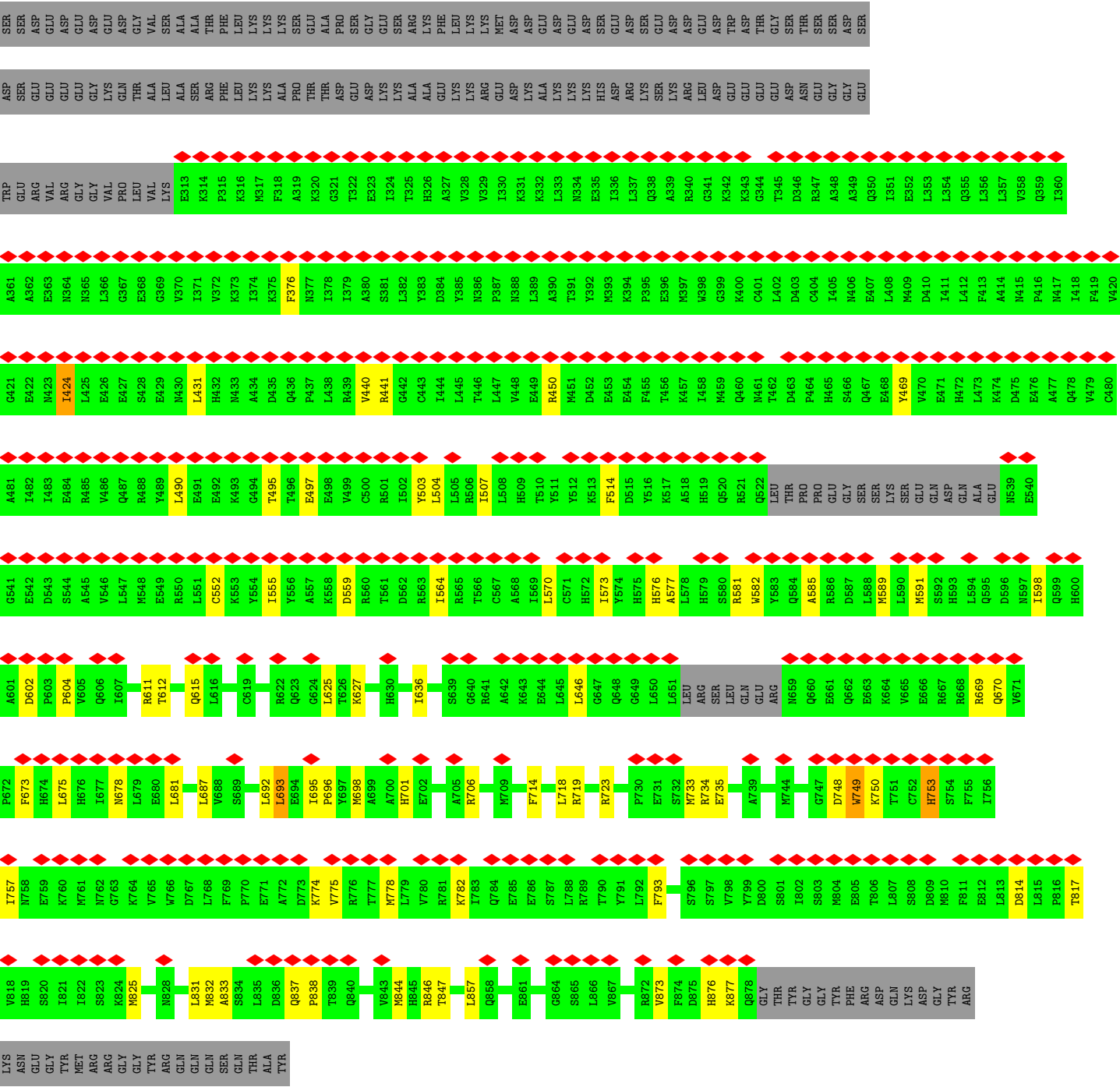
[illegible]

- Molecule 40: Eukaryotic translation initiation factor 3 subunit E

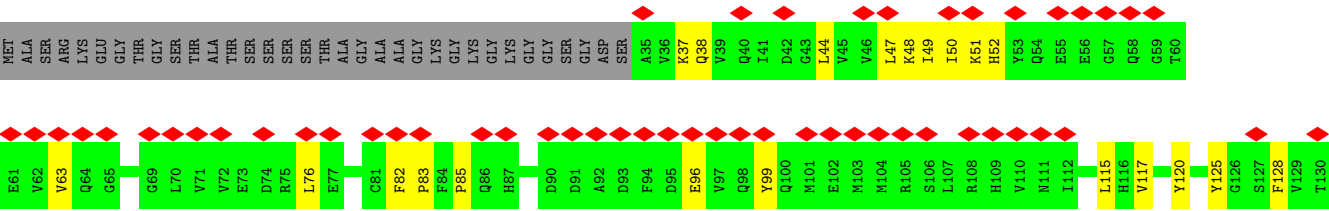


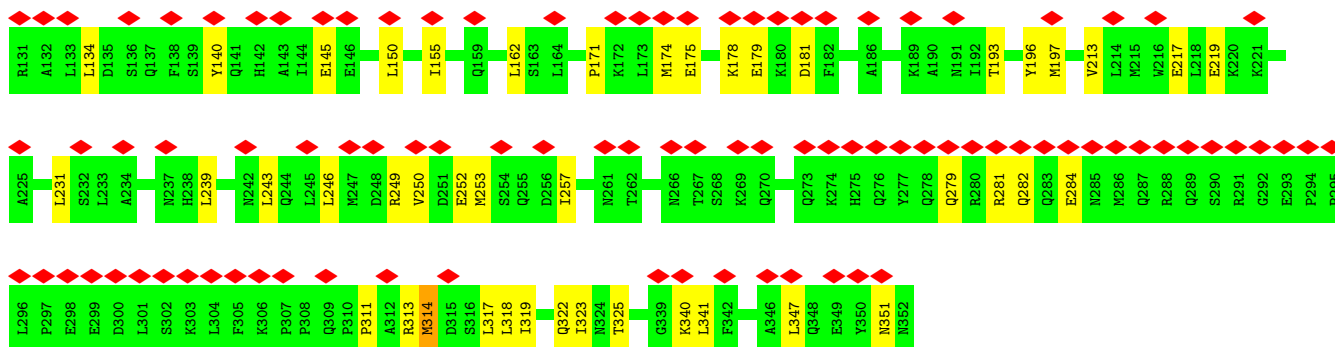
- Molecule 41: Eukaryotic translation initiation factor 3 subunit C

[illegible]

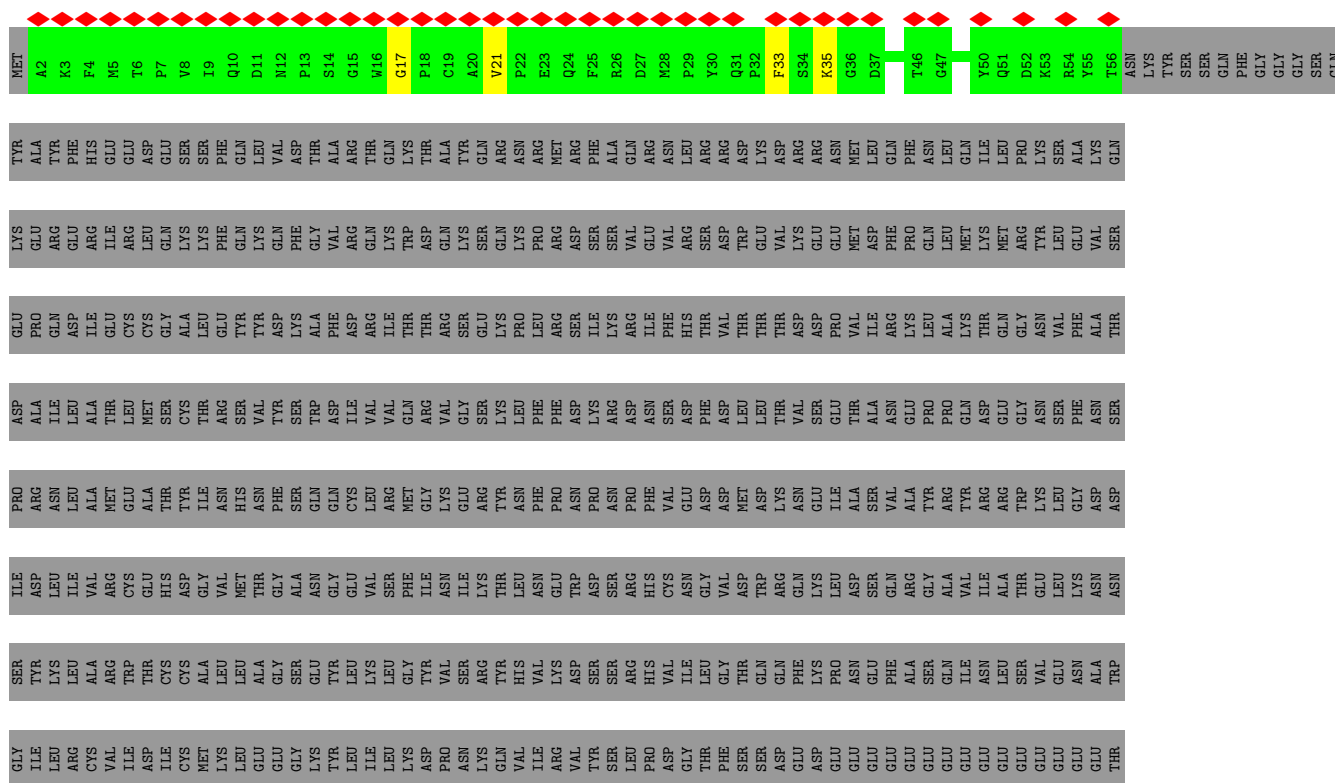


● Molecule 42: Eukaryotic translation initiation factor 3 subunit H

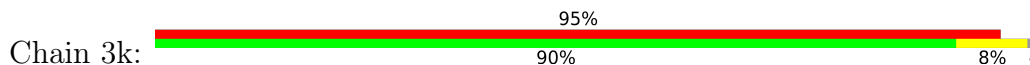


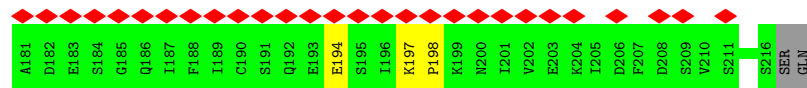


• Molecule 43: Eukaryotic translation initiation factor 3 subunit D

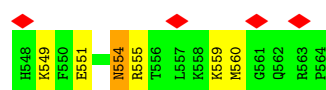
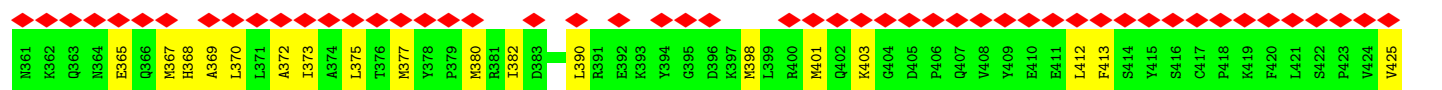
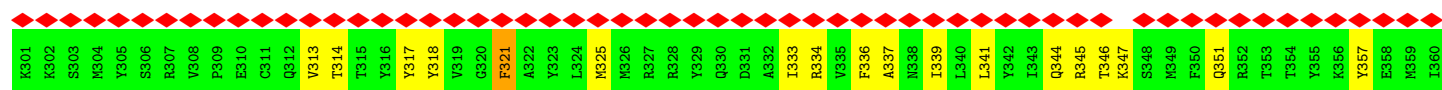
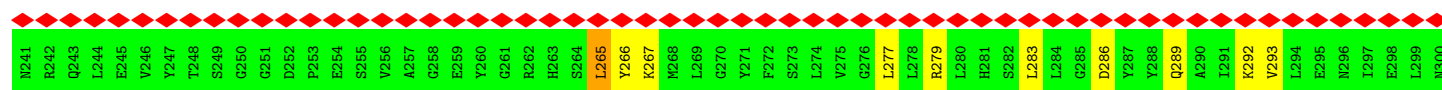
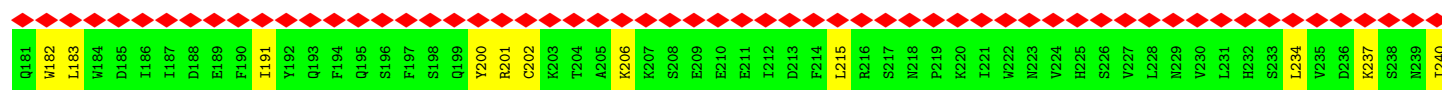
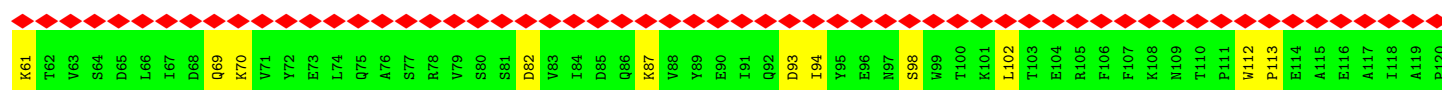
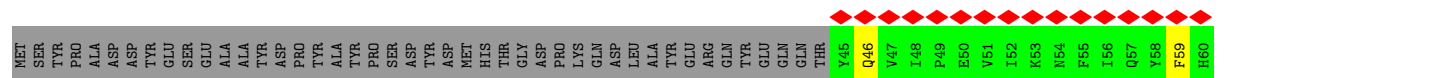
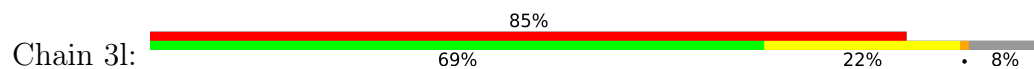


• Molecule 44: Eukaryotic translation initiation factor 3 subunit K





• Molecule 45: Eukaryotic translation initiation factor 3 subunit L



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24675	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	0.096	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (\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 (\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	SA	0.22	0/1742	0.37	0/2367
2	SB	0.21	0/1749	0.43	0/2340
3	SC	0.23	0/1737	0.40	0/2347
4	SD	0.17	0/1784	0.34	0/2402
5	SE	0.23	0/2107	0.43	1/2836 (0.0%)
6	SF	0.23	0/1540	0.50	2/2071 (0.1%)
7	SG	0.17	0/1946	0.34	0/2590
8	SH	0.20	0/1529	0.43	0/2048
9	SI	0.20	0/1711	0.35	0/2282
10	SJ	0.22	0/1524	0.38	0/2035
11	SK	0.19	0/834	0.49	0/1125
12	SL	0.24	0/1241	0.38	0/1662
13	Sf	0.19	0/945	0.53	0/1269
14	SN	0.24	0/1226	0.45	0/1649
15	SO	0.22	0/1020	0.38	0/1368
16	SP	0.19	0/1003	0.49	0/1340
17	SQ	0.23	0/1133	0.51	0/1517
18	SR	0.21	0/1082	0.48	0/1452
19	SS	0.17	0/1202	0.41	0/1610
20	ST	0.18	0/1122	0.37	0/1504
21	SU	0.19	0/813	0.47	0/1092
22	SV	0.22	0/643	0.50	0/860
23	SW	0.25	0/1051	0.36	0/1406
24	SX	0.24	0/1116	0.44	0/1490
25	SY	0.20	0/1031	0.37	0/1370
26	SZ	0.22	0/607	0.52	0/815
27	Sa	0.23	0/817	0.35	0/1095
28	Sb	0.21	0/665	0.41	0/891
29	Sc	0.22	0/490	0.49	0/656
30	Sd	0.22	0/470	0.47	0/623
31	Se	0.21	0/422	0.42	0/555
32	sh	0.18	0/533	0.45	0/706

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sg	0.17	0/2493	0.40	0/3394
34	Ln	0.22	0/231	0.59	0/294
35	S2	0.22	0/42121	0.31	0/65651
36	zz	0.16	0/7199	0.33	0/11223
37	3m	0.12	0/2676	0.36	0/3635
38	3f	0.12	0/2099	0.35	0/2856
39	3a	0.14	0/4583	0.40	0/6237
40	3e	0.12	0/3288	0.33	0/4475
41	3c	0.14	0/3990	0.39	1/5424 (0.0%)
42	3h	0.13	0/2571	0.37	0/3484
43	3d	0.11	0/358	0.30	0/493
44	3k	0.13	0/1502	0.34	0/2052
45	3l	0.13	0/4446	0.35	0/6013
All	All	0.20	0/114392	0.36	4/164604 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	3c	424	ILE	N-CA-C	6.65	113.33	106.21
5	SE	19	MET	CB-CG-SD	-5.60	95.90	112.70
6	SF	78	MET	CA-C-N	5.37	130.47	122.74
6	SF	78	MET	C-N-CA	5.37	130.47	122.74

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	SA	1705	0	1706	23	0
2	SB	1722	0	1794	15	0
3	SC	1700	0	1784	24	0
4	SD	1756	0	1851	20	0
5	SE	2065	0	2169	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	SF	1518	0	1569	13	0
7	SG	1923	0	2089	21	0
8	SH	1506	0	1603	19	0
9	SI	1682	0	1769	16	0
10	SJ	1499	0	1618	7	0
11	SK	810	0	836	15	0
12	SL	1220	0	1289	9	0
13	Sf	935	0	964	18	0
14	SN	1202	0	1289	7	0
15	SO	1007	0	1032	13	0
16	SP	984	0	1033	10	0
17	SQ	1116	0	1185	17	0
18	SR	1068	0	1121	11	0
19	SS	1184	0	1244	14	0
20	ST	1103	0	1133	11	0
21	SU	803	0	873	9	0
22	SV	636	0	637	7	0
23	SW	1034	0	1080	6	0
24	SX	1098	0	1167	12	0
25	SY	1014	0	1082	11	0
26	SZ	601	0	662	9	0
27	Sa	803	0	850	4	0
28	Sb	651	0	672	6	0
29	Sc	488	0	514	9	0
30	Sd	459	0	452	7	0
31	Se	417	0	463	3	0
32	sh	522	0	530	9	0
33	Sg	2436	0	2393	45	0
34	Ln	230	0	276	2	0
35	S2	37669	0	19037	276	0
36	zz	6443	0	3259	82	0
37	3m	2639	0	2442	32	0
38	3f	2063	0	2054	28	0
39	3a	4497	0	4224	64	0
40	3e	3224	0	2925	18	0
41	3c	3924	0	3512	51	0
42	3h	2520	0	2445	46	0
43	3d	347	0	259	2	0
44	3k	1475	0	1239	10	0
45	3l	4335	0	4272	76	0
46	Sa	1	0	0	0	0
46	sh	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	S2	8	0	0	0	0
All	All	108043	0	86397	1035	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1035) 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)
36:zz:61:U:H3	36:zz:107:G:H1	1.12	0.94
36:zz:145:G:H1	36:zz:248:U:H3	1.11	0.93
35:S2:172:U:H3	35:S2:174:C:H41	1.18	0.90
36:zz:52:G:N2	36:zz:111:C:O2	2.06	0.88
41:3c:573:ILE:HD13	41:3c:589:MET:HE3	1.60	0.82
35:S2:197:U:H3	35:S2:202:G:H1	1.36	0.74
24:SX:68:LYS:HB3	24:SX:91:LEU:HD12	1.69	0.73
17:SQ:108:ILE:HA	17:SQ:111:ILE:HD12	1.70	0.73
20:ST:85:ASN:HB2	20:ST:88:MET:HB2	1.69	0.73
33:Sg:87:LEU:HB2	33:Sg:101:PHE:HB2	1.70	0.73
17:SQ:40:GLU:HA	17:SQ:48:GLN:HE22	1.54	0.72
38:3f:206:LEU:HD23	39:3a:554:VAL:HG13	1.71	0.72
35:S2:1286:G:N2	35:S2:1313:A:H62	1.88	0.71
35:S2:669:A:H8	35:S2:1164:G:HO2'	1.39	0.71
33:Sg:109:LEU:HD11	33:Sg:125:ARG:HG3	1.72	0.71
33:Sg:5:MET:HB3	33:Sg:270:LEU:HD21	1.72	0.70
30:Sd:31:ILE:HG21	30:Sd:36:LEU:HD12	1.72	0.70
36:zz:259:U:O2	36:zz:274:A:N7	2.25	0.70
36:zz:193:C:H42	36:zz:202:A:H61	1.39	0.69
39:3a:47:HIS:HA	39:3a:50:ILE:HD12	1.75	0.69
39:3a:186:LEU:HD21	39:3a:239:SER:HA	1.76	0.68
16:SP:118:GLU:HB2	19:SS:120:HIS:H	1.58	0.68
19:SS:36:VAL:HG23	19:SS:40:TYR:HB3	1.75	0.68
37:3m:49:CYS:HA	37:3m:52:CYS:HB3	1.76	0.67
35:S2:1756:C:H2'	35:S2:1757:G:H8	1.58	0.67
35:S2:1824:A:H2'	35:S2:1825:A:H2'	1.76	0.67
19:SS:130:ARG:HD2	19:SS:134:GLN:HE21	1.59	0.66
35:S2:1286:G:N2	35:S2:1313:A:N6	2.43	0.66
13:Sf:93:LYS:HB3	13:Sf:102:LYS:HB2	1.76	0.66
18:SR:106:LEU:HA	18:SR:109:LEU:HB2	1.76	0.66
35:S2:172:U:H3	35:S2:174:C:N4	1.90	0.66
42:3h:253:MET:HE3	42:3h:319:ILE:HG22	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:34:MET:HE2	1:SA:154:LEU:HD21	1.78	0.66
36:zz:252:A:H4'	36:zz:253:G:H5'	1.78	0.65
42:3h:243:LEU:HD12	42:3h:246:LEU:HD21	1.77	0.65
36:zz:59:U:H3	36:zz:109:A:H62	1.44	0.64
4:SD:25:LEU:HD13	4:SD:50:ILE:HD11	1.79	0.64
35:S2:230:A:H62	35:S2:887:U:H3	1.44	0.64
10:SJ:79:ARG:HH22	10:SJ:83:ARG:HD3	1.63	0.64
41:3c:678:ASN:HB3	41:3c:681:LEU:HB3	1.79	0.64
12:SL:4:ILE:HD11	12:SL:55:TYR:HA	1.80	0.63
35:S2:1286:G:H21	35:S2:1313:A:N6	1.96	0.63
35:S2:1417:C:H42	35:S2:1422:G:H22	1.45	0.63
39:3a:385:PRO:HA	39:3a:388:LYS:HB2	1.81	0.63
24:SX:88:ASP:HB3	35:S2:617:G:H4'	1.81	0.63
40:3e:255:ARG:HG3	40:3e:292:ILE:HG21	1.80	0.63
45:3l:202:CYS:HA	45:3l:426:PRO:HG2	1.81	0.63
35:S2:1536:G:H2'	35:S2:1537:A:H8	1.64	0.62
35:S2:239:C:H42	35:S2:278:C:H42	1.48	0.62
35:S2:241:G:H22	35:S2:276:G:H22	1.47	0.62
39:3a:183:LYS:HA	39:3a:186:LEU:HD12	1.82	0.62
2:SB:171:ILE:HD11	2:SB:197:ILE:HG12	1.82	0.62
37:3m:189:LEU:HG	37:3m:228:PRO:HG2	1.82	0.62
33:Sg:251:ALA:HA	33:Sg:256:ILE:HG22	1.81	0.62
37:3m:189:LEU:HD23	37:3m:226:LEU:HD13	1.82	0.61
44:3k:71:LEU:HA	44:3k:74:LEU:HD12	1.82	0.61
24:SX:54:LYS:HD3	24:SX:91:LEU:HD21	1.80	0.61
45:3l:344:GLN:HA	45:3l:347:LYS:HD2	1.82	0.61
15:SO:52:THR:HG21	35:S2:952:G:H21	1.66	0.61
17:SQ:78:VAL:HG22	35:S2:1673:U:H5''	1.83	0.61
42:3h:197:MET:HE3	42:3h:317:LEU:HG	1.82	0.61
35:S2:698:G:H5'	35:S2:733:C:H42	1.64	0.61
45:3l:337:ALA:HB2	45:3l:382:ILE:HD11	1.82	0.61
23:SW:8:ALA:HA	23:SW:74:VAL:HG11	1.82	0.61
17:SQ:27:ARG:HA	17:SQ:66:VAL:HG12	1.82	0.60
36:zz:248:U:H2'	36:zz:249:G:H8	1.66	0.60
6:SF:142:SER:HB2	29:Sc:50:VAL:HG22	1.81	0.60
26:SZ:64:ASN:HA	26:SZ:111:ARG:HD3	1.84	0.60
35:S2:870:A:H4'	35:S2:871:U:H3'	1.82	0.60
41:3c:627:LYS:HE3	41:3c:693:LEU:HB3	1.82	0.60
1:SA:71:PRO:HB3	1:SA:186:ARG:HH22	1.66	0.60
38:3f:242:TYR:H	38:3f:245:GLU:HB2	1.66	0.60
39:3a:526:MET:HG2	42:3h:347:LEU:HD11	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:zz:59:U:H3	36:zz:109:A:N6	2.00	0.60
11:SK:71:LEU:HD12	11:SK:76:ILE:HG12	1.83	0.60
37:3m:46:ILE:HG13	37:3m:89:LYS:HD3	1.84	0.60
13:Sf:117:GLU:HG2	13:Sf:120:ALA:H	1.67	0.59
17:SQ:19:ALA:HB2	17:SQ:75:GLY:HA3	1.83	0.59
3:SC:167:ARG:HB3	3:SC:177:PRO:HB2	1.84	0.59
35:S2:1723:G:H2'	35:S2:1724:A:H8	1.67	0.59
45:3l:191:ILE:HG21	45:3l:279:ARG:HD3	1.83	0.59
36:zz:118:G:H3'	36:zz:119:A:H8	1.68	0.59
38:3f:163:VAL:HG22	42:3h:85:PRO:HG3	1.84	0.59
39:3a:276:TYR:HE2	39:3a:302:LEU:HD12	1.68	0.59
40:3e:176:GLU:HA	40:3e:179:MET:HE2	1.85	0.59
1:SA:184:ARG:HD2	1:SA:191:ARG:HG2	1.83	0.59
36:zz:61:U:O2	36:zz:107:G:N2	2.28	0.58
42:3h:311:PRO:HG2	42:3h:313:ARG:HH12	1.67	0.58
35:S2:844:U:H2'	35:S2:845:G:H8	1.68	0.58
41:3c:775:VAL:HA	41:3c:778:MET:HE2	1.86	0.58
16:SP:52:LYS:HE2	16:SP:80:LEU:HD21	1.85	0.58
9:SI:141:ARG:HB3	9:SI:145:ILE:HB	1.86	0.58
35:S2:1536:G:H2'	35:S2:1537:A:C8	2.39	0.58
37:3m:257:GLN:HA	37:3m:260:LYS:HE3	1.85	0.58
41:3c:495:THR:HG22	41:3c:497:GLU:H	1.67	0.58
41:3c:844:MET:HG2	41:3c:846:ARG:H	1.68	0.57
19:SS:16:LEU:HD23	19:SS:100:ALA:HB2	1.86	0.57
35:S2:546:G:H4'	35:S2:547:G:H5'	1.86	0.57
38:3f:357:LEU:HD11	40:3e:422:ILE:HD11	1.87	0.57
35:S2:1174:U:H2'	35:S2:1175:G:H8	1.68	0.57
44:3k:43:ASP:H	44:3k:72:LYS:HD2	1.69	0.57
35:S2:1183:A:H2'	35:S2:1184:G:H8	1.68	0.57
38:3f:331:ILE:HG13	42:3h:341:LEU:HD13	1.85	0.57
6:SF:59:LYS:HD2	6:SF:62:ARG:HH21	1.69	0.57
13:Sf:85:LEU:HA	13:Sf:88:TRP:HB2	1.85	0.57
42:3h:44:LEU:HD12	42:3h:47:LEU:HD11	1.87	0.57
35:S2:1189:A:H2'	35:S2:1190:A:H8	1.69	0.56
36:zz:98:G:H2'	36:zz:99:A:C8	2.40	0.56
38:3f:206:LEU:HD21	42:3h:213:VAL:HG11	1.85	0.56
21:SU:98:VAL:HA	21:SU:101:ILE:HD12	1.85	0.56
39:3a:195:ARG:HH21	39:3a:245:LEU:HD13	1.69	0.56
15:SO:143:LYS:HG2	35:S2:1047:C:H5''	1.86	0.56
29:Sc:12:ALA:HB1	29:Sc:32:VAL:HB	1.88	0.56
33:Sg:111:VAL:HG12	33:Sg:122:SER:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:851:C:H5'	35:S2:852:G:H5'	1.88	0.56
45:3l:498:LYS:HG2	45:3l:513:PHE:HB3	1.88	0.56
35:S2:1723:G:H2'	35:S2:1724:A:C8	2.40	0.56
28:Sb:67:THR:HG23	28:Sb:69:GLY:H	1.71	0.56
29:Sc:17:VAL:HA	29:Sc:30:VAL:HG12	1.88	0.56
5:SE:107:GLY:HA2	5:SE:189:LEU:HB3	1.88	0.56
45:3l:313:VAL:HA	45:3l:339:ILE:HD11	1.88	0.56
10:SJ:60:LEU:HA	10:SJ:63:LEU:HD12	1.88	0.56
30:Sd:50:ILE:HD12	30:Sd:50:ILE:H	1.70	0.56
31:Se:39:ASN:HA	31:Se:43:VAL:HG12	1.87	0.56
35:S2:1513:C:H2'	35:S2:1514:G:H8	1.71	0.56
37:3m:113:MET:HE1	37:3m:123:VAL:HG21	1.88	0.56
3:SC:70:VAL:HG11	3:SC:93:ILE:HG23	1.88	0.55
35:S2:907:G:H2'	35:S2:908:A:C8	2.40	0.55
40:3e:376:ARG:HG2	45:3l:466:LEU:HD11	1.87	0.55
45:3l:461:ARG:HA	45:3l:464:LEU:HB2	1.88	0.55
4:SD:106:ARG:HG3	4:SD:175:VAL:HG22	1.87	0.55
9:SI:142:SER:H	9:SI:145:ILE:HD12	1.71	0.55
18:SR:100:PRO:HD3	18:SR:119:VAL:HG13	1.87	0.55
11:SK:3:MET:HE1	11:SK:8:ARG:HG2	1.88	0.55
17:SQ:102:GLU:HA	17:SQ:105:LYS:HB3	1.87	0.55
35:S2:736:C:H2'	35:S2:737:G:C8	2.42	0.55
45:3l:454:GLN:HA	45:3l:457:LEU:HD13	1.88	0.55
9:SI:57:ALA:HB2	9:SI:183:GLY:HA2	1.87	0.55
36:zz:336:U:HO2'	36:zz:337:G:H8	1.54	0.55
39:3a:205:LEU:HD21	39:3a:229:HIS:HE2	1.70	0.55
35:S2:649:U:H2'	35:S2:650:A:H8	1.71	0.55
4:SD:15:GLY:HA3	30:Sd:50:ILE:HG23	1.88	0.55
35:S2:186:C:H2'	35:S2:187:G:H8	1.72	0.55
2:SB:62:LEU:HA	2:SB:65:ARG:HE	1.72	0.55
35:S2:1228:A:H2'	35:S2:1229:G:C8	2.42	0.55
36:zz:259:U:C2	36:zz:274:A:N7	2.75	0.55
37:3m:14:GLN:HE21	38:3f:226:ARG:HH21	1.55	0.55
36:zz:51:G:O6	36:zz:113:U:O4	2.24	0.55
15:SO:34:PHE:HB3	15:SO:41:PHE:HB2	1.89	0.55
35:S2:874:G:H2'	35:S2:875:A:H8	1.70	0.55
35:S2:1714:U:H2'	35:S2:1715:A:C8	2.42	0.55
39:3a:48:GLU:HA	39:3a:51:MET:HE1	1.89	0.55
42:3h:281:ARG:HA	42:3h:284:GLU:HB3	1.88	0.55
42:3h:175:GLU:HA	42:3h:178:LYS:HE2	1.89	0.54
45:3l:150:LEU:HA	45:3l:153:ARG:HE	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Sc:46:VAL:HG21	29:Sc:50:VAL:HG21	1.89	0.54
39:3a:341:LEU:HG	41:3c:698:MET:HG3	1.89	0.54
33:Sg:125:ARG:HA	33:Sg:150:TRP:HB3	1.89	0.54
39:3a:353:ARG:HH21	39:3a:354:ARG:HB3	1.72	0.54
45:3l:535:VAL:HG12	45:3l:538:ARG:H	1.72	0.54
4:SD:161:GLY:HA3	35:S2:1388:A:H61	1.71	0.54
35:S2:28:U:H2'	35:S2:29:G:H8	1.73	0.54
35:S2:1677:U:H2'	35:S2:1678:A:H8	1.72	0.54
7:SG:2:LYS:HB3	7:SG:15:LEU:HD11	1.89	0.54
23:SW:3:ARG:HD3	23:SW:6:VAL:HG23	1.89	0.54
35:S2:1756:C:H2'	35:S2:1757:G:C8	2.42	0.54
35:S2:746:C:H1'	35:S2:747:U:H5	1.71	0.54
35:S2:960:U:H1'	35:S2:963:A:H62	1.73	0.54
35:S2:792:C:H2'	35:S2:793:G:C8	2.43	0.54
35:S2:1228:A:H2'	35:S2:1229:G:H8	1.72	0.54
41:3c:573:ILE:HG13	41:3c:585:ALA:HB1	1.90	0.54
44:3k:146:VAL:HA	44:3k:149:THR:HG22	1.90	0.54
13:Sf:56:CYS:HB2	13:Sf:61:TYR:HD2	1.73	0.53
36:zz:240:C:H2'	36:zz:241:G:C8	2.44	0.53
16:SP:51:ARG:HH21	16:SP:55:SER:HB2	1.74	0.53
33:Sg:127:LYS:HG2	33:Sg:149:GLU:HA	1.90	0.53
39:3a:307:ARG:HH22	39:3a:315:MET:HE2	1.73	0.53
41:3c:833:ALA:HA	41:3c:844:MET:HA	1.90	0.53
42:3h:120:TYR:HB2	42:3h:150:LEU:HD22	1.90	0.53
45:3l:179:PRO:HD2	45:3l:182:TRP:HE3	1.73	0.53
38:3f:98:ILE:HD12	38:3f:131:VAL:HG13	1.89	0.53
13:Sf:22:LEU:HD21	13:Sf:89:VAL:HA	1.90	0.53
17:SQ:31:LEU:HB3	17:SQ:67:ASP:HB2	1.91	0.53
35:S2:1232:U:H2'	35:S2:1233:G:H8	1.73	0.53
36:zz:175:U:H3'	36:zz:176:G:H8	1.74	0.53
38:3f:304:VAL:HG22	39:3a:536:VAL:HG12	1.91	0.53
39:3a:93:TYR:HA	39:3a:96:MET:HE2	1.91	0.53
44:3k:161:MET:HE3	44:3k:162:LEU:HB3	1.90	0.53
15:SO:31:CYS:HB2	15:SO:44:VAL:HG22	1.91	0.53
15:SO:147:ARG:HB2	15:SO:150:ARG:HH11	1.74	0.53
38:3f:124:VAL:HG23	38:3f:129:VAL:HG23	1.91	0.53
2:SB:136:ARG:HB2	2:SB:218:LEU:HD21	1.91	0.53
6:SF:50:PRO:HB3	6:SF:69:VAL:HG23	1.90	0.53
12:SL:139:ARG:HD3	35:S2:352:U:H5''	1.91	0.53
18:SR:8:THR:HG21	35:S2:1387:G:H21	1.73	0.53
20:ST:14:PHE:HE1	20:ST:135:ALA:HB2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:1545:A:H2'	35:S2:1546:G:C8	2.44	0.53
3:SC:114:LYS:HE3	35:S2:1358:U:H5'	1.89	0.53
5:SE:192:ILE:HB	5:SE:243:GLY:HA3	1.91	0.53
36:zz:73:A:H2'	36:zz:74:A:H8	1.73	0.53
35:S2:1628:C:H2'	35:S2:1629:C:H6	1.74	0.53
1:SA:25:LEU:HD12	1:SA:46:ILE:HG21	1.91	0.52
11:SK:80:ARG:HH12	11:SK:89:ILE:HG23	1.74	0.52
33:Sg:87:LEU:HD21	33:Sg:111:VAL:HG11	1.90	0.52
19:SS:138:THR:HA	19:SS:141:ARG:HH21	1.73	0.52
35:S2:5:U:H2'	35:S2:6:G:H8	1.73	0.52
39:3a:296:LEU:HA	39:3a:299:LEU:HD13	1.92	0.52
44:3k:198:PRO:HB3	45:3l:533:THR:HG23	1.91	0.52
36:zz:125:C:H2'	36:zz:126:C:C6	2.44	0.52
39:3a:12:LEU:HD21	39:3a:50:ILE:HA	1.90	0.52
29:Sc:66:ARG:HB2	36:zz:334:C:H41	1.75	0.52
35:S2:1813:A:H3'	35:S2:1814:G:H8	1.74	0.52
37:3m:165:LEU:HA	37:3m:168:LEU:HD12	1.91	0.52
5:SE:72:ILE:HG12	5:SE:90:ILE:HD13	1.91	0.52
41:3c:636:ILE:HD11	41:3c:646:LEU:HD21	1.91	0.52
42:3h:134:LEU:HD22	42:3h:318:LEU:HD11	1.91	0.52
7:SG:22:ARG:HA	7:SG:25:ARG:HE	1.74	0.52
36:zz:65:C:H2'	36:zz:66:A:H8	1.74	0.52
35:S2:388:U:H2'	35:S2:389:A:H8	1.75	0.52
35:S2:1288:U:H3	35:S2:1311:C:H42	1.56	0.52
35:S2:1842:C:H2'	35:S2:1843:G:H8	1.74	0.52
36:zz:65:C:H2'	36:zz:66:A:C8	2.45	0.52
45:3l:201:ARG:HD3	45:3l:425:VAL:HA	1.92	0.52
1:SA:18:PHE:CZ	1:SA:177:MET:HE1	2.45	0.52
8:SH:160:LYS:HE2	8:SH:189:PHE:HB3	1.92	0.52
20:ST:4:VAL:HG11	20:ST:136:GLY:HA2	1.91	0.52
35:S2:595:U:H2'	35:S2:596:U:C6	2.45	0.52
12:SL:33:LEU:HD23	12:SL:34:PRO:HD2	1.91	0.52
33:Sg:101:PHE:HE1	33:Sg:136:GLY:HA2	1.75	0.52
35:S2:1776:G:H2'	35:S2:1777:G:H4'	1.91	0.52
42:3h:44:LEU:HG	42:3h:48:LYS:HE3	1.91	0.52
3:SC:209:VAL:HG21	3:SC:233:LEU:HD21	1.91	0.52
22:SV:14:PRO:HG2	22:SV:23:ILE:HD11	1.92	0.52
35:S2:1101:U:H2'	35:S2:1102:G:C8	2.45	0.52
40:3e:397:ALA:HB1	41:3c:847:THR:HG21	1.92	0.52
41:3c:687:LEU:HD12	41:3c:733:MET:HE1	1.92	0.52
7:SG:31:ARG:HH12	35:S2:1745:A:H4'	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:791:C:H2'	35:S2:792:C:C6	2.45	0.51
36:zz:185:A:H1'	36:zz:186:C:H5	1.75	0.51
36:zz:206:A:H1'	36:zz:207:C:H5'	1.92	0.51
38:3f:335:LEU:HD12	45:3l:544:ILE:HD11	1.93	0.51
35:S2:885:U:H3	35:S2:901:G:H22	1.59	0.51
39:3a:223:PRO:HA	39:3a:226:GLN:HB2	1.91	0.51
3:SC:102:LEU:HD12	3:SC:130:ILE:HG12	1.91	0.51
16:SP:96:VAL:HG11	16:SP:116:LEU:HB3	1.91	0.51
33:Sg:89:LEU:HD13	33:Sg:99:ARG:HB3	1.93	0.51
35:S2:146:G:H1	35:S2:173:A:H61	1.58	0.51
35:S2:587:A:H5'	35:S2:592:C:H41	1.74	0.51
1:SA:7:VAL:HG13	1:SA:8:LEU:HD12	1.91	0.51
35:S2:898:U:H2'	35:S2:899:U:H6	1.75	0.51
35:S2:1098:C:H2'	35:S2:1099:G:C8	2.45	0.51
24:SX:101:LEU:HB3	24:SX:124:LYS:HB2	1.92	0.51
45:3l:469:THR:HA	45:3l:527:MET:HE1	1.92	0.51
35:S2:981:A:H2'	35:S2:982:G:C8	2.45	0.51
35:S2:746:C:H4'	35:S2:747:U:H5'	1.92	0.51
35:S2:1531:A:H2'	35:S2:1532:C:C6	2.45	0.51
32:sh:121:CYS:HB3	32:sh:130:VAL:HG23	1.92	0.51
35:S2:1317:C:H2'	35:S2:1318:G:H8	1.76	0.51
35:S2:1844:U:H2'	35:S2:1845:A:C8	2.46	0.51
36:zz:141:U:H2'	36:zz:142:A:H8	1.75	0.51
39:3a:462:VAL:HG21	39:3a:467:LEU:HD13	1.92	0.51
45:3l:279:ARG:HG3	45:3l:318:TYR:CZ	2.45	0.51
15:SO:44:VAL:HG12	15:SO:53:ILE:HB	1.93	0.51
22:SV:81:LYS:N	22:SV:81:LYS:HE2	2.26	0.51
35:S2:866:U:H2'	35:S2:867:G:C8	2.46	0.51
35:S2:877:C:H2'	35:S2:878:G:C8	2.45	0.51
37:3m:355:ASN:HA	38:3f:287:LEU:HD11	1.92	0.51
38:3f:357:LEU:HD22	41:3c:877:LYS:HD2	1.92	0.51
23:SW:34:ILE:O	23:SW:38:LEU:HD12	2.11	0.51
36:zz:220:U:H2'	36:zz:221:G:C8	2.46	0.51
37:3m:57:ASP:HA	37:3m:101:LEU:HD11	1.91	0.51
45:3l:546:GLN:HA	45:3l:549:LYS:HE2	1.93	0.51
35:S2:388:U:H2'	35:S2:389:A:C8	2.45	0.50
35:S2:1588:A:H2'	35:S2:1589:A:C8	2.45	0.50
36:zz:259:U:N3	36:zz:274:A:C8	2.73	0.50
36:zz:262:U:H2'	36:zz:263:G:C8	2.46	0.50
39:3a:55:LEU:HD13	39:3a:93:TYR:HB2	1.93	0.50
1:SA:119:PRO:HG2	1:SA:142:LEU:HD21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:SR:28:PHE:HA	18:SR:55:THR:HG21	1.93	0.50
35:S2:959:G:H2'	35:S2:960:U:C6	2.46	0.50
35:S2:1420:G:H21	35:S2:1421:A:H1'	1.76	0.50
35:S2:1764:G:O6	35:S2:1768:A:N7	2.44	0.50
45:3l:177:GLU:HA	45:3l:265:LEU:HG	1.93	0.50
45:3l:351:GLN:HA	45:3l:357:TYR:HB2	1.93	0.50
1:SA:77:ILE:HG13	1:SA:99:ILE:HB	1.93	0.50
8:SH:61:ILE:HG23	8:SH:93:VAL:HG23	1.94	0.50
33:Sg:125:ARG:HG2	33:Sg:150:TRP:CG	2.47	0.50
33:Sg:238:ALA:H	33:Sg:251:ALA:HB3	1.75	0.50
35:S2:538:U:H2'	35:S2:539:C:O4'	2.12	0.50
36:zz:185:A:H1'	36:zz:186:C:C5	2.47	0.50
17:SQ:74:GLY:HA2	35:S2:1545:A:H4'	1.92	0.50
37:3m:137:ILE:HD11	37:3m:175:CYS:HB2	1.93	0.50
45:3l:318:TYR:HA	45:3l:321:PHE:HB2	1.93	0.50
45:3l:551:GLU:HB3	45:3l:555:ARG:HH21	1.77	0.50
13:Sf:66:GLU:HG3	13:Sf:76:LEU:HD13	1.92	0.50
24:SX:90:CYS:HA	24:SX:93:PHE:HD2	1.76	0.50
36:zz:164:U:H1'	36:zz:165:A:C5	2.46	0.50
37:3m:68:VAL:HG13	37:3m:109:LEU:HG	1.93	0.50
42:3h:231:LEU:HA	42:3h:340:LYS:HD2	1.92	0.50
45:3l:70:LYS:HD3	45:3l:177:GLU:HG3	1.93	0.50
4:SD:55:THR:HA	4:SD:58:VAL:HG22	1.92	0.50
33:Sg:269:GLU:HG2	33:Sg:271:LYS:NZ	2.27	0.50
33:Sg:313:THR:HG22	33:Sg:314:ILE:HD12	1.94	0.50
40:3e:118:ALA:HA	40:3e:123:PHE:H	1.76	0.50
45:3l:345:ARG:HG3	45:3l:346:THR:HG23	1.92	0.50
3:SC:88:ILE:HD11	3:SC:93:ILE:HB	1.94	0.50
3:SC:191:VAL:HG11	3:SC:236:PHE:HA	1.94	0.50
3:SC:204:ILE:HD13	3:SC:215:MET:HG2	1.93	0.50
35:S2:201:C:H3'	35:S2:202:G:H8	1.77	0.50
39:3a:342:LEU:HD21	41:3c:719:ARG:HA	1.92	0.50
39:3a:400:PRO:HB3	39:3a:442:GLN:HB3	1.94	0.50
41:3c:831:LEU:O	41:3c:832:MET:HE3	2.12	0.50
38:3f:350:LEU:HA	38:3f:353:LYS:HE3	1.94	0.49
26:SZ:39:LYS:HG2	36:zz:94:G:H5''	1.94	0.49
30:Sd:22:ARG:HH21	30:Sd:37:ASN:HB2	1.77	0.49
33:Sg:230:LEU:HD21	33:Sg:259:TRP:CG	2.47	0.49
39:3a:253:VAL:HG12	39:3a:358:LEU:HD22	1.94	0.49
39:3a:307:ARG:HG2	39:3a:309:ASN:H	1.76	0.49
45:3l:317:TYR:HD1	45:3l:367:MET:HE1	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:32:PHE:CD2	35:S2:1097:G:H4'	2.48	0.49
22:SV:68:SER:O	22:SV:72:LEU:HD12	2.12	0.49
35:S2:1714:U:H2'	35:S2:1715:A:H8	1.77	0.49
36:zz:259:U:H2'	36:zz:260:A:H8	1.76	0.49
38:3f:348:ILE:HG21	42:3h:323:ILE:HG21	1.93	0.49
1:SA:30:LEU:HB2	1:SA:47:TYR:CE2	2.48	0.49
13:Sf:58:GLU:HG3	13:Sf:60:MET:H	1.77	0.49
32:sh:108:VAL:HB	32:sh:114:ILE:HG12	1.94	0.49
35:S2:669:A:H3'	35:S2:670:A:C8	2.47	0.49
25:SY:110:ARG:HG2	25:SY:114:MET:HE3	1.95	0.49
35:S2:527:C:H2'	35:S2:528:A:H8	1.77	0.49
39:3a:43:TRP:HE1	39:3a:74:TYR:HE2	1.61	0.49
45:3l:279:ARG:HH11	45:3l:283:LEU:HD11	1.78	0.49
45:3l:333:ILE:HG12	45:3l:380:MET:HG2	1.95	0.49
15:SO:136:PRO:HB2	15:SO:139:SER:HB3	1.93	0.49
35:S2:935:G:H2'	35:S2:936:G:H8	1.78	0.49
38:3f:137:VAL:HG13	38:3f:152:PHE:CD1	2.48	0.49
39:3a:175:HIS:CE1	39:3a:229:HIS:HA	2.48	0.49
8:SH:70:LYS:HA	8:SH:73:GLN:HB2	1.95	0.49
13:Sf:32:ALA:HB3	13:Sf:110:VAL:HB	1.95	0.49
35:S2:857:U:H2'	35:S2:858:A:C8	2.48	0.49
37:3m:71:LEU:HD22	37:3m:83:ILE:HG12	1.95	0.49
38:3f:211:MET:HB2	42:3h:217:GLU:HG3	1.95	0.49
42:3h:37:LYS:HD2	42:3h:38:GLN:HB3	1.94	0.49
42:3h:179:GLU:HG3	42:3h:181:ASP:H	1.78	0.49
42:3h:197:MET:HE1	42:3h:318:LEU:HA	1.94	0.49
44:3k:139:ARG:HH21	44:3k:173:TRP:HE1	1.60	0.49
5:SE:146:THR:HG21	35:S2:122:G:H21	1.78	0.49
18:SR:100:PRO:HA	18:SR:103:LYS:HB3	1.95	0.49
20:ST:104:LEU:HD23	20:ST:121:ARG:HH11	1.78	0.49
27:Sa:7:ASN:OD1	35:S2:1865:C:H1'	2.13	0.49
35:S2:508:A:H3'	35:S2:509:G:H8	1.78	0.49
35:S2:1562:C:H2'	35:S2:1563:G:H8	1.78	0.49
36:zz:180:G:H2'	36:zz:181:G:C8	2.48	0.49
21:SU:26:SER:HB2	21:SU:110:VAL:HA	1.95	0.48
33:Sg:228:TYR:HD2	33:Sg:264:LYS:HG2	1.78	0.48
35:S2:116:U:H3	35:S2:347:G:H1	1.60	0.48
36:zz:179:A:H2'	36:zz:180:G:C8	2.48	0.48
2:SB:168:MET:HG2	2:SB:197:ILE:HD13	1.95	0.48
36:zz:59:U:H2'	36:zz:60:G:C8	2.48	0.48
36:zz:154:A:H61	36:zz:173:A:H1'	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Sf:89:VAL:HG13	13:Sf:91:LEU:H	1.78	0.48
33:Sg:163:PRO:HB2	33:Sg:179:LEU:HB2	1.95	0.48
36:zz:163:G:H1'	36:zz:164:U:C5	2.49	0.48
42:3h:76:LEU:HD11	42:3h:117:VAL:HG11	1.95	0.48
3:SC:246:LYS:HE3	3:SC:246:LYS:HB2	1.72	0.48
7:SG:52:ILE:HD12	7:SG:52:ILE:H	1.77	0.48
8:SH:100:ILE:HG12	8:SH:125:VAL:HG21	1.94	0.48
35:S2:1413:G:H2'	35:S2:1414:A:H8	1.78	0.48
35:S2:1751:C:H3'	35:S2:1752:C:H4'	1.95	0.48
35:S2:863:U:H2'	35:S2:864:A:H8	1.79	0.48
36:zz:172:A:H2'	36:zz:173:A:C8	2.48	0.48
37:3m:46:ILE:HD11	37:3m:86:LEU:HD12	1.95	0.48
41:3c:814:ASP:HB3	41:3c:817:THR:HG23	1.95	0.48
2:SB:164:ILE:HG22	2:SB:168:MET:HE3	1.96	0.48
44:3k:125:MET:HE3	44:3k:125:MET:O	2.14	0.48
2:SB:87:ILE:HG22	2:SB:101:HIS:HB2	1.95	0.48
3:SC:65:LYS:HD2	3:SC:273:LEU:HD21	1.96	0.48
7:SG:175:LYS:HB2	35:S2:78:C:H1'	1.94	0.48
8:SH:145:ARG:HE	23:SW:51:GLU:CD	2.22	0.48
24:SX:60:LYS:HE3	24:SX:116:PRO:HB3	1.96	0.48
33:Sg:24:THR:HG23	33:Sg:27:PHE:H	1.79	0.48
35:S2:12:U:H2'	35:S2:13:C:C6	2.49	0.48
36:zz:205:A:H2'	36:zz:206:A:C8	2.48	0.48
38:3f:206:LEU:HD22	39:3a:557:TYR:HD2	1.79	0.48
21:SU:56:MET:HE3	21:SU:56:MET:HA	1.95	0.48
23:SW:6:VAL:HG13	23:SW:34:ILE:HD11	1.95	0.48
36:zz:87:G:H2'	36:zz:88:G:H8	1.79	0.48
36:zz:118:G:H3'	36:zz:119:A:C8	2.48	0.48
6:SF:40:ALA:HB3	6:SF:67:PRO:HA	1.96	0.48
36:zz:89:C:H2'	36:zz:90:G:H8	1.78	0.48
36:zz:259:U:H2'	36:zz:260:A:C8	2.48	0.48
37:3m:227:LYS:HB2	37:3m:227:LYS:HE2	1.63	0.48
8:SH:38:ALA:HA	8:SH:41:ARG:HH12	1.79	0.47
35:S2:5:U:H2'	35:S2:6:G:C8	2.49	0.47
35:S2:793:G:H2'	35:S2:794:A:O4'	2.14	0.47
35:S2:963:A:H2'	35:S2:964:A:C8	2.49	0.47
36:zz:215:A:H5''	36:zz:216:U:H5''	1.96	0.47
4:SD:10:LYS:HE3	4:SD:10:LYS:HB2	1.71	0.47
4:SD:117:ARG:HD3	4:SD:117:ARG:HA	1.65	0.47
7:SG:5:ILE:HD12	7:SG:111:LEU:HB2	1.96	0.47
23:SW:30:CYS:HB2	23:SW:61:ILE:HG13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24: SX:18: ARG: HD3	35: S2:359: U: OP2	2.14	0.47
4: SD:108: LYS: HA	4: SD:108: LYS: HD3	1.75	0.47
35: S2:647: U: H2'	35: S2:648: A: H8	1.79	0.47
35: S2:804: U: H2'	35: S2:805: U: C6	2.48	0.47
37: 3m:137: ILE: HG21	37: 3m:171: ALA: HB1	1.96	0.47
42: 3h:52: HIS: ND1	42: 3h:63: VAL: HB	2.29	0.47
6: SF:134: VAL: HG21	36: zz:87: G: H4'	1.95	0.47
35: S2:191: A: H62	35: S2:208: G: H21	1.61	0.47
35: S2:1286: G: C2	35: S2:1313: A: N6	2.82	0.47
36: zz:179: A: H2'	36: zz:180: G: H8	1.79	0.47
39: 3a:408: THR: HA	39: 3a:411: LEU: HB2	1.96	0.47
8: SH:43: LEU: HB3	8: SH:72: PHE: HE1	1.79	0.47
35: S2:171: A: H3'	35: S2:172: U: C6	2.50	0.47
35: S2:756: C: H2'	35: S2:757: C: H6	1.78	0.47
41: 3c:698: MET: HA	41: 3c:701: HIS: CE1	2.49	0.47
7: SG:52: ILE: HA	7: SG:111: LEU: HD23	1.96	0.47
9: SI:64: ASN: HA	9: SI:75: LYS: HA	1.97	0.47
17: SQ:39: LEU: HD12	17: SQ:39: LEU: H	1.80	0.47
19: SS:132: ARG: HD3	35: S2:1623[A]: A: N6	2.29	0.47
25: SY:87: PRO: HG2	25: SY:90: ARG: HB2	1.97	0.47
33: Sg:252: THR: HG22	33: Sg:254: PRO: HD2	1.95	0.47
35: S2:1144: A: H2'	35: S2:1145: A: C8	2.50	0.47
42: 3h:249: ARG: NE	42: 3h:322: GLN: HB3	2.30	0.47
44: 3k:139: ARG: HD2	44: 3k:162: LEU: HD12	1.97	0.47
45: 3l:168: LEU: HD23	45: 3l:237: LYS: HD2	1.97	0.47
4: SD:142: LEU: HD11	4: SD:148: LYS: HB2	1.96	0.47
5: SE:3: ARG: HG2	35: S2:447: A: H4'	1.97	0.47
16: SP:62: LYS: HA	16: SP:62: LYS: HD3	1.73	0.47
19: SS:130: ARG: HB3	19: SS:134: GLN: HE21	1.80	0.47
33: Sg:291: TRP: CD2	33: Sg:298: LEU: HD23	2.49	0.47
35: S2:1758: G: H2'	35: S2:1759: G: H8	1.80	0.47
38: 3f:137: VAL: HG13	38: 3f:152: PHE: HD1	1.79	0.47
40: 3e:152: TYR: HB2	40: 3e:172: LYS: HE3	1.97	0.47
6: SF:91: ARG: HD2	26: SZ:103: HIS: CE1	2.50	0.47
35: S2:695: C: H5''	35: S2:696: G: C8	2.50	0.47
35: S2:928: G: H2'	35: S2:929: G: C8	2.50	0.47
15: SO:97: LEU: HD13	27: Sa:44: ILE: HD11	1.97	0.47
32: sh:99: LYS: HD2	32: sh:99: LYS: HA	1.75	0.47
36: zz:181: G: H2'	36: zz:182: A: C8	2.50	0.47
39: 3a:239: SER: O	39: 3a:243: MET: HG2	2.14	0.47
41: 3c:469: TYR: HE2	41: 3c:673: PHE: HB3	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3c:714:PHE:CE2	41:3c:718:LEU:HD21	2.50	0.47
8:SH:160:LYS:HD3	8:SH:160:LYS:HA	1.71	0.46
35:S2:525:A:H2'	35:S2:526:A:H8	1.79	0.46
35:S2:669:A:H8	35:S2:1164:G:O2'	1.97	0.46
45:3l:398:MET:HA	45:3l:401:MET:HE3	1.96	0.46
35:S2:958:G:H2'	35:S2:959:G:C8	2.51	0.46
35:S2:1769:C:H2'	35:S2:1770:G:C8	2.50	0.46
38:3f:272:VAL:HG13	42:3h:340:LYS:HE3	1.97	0.46
1:SA:39:TYR:CE1	1:SA:40:LYS:HG2	2.51	0.46
5:SE:29:PRO:HG2	5:SE:46:ILE:HD11	1.98	0.46
15:SO:97:LEU:HD11	15:SO:112:ALA:HB1	1.98	0.46
35:S2:1101:U:H2'	35:S2:1102:G:H8	1.80	0.46
35:S2:1232:U:H2'	35:S2:1233:G:C8	2.51	0.46
39:3a:44:GLN:NE2	39:3a:47:HIS:HE1	2.13	0.46
42:3h:171:PRO:HA	42:3h:174:MET:HG2	1.96	0.46
21:SU:24:LEU:HB3	21:SU:32:LEU:HD11	1.96	0.46
35:S2:223:C:H2'	35:S2:224:A:C8	2.50	0.46
35:S2:1189:A:H2'	35:S2:1190:A:C8	2.49	0.46
35:S2:1413:G:H2'	35:S2:1414:A:C8	2.51	0.46
35:S2:1716:C:H2'	35:S2:1717:C:H6	1.80	0.46
35:S2:1845:A:H2'	35:S2:1846:G:C8	2.51	0.46
38:3f:141:GLU:HA	38:3f:146:VAL:HG23	1.98	0.46
42:3h:193:THR:H	42:3h:196:TYR:HD2	1.61	0.46
45:3l:375:LEU:HD13	45:3l:380:MET:HE3	1.97	0.46
35:S2:349:A:H2'	35:S2:350:C:C6	2.50	0.46
9:SI:26:LYS:HD2	9:SI:29:LEU:HD23	1.97	0.46
12:SL:99:TYR:CE1	24:SX:13:LEU:HB3	2.51	0.46
33:Sg:32:LEU:HD11	33:Sg:92:LEU:HD21	1.97	0.46
35:S2:1405:A:H2'	35:S2:1406:G:O4'	2.15	0.46
36:zz:262:U:H2'	36:zz:263:G:H8	1.80	0.46
39:3a:347:ILE:HD11	41:3c:723:ARG:HA	1.98	0.46
13:Sf:23:LYS:HD3	13:Sf:23:LYS:HA	1.74	0.46
21:SU:39:LEU:HD12	21:SU:101:ILE:HG22	1.97	0.46
33:Sg:5:MET:HE1	33:Sg:312:VAL:HG22	1.98	0.46
35:S2:825:A:H2'	35:S2:826:A:C8	2.51	0.46
42:3h:279:GLN:HA	42:3h:282:GLN:HG3	1.96	0.46
45:3l:314:THR:HG23	45:3l:318:TYR:HE2	1.81	0.46
45:3l:372:ALA:HA	45:3l:390:LEU:HD21	1.98	0.46
45:3l:559:LYS:HG3	45:3l:560:MET:HE2	1.97	0.46
13:Sf:94:ILE:HA	13:Sf:100:PRO:HA	1.97	0.46
20:ST:112:MET:SD	20:ST:127:GLY:HA2	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:696:G:H4'	35:S2:735:C:H5	1.80	0.46
36:zz:180:G:H2'	36:zz:181:G:H8	1.81	0.46
44:3k:104:TYR:O	44:3k:108:LEU:HD12	2.16	0.46
4:SD:105:LEU:HB2	4:SD:122:VAL:HG21	1.98	0.46
9:SI:106:SER:HB3	9:SI:171:LEU:HG	1.97	0.46
25:SY:20:ARG:NH1	25:SY:74:MET:HE1	2.30	0.46
25:SY:101:LYS:HE2	25:SY:101:LYS:HB2	1.72	0.46
35:S2:1858:G:H2'	35:S2:1859:A:H8	1.80	0.46
36:zz:116:A:H3'	36:zz:117:G:H8	1.81	0.46
45:3l:380:MET:HE1	45:3l:382:ILE:HB	1.98	0.46
2:SB:116:LYS:HG3	35:S2:988:C:H5''	1.98	0.45
4:SD:56:GLN:CD	4:SD:56:GLN:H	2.24	0.45
17:SQ:40:GLU:HA	17:SQ:48:GLN:NE2	2.29	0.45
33:Sg:194:TYR:HE1	33:Sg:212:LYS:HD3	1.80	0.45
35:S2:644:G:H2'	35:S2:645:C:C6	2.51	0.45
39:3a:41:ARG:HE	39:3a:41:ARG:HB3	1.57	0.45
20:ST:39:LEU:HD12	20:ST:39:LEU:H	1.80	0.45
35:S2:106:C:H2'	35:S2:107:A:H8	1.80	0.45
35:S2:155:G:H2'	35:S2:156:G:H8	1.81	0.45
35:S2:321:C:H2'	35:S2:322:C:C6	2.52	0.45
39:3a:269:PRO:HB2	39:3a:306:MET:SD	2.56	0.45
4:SD:214:LYS:HE3	4:SD:214:LYS:HB3	1.72	0.45
11:SK:60:GLU:HB3	11:SK:69:TRP:CD1	2.51	0.45
16:SP:52:LYS:NZ	35:S2:1298:G:H21	2.14	0.45
25:SY:55:ILE:HG12	25:SY:75:ILE:HG22	1.97	0.45
33:Sg:23:THR:HG22	33:Sg:31:ILE:HG23	1.98	0.45
35:S2:496:C:H2'	35:S2:497:C:H6	1.81	0.45
35:S2:656:G:H21	35:S2:663:C:H5''	1.81	0.45
36:zz:224:G:H2'	36:zz:225:A:C8	2.51	0.45
10:SJ:114:VAL:HG21	10:SJ:130:ILE:HD11	1.98	0.45
24:SX:48:LYS:HB3	24:SX:75:ILE:HD11	1.97	0.45
33:Sg:101:PHE:CE1	33:Sg:136:GLY:HA2	2.51	0.45
35:S2:375:U:H2'	35:S2:376:A:C8	2.51	0.45
35:S2:610:G:H2'	35:S2:611:G:H8	1.81	0.45
35:S2:1382:A:H2'	35:S2:1383:A:H8	1.81	0.45
35:S2:1568:C:H2'	35:S2:1569:A:C8	2.51	0.45
37:3m:182:SER:HA	37:3m:185:MET:HE2	1.98	0.45
13:Sf:116:LYS:HA	13:Sf:116:LYS:HD3	1.73	0.45
37:3m:353:THR:HB	42:3h:351:ASN:HD21	1.82	0.45
39:3a:158:ARG:HE	39:3a:158:ARG:HB3	1.69	0.45
39:3a:165:ARG:HD2	39:3a:166:ASN:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:3e:404:VAL:HG22	41:3c:857:LEU:HD13	1.98	0.45
3:SC:86:LEU:HD11	3:SC:265:PRO:HG2	1.98	0.45
3:SC:202:THR:HG22	3:SC:221:ASP:HB3	1.97	0.45
7:SG:51:ARG:HH21	7:SG:112:VAL:HG11	1.82	0.45
11:SK:5:LYS:HE3	35:S2:1313:A:H5''	1.97	0.45
14:SN:23:PRO:HG2	14:SN:26:LEU:HB2	1.97	0.45
25:SY:21:LYS:HD2	25:SY:75:ILE:HD11	1.98	0.45
32:sh:100:LEU:O	32:sh:103:LEU:HG	2.17	0.45
35:S2:803:C:H2'	35:S2:804:U:C6	2.52	0.45
36:zz:82:G:H1'	36:zz:83:C:H5''	1.97	0.45
39:3a:28:LEU:HD23	39:3a:57:LEU:HD13	1.98	0.45
41:3c:734:ARG:HH21	41:3c:735:GLU:HG2	1.82	0.45
3:SC:91:SER:HB2	3:SC:156:ILE:HG23	1.99	0.45
4:SD:105:LEU:HD12	4:SD:122:VAL:HG21	1.99	0.45
31:Se:53:LYS:HA	31:Se:53:LYS:HD3	1.74	0.45
35:S2:1850:A:H2'	35:S2:1851:A:C8	2.52	0.45
36:zz:294:U:H2'	36:zz:295:G:H2'	1.98	0.45
45:3l:277:LEU:HD23	45:3l:277:LEU:HA	1.87	0.45
45:3l:540:GLY:HA2	45:3l:543:PHE:CZ	2.52	0.45
29:Sc:59:LEU:HD12	29:Sc:59:LEU:H	1.81	0.45
35:S2:953:C:H2'	35:S2:954:U:O4'	2.17	0.45
35:S2:1671:G:H2'	35:S2:1672:U:C6	2.51	0.45
39:3a:507:ILE:HD11	39:3a:510:HIS:HB2	1.98	0.45
8:SH:154:ILE:HB	8:SH:185:VAL:HG22	1.97	0.45
21:SU:17:ILE:HD13	21:SU:93:SER:HA	1.99	0.45
35:S2:874:G:H2'	35:S2:875:A:C8	2.51	0.45
36:zz:287:U:H2'	36:zz:288:A:H8	1.81	0.45
37:3m:176:LYS:HA	37:3m:176:LYS:HD2	1.62	0.45
39:3a:318:MET:HE3	39:3a:318:MET:O	2.17	0.45
40:3e:362:MET:SD	40:3e:366:GLU:HG3	2.57	0.45
41:3c:503:TYR:HB3	41:3c:555:ILE:HD11	1.99	0.45
45:3l:403:LYS:HD2	45:3l:403:LYS:HA	1.74	0.45
1:SA:70:ASN:HD21	1:SA:72:ALA:HB3	1.82	0.45
11:SK:16:PHE:CD1	11:SK:79:LEU:HD23	2.52	0.45
17:SQ:82:TYR:HA	17:SQ:85:ARG:HG2	1.98	0.45
36:zz:52:G:N2	36:zz:53:A:H1'	2.32	0.45
36:zz:107:G:H2'	36:zz:108:C:C6	2.52	0.45
2:SB:122:GLU:HG2	2:SB:140:VAL:HG22	1.98	0.44
19:SS:132:ARG:HB3	35:S2:1623[B]:A:N7	2.33	0.44
28:Sb:8:LEU:HD23	28:Sb:8:LEU:HA	1.83	0.44
29:Sc:14:VAL:HG22	29:Sc:54:ASP:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:1762:C:H2'	35:S2:1763:G:C8	2.52	0.44
41:3c:504:LEU:HD12	41:3c:507:ILE:HD11	1.97	0.44
41:3c:577:ALA:HB3	41:3c:615:GLN:HG3	1.99	0.44
41:3c:825:MET:HG3	41:3c:831:LEU:HD22	1.99	0.44
45:3l:454:GLN:HG2	45:3l:496:LYS:HD3	1.99	0.44
1:SA:51:LEU:HD23	18:SR:105:MET:HE1	1.98	0.44
35:S2:106:C:H2'	35:S2:107:A:C8	2.53	0.44
35:S2:946:U:H2'	35:S2:947:G:H8	1.83	0.44
35:S2:1317:C:H2'	35:S2:1318:G:C8	2.52	0.44
35:S2:1595:U:H2'	35:S2:1596:U:C6	2.51	0.44
35:S2:1753:C:H4'	35:S2:1754:G:C8	2.52	0.44
36:zz:235:G:H2'	36:zz:236:C:C6	2.53	0.44
10:SJ:35:TYR:CG	10:SJ:106:LEU:HD23	2.53	0.44
35:S2:107:A:H2'	35:S2:108:G:H8	1.83	0.44
35:S2:1134:G:H2'	35:S2:1135:C:C6	2.52	0.44
3:SC:198:ALA:HB1	3:SC:202:THR:HG21	1.99	0.44
25:SY:23:MET:HE3	25:SY:23:MET:HB2	1.72	0.44
35:S2:235:A:H2'	35:S2:236:A:C8	2.52	0.44
35:S2:803:C:H2'	35:S2:804:U:H6	1.82	0.44
35:S2:1010:G:H2'	35:S2:1011:A:H8	1.82	0.44
35:S2:1842:C:H2'	35:S2:1843:G:C8	2.52	0.44
42:3h:128:PHE:HE1	42:3h:325:THR:HG21	1.82	0.44
45:3l:240:ILE:HD11	45:3l:267:LYS:HA	1.99	0.44
45:3l:522:TYR:CE1	45:3l:529:HIS:HB3	2.52	0.44
1:SA:89:LYS:HB2	1:SA:202:TYR:CE2	2.53	0.44
5:SE:192:ILE:HD13	5:SE:192:ILE:HA	1.77	0.44
7:SG:223:LYS:HA	7:SG:223:LYS:HD3	1.61	0.44
16:SP:85:ILE:HD12	16:SP:111:MET:HB3	1.99	0.44
32:sh:133:ALA:HB2	35:S2:1309:C:O4'	2.18	0.44
35:S2:102:A:H4'	35:S2:104:A:C8	2.52	0.44
35:S2:952:G:H2'	35:S2:953:C:C6	2.52	0.44
35:S2:1776:G:N2	35:S2:1778:C:H41	2.16	0.44
37:3m:21:TYR:CZ	37:3m:63:VAL:HG22	2.52	0.44
37:3m:149:LYS:HE3	37:3m:149:LYS:HB3	1.77	0.44
39:3a:55:LEU:HD11	39:3a:71:LEU:HD21	1.99	0.44
2:SB:86:LEU:HB3	2:SB:98:THR:HG21	1.98	0.44
4:SD:173:ARG:HD3	4:SD:173:ARG:HA	1.92	0.44
11:SK:49:MET:H	11:SK:49:MET:HG2	1.48	0.44
33:Sg:147:HIS:HD2	33:Sg:151:VAL:HG12	1.82	0.44
35:S2:107:A:H2'	35:S2:108:G:C8	2.53	0.44
35:S2:909:G:H2'	35:S2:910:G:H8	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:982:G:H2'	35:S2:983:A:H8	1.83	0.44
35:S2:1491:G:H2'	35:S2:1492:U:C6	2.52	0.44
36:zz:231:G:H22	36:zz:233:G:H1	1.65	0.44
36:zz:242:C:H2'	36:zz:243:G:C8	2.52	0.44
38:3f:222:GLY:HA3	38:3f:226:ARG:HD2	2.00	0.44
45:3l:457:LEU:HD11	45:3l:492:VAL:HG12	1.98	0.44
3:SC:82:TYR:CZ	3:SC:164:PRO:HD3	2.52	0.44
6:SF:123:GLU:HB2	29:Sc:59:LEU:HD13	2.00	0.44
10:SJ:131:ARG:HD2	10:SJ:131:ARG:HA	1.80	0.44
13:Sf:35:ILE:HD12	13:Sf:36:ARG:N	2.33	0.44
15:SO:99:ALA:H	15:SO:133:THR:HB	1.82	0.44
19:SS:15:VAL:HG13	19:SS:68:ILE:HD11	1.99	0.44
20:ST:40:ALA:HB3	20:ST:43:LYS:HG2	1.99	0.44
35:S2:528:A:H2'	35:S2:529:A:C8	2.52	0.44
35:S2:1628:C:H2'	35:S2:1629:C:C6	2.52	0.44
35:S2:1643:U:H2'	35:S2:1644:C:C6	2.52	0.44
37:3m:128:ILE:HD13	37:3m:167:LEU:HB3	1.99	0.44
5:SE:191:ARG:HD3	5:SE:245:ARG:HB2	2.00	0.44
17:SQ:32:ILE:HD12	17:SQ:32:ILE:HA	1.83	0.44
17:SQ:113:ILE:HD13	17:SQ:113:ILE:HA	1.84	0.44
33:Sg:228:TYR:CD2	33:Sg:264:LYS:HG2	2.52	0.44
35:S2:1845:A:H2'	35:S2:1846:G:H8	1.82	0.44
36:zz:141:U:H2'	36:zz:142:A:C8	2.52	0.44
38:3f:334:LEU:HD22	42:3h:239:LEU:HD23	1.99	0.44
38:3f:353:LYS:HA	38:3f:356:ASN:HB2	1.99	0.44
35:S2:649:U:H2'	35:S2:650:A:C8	2.52	0.44
35:S2:1244:U:H2'	35:S2:1245:G:H8	1.83	0.44
35:S2:1811:C:H2'	35:S2:1812:U:C6	2.53	0.44
35:S2:1844:U:H2'	35:S2:1845:A:H8	1.80	0.44
40:3e:372:VAL:HG22	45:3l:463:PHE:CE1	2.53	0.44
45:3l:341:LEU:HD11	45:3l:549:LYS:HE3	2.00	0.44
1:SA:85:ARG:O	1:SA:89:LYS:HG2	2.18	0.43
7:SG:175:LYS:HG3	35:S2:77:A:H2	1.83	0.43
11:SK:14:LEU:HA	11:SK:17:LYS:HB3	2.00	0.43
35:S2:70:G:H21	35:S2:79:A:H62	1.64	0.43
36:zz:61:U:H2'	36:zz:62:C:C6	2.53	0.43
36:zz:220:U:H2'	36:zz:221:G:H8	1.81	0.43
41:3c:692:LEU:HD21	41:3c:782:LYS:HB3	2.00	0.43
42:3h:249:ARG:HH21	42:3h:319:ILE:HA	1.83	0.43
45:3l:160:TYR:HD1	45:3l:160:TYR:HA	1.71	0.43
45:3l:377:MET:HE2	45:3l:454:GLN:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SG:154:ARG:HG2	35:S2:77:A:C8	2.53	0.43
7:SG:211:LYS:HB2	7:SG:211:LYS:HE2	1.81	0.43
14:SN:88:LEU:HD22	14:SN:125:LEU:HD23	2.00	0.43
33:Sg:197:THR:HG21	33:Sg:238:ALA:HA	2.00	0.43
41:3c:749:TRP:CD1	41:3c:750:LYS:HG3	2.53	0.43
42:3h:51:LYS:HE3	42:3h:51:LYS:HB3	1.75	0.43
5:SE:248:ILE:HD11	35:S2:848:U:H4'	2.01	0.43
8:SH:138:GLU:OE2	14:SN:19:ARG:HD2	2.18	0.43
33:Sg:54:ILE:HD13	33:Sg:54:ILE:HA	1.83	0.43
35:S2:527:C:H2'	35:S2:528:A:C8	2.52	0.43
35:S2:982:G:H2'	35:S2:983:A:C8	2.52	0.43
37:3m:39:HIS:CE1	37:3m:40:VAL:HG23	2.54	0.43
39:3a:95:LYS:HA	39:3a:95:LYS:HD3	1.84	0.43
41:3c:504:LEU:HD22	41:3c:564:ILE:HG23	1.99	0.43
41:3c:591:MET:HA	41:3c:591:MET:HE2	2.00	0.43
41:3c:774:LYS:HE3	41:3c:774:LYS:HB3	1.62	0.43
42:3h:44:LEU:O	42:3h:48:LYS:HG2	2.18	0.43
26:SZ:102:LYS:HD2	26:SZ:107:VAL:HG12	2.01	0.43
35:S2:241:G:H1	35:S2:276:G:H1	1.67	0.43
35:S2:942:G:H2'	35:S2:943:U:C6	2.53	0.43
39:3a:92:ALA:O	39:3a:96:MET:HG2	2.18	0.43
41:3c:376:PHE:HE2	41:3c:441:ARG:HH11	1.66	0.43
4:SD:61:GLU:H	4:SD:61:GLU:HG3	1.67	0.43
8:SH:115:LYS:HG3	35:S2:868:G:C5	2.53	0.43
13:Sf:85:LEU:O	13:Sf:89:VAL:HG12	2.18	0.43
18:SR:31:ASN:ND2	18:SR:55:THR:HG22	2.33	0.43
20:ST:78:ILE:HD11	35:S2:1587:G:C5	2.54	0.43
25:SY:68:LYS:HE2	25:SY:68:LYS:HB3	1.67	0.43
33:Sg:62:HIS:CE1	33:Sg:88:ARG:HG3	2.53	0.43
35:S2:551:U:H2'	35:S2:552:G:C8	2.54	0.43
36:zz:73:A:H2'	36:zz:74:A:C8	2.54	0.43
39:3a:384:VAL:HG12	39:3a:386:GLU:H	1.83	0.43
45:3l:237:LYS:HB3	45:3l:237:LYS:HE2	1.90	0.43
1:SA:142:LEU:HD12	1:SA:142:LEU:HA	1.77	0.43
8:SH:27:LEU:HD13	8:SH:27:LEU:HA	1.85	0.43
8:SH:110:THR:HG21	35:S2:744:G:H21	1.84	0.43
12:SL:13:GLN:NE2	12:SL:36:TYR:HB3	2.33	0.43
33:Sg:234:ASP:C	33:Sg:235:ILE:HD13	2.43	0.43
35:S2:1407:U:H2'	35:S2:1408:U:C6	2.54	0.43
35:S2:1817:G:H2'	35:S2:1818:A:C8	2.54	0.43
37:3m:169:TYR:O	37:3m:173:VAL:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3a:402:LYS:HG3	39:3a:406:ARG:HE	1.83	0.43
41:3c:552:CYS:HA	41:3c:555:ILE:HD12	1.99	0.43
42:3h:50:ILE:HD11	42:3h:162:LEU:HD21	2.00	0.43
42:3h:246:LEU:O	42:3h:250:VAL:HG23	2.18	0.43
45:3l:61:LYS:HD2	45:3l:61:LYS:HA	1.91	0.43
7:SG:119:LYS:HE2	7:SG:119:LYS:HB2	1.82	0.43
12:SL:75:GLY:HA3	12:SL:88:ILE:HD12	2.01	0.43
12:SL:128:VAL:HB	12:SL:140:PHE:HB3	2.01	0.43
27:Sa:37:LYS:HE2	27:Sa:37:LYS:HB2	1.76	0.43
37:3m:280:LEU:HD22	37:3m:339:HIS:CE1	2.53	0.43
41:3c:753:HIS:CE1	41:3c:757:ILE:HG12	2.54	0.43
42:3h:252:GLU:HB3	42:3h:319:ILE:HG21	2.00	0.43
2:SB:217:MET:HE3	2:SB:217:MET:HB3	1.74	0.43
3:SC:211:LYS:O	3:SC:215:MET:HG3	2.19	0.43
8:SH:24:SER:O	8:SH:28:LEU:HG	2.19	0.43
8:SH:27:LEU:HD12	8:SH:40:LEU:HD21	2.01	0.43
10:SJ:37:LEU:HD12	10:SJ:43:VAL:HG23	2.00	0.43
11:SK:47:LYS:HE3	11:SK:47:LYS:HB3	1.88	0.43
41:3c:706:ARG:HA	41:3c:706:ARG:HD2	1.87	0.43
45:3l:334:ARG:HA	45:3l:334:ARG:HD2	1.76	0.43
5:SE:6:LYS:H	5:SE:6:LYS:HG2	1.70	0.43
5:SE:189:LEU:HD12	5:SE:189:LEU:HA	1.87	0.43
11:SK:32:HIS:HD2	11:SK:45:VAL:HG11	1.83	0.43
20:ST:39:LEU:HD13	35:S2:1540:G:OP1	2.18	0.43
21:SU:80:PHE:HB3	30:Sd:52:PHE:HB3	2.01	0.43
36:zz:57:A:H3'	36:zz:58:C:H4'	2.01	0.43
37:3m:237:ILE:HD13	37:3m:262:PHE:HZ	1.84	0.43
42:3h:125:TYR:HE1	42:3h:155:ILE:HG21	1.83	0.43
44:3k:197:LYS:HB2	44:3k:197:LYS:HE2	1.87	0.43
45:3l:325:MET:HE1	45:3l:413:PHE:HZ	1.83	0.43
7:SG:7:PHE:HD2	7:SG:10:THR:HG22	1.84	0.43
8:SH:130:LEU:HD11	8:SH:156:VAL:HG21	2.01	0.43
11:SK:58:VAL:HG12	11:SK:71:LEU:HD22	2.01	0.43
33:Sg:45:LEU:HD22	33:Sg:52:TYR:HD1	1.83	0.43
33:Sg:129:ILE:HD11	33:Sg:151:VAL:HG11	2.00	0.43
35:S2:639:C:H2'	35:S2:640:A:C8	2.54	0.43
35:S2:845:G:H2'	35:S2:846:G:C8	2.54	0.43
35:S2:1217:A:H2'	35:S2:1218:C:C6	2.54	0.43
35:S2:1415:C:H2'	35:S2:1416:C:C6	2.54	0.43
37:3m:177:LYS:HB3	37:3m:177:LYS:HE2	1.82	0.43
39:3a:220:LEU:HD13	39:3a:220:LEU:HA	1.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3a:523:LEU:HD22	42:3h:231:LEU:HB3	2.00	0.43
45:3l:490:LEU:HD12	45:3l:490:LEU:HA	1.83	0.43
3:SC:133:TYR:CD1	3:SC:216:MET:HA	2.54	0.42
13:Sf:24:THR:O	13:Sf:27:ILE:HG13	2.19	0.42
14:SN:141:TYR:HE2	14:SN:146:ALA:HB2	1.84	0.42
26:SZ:100:VAL:HG22	26:SZ:110:THR:HG22	2.01	0.42
35:S2:239:C:H42	35:S2:278:C:N4	2.13	0.42
35:S2:909:G:H2'	35:S2:910:G:C8	2.54	0.42
35:S2:1174:U:H2'	35:S2:1175:G:C8	2.50	0.42
35:S2:1759:G:H2'	35:S2:1760:G:H8	1.83	0.42
35:S2:1797:U:H2'	35:S2:1798:C:C6	2.54	0.42
36:zz:173:A:H2'	36:zz:174:U:C6	2.54	0.42
41:3c:611:ARG:HH21	41:3c:675:LEU:HD12	1.83	0.42
4:SD:109:LEU:HD23	4:SD:109:LEU:HA	1.87	0.42
16:SP:15:PHE:HB3	16:SP:22:LEU:HD11	2.00	0.42
33:Sg:131:LEU:HD21	33:Sg:140:TYR:HB3	2.01	0.42
35:S2:240:G:H2'	35:S2:241:G:C8	2.53	0.42
35:S2:634:A:H2'	35:S2:635:G:H8	1.84	0.42
35:S2:1565:C:H2'	35:S2:1566:G:H8	1.84	0.42
35:S2:1629:C:C2	35:S2:1630:A:C8	3.07	0.42
45:3l:69:GLN:HE22	45:3l:87:LYS:HE3	1.84	0.42
45:3l:369:ALA:HB1	45:3l:412:LEU:HD21	2.01	0.42
1:SA:155:ARG:HG2	1:SA:156:TYR:CD1	2.54	0.42
6:SF:76:MET:HE2	6:SF:76:MET:HB2	1.81	0.42
7:SG:237:LEU:HD23	7:SG:237:LEU:HA	1.88	0.42
15:SO:143:LYS:HB3	15:SO:143:LYS:HE3	1.82	0.42
32:sh:94:LYS:HB3	32:sh:94:LYS:HE3	1.83	0.42
35:S2:550:C:H2'	35:S2:551:U:C6	2.54	0.42
35:S2:864:A:H2'	35:S2:865:A:H8	1.83	0.42
35:S2:1593:C:H2'	35:S2:1594:A:H8	1.84	0.42
35:S2:1798:C:H2'	35:S2:1799:G:O4'	2.20	0.42
37:3m:38:LEU:HD21	37:3m:74:LEU:HD13	2.01	0.42
42:3h:49:ILE:HG12	42:3h:120:TYR:CE2	2.54	0.42
45:3l:292:LYS:HB2	45:3l:292:LYS:HE3	1.82	0.42
3:SC:117:ARG:H	3:SC:117:ARG:HD3	1.84	0.42
6:SF:134:VAL:HG11	36:zz:87:G:O4'	2.18	0.42
7:SG:203:LYS:HB3	7:SG:203:LYS:HE2	1.81	0.42
11:SK:32:HIS:HE1	11:SK:34:GLU:HB3	1.83	0.42
12:SL:101:ARG:HH21	24:SX:5:ARG:HG3	1.85	0.42
28:Sb:54:VAL:HG23	28:Sb:63:LEU:HD13	2.01	0.42
36:zz:216:U:C4	39:3a:69:GLU:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:zz:265:U:O2'	36:zz:266:G:H8	2.03	0.42
39:3a:352:GLN:HE22	39:3a:364:PRO:HG3	1.85	0.42
2:SB:103:MET:HB3	2:SB:215:VAL:HB	2.01	0.42
3:SC:114:LYS:HD2	3:SC:121:ARG:CZ	2.50	0.42
9:SI:141:ARG:HB2	9:SI:146:GLN:HG2	2.01	0.42
32:sh:118:ARG:HA	32:sh:118:ARG:NH1	2.34	0.42
35:S2:495:U:H2'	35:S2:496:C:O4'	2.20	0.42
35:S2:1808:U:H2'	35:S2:1809:A:C8	2.55	0.42
36:zz:127:U:H3	36:zz:321:A:H2	1.67	0.42
42:3h:243:LEU:O	42:3h:246:LEU:HG	2.19	0.42
45:3l:112:TRP:CE3	45:3l:113:PRO:HD2	2.54	0.42
45:3l:491:LEU:O	45:3l:495:HIS:HB3	2.19	0.42
5:SE:153:LEU:HG	7:SG:216:ARG:HE	1.84	0.42
9:SI:150:ASP:HA	9:SI:153:LYS:HE2	2.02	0.42
35:S2:562:U:H2'	35:S2:563:G:C8	2.54	0.42
35:S2:1758:G:H2'	35:S2:1759:G:C8	2.54	0.42
41:3c:576:HIS:O	41:3c:581:ARG:HG2	2.19	0.42
42:3h:314:MET:HE2	42:3h:314:MET:HB3	1.75	0.42
45:3l:130:ILE:HG21	45:3l:163:LEU:HB2	2.02	0.42
45:3l:367:MET:HA	45:3l:370:LEU:HB2	2.00	0.42
45:3l:544:ILE:HD12	45:3l:544:ILE:HA	1.91	0.42
2:SB:78:GLU:HB2	2:SB:79:VAL:H	1.68	0.42
16:SP:60:LEU:HD11	16:SP:89:MET:HB3	2.01	0.42
33:Sg:171:ASP:O	33:Sg:173:LEU:HD12	2.20	0.42
33:Sg:269:GLU:HG2	33:Sg:271:LYS:HZ1	1.83	0.42
35:S2:186:C:H2'	35:S2:187:G:C8	2.52	0.42
42:3h:50:ILE:HD11	42:3h:162:LEU:HD11	2.01	0.42
45:3l:98:SER:O	45:3l:102:LEU:HD23	2.20	0.42
45:3l:200:TYR:CE1	45:3l:206:LYS:HG3	2.55	0.42
45:3l:549:LYS:HE2	45:3l:549:LYS:HB2	1.71	0.42
1:SA:89:LYS:NZ	1:SA:201:LEU:HG	2.35	0.42
9:SI:135:GLU:O	9:SI:139:LYS:HB2	2.19	0.42
14:SN:52:VAL:HG23	14:SN:55:ARG:NH2	2.35	0.42
21:SU:98:VAL:O	21:SU:102:THR:HG23	2.20	0.42
24:SX:90:CYS:HA	24:SX:93:PHE:CD2	2.55	0.42
35:S2:96:C:H2'	35:S2:97:U:C6	2.55	0.42
35:S2:160:U:O2'	35:S2:161:U:H3'	2.20	0.42
35:S2:441:C:H2'	35:S2:442:C:C6	2.55	0.42
35:S2:756:C:H2'	35:S2:757:C:C6	2.54	0.42
35:S2:1415:C:H2'	35:S2:1416:C:H6	1.84	0.42
35:S2:1759:G:H2'	35:S2:1760:G:C8	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:1862:G:H1'	35:S2:1863:A:H2'	2.02	0.42
36:zz:78:U:H2'	36:zz:79:C:C6	2.55	0.42
38:3f:206:LEU:HD22	39:3a:557:TYR:CD2	2.54	0.42
41:3c:687:LEU:HD23	41:3c:687:LEU:HA	1.87	0.42
45:3l:365:GLU:HA	45:3l:368:HIS:HB3	2.01	0.42
45:3l:427:ASN:HB2	45:3l:430:ASN:OD1	2.20	0.42
4:SD:136:VAL:HG22	4:SD:186:VAL:HG22	2.02	0.42
18:SR:71:ILE:HG23	18:SR:74:GLN:HB2	2.01	0.42
33:Sg:280:LYS:HA	33:Sg:280:LYS:HD3	1.79	0.42
35:S2:563:G:O2'	35:S2:564:A:H8	2.03	0.42
35:S2:1116:C:H2'	35:S2:1117:C:H5''	2.01	0.42
35:S2:1769:C:H2'	35:S2:1770:G:H8	1.84	0.42
39:3a:62:ARG:HD3	39:3a:152:PHE:HB2	2.02	0.42
39:3a:165:ARG:HA	39:3a:204:HIS:CE1	2.55	0.42
39:3a:191:LYS:HG2	39:3a:245:LEU:HD11	2.01	0.42
39:3a:205:LEU:HD21	39:3a:229:HIS:NE2	2.35	0.42
40:3e:367:ALA:O	40:3e:371:ILE:HG12	2.19	0.42
43:3d:33:PHE:CE2	43:3d:35:LYS:HG3	2.55	0.42
3:SC:68:ARG:HG2	3:SC:277:HIS:CE1	2.55	0.42
5:SE:139:LEU:HD12	5:SE:150:PRO:HB3	2.02	0.42
6:SF:59:LYS:HB3	6:SF:62:ARG:HE	1.84	0.42
22:SV:41:LYS:HA	22:SV:41:LYS:HD3	1.81	0.42
35:S2:788:G:H2'	35:S2:789:G:C8	2.55	0.42
39:3a:317:ARG:HH12	39:3a:424:LEU:HD21	1.84	0.42
40:3e:360:LEU:HD12	40:3e:360:LEU:HA	1.87	0.42
45:3l:149:SER:O	45:3l:153:ARG:HG2	2.19	0.42
1:SA:78:SER:HB3	1:SA:87:VAL:HG21	2.01	0.41
1:SA:154:LEU:HD13	1:SA:154:LEU:HA	1.87	0.41
5:SE:126:VAL:HG12	5:SE:158:ASP:O	2.20	0.41
8:SH:109:ARG:NE	35:S2:799:U:H5'	2.35	0.41
19:SS:132:ARG:HD3	35:S2:1623[B]:A:C6	2.55	0.41
25:SY:74:MET:HE3	25:SY:74:MET:HB3	1.91	0.41
35:S2:1560:U:O2	35:S2:1575:G:O6	2.38	0.41
35:S2:1763:G:H2'	35:S2:1764:G:H8	1.85	0.41
36:zz:240:C:H2'	36:zz:241:G:H8	1.83	0.41
37:3m:74:LEU:HD11	37:3m:78:LYS:HB2	2.02	0.41
39:3a:455:LEU:HD12	39:3a:455:LEU:HA	1.89	0.41
45:3l:481:LEU:HD21	45:3l:485:GLU:HG3	2.02	0.41
35:S2:811[A]:A:H2'	35:S2:812:A:H8	1.84	0.41
35:S2:1362:U:H5''	35:S2:1363:C:C5	2.55	0.41
45:3l:474:LYS:HB3	45:3l:474:LYS:HE3	1.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SC:84:PHE:CD1	3:SC:265:PRO:HD3	2.56	0.41
4:SD:69:LEU:HD13	4:SD:69:LEU:HA	1.89	0.41
5:SE:51:ARG:HA	5:SE:51:ARG:HD3	1.84	0.41
5:SE:68:ARG:HB3	5:SE:76:VAL:HG11	2.01	0.41
28:Sb:46:VAL:HG11	28:Sb:54:VAL:HG21	2.03	0.41
35:S2:811[A]:A:H2'	35:S2:812:A:C8	2.54	0.41
35:S2:980:A:H2'	35:S2:981:A:C8	2.55	0.41
35:S2:1470:C:H2'	35:S2:1471:C:H6	1.85	0.41
35:S2:1768:A:H2'	35:S2:1769:C:C6	2.54	0.41
36:zz:66:A:H2'	36:zz:67:C:C6	2.56	0.41
41:3c:602:ASP:HB3	41:3c:604:PRO:HD2	2.02	0.41
42:3h:313:ARG:HD3	42:3h:313:ARG:HA	1.69	0.41
3:SC:212:LYS:HA	3:SC:212:LYS:HD2	1.67	0.41
6:SF:76:MET:HB3	6:SF:89:THR:HG21	2.02	0.41
27:Sa:18:VAL:HG21	27:Sa:33:ASP:OD2	2.20	0.41
33:Sg:77:PHE:HD1	33:Sg:77:PHE:HA	1.72	0.41
35:S2:5:U:O2'	35:S2:602:G:H4'	2.21	0.41
35:S2:889:U:H2'	35:S2:890:U:C5	2.55	0.41
36:zz:276:A:H2'	36:zz:277:G:C8	2.55	0.41
39:3a:98:GLU:HG2	39:3a:184:PHE:CE2	2.55	0.41
40:3e:167:SER:HB3	43:3d:17:GLY:H	1.85	0.41
40:3e:186:MET:HA	40:3e:189:LEU:HB3	2.03	0.41
41:3c:450:ARG:HD2	41:3c:450:ARG:HA	1.84	0.41
45:3l:59:PHE:CD1	45:3l:94:ILE:HD13	2.55	0.41
13:Sf:78:LYS:HB2	13:Sf:78:LYS:HE2	1.71	0.41
33:Sg:275:ILE:HG23	33:Sg:278:SER:H	1.85	0.41
35:S2:319:C:H2'	35:S2:320:G:O4'	2.21	0.41
35:S2:528:A:H2'	35:S2:529:A:H8	1.85	0.41
35:S2:1134:G:H2'	35:S2:1135:C:H6	1.85	0.41
35:S2:1539:U:H2'	35:S2:1540:G:C8	2.56	0.41
35:S2:1562:C:H2'	35:S2:1563:G:C8	2.56	0.41
39:3a:469:ARG:NH2	41:3c:748:ASP:HA	2.35	0.41
40:3e:17:HIS:NE2	40:3e:140:GLU:HA	2.36	0.41
45:3l:127:VAL:HG11	45:3l:176:LEU:HD21	2.03	0.41
2:SB:153:THR:HB	2:SB:155:TYR:CE1	2.56	0.41
10:SJ:92:MET:HE3	10:SJ:92:MET:HB3	1.74	0.41
19:SS:3:LEU:O	26:SZ:50:PHE:HB2	2.20	0.41
33:Sg:191:HIS:CD2	33:Sg:195:LEU:HD21	2.55	0.41
35:S2:191:A:H2'	35:S2:192:C:O4'	2.21	0.41
35:S2:799:U:O2'	35:S2:800:U:H5''	2.20	0.41
35:S2:1406:G:H2'	35:S2:1407:U:C6	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:1774:C:H2'	35:S2:1775:U:C6	2.56	0.41
36:zz:181:G:H2'	36:zz:182:A:H8	1.86	0.41
37:3m:213:LYS:HB2	37:3m:213:LYS:HE3	1.65	0.41
38:3f:126:LYS:H	38:3f:126:LYS:HG2	1.63	0.41
40:3e:169:LEU:HD12	40:3e:169:LEU:HA	1.93	0.41
41:3c:555:ILE:O	41:3c:559:ASP:HB2	2.21	0.41
45:3l:336:PHE:CE2	45:3l:370:LEU:HB3	2.55	0.41
2:SB:89:GLU:OE2	2:SB:228:LEU:HD21	2.21	0.41
4:SD:31:GLU:HA	4:SD:107:TYR:CE1	2.55	0.41
18:SR:73:LEU:HD13	18:SR:73:LEU:HA	1.89	0.41
21:SU:67:LYS:HG2	30:Sd:44:ARG:NH1	2.36	0.41
35:S2:1244:U:H2'	35:S2:1245:G:C8	2.56	0.41
37:3m:227:LYS:O	37:3m:230:LYS:HG2	2.20	0.41
41:3c:670:GLN:H	41:3c:670:GLN:HG2	1.75	0.41
17:SQ:106:LYS:HE3	17:SQ:106:LYS:HB3	1.83	0.41
1:SA:210:ILE:O	1:SA:214:GLU:HG2	2.21	0.41
3:SC:135:GLY:HA2	3:SC:165:VAL:HG12	2.03	0.41
4:SD:66:ILE:HD12	4:SD:66:ILE:HA	1.91	0.41
5:SE:64:ILE:HG13	25:SY:18:LEU:HD13	2.01	0.41
7:SG:164:LYS:HB2	35:S2:67:C:H41	1.86	0.41
8:SH:142:LYS:HB2	8:SH:142:LYS:HE3	1.90	0.41
12:SL:4:ILE:HD12	12:SL:56:ILE:HG22	2.03	0.41
15:SO:74:ALA:HB1	15:SO:115:ALA:HB2	2.01	0.41
17:SQ:32:ILE:HG13	17:SQ:39:LEU:HD11	2.02	0.41
18:SR:78:ARG:HB2	18:SR:81:ARG:NH2	2.35	0.41
19:SS:60:THR:O	19:SS:64:VAL:HG12	2.20	0.41
22:SV:59:ILE:HD13	22:SV:59:ILE:HA	1.91	0.41
22:SV:81:LYS:HE2	22:SV:81:LYS:H	1.85	0.41
26:SZ:77:LEU:HB3	26:SZ:79:ILE:HG12	2.02	0.41
29:Sc:22:GLY:HA2	29:Sc:68:LEU:HB2	2.02	0.41
35:S2:115:U:H2'	35:S2:116:U:C6	2.55	0.41
35:S2:386:C:H2'	35:S2:387:C:C6	2.56	0.41
35:S2:641:A:H2'	35:S2:642:U:O4'	2.19	0.41
36:zz:178:C:H2'	36:zz:179:A:C8	2.55	0.41
36:zz:336:U:O2'	36:zz:337:G:H8	2.04	0.41
39:3a:36:LYS:HA	39:3a:36:LYS:HD2	1.83	0.41
40:3e:405:ILE:HA	40:3e:408:THR:HG22	2.02	0.41
42:3h:82:PHE:HA	42:3h:83:PRO:HD3	1.94	0.41
45:3l:178:LEU:H	45:3l:265:LEU:HD21	1.85	0.41
45:3l:493:PHE:O	45:3l:497:MET:HG3	2.21	0.41
2:SB:97:LEU:HB3	2:SB:228:LEU:HD22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SF:178:ILE:HD13	6:SF:178:ILE:HA	1.85	0.41
9:SI:66:SER:O	9:SI:189:VAL:HG12	2.21	0.41
17:SQ:15:ARG:HH22	35:S2:1444:U:P	2.43	0.41
22:SV:17:CYS:HB2	22:SV:56:CYS:HB3	2.02	0.41
30:Sd:17:GLY:HA2	30:Sd:27:ARG:HD3	2.03	0.41
33:Sg:8:ARG:HB3	33:Sg:309:VAL:HG23	2.03	0.41
35:S2:891:G:H2'	35:S2:892:U:C6	2.56	0.41
35:S2:935:G:H2'	35:S2:936:G:C8	2.56	0.41
35:S2:1139:C:H2'	35:S2:1140:G:O4'	2.21	0.41
39:3a:18:PHE:CG	39:3a:23:LYS:HD3	2.56	0.41
39:3a:164:LEU:HB3	39:3a:174:TYR:HB2	2.02	0.41
40:3e:319:LEU:HD23	40:3e:325:LEU:HB3	2.02	0.41
45:3l:200:TYR:HE1	45:3l:206:LYS:HG3	1.86	0.41
45:3l:286:ASP:HB3	45:3l:289:GLN:HB2	2.03	0.41
5:SE:61:VAL:HA	5:SE:64:ILE:HG22	2.03	0.40
7:SG:224:ARG:O	7:SG:228:ILE:HG12	2.20	0.40
9:SI:139:LYS:HA	9:SI:139:LYS:HD2	1.82	0.40
9:SI:158:ILE:HD12	9:SI:158:ILE:HA	1.95	0.40
11:SK:24:LYS:O	11:SK:24:LYS:HD2	2.20	0.40
14:SN:17:PRO:HG3	28:Sb:28:PRO:HG3	2.02	0.40
16:SP:64:LYS:HD3	16:SP:64:LYS:HA	1.89	0.40
19:SS:67:VAL:O	19:SS:71:MET:HG3	2.21	0.40
19:SS:118:ARG:HE	19:SS:118:ARG:HB3	1.78	0.40
24:SX:132:ALA:HB1	24:SX:137:LYS:HB2	2.03	0.40
31:Se:26:LYS:HE3	35:S2:593:C:H4'	2.02	0.40
33:Sg:225:LYS:HE2	33:Sg:225:LYS:HB3	1.78	0.40
35:S2:29:G:H2'	35:S2:30:C:C6	2.56	0.40
35:S2:754:G:C6	35:S2:791:C:H1'	2.55	0.40
35:S2:825:A:H2'	35:S2:826:A:H8	1.87	0.40
35:S2:1018:U:H2'	35:S2:1019:C:H6	1.86	0.40
35:S2:1395:C:H2'	35:S2:1396:A:N3	2.37	0.40
35:S2:1410:C:H2'	35:S2:1411:G:C8	2.56	0.40
36:zz:200:G:H2'	36:zz:201:G:C8	2.56	0.40
38:3f:268:ASP:O	38:3f:272:VAL:HG23	2.21	0.40
41:3c:604:PRO:HG3	41:3c:669:ARG:HD2	2.03	0.40
5:SE:44:LEU:HD23	5:SE:72:ILE:HD11	2.03	0.40
7:SG:7:PHE:HD1	7:SG:113:ILE:HB	1.86	0.40
15:SO:65:ASP:HB3	35:S2:963:A:OP1	2.22	0.40
28:Sb:24:LEU:HD12	28:Sb:24:LEU:HA	1.90	0.40
34:Ln:2:ARG:HB3	34:Ln:5:TRP:CD1	2.55	0.40
35:S2:566:U:H2'	35:S2:567:C:O4'	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:1541:G:H2'	35:S2:1542:C:C6	2.57	0.40
36:zz:80:U:H3	36:zz:85:A:H2	1.68	0.40
38:3f:91:VAL:HA	38:3f:236:THR:HB	2.03	0.40
39:3a:63:LYS:HD2	39:3a:66:LEU:HD12	2.04	0.40
39:3a:278:LYS:O	39:3a:282:VAL:HG12	2.20	0.40
41:3c:695:ILE:HG23	41:3c:696:PRO:HD3	2.03	0.40
41:3c:837:GLN:HG2	41:3c:838:PRO:HD3	2.03	0.40
8:SH:9:VAL:HG22	8:SH:45:ILE:HD11	2.03	0.40
13:Sf:39:ALA:O	13:Sf:43:ASP:HB2	2.21	0.40
20:ST:116:ASP:HA	20:ST:122:LYS:HZ2	1.86	0.40
26:SZ:99:LEU:HD23	26:SZ:109:TYR:CE1	2.57	0.40
32:sh:121:CYS:HB2	32:sh:132:MET:HE1	2.03	0.40
33:Sg:299:PHE:CD1	33:Sg:309:VAL:HG12	2.57	0.40
35:S2:753:C:H2'	35:S2:754:G:H8	1.86	0.40
35:S2:848:U:H2'	35:S2:849:A:H8	1.87	0.40
35:S2:1365:G:H2'	35:S2:1366:G:H8	1.87	0.40
35:S2:1438:A:H2'	35:S2:1439:A:C8	2.57	0.40
36:zz:178:C:H2'	36:zz:179:A:H8	1.86	0.40
39:3a:331:ILE:HD12	39:3a:437:LEU:HD22	2.03	0.40
39:3a:411:LEU:HG	39:3a:428:VAL:HG13	2.03	0.40
41:3c:431:LEU:HD23	41:3c:440:VAL:HG12	2.03	0.40
41:3c:576:HIS:ND1	41:3c:581:ARG:HG3	2.35	0.40
1:SA:39:TYR:CD1	1:SA:40:LYS:HG2	2.56	0.40
3:SC:187:ARG:HE	3:SC:192:LEU:HD12	1.87	0.40
9:SI:66:SER:HA	9:SI:73:THR:HG22	2.03	0.40
9:SI:137:LEU:HD23	9:SI:137:LEU:HA	1.91	0.40
11:SK:32:HIS:CD2	11:SK:45:VAL:HG11	2.56	0.40
14:SN:76:LYS:HB2	14:SN:76:LYS:HE2	1.79	0.40
18:SR:51:ALA:HA	18:SR:54:VAL:HG12	2.03	0.40
20:ST:104:LEU:HD23	20:ST:121:ARG:HD2	2.03	0.40
25:SY:20:ARG:CZ	25:SY:74:MET:HE1	2.51	0.40
33:Sg:172:LYS:HD3	33:Sg:193:GLY:H	1.86	0.40
34:Ln:2:ARG:HD2	35:S2:1841:C:P	2.62	0.40
35:S2:647:U:H2'	35:S2:648:A:C8	2.56	0.40
35:S2:1216:C:H42	35:S2:1342:U:P	2.44	0.40
36:zz:89:C:H2'	36:zz:90:G:C8	2.55	0.40
36:zz:215:A:N7	36:zz:217:G:H1'	2.36	0.40
37:3m:124:TYR:HB3	37:3m:154:TRP:HH2	1.86	0.40
39:3a:302:LEU:HD23	39:3a:302:LEU:HA	1.88	0.40
41:3c:570:LEU:HD22	41:3c:612:THR:HG21	2.02	0.40
41:3c:598:ILE:HD12	41:3c:598:ILE:HA	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3l:554:ASN:HD22	45:3l:554:ASN:HA	1.69	0.40
1:SA:37:TYR:HA	1:SA:53:ARG:HD2	2.04	0.40
6:SF:91:ARG:HD2	26:SZ:103:HIS:NE2	2.36	0.40
7:SG:214:ALA:O	7:SG:218:LYS:HG2	2.22	0.40
9:SI:27:TYR:HB2	35:S2:381:C:H41	1.86	0.40
9:SI:27:TYR:HB2	35:S2:381:C:N4	2.36	0.40
11:SK:25:LYS:HD2	11:SK:25:LYS:C	2.47	0.40
13:Sf:44:LYS:HD3	32:sh:129:GLY:H	1.85	0.40
17:SQ:12:VAL:HG11	17:SQ:90:LYS:HB3	2.03	0.40
33:Sg:45:LEU:HD22	33:Sg:52:TYR:CD1	2.56	0.40
35:S2:45:A:H4'	35:S2:46:A:H5'	2.04	0.40
35:S2:1103:C:H2'	35:S2:1104:G:C8	2.57	0.40
35:S2:1736:G:H2'	35:S2:1737:G:H8	1.86	0.40
36:zz:121:C:H2'	36:zz:122:C:O4'	2.22	0.40
41:3c:873:VAL:HA	41:3c:876:HIS:NE2	2.36	0.40
42:3h:96:GLU:HA	42:3h:99:TYR:HB3	2.04	0.40
42:3h:257:ILE:HA	42:3h:257:ILE:HD12	1.87	0.40
45:3l:336:PHE:HA	45:3l:339:ILE:HG22	2.03	0.40
45:3l:555:ARG:O	45:3l:559:LYS:HG2	2.21	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	SA	214/295 (72%)	207 (97%)	7 (3%)	0	100	100
2	SB	210/264 (80%)	204 (97%)	6 (3%)	0	100	100
3	SC	217/293 (74%)	209 (96%)	8 (4%)	0	100	100
4	SD	224/243 (92%)	222 (99%)	2 (1%)	0	100	100
5	SE	258/263 (98%)	243 (94%)	15 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	SF	190/204 (93%)	181 (95%)	9 (5%)	0	100	100
7	SG	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
8	SH	185/194 (95%)	175 (95%)	10 (5%)	0	100	100
9	SI	203/208 (98%)	195 (96%)	8 (4%)	0	100	100
10	SJ	178/194 (92%)	174 (98%)	4 (2%)	0	100	100
11	SK	94/165 (57%)	87 (93%)	7 (7%)	0	100	100
12	SL	148/158 (94%)	143 (97%)	5 (3%)	0	100	100
13	Sf	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
14	SN	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
15	SO	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
16	SP	117/145 (81%)	115 (98%)	2 (2%)	0	100	100
17	SQ	138/146 (94%)	133 (96%)	5 (4%)	0	100	100
18	SR	130/135 (96%)	124 (95%)	6 (5%)	0	100	100
19	SS	141/152 (93%)	134 (95%)	7 (5%)	0	100	100
20	ST	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
21	SU	99/119 (83%)	98 (99%)	1 (1%)	0	100	100
22	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
23	SW	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
24	SX	139/143 (97%)	129 (93%)	10 (7%)	0	100	100
25	SY	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
26	SZ	73/125 (58%)	69 (94%)	4 (6%)	0	100	100
27	Sa	98/115 (85%)	95 (97%)	3 (3%)	0	100	100
28	Sb	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
29	Sc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
30	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
31	Se	50/59 (85%)	49 (98%)	1 (2%)	0	100	100
32	sh	62/156 (40%)	56 (90%)	6 (10%)	0	100	100
33	Sg	311/317 (98%)	296 (95%)	15 (5%)	0	100	100
34	Ln	22/25 (88%)	20 (91%)	2 (9%)	0	100	100
37	3m	361/374 (96%)	347 (96%)	14 (4%)	0	100	100
38	3f	267/357 (75%)	261 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	3a	590/1382 (43%)	567 (96%)	23 (4%)	0	100	100
40	3e	428/445 (96%)	419 (98%)	8 (2%)	1 (0%)	44	71
41	3c	537/913 (59%)	522 (97%)	15 (3%)	0	100	100
42	3h	316/352 (90%)	306 (97%)	10 (3%)	0	100	100
43	3d	53/548 (10%)	49 (92%)	4 (8%)	0	100	100
44	3k	213/218 (98%)	210 (99%)	3 (1%)	0	100	100
45	3l	518/564 (92%)	506 (98%)	12 (2%)	0	100	100
All	All	8082/10654 (76%)	7808 (97%)	273 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	3e	264	ASN

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	SA	180/243 (74%)	172 (96%)	8 (4%)	24	52
2	SB	193/231 (84%)	187 (97%)	6 (3%)	35	61
3	SC	185/225 (82%)	177 (96%)	8 (4%)	25	53
4	SD	189/202 (94%)	180 (95%)	9 (5%)	21	50
5	SE	223/225 (99%)	215 (96%)	8 (4%)	30	57
6	SF	162/170 (95%)	155 (96%)	7 (4%)	25	53
7	SG	207/218 (95%)	202 (98%)	5 (2%)	44	68
8	SH	167/174 (96%)	159 (95%)	8 (5%)	21	50
9	SI	178/180 (99%)	173 (97%)	5 (3%)	38	64
10	SJ	160/168 (95%)	151 (94%)	9 (6%)	17	45
11	SK	87/136 (64%)	79 (91%)	8 (9%)	7	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	SL	134/142 (94%)	127 (95%)	7 (5%)	19	47
13	Sf	102/108 (94%)	97 (95%)	5 (5%)	21	49
14	SN	130/131 (99%)	125 (96%)	5 (4%)	28	56
15	SO	104/119 (87%)	99 (95%)	5 (5%)	21	50
16	SP	107/130 (82%)	106 (99%)	1 (1%)	75	85
17	SQ	116/121 (96%)	109 (94%)	7 (6%)	16	42
18	SR	119/122 (98%)	110 (92%)	9 (8%)	11	34
19	SS	124/132 (94%)	110 (89%)	14 (11%)	4	18
20	ST	112/115 (97%)	106 (95%)	6 (5%)	18	46
21	SU	93/107 (87%)	89 (96%)	4 (4%)	25	53
22	SV	67/67 (100%)	65 (97%)	2 (3%)	36	62
23	SW	112/113 (99%)	109 (97%)	3 (3%)	40	65
24	SX	113/115 (98%)	104 (92%)	9 (8%)	10	32
25	SY	108/115 (94%)	104 (96%)	4 (4%)	29	56
26	SZ	67/103 (65%)	62 (92%)	5 (8%)	11	34
27	Sa	87/98 (89%)	84 (97%)	3 (3%)	32	59
28	Sb	75/76 (99%)	71 (95%)	4 (5%)	19	47
29	Sc	55/62 (89%)	53 (96%)	2 (4%)	30	57
30	Sd	48/49 (98%)	47 (98%)	1 (2%)	48	70
31	Se	42/48 (88%)	39 (93%)	3 (7%)	12	37
32	sh	57/140 (41%)	54 (95%)	3 (5%)	19	47
33	Sg	272/275 (99%)	256 (94%)	16 (6%)	16	43
34	Ln	23/24 (96%)	23 (100%)	0	100	100
37	3m	252/335 (75%)	237 (94%)	15 (6%)	16	42
38	3f	229/289 (79%)	221 (96%)	8 (4%)	31	58
39	3a	439/1259 (35%)	422 (96%)	17 (4%)	27	55
40	3e	302/406 (74%)	296 (98%)	6 (2%)	50	71
41	3c	347/811 (43%)	338 (97%)	9 (3%)	41	66
42	3h	272/310 (88%)	267 (98%)	5 (2%)	54	74
43	3d	20/494 (4%)	19 (95%)	1 (5%)	20	48
44	3k	121/193 (63%)	118 (98%)	3 (2%)	42	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	3I	475/515 (92%)	451 (95%)	24 (5%)	20	48
All	All	6655/9296 (72%)	6368 (96%)	287 (4%)	27	53

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	SA	88	LEU
1	SA	122	LEU
1	SA	148	CYS
1	SA	154	LEU
1	SA	178	LEU
1	SA	181	GLU
1	SA	197	VAL
1	SA	198	MET
2	SB	29	ASP
2	SB	38	MET
2	SB	48	LEU
2	SB	153	THR
2	SB	189	ILE
2	SB	218	LEU
3	SC	80	GLU
3	SC	105	GLU
3	SC	112	VAL
3	SC	152	ARG
3	SC	157	LEU
3	SC	160	LEU
3	SC	213	LEU
3	SC	233	LEU
4	SD	42	THR
4	SD	50	ILE
4	SD	69	LEU
4	SD	73	VAL
4	SD	142	LEU
4	SD	153	VAL
4	SD	156	LEU
4	SD	160	SER
4	SD	176	LEU
5	SE	12	VAL
5	SE	16	LYS
5	SE	23	LEU
5	SE	40	GLU
5	SE	65	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	SE	183	VAL
5	SE	236	ILE
5	SE	238	LEU
6	SF	28	VAL
6	SF	32	ASP
6	SF	41	VAL
6	SF	52	SER
6	SF	78	MET
6	SF	79	HIS
6	SF	172	CYS
7	SG	114	VAL
7	SG	144	LEU
7	SG	158	VAL
7	SG	162	LEU
7	SG	179	LEU
8	SH	27	LEU
8	SH	30	LEU
8	SH	40	LEU
8	SH	45	ILE
8	SH	97	GLN
8	SH	109	ARG
8	SH	118	ARG
8	SH	130	LEU
9	SI	92	ARG
9	SI	130	THR
9	SI	164	GLU
9	SI	189	VAL
9	SI	195	LEU
10	SJ	12	THR
10	SJ	20	PHE
10	SJ	21	GLU
10	SJ	29	LEU
10	SJ	73	GLU
10	SJ	122	SER
10	SJ	137	VAL
10	SJ	151	LEU
10	SJ	163	SER
11	SK	2	LEU
11	SK	16	PHE
11	SK	40	VAL
11	SK	49	MET
11	SK	59	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	SK	65	ARG
11	SK	71	LEU
11	SK	73	ASN
12	SL	4	ILE
12	SL	33	LEU
12	SL	40	ILE
12	SL	74	SER
12	SL	76	VAL
12	SL	145	VAL
12	SL	146	THR
13	Sf	35	ILE
13	Sf	42	LEU
13	Sf	43	ASP
13	Sf	66	GLU
13	Sf	80	ASP
14	SN	4	MET
14	SN	60	VAL
14	SN	67	THR
14	SN	117	LEU
14	SN	118	ILE
15	SO	40	THR
15	SO	88	LEU
15	SO	100	THR
15	SO	116	LEU
15	SO	119	LEU
16	SP	82	ASP
17	SQ	18	THR
17	SQ	20	THR
17	SQ	34	VAL
17	SQ	39	LEU
17	SQ	53	GLU
17	SQ	127	CYS
17	SQ	144	SER
18	SR	16	ILE
18	SR	62	GLN
18	SR	69	ILE
18	SR	73	LEU
18	SR	91	LEU
18	SR	109	LEU
18	SR	120	THR
18	SR	124	VAL
18	SR	130	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	SS	33	ILE
19	SS	36	VAL
19	SS	44	VAL
19	SS	60	THR
19	SS	65	GLU
19	SS	83	PHE
19	SS	85	ASN
19	SS	103	LEU
19	SS	107	LEU
19	SS	112	GLU
19	SS	131	VAL
19	SS	136	THR
19	SS	142	ARG
19	SS	145	THR
20	ST	4	VAL
20	ST	5	THR
20	ST	50	GLU
20	ST	76	THR
20	ST	110	LEU
20	ST	113	VAL
21	SU	55	ARG
21	SU	68	THR
21	SU	91	LEU
21	SU	110	VAL
22	SV	13	VAL
22	SV	70	LEU
23	SW	25	VAL
23	SW	74	VAL
23	SW	111	MET
24	SX	5	ARG
24	SX	9	THR
24	SX	12	LYS
24	SX	52	LEU
24	SX	53	GLU
24	SX	72	VAL
24	SX	118	VAL
24	SX	123	VAL
24	SX	128	VAL
25	SY	18	LEU
25	SY	25	ILE
25	SY	120	THR
25	SY	125	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	SZ	49	LEU
26	SZ	65	TYR
26	SZ	68	ILE
26	SZ	92	LEU
26	SZ	100	VAL
27	Sa	55	GLU
27	Sa	63	VAL
27	Sa	89	ARG
28	Sb	11	SER
28	Sb	57	VAL
28	Sb	70	LYS
28	Sb	72	ARG
29	Sc	15	THR
29	Sc	43	ILE
30	Sd	7	TYR
31	Se	33	LYS
31	Se	45	VAL
31	Se	48	THR
32	sh	102	VAL
32	sh	107	LYS
32	sh	119	ARG
33	Sg	40	ILE
33	Sg	54	ILE
33	Sg	64	HIS
33	Sg	71	ILE
33	Sg	77	PHE
33	Sg	98	THR
33	Sg	113	PHE
33	Sg	132	TRP
33	Sg	150	TRP
33	Sg	151	VAL
33	Sg	179	LEU
33	Sg	226	HIS
33	Sg	256	ILE
33	Sg	267	VAL
33	Sg	297	THR
33	Sg	298	LEU
37	3m	21	TYR
37	3m	31	GLU
37	3m	46	ILE
37	3m	86	LEU
37	3m	95	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	3m	97	GLU
37	3m	103	LEU
37	3m	116	ASN
37	3m	176	LYS
37	3m	195	ASP
37	3m	199	GLN
37	3m	208	ILE
37	3m	212	LEU
37	3m	232	LEU
37	3m	282	PHE
38	3f	127	HIS
38	3f	131	VAL
38	3f	148	VAL
38	3f	232	PHE
38	3f	236	THR
38	3f	238	LYS
38	3f	262	VAL
38	3f	355	VAL
39	3a	35	MET
39	3a	65	HIS
39	3a	158	ARG
39	3a	220	LEU
39	3a	225	SER
39	3a	268	LYS
39	3a	285	LYS
39	3a	315	MET
39	3a	331	ILE
39	3a	341	LEU
39	3a	397	GLU
39	3a	410	VAL
39	3a	420	LYS
39	3a	425	GLN
39	3a	452	PHE
39	3a	529	VAL
39	3a	535	GLU
40	3e	189	LEU
40	3e	205	LEU
40	3e	232	ILE
40	3e	343	THR
40	3e	356	LEU
40	3e	392	VAL
41	3c	424	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	3c	490	LEU
41	3c	514	PHE
41	3c	582	TRP
41	3c	625	LEU
41	3c	693	LEU
41	3c	749	TRP
41	3c	753	HIS
41	3c	793	PHE
42	3h	115	LEU
42	3h	140	TYR
42	3h	145	GLU
42	3h	219	GLU
42	3h	314	MET
43	3d	21	VAL
44	3k	128	LEU
44	3k	150	TYR
44	3k	194	GLU
45	3l	46	GLN
45	3l	82	ASP
45	3l	93	ASP
45	3l	136	TYR
45	3l	145	SER
45	3l	151	GLU
45	3l	160	TYR
45	3l	183	LEU
45	3l	215	LEU
45	3l	234	LEU
45	3l	265	LEU
45	3l	266	TYR
45	3l	293	VAL
45	3l	321	PHE
45	3l	373	ILE
45	3l	427	ASN
45	3l	431	VAL
45	3l	436	HIS
45	3l	456	GLN
45	3l	459	THR
45	3l	495	HIS
45	3l	503	THR
45	3l	547	ILE
45	3l	554	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60)

such sidechains are listed below:

Mol	Chain	Res	Type
1	SA	81	ASN
1	SA	113	GLN
2	SB	101	HIS
2	SB	163	GLN
2	SB	177	GLN
3	SC	120	GLN
5	SE	138	HIS
5	SE	197	ASN
6	SF	79	HIS
7	SG	163	ASN
7	SG	177	GLN
9	SI	22	HIS
11	SK	66	HIS
12	SL	39	ASN
13	Sf	119	GLN
14	SN	138	ASN
16	SP	103	ASN
17	SQ	11	GLN
17	SQ	114	GLN
18	SR	26	ASN
19	SS	11	HIS
19	SS	42	HIS
19	SS	134	GLN
20	ST	63	HIS
20	ST	83	GLN
22	SV	3	ASN
23	SW	98	GLN
30	Sd	37	ASN
31	Se	37	GLN
37	3m	116	ASN
37	3m	196	ASN
37	3m	205	HIS
37	3m	257	GLN
39	3a	44	GLN
39	3a	175	HIS
39	3a	180	GLN
39	3a	187	GLN
39	3a	301	HIS
41	3c	461	ASN
41	3c	465	HIS
41	3c	579	HIS
41	3c	597	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	3c	615	GLN
41	3c	753	HIS
41	3c	828	ASN
42	3h	159	GLN
42	3h	255	GLN
42	3h	261	ASN
42	3h	270	GLN
42	3h	276	GLN
44	3k	151	GLN
45	3l	109	ASN
45	3l	139	HIS
45	3l	223	ASN
45	3l	225	HIS
45	3l	229	ASN
45	3l	239	ASN
45	3l	296	ASN
45	3l	452	GLN
45	3l	546	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	S2	1746/1869 (93%)	325 (18%)	6 (0%)
36	zz	301/332 (90%)	117 (38%)	0
All	All	2047/2201 (93%)	442 (21%)	6 (0%)

All (442) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	S2	2	A
35	S2	17	C
35	S2	33	G
35	S2	41	G
35	S2	42	A
35	S2	44	U
35	S2	46	A
35	S2	56	G
35	S2	59	U
35	S2	62	G
35	S2	65	C
35	S2	67	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	S2	68	A
35	S2	73	C
35	S2	74	G
35	S2	75	G
35	S2	99	A
35	S2	103	A
35	S2	113	G
35	S2	114	G
35	S2	115	U
35	S2	126	G
35	S2	130	G
35	S2	143	U
35	S2	155	G
35	S2	163	U
35	S2	166	A
35	S2	172	U
35	S2	175	A
35	S2	178	C
35	S2	191	A
35	S2	193	C
35	S2	196	C
35	S2	199	C
35	S2	200	G
35	S2	202	G
35	S2	204	G
35	S2	205	G
35	S2	211	G
35	S2	226	A
35	S2	228	C
35	S2	238	C
35	S2	281	C
35	S2	282	G
35	S2	283	G
35	S2	294	U
35	S2	302	A
35	S2	306	C
35	S2	309	G
35	S2	319	C
35	S2	320	G
35	S2	321	C
35	S2	325	C
35	S2	326	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	S2	327	G
35	S2	328	U
35	S2	329	G
35	S2	332	G
35	S2	339	A
35	S2	347	G
35	S2	362	C
35	S2	364	A
35	S2	368	U
35	S2	370	G
35	S2	383	G
35	S2	385	G
35	S2	386	C
35	S2	400	C
35	S2	407	G
35	S2	409	C
35	S2	418	A
35	S2	435	A
35	S2	448	A
35	S2	449	A
35	S2	450	C
35	S2	465	A
35	S2	471	G
35	S2	472	C
35	S2	474	G
35	S2	482	G
35	S2	487	U
35	S2	492	C
35	S2	493	A
35	S2	516	A
35	S2	517	C
35	S2	518	G
35	S2	532	C
35	S2	536	A
35	S2	537	C
35	S2	538	U
35	S2	539	C
35	S2	541	U
35	S2	543	C
35	S2	544	G
35	S2	545	A
35	S2	546	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	S2	547	G
35	S2	548	C
35	S2	549	C
35	S2	550	C
35	S2	554	A
35	S2	555	A
35	S2	564	A
35	S2	568	C
35	S2	569	A
35	S2	576	A
35	S2	583	A
35	S2	587	A
35	S2	589	G
35	S2	590	A
35	S2	591	U
35	S2	593	C
35	S2	607	U
35	S2	614	C
35	S2	615	C
35	S2	617	G
35	S2	629	A
35	S2	643	A
35	S2	644	G
35	S2	655	A
35	S2	659	G
35	S2	660	C
35	S2	668	A
35	S2	669	A
35	S2	670	A
35	S2	671	A
35	S2	672	A
35	S2	673	G
35	S2	684	G
35	S2	688	U
35	S2	690	G
35	S2	692	G
35	S2	693	A
35	S2	695	C
35	S2	696	G
35	S2	697	G
35	S2	698	G
35	S2	731	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	S2	732	U
35	S2	733	C
35	S2	735	C
35	S2	736	C
35	S2	738	C
35	S2	746	C
35	S2	749	U
35	S2	790	C
35	S2	795	A
35	S2	796	G
35	S2	799	U
35	S2	801	U
35	S2	821	G
35	S2	822	U
35	S2	834	C
35	S2	847	A
35	S2	869	A
35	S2	870	A
35	S2	871	U
35	S2	872	A
35	S2	878	G
35	S2	886	A
35	S2	890	U
35	S2	891	G
35	S2	894	G
35	S2	895	G
35	S2	896	U
35	S2	897	U
35	S2	906	U
35	S2	913	A
35	S2	914	U
35	S2	920	A
35	S2	921	G
35	S2	922	A
35	S2	933	G
35	S2	943	U
35	S2	963	A
35	S2	971	G
35	S2	985	G
35	S2	990	A
35	S2	992	A
35	S2	1002	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	S2	1017	U
35	S2	1023	A
35	S2	1027	A
35	S2	1045	U
35	S2	1061	U
35	S2	1062	A
35	S2	1078	C
35	S2	1081	U
35	S2	1082	A
35	S2	1083	A
35	S2	1085	C
35	S2	1109	C
35	S2	1114	U
35	S2	1115	U
35	S2	1117	C
35	S2	1118	C
35	S2	1119	A
35	S2	1121	G
35	S2	1133	A
35	S2	1135	C
35	S2	1138	C
35	S2	1139	C
35	S2	1149	A
35	S2	1153	C
35	S2	1154	U
35	S2	1171	G
35	S2	1195	A
35	S2	1201	U
35	S2	1207	G
35	S2	1215	C
35	S2	1242	U
35	S2	1243	U
35	S2	1249	C
35	S2	1251	A
35	S2	1253	A
35	S2	1255	G
35	S2	1256	G
35	S2	1257	G
35	S2	1259	A
35	S2	1264	C
35	S2	1274	G
35	S2	1275	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	S2	1285	G
35	S2	1286	G
35	S2	1287	A
35	S2	1288	U
35	S2	1301	A
35	S2	1302	G
35	S2	1303	C
35	S2	1306	U
35	S2	1308	U
35	S2	1309	C
35	S2	1322	G
35	S2	1326	U
35	S2	1327	G
35	S2	1342	U
35	S2	1348	G
35	S2	1364	U
35	S2	1371	U
35	S2	1372	U
35	S2	1378	A
35	S2	1382	A
35	S2	1397	U
35	S2	1401	A
35	S2	1404	U
35	S2	1417	C
35	S2	1418	C
35	S2	1419	C
35	S2	1420	G
35	S2	1421	A
35	S2	1422	G
35	S2	1423	C
35	S2	1424	G
35	S2	1428	G
35	S2	1435	C
35	S2	1436	C
35	S2	1438	A
35	S2	1442	U
35	S2	1454	A
35	S2	1462	U
35	S2	1463	U
35	S2	1464	C
35	S2	1489	A
35	S2	1490	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	S2	1494	U
35	S2	1495	G
35	S2	1497	G
35	S2	1498	A
35	S2	1508	A
35	S2	1520	G
35	S2	1521	C
35	S2	1533	A
35	S2	1553	C
35	S2	1555	U
35	S2	1556	A
35	S2	1580	A
35	S2	1588	A
35	S2	1601	A
35	S2	1606	G
35	S2	1621	U
35	S2	1646	C
35	S2	1654	G
35	S2	1665	G
35	S2	1699	A
35	S2	1706	G
35	S2	1712	A
35	S2	1713	C
35	S2	1714	U
35	S2	1719	A
35	S2	1721	U
35	S2	1722	G
35	S2	1723	G
35	S2	1744	G
35	S2	1745	A
35	S2	1748	G
35	S2	1752	C
35	S2	1753	C
35	S2	1754	G
35	S2	1768	A
35	S2	1776	G
35	S2	1777	G
35	S2	1778	C
35	S2	1780	G
35	S2	1781	A
35	S2	1782	G
35	S2	1783	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	S2	1784	G
35	S2	1812	U
35	S2	1813	A
35	S2	1820	G
35	S2	1823	A
35	S2	1824	A
35	S2	1825	A
35	S2	1826	G
35	S2	1829	G
35	S2	1835	A
35	S2	1837	G
35	S2	1838	U
35	S2	1849	G
35	S2	1851	A
35	S2	1861	G
35	S2	1862	G
35	S2	1863	A
35	S2	1864	U
35	S2	1865	C
36	zz	45	C
36	zz	46	U
36	zz	47	G
36	zz	48	U
36	zz	49	G
36	zz	51	G
36	zz	54	A
36	zz	56	U
36	zz	57	A
36	zz	58	C
36	zz	60	G
36	zz	64	U
36	zz	82	G
36	zz	83	C
36	zz	84	C
36	zz	85	A
36	zz	86	U
36	zz	94	G
36	zz	102	G
36	zz	104	C
36	zz	105	G
36	zz	106	U
36	zz	107	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	zz	110	G
36	zz	111	C
36	zz	112	C
36	zz	113	U
36	zz	115	C
36	zz	118	G
36	zz	120	C
36	zz	125	C
36	zz	129	C
36	zz	137	G
36	zz	145	G
36	zz	146	G
36	zz	151	C
36	zz	154	A
36	zz	156	C
36	zz	157	C
36	zz	160	U
36	zz	161	G
36	zz	162	A
36	zz	163	G
36	zz	164	U
36	zz	166	C
36	zz	168	C
36	zz	169	C
36	zz	172	A
36	zz	175	U
36	zz	185	A
36	zz	186	C
36	zz	188	G
36	zz	189	G
36	zz	191	U
36	zz	192	C
36	zz	195	U
36	zz	196	U
36	zz	197	C
36	zz	198	U
36	zz	202	A
36	zz	204	C
36	zz	207	C
36	zz	208	C
36	zz	209	C
36	zz	210	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	zz	211	C
36	zz	213	C
36	zz	216	U
36	zz	217	G
36	zz	222	G
36	zz	223	A
36	zz	224	G
36	zz	225	A
36	zz	229	G
36	zz	233	G
36	zz	234	U
36	zz	235	G
36	zz	236	C
36	zz	237	C
36	zz	244	A
36	zz	245	G
36	zz	247	C
36	zz	253	G
36	zz	258	G
36	zz	260	A
36	zz	263	G
36	zz	265	U
36	zz	266	G
36	zz	270	C
36	zz	276	A
36	zz	280	C
36	zz	281	U
36	zz	282	U
36	zz	283	G
36	zz	284	U
36	zz	286	G
36	zz	288	A
36	zz	289	C
36	zz	290	U
36	zz	295	G
36	zz	296	A
36	zz	297	U
36	zz	303	G
36	zz	306	U
36	zz	311	G
36	zz	318	G
36	zz	323	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	zz	330	A
36	zz	331	G
36	zz	332	A
36	zz	334	C
36	zz	335	G
36	zz	336	U
36	zz	337	G
36	zz	339	A
36	zz	344	G
36	zz	345	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	S2	174	C
35	S2	517	C
35	S2	531	A
35	S2	871	U
35	S2	1326	U
35	S2	1434	C

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

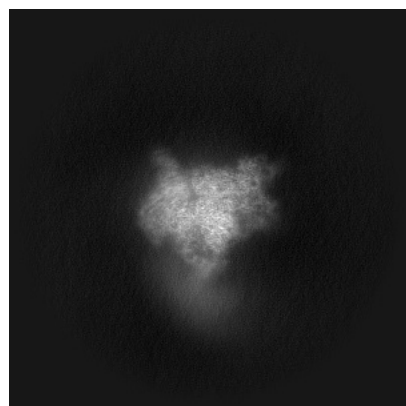
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62386. These allow visual inspection of the internal detail of the map and identification of artifacts.

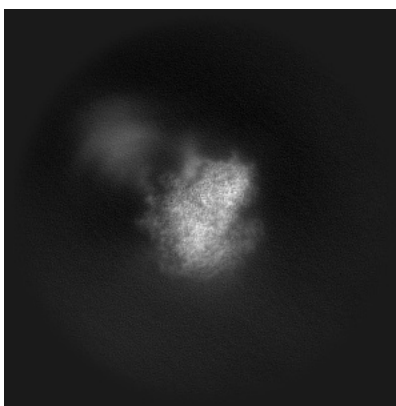
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

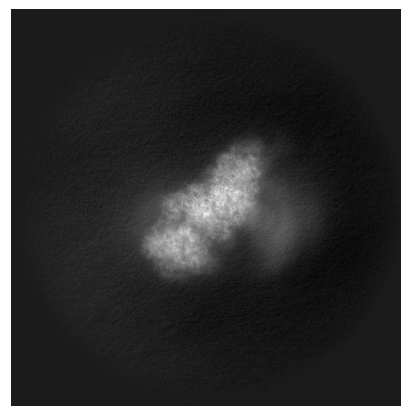
6.1.1 Primary map



X

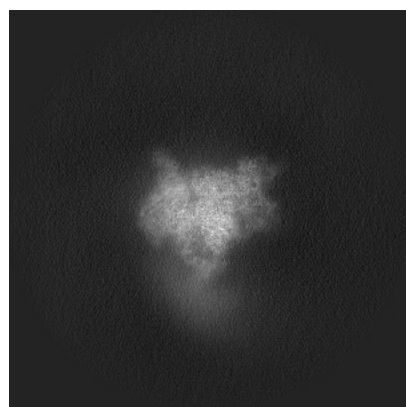


Y

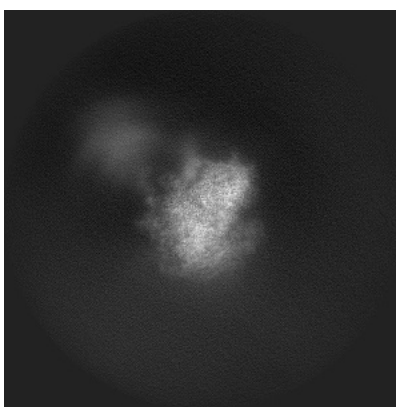


Z

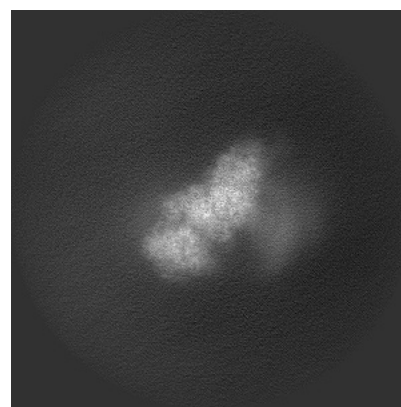
6.1.2 Raw map



X



Y

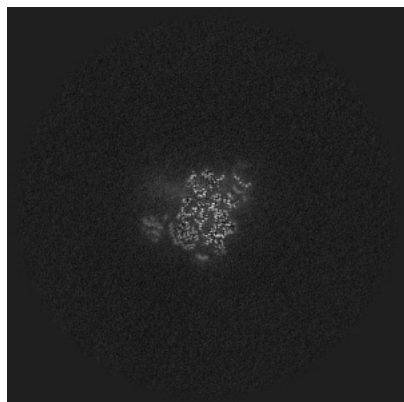


Z

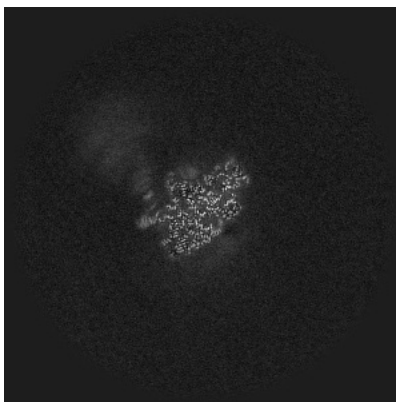
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

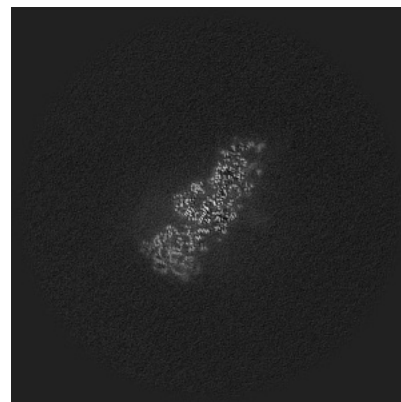
6.2.1 Primary map



X Index: 250

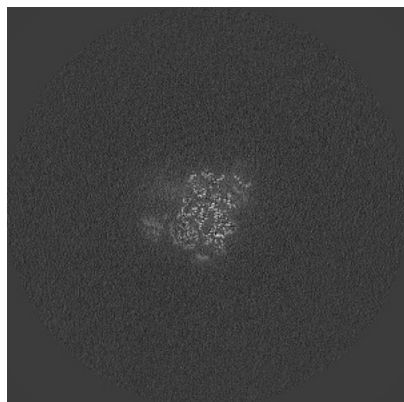


Y Index: 250

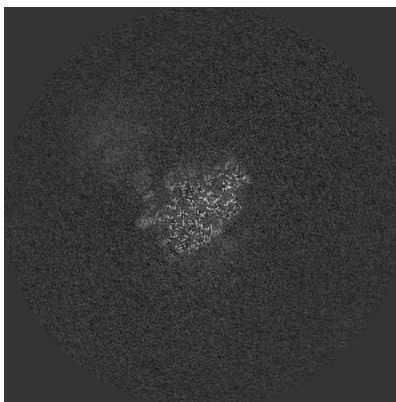


Z Index: 250

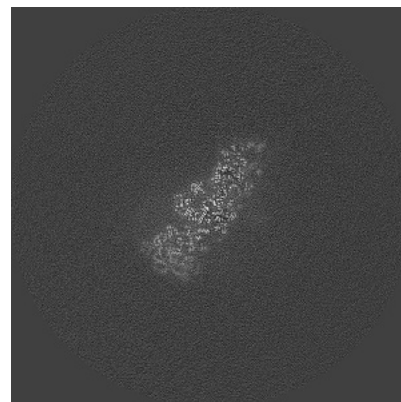
6.2.2 Raw map



X Index: 250



Y Index: 250

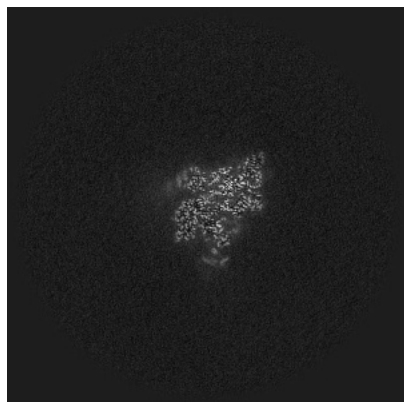


Z Index: 250

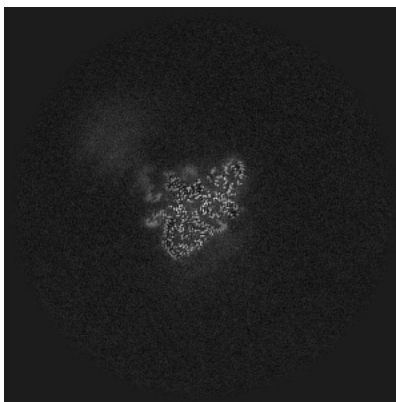
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

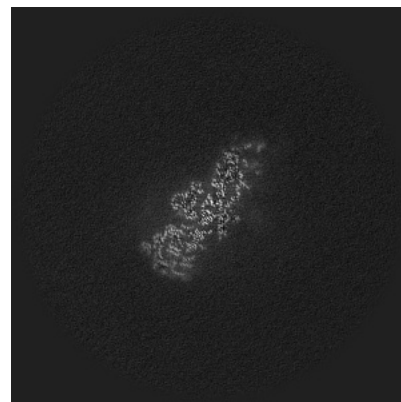
6.3.1 Primary map



X Index: 267

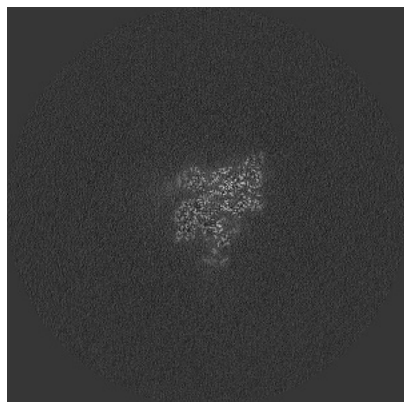


Y Index: 255

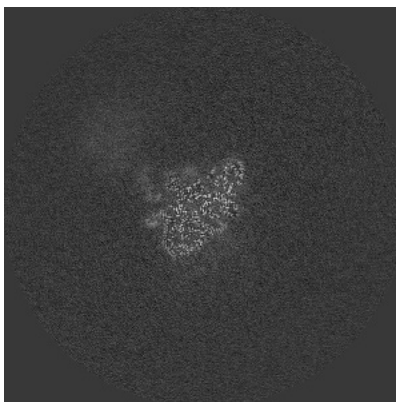


Z Index: 248

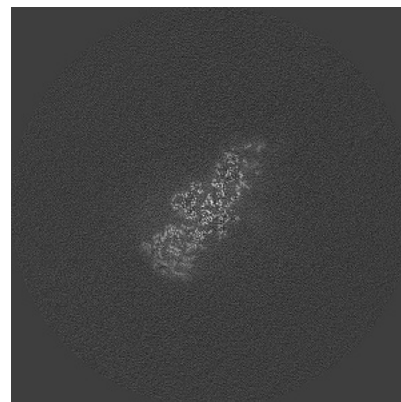
6.3.2 Raw map



X Index: 267



Y Index: 255

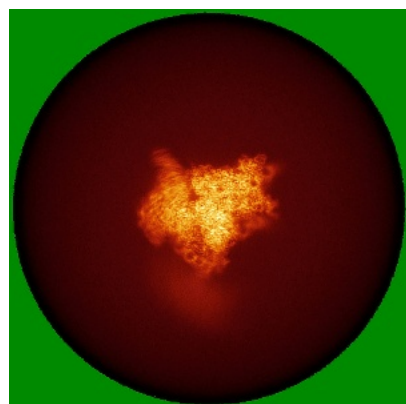


Z Index: 248

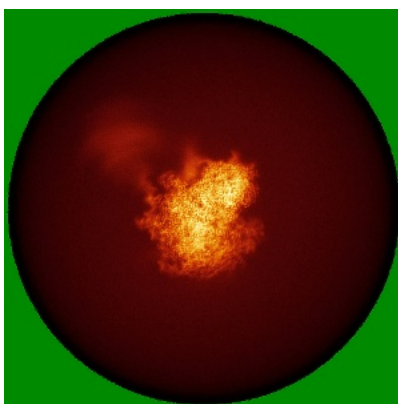
The images above show the largest variance slices of the map in three orthogonal directions.

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

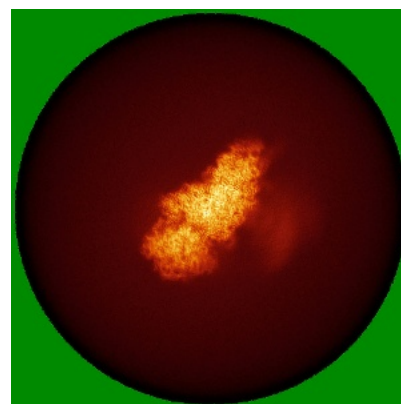
6.4.1 Primary map



X

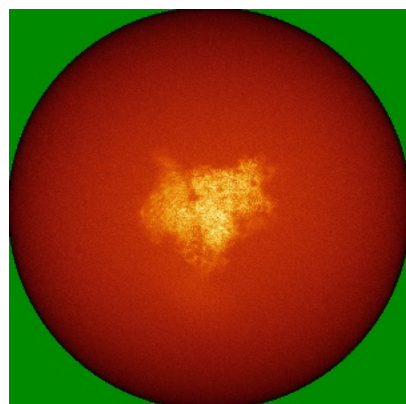


Y

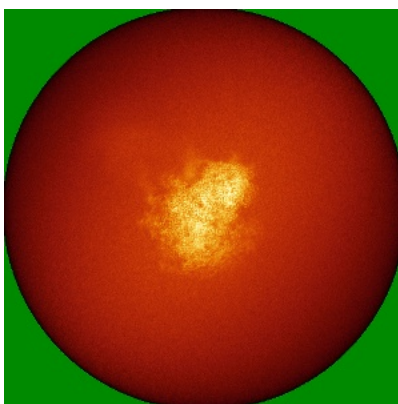


Z

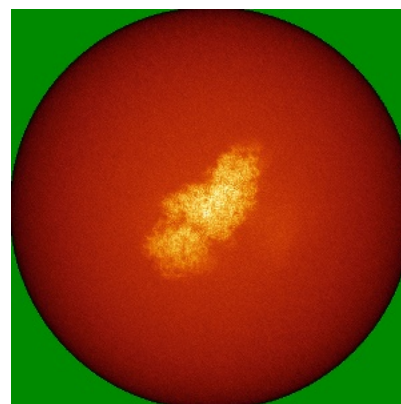
6.4.2 Raw map



X



Y

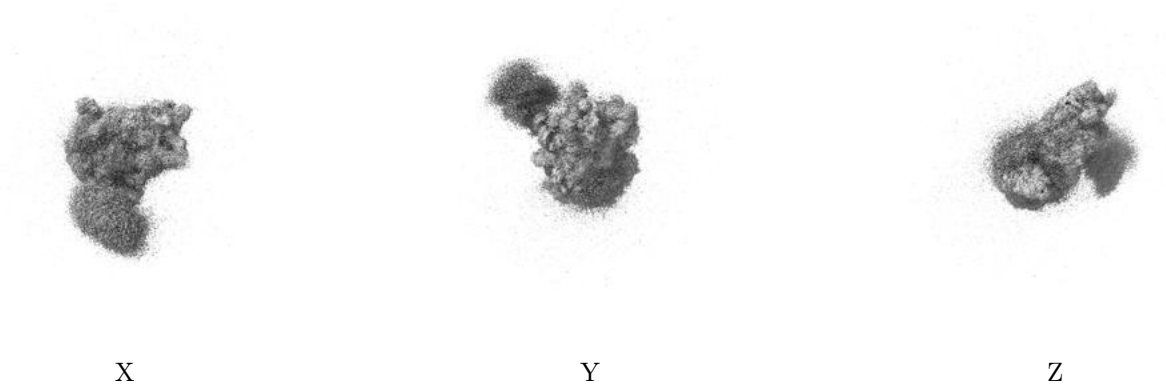


Z

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.

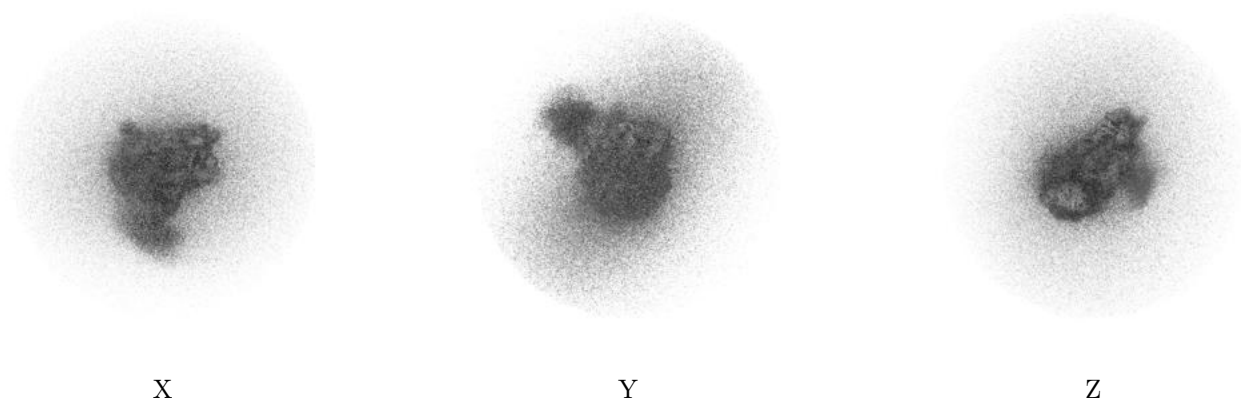
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

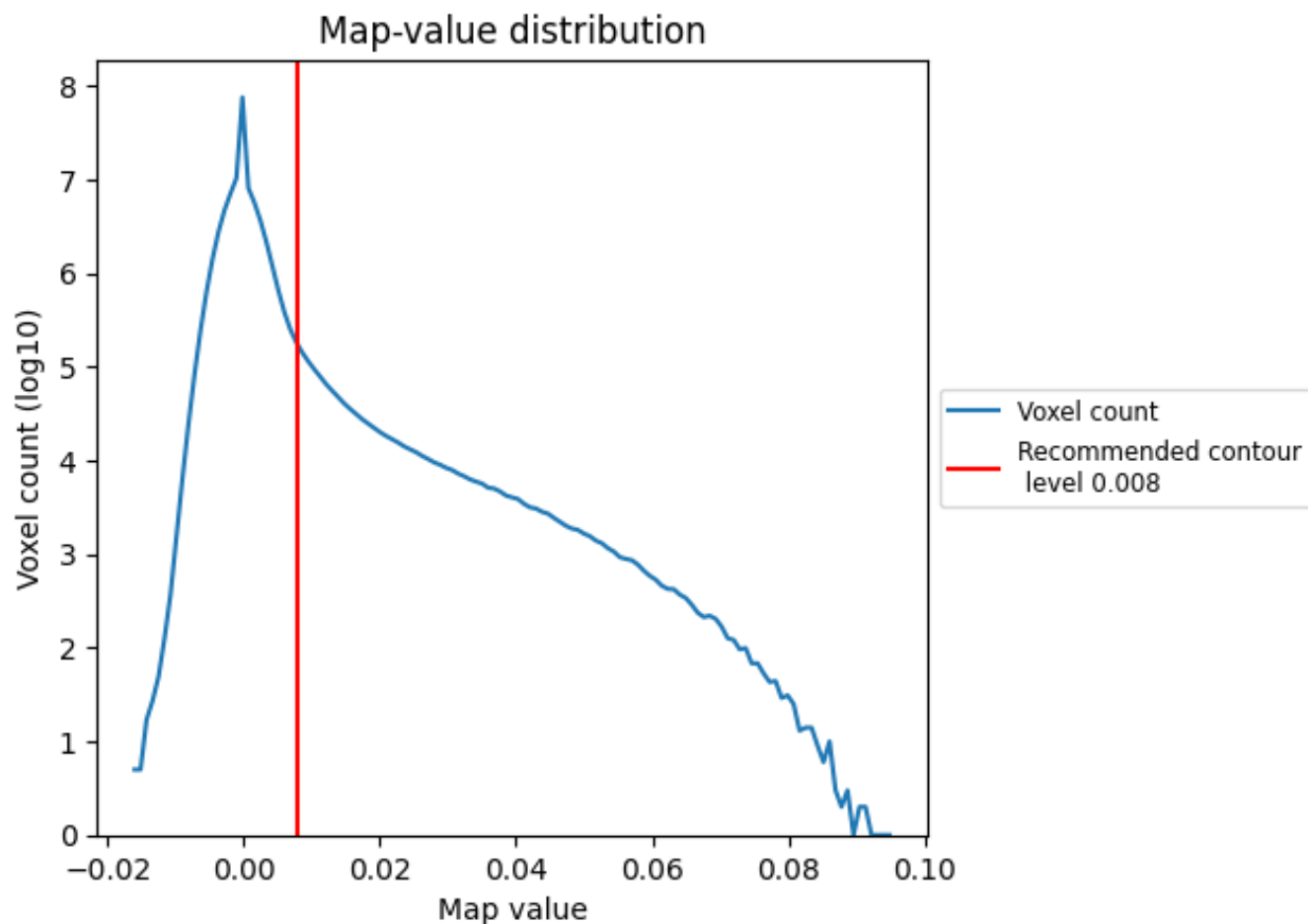
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

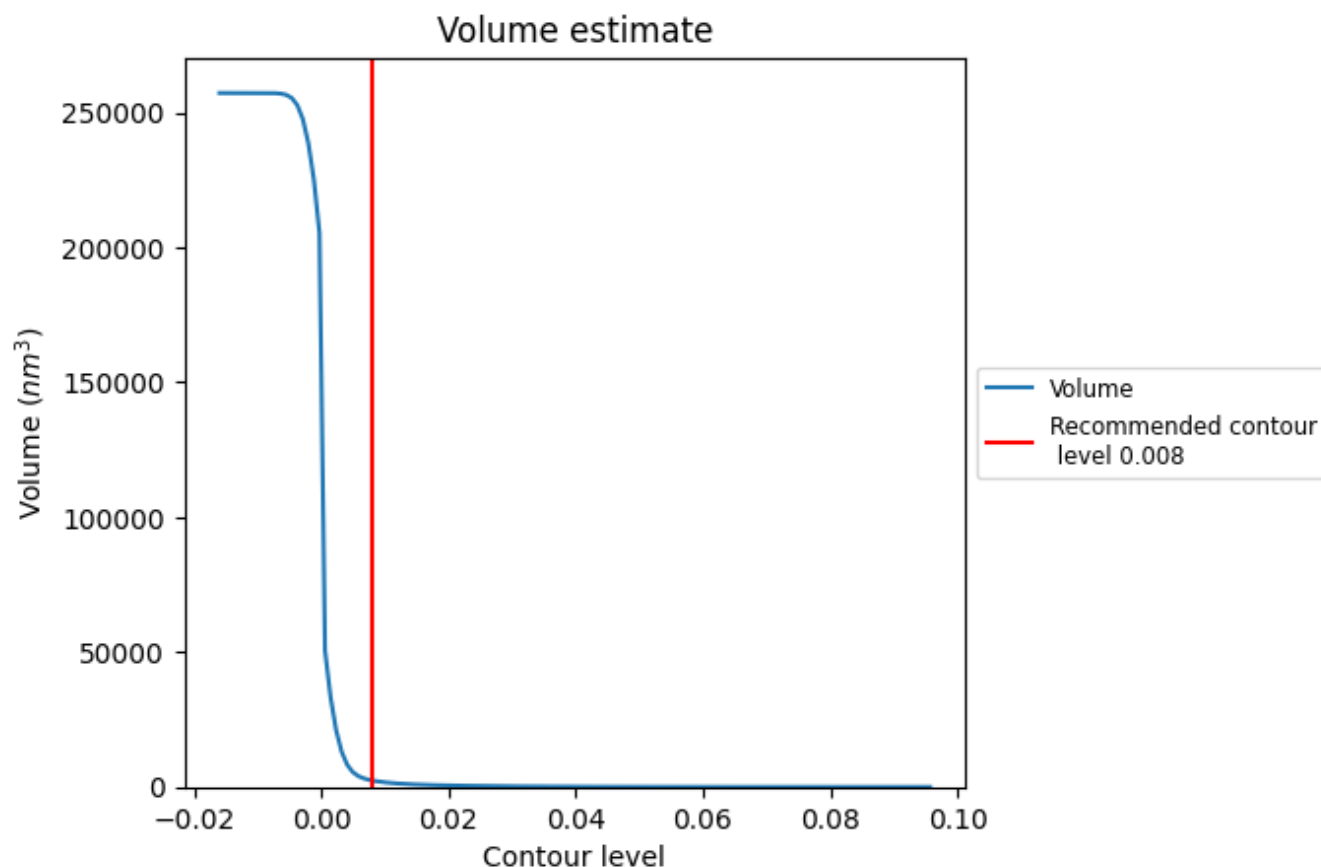
This section contains the results of statistical analysis of the map.

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.

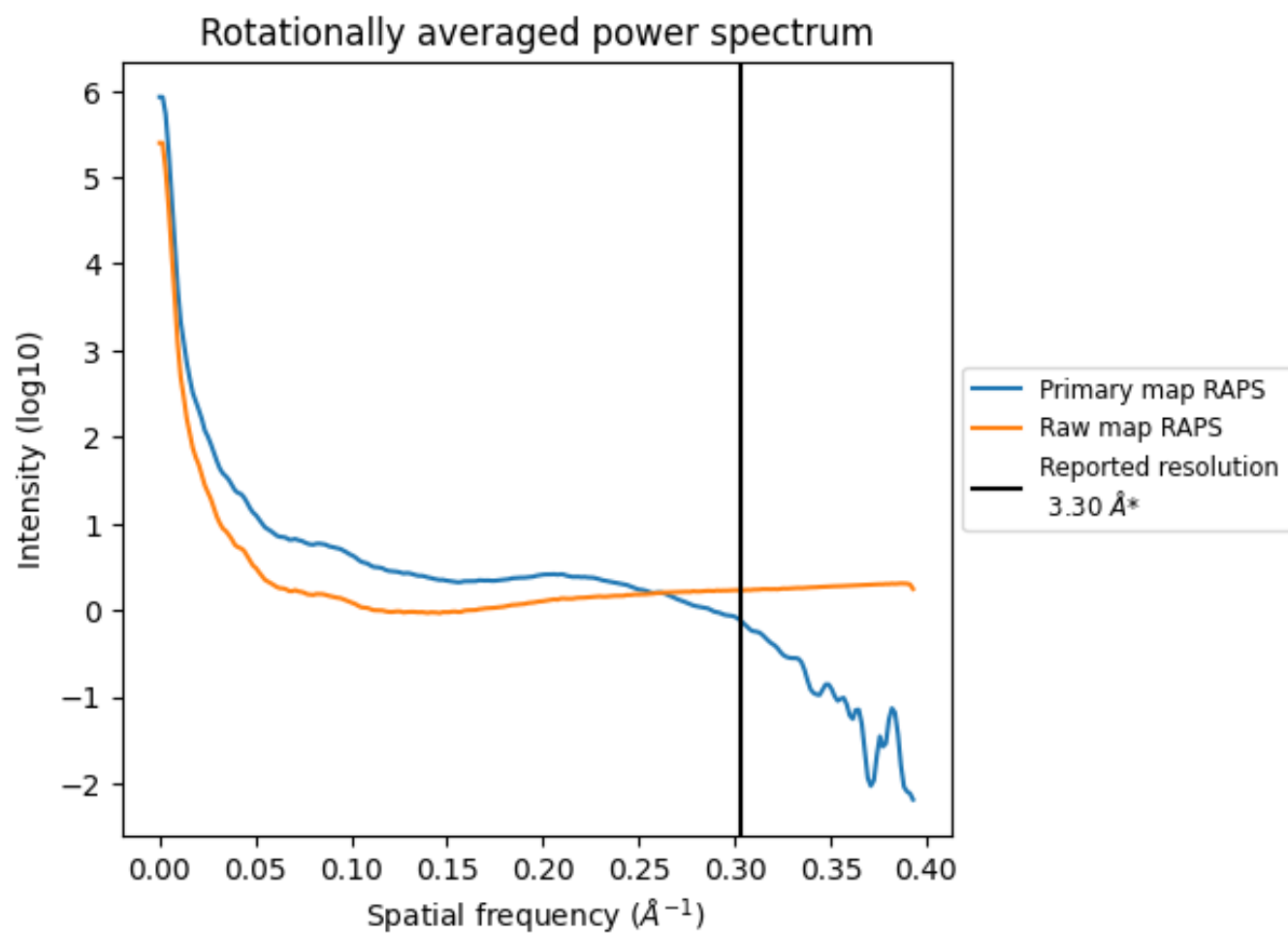
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2406 nm^3 ; this corresponds to an approximate mass of 2173 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 ⓘ

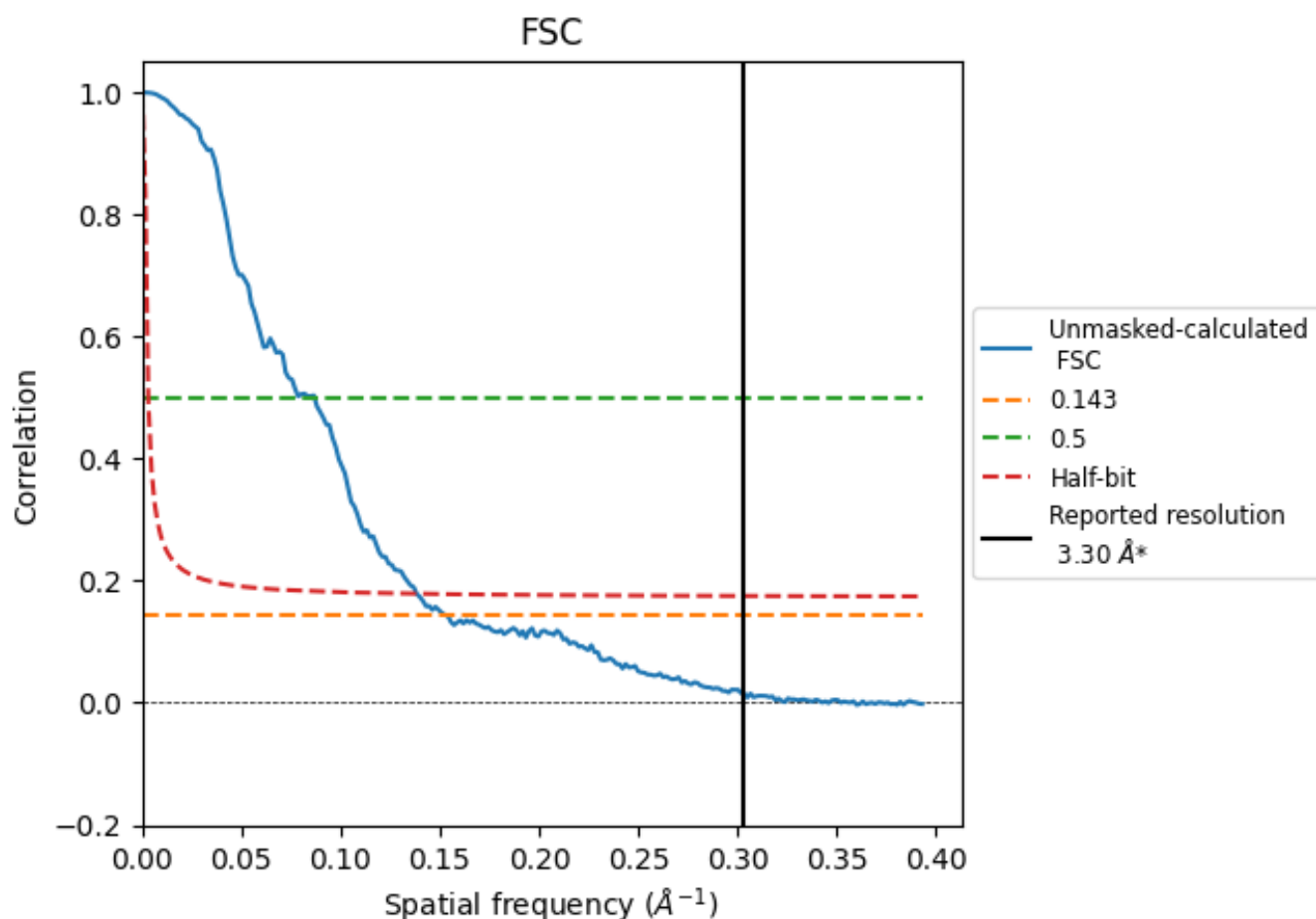


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

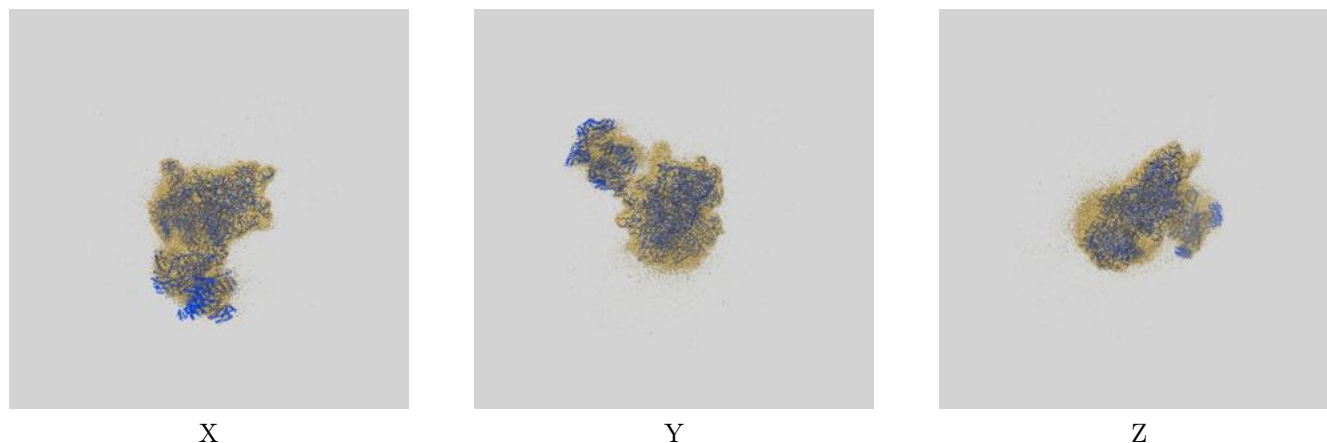
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.53	11.53	7.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.53 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

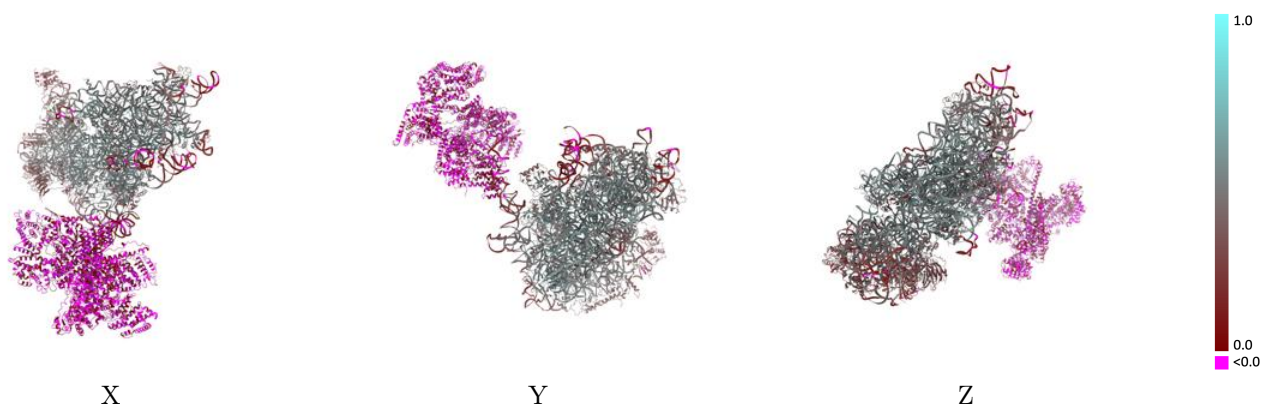
This section contains information regarding the fit between EMDB map EMD-62386 and PDB model 9KKF. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



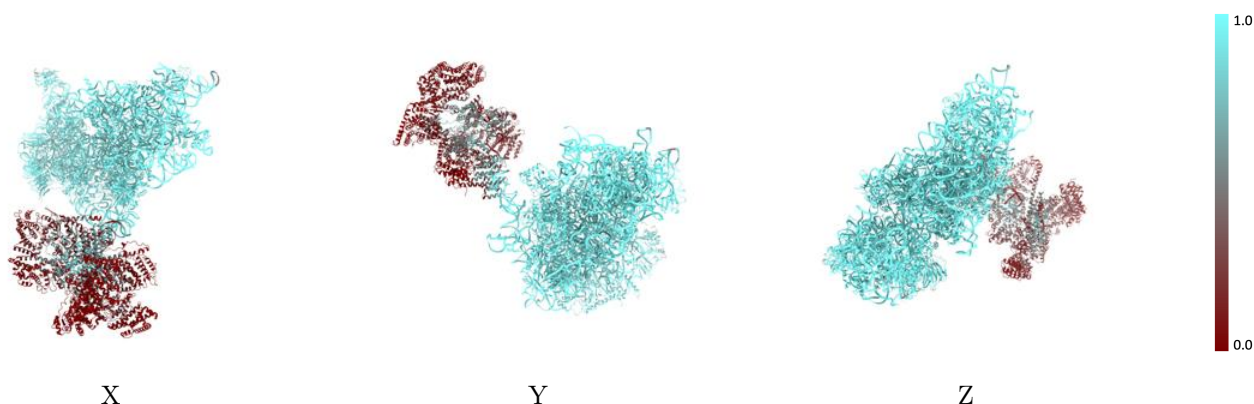
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



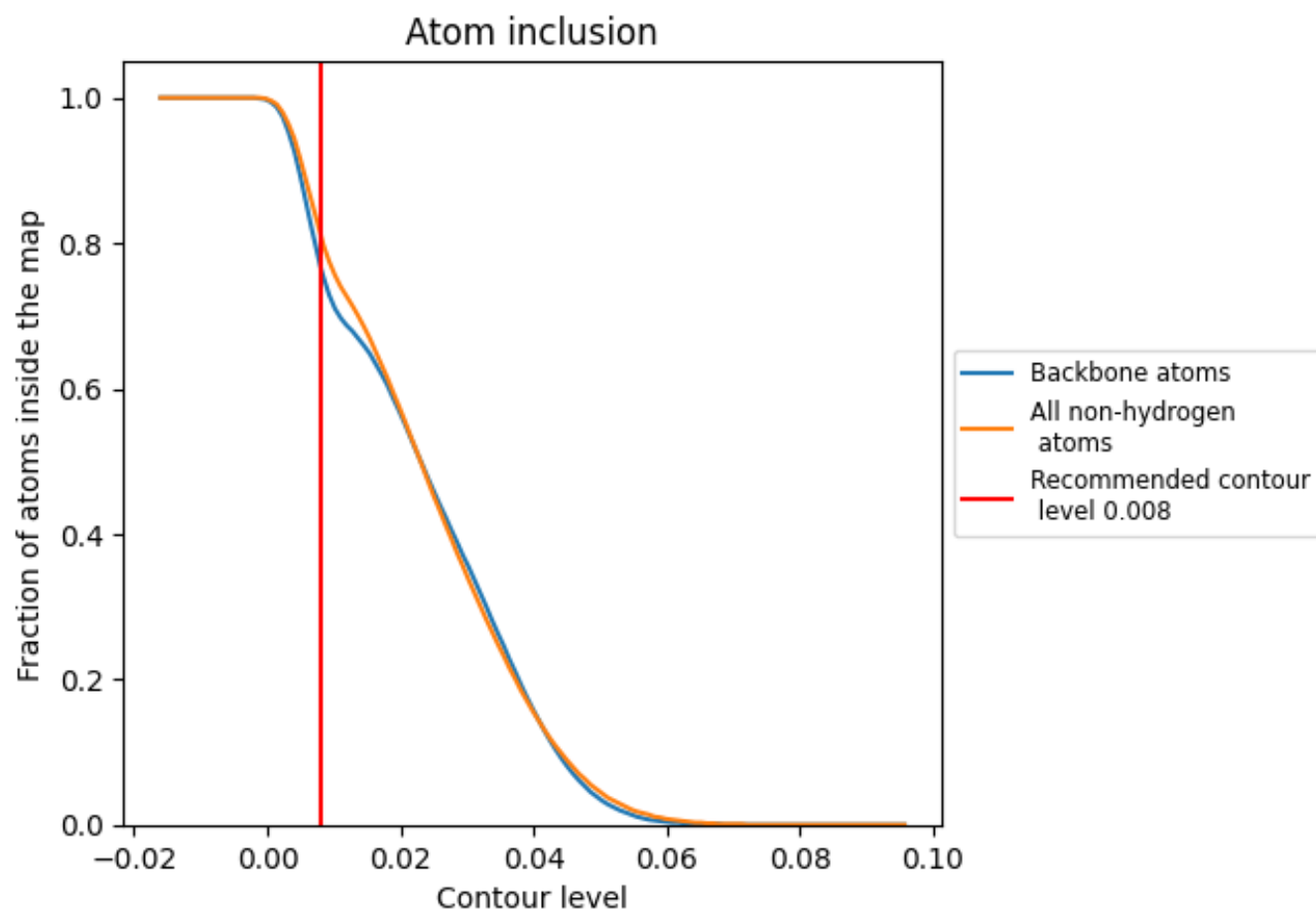
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 81% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8110	 0.3360
3a	 0.3820	 0.0180
3c	 0.2760	 -0.0020
3d	 0.2020	 0.0300
3e	 0.1760	 0.0030
3f	 0.3100	 0.0060
3h	 0.4350	 0.0140
3k	 0.0380	 -0.0160
3l	 0.0860	 -0.0050
3m	 0.0720	 -0.0110
Ln	 1.0000	 0.5090
S2	 0.9960	 0.4550
SA	 0.9950	 0.5030
SB	 0.9880	 0.5000
SC	 0.9960	 0.5170
SD	 0.9940	 0.4090
SE	 0.9950	 0.4970
SF	 0.9960	 0.4770
SG	 0.9790	 0.4050
SH	 0.9870	 0.4450
SI	 0.9880	 0.4930
SJ	 0.9950	 0.5060
SK	 0.9920	 0.3470
SL	 0.9940	 0.5010
SN	 0.9950	 0.4950
SO	 0.9960	 0.5260
SP	 0.9780	 0.3210
SQ	 0.9950	 0.4310
SR	 0.9830	 0.4480
SS	 0.9750	 0.3650
ST	 0.9910	 0.3840
SU	 0.9940	 0.3800
SV	 0.9890	 0.5010
SW	 1.0000	 0.5040
SX	 0.9980	 0.5080



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SY	 0.9880	 0.4480
SZ	 0.9980	 0.4390
Sa	 1.0000	 0.5340
Sb	 0.9950	 0.5070
Sc	 1.0000	 0.5000
Sd	 0.9980	 0.4190
Se	 0.9950	 0.4710
Sf	 0.8830	 0.2190
Sg	 0.9770	 0.3200
sh	 0.9060	 0.2140
zz	 0.9130	 0.2920